wwPDB EM Validation Summary Report (i)

Mar 6, 2026 – 03:33 AM UTC

PDB ID	:	8IYJ / pdb_00008iyj
EMDB ID	:	EMD-35823
Title	:	Cryo-EM structure of the 48-nm repeat doublet microtubule from mouse sperm
Authors	:	Zhou, L.N.; Gui, M.; Wu, J.P.
Deposited on	:	2023-04-05
Resolution	:	3.50 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:

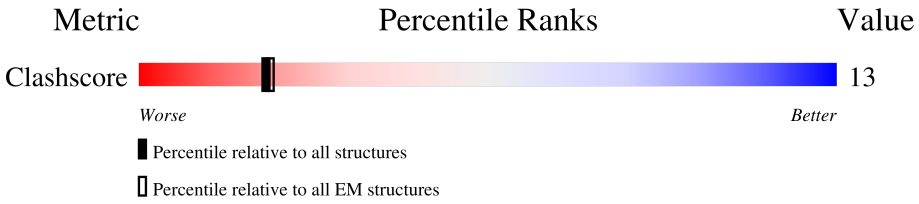
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

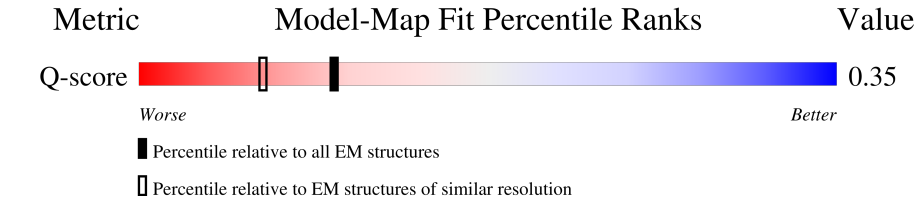
1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	228	21% 15% 64%
1	7	228	42% 20% 38%
2	1	853	41% 13% 46%
2	2	853	22% 10% 68%
3	3	514	65% 27% 8%
3	4	514	20% 9% 71%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	5	395	68% 27% 5%
4	6	395	71% 24% 5%
4	j1	395	61% 34% 5%
5	8	196	64% 25% 10%
6	A	101	5% 67% 26% 7%
6	N1	101	61% 31% 7%
7	A0	418	8% 5% 87%
7	A1	418	67% 18% 14%
7	A2	418	78% 18%
7	A3	418	80% 16%
7	A4	418	82% 13% 5%
7	A5	418	30% 11% 60%
8	AA	450	73% 25%
8	AC	450	73% 24%
8	AE	450	69% 28%
8	AG	450	73% 25%
8	AI	450	75% 23%
8	AK	450	71% 27%
8	AM	450	71% 26%
8	AO	450	68% 30%
8	BC	450	70% 26%
8	BE	450	68% 30%
8	BG	450	74% 23%
8	BI	450	76% 22%
8	BK	450	71% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	BM	450	71% 27%
8	BO	450	70% 26%
8	CC	450	70% 27%
8	CE	450	72% 25%
8	CG	450	71% 26%
8	CI	450	75% 22%
8	CK	450	75% 22%
8	CM	450	66% 31%
8	CO	450	70% 28%
8	CQ	450	8% 71% 26%
8	DC	450	64% 32%
8	DE	450	73% 22%
8	DG	450	73% 22%
8	DI	450	71% 25%
8	DK	450	72% 24%
8	DM	450	72% 24%
8	DO	450	73% 23%
8	DQ	450	5% 71% 24% 5%
8	EA	450	74% 23%
8	EC	450	71% 26%
8	EE	450	74% 23%
8	EG	450	74% 23%
8	EI	450	72% 25%
8	EK	450	75% 22%
8	EM	450	72% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	EO	450	5% 70% 27%
8	FA	450	62% 33%
8	FC	450	70% 26%
8	FE	450	68% 28%
8	FG	450	70% 25% 5%
8	FI	450	67% 29%
8	FK	450	68% 28%
8	FM	450	68% 27%
8	FO	450	66% 29% 5%
8	GA	450	68% 27%
8	GC	450	65% 30%
8	GE	450	64% 32%
8	GG	450	61% 37%
8	GI	450	66% 30%
8	GK	450	67% 29%
8	GM	450	62% 35%
8	GO	450	70% 26%
8	HA	450	67% 28%
8	HC	450	60% 36%
8	HE	450	69% 28%
8	HG	450	66% 31%
8	HI	450	70% 27%
8	HK	450	65% 30%
8	HM	450	63% 33%
8	HO	450	63% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	IA	450	62% 34%
8	IC	450	63% 35%
8	IE	450	62% 36%
8	IG	450	59% 37%
8	II	450	67% 30%
8	IK	450	59% 38%
8	IM	450	65% 30%
8	IO	450	60% 37%
8	JC	450	64% 33%
8	JE	450	64% 33%
8	JG	450	70% 25% 5%
8	JI	450	65% 31%
8	JK	450	67% 29%
8	JM	450	66% 29%
8	JO	450	61% 35%
8	JQ	450	67% 30%
8	KA	450	67% 29%
8	KC	450	69% 27%
8	KE	450	65% 31%
8	KG	450	68% 27%
8	KI	450	67% 29%
8	KK	450	68% 28%
8	KM	450	65% 31%
8	KO	450	68% 29%
8	LA	450	67% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	LC	450	71% 25%
8	LE	450	73% 23%
8	LG	450	74% 24%
8	LI	450	77% 21%
8	LK	450	71% 27%
8	LM	450	70% 27%
8	LO	450	65% 30%
8	MA	450	74% 22%
8	MC	450	76% 20%
8	ME	450	76% 22%
8	MG	450	67% 29%
8	MI	450	70% 26%
8	MK	450	70% 26%
8	MM	450	70% 26%
8	MO	450	64% 31% 5%
8	NA	450	5% 66% 29% 5%
8	NC	450	6% 66% 29% 5%
8	NE	450	66% 30%
8	NG	450	62% 34%
8	NI	450	66% 29%
8	NK	450	58% 37%
8	NM	450	58% 38%
8	NO	450	64% 32%
8	OA	450	19% 68% 28%
8	OC	450	6% 64% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	OE	450	67% 29%
8	OG	450	67% 28%
8	OI	450	67% 28% 5%
8	OK	450	63% 33%
8	OM	450	66% 29% 5%
8	OO	450	5% 62% 32% 6%
8	PC	450	65% 30% 5%
8	PE	450	68% 27% 6%
8	PG	450	68% 27%
8	PI	450	63% 32%
8	PK	450	63% 32%
8	PM	450	65% 31%
8	PO	450	5% 69% 27%
8	QC	450	8% 68% 28% 5%
8	QE	450	68% 28%
8	QG	450	5% 68% 28% 5%
8	QI	450	64% 31% 5%
8	QK	450	69% 26% 5%
8	QM	450	61% 33% 5%
8	QO	450	5% 67% 28% 5%
8	RC	450	69% 26% 5%
8	RE	450	68% 27% 5%
8	RG	450	64% 31% 5%
8	RI	450	68% 27% 5%
8	RK	450	67% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	RM	450	65% 30% 5%
8	RO	450	66% 28% 5%
8	SA	450	9% 69% 26% 5%
8	SC	450	65% 30% 5%
8	SE	450	64% 31% 5%
8	SG	450	65% 30% 5%
8	SI	450	66% 29% 5%
8	SK	450	67% 28% 5%
8	SM	450	66% 28% 6%
8	TA	450	8% 67% 28% 5%
8	TC	450	61% 34% 5%
8	TE	450	66% 29% 5%
8	TG	450	68% 27% 5%
8	TI	450	66% 29% 5%
8	TK	450	69% 26% 5%
8	TM	450	64% 31% 5%
8	UA	450	7% 64% 30% 6%
8	UC	450	66% 29% 5%
8	UE	450	63% 32% 5%
8	UG	450	72% 23% 5%
8	UI	450	70% 25% 5%
8	UK	450	68% 27% 5%
8	UM	450	8% 66% 29% 5%
8	UO	450	23% 64% 31% 5%
8	VA	450	8% 70% 25% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	VC	450	74% 24%
8	VE	450	68% 27% 5%
8	VG	450	63% 34%
8	VI	450	62% 33% 5%
8	VK	450	67% 30%
8	VM	450	66% 29% 5%
8	VO	450	7% 68% 28%
8	WA	450	6% 68% 29%
8	WC	450	73% 24%
8	WE	450	68% 28%
8	WG	450	72% 26%
8	WI	450	72% 25%
8	WK	450	70% 27%
8	WM	450	71% 24%
8	WO	450	68% 27% 5%
9	AB	445	71% 26%
9	AD	445	69% 28%
9	AF	445	68% 28%
9	AH	445	75% 23%
9	AJ	445	73% 24%
9	AL	445	68% 29%
9	AN	445	68% 29%
9	AP	445	70% 27%
9	BB	445	71% 25%
9	BD	445	75% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	BF	445	71% 25%
9	BH	445	72% 24%
9	BJ	445	72% 25%
9	BL	445	67% 29%
9	BN	445	73% 24%
9	BP	445	70% 27%
9	CB	445	68% 28%
9	CD	445	70% 27%
9	CF	445	75% 22%
9	CH	445	76% 20%
9	CJ	445	77% 19%
9	CL	445	68% 28%
9	CN	445	68% 29%
9	CP	445	72% 24%
9	DB	445	9% 69% 27%
9	DD	445	72% 24%
9	DF	445	74% 22%
9	DH	445	74% 22%
9	DJ	445	77% 20%
9	DL	445	74% 23%
9	DN	445	76% 20%
9	DP	445	75% 22%
9	EB	445	69% 27%
9	ED	445	72% 24%
9	EF	445	71% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	EH	445	71% 25%
9	EJ	445	74% 22%
9	EL	445	71% 26%
9	EN	445	69% 27%
9	FB	445	68% 28%
9	FD	445	74% 22%
9	FF	445	73% 23%
9	FH	445	71% 26%
9	FJ	445	71% 26%
9	FL	445	70% 26%
9	FN	445	65% 32%
9	GB	445	63% 32%
9	GD	445	66% 31%
9	GF	445	67% 29%
9	GH	445	66% 30%
9	GJ	445	70% 27%
9	GL	445	65% 32%
9	GN	445	70% 27%
9	HB	445	63% 33%
9	HD	445	58% 38%
9	HF	445	70% 26%
9	HH	445	67% 29%
9	HJ	445	61% 36%
9	HL	445	61% 36%
9	HN	445	68% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	HP	445	68% 28%
9	IB	445	61% 36%
9	ID	445	62% 34%
9	IF	445	63% 33%
9	IH	445	62% 34%
9	IJ	445	64% 32%
9	IL	445	62% 35%
9	IN	445	62% 35%
9	IP	445	63% 33%
9	JB	445	5% 67% 29%
9	JD	445	64% 32%
9	JF	445	63% 32%
9	JH	445	65% 31%
9	JJ	445	63% 33%
9	JL	445	64% 32%
9	JN	445	66% 30%
9	JP	445	68% 28%
9	KB	445	67% 29%
9	KD	445	65% 32%
9	KF	445	73% 24%
9	KH	445	62% 35%
9	KJ	445	70% 27%
9	KL	445	66% 30%
9	KN	445	62% 34%
9	KP	445	65% 31%

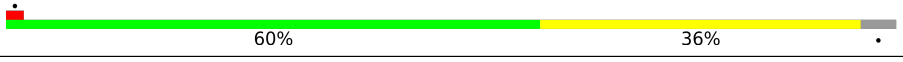
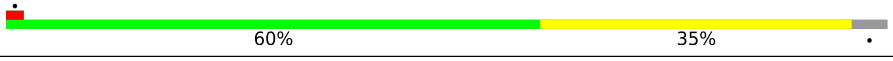
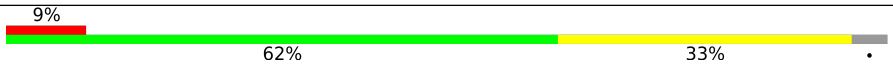
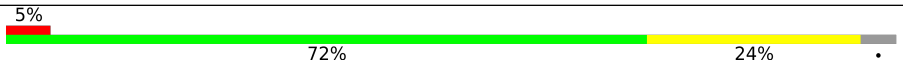
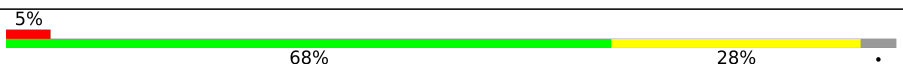
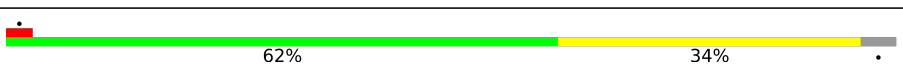
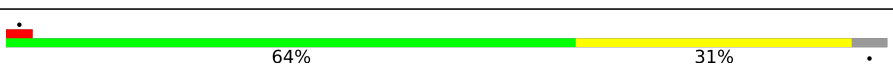
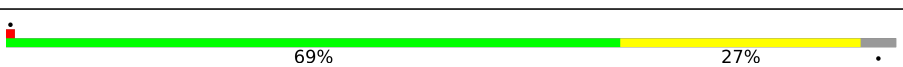
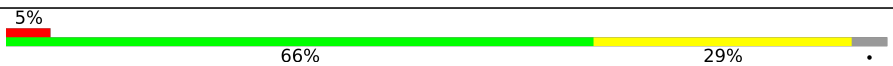
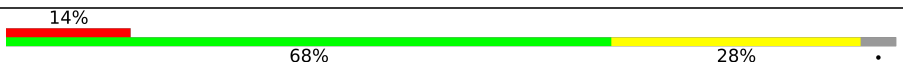
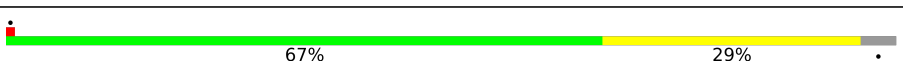
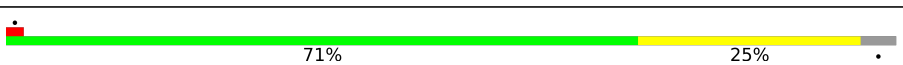
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	LB	445	69% 29%
9	LD	445	70% 27%
9	LF	445	74% 24%
9	LH	445	71% 26%
9	LJ	445	71% 27%
9	LL	445	67% 29%
9	LN	445	69% 28%
9	LP	445	73% 23%
9	MB	445	74% 22%
9	MD	445	70% 27%
9	MF	445	74% 22%
9	MH	445	70% 27%
9	MJ	445	79% 17%
9	ML	445	69% 28%
9	MN	445	74% 23%
9	MP	445	68% 29%
9	NB	445	63% 33%
9	ND	445	5% 69% 27%
9	NF	445	60% 36%
9	NH	445	61% 35%
9	NJ	445	60% 36%
9	NL	445	62% 34%
9	NN	445	62% 34%
9	NP	445	67% 29%
9	OB	445	6% 60% 36%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	OD	445	
9	OF	445	
9	OH	445	
9	OJ	445	
9	OL	445	
9	ON	445	
9	OP	445	
9	PB	445	
9	PD	445	
9	PF	445	
9	PH	445	
9	PJ	445	
9	PL	445	
9	PN	445	
9	PP	445	
9	QB	445	
9	QD	445	
9	QF	445	
9	QH	445	
9	QJ	445	
9	QL	445	
9	QN	445	
9	QP	445	
9	RD	445	
9	RF	445	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	RH	445	67% 29%
9	RJ	445	66% 30%
9	RL	445	68% 28%
9	RN	445	72% 24%
9	RP	445	10% 75% 22%
9	SB	445	68% 28%
9	SD	445	68% 28%
9	SF	445	63% 33%
9	SH	445	64% 31%
9	SJ	445	62% 34%
9	SL	445	66% 30%
9	SN	445	9% 66% 30%
9	TB	445	66% 29%
9	TD	445	68% 28%
9	TF	445	67% 29%
9	TH	445	64% 32%
9	TJ	445	63% 33%
9	TL	445	67% 28%
9	TN	445	5% 67% 28%
9	UB	445	66% 29%
9	UD	445	68% 28%
9	UF	445	69% 27%
9	UH	445	67% 29%
9	UJ	445	69% 27%
9	UL	445	6% 65% 30%

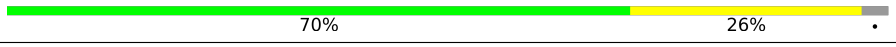
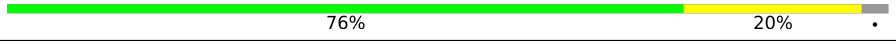
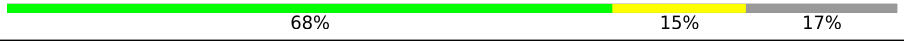
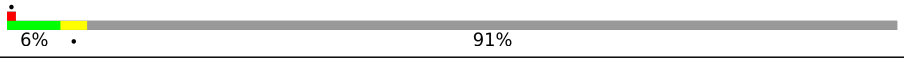
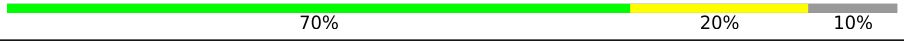
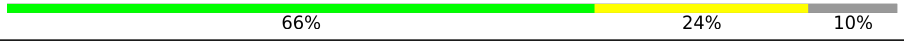
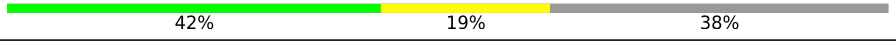
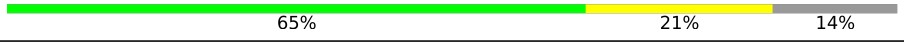
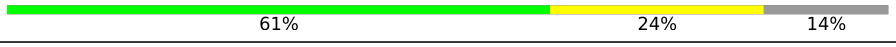
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	UN	445	10% 67% 29%
9	VB	445	67% 28%
9	VD	445	73% 23%
9	VF	445	67% 29%
9	VH	445	61% 35%
9	VJ	445	67% 28%
9	VL	445	69% 27%
9	VN	445	65% 31%
9	WB	445	69% 27%
9	WD	445	72% 24%
9	WF	445	72% 24%
9	WH	445	71% 25%
9	WJ	445	72% 24%
9	WL	445	72% 24%
9	WN	445	68% 28%
9	WP	445	6% 69% 27%
10	B	491	49% 15% 35%
10	C	491	39% 18% 43%
11	B0	430	6% 91%
11	B1	430	65% 19% 15%
11	B2	430	77% 20%
11	B3	430	74% 22%
11	B4	430	75% 21%
11	B5	430	30% 17% 53%
11	R0	430	30% 16% 54%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	R1	430	
11	R2	430	
11	R3	430	
11	R4	430	
11	R5	430	
12	C0	490	
12	C1	490	
12	C2	490	
12	C3	490	
12	C4	490	
12	C5	490	
12	C6	490	
12	S0	490	
12	S1	490	
12	S2	490	
12	S3	490	
12	S4	490	
12	S5	490	
12	S6	490	
12	S7	490	
12	S8	490	
12	S9	490	
13	D	470	
13	K3	470	
14	D0	447	

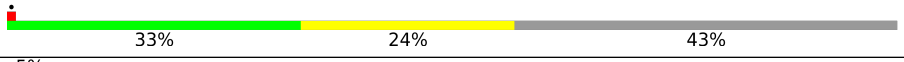
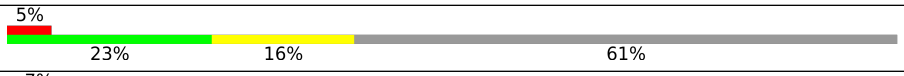
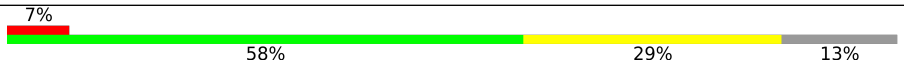
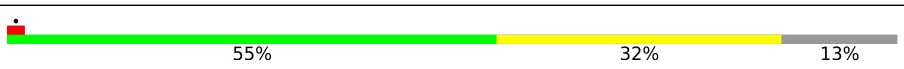
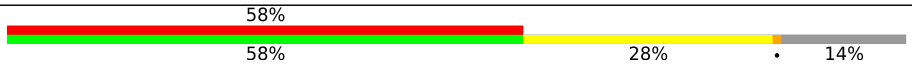
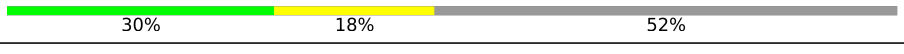
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	D1	447	74% 18% 8%
14	D2	447	77% 18% 5%
14	D3	447	73% 22% 5%
14	D4	447	73% 21% 5%
14	D5	447	11% 7% 81%
14	T0	447	18% 8% 73%
14	T1	447	68% 31%
14	T2	447	70% 28%
14	T3	447	79% 20%
14	T4	447	66% 23% 12%
14	T5	447	13% 13% 73%
15	E	303	73% 25%
15	F	303	13% 75% 23%
15	N2	303	74% 24%
16	G	122	9% 55% 20% 25%
17	H	319	37% 14% 49%
17	I	319	39% 16% 45%
17	J	319	41% 9% 50%
17	K	319	44% 11% 45%
17	L	319	37% 14% 49%
17	M	319	41% 13% 46%
17	N	319	37% 14% 49%
17	O7	319	35% 19% 46%
17	O8	319	21% 11% 68%
17	O9	319	24% 8% 68%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	P8	319	
17	P9	319	
17	Z2	319	
17	Z3	319	
17	Z4	319	
17	Z5	319	
18	I1	166	
19	J1	283	
19	J2	283	
19	J3	283	
19	J4	283	
19	J5	283	
20	K1	137	
20	K2	137	
21	L1	182	
22	M1	200	
22	M2	200	
22	M3	200	
22	M4	200	
23	O	379	
23	P	379	
23	Q	379	
24	O1	189	
24	O2	189	
24	O3	189	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
24	O4	189	68% 21% 12%
25	O5	648	56% 20% 24%
25	O6	648	93%
25	T	648	28% 15% 57%
25	U	648	52% 25% 22%
25	V	648	56% 24% 19%
26	P1	131	39% 19% 42%
26	P2	131	38% 37% 25%
27	P3	180	7% 45% 29% 25%
27	P4	180	64% 22% 14%
27	P5	180	61% 25% 14%
27	P6	180	58% 27% 14%
27	P7	180	6% 23% 7% 71%
28	Q1	206	72% 23%
28	Q2	206	68% 28%
28	Q3	206	73% 22%
28	Q4	206	7% 67% 29%
28	Q5	206	5% 91%
29	R	377	38% 13% 48%
29	S	377	67% 19% 14%
30	U0	557	49% 15% 36%
30	U1	557	57% 17% 25%
30	U2	557	60% 14% 25%
30	U3	557	59% 15% 25%
30	U4	557	28% 8% 64%

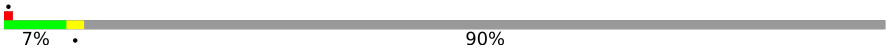
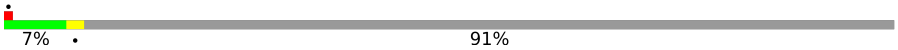
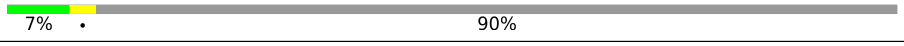
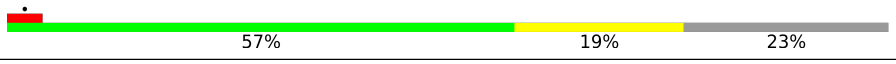
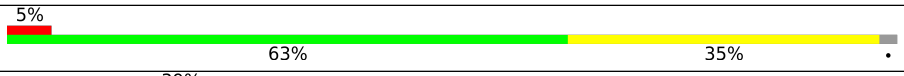
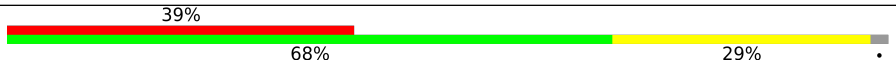
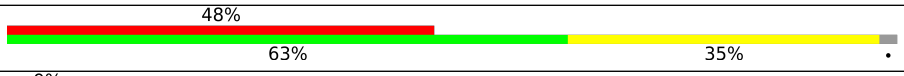
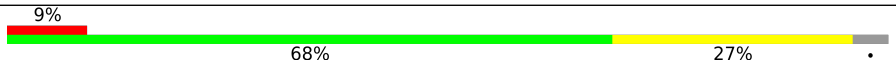
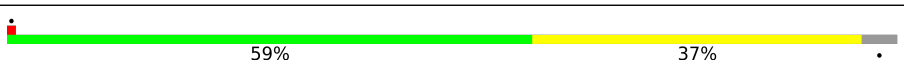
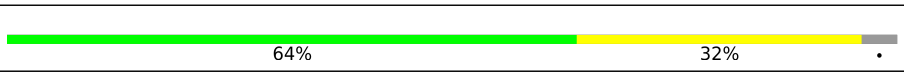
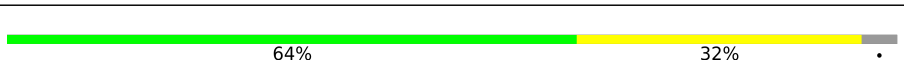
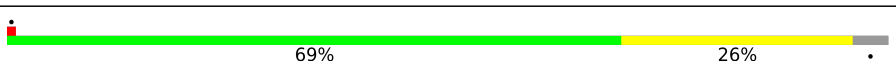
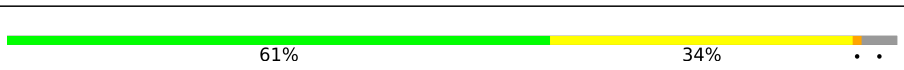
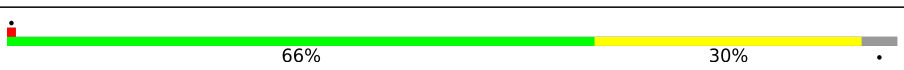
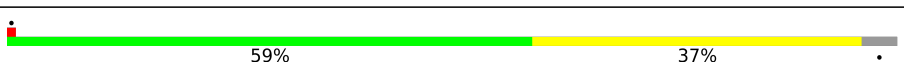
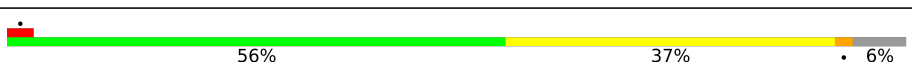
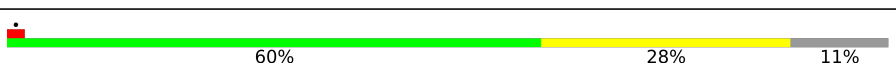
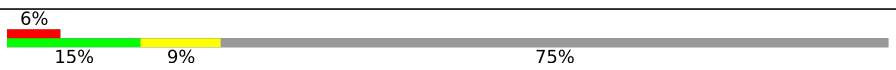
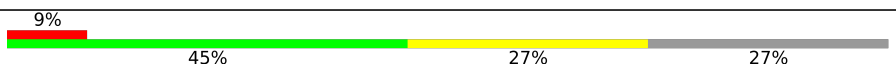
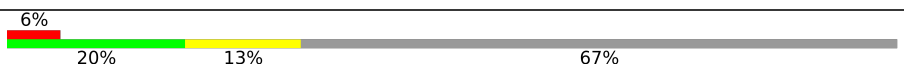
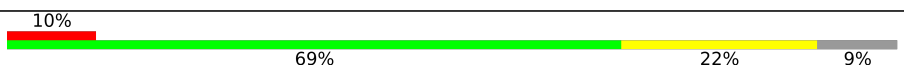
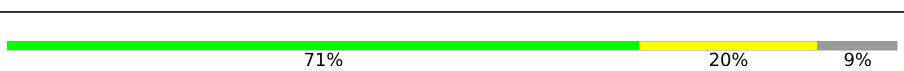
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	U5	557	8% 40% 17% 43%
30	U6	557	5% 55% 18% 26%
30	U7	557	55% 18% 26%
30	U8	557	8% 53% 20% 26%
30	U9	557	6% 22% 10% 67%
30	V0	557	26% 25% 12% 63%
30	V1	557	12% 48% 21% 30%
30	V2	557	50% 19% 30%
30	V3	557	11% 48% 21% 30%
30	V4	557	11% 36% 15% 49%
30	V5	557	37% 16% 47%
30	V6	557	50% 15% 35%
30	V7	557	38% 22% 40%
30	V8	557	41% 13% 46%
30	V9	557	12% 5% 82%
30	W0	557	35% 31% 22% 46%
30	W2	557	8% 38% 16% 46%
30	W4	557	47% 11% 42%
30	W5	557	44% 14% 42%
30	W6	557	50% 8% 42%
30	W7	557	44% 14% 42%
31	W	750	74% 25%
31	X	750	78% 21%
31	Y	750	74% 24%
31	Z	750	77% 21%

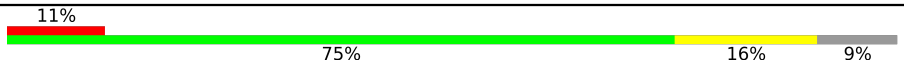
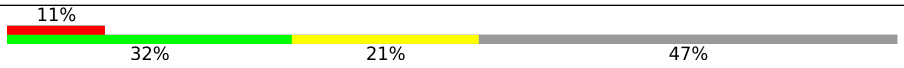
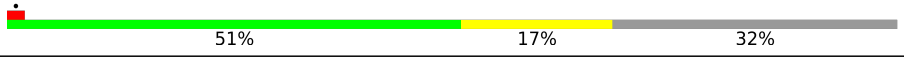
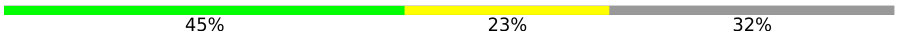
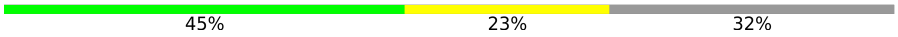
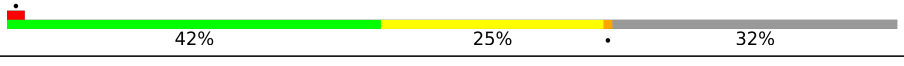
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
32	X0	260	
32	X1	260	
32	X2	260	
32	X3	260	
33	X4	427	
33	X5	427	
34	X6	273	
34	X7	273	
34	X8	273	
35	XA	193	
35	XB	193	
35	XC	193	
35	XD	193	
35	XE	193	
35	XF	193	
35	XG	193	
35	XH	193	
36	Y0	254	
36	Y1	254	
36	Y2	254	
36	Y3	254	
36	Y4	254	
36	Y5	254	
37	YA	241	
37	YB	241	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
37	YC	241	
37	YD	241	
37	YE	241	
37	YF	241	
37	YG	241	
37	YH	241	
38	Z1	216	
39	a	551	
39	a6	551	
39	b	551	
39	c	551	
39	d	551	
40	a1	229	
40	a2	229	
40	a3	229	
40	a4	229	
41	b1	499	
41	b2	499	
41	b3	499	
41	b4	499	
41	b5	499	
42	e	620	
42	f	620	
42	g	620	
43	h	255	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
43	i	255	72% 24%
43	j	255	73% 23%
43	k	255	65% 31%
44	h1	141	45% 24% 31%
44	h2	141	43% 27% 30%
44	h3	141	44% 26% 30%
44	h4	141	43% 27% 30%
45	i1	189	44% 17% 39%
45	l	189	43% 19% 39%
45	m	189	44% 17% 39%
45	n	189	42% 20% 39%
46	i2	1516	7% 88%
46	i3	1516	7% 88%
46	i4	1516	7% 88%
47	o	547	16% 24% 12% 64%
47	p	547	21% 51% 21% 28%
48	q	168	33% 11% 55%
48	r	168	36% 10% 54%
48	s	168	29% 17% 54%
49	y	167	42% 24% 34%

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 1650085 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	81	Total	C	N	O	S	0	0
			670	422	120	123	5		
1	7	141	Total	C	N	O	S	0	0
			1174	741	210	217	6		

- Molecule 2 is a protein called EF-hand domain-containing family member B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	462	Total	C	N	O	S	0	0
			3738	2356	672	700	10		
2	2	270	Total	C	N	O	S	0	0
			2160	1381	385	386	8		

- Molecule 3 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	475	Total	C	N	O	S	0	0
			4023	2453	784	770	16		
3	4	148	Total	C	N	O	S	0	0
			1230	747	241	235	7		

- Molecule 4 is a protein called Nucleoside diphosphate kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	376	Total	C	N	O	S	0	0
			2975	1885	517	553	20		
4	6	376	Total	C	N	O	S	0	0
			2975	1885	517	553	20		
4	j1	376	Total	C	N	O	S	0	0
			2975	1885	517	553	20		

- Molecule 5 is a protein called Cilia- and flagella-associated protein 107.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	176	Total	C	N	O	S	0	0
			1470	949	257	259	5		

- Molecule 6 is a protein called Cilia- and flagella-associated protein 141.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	94	Total	C	N	O	S	0	0
			806	507	150	145	4		
6	N1	94	Total	C	N	O	S	0	0
			806	507	150	145	4		

- Molecule 7 is a protein called Tektin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A0	54	Total	C	N	O	S	0	0
			444	271	89	83	1		
7	A1	359	Total	C	N	O	S	0	0
			2935	1818	527	580	10		
7	A2	401	Total	C	N	O	S	0	0
			3288	2038	595	645	10		
7	A3	401	Total	C	N	O	S	0	0
			3288	2038	595	645	10		
7	A4	399	Total	C	N	O	S	0	0
			3274	2029	592	643	10		
7	A5	169	Total	C	N	O	S	0	0
			1400	868	252	279	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AA	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	AC	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	AE	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	AG	441	Total	C	N	O	S	0	0
			3440	2179	584	655	22		
8	AI	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	AK	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AM	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	AO	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	BC	431	Total	C	N	O	S	0	0
			3374	2140	573	639	22		
8	BE	441	Total	C	N	O	S	0	0
			3440	2179	584	655	22		
8	BG	434	Total	C	N	O	S	0	0
			3396	2153	576	645	22		
8	BI	441	Total	C	N	O	S	0	0
			3440	2179	584	655	22		
8	BK	433	Total	C	N	O	S	0	0
			3390	2150	575	643	22		
8	BM	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	BO	434	Total	C	N	O	S	0	0
			3396	2153	576	645	22		
8	CC	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	CE	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	CG	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	CI	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	CK	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	CM	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	CO	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	CQ	437	Total	C	N	O	S	0	0
			3410	2162	580	646	22		
8	DC	432	Total	C	N	O	S	0	0
			3382	2146	574	640	22		
8	DE	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	DG	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	DI	431	Total	C	N	O	S	0	0
			3374	2142	573	637	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DK	431	Total	C	N	O	S	0	0
			3373	2141	573	637	22		
8	DM	432	Total	C	N	O	S	0	0
			3380	2143	574	641	22		
8	DO	431	Total	C	N	O	S	0	0
			3372	2139	573	638	22		
8	DQ	429	Total	C	N	O	S	0	0
			3360	2133	571	634	22		
8	EA	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	EC	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
8	EE	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	EG	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	EI	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	EK	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	EM	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	EO	437	Total	C	N	O	S	0	0
			3410	2162	580	646	22		
8	FA	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	FC	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	FE	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	FG	428	Total	C	N	O	S	0	0
			3351	2127	570	632	22		
8	FI	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	FK	431	Total	C	N	O	S	0	0
			3373	2141	573	637	22		
8	FM	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	FO	428	Total	C	N	O	S	0	0
			3355	2129	570	634	22		
8	GA	430	Total	C	N	O	S	0	0
			3368	2137	572	637	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	GC	431	Total	C	N	O	S	0	0
			3373	2141	573	637	22		
8	GE	431	Total	C	N	O	S	0	0
			3373	2141	573	637	22		
8	GG	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	GI	433	Total	C	N	O	S	0	0
			3387	2148	575	642	22		
8	GK	433	Total	C	N	O	S	0	0
			3387	2148	575	642	22		
8	GM	434	Total	C	N	O	S	0	0
			3395	2152	576	645	22		
8	GO	434	Total	C	N	O	S	0	0
			3395	2152	576	645	22		
8	HA	431	Total	C	N	O	S	0	0
			3371	2140	573	636	22		
8	HC	434	Total	C	N	O	S	0	0
			3389	2149	576	642	22		
8	HE	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	HG	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	HI	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	HK	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	HM	434	Total	C	N	O	S	0	0
			3389	2149	576	642	22		
8	HO	432	Total	C	N	O	S	0	0
			3381	2145	574	640	22		
8	IA	432	Total	C	N	O	S	0	0
			3380	2143	574	641	22		
8	IC	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	IE	441	Total	C	N	O	S	0	0
			3440	2179	584	655	22		
8	IG	433	Total	C	N	O	S	0	0
			3387	2148	575	642	22		
8	II	435	Total	C	N	O	S	0	0
			3399	2154	577	646	22		
8	IK	436	Total	C	N	O	S	0	0
			3411	2162	579	648	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	IM	434	Total	C	N	O	S	0	0
			3391	2150	576	643	22		
8	IO	440	Total	C	N	O	S	0	0
			3431	2174	583	652	22		
8	JC	434	Total	C	N	O	S	0	0
			3388	2147	576	643	22		
8	JE	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	JG	429	Total	C	N	O	S	0	0
			3360	2133	571	634	22		
8	JI	433	Total	C	N	O	S	0	0
			3390	2150	575	643	22		
8	JK	432	Total	C	N	O	S	0	0
			3381	2145	574	640	22		
8	JM	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	JO	432	Total	C	N	O	S	0	0
			3379	2144	574	639	22		
8	JQ	435	Total	C	N	O	S	0	0
			3403	2158	578	645	22		
8	KA	432	Total	C	N	O	S	0	0
			3380	2143	574	641	22		
8	KC	433	Total	C	N	O	S	0	0
			3389	2149	576	642	22		
8	KE	434	Total	C	N	O	S	0	0
			3397	2153	577	645	22		
8	KG	432	Total	C	N	O	S	0	0
			3380	2143	574	641	22		
8	KI	431	Total	C	N	O	S	0	0
			3374	2140	573	639	22		
8	KK	431	Total	C	N	O	S	0	0
			3372	2139	573	638	22		
8	KM	432	Total	C	N	O	S	0	0
			3380	2143	574	641	22		
8	KO	433	Total	C	N	O	S	0	0
			3389	2149	576	642	22		
8	LA	434	Total	C	N	O	S	0	0
			3396	2153	576	645	22		
8	LC	431	Total	C	N	O	S	0	0
			3374	2140	573	639	22		
8	LE	433	Total	C	N	O	S	0	0
			3388	2149	575	642	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LG	441	Total	C	N	O	S	0	0
			3440	2179	584	655	22		
8	LI	441	Total	C	N	O	S	0	0
			3440	2179	584	655	22		
8	LK	441	Total	C	N	O	S	0	0
			3440	2179	584	655	22		
8	LM	435	Total	C	N	O	S	0	0
			3404	2157	577	648	22		
8	LO	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	MA	431	Total	C	N	O	S	0	0
			3374	2140	573	639	22		
8	MC	431	Total	C	N	O	S	0	0
			3374	2140	573	639	22		
8	ME	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	MG	432	Total	C	N	O	S	0	0
			3380	2143	574	641	22		
8	MI	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
8	MK	433	Total	C	N	O	S	0	0
			3390	2150	575	643	22		
8	MM	432	Total	C	N	O	S	0	0
			3380	2143	574	641	22		
8	MO	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	NA	428	Total	C	N	O	S	0	0
			3353	2128	570	633	22		
8	NC	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	NE	434	Total	C	N	O	S	0	0
			3394	2152	576	644	22		
8	NG	432	Total	C	N	O	S	0	0
			3382	2146	574	640	22		
8	NI	431	Total	C	N	O	S	0	0
			3373	2141	573	637	22		
8	NK	431	Total	C	N	O	S	0	0
			3373	2141	573	637	22		
8	NM	432	Total	C	N	O	S	0	0
			3382	2146	574	640	22		
8	NO	432	Total	C	N	O	S	0	0
			3382	2146	574	640	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	OA	431	Total	C	N	O	S	0	0
			3374	2140	573	639	22		
8	OC	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	OE	431	Total	C	N	O	S	0	0
			3372	2139	573	638	22		
8	OG	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	OI	429	Total	C	N	O	S	0	0
			3360	2133	571	634	22		
8	OK	431	Total	C	N	O	S	0	0
			3374	2140	573	639	22		
8	OM	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	OO	425	Total	C	N	O	S	0	0
			3330	2114	567	628	21		
8	PC	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	PE	425	Total	C	N	O	S	0	0
			3330	2115	566	628	21		
8	PG	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	PI	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	PK	430	Total	C	N	O	S	0	0
			3367	2135	572	638	22		
8	PM	432	Total	C	N	O	S	0	0
			3380	2143	574	641	22		
8	PO	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	QC	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	QE	430	Total	C	N	O	S	0	0
			3366	2136	572	636	22		
8	QG	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	QI	427	Total	C	N	O	S	0	0
			3345	2124	569	630	22		
8	QK	427	Total	C	N	O	S	0	0
			3345	2124	569	630	22		
8	QM	426	Total	C	N	O	S	0	0
			3338	2119	568	629	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	QO	427	Total	C	N	O	S	0	0
			3345	2124	569	630	22		
8	RC	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	RE	428	Total	C	N	O	S	0	0
			3353	2128	570	633	22		
8	RG	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	RI	429	Total	C	N	O	S	0	0
			3360	2133	571	634	22		
8	RK	430	Total	C	N	O	S	0	0
			3368	2137	572	637	22		
8	RM	429	Total	C	N	O	S	0	0
			3361	2132	571	636	22		
8	RO	428	Total	C	N	O	S	0	0
			3353	2128	570	633	22		
8	SA	429	Total	C	N	O	S	0	0
			3359	2131	571	635	22		
8	SC	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	SE	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	SG	427	Total	C	N	O	S	0	0
			3345	2124	569	630	22		
8	SI	429	Total	C	N	O	S	0	0
			3360	2133	571	634	22		
8	SK	427	Total	C	N	O	S	0	0
			3345	2124	569	630	22		
8	SM	425	Total	C	N	O	S	0	0
			3333	2118	567	626	22		
8	TA	426	Total	C	N	O	S	0	0
			3342	2121	568	631	22		
8	TC	426	Total	C	N	O	S	0	0
			3337	2120	568	627	22		
8	TE	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	TG	426	Total	C	N	O	S	0	0
			3341	2122	568	629	22		
8	TI	427	Total	C	N	O	S	0	0
			3349	2126	569	632	22		
8	TK	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	TM	426	Total	C	N	O	S	0	0
			3341	2122	568	629	22		
8	UA	424	Total	C	N	O	S	0	0
			3327	2112	566	627	22		
8	UC	428	Total	C	N	O	S	0	0
			3351	2127	570	632	22		
8	UE	428	Total	C	N	O	S	0	0
			3351	2127	570	632	22		
8	UG	428	Total	C	N	O	S	0	0
			3353	2128	570	633	22		
8	UI	428	Total	C	N	O	S	0	0
			3352	2129	570	631	22		
8	UK	428	Total	C	N	O	S	0	0
			3353	2128	570	633	22		
8	UM	429	Total	C	N	O	S	0	0
			3359	2131	571	635	22		
8	UO	427	Total	C	N	O	S	0	0
			3347	2125	569	631	22		
8	VA	427	Total	C	N	O	S	0	0
			3345	2124	569	630	22		
8	VC	437	Total	C	N	O	S	0	0
			3410	2162	580	646	22		
8	VE	429	Total	C	N	O	S	0	0
			3358	2132	571	633	22		
8	VG	437	Total	C	N	O	S	0	0
			3410	2162	580	646	22		
8	VI	429	Total	C	N	O	S	0	0
			3360	2133	571	634	22		
8	VK	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
8	VM	429	Total	C	N	O	S	0	0
			3359	2131	571	635	22		
8	VO	436	Total	C	N	O	S	0	0
			3403	2157	579	645	22		
8	WA	436	Total	C	N	O	S	0	0
			3403	2157	579	645	22		
8	WC	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	WE	433	Total	C	N	O	S	0	0
			3382	2144	575	641	22		
8	WG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	WI	439	Total	C	N	O	S	0	0
			3424	2169	582	651	22		
8	WK	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
8	WM	431	Total	C	N	O	S	0	0
			3374	2140	573	639	22		
8	WO	429	Total	C	N	O	S	0	0
			3358	2132	571	633	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AB	432	Total	C	N	O	S	0	0
			3391	2129	580	656	26		
9	AD	435	Total	C	N	O	S	0	0
			3413	2141	583	663	26		
9	AF	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	AH	434	Total	C	N	O	S	0	0
			3404	2136	582	660	26		
9	AJ	434	Total	C	N	O	S	0	0
			3404	2136	582	660	26		
9	AL	434	Total	C	N	O	S	0	0
			3404	2136	582	660	26		
9	AN	434	Total	C	N	O	S	0	0
			3404	2136	582	660	26		
9	AP	432	Total	C	N	O	S	0	0
			3391	2129	580	656	26		
9	BB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	BD	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	BF	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	BH	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	BJ	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	BL	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	BN	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BP	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	CB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	CD	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	CF	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	CH	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	CJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	CL	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	CN	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	CP	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	DB	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	DD	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	DF	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	DH	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	DJ	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	DL	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	DN	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	DP	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	EB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	ED	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	EF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	EH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	EJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	EL	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	EN	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	FB	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	FD	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	FF	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	FH	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	FJ	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	FL	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	FN	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	GB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	GD	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	GF	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	GH	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	GJ	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	GL	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	GN	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	HB	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	HD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	HF	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	HH	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	HJ	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	HL	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	HN	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	HP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	IB	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	ID	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	IF	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	IH	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	IJ	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	IL	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	IN	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	IP	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	JB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	JD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	JF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	JH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	JJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	JL	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	JN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	JP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	KB	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	KD	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	KF	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	KH	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	KJ	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	KL	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	KN	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	KP	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	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	LF	439	Total	C	N	O	S	0	0
			3451	2165	587	673	26		
9	LH	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	LJ	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		
9	LL	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	LN	432	Total	C	N	O	S	0	0
			3391	2129	580	656	26		
9	LP	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	MB	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	MD	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	MF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	MH	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	MJ	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	ML	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	MN	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	MP	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	NB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	ND	431	Total	C	N	O	S	0	0
			3382	2124	579	653	26		
9	NF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	NH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	NJ	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	NL	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	NN	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	NP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	OB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	OD	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	OF	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	OH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	OJ	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	OL	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	ON	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	OP	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	PB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	PD	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	PF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	PH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	PJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	PL	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	PN	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	PP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	QB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	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	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	QJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	QL	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	QN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	QP	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	RD	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	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	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	RP	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SD	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	SH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	SJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	SL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	SN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	TB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	TD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	TF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	TH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	TJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	TL	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	TN	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	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	UF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	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	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	VB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	VJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	VL	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	VN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	WD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	WF	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
9	WH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	WJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	WL	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	WN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	WP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

- Molecule 10 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	319	Total	C	N	O	S	0	0
			2769	1697	520	539	13		
10	C	279	Total	C	N	O	S	0	0
			2408	1493	445	459	11		

- Molecule 11 is a protein called Tektin-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	B0	39	Total	C	N	O	0	0
			334	203	66	65		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
11	B1	364	Total C N O S 2984 1840 547 586 11	0	0
11	B2	414	Total C N O S 3401 2093 627 667 14	0	0
11	B3	414	Total C N O S 3401 2093 627 667 14	0	0
11	B4	415	Total C N O S 3412 2099 631 668 14	0	0
11	B5	203	Total C N O S 1675 1036 305 325 9	0	0
11	R0	196	Total C N O S 1612 996 294 313 9	0	0
11	R1	415	Total C N O S 3412 2099 631 668 14	0	0
11	R2	415	Total C N O S 3412 2099 631 668 14	0	0
11	R3	415	Total C N O S 3412 2099 631 668 14	0	0
11	R4	369	Total C N O S 3025 1864 555 595 11	0	0
11	R5	43	Total C N O 366 224 73 69	0	0

- Molecule 12 is a protein called Tektin-3.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	C0	179	Total C N O S 1453 887 270 293 3	0	0
12	C1	411	Total C N O S 3354 2064 616 658 16	0	0
12	C2	411	Total C N O S 3354 2064 616 658 16	0	0
12	C3	408	Total C N O S 3332 2050 613 654 15	0	0
12	C4	363	Total C N O S 2944 1810 539 580 15	0	0
12	C5	51	Total C N O S 420 259 78 81 2	0	0
12	C6	42	Total C N O S 354 220 69 63 2	0	0
12	S0	325	Total C N O S 2675 1642 499 521 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S1	441	Total	C	N	O	S	0	0
			3613	2223	669	705	16		
12	S2	441	Total	C	N	O	S	0	0
			3613	2223	669	705	16		
12	S3	441	Total	C	N	O	S	0	0
			3613	2223	669	705	16		
12	S4	303	Total	C	N	O	S	0	0
			2459	1515	446	485	13		
12	S5	313	Total	C	N	O	S	0	0
			2568	1581	472	504	11		
12	S6	422	Total	C	N	O	S	0	0
			3453	2130	633	676	14		
12	S7	422	Total	C	N	O	S	0	0
			3453	2130	633	676	14		
12	S8	420	Total	C	N	O	S	0	0
			3435	2117	631	673	14		
12	S9	276	Total	C	N	O	S	0	0
			2232	1370	409	440	13		

- Molecule 13 is a protein called Sperm-associated antigen 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	77	Total	C	N	O	S	0	0
			622	393	112	116	1		
13	K3	179	Total	C	N	O	S	0	0
			1460	911	268	274	7		

- Molecule 14 is a protein called Tektin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D0	109	Total	C	N	O	S	0	0
			889	545	164	178	2		
14	D1	411	Total	C	N	O	S	0	0
			3370	2070	621	663	16		
14	D2	424	Total	C	N	O	S	0	0
			3480	2133	647	683	17		
14	D3	424	Total	C	N	O	S	0	0
			3480	2133	647	683	17		
14	D4	424	Total	C	N	O	S	0	0
			3480	2133	647	683	17		
14	D5	87	Total	C	N	O	S	0	0
			715	436	139	138	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T0	119	Total	C	N	O	S	0	0
			957	588	173	193	3		
14	T1	440	Total	C	N	O	S	0	0
			3594	2206	664	706	18		
14	T2	440	Total	C	N	O	S	0	0
			3594	2206	664	706	18		
14	T3	441	Total	C	N	O	S	0	0
			3606	2215	665	708	18		
14	T4	395	Total	C	N	O	S	0	0
			3260	1997	608	639	16		
14	T5	119	Total	C	N	O	S	0	0
			975	600	180	191	4		

- Molecule 15 is a protein called Cilia- and flagella-associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	298	Total	C	N	O	S	0	0
			2372	1486	423	446	17		
15	F	297	Total	C	N	O	S	0	0
			2363	1481	421	444	17		
15	N2	297	Total	C	N	O	S	0	0
			2363	1481	421	444	17		

- Molecule 16 is a protein called Piercer of microtubule wall 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	91	Total	C	N	O	S	0	0
			724	462	123	134	5		

- Molecule 17 is a protein called Protein FAM166A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	162	Total	C	N	O	S	0	0
			1316	841	234	233	8		
17	I	175	Total	C	N	O	S	0	0
			1429	912	259	250	8		
17	J	161	Total	C	N	O	S	0	0
			1307	835	232	232	8		
17	K	174	Total	C	N	O	S	0	0
			1420	906	257	249	8		
17	L	162	Total	C	N	O	S	0	0
			1316	841	234	233	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	173	Total	C	N	O	S	0	0
			1413	902	256	247	8		
17	N	162	Total	C	N	O	S	0	0
			1316	841	234	233	8		
17	O7	173	Total	C	N	O	S	0	0
			1413	902	256	247	8		
17	O8	103	Total	C	N	O	S	0	0
			837	539	141	153	4		
17	O9	103	Total	C	N	O	S	0	0
			837	539	141	153	4		
17	P8	103	Total	C	N	O	S	0	0
			837	539	141	153	4		
17	P9	103	Total	C	N	O	S	0	0
			837	539	141	153	4		
17	Z2	51	Total	C	N	O	S	0	0
			412	265	74	69	4		
17	Z3	51	Total	C	N	O	S	0	0
			412	265	74	69	4		
17	Z4	51	Total	C	N	O	S	0	0
			412	265	74	69	4		
17	Z5	50	Total	C	N	O	S	0	0
			405	260	73	68	4		

- Molecule 18 is a protein called Cilia- and flagella-associated protein 68.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I1	94	Total	C	N	O	S	0	0
			796	503	145	145	3		

- Molecule 19 is a protein called Cilia and flagella-associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J1	111	Total	C	N	O	S	0	0
			934	596	177	158	3		
19	J2	247	Total	C	N	O	S	0	0
			2010	1269	377	353	11		
19	J3	247	Total	C	N	O	S	0	0
			2010	1269	377	353	11		
19	J4	245	Total	C	N	O	S	0	0
			1992	1259	374	348	11		
19	J5	126	Total	C	N	O	S	0	0
			1001	626	188	180	7		

- Molecule 20 is a protein called Family with sequence similarity 183, member B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K1	118	Total	C	N	O	S	0	0
			1009	640	187	181	1		
20	K2	118	Total	C	N	O	S	0	0
			1009	640	187	181	1		

- Molecule 21 is a protein called Cilia- and flagella-associated protein 90.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L1	126	Total	C	N	O	S	0	0
			1034	652	193	187	2		

- Molecule 22 is a protein called Protein FAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M1	96	Total	C	N	O		0	0
			826	529	148	149			
22	M2	96	Total	C	N	O		0	0
			826	529	148	149			
22	M3	156	Total	C	N	O	S	0	0
			1280	821	223	233	3		
22	M4	96	Total	C	N	O		0	0
			826	529	148	149			

- Molecule 23 is a protein called RIB43A-like with coiled-coils protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	74	Total	C	N	O	S	0	0
			627	386	124	115	2		
23	P	347	Total	C	N	O	S	0	0
			2875	1751	564	549	11		
23	Q	103	Total	C	N	O	S	0	0
			858	522	165	169	2		

- Molecule 24 is a protein called Dual specificity phosphatase 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O1	166	Total	C	N	O	S	0	0
			1332	856	225	244	7		
24	O2	167	Total	C	N	O	S	0	0
			1344	865	226	246	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O3	167	Total	C	N	O	S	0	0
			1344	865	226	246	7		
24	O4	167	Total	C	N	O	S	0	0
			1344	865	226	246	7		

- Molecule 25 is a protein called EF-hand domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O5	491	Total	C	N	O	S	0	0
			4047	2608	682	740	17		
25	O6	48	Total	C	N	O	S	0	0
			383	240	73	69	1		
25	T	280	Total	C	N	O	S	0	0
			2365	1525	396	433	11		
25	U	503	Total	C	N	O	S	0	0
			4138	2671	694	756	17		
25	V	524	Total	C	N	O	S	0	0
			4299	2773	720	789	17		

- Molecule 26 is a protein called Testis expressed 49.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P1	76	Total	C	N	O	S	0	0
			637	409	117	109	2		
26	P2	98	Total	C	N	O	S	0	0
			825	531	152	140	2		

- Molecule 27 is a protein called Testis-expressed sequence 37 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P3	135	Total	C	N	O	S	0	0
			1103	719	187	190	7		
27	P4	155	Total	C	N	O	S	0	0
			1272	829	211	224	8		
27	P5	155	Total	C	N	O	S	0	0
			1272	829	211	224	8		
27	P6	154	Total	C	N	O	S	0	0
			1263	824	210	221	8		
27	P7	53	Total	C	N	O	S	0	0
			447	293	70	82	2		

- Molecule 28 is a protein called Tektin bundle-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q1	199	Total	C	N	O	S	0	0
			1634	1046	305	277	6		
28	Q2	199	Total	C	N	O	S	0	0
			1634	1046	305	277	6		
28	Q3	199	Total	C	N	O	S	0	0
			1634	1046	305	277	6		
28	Q4	199	Total	C	N	O	S	0	0
			1634	1046	305	277	6		
28	Q5	18	Total	C	N	O	S	0	0
			152	101	28	22	1		

- Molecule 29 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	R	195	Total	C	N	O	S	0	0
			1648	1010	324	304	10		
29	S	323	Total	C	N	O	S	0	0
			2728	1662	539	512	15		

- Molecule 30 is a protein called Tektin-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U0	355	Total	C	N	O	S	0	0
			2897	1793	524	557	23		
30	U1	415	Total	C	N	O	S	0	0
			3396	2101	624	646	25		
30	U2	415	Total	C	N	O	S	0	0
			3396	2101	624	646	25		
30	U3	415	Total	C	N	O	S	0	0
			3396	2101	624	646	25		
30	U4	201	Total	C	N	O	S	0	0
			1664	1019	319	319	7		
30	U5	318	Total	C	N	O	S	0	0
			2607	1604	484	501	18		
30	U6	410	Total	C	N	O	S	0	0
			3360	2079	619	638	24		
30	U7	410	Total	C	N	O	S	0	0
			3360	2079	619	638	24		
30	U8	410	Total	C	N	O	S	0	0
			3360	2079	619	638	24		
30	U9	182	Total	C	N	O	S	0	0
			1486	932	266	275	13		
30	V0	208	Total	C	N	O	S	0	0
			1695	1061	300	319	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V1	389	Total	C	N	O	S	0	0
			3185	1967	583	612	23		
30	V2	389	Total	C	N	O	S	0	0
			3185	1967	583	612	23		
30	V3	389	Total	C	N	O	S	0	0
			3185	1967	583	612	23		
30	V4	284	Total	C	N	O	S	0	0
			2325	1425	429	454	17		
30	V5	294	Total	C	N	O	S	0	0
			2408	1493	432	466	17		
30	V6	364	Total	C	N	O	S	0	0
			2980	1841	542	577	20		
30	V7	334	Total	C	N	O	S	0	0
			2736	1700	493	522	21		
30	V8	303	Total	C	N	O	S	0	0
			2477	1539	442	479	17		
30	V9	99	Total	C	N	O	S	0	0
			800	507	136	153	4		
30	W0	298	Total	C	N	O	S	0	0
			2447	1513	449	465	20		
30	W2	300	Total	C	N	O	S	0	0
			2458	1522	447	469	20		
30	W4	323	Total	C	N	O	S	0	0
			2662	1655	486	502	19		
30	W5	323	Total	C	N	O	S	0	0
			2662	1655	486	502	19		
30	W6	323	Total	C	N	O	S	0	0
			2662	1655	486	502	19		
30	W7	323	Total	C	N	O	S	0	0
			2662	1655	486	502	19		

- Molecule 31 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	741	Total	C	N	O	S	0	0
			6116	3950	1019	1119	28		
31	X	741	Total	C	N	O	S	0	0
			6116	3950	1019	1119	28		
31	Y	742	Total	C	N	O	S	0	0
			6124	3954	1021	1121	28		
31	Z	741	Total	C	N	O	S	0	0
			6116	3950	1019	1119	28		

- Molecule 32 is a protein called Spermatid-specific manchette-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X0	25	Total	C	N	O	S	0	0
			200	124	34	38	4		
32	X1	24	Total	C	N	O	S	0	0
			192	118	33	37	4		
32	X2	24	Total	C	N	O	S	0	0
			192	118	33	37	4		
32	X3	25	Total	C	N	O	S	0	0
			200	124	34	38	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	X4	330	Total	C	N	O	S	0	0
			2619	1638	471	509	1		
33	X5	133	Total	C	N	O	S	0	0
			1041	658	182	196	5		

- Molecule 34 is a protein called Testis-specific serine/threonine-protein kinase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	X6	267	Total	C	N	O	S	0	0
			2097	1335	380	374	8		
34	X7	267	Total	C	N	O	S	0	0
			2097	1335	380	374	8		
34	X8	267	Total	C	N	O	S	0	0
			2097	1335	380	374	8		

- Molecule 35 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	XA	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
35	XB	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
35	XC	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
35	XD	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
35	XE	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
35	XF	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
35	XG	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
35	XH	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		

- Molecule 36 is a protein called Outer dense fiber protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Y0	63	Total	C	N	O	S	0	0
			483	313	87	80	3		
36	Y1	240	Total	C	N	O	S	0	0
			1828	1176	317	327	8		
36	Y2	225	Total	C	N	O	S	0	0
			1711	1101	294	309	7		
36	Y3	63	Total	C	N	O	S	0	0
			483	313	87	80	3		
36	Y4	185	Total	C	N	O	S	0	0
			1412	910	241	255	6		
36	Y5	85	Total	C	N	O	S	0	0
			644	411	110	120	3		

- Molecule 37 is a protein called Parkin coregulated gene protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	YA	220	Total	C	N	O	S	0	0
			1775	1148	300	317	10		
37	YB	220	Total	C	N	O	S	0	0
			1775	1148	300	317	10		
37	YC	220	Total	C	N	O	S	0	0
			1775	1148	300	317	10		
37	YD	220	Total	C	N	O	S	0	0
			1775	1148	300	317	10		
37	YE	220	Total	C	N	O	S	0	0
			1775	1148	300	317	10		
37	YF	220	Total	C	N	O	S	0	0
			1775	1148	300	317	10		
37	YG	220	Total	C	N	O	S	0	0
			1775	1148	300	317	10		
37	YH	220	Total	C	N	O	S	0	0
			1775	1148	300	317	10		

- Molecule 38 is a protein called Testis, prostate and placenta-expressed protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Z1	33	Total	C	N	O	S	0	0
			279	181	48	48	2		

- Molecule 39 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a	294	Total	C	N	O	S	0	0
			2499	1522	478	485	14		
39	a6	70	Total	C	N	O	S	0	0
			572	363	99	108	2		
39	b	244	Total	C	N	O	S	0	0
			2092	1266	420	399	7		
39	c	413	Total	C	N	O	S	0	0
			3528	2141	692	680	15		
39	d	135	Total	C	N	O	S	0	0
			1155	701	233	219	2		

- Molecule 40 is a protein called Uncharacterized protein C10orf82 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	a1	156	Total	C	N	O	S	0	0
			1277	818	218	231	10		
40	a2	156	Total	C	N	O	S	0	0
			1277	818	218	231	10		
40	a3	156	Total	C	N	O	S	0	0
			1277	818	218	231	10		
40	a4	156	Total	C	N	O	S	0	0
			1277	818	218	231	10		

- Molecule 41 is a protein called Coiled-coil domain-containing protein 105.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	b1	132	Total	C	N	O	S	0	0
			1081	670	212	188	11		
41	b2	381	Total	C	N	O	S	0	0
			3091	1915	598	555	23		
41	b3	382	Total	C	N	O	S	0	0
			3102	1921	602	556	23		
41	b4	382	Total	C	N	O	S	0	0
			3102	1921	602	556	23		
41	b5	333	Total	C	N	O	S	0	0
			2705	1675	519	489	22		

- Molecule 42 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	e	607	Total	C	N	O	S	0	0
			4689	2967	818	872	32		
42	f	607	Total	C	N	O	S	0	0
			4689	2967	818	872	32		
42	g	607	Total	C	N	O	S	0	0
			4689	2967	818	872	32		

- Molecule 43 is a protein called Enkurin.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	247	Total	C	N	O	S	0	0
			2014	1287	351	367	9		
43	i	245	Total	C	N	O	S	0	0
			1999	1279	349	362	9		
43	j	244	Total	C	N	O	S	0	0
			1993	1276	348	360	9		
43	k	245	Total	C	N	O	S	0	0
			1999	1279	349	362	9		

- Molecule 44 is a protein called Testis-expressed protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h1	97	Total	C	N	O	S	0	0
			787	506	139	136	6		
44	h2	99	Total	C	N	O	S	0	0
			809	518	147	138	6		
44	h3	99	Total	C	N	O	S	0	0
			809	518	147	138	6		
44	h4	98	Total	C	N	O	S	0	0
			798	512	143	137	6		

- Molecule 45 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i1	116	Total	C	N	O	S	0	0
			909	579	162	165	3		
45	l	116	Total	C	N	O	S	0	0
			909	579	162	165	3		
45	m	116	Total	C	N	O	S	0	0
			909	579	162	165	3		
45	n	116	Total	C	N	O	S	0	0
			909	579	162	165	3		

- Molecule 46 is a protein called EF-hand calcium-binding domain-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	i2	180	Total	C	N	O	S	0	0
			1500	956	263	271	10		
46	i3	180	Total	C	N	O	S	0	0
			1500	956	263	271	10		
46	i4	180	Total	C	N	O	S	0	0
			1500	956	263	271	10		

- Molecule 47 is a protein called Cilia- and flagella-associated protein 210.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	199	Total	C	N	O	S	0	0
			1688	1040	321	322	5		
47	p	395	Total	C	N	O	S	0	0
			3300	2045	601	643	11		

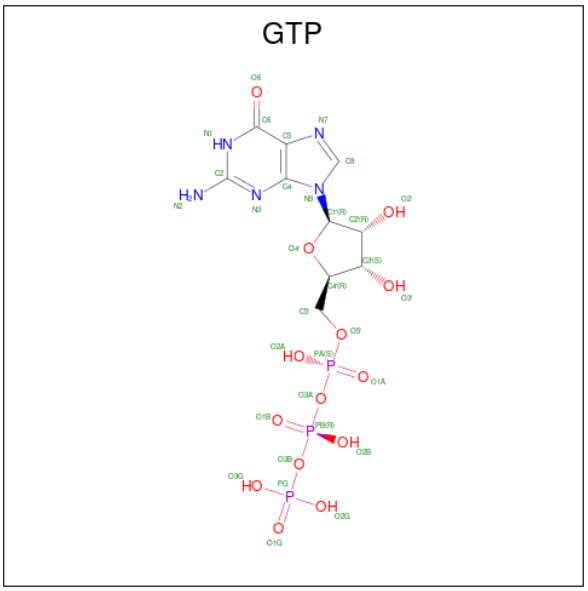
- Molecule 48 is a protein called Cilia- and flagella-associated protein 276.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	q	75	Total	C	N	O	0	0
			599	379	108	112		
48	r	78	Total	C	N	O	0	0
			625	395	114	116		
48	s	78	Total	C	N	O	0	0
			625	395	114	116		

- Molecule 49 is a protein called Piercer of microtubule wall 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	111	Total	C	N	O	S	0	0
			911	577	165	166	3		

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
50	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	AM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	AO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	BM	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
50	BO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	CC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	CE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	CG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	CI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	CK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	CM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	CO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	CQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	DC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	DE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	DG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	DI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	DK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	DM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	DO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	DQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	EA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	EC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	EE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	EG	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
50	EI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	EK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	EM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	EO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	FA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	FC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	FE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	FG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	FI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	FK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	FM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	FO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	GA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	GC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	GE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	GG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	GI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	GK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	GM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	GO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	HA	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
50	HC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	HE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	HG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	HI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	HK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	HM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	HO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	IA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	IC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	IE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	IG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	II	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	IK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	IM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	IO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	JC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	JE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	JG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	JI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	JK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	JM	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
50	JO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	JQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	KA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	KC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	KE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	KG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	KI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	KK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	KM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	KO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	LA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	LC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	LE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	LG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	LI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	LK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	LM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	LO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	MA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	MC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	ME	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
50	MG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	MI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	MK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	MM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	MO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	NA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	NC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	NE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	NG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	NI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	NK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	NM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	NO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	OA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	OC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	OE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	OG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	OI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	OK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	OM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	OO	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
50	PC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	PE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	PG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	PI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	PK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	PM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	PO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	QC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	QE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	QG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	QI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	QK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	QM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	QO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	RC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	RE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	RG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	RI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	RK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	RM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	RO	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
50	SA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	SC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	SE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	SG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	SK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	SM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	TA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	TC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	TE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	TG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	TI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	TK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	TM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	UA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	UC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	UE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	UG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	UI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	UK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	UM	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
50	UO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	VA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	VC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	VE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	VG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	VI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	VK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	VM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	VO	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	WA	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	WC	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	WE	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	WG	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	WI	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	WK	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	WM	1	Total	C	N	O	P	0
			32	10	5	14	3	
50	WO	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	AA	1	Total	Mg	0
			1	1	
51	AC	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
51	AE	1	Total Mg 1 1	0
51	AG	1	Total Mg 1 1	0
51	AI	1	Total Mg 1 1	0
51	AK	1	Total Mg 1 1	0
51	AM	1	Total Mg 1 1	0
51	AO	1	Total Mg 1 1	0
51	BC	1	Total Mg 1 1	0
51	BE	1	Total Mg 1 1	0
51	BG	1	Total Mg 1 1	0
51	BI	1	Total Mg 1 1	0
51	BK	1	Total Mg 1 1	0
51	BM	1	Total Mg 1 1	0
51	BO	1	Total Mg 1 1	0
51	CC	1	Total Mg 1 1	0
51	CE	1	Total Mg 1 1	0
51	CG	1	Total Mg 1 1	0
51	CI	1	Total Mg 1 1	0
51	CK	1	Total Mg 1 1	0
51	CM	1	Total Mg 1 1	0
51	CO	1	Total Mg 1 1	0
51	CQ	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
51	DC	1	Total Mg 1 1	0
51	DE	1	Total Mg 1 1	0
51	DG	1	Total Mg 1 1	0
51	DI	1	Total Mg 1 1	0
51	DK	1	Total Mg 1 1	0
51	DM	1	Total Mg 1 1	0
51	DO	1	Total Mg 1 1	0
51	DQ	1	Total Mg 1 1	0
51	EA	1	Total Mg 1 1	0
51	EC	1	Total Mg 1 1	0
51	EE	1	Total Mg 1 1	0
51	EG	1	Total Mg 1 1	0
51	EI	1	Total Mg 1 1	0
51	EK	1	Total Mg 1 1	0
51	EM	1	Total Mg 1 1	0
51	EO	1	Total Mg 1 1	0
51	FA	1	Total Mg 1 1	0
51	FC	1	Total Mg 1 1	0
51	FE	1	Total Mg 1 1	0
51	FG	1	Total Mg 1 1	0
51	FI	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
51	FK	1	Total Mg 1 1	0
51	FM	1	Total Mg 1 1	0
51	FO	1	Total Mg 1 1	0
51	GA	1	Total Mg 1 1	0
51	GC	1	Total Mg 1 1	0
51	GE	1	Total Mg 1 1	0
51	GG	1	Total Mg 1 1	0
51	GI	1	Total Mg 1 1	0
51	GK	1	Total Mg 1 1	0
51	GM	1	Total Mg 1 1	0
51	GO	1	Total Mg 1 1	0
51	HA	1	Total Mg 1 1	0
51	HC	1	Total Mg 1 1	0
51	HE	1	Total Mg 1 1	0
51	HG	1	Total Mg 1 1	0
51	HI	1	Total Mg 1 1	0
51	HK	1	Total Mg 1 1	0
51	HM	1	Total Mg 1 1	0
51	HO	1	Total Mg 1 1	0
51	IA	1	Total Mg 1 1	0
51	IC	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
51	IE	1	Total Mg 1 1	0
51	IG	1	Total Mg 1 1	0
51	II	1	Total Mg 1 1	0
51	IK	1	Total Mg 1 1	0
51	IM	1	Total Mg 1 1	0
51	IO	1	Total Mg 1 1	0
51	JC	1	Total Mg 1 1	0
51	JE	1	Total Mg 1 1	0
51	JG	1	Total Mg 1 1	0
51	JI	1	Total Mg 1 1	0
51	JK	1	Total Mg 1 1	0
51	JM	1	Total Mg 1 1	0
51	JO	1	Total Mg 1 1	0
51	JQ	1	Total Mg 1 1	0
51	KA	1	Total Mg 1 1	0
51	KC	1	Total Mg 1 1	0
51	KE	1	Total Mg 1 1	0
51	KG	1	Total Mg 1 1	0
51	KI	1	Total Mg 1 1	0
51	KK	1	Total Mg 1 1	0
51	KM	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
51	KO	1	Total Mg 1 1	0
51	LA	1	Total Mg 1 1	0
51	LC	1	Total Mg 1 1	0
51	LE	1	Total Mg 1 1	0
51	LG	1	Total Mg 1 1	0
51	LI	1	Total Mg 1 1	0
51	LK	1	Total Mg 1 1	0
51	LM	1	Total Mg 1 1	0
51	LO	1	Total Mg 1 1	0
51	MA	1	Total Mg 1 1	0
51	MC	1	Total Mg 1 1	0
51	ME	1	Total Mg 1 1	0
51	MG	1	Total Mg 1 1	0
51	MI	1	Total Mg 1 1	0
51	MK	1	Total Mg 1 1	0
51	MM	1	Total Mg 1 1	0
51	MO	1	Total Mg 1 1	0
51	NA	1	Total Mg 1 1	0
51	NC	1	Total Mg 1 1	0
51	NE	1	Total Mg 1 1	0
51	NG	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
51	NI	1	Total Mg 1 1	0
51	NK	1	Total Mg 1 1	0
51	NM	1	Total Mg 1 1	0
51	NO	1	Total Mg 1 1	0
51	OA	1	Total Mg 1 1	0
51	OC	1	Total Mg 1 1	0
51	OE	1	Total Mg 1 1	0
51	OG	1	Total Mg 1 1	0
51	OI	1	Total Mg 1 1	0
51	OK	1	Total Mg 1 1	0
51	OM	1	Total Mg 1 1	0
51	OO	1	Total Mg 1 1	0
51	PC	1	Total Mg 1 1	0
51	PE	1	Total Mg 1 1	0
51	PG	1	Total Mg 1 1	0
51	PI	1	Total Mg 1 1	0
51	PK	1	Total Mg 1 1	0
51	PM	1	Total Mg 1 1	0
51	PO	1	Total Mg 1 1	0
51	QC	1	Total Mg 1 1	0
51	QE	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
51	QG	1	Total Mg 1 1	0
51	QI	1	Total Mg 1 1	0
51	QK	1	Total Mg 1 1	0
51	QM	1	Total Mg 1 1	0
51	QO	1	Total Mg 1 1	0
51	RC	1	Total Mg 1 1	0
51	RE	1	Total Mg 1 1	0
51	RG	1	Total Mg 1 1	0
51	RI	1	Total Mg 1 1	0
51	RK	1	Total Mg 1 1	0
51	RM	1	Total Mg 1 1	0
51	RO	1	Total Mg 1 1	0
51	SA	1	Total Mg 1 1	0
51	SC	1	Total Mg 1 1	0
51	SE	1	Total Mg 1 1	0
51	SG	1	Total Mg 1 1	0
51	SI	1	Total Mg 1 1	0
51	SK	1	Total Mg 1 1	0
51	SM	1	Total Mg 1 1	0
51	TA	1	Total Mg 1 1	0
51	TC	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

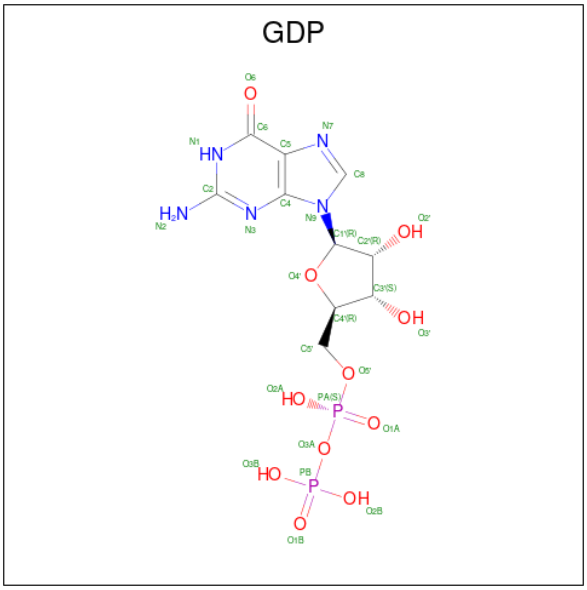
Mol	Chain	Residues	Atoms	AltConf
51	TE	1	Total Mg 1 1	0
51	TG	1	Total Mg 1 1	0
51	TI	1	Total Mg 1 1	0
51	TK	1	Total Mg 1 1	0
51	TM	1	Total Mg 1 1	0
51	UA	1	Total Mg 1 1	0
51	UC	1	Total Mg 1 1	0
51	UE	1	Total Mg 1 1	0
51	UG	1	Total Mg 1 1	0
51	UI	1	Total Mg 1 1	0
51	UK	1	Total Mg 1 1	0
51	UM	1	Total Mg 1 1	0
51	UO	1	Total Mg 1 1	0
51	VA	1	Total Mg 1 1	0
51	VC	1	Total Mg 1 1	0
51	VE	1	Total Mg 1 1	0
51	VG	1	Total Mg 1 1	0
51	VI	1	Total Mg 1 1	0
51	VK	1	Total Mg 1 1	0
51	VM	1	Total Mg 1 1	0
51	VO	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
51	WA	1	Total Mg 1 1	0
51	WC	1	Total Mg 1 1	0
51	WE	1	Total Mg 1 1	0
51	WG	1	Total Mg 1 1	0
51	WI	1	Total Mg 1 1	0
51	WK	1	Total Mg 1 1	0
51	WM	1	Total Mg 1 1	0
51	WO	1	Total Mg 1 1	0

- Molecule 52 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	AH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	AJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	AL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	AN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	AP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	BB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	BH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	BJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	BL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	BN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	BP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	CH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	CJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	CL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	CN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	CP	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	DB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	DF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	DH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	DJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	DL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	DN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	DP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	EB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	ED	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	EH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	EJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	EL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	EN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	FB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	FH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	FJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	FL	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	FN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	GB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	GH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	GJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	GL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	GN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	HB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	HH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	HJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	HL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	HN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	HP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	IB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	IH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	IJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	IL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	IN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	IP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	JB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	JD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	JF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	JH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	JJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	JL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	JN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	JP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	KB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	KD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	KF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	KH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	KJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	KL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	KN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	KP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	LD	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	LF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	LH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	LJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	LL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	LN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	LP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	MB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	MD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	MF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	MH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	MJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	ML	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	MN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	MP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	NB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	ND	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	NF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	NH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	NJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	NL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	NN	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	NP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	OB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	OD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	OF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	OH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	OJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	OL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	ON	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	OP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	PB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	PD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	PF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	PH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	PJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	PL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	PN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	PP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	QB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	QD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	QF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	QH	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	QJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	QL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	QN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	QP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	RD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	RF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	RH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	RJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	RL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	RN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	RP	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	SB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	SD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	SF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	SH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	SJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	SL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	SN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	TB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	TD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	TF	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	TH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	TJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	TL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	TN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	UB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	UD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	UF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	UH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	UJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	UL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	UN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	VB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	VD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	VF	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	VH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	VJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	VL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	VN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	WB	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	WD	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	WF	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

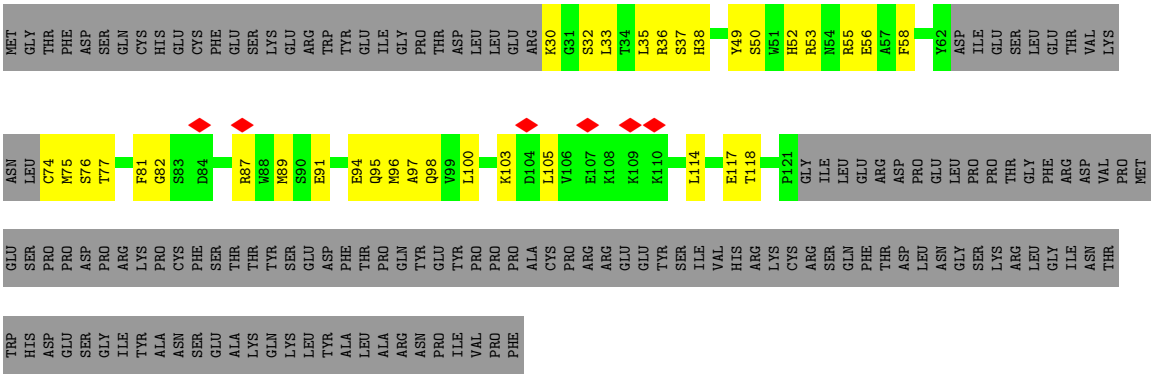
Mol	Chain	Residues	Atoms					AltConf
52	WH	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	WN	1	Total	C	N	O	P	0
			28	10	5	11	2	
52	WP	1	Total	C	N	O	P	0
			28	10	5	11	2	

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.

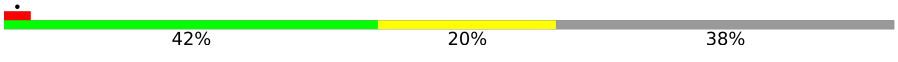
• Molecule 1: Cilia- and flagella-associated protein 95

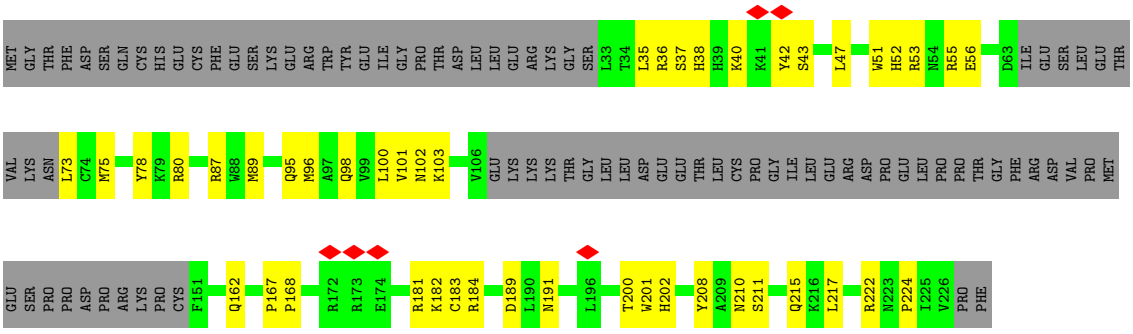
Chain 0:



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

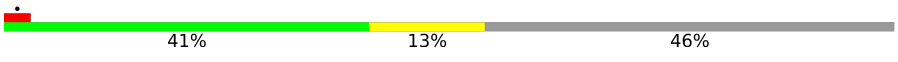
Chain 7:

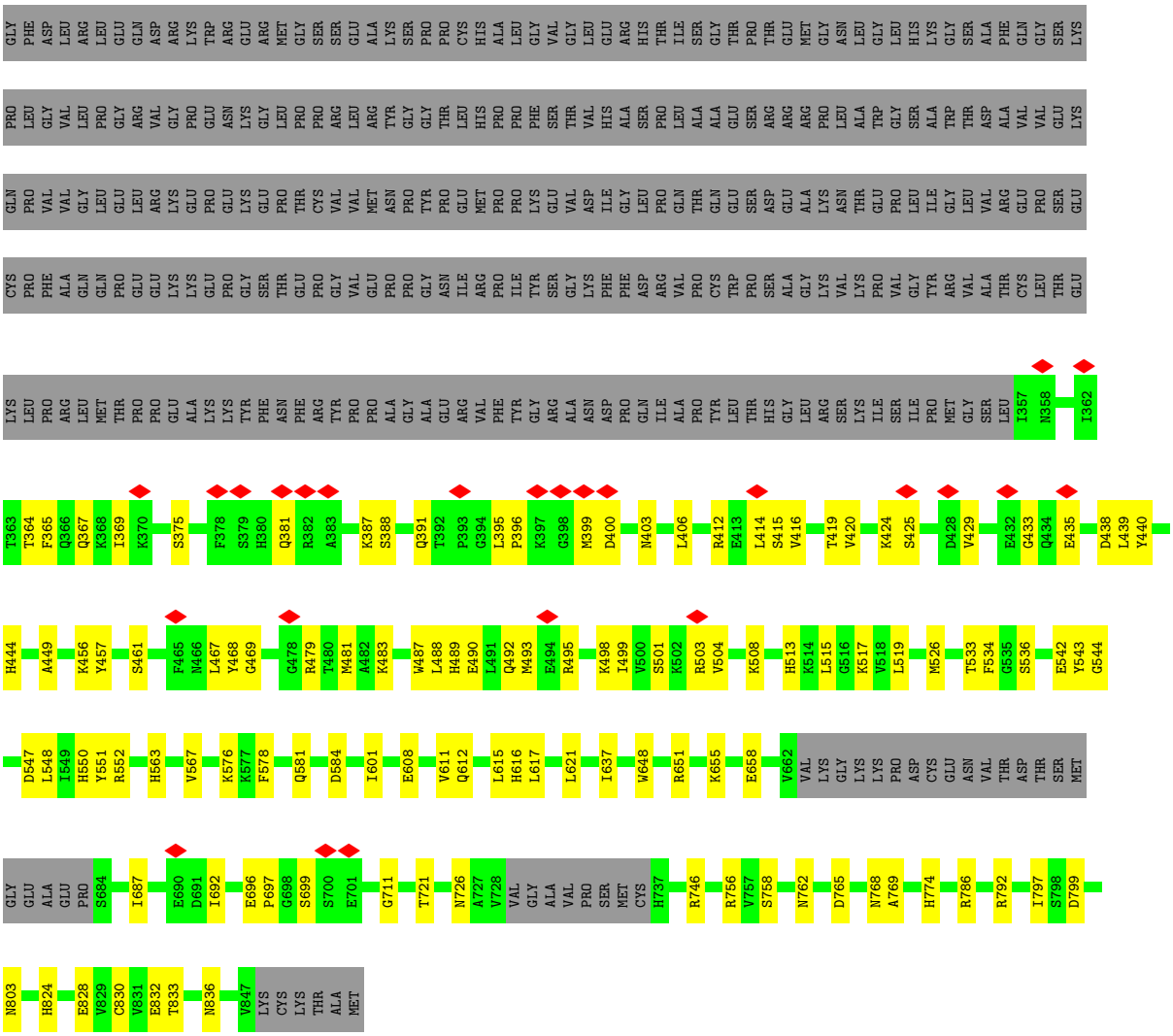




• Molecule 2: EF-hand domain-containing family member B

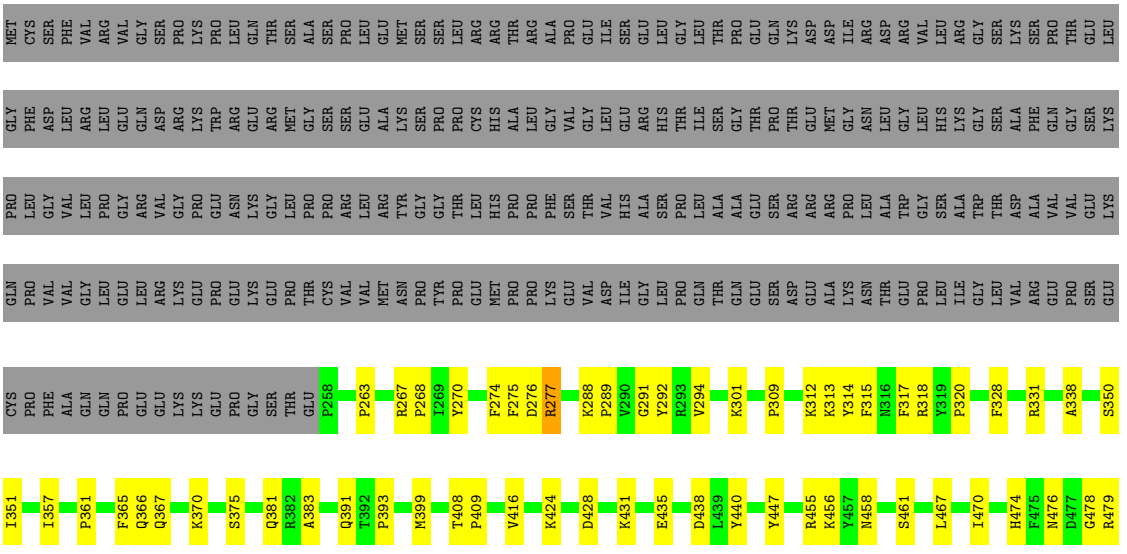
Chain 1:

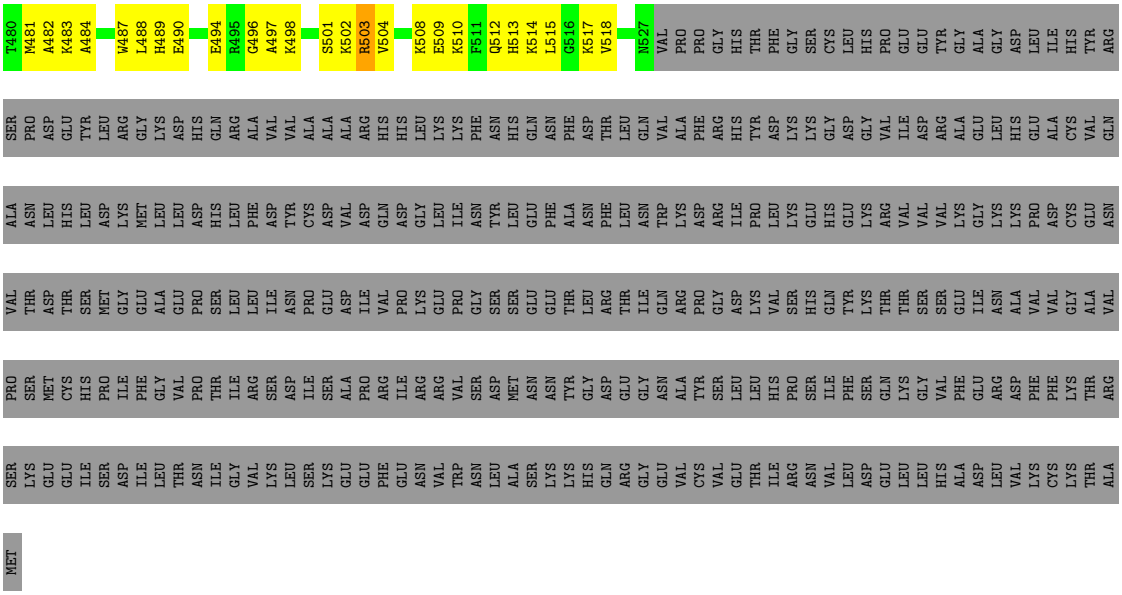




• Molecule 2: EF-hand domain-containing family member B

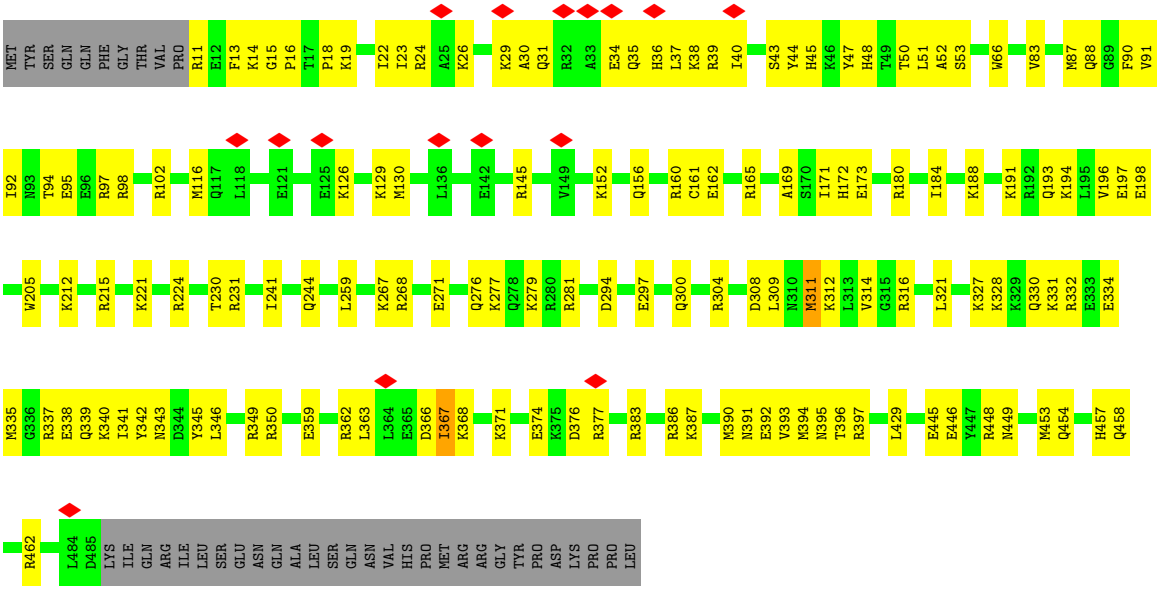
Chain 2:





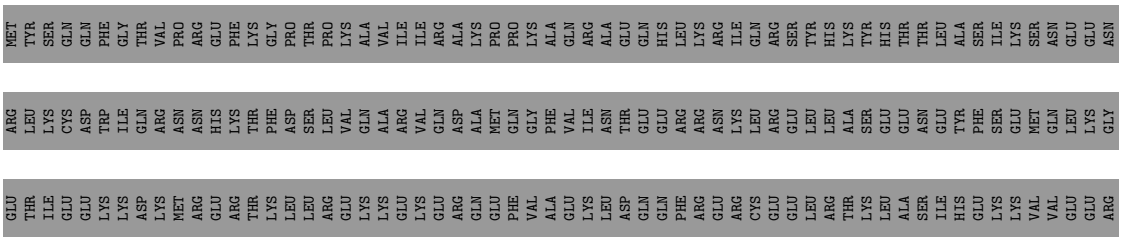
• Molecule 3: Cilia- and flagella-associated protein 53

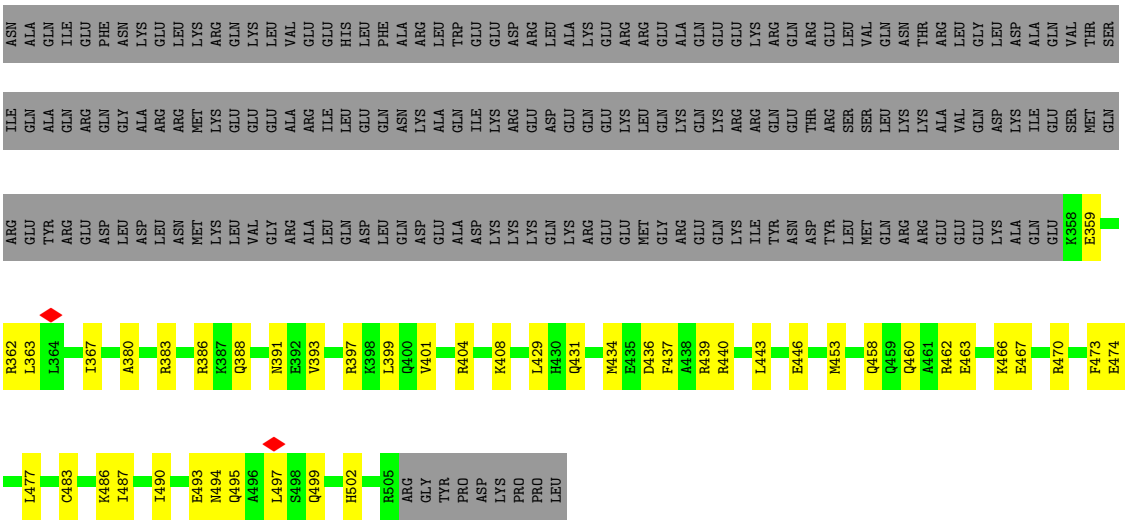
Chain 3:



• Molecule 3: Cilia- and flagella-associated protein 53

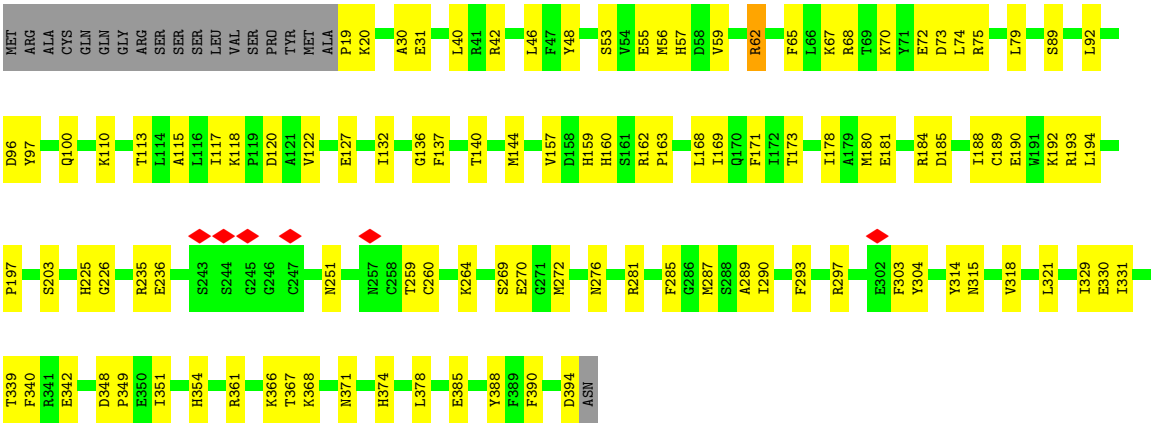
Chain 4:





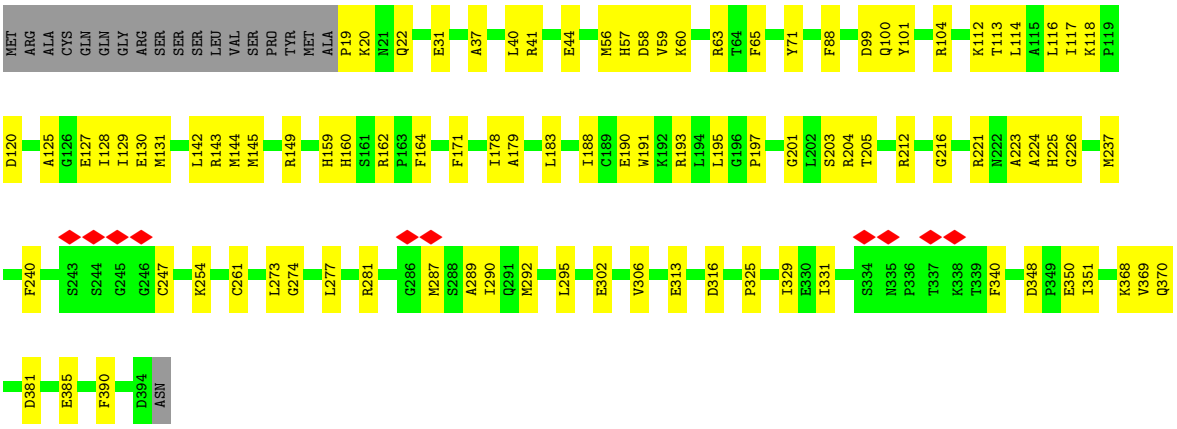
• Molecule 4: Nucleoside diphosphate kinase 7

Chain 5:



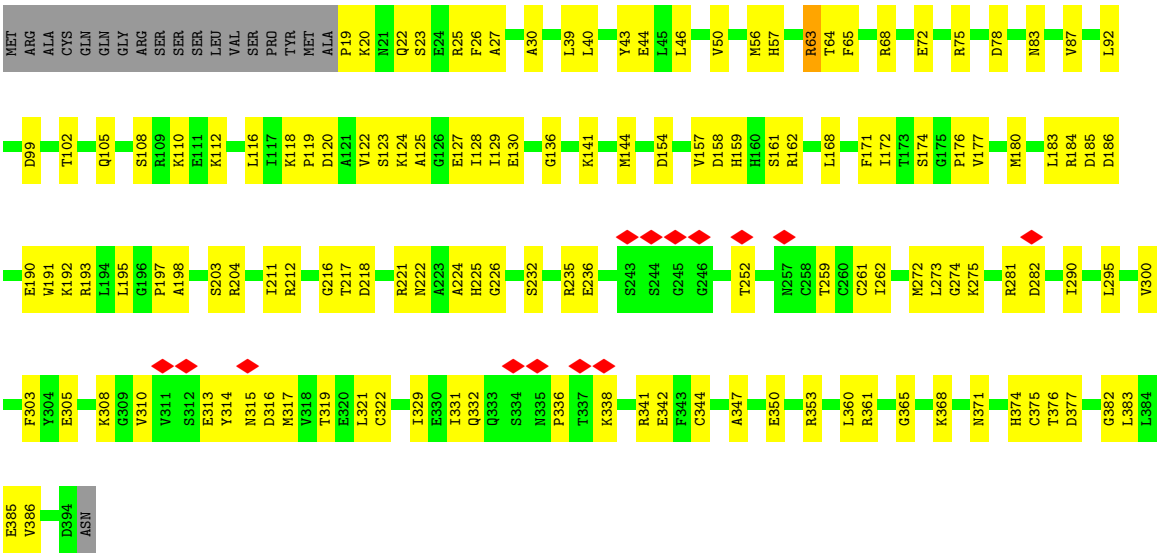
• Molecule 4: Nucleoside diphosphate kinase 7

Chain 6:



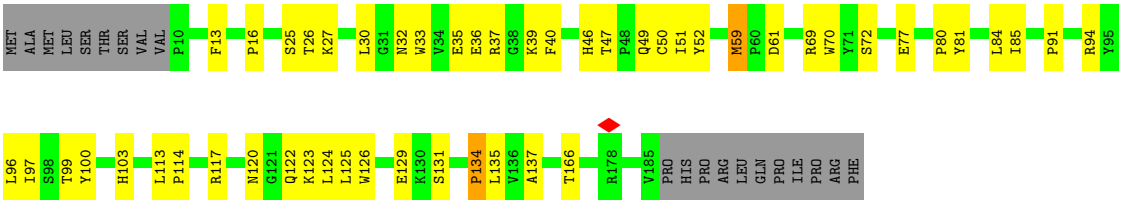
• Molecule 4: Nucleoside diphosphate kinase 7

Chain j1:



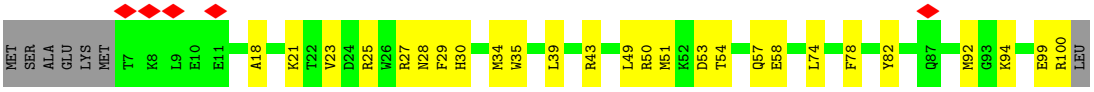
• Molecule 5: Cilia- and flagella-associated protein 107

Chain 8:



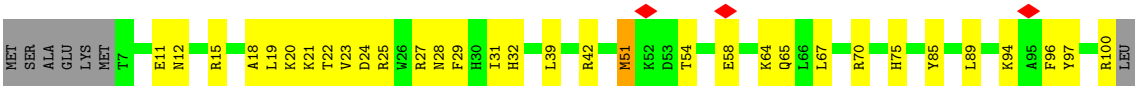
• Molecule 6: Cilia- and flagella-associated protein 141

Chain A:



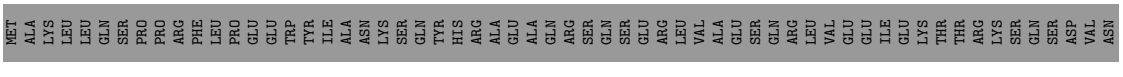
• Molecule 6: Cilia- and flagella-associated protein 141

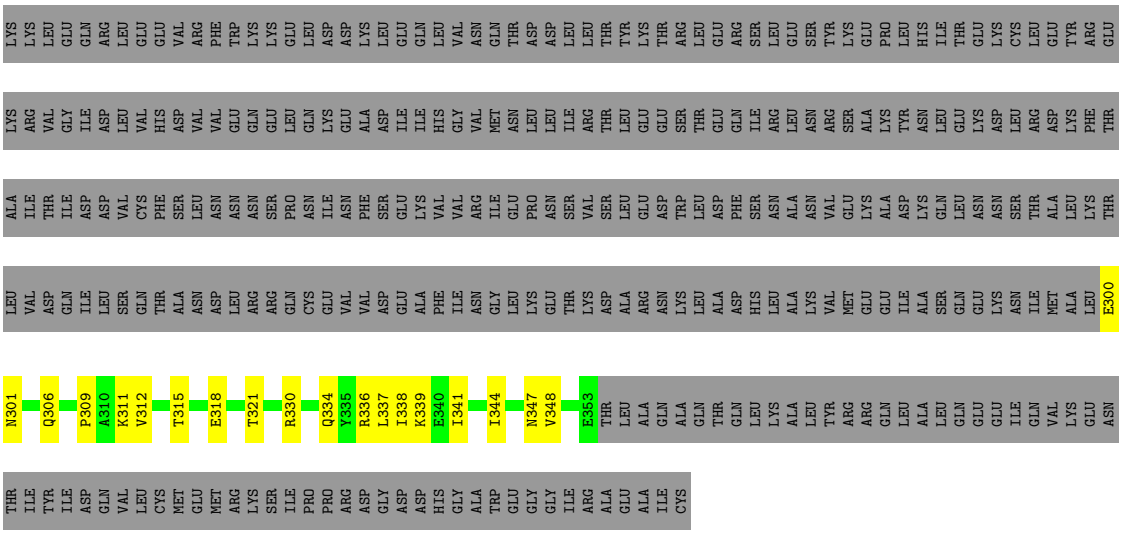
Chain N1:



• Molecule 7: Tektin-1

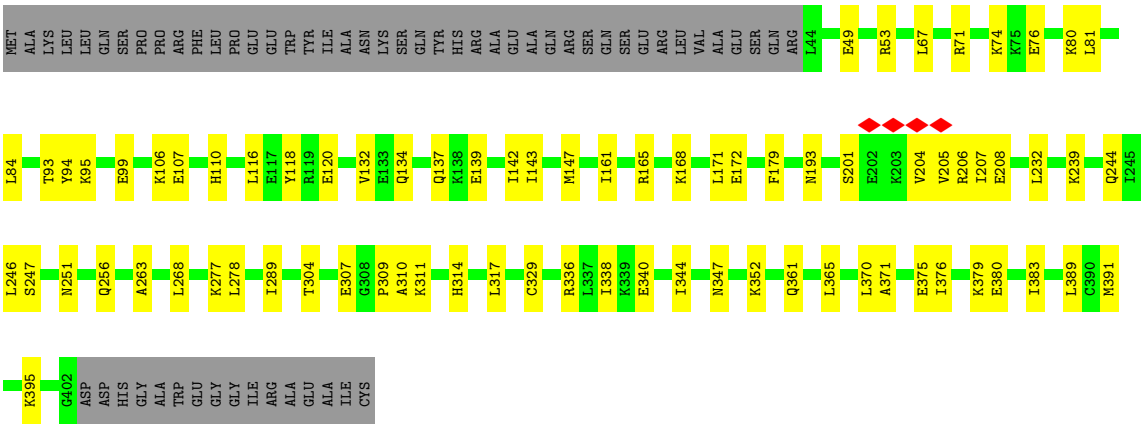
Chain A0:





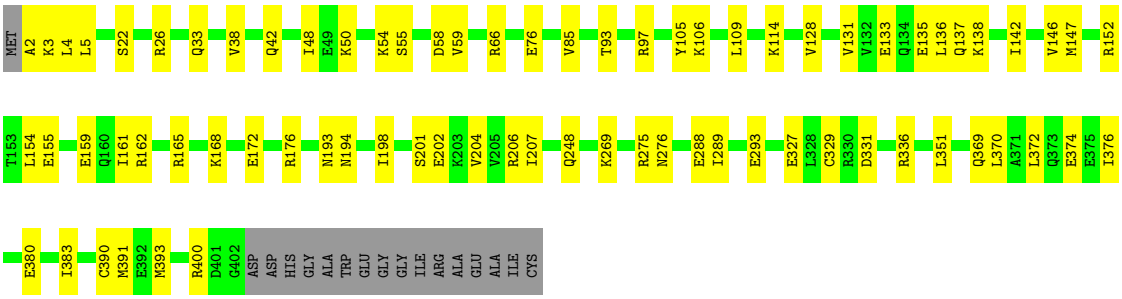
• Molecule 7: Tektin-1

Chain A1:



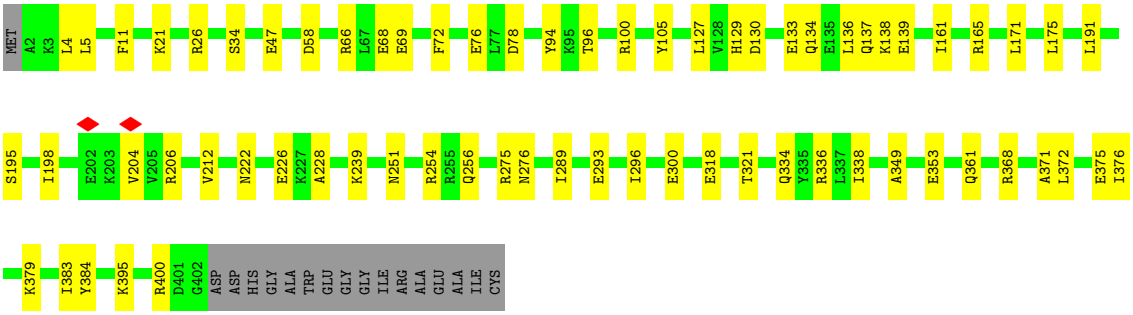
• Molecule 7: Tektin-1

Chain A2:



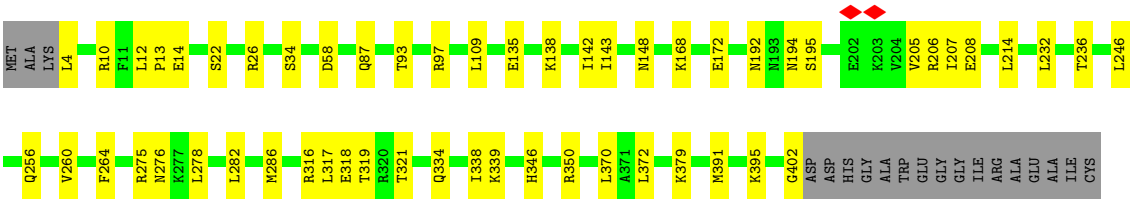
• Molecule 7: Tektin-1

Chain A3:



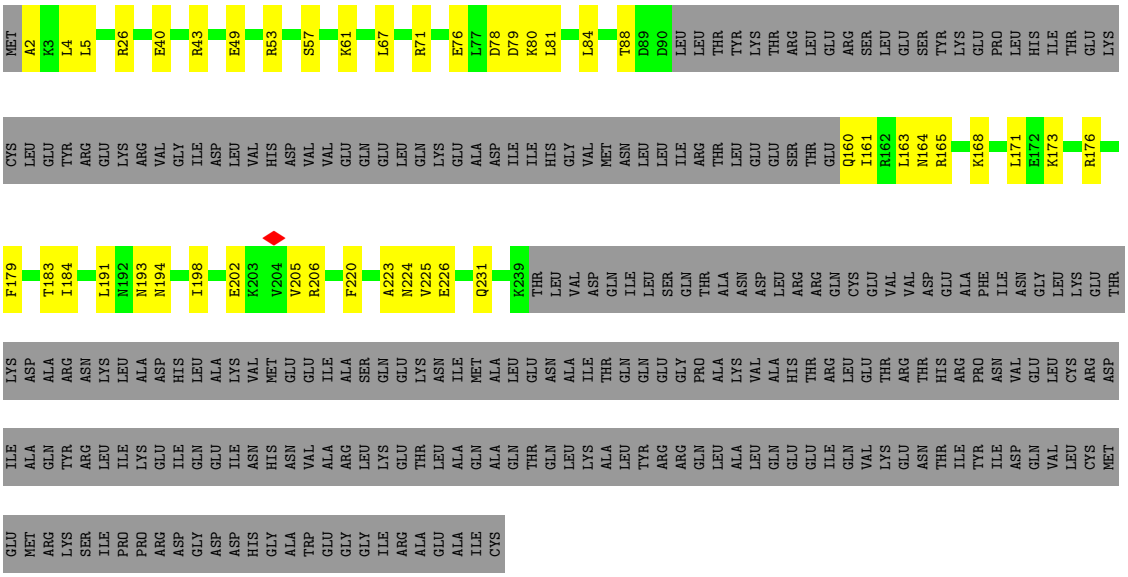
• Molecule 7: Tektin-1

Chain A4:



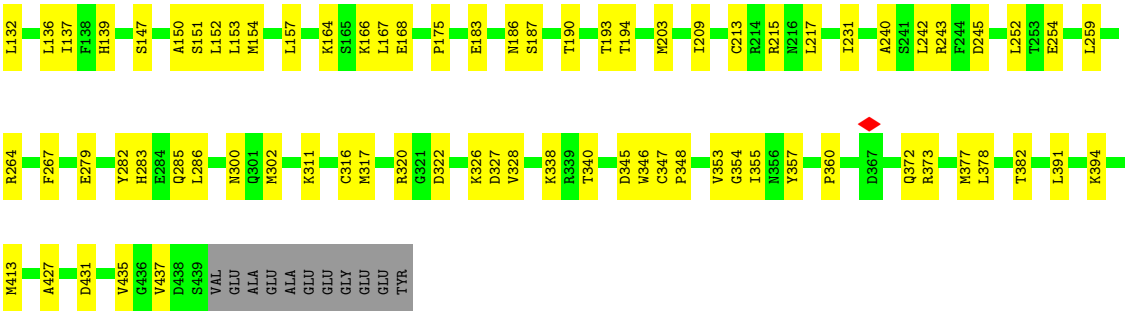
• Molecule 7: Tektin-1

Chain A5:



• Molecule 8: Tubulin alpha-3 chain

Chain AA:

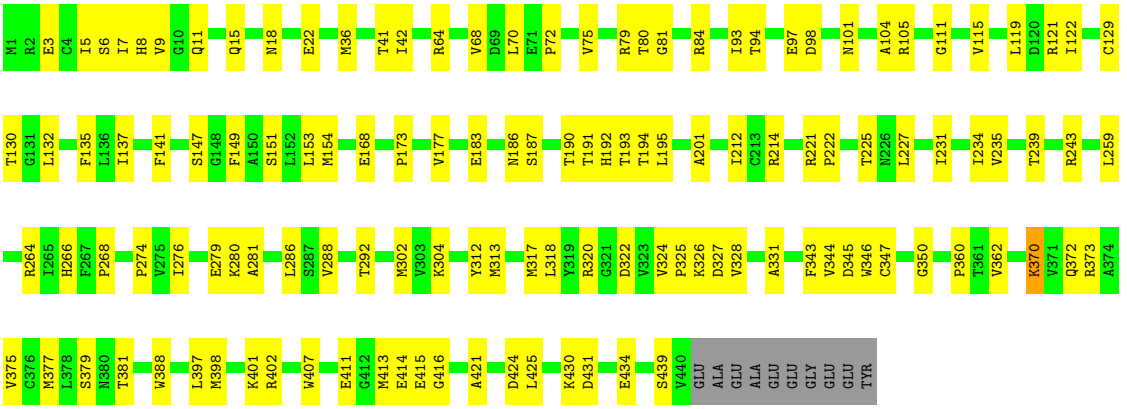


• Molecule 8: Tubulin alpha-3 chain

Chain AC:

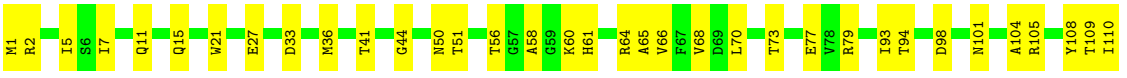
• Molecule 8: Tubulin alpha-3 chain

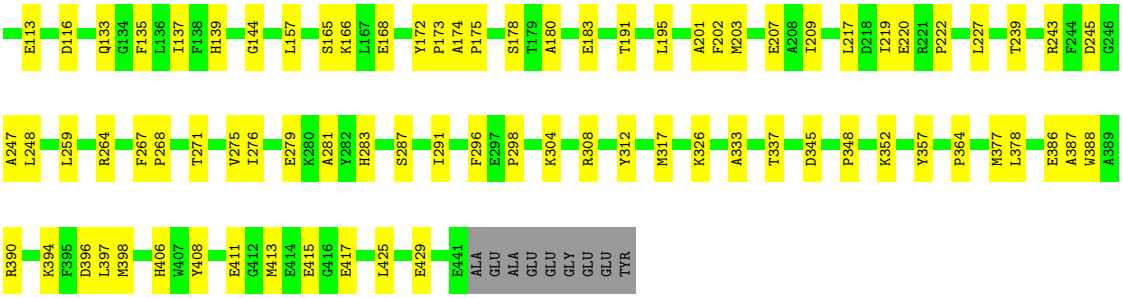
Chain AE:



• Molecule 8: Tubulin alpha-3 chain

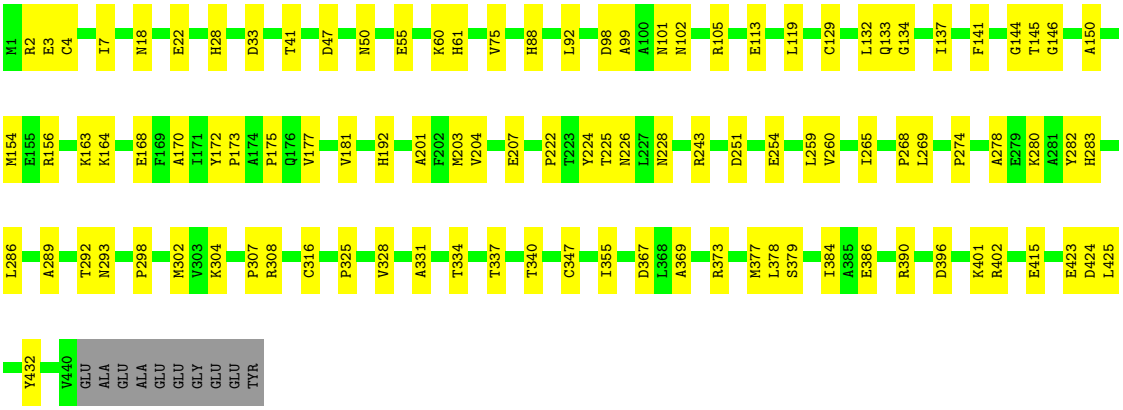
Chain AG:





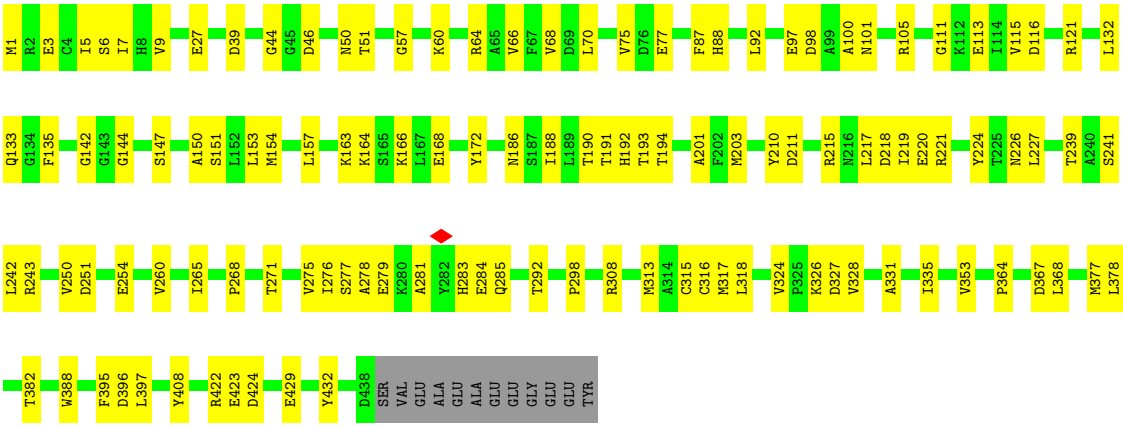
• Molecule 8: Tubulin alpha-3 chain

Chain AI:



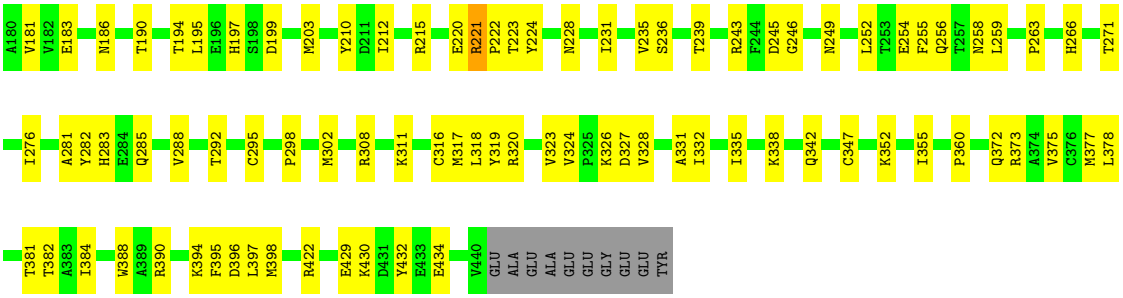
• Molecule 8: Tubulin alpha-3 chain

Chain AK:



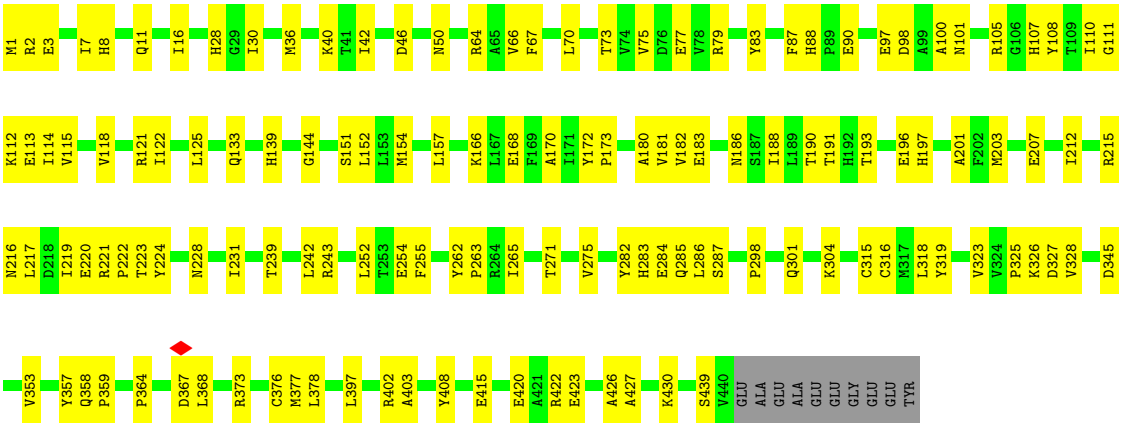
• Molecule 8: Tubulin alpha-3 chain

Chain AM:



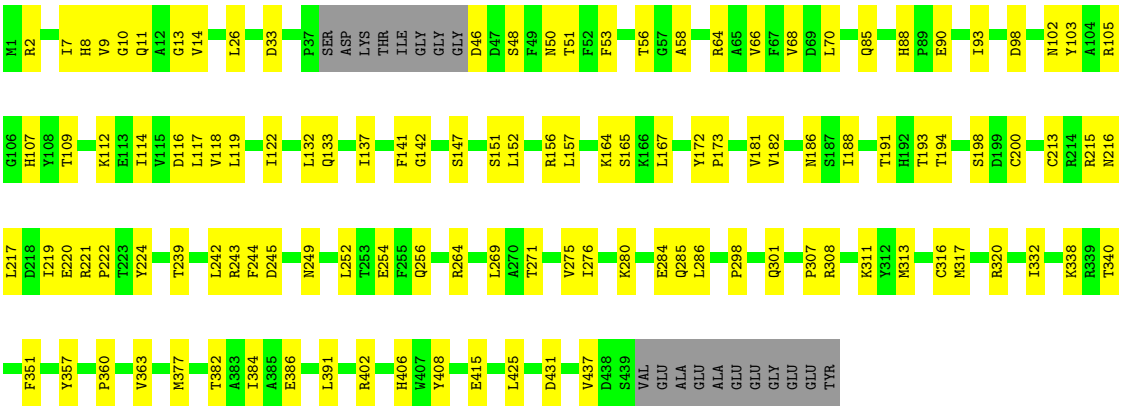
• Molecule 8: Tubulin alpha-3 chain

Chain AO:



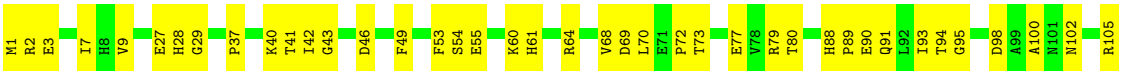
• Molecule 8: Tubulin alpha-3 chain

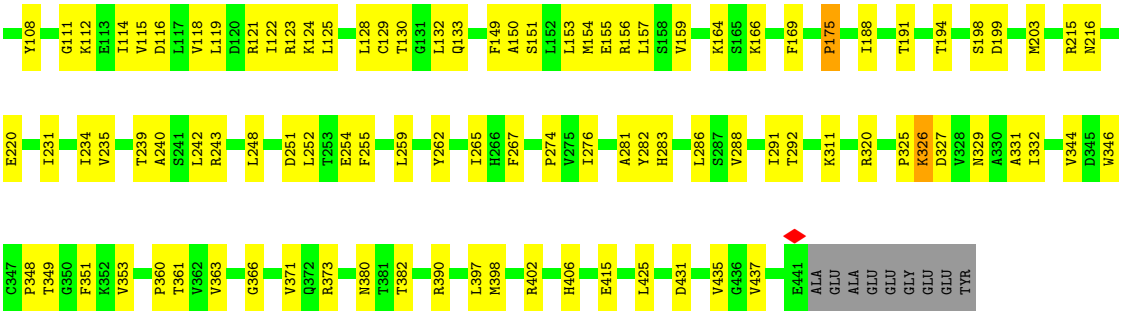
Chain BC:



• Molecule 8: Tubulin alpha-3 chain

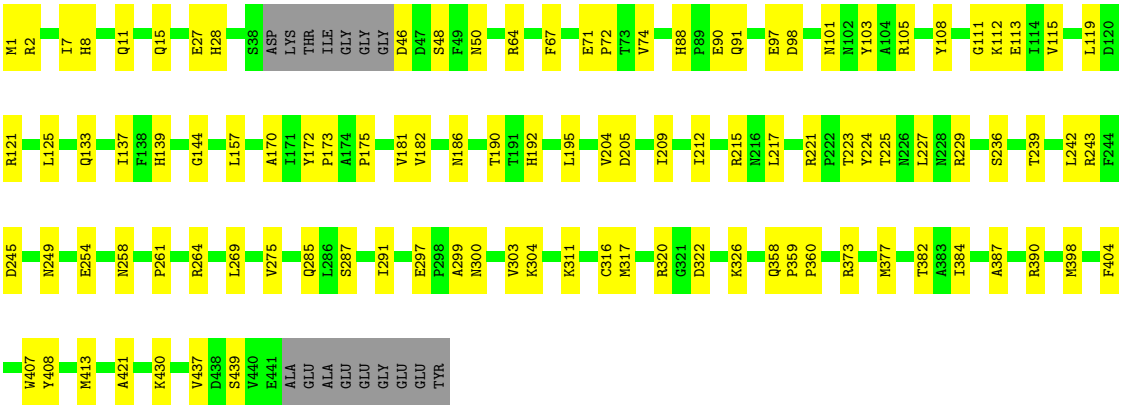
Chain BE:





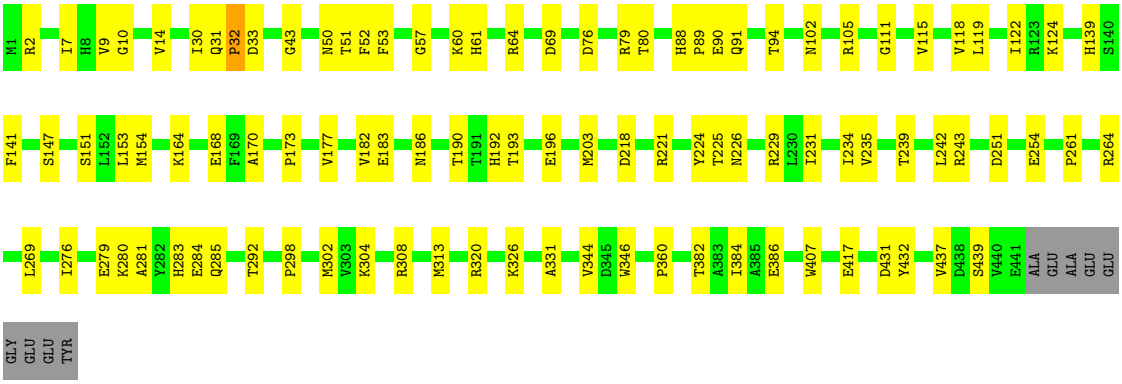
• Molecule 8: Tubulin alpha-3 chain

Chain BG:



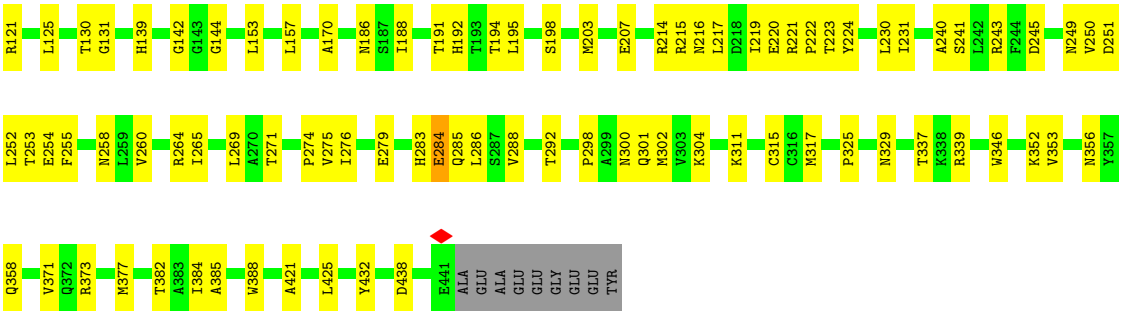
• Molecule 8: Tubulin alpha-3 chain

Chain BI:



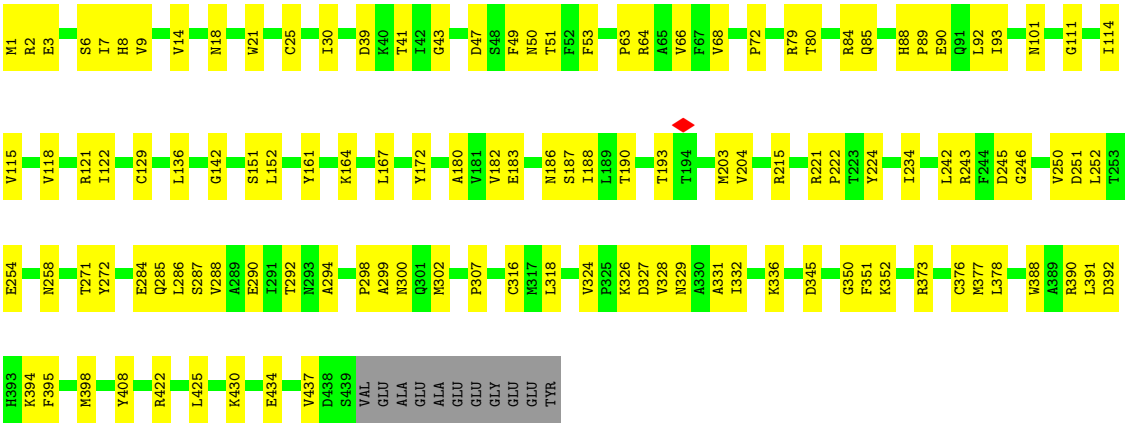
• Molecule 8: Tubulin alpha-3 chain

Chain BK:



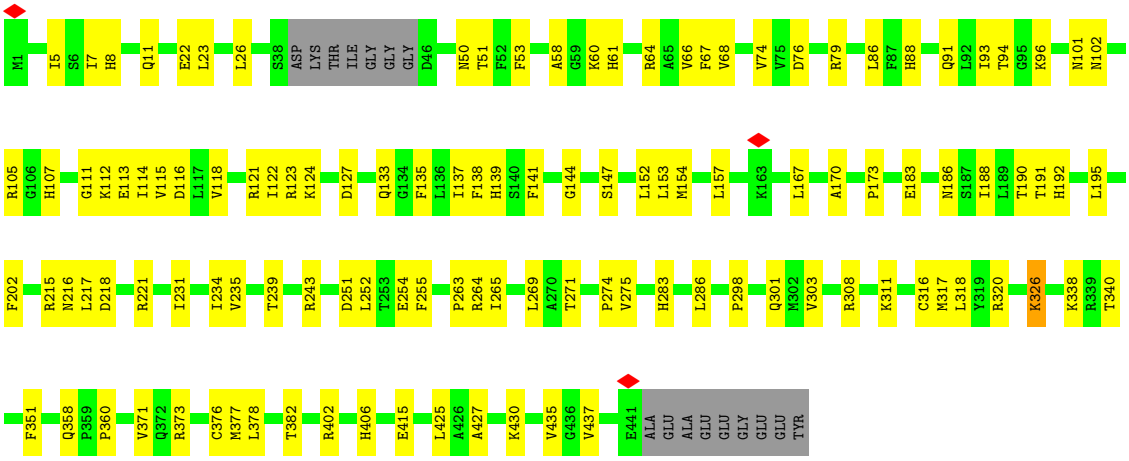
• Molecule 8: Tubulin alpha-3 chain

Chain BM:



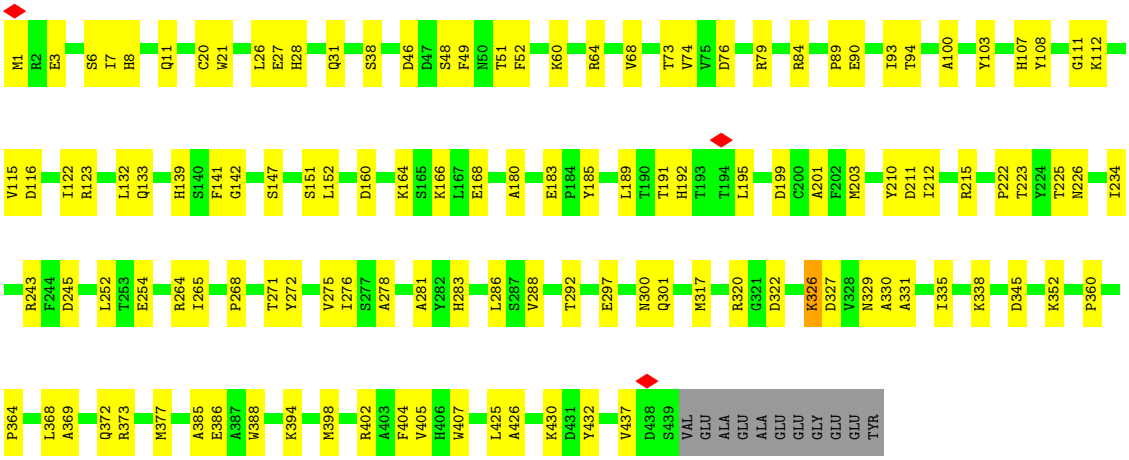
• Molecule 8: Tubulin alpha-3 chain

Chain BO:



• Molecule 8: Tubulin alpha-3 chain

Chain CC:

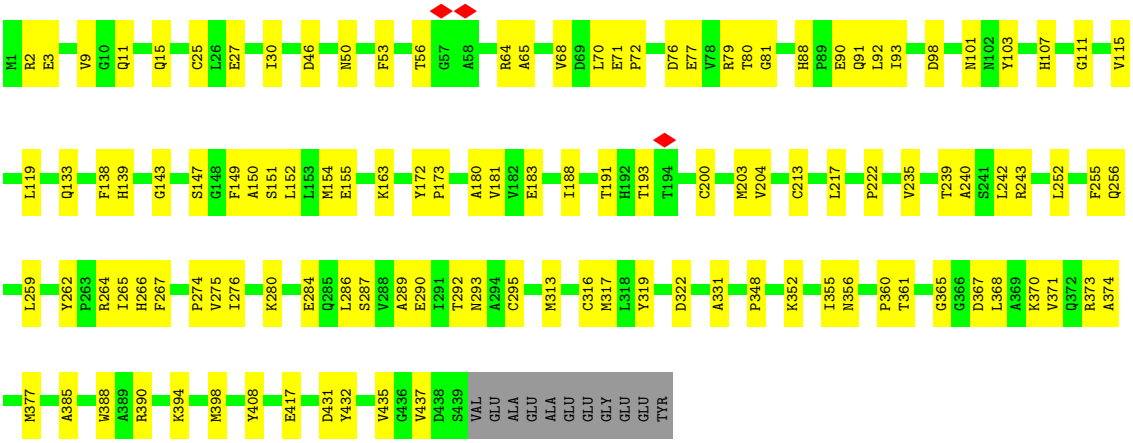


• Molecule 8: Tubulin alpha-3 chain

Chain CE:

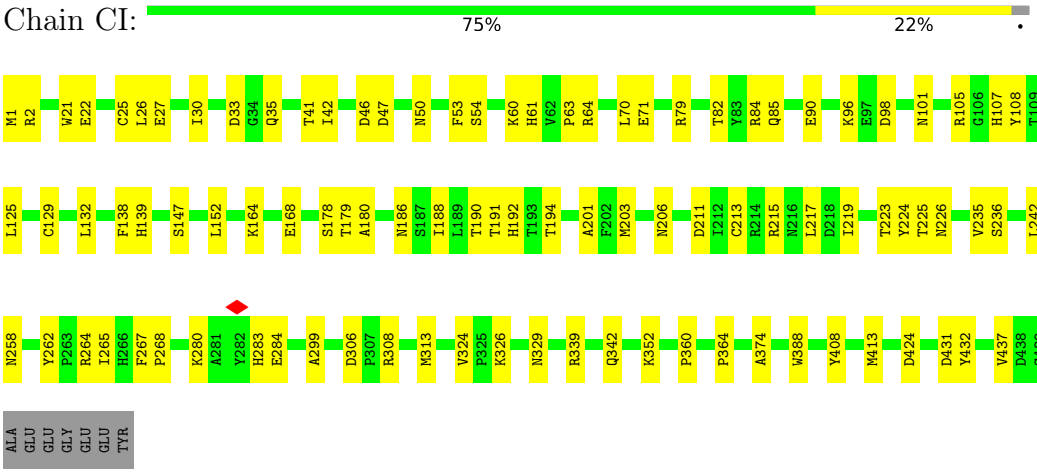
• Molecule 8: Tubulin alpha-3 chain

Chain CG:



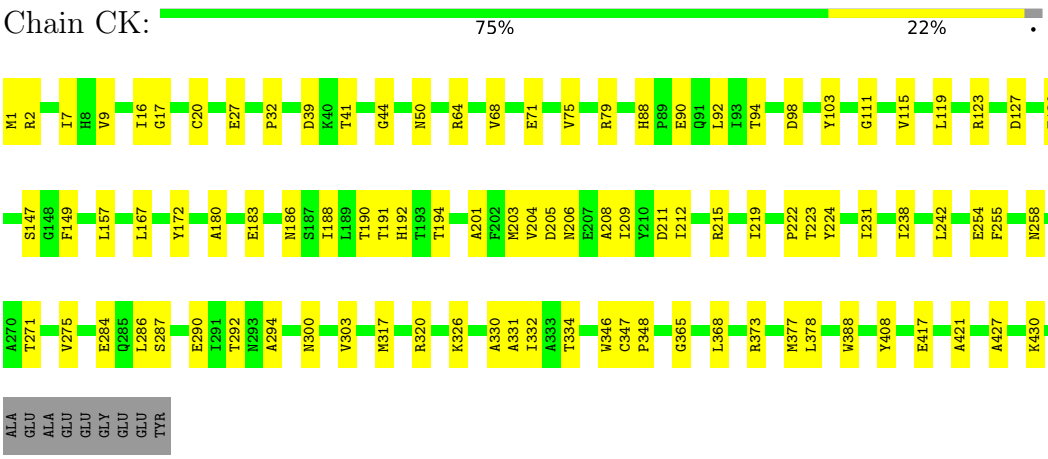
• Molecule 8: Tubulin alpha-3 chain

Chain CI:



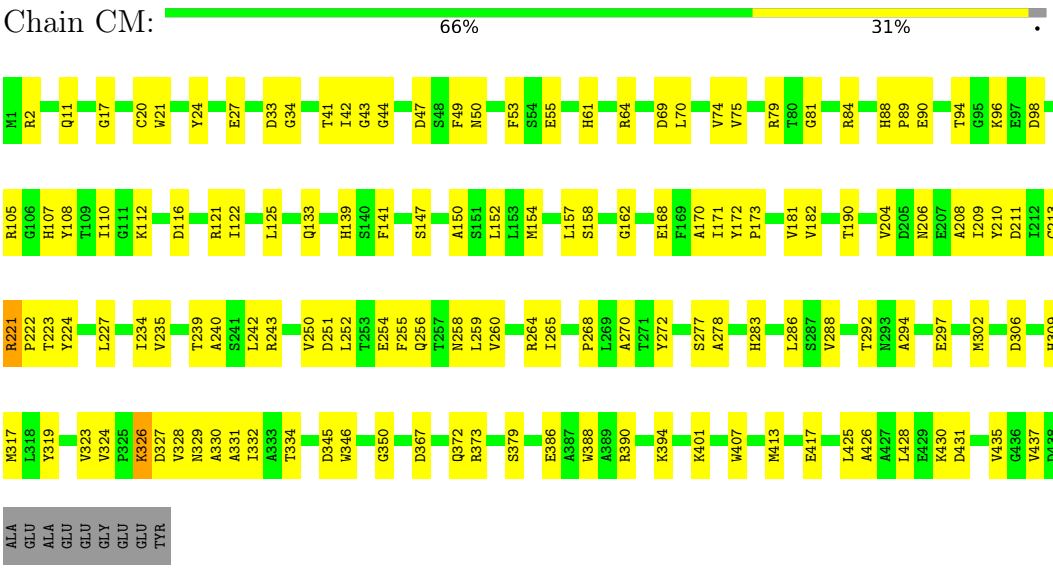
- Molecule 8: Tubulin alpha-3 chain

Chain CK:



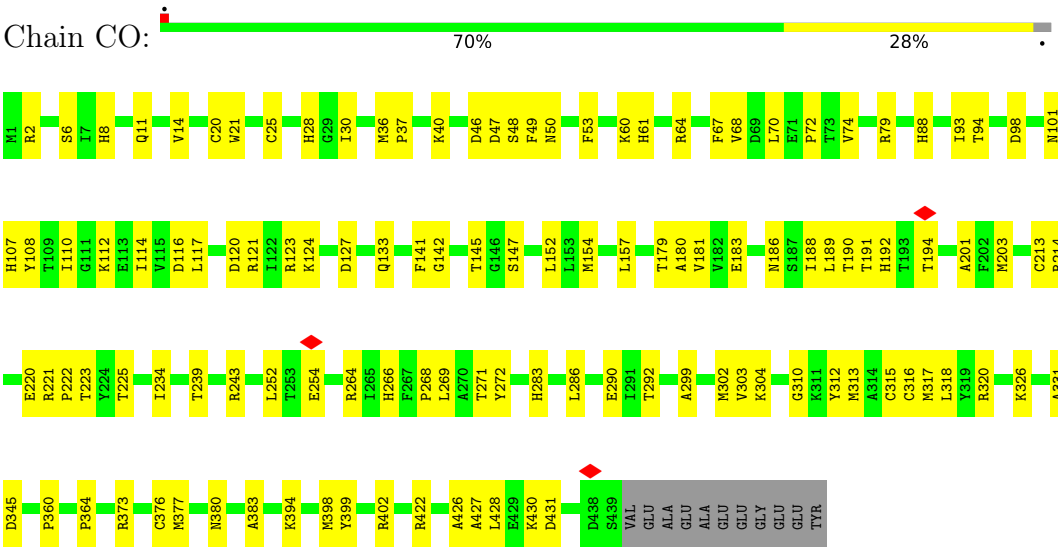
- Molecule 8: Tubulin alpha-3 chain

Chain CM:



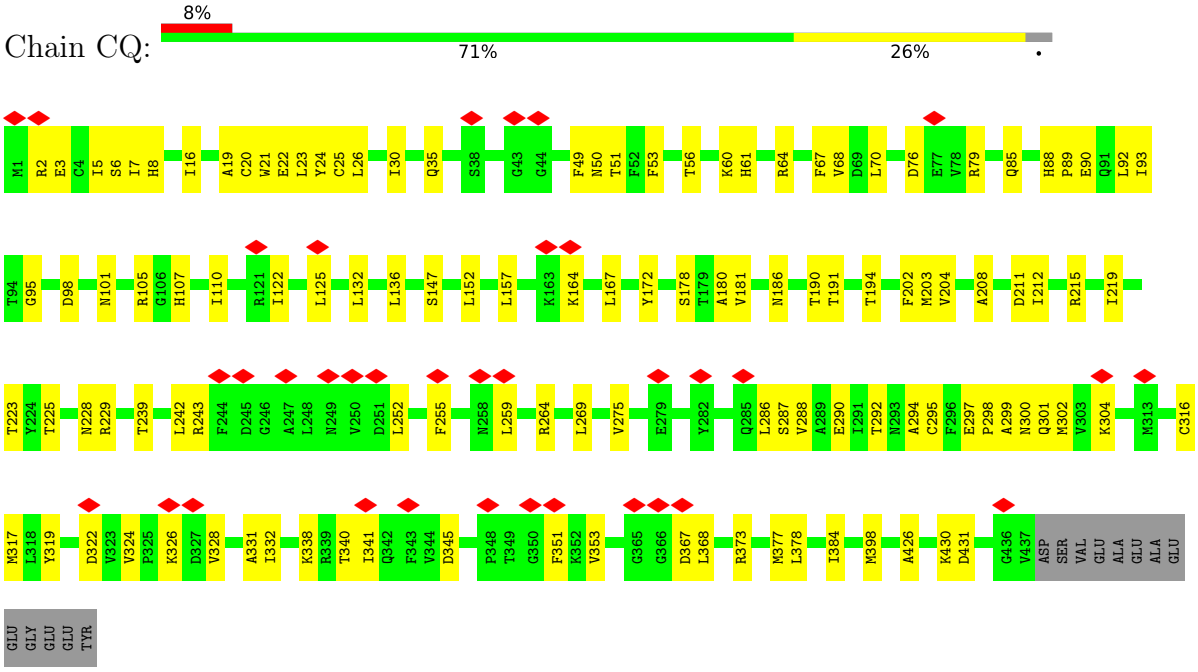
- Molecule 8: Tubulin alpha-3 chain

Chain CO:



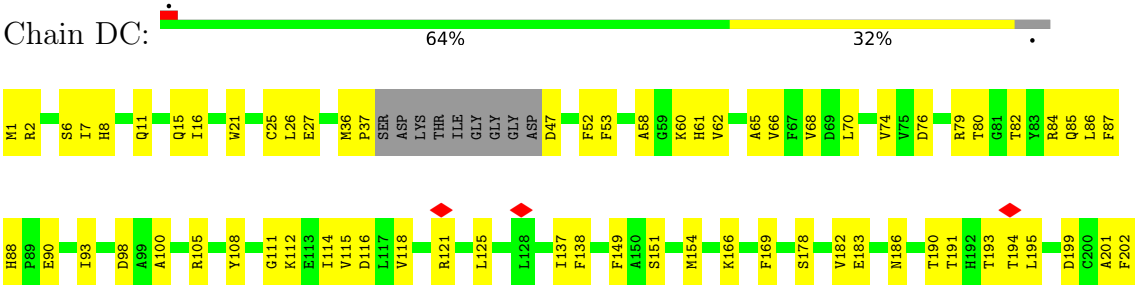
• Molecule 8: Tubulin alpha-3 chain

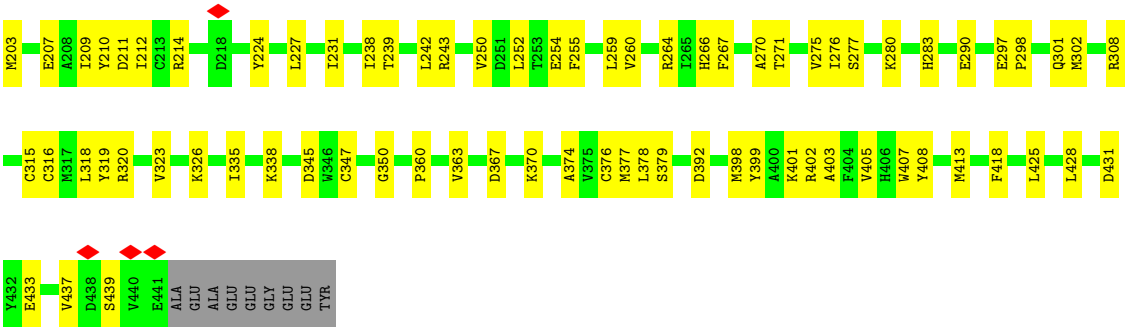
Chain CQ:



• Molecule 8: Tubulin alpha-3 chain

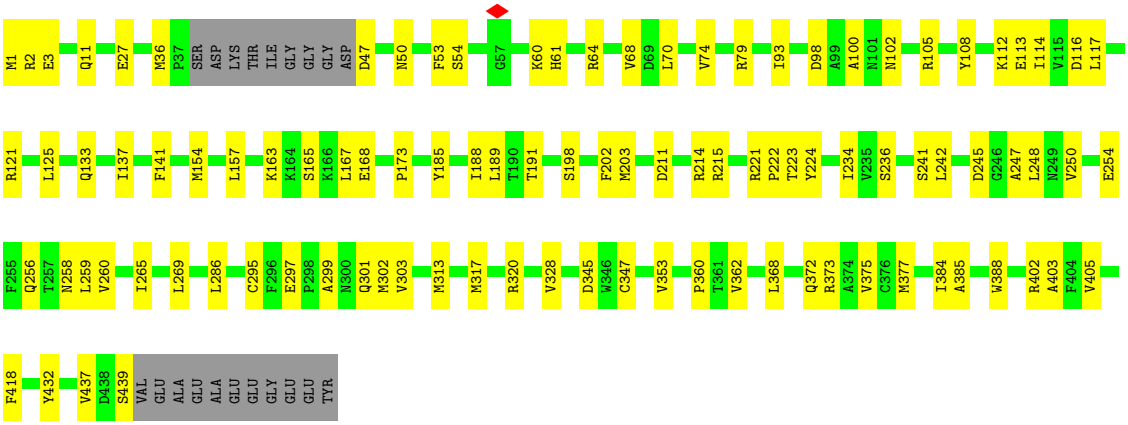
Chain DC:





• Molecule 8: Tubulin alpha-3 chain

Chain DE:

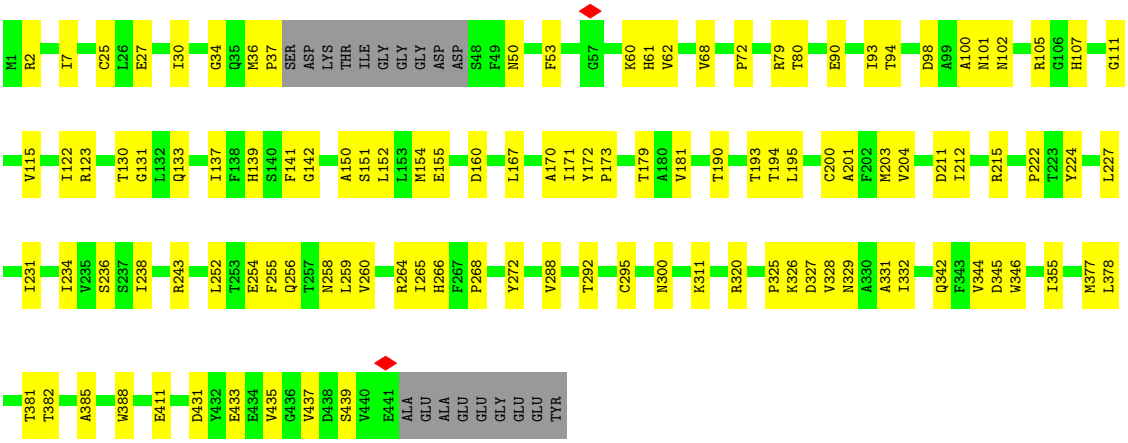


• Molecule 8: Tubulin alpha-3 chain

Chain DG:

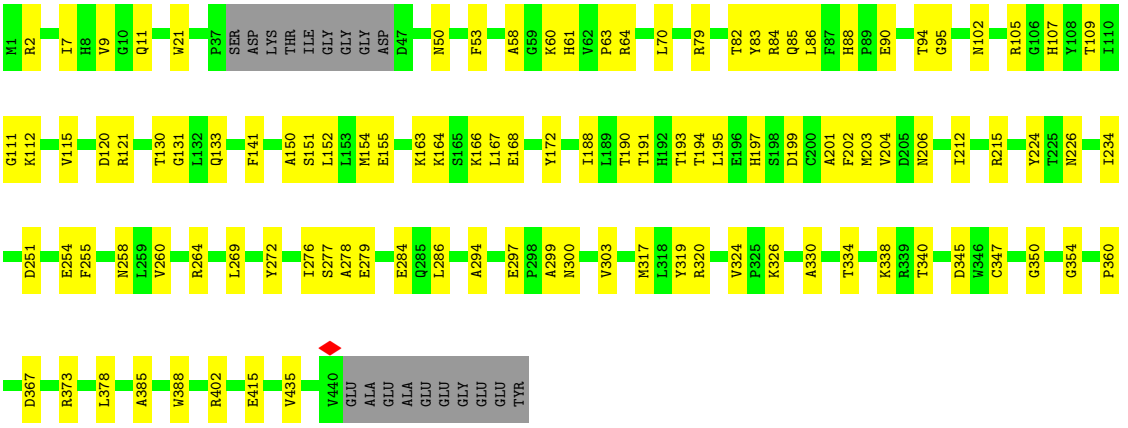
• Molecule 8: Tubulin alpha-3 chain

Chain DI:



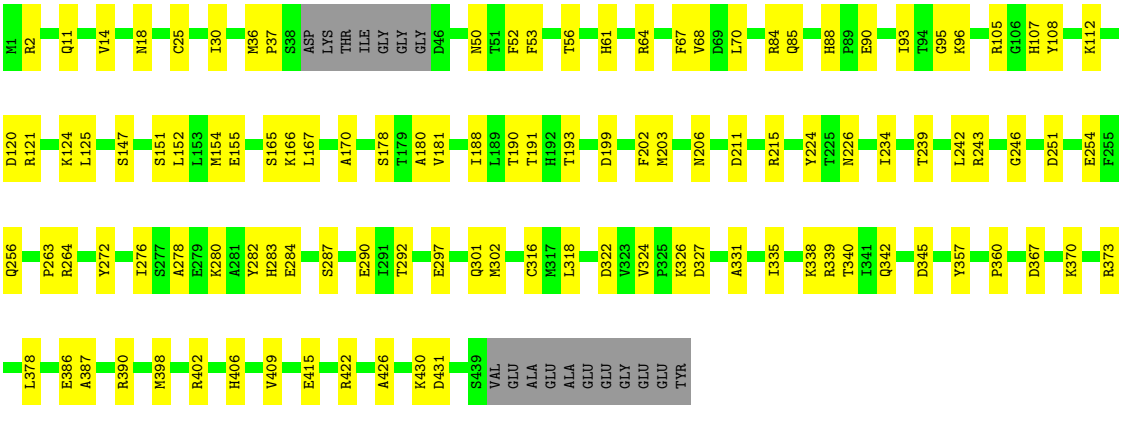
• Molecule 8: Tubulin alpha-3 chain

Chain DK:



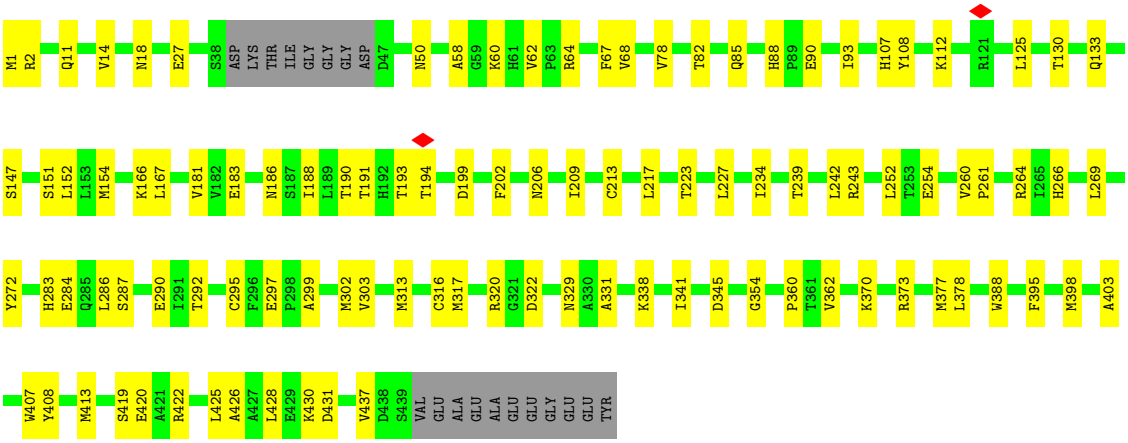
• Molecule 8: Tubulin alpha-3 chain

Chain DM:



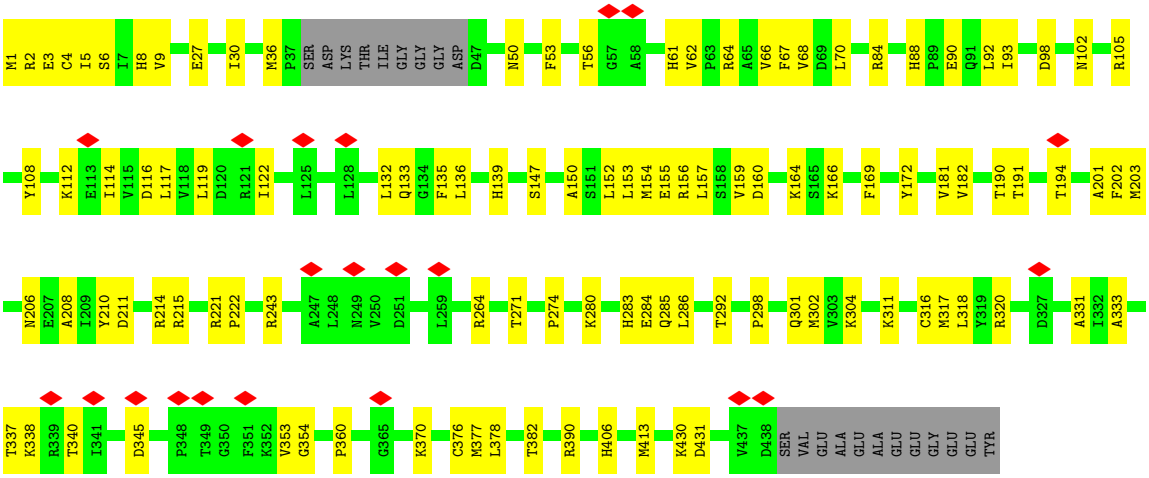
• Molecule 8: Tubulin alpha-3 chain

Chain DO:



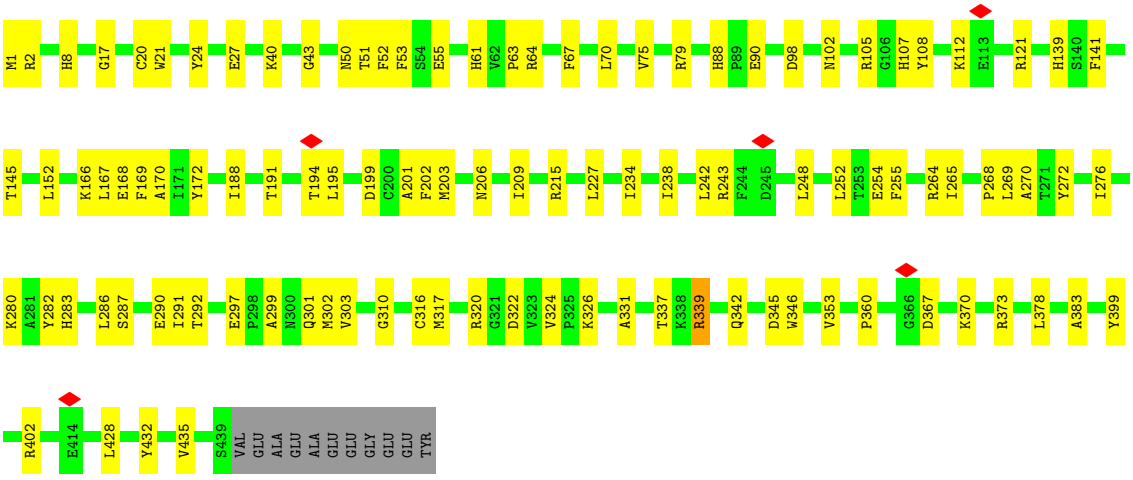
• Molecule 8: Tubulin alpha-3 chain

Chain DQ:



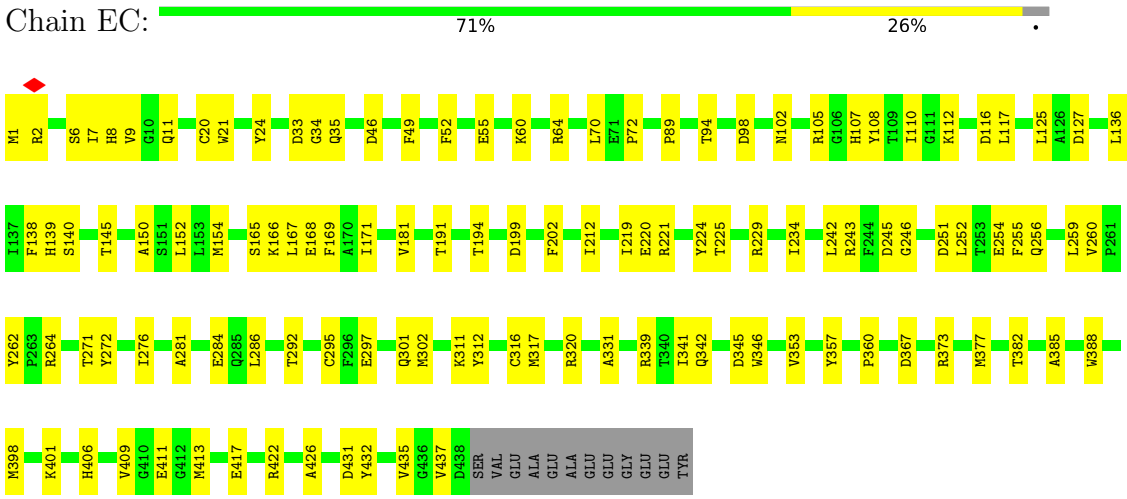
• Molecule 8: Tubulin alpha-3 chain

Chain EA:



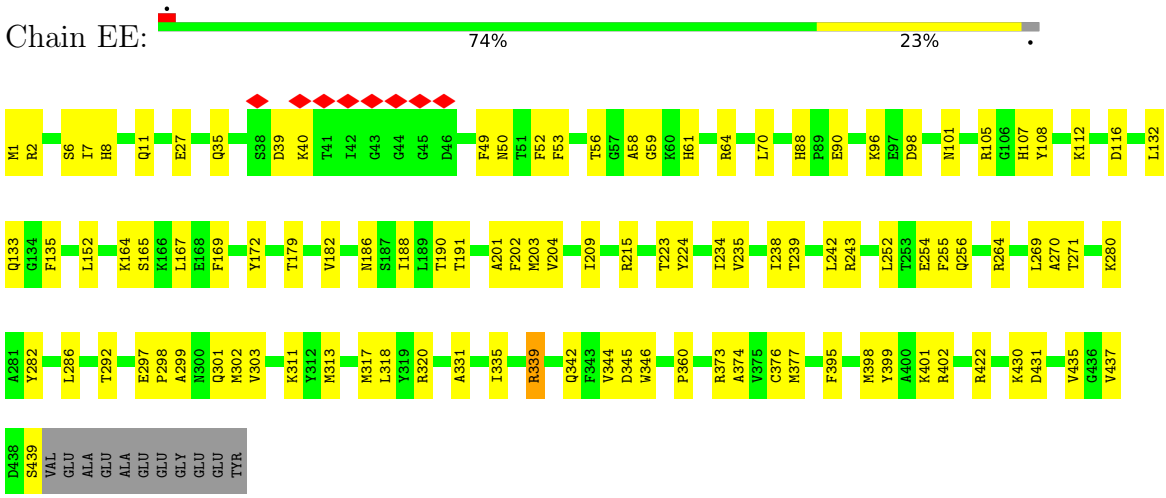
• Molecule 8: Tubulin alpha-3 chain

Chain EC:



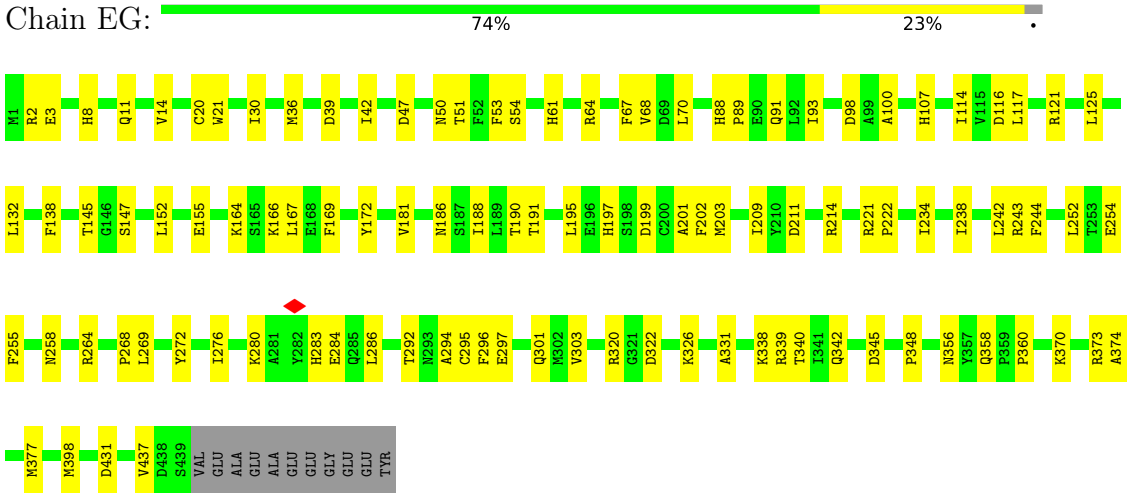
• Molecule 8: Tubulin alpha-3 chain

Chain EE:



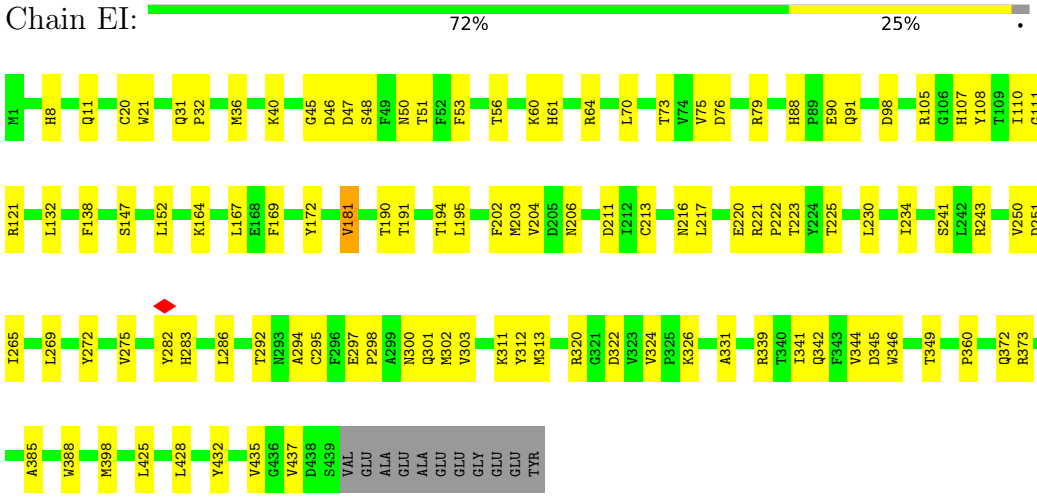
• Molecule 8: Tubulin alpha-3 chain

Chain EG:



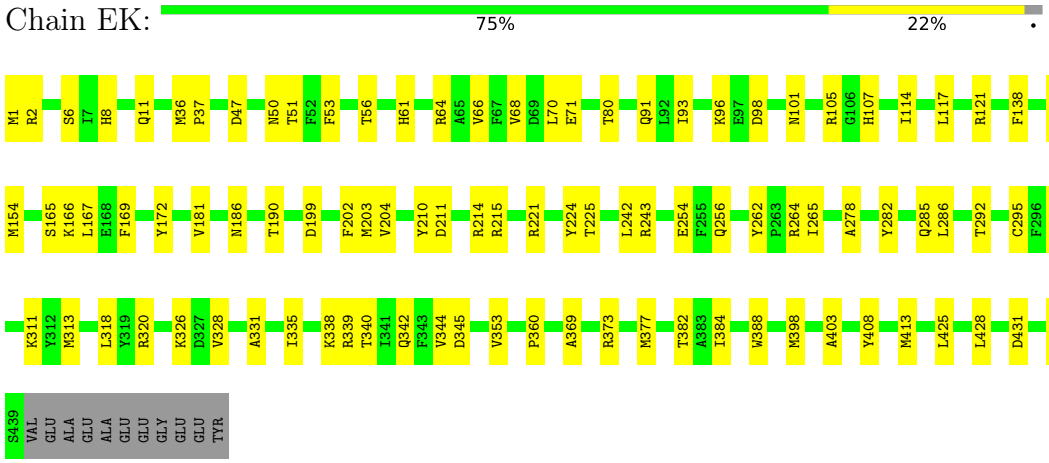
• Molecule 8: Tubulin alpha-3 chain

Chain EI:



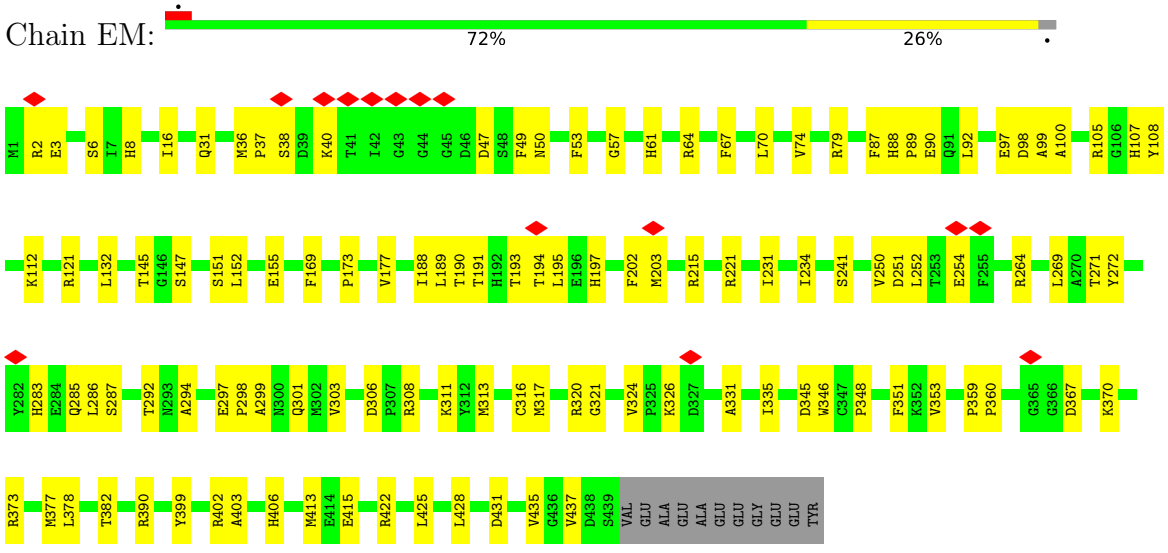
• Molecule 8: Tubulin alpha-3 chain

Chain EK:



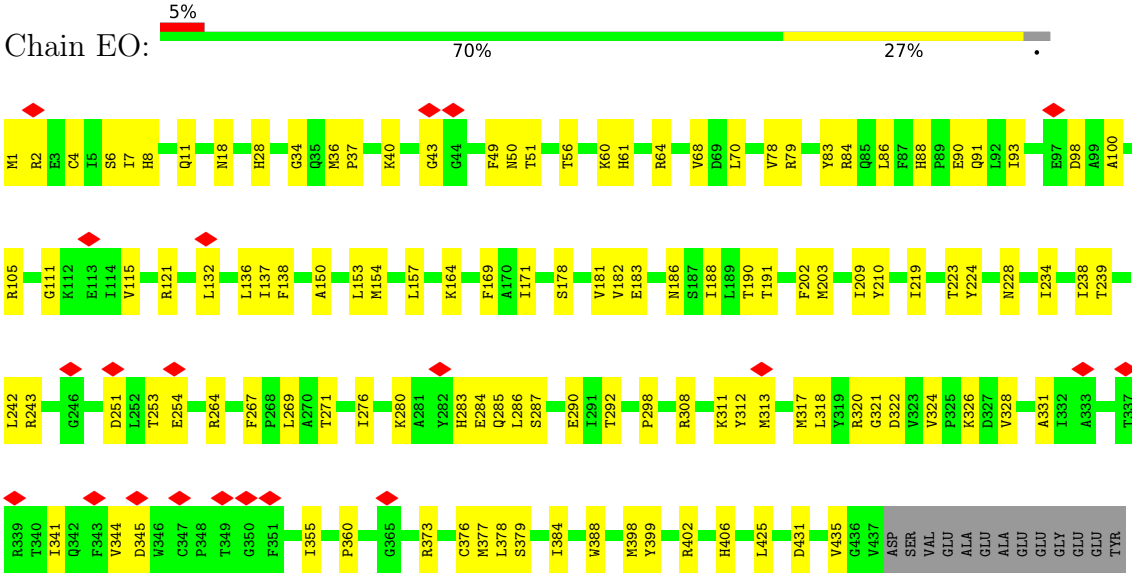
• Molecule 8: Tubulin alpha-3 chain

Chain EM:



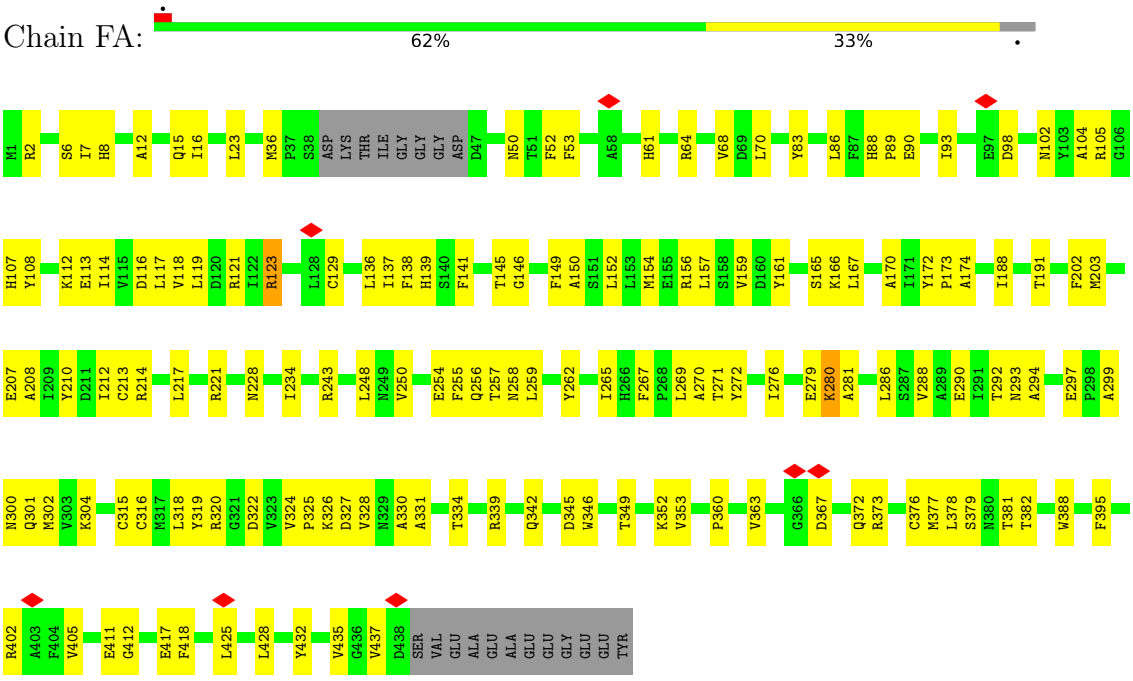
• Molecule 8: Tubulin alpha-3 chain

Chain EO:



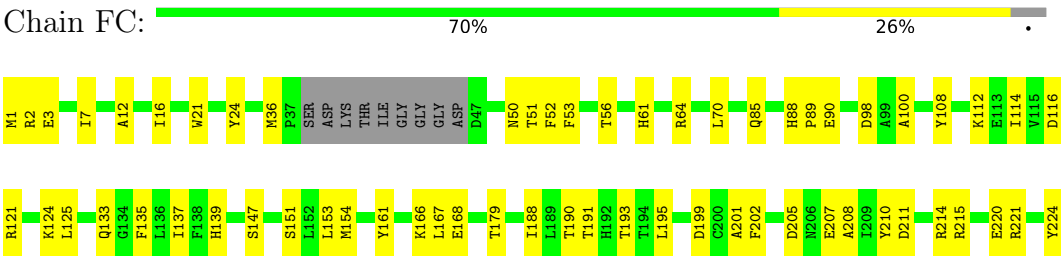
• Molecule 8: Tubulin alpha-3 chain

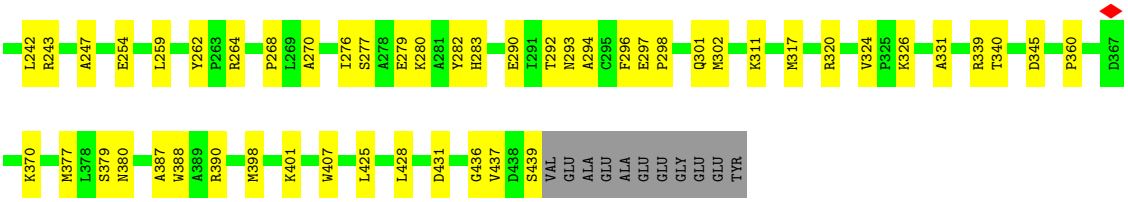
Chain FA:



• Molecule 8: Tubulin alpha-3 chain

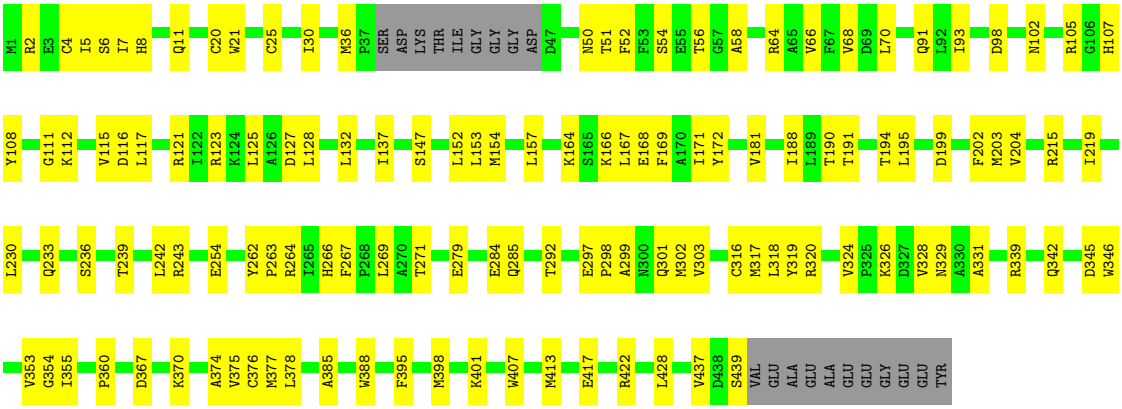
Chain FC:





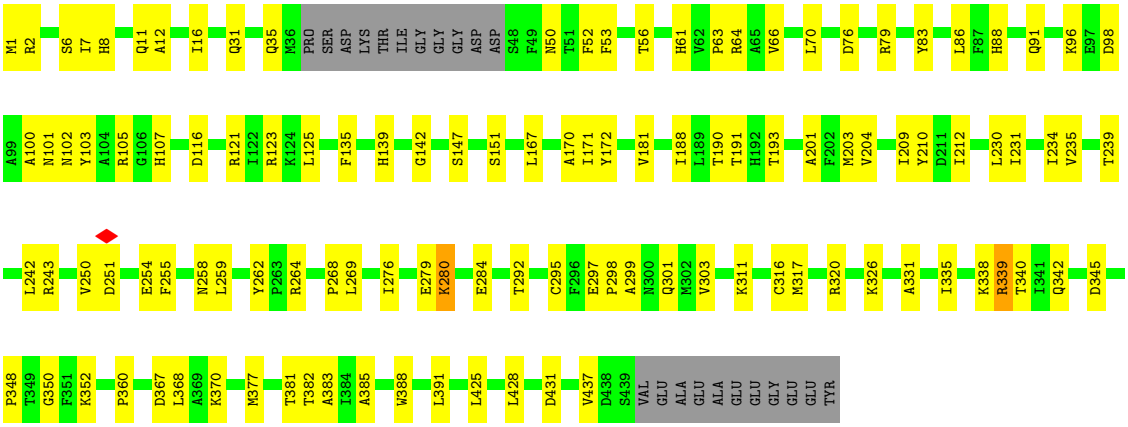
• Molecule 8: Tubulin alpha-3 chain

Chain FE:



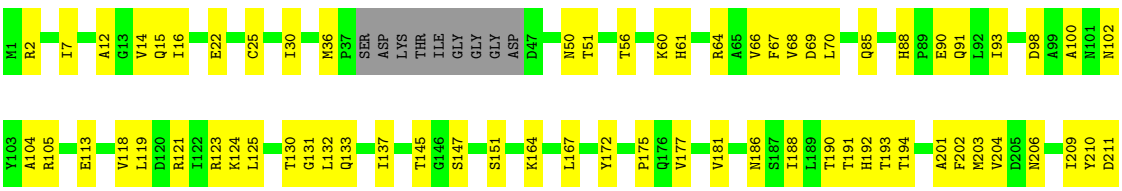
• Molecule 8: Tubulin alpha-3 chain

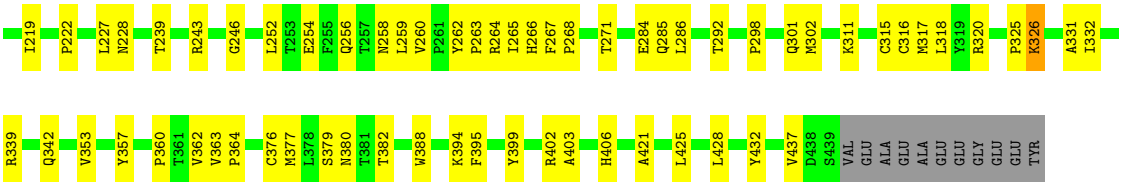
Chain FG:



• Molecule 8: Tubulin alpha-3 chain

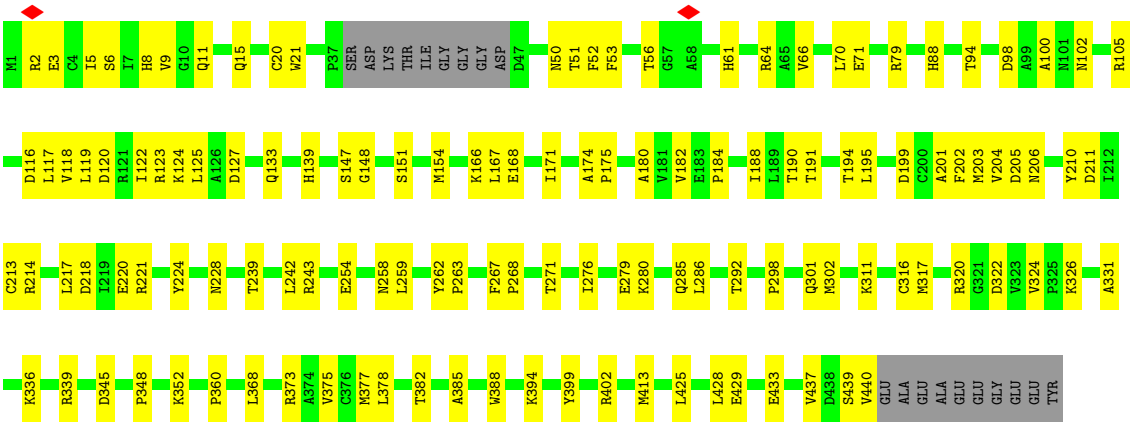
Chain FI:





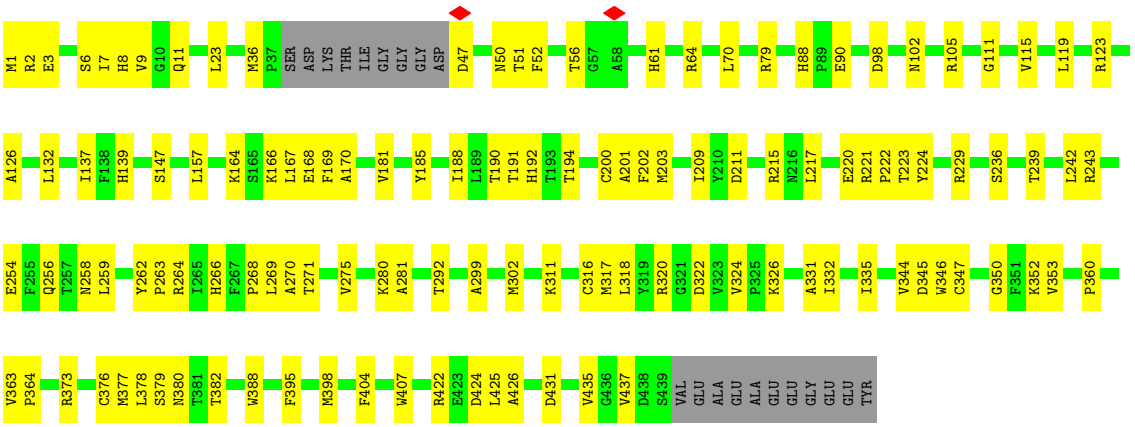
• Molecule 8: Tubulin alpha-3 chain

Chain FK:



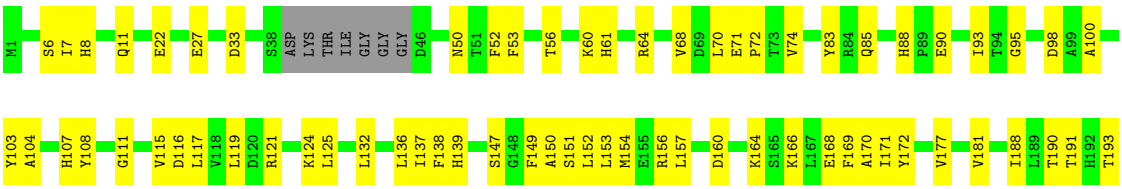
• Molecule 8: Tubulin alpha-3 chain

Chain FM:



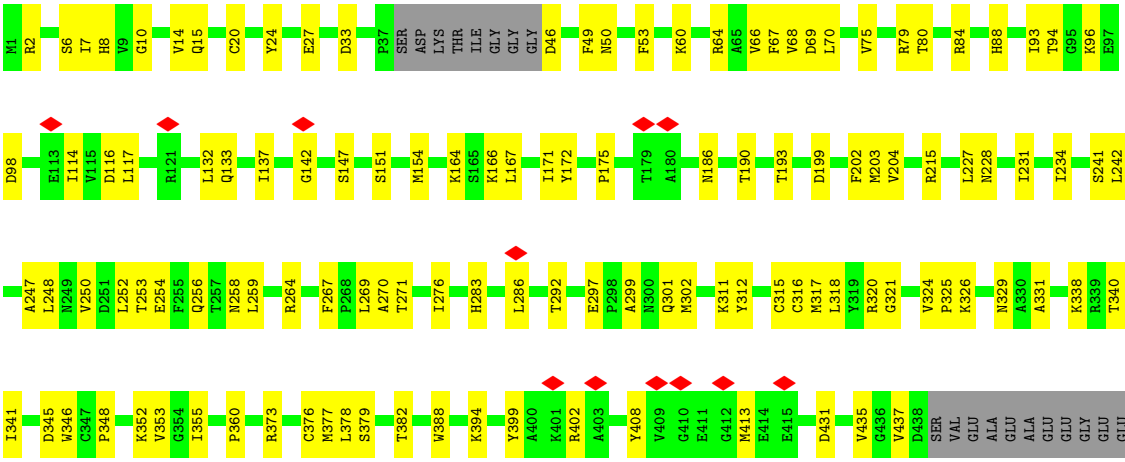
• Molecule 8: Tubulin alpha-3 chain

Chain FO:



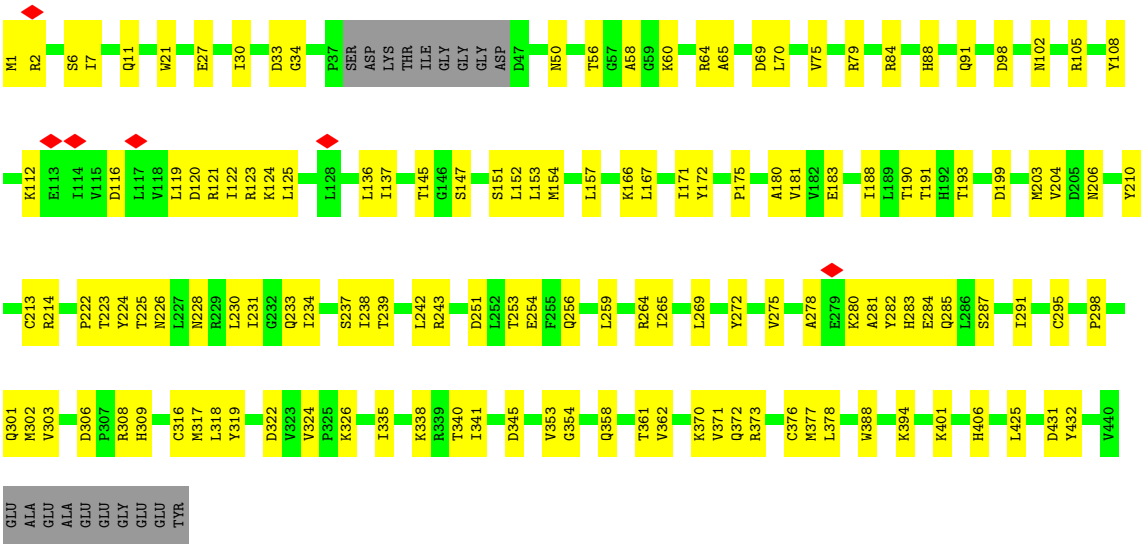
• Molecule 8: Tubulin alpha-3 chain

Chain GA:



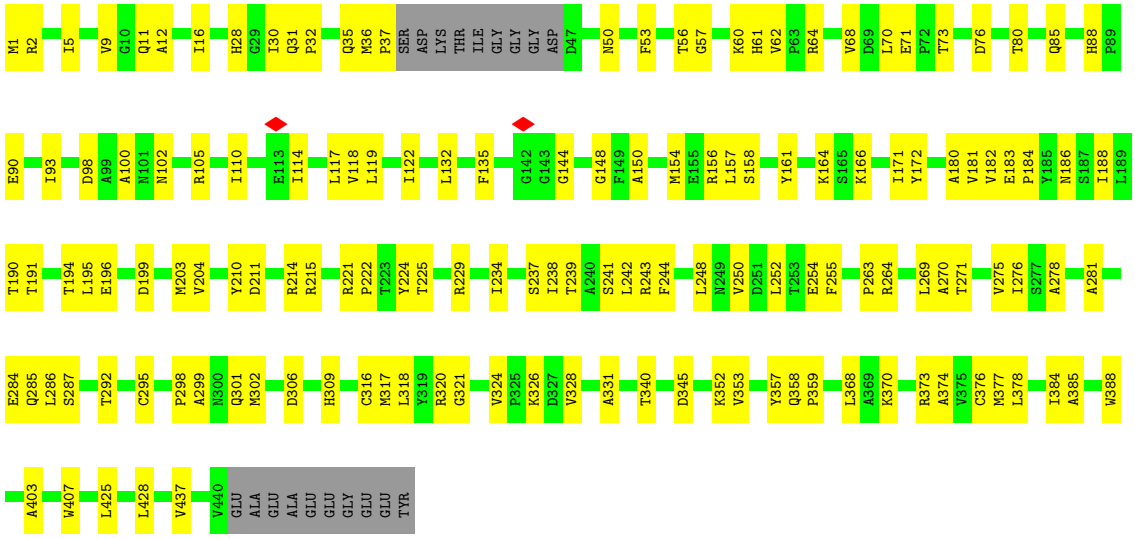
• Molecule 8: Tubulin alpha-3 chain

Chain GC:



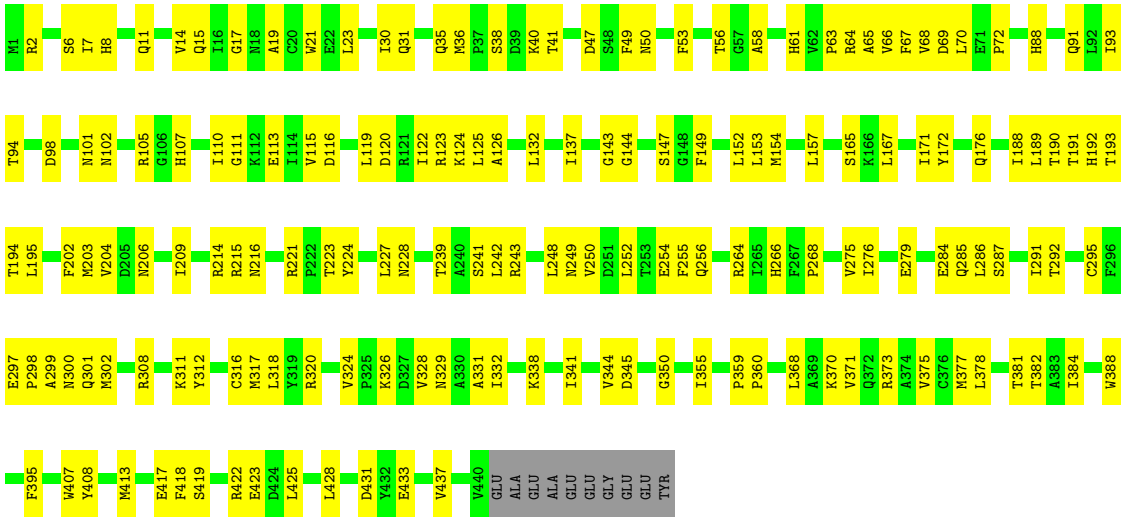
• Molecule 8: Tubulin alpha-3 chain

Chain GE:



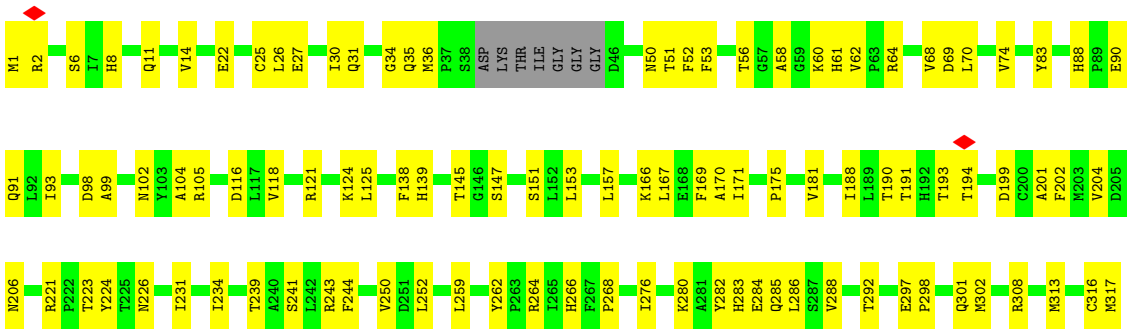
• Molecule 8: Tubulin alpha-3 chain

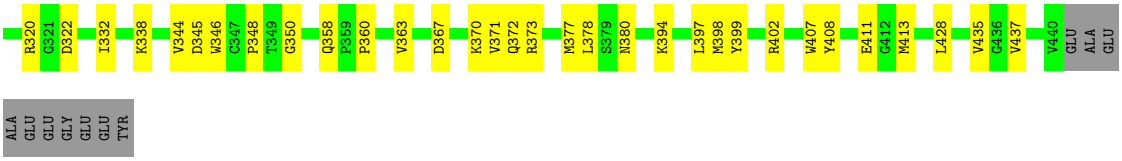
Chain GG:



• Molecule 8: Tubulin alpha-3 chain

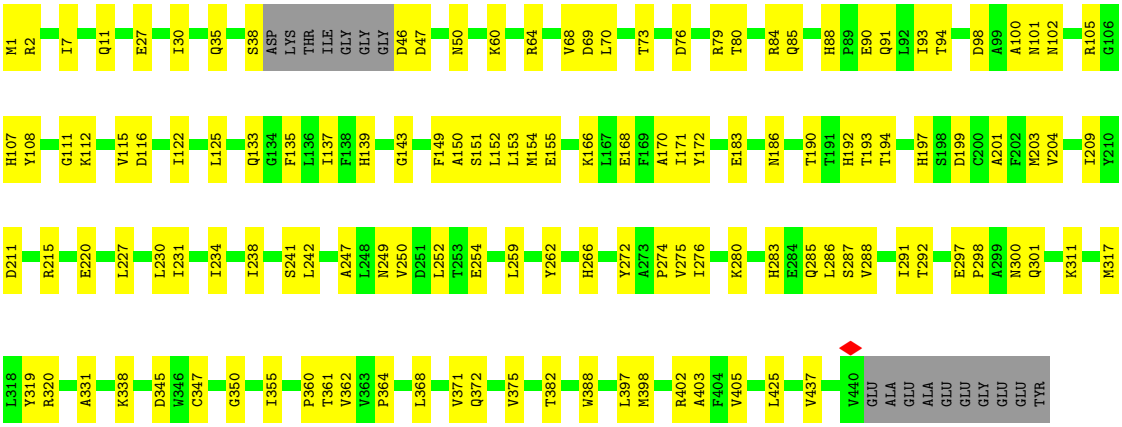
Chain GI:





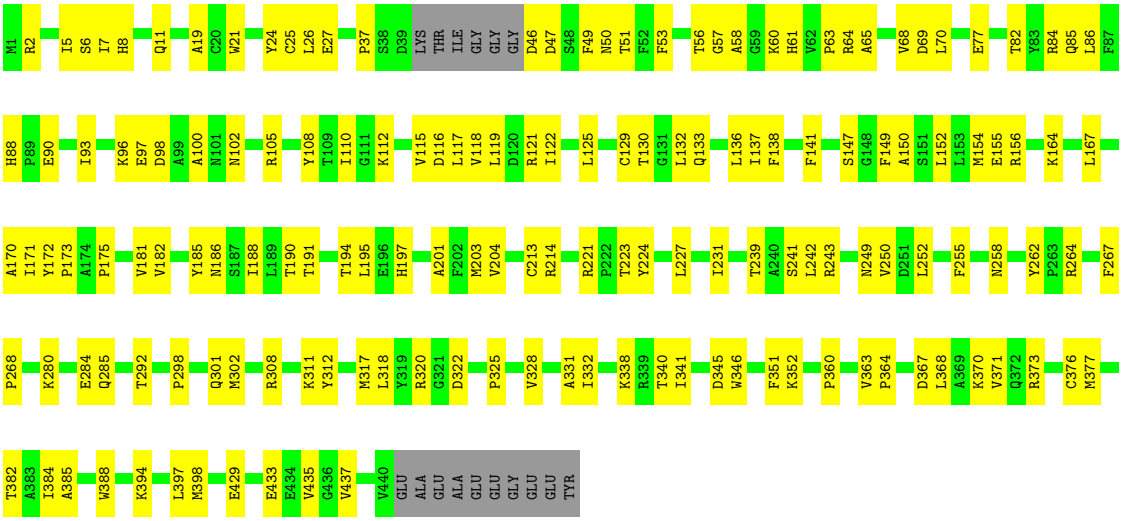
• Molecule 8: Tubulin alpha-3 chain

Chain GK:



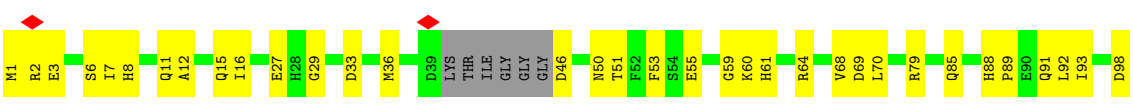
• Molecule 8: Tubulin alpha-3 chain

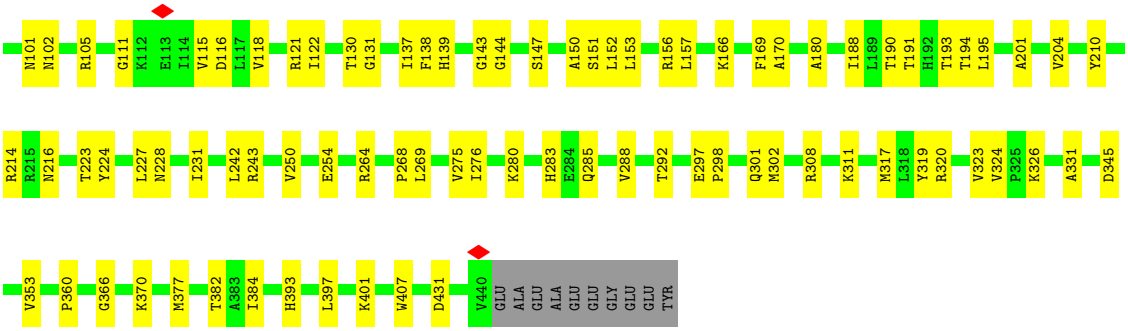
Chain GM:



• Molecule 8: Tubulin alpha-3 chain

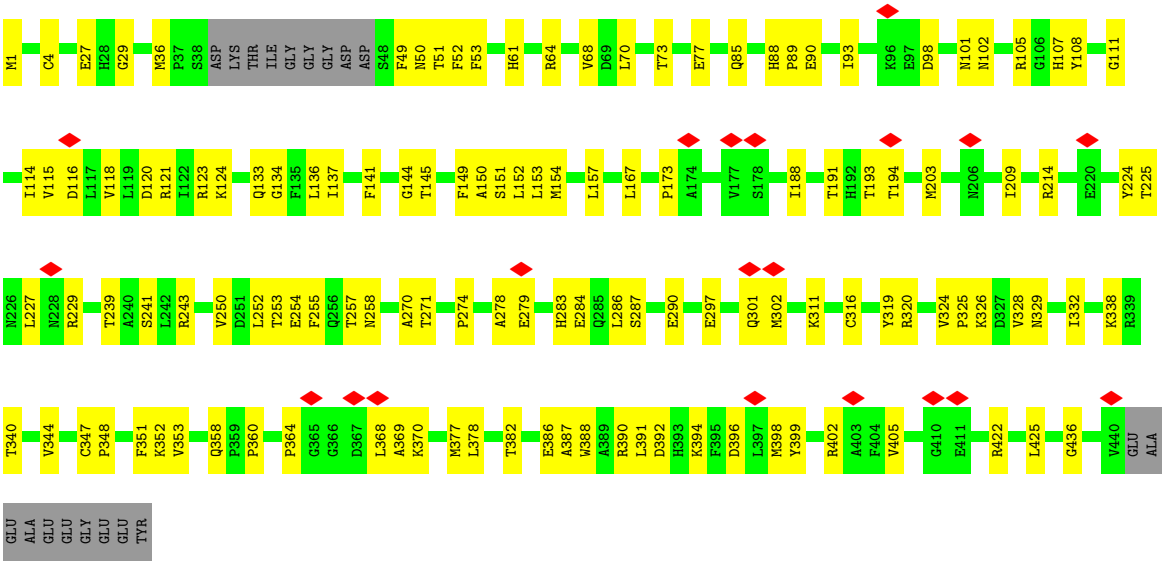
Chain GO:





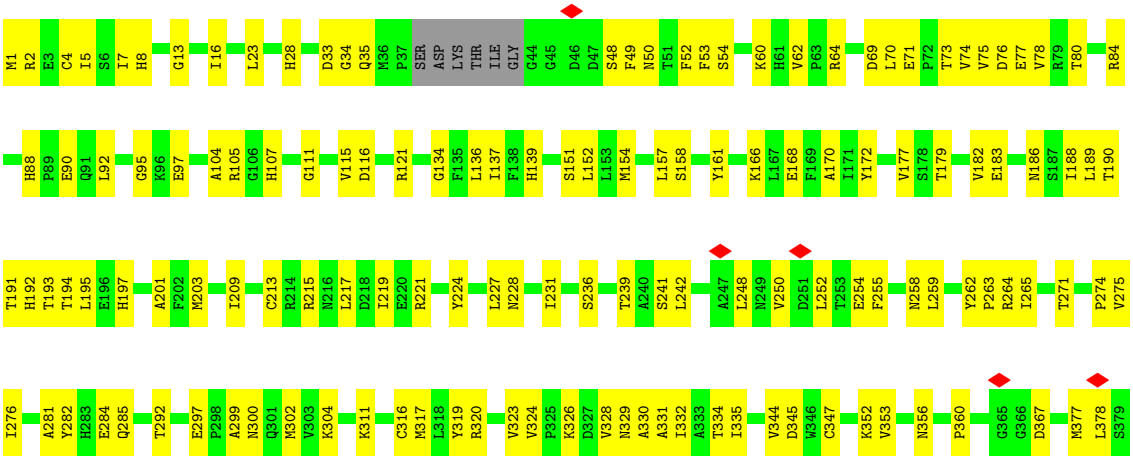
• Molecule 8: Tubulin alpha-3 chain

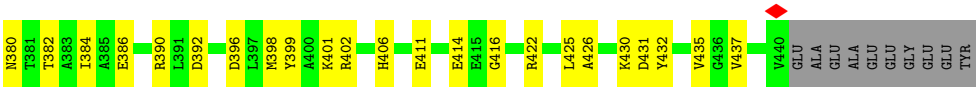
Chain HA:



• Molecule 8: Tubulin alpha-3 chain

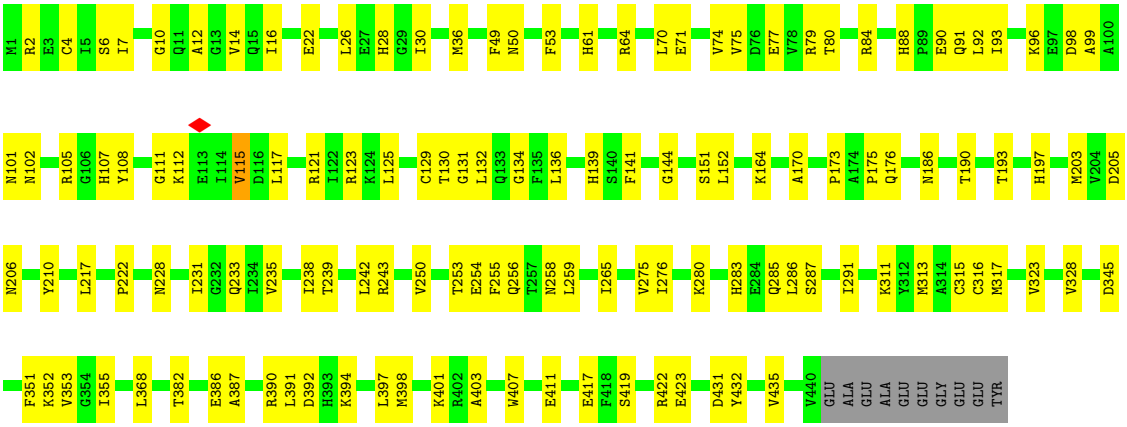
Chain HC:





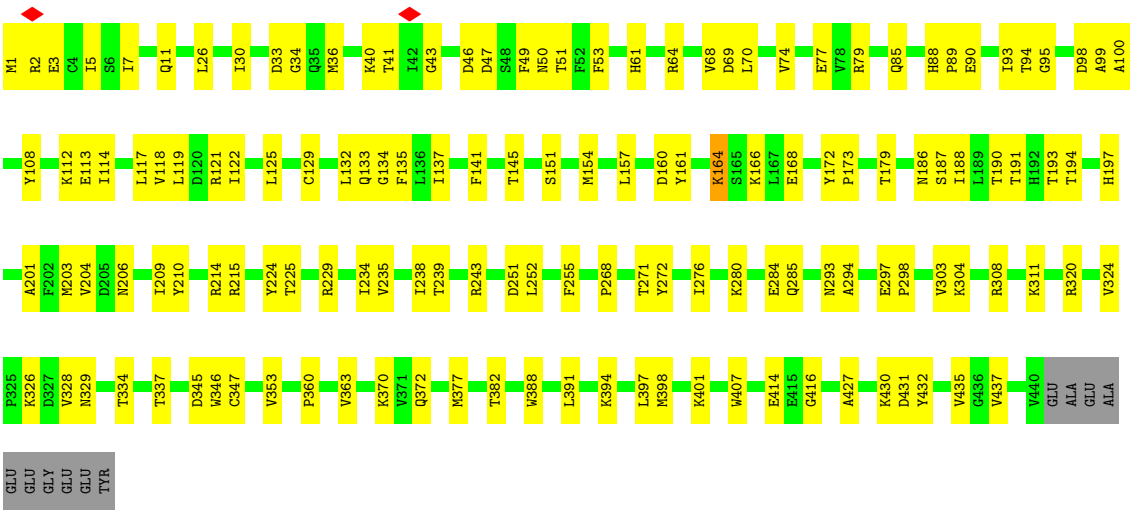
• Molecule 8: Tubulin alpha-3 chain

Chain HE:



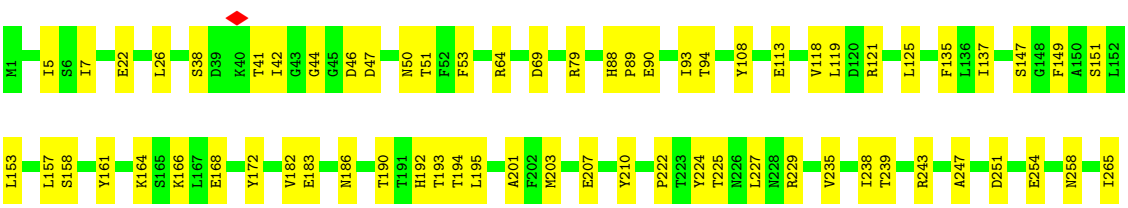
• Molecule 8: Tubulin alpha-3 chain

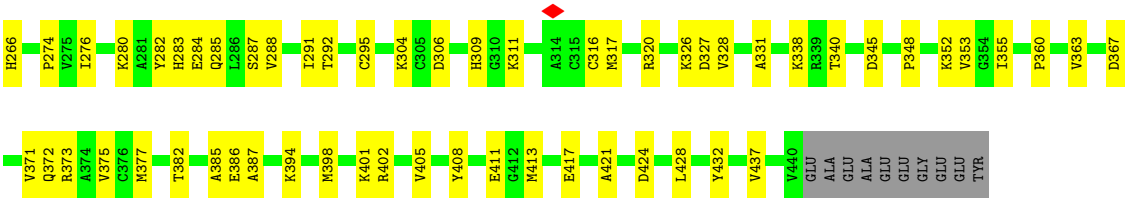
Chain HG:



• Molecule 8: Tubulin alpha-3 chain

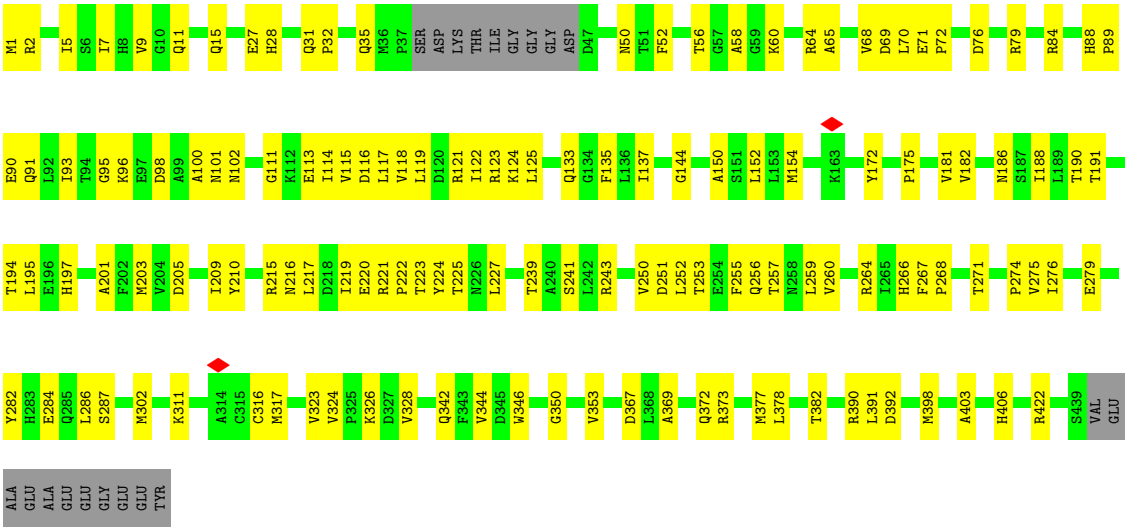
Chain HI:





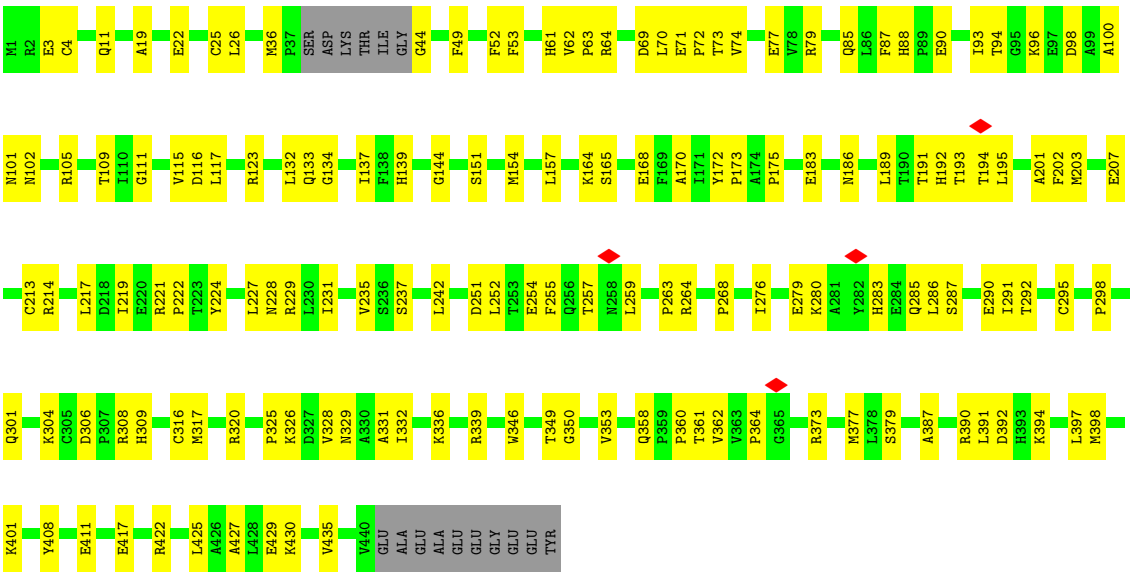
• Molecule 8: Tubulin alpha-3 chain

Chain HK:



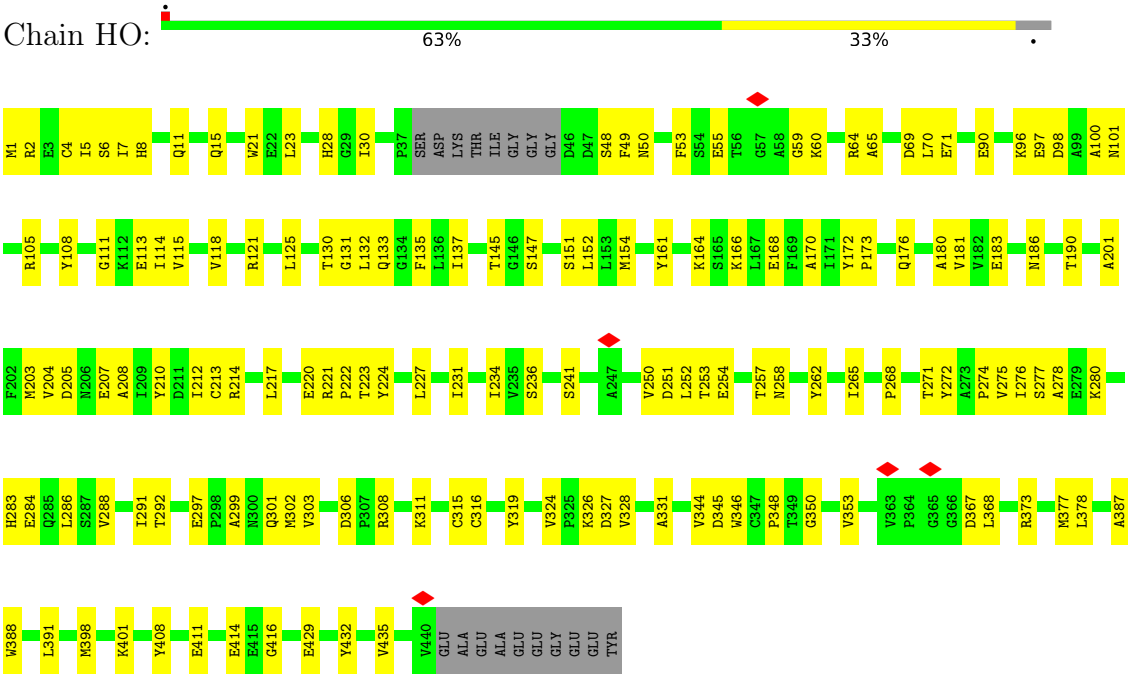
• Molecule 8: Tubulin alpha-3 chain

Chain HM:



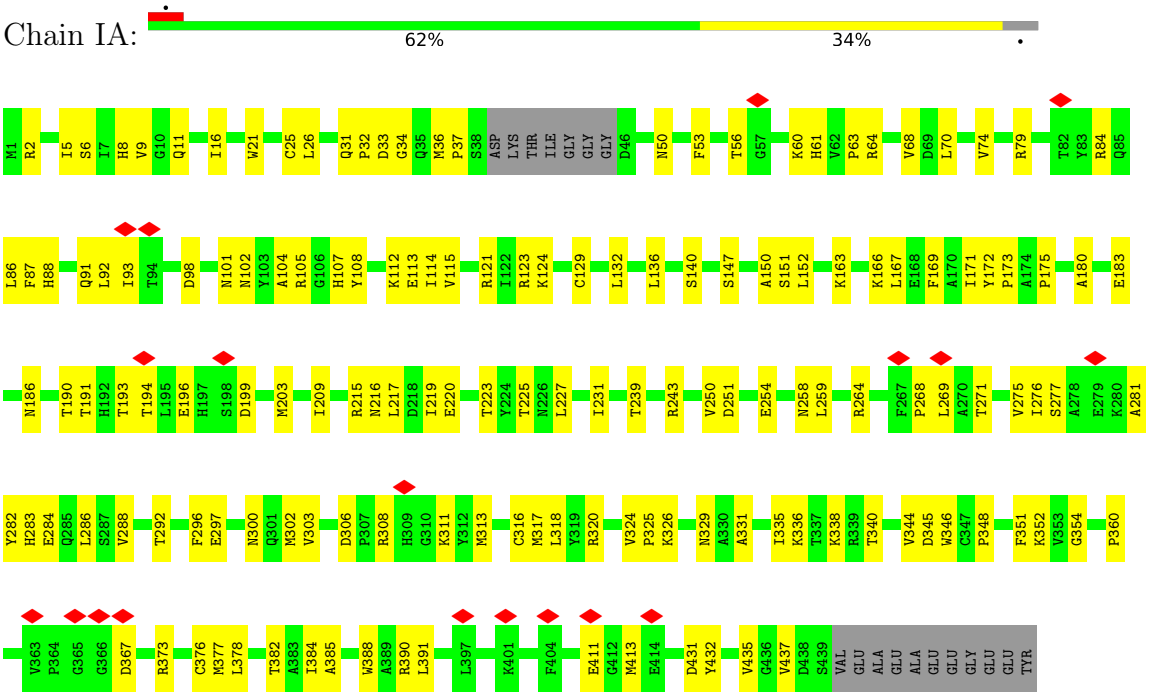
• Molecule 8: Tubulin alpha-3 chain

Chain HO:



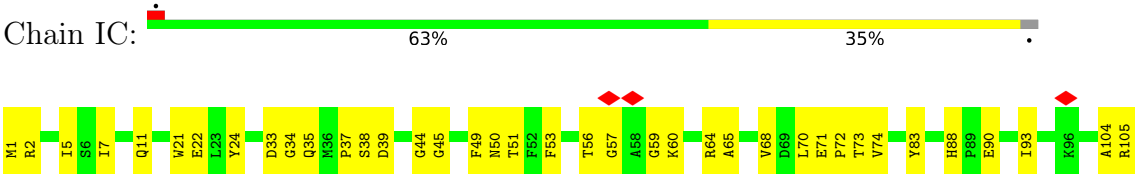
• Molecule 8: Tubulin alpha-3 chain

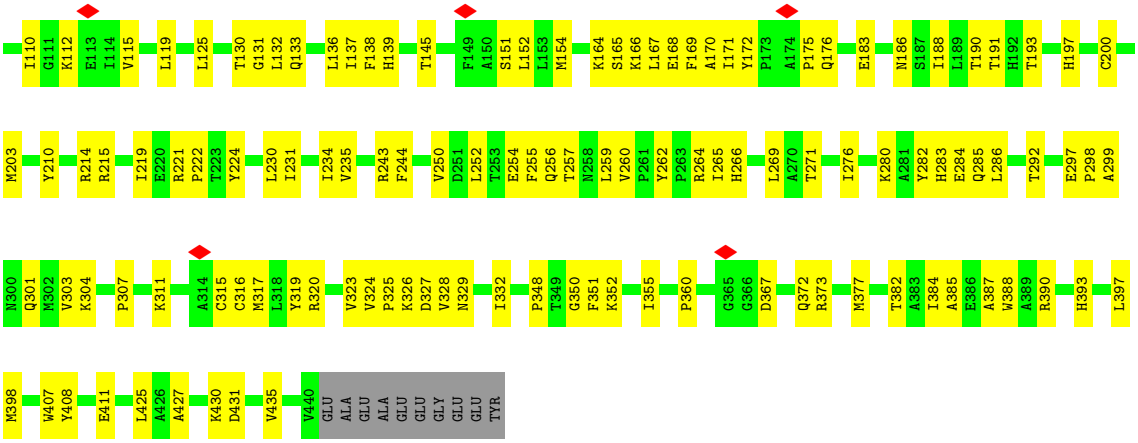
Chain IA:



• Molecule 8: Tubulin alpha-3 chain

Chain IC:



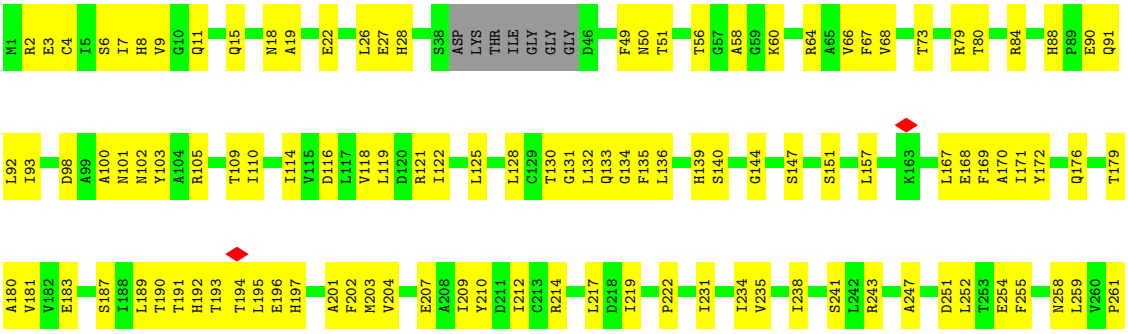


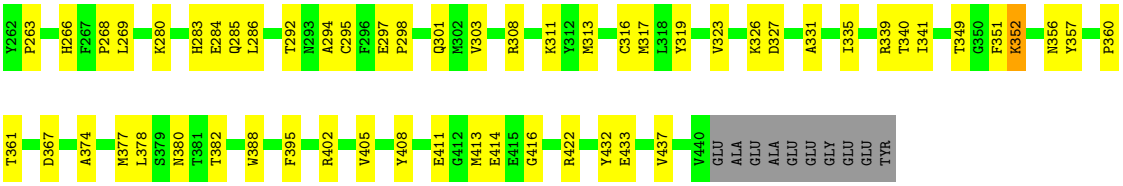
• Molecule 8: Tubulin alpha-3 chain

Chain IE:

• Molecule 8: Tubulin alpha-3 chain

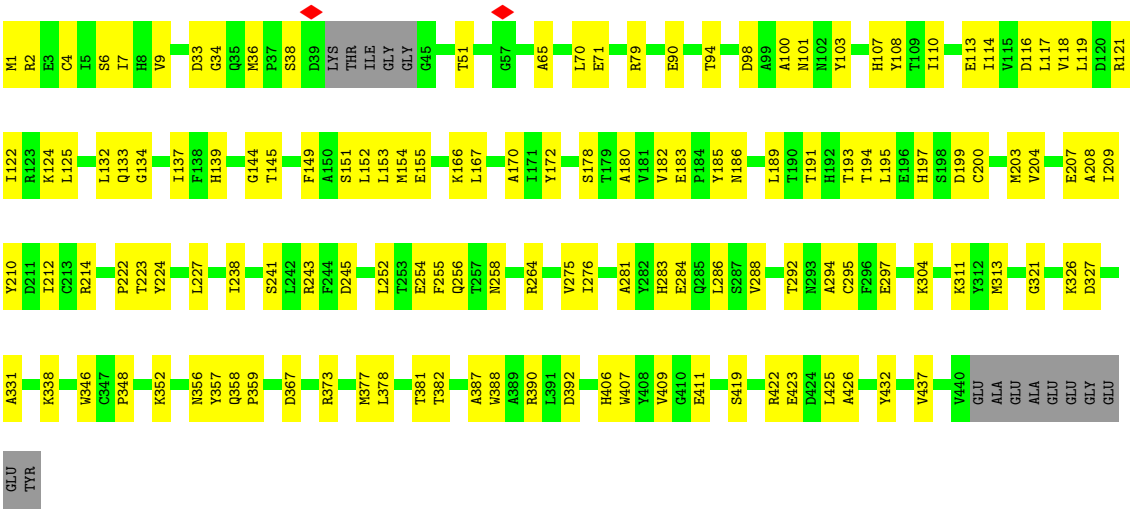
Chain IG:





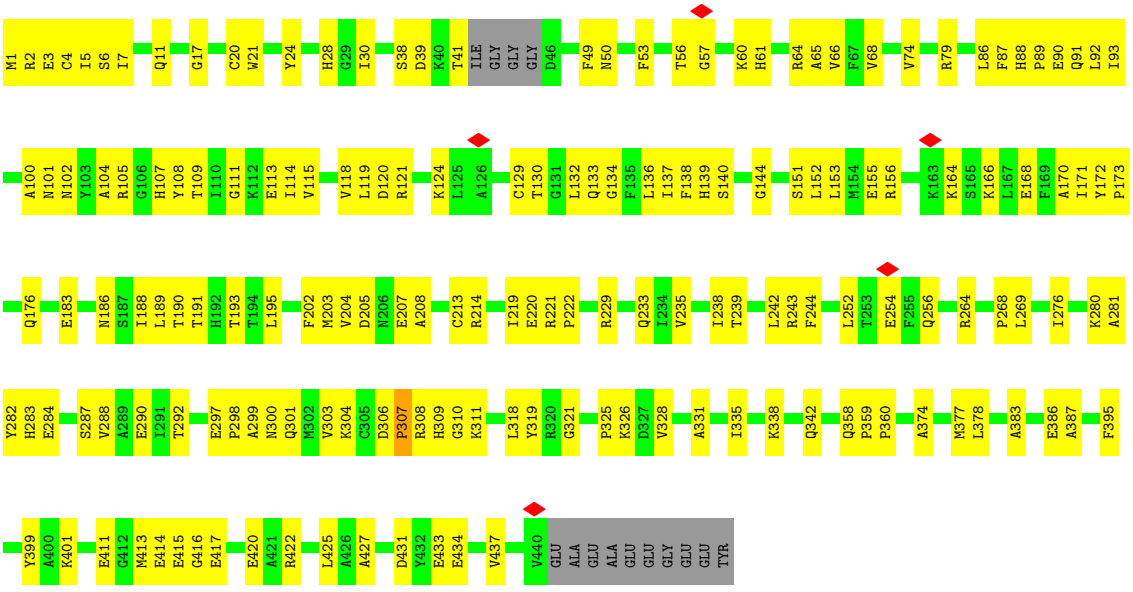
• Molecule 8: Tubulin alpha-3 chain

Chain II:



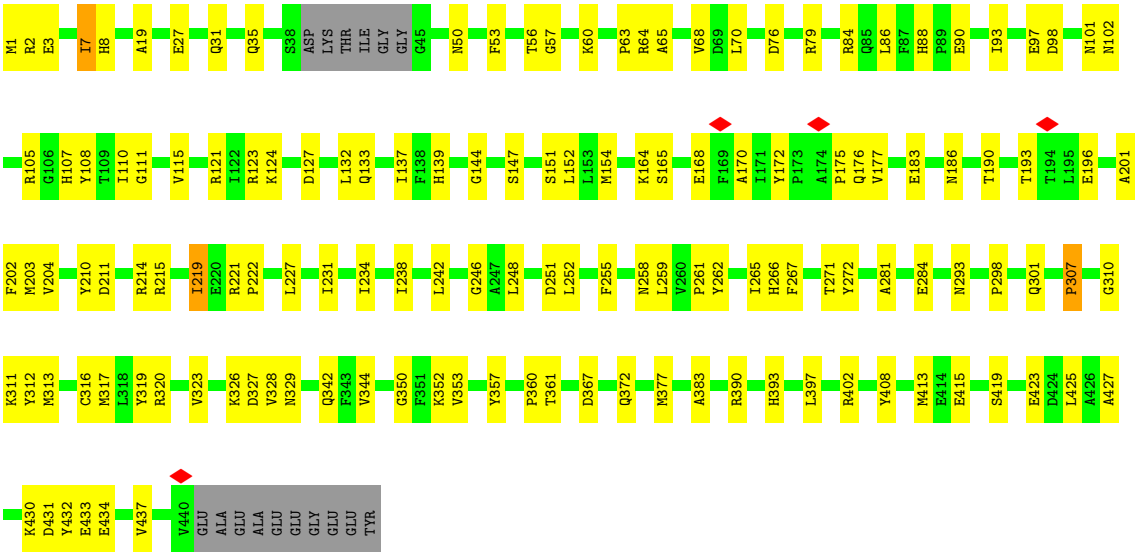
• Molecule 8: Tubulin alpha-3 chain

Chain IK:



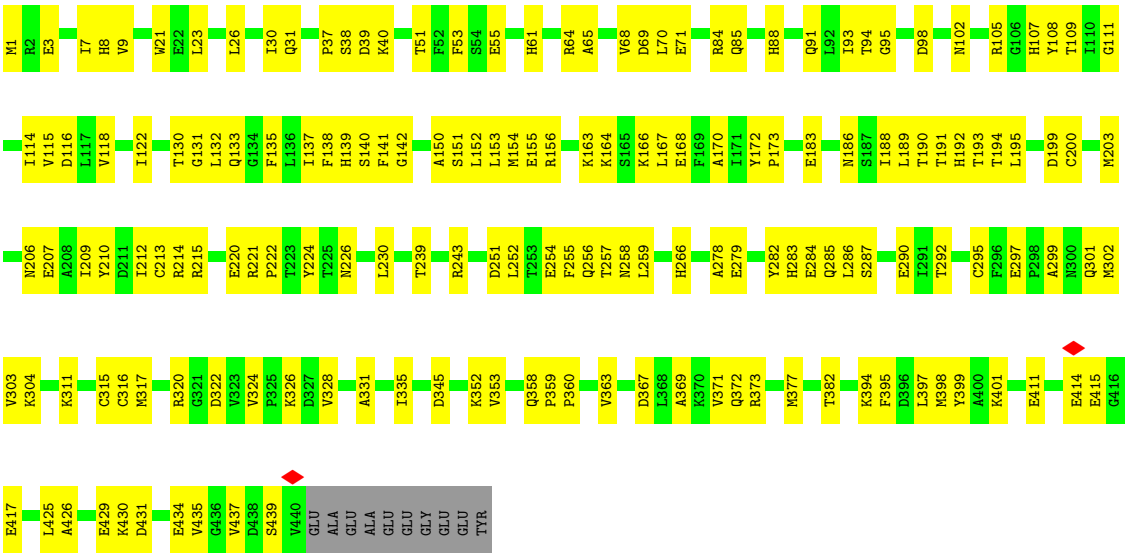
• Molecule 8: Tubulin alpha-3 chain

Chain IM:



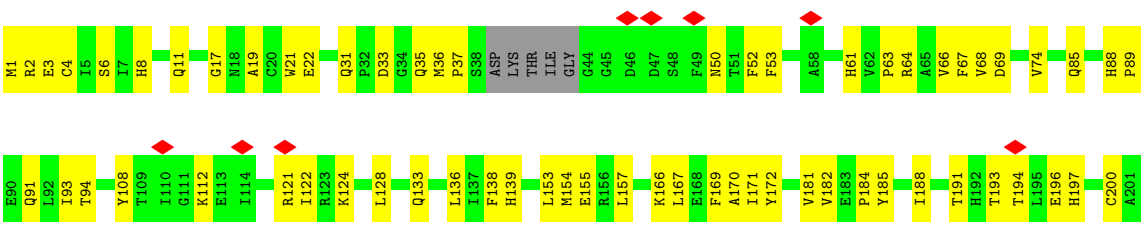
• Molecule 8: Tubulin alpha-3 chain

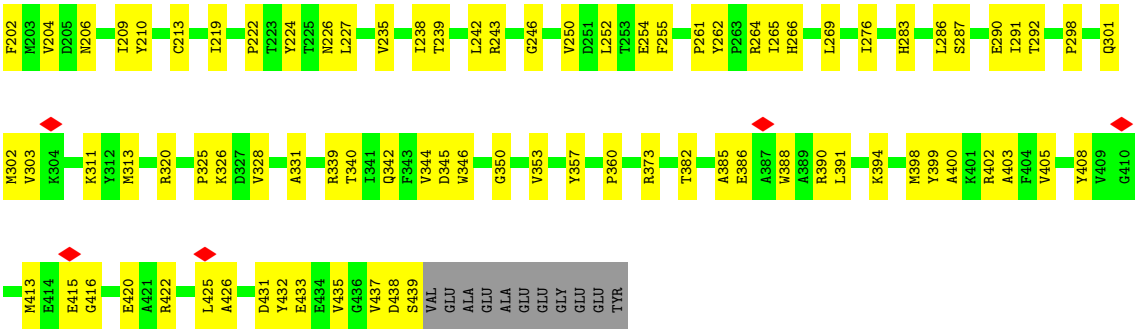
Chain IO:



• Molecule 8: Tubulin alpha-3 chain

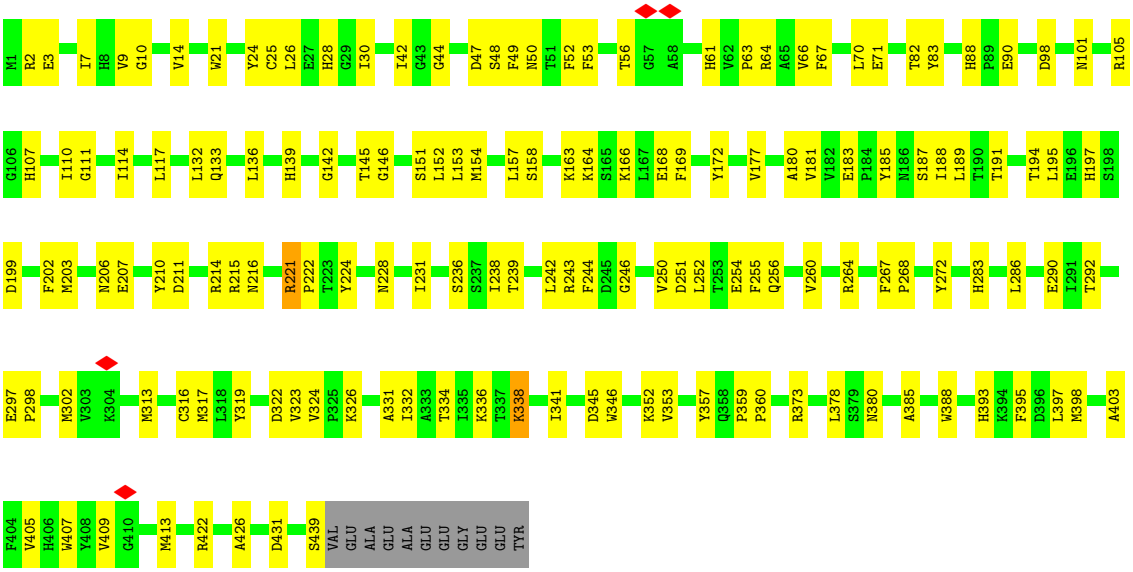
Chain JC:





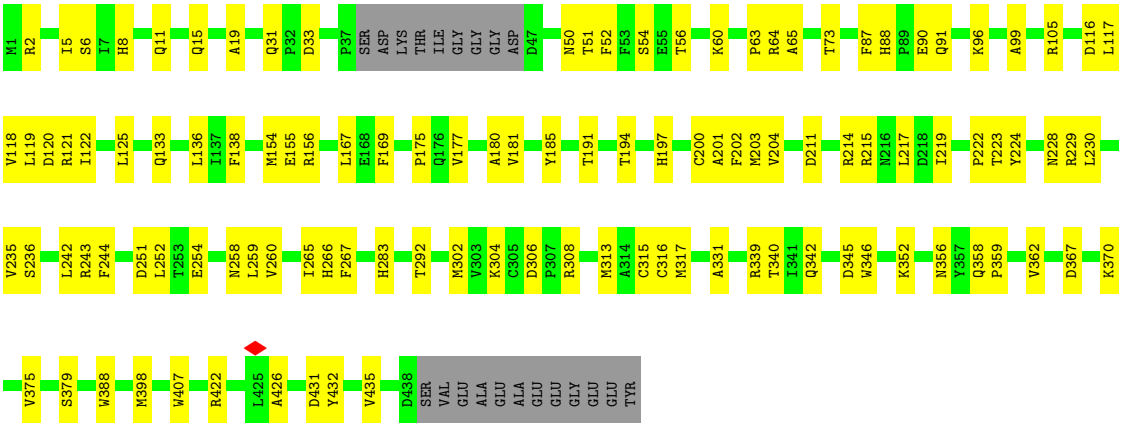
• Molecule 8: Tubulin alpha-3 chain

Chain JE:



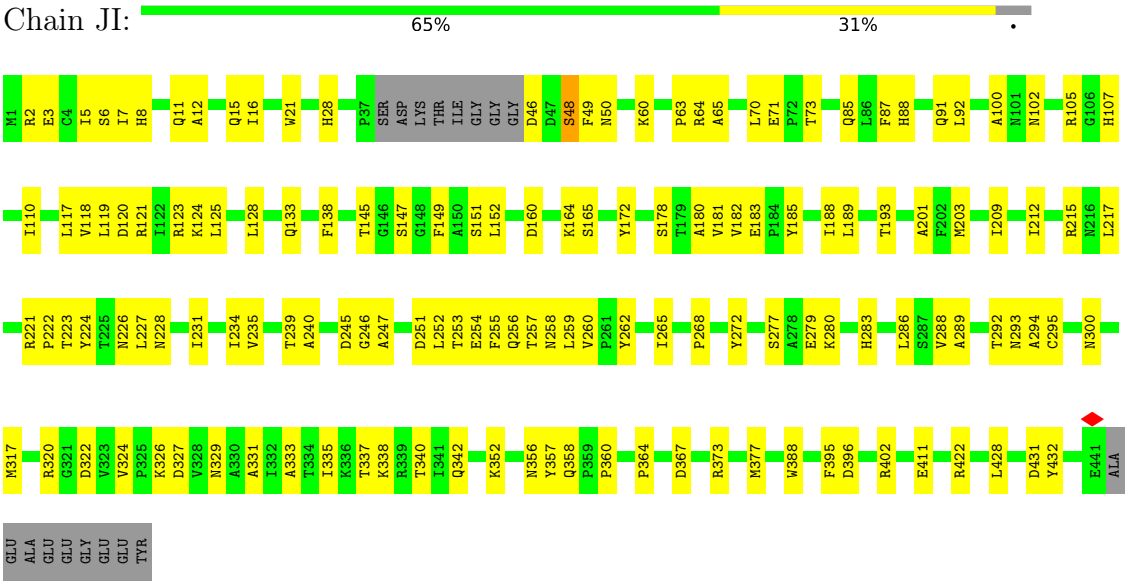
• Molecule 8: Tubulin alpha-3 chain

Chain JG:



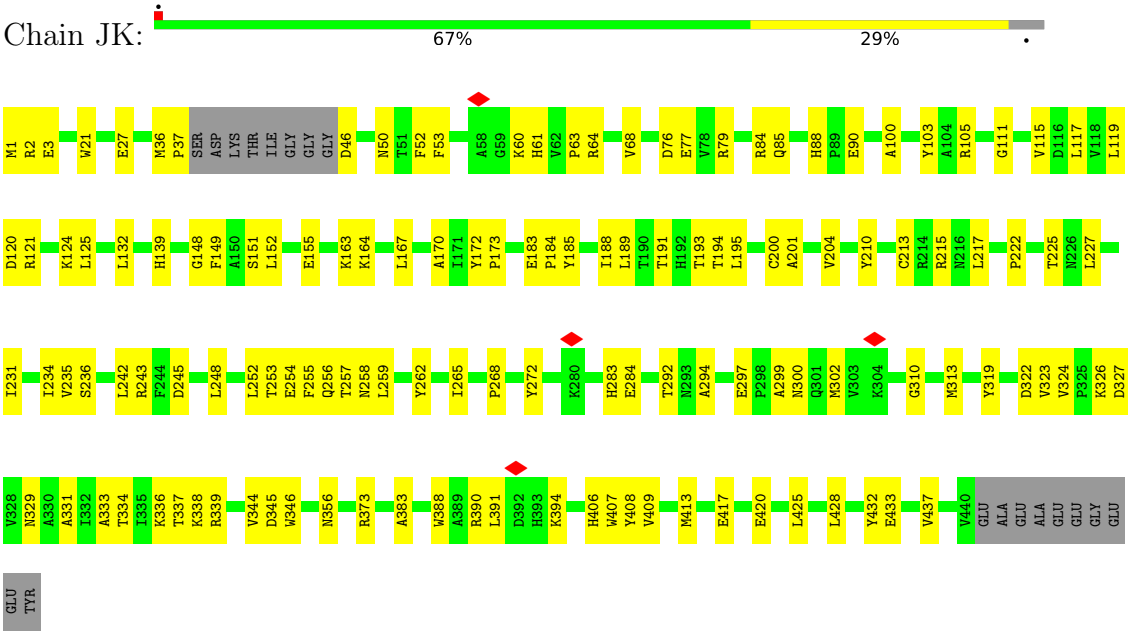
• Molecule 8: Tubulin alpha-3 chain

Chain JI:



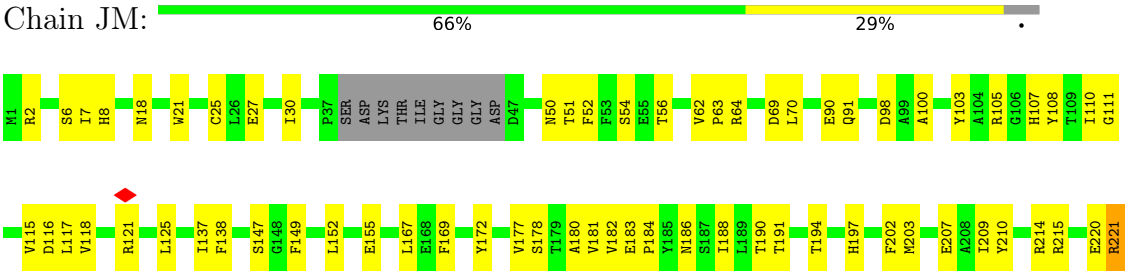
• Molecule 8: Tubulin alpha-3 chain

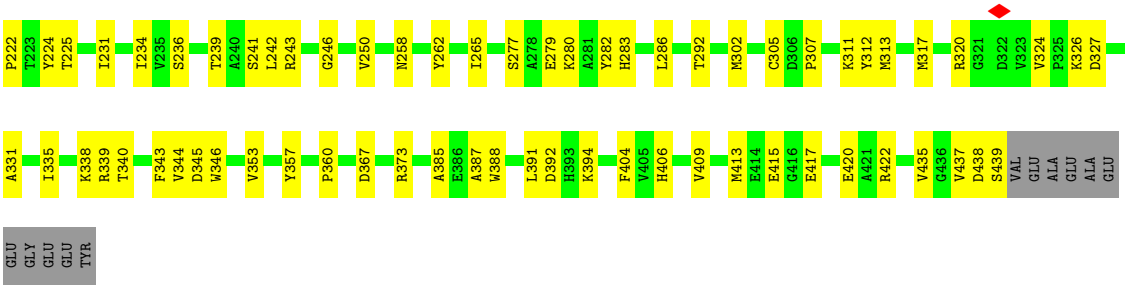
Chain JK:



• Molecule 8: Tubulin alpha-3 chain

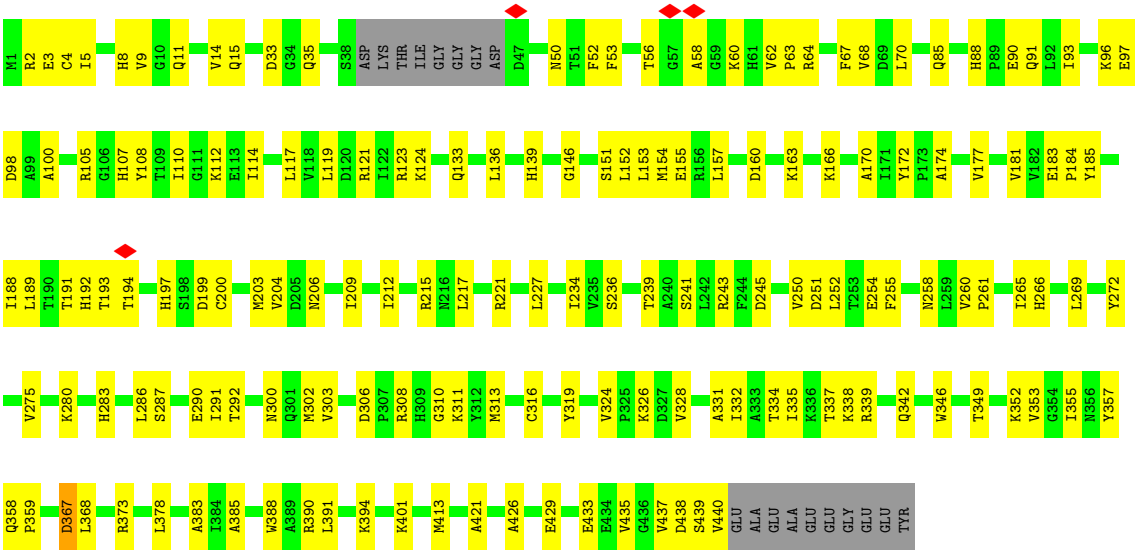
Chain JM:





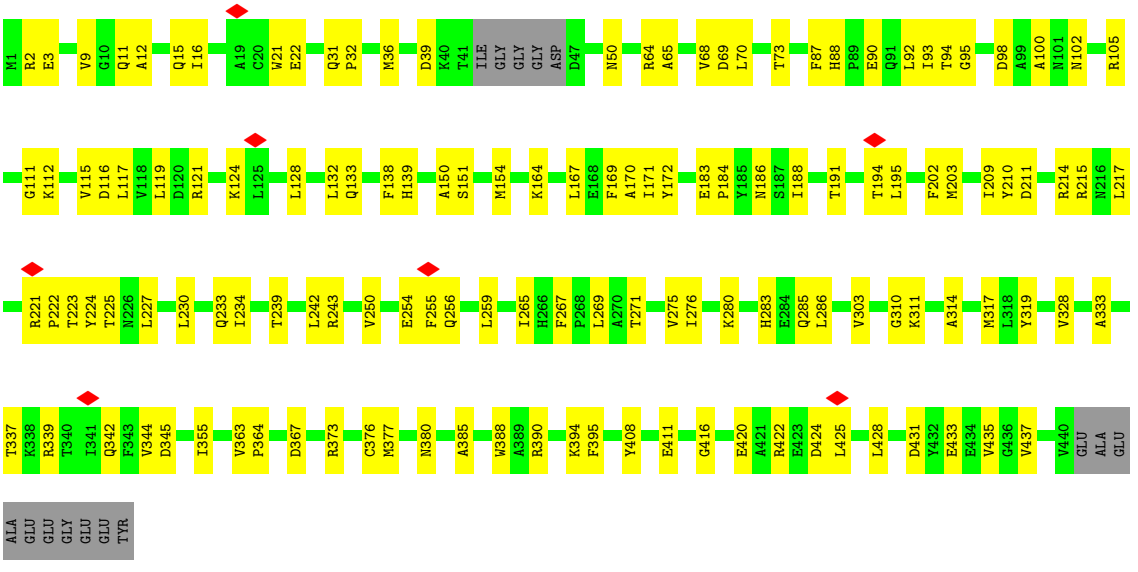
• Molecule 8: Tubulin alpha-3 chain

Chain JO:



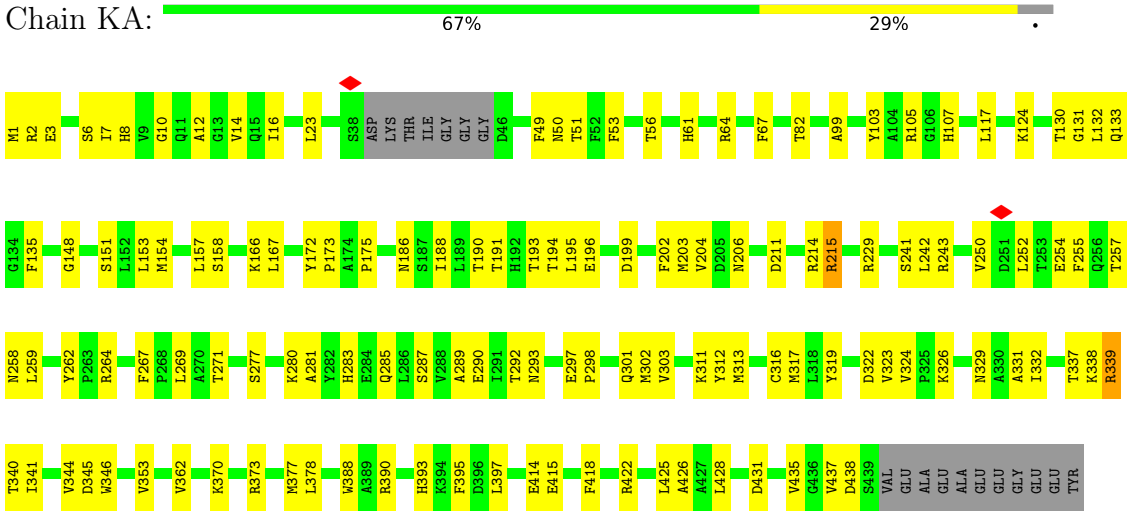
• Molecule 8: Tubulin alpha-3 chain

Chain JQ:



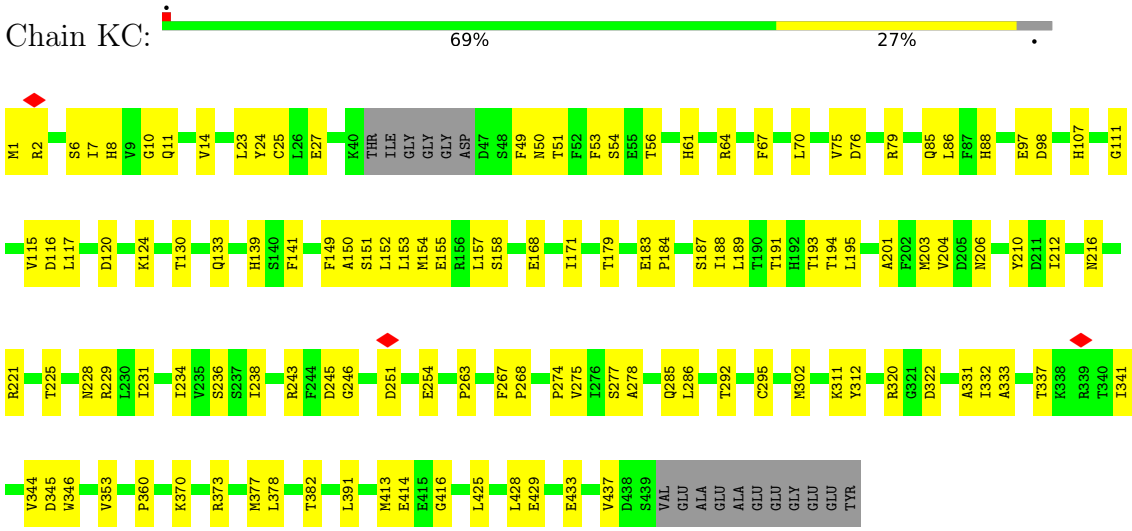
• Molecule 8: Tubulin alpha-3 chain

Chain KA:



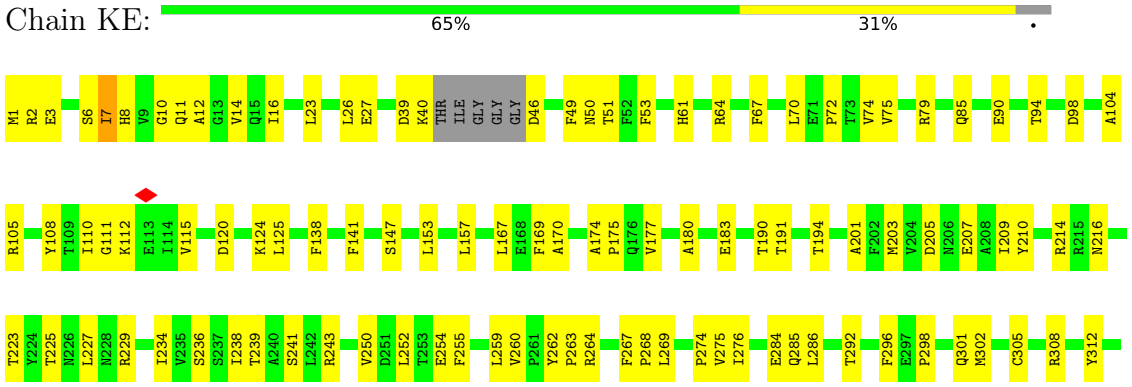
• Molecule 8: Tubulin alpha-3 chain

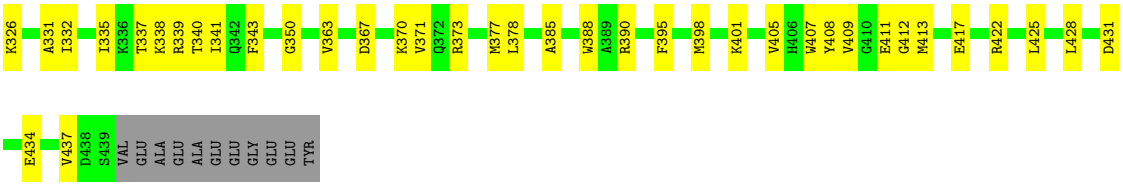
Chain KC:



• Molecule 8: Tubulin alpha-3 chain

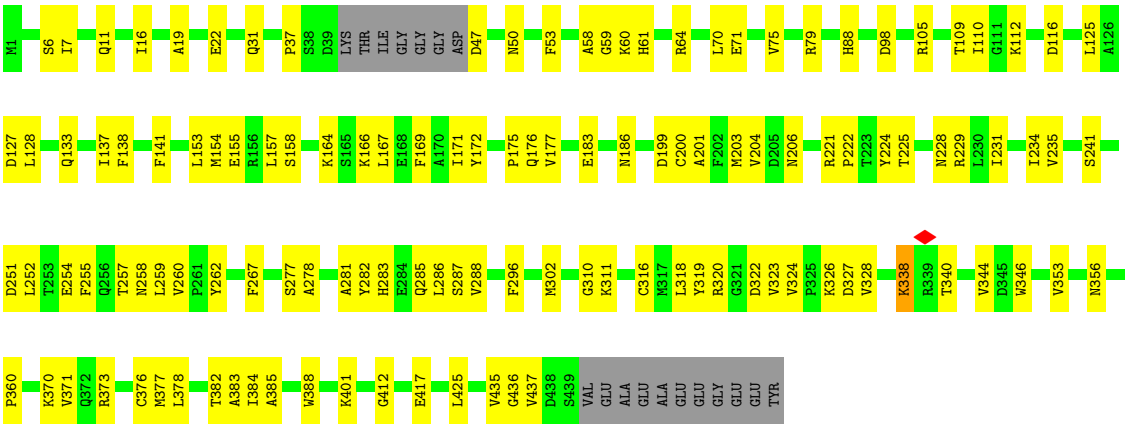
Chain KE:





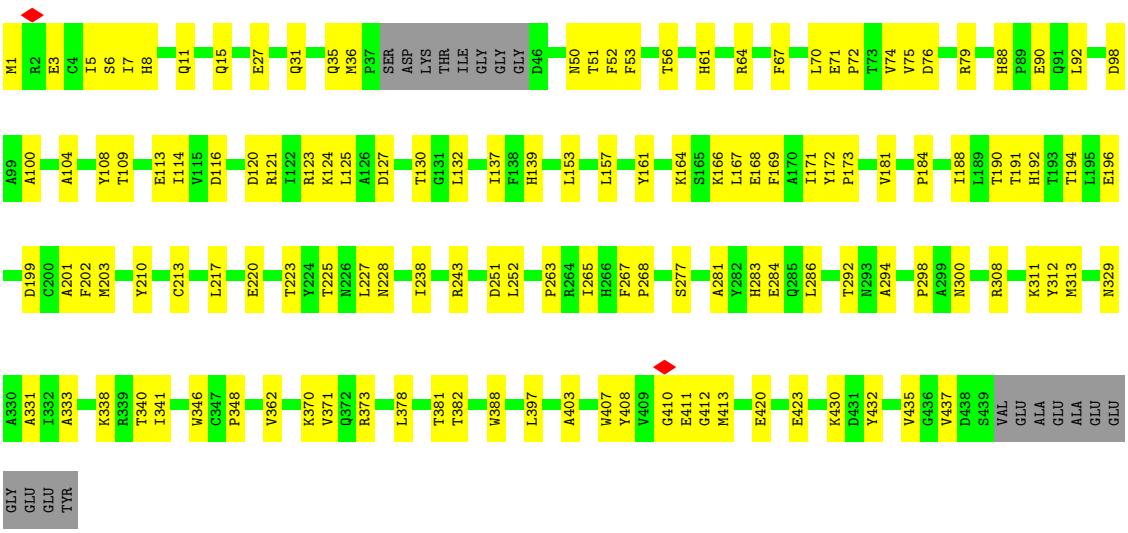
• Molecule 8: Tubulin alpha-3 chain

Chain KG:



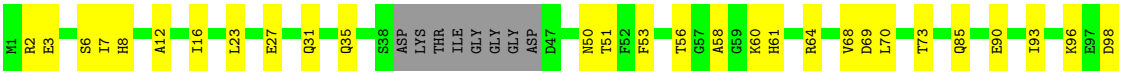
• Molecule 8: Tubulin alpha-3 chain

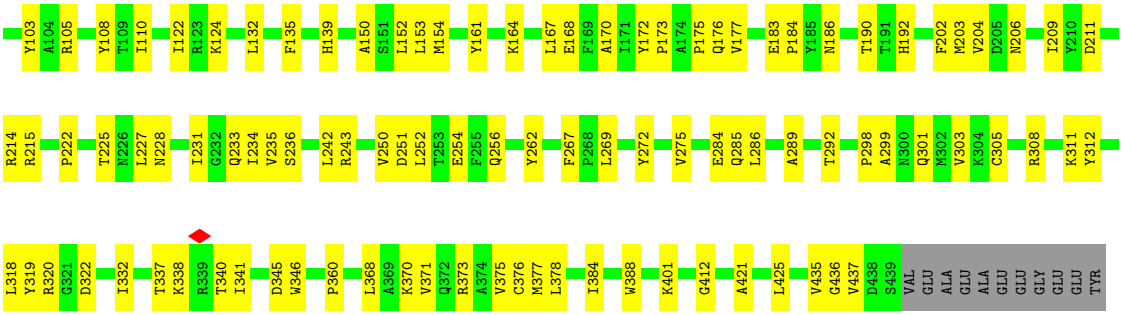
Chain KI:



• Molecule 8: Tubulin alpha-3 chain

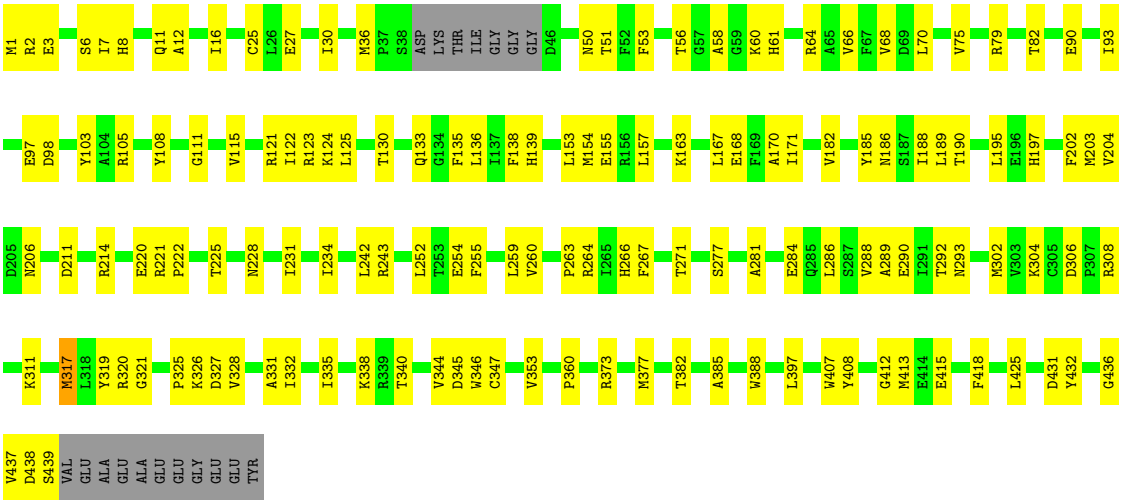
Chain KK:





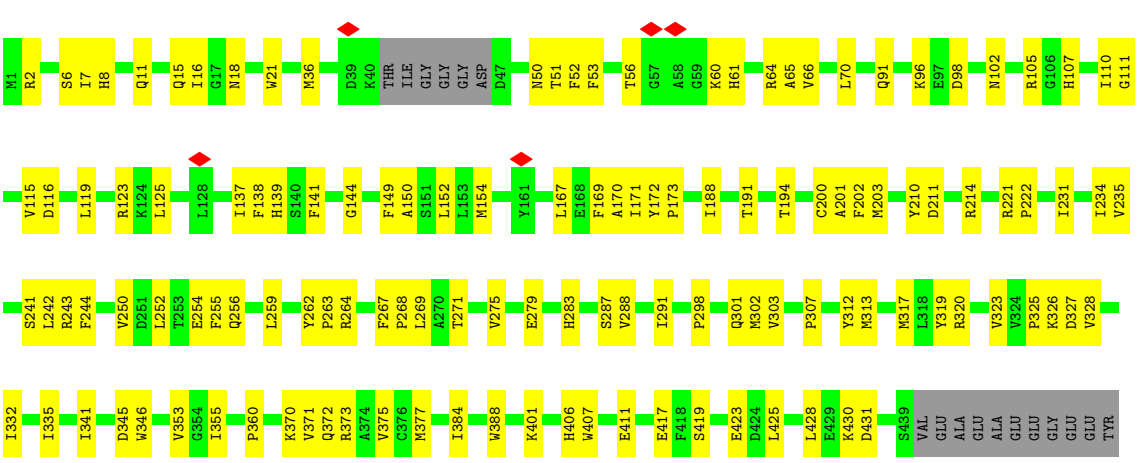
• Molecule 8: Tubulin alpha-3 chain

Chain KM:



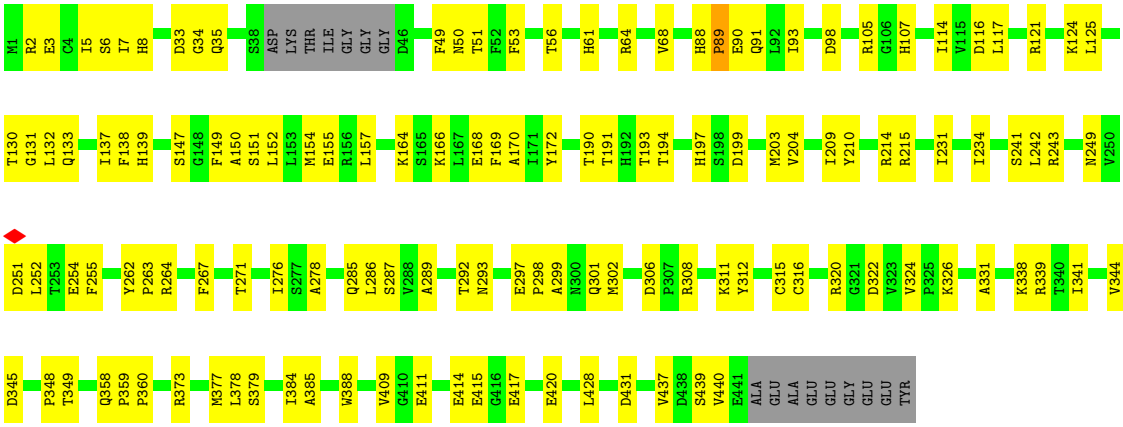
• Molecule 8: Tubulin alpha-3 chain

Chain KO:



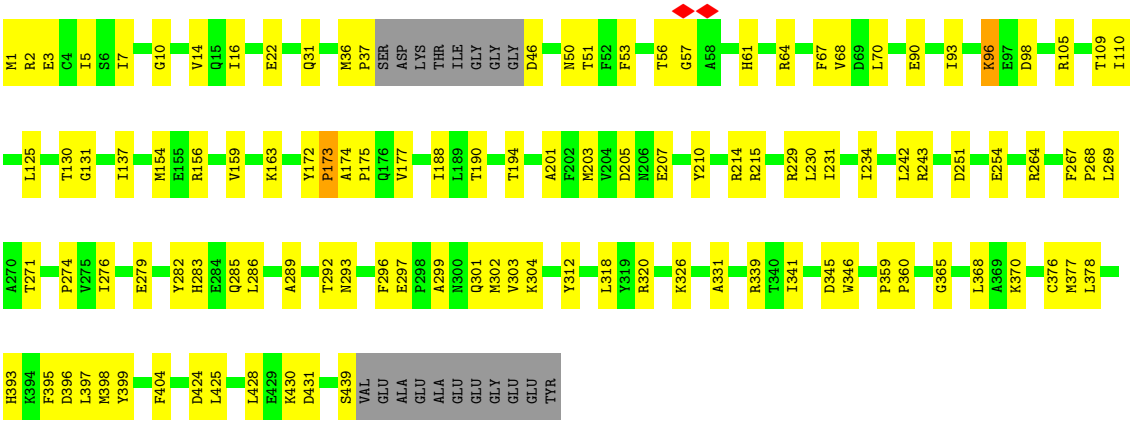
• Molecule 8: Tubulin alpha-3 chain

Chain LA:



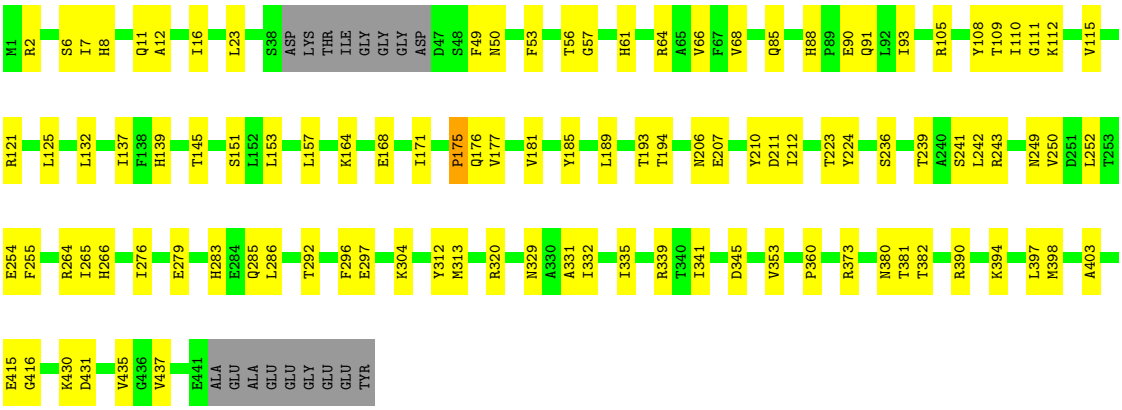
• Molecule 8: Tubulin alpha-3 chain

Chain LC:



• Molecule 8: Tubulin alpha-3 chain

Chain LE:

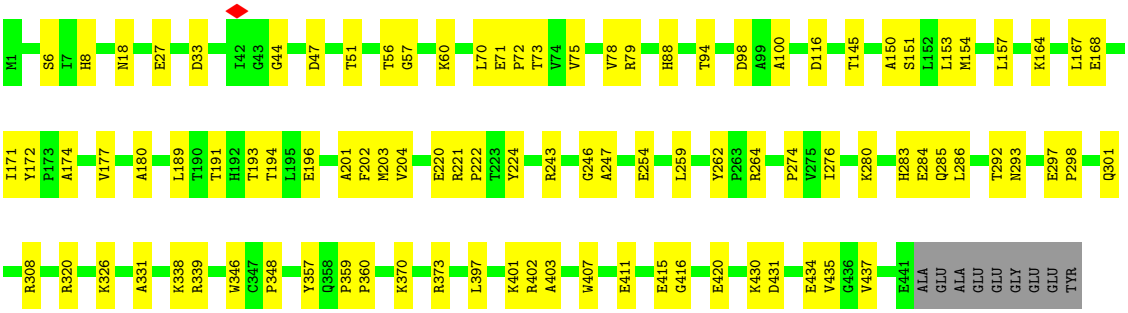


• Molecule 8: Tubulin alpha-3 chain

Chain LG:

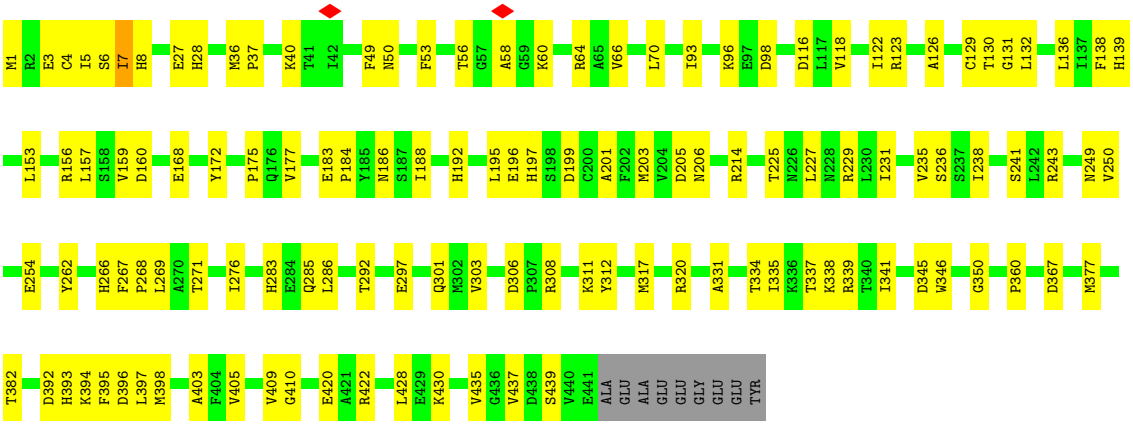
• Molecule 8: Tubulin alpha-3 chain

Chain LI:



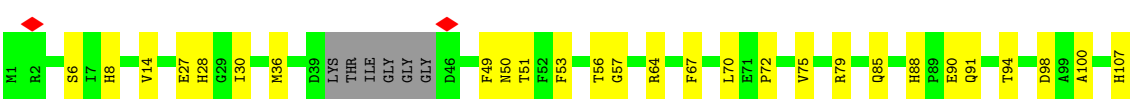
• Molecule 8: Tubulin alpha-3 chain

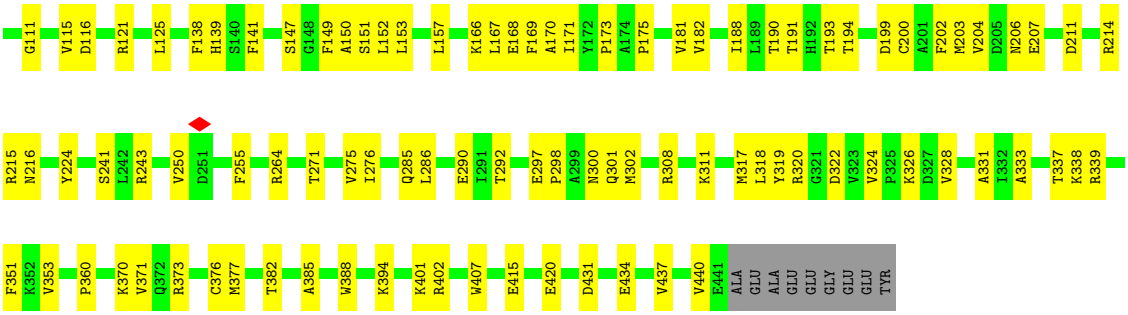
Chain LK:



• Molecule 8: Tubulin alpha-3 chain

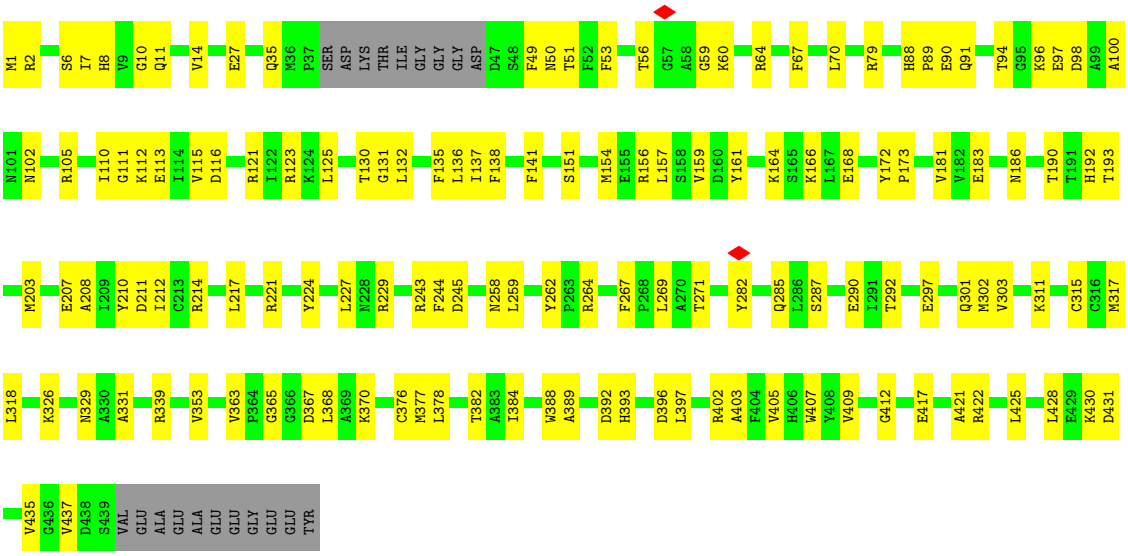
Chain LM:





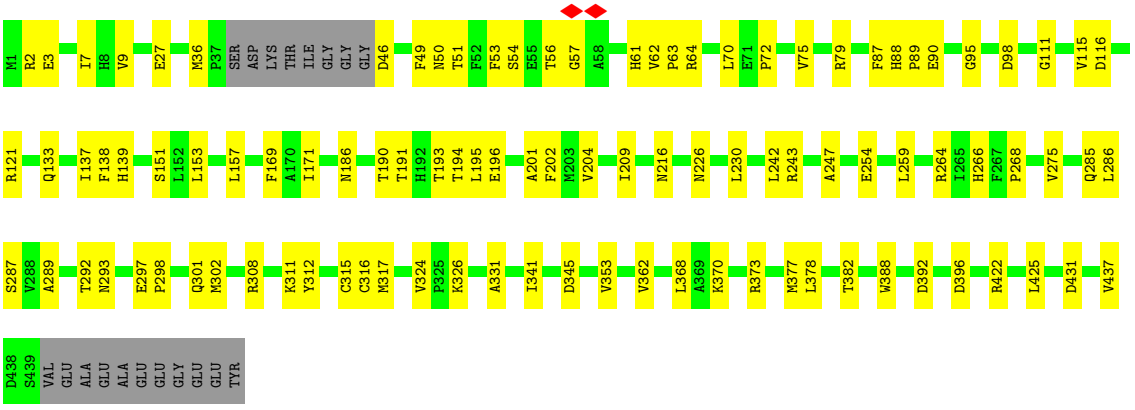
• Molecule 8: Tubulin alpha-3 chain

Chain LO:



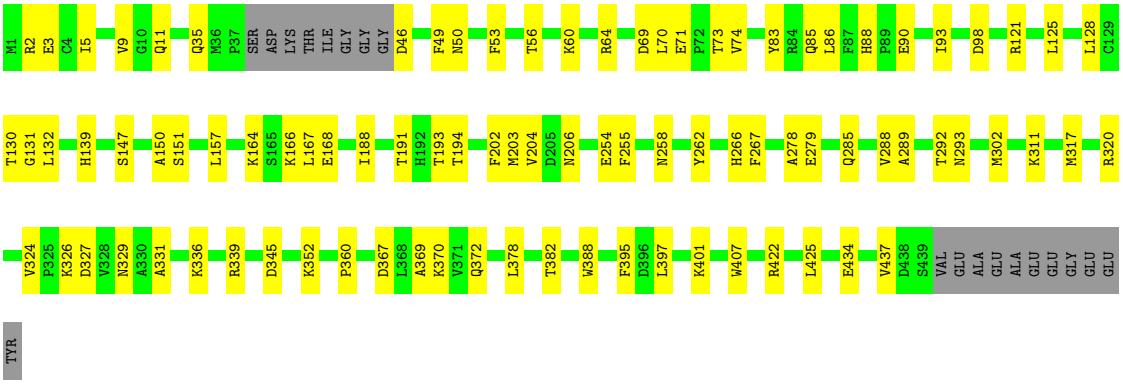
• Molecule 8: Tubulin alpha-3 chain

Chain MA:



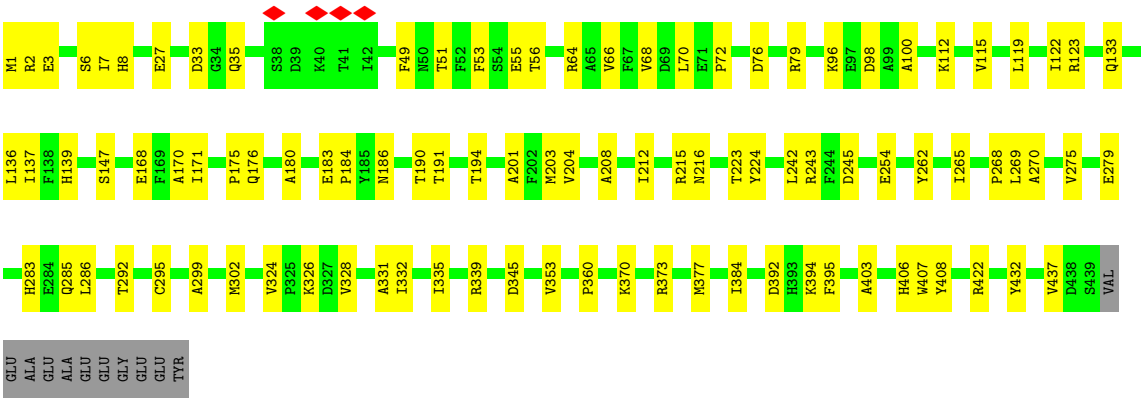
• Molecule 8: Tubulin alpha-3 chain

Chain MC:



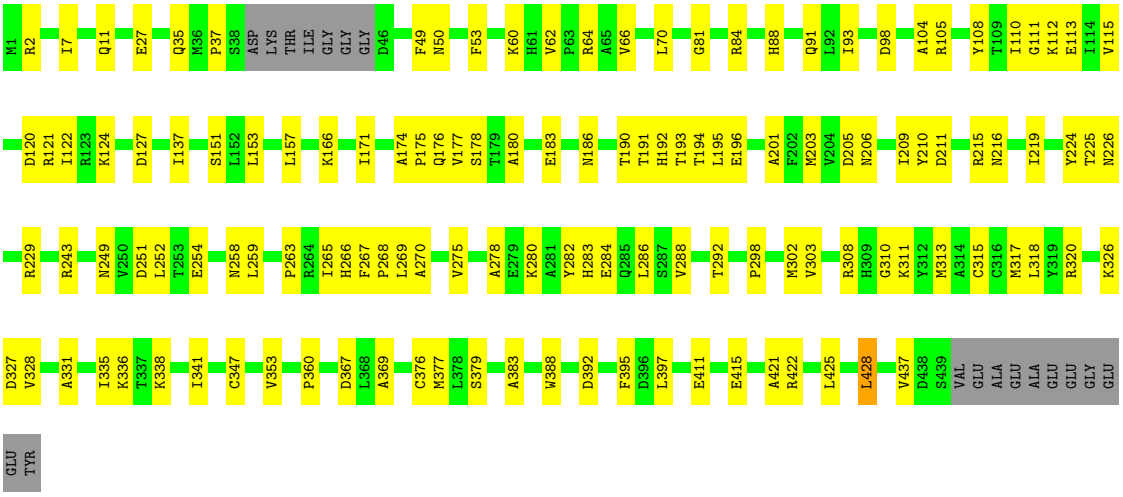
• Molecule 8: Tubulin alpha-3 chain

Chain ME:



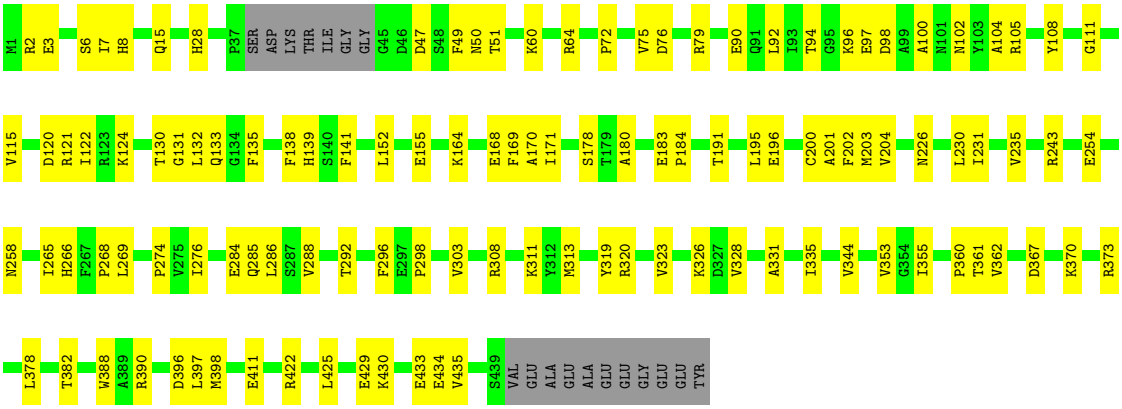
• Molecule 8: Tubulin alpha-3 chain

Chain MG:



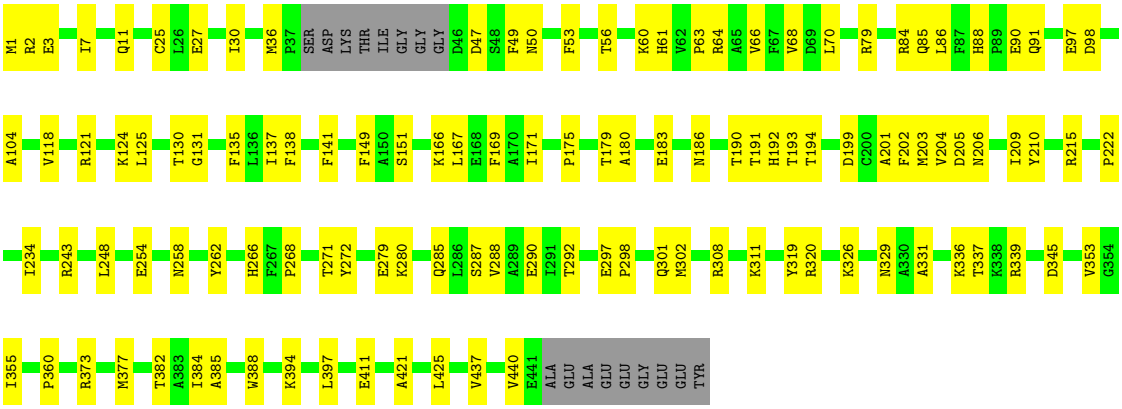
• Molecule 8: Tubulin alpha-3 chain

Chain MI:



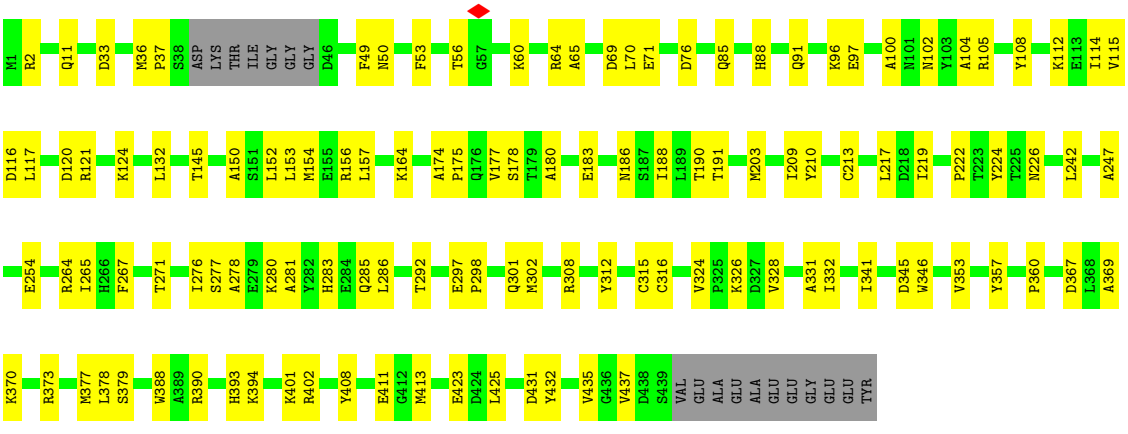
• Molecule 8: Tubulin alpha-3 chain

Chain MK:



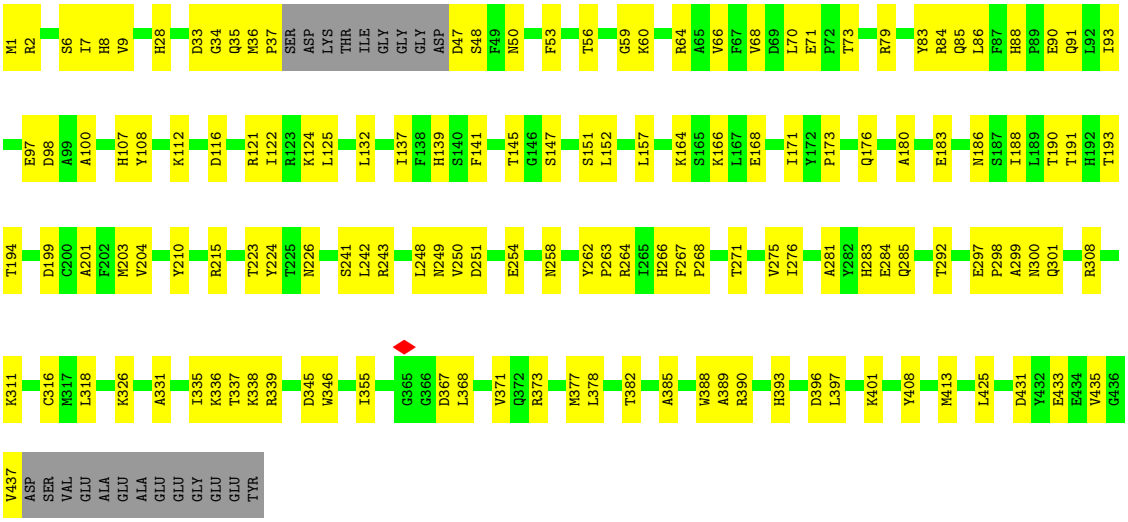
• Molecule 8: Tubulin alpha-3 chain

Chain MM:



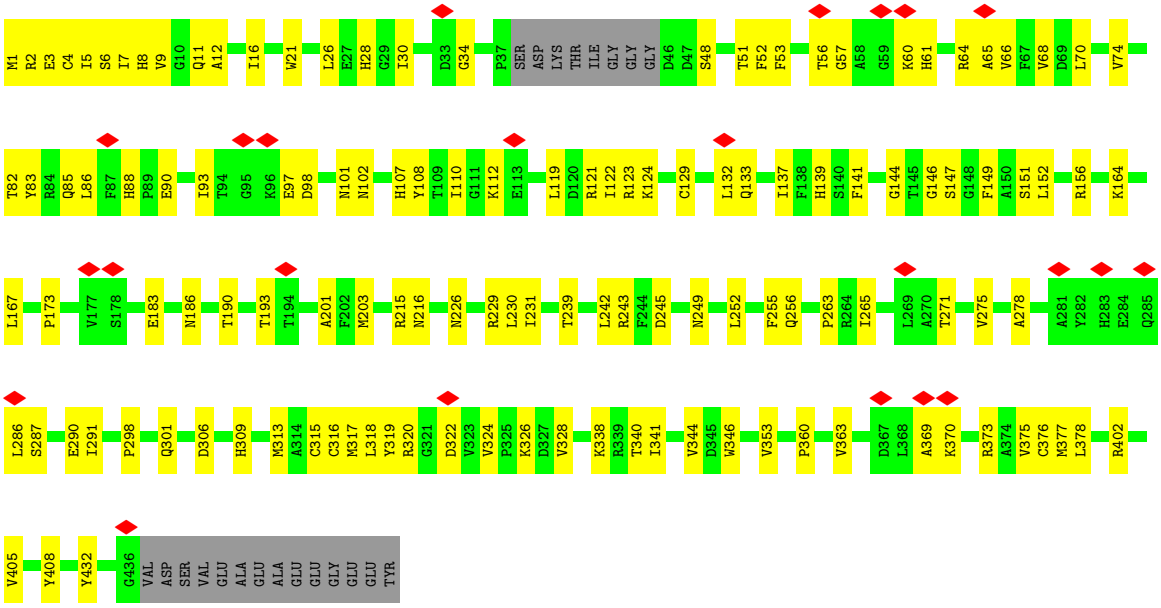
• Molecule 8: Tubulin alpha-3 chain

Chain MO:



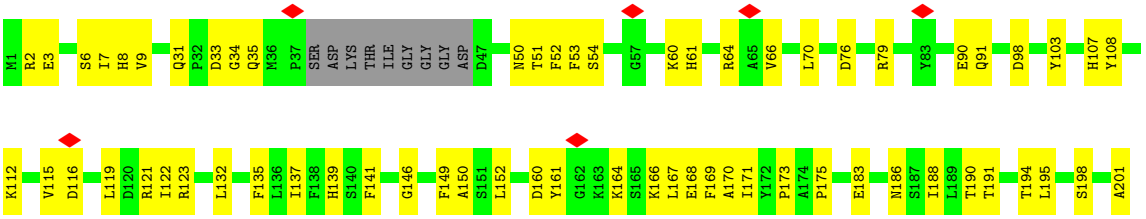
• Molecule 8: Tubulin alpha-3 chain

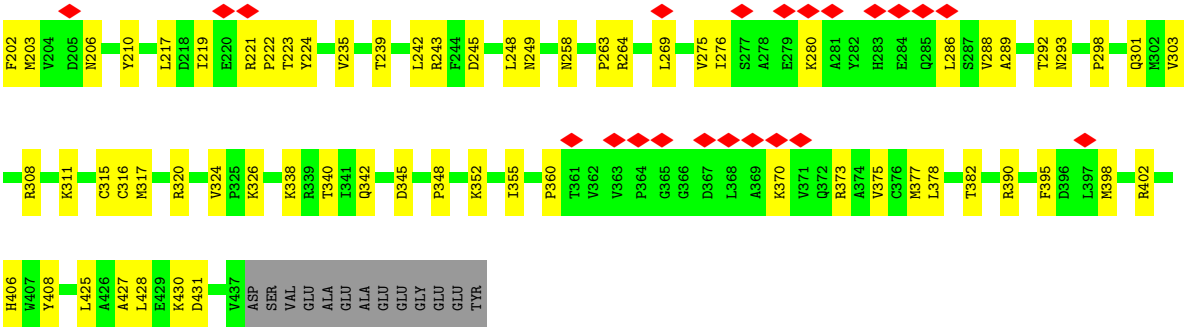
Chain NA:



• Molecule 8: Tubulin alpha-3 chain

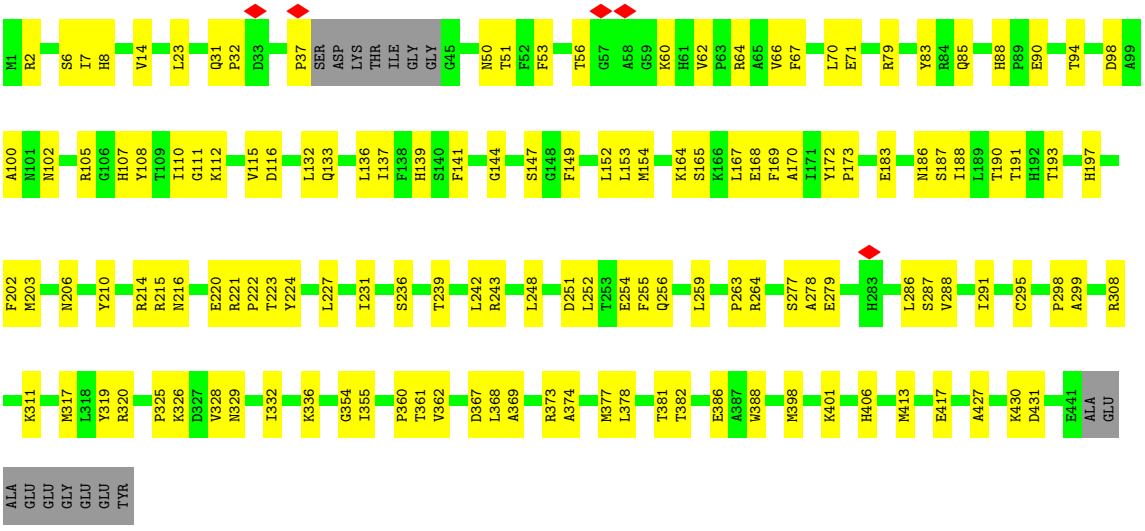
Chain NC:





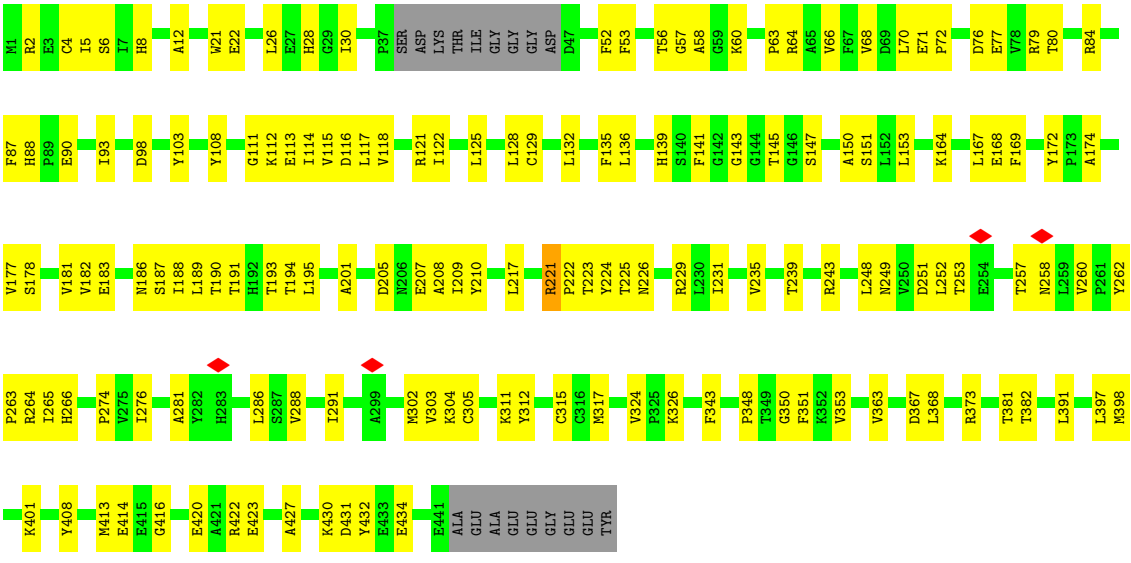
• Molecule 8: Tubulin alpha-3 chain

Chain NE:



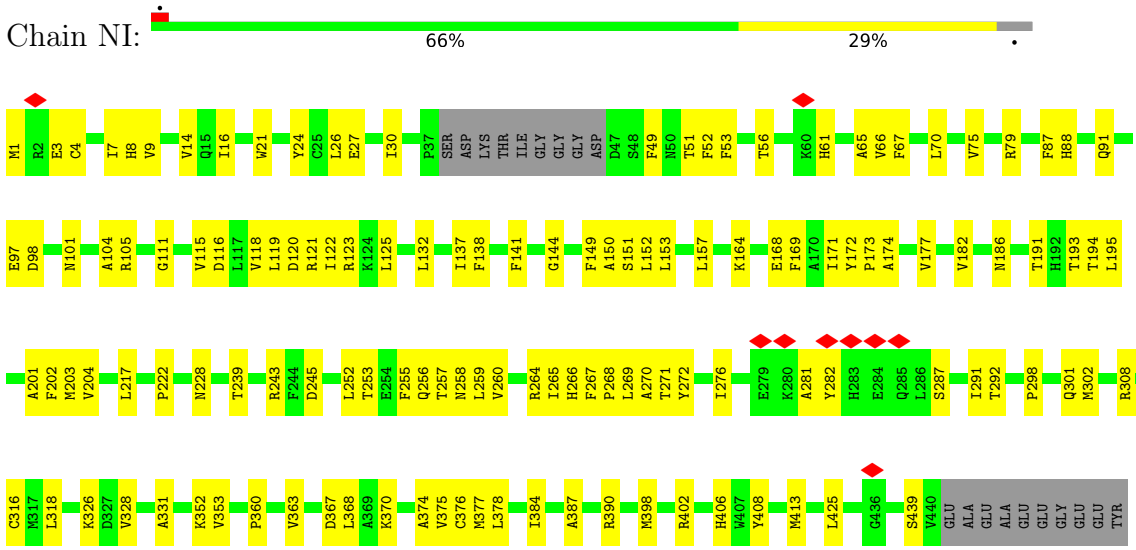
• Molecule 8: Tubulin alpha-3 chain

Chain NG:



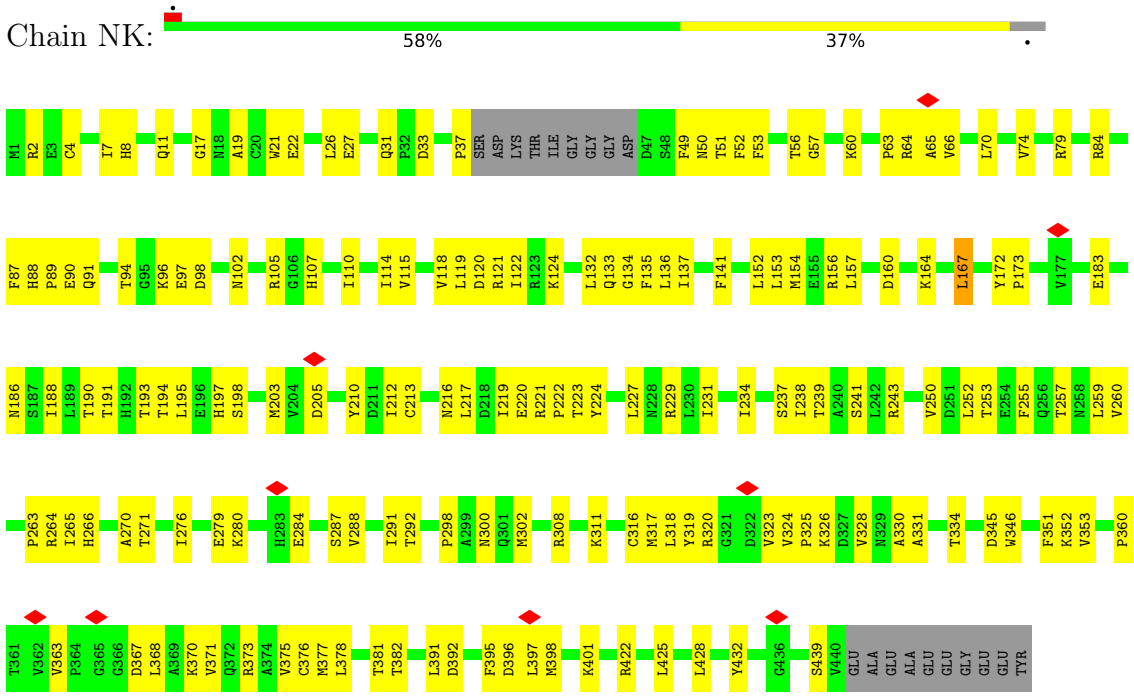
• Molecule 8: Tubulin alpha-3 chain

Chain NI:



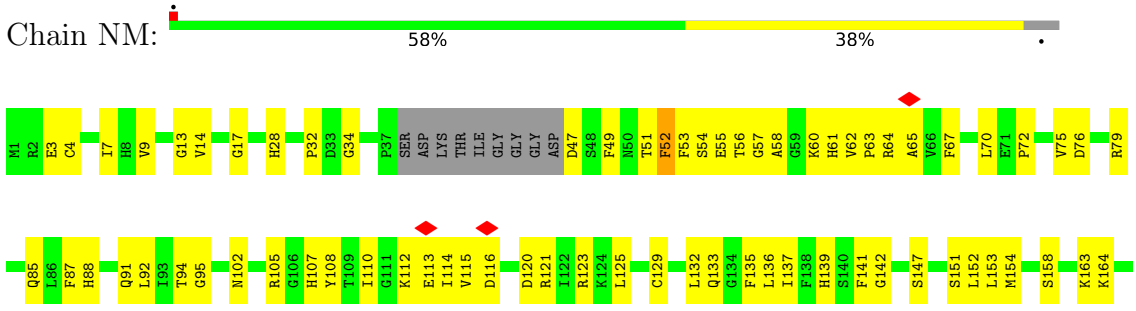
• Molecule 8: Tubulin alpha-3 chain

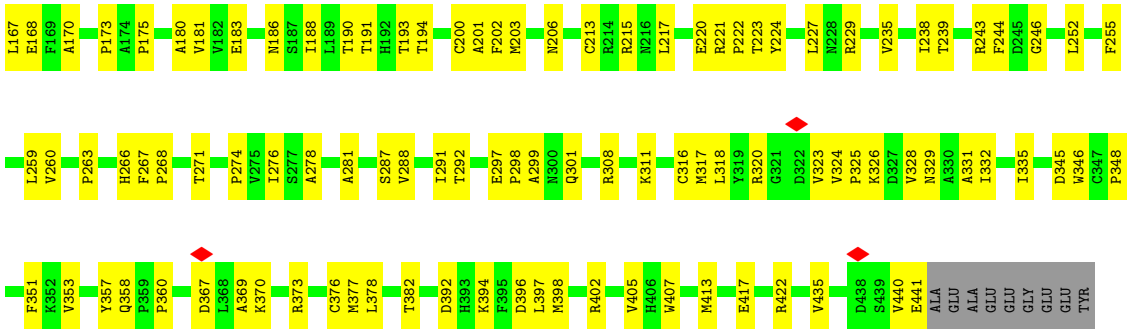
Chain NK:



• Molecule 8: Tubulin alpha-3 chain

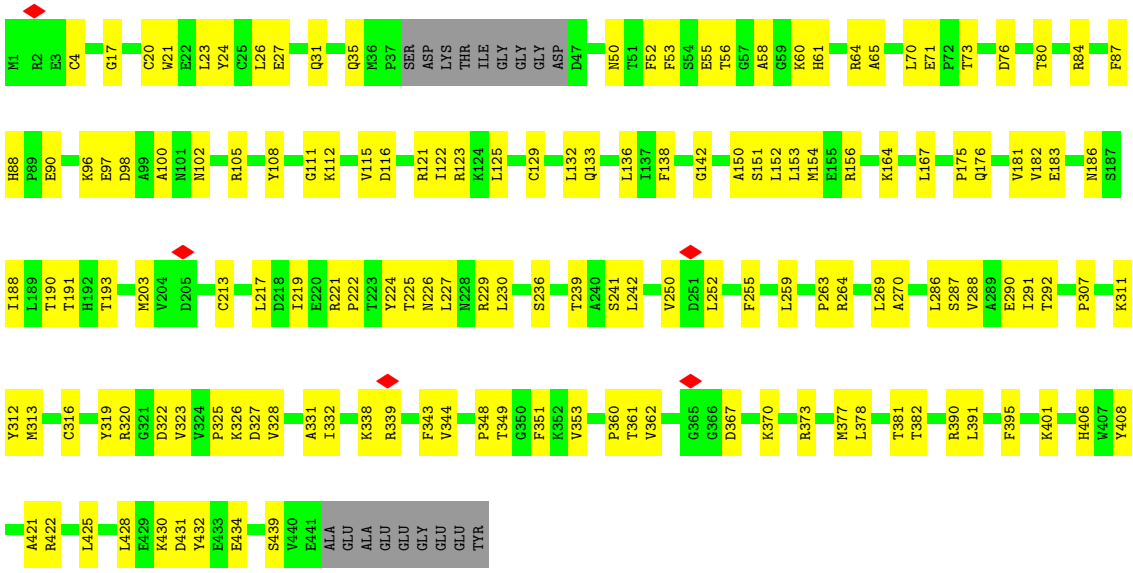
Chain NM:





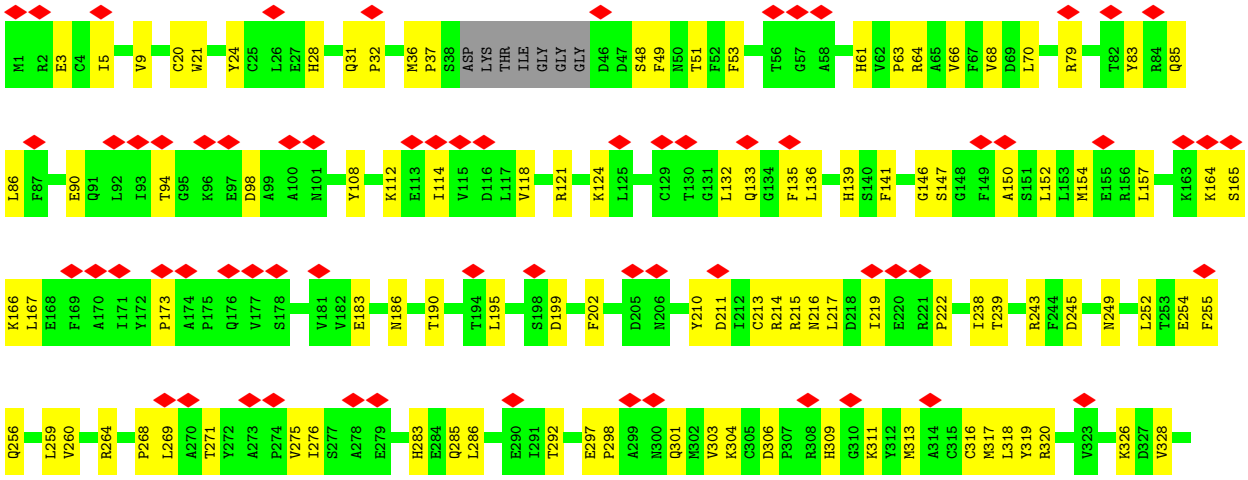
• Molecule 8: Tubulin alpha-3 chain

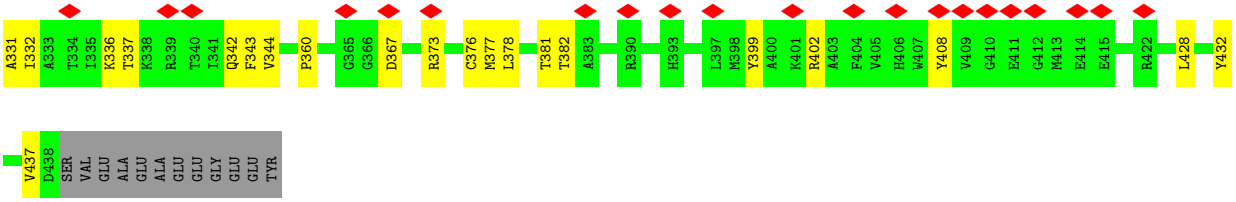
Chain NO:



• Molecule 8: Tubulin alpha-3 chain

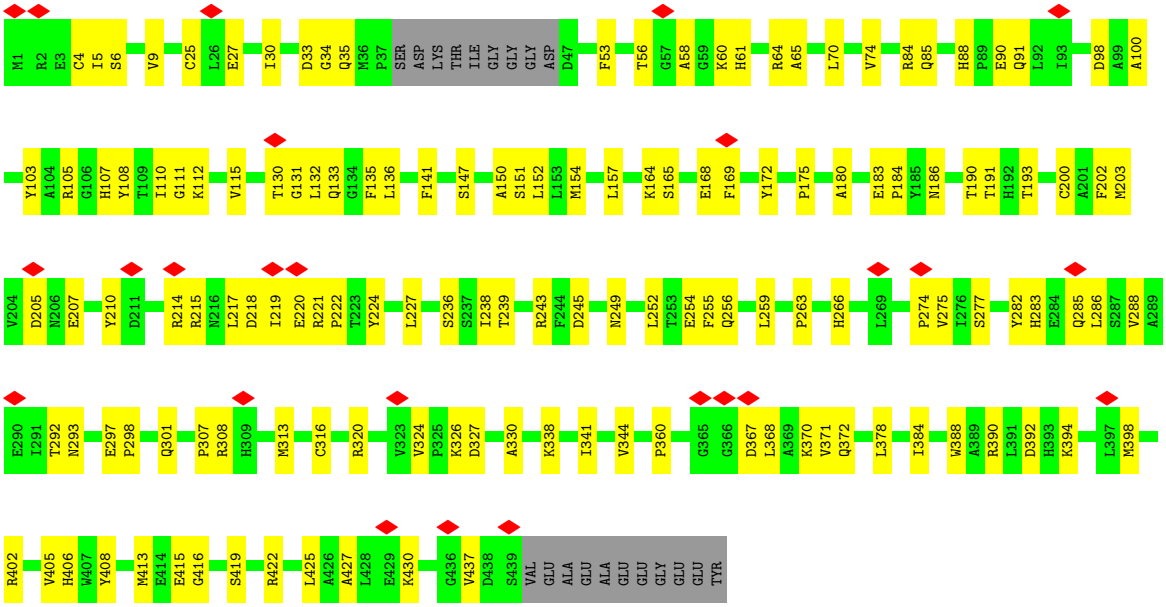
Chain OA:





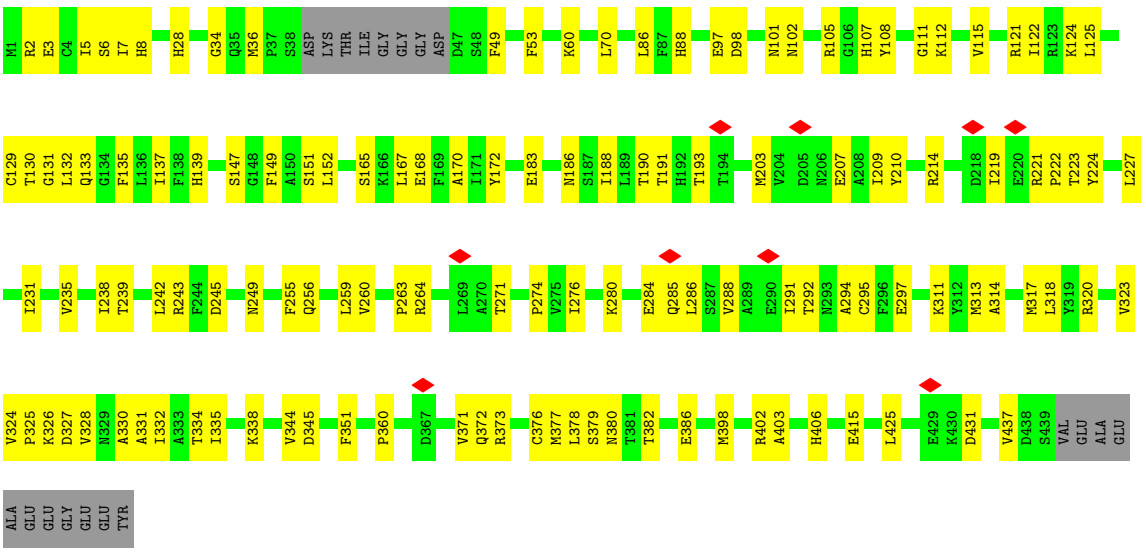
• Molecule 8: Tubulin alpha-3 chain

Chain OC:



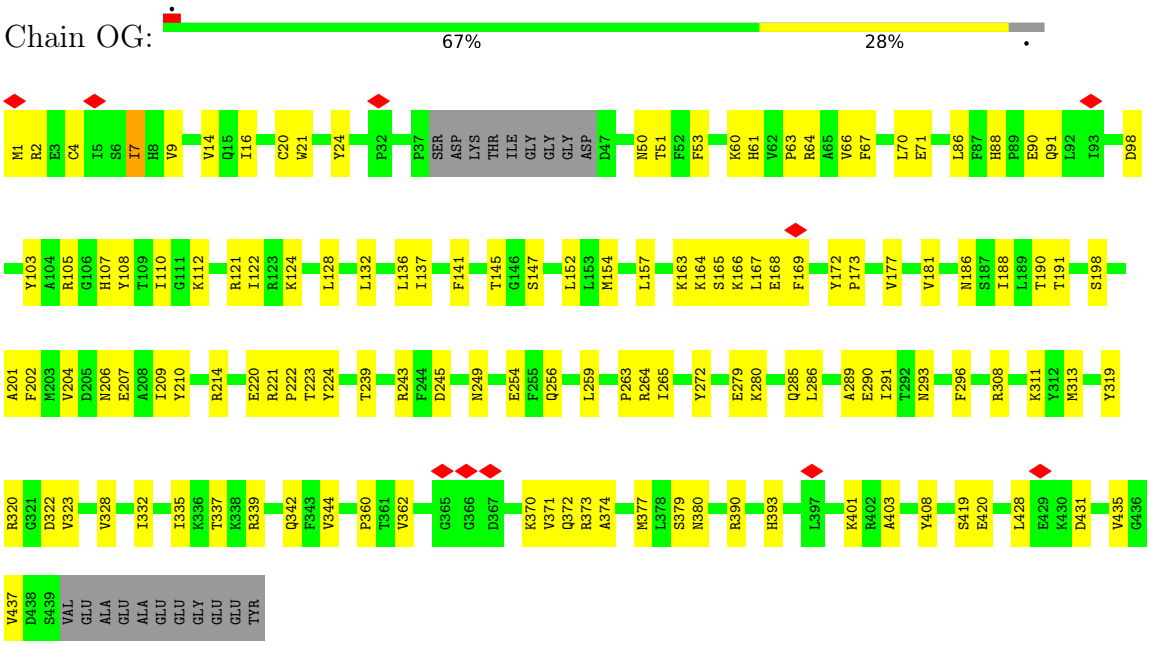
• Molecule 8: Tubulin alpha-3 chain

Chain OE:



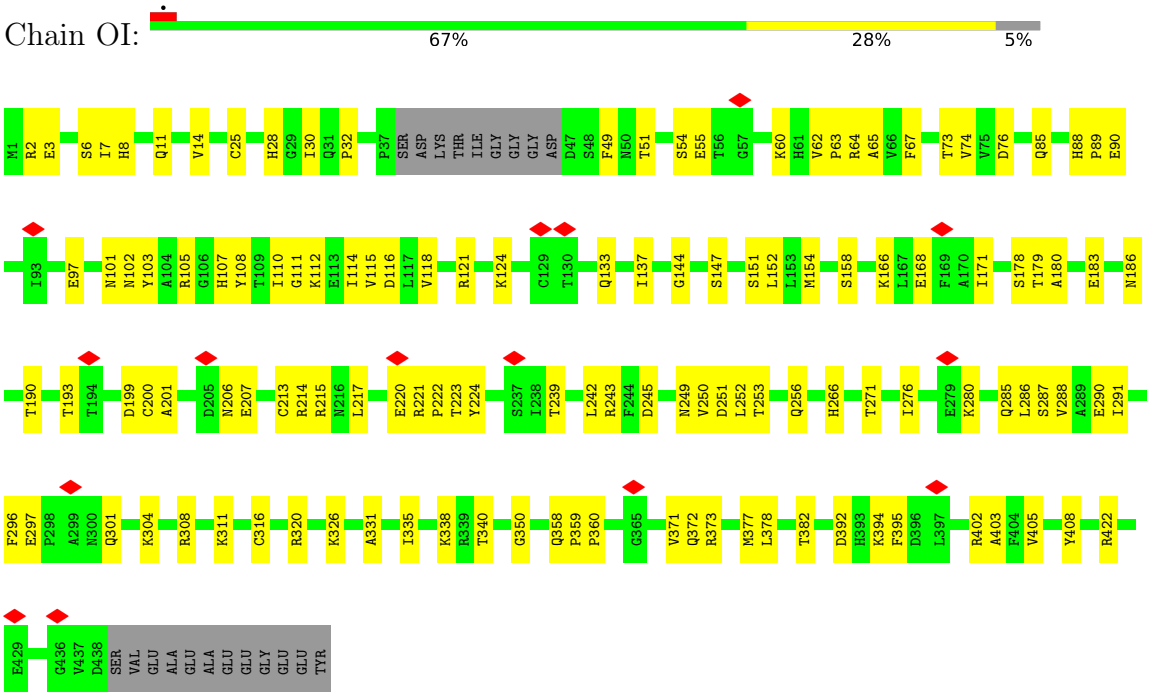
• Molecule 8: Tubulin alpha-3 chain

Chain OG:



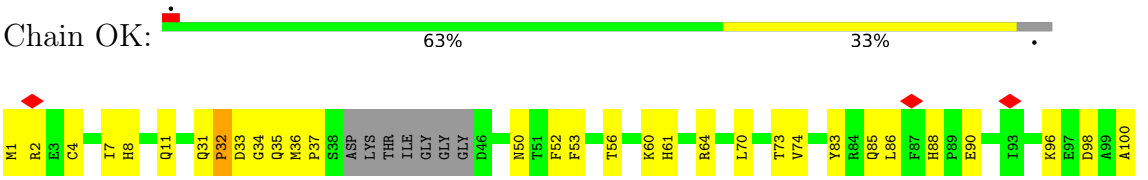
• Molecule 8: Tubulin alpha-3 chain

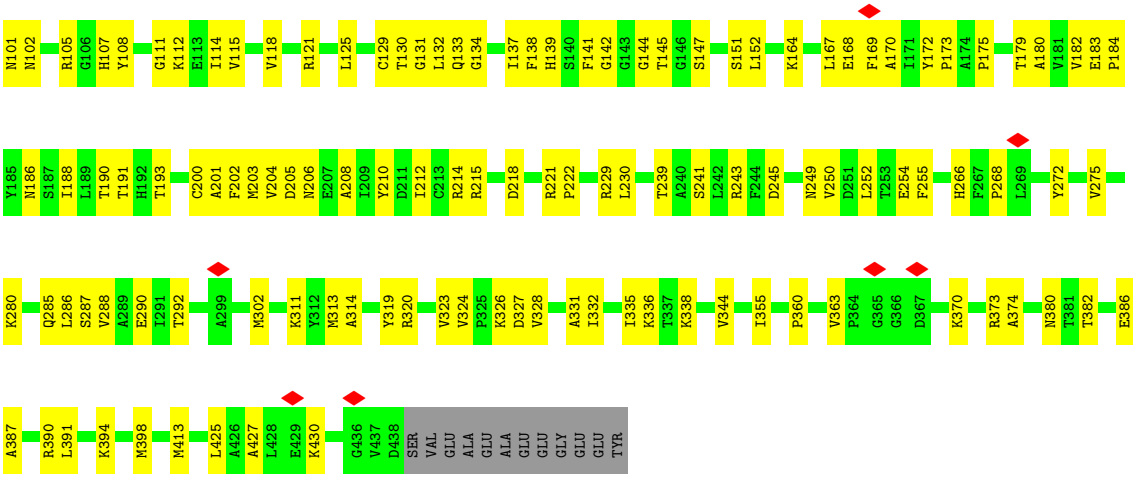
Chain OI:



• Molecule 8: Tubulin alpha-3 chain

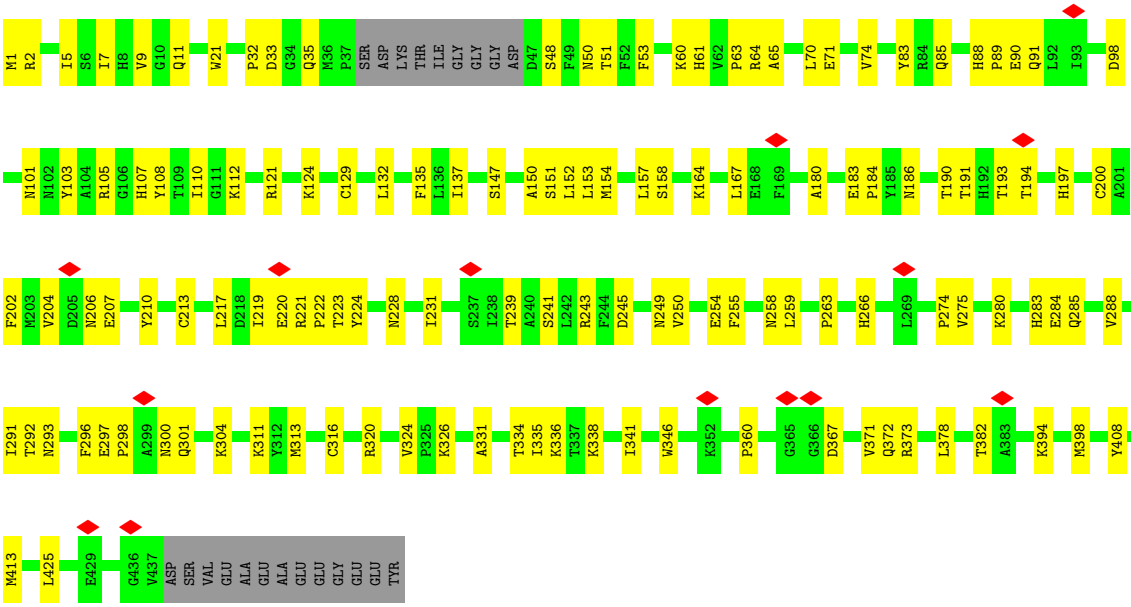
Chain OK:





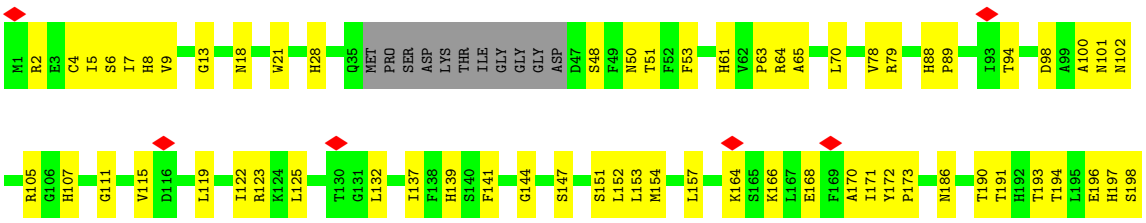
• Molecule 8: Tubulin alpha-3 chain

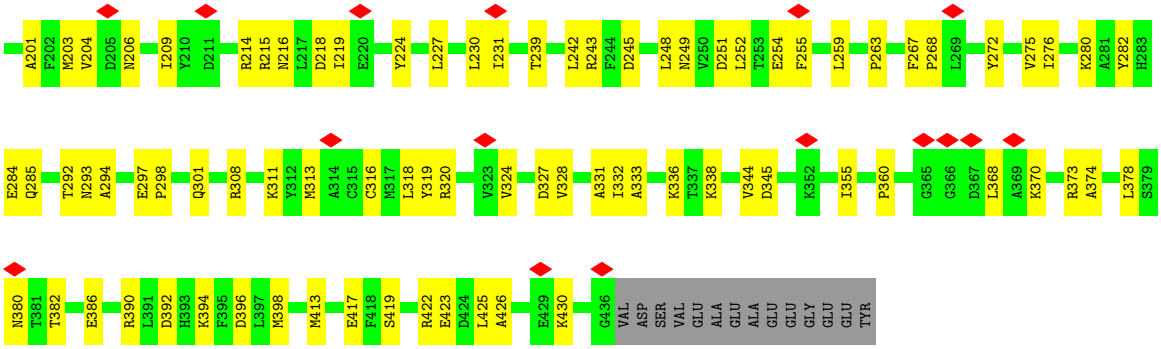
Chain OM:



• Molecule 8: Tubulin alpha-3 chain

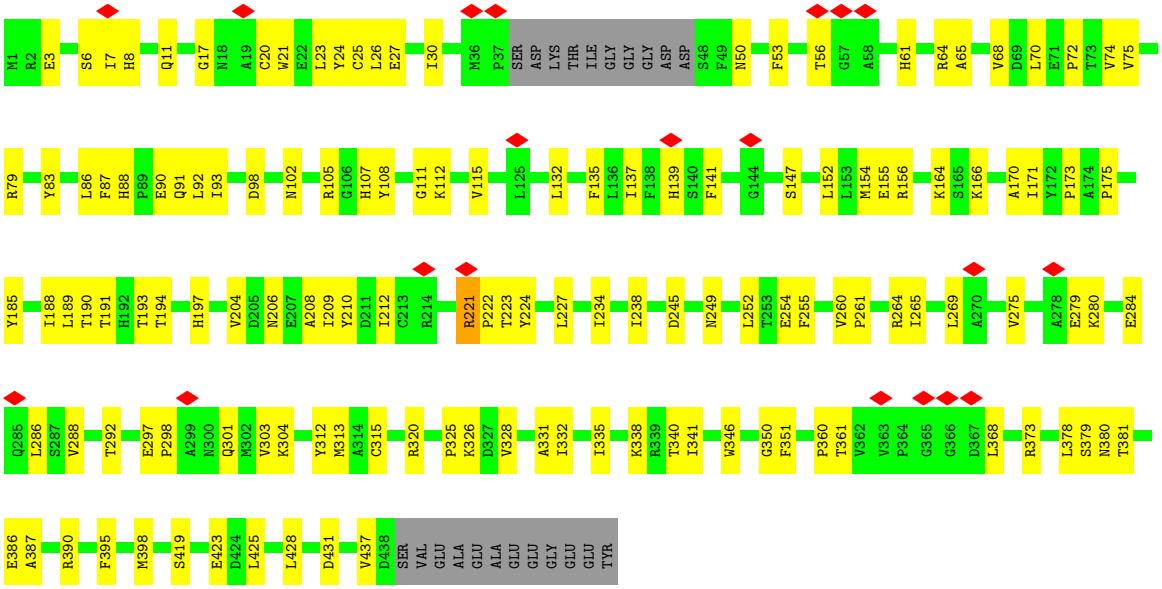
Chain OO:





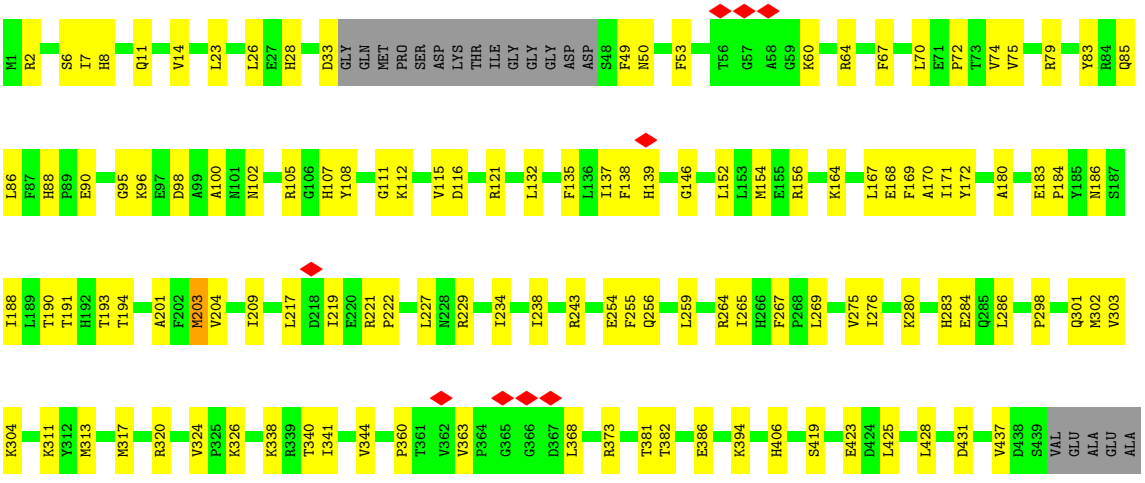
• Molecule 8: Tubulin alpha-3 chain

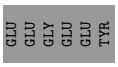
Chain PC:



• Molecule 8: Tubulin alpha-3 chain

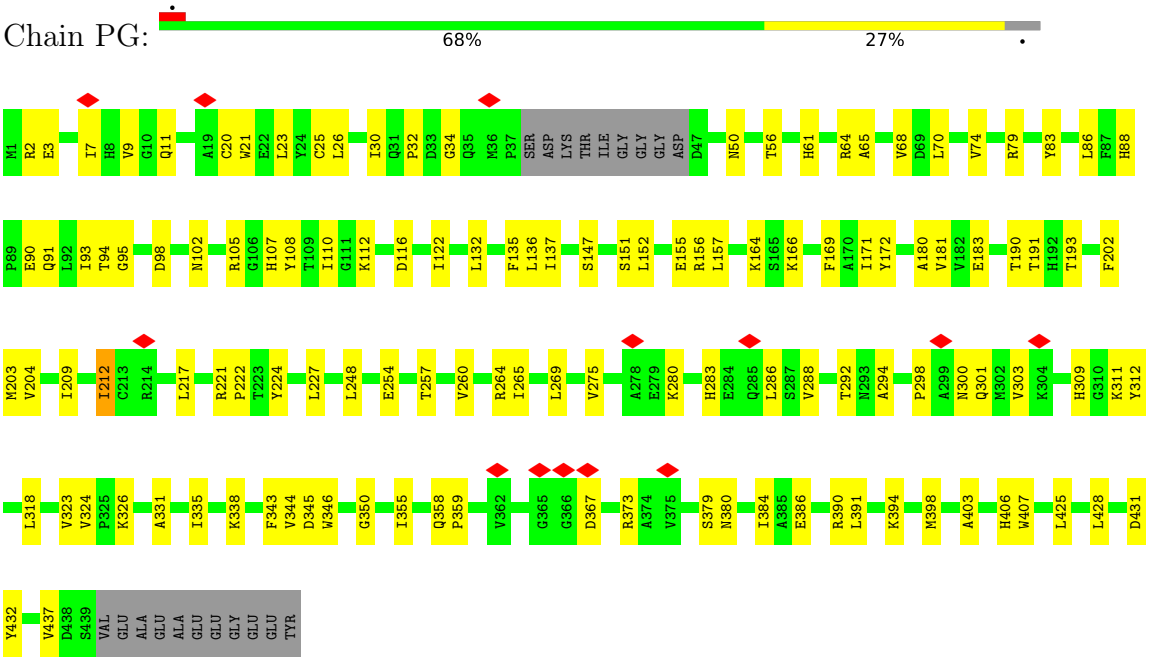
Chain PE:





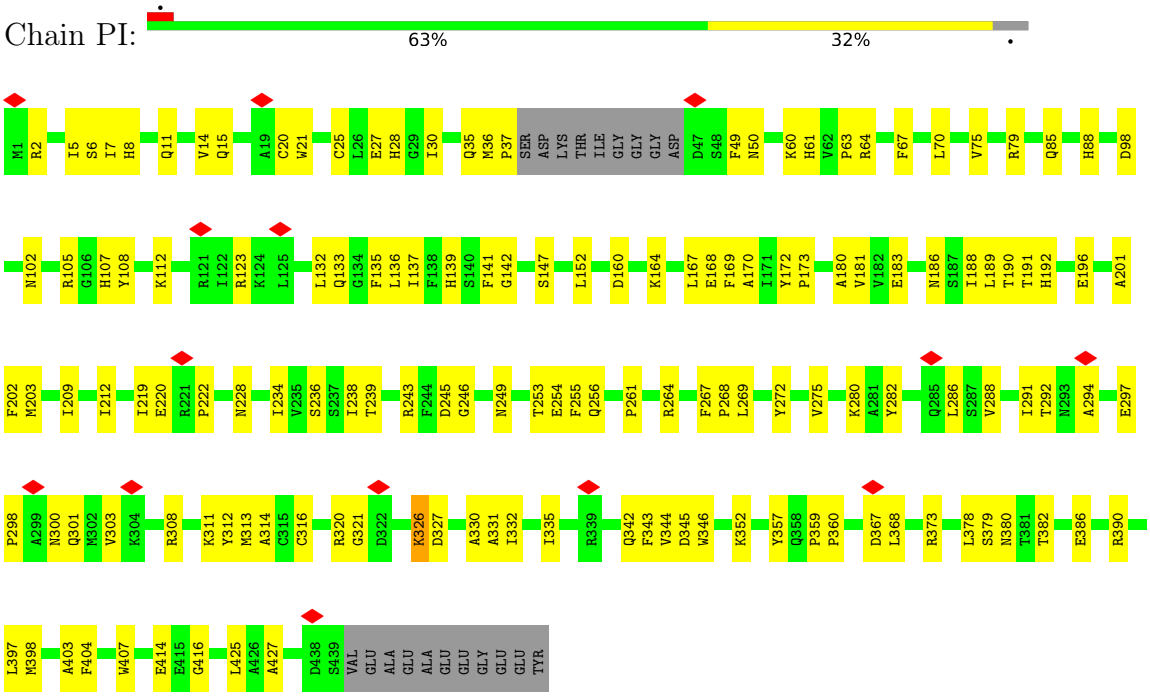
• Molecule 8: Tubulin alpha-3 chain

Chain PG:



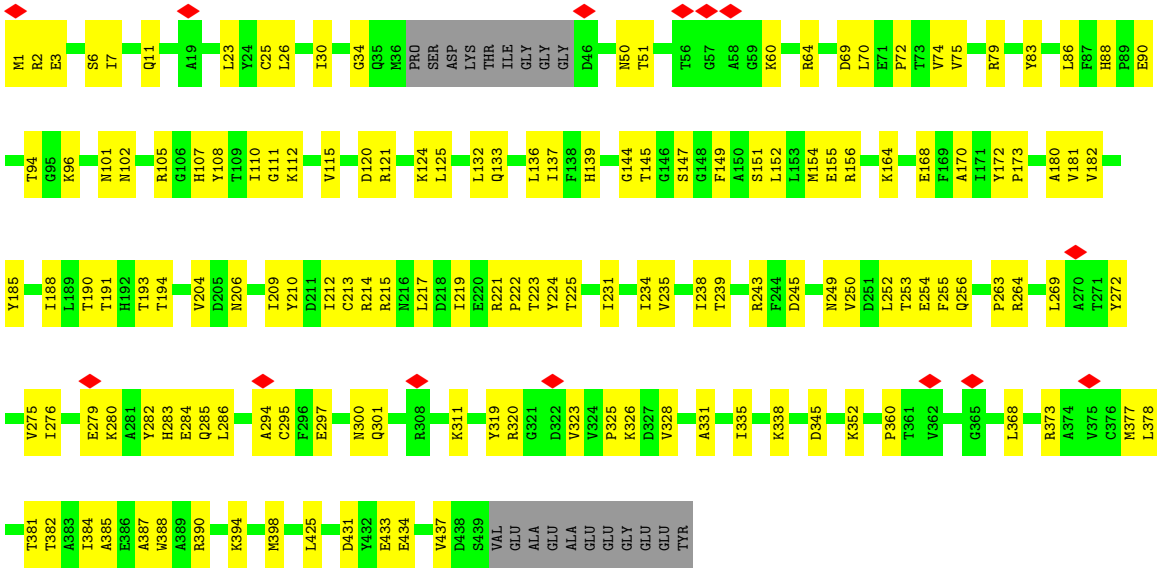
• Molecule 8: Tubulin alpha-3 chain

Chain PI:



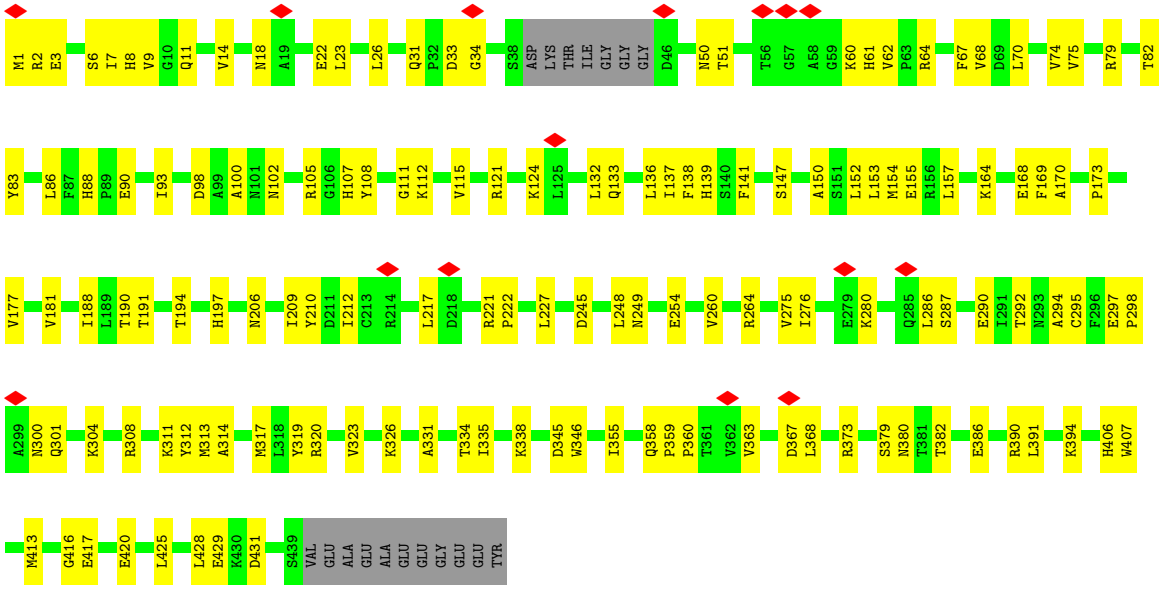
• Molecule 8: Tubulin alpha-3 chain

Chain PK:



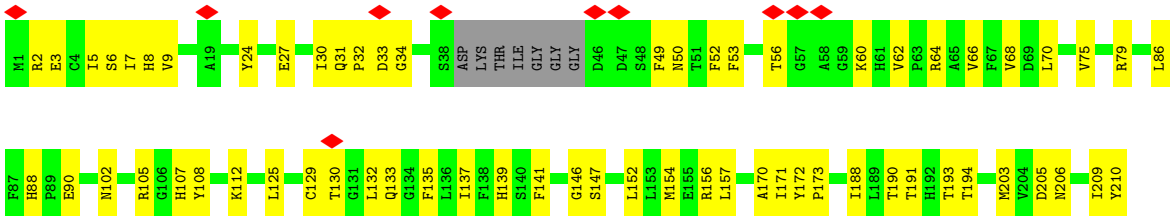
• Molecule 8: Tubulin alpha-3 chain

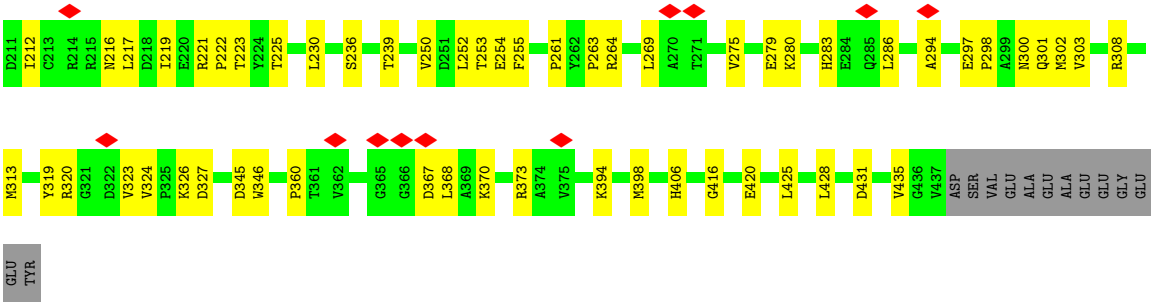
Chain PM:



• Molecule 8: Tubulin alpha-3 chain

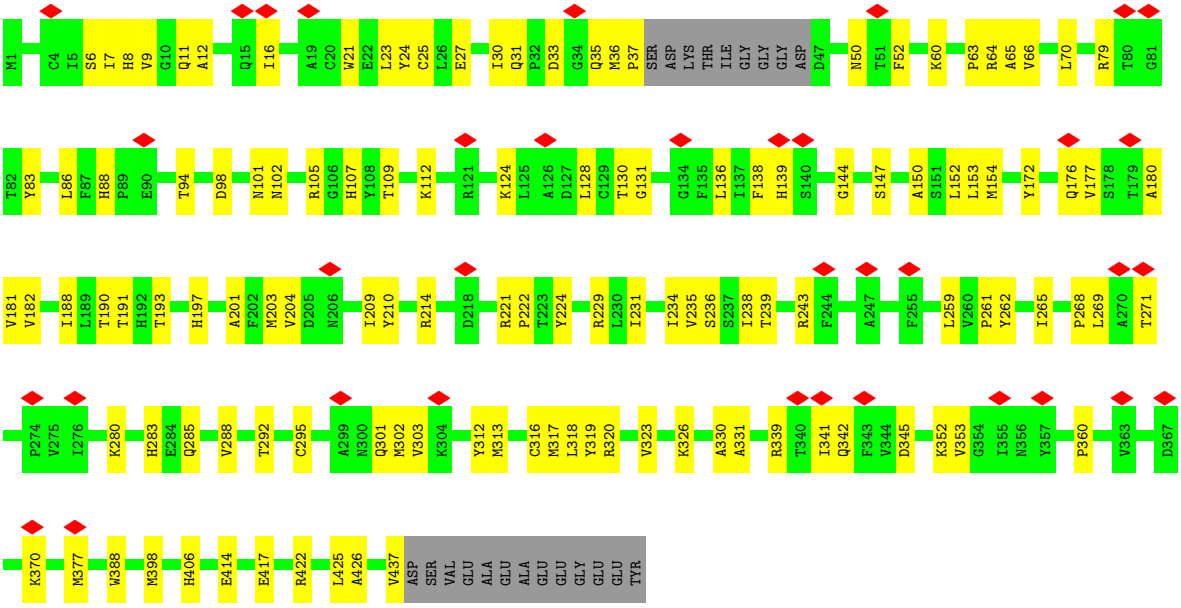
Chain PO:





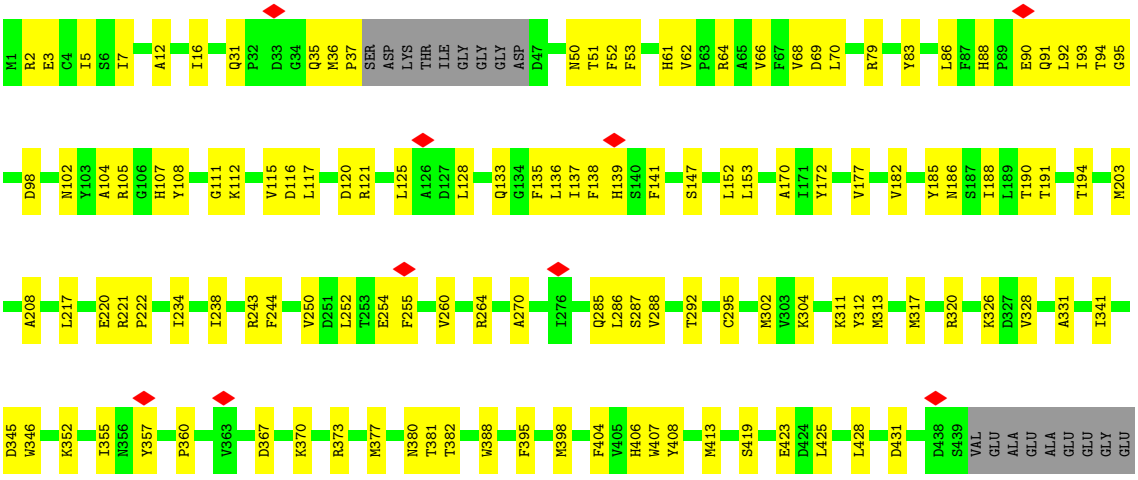
• Molecule 8: Tubulin alpha-3 chain

Chain QC:



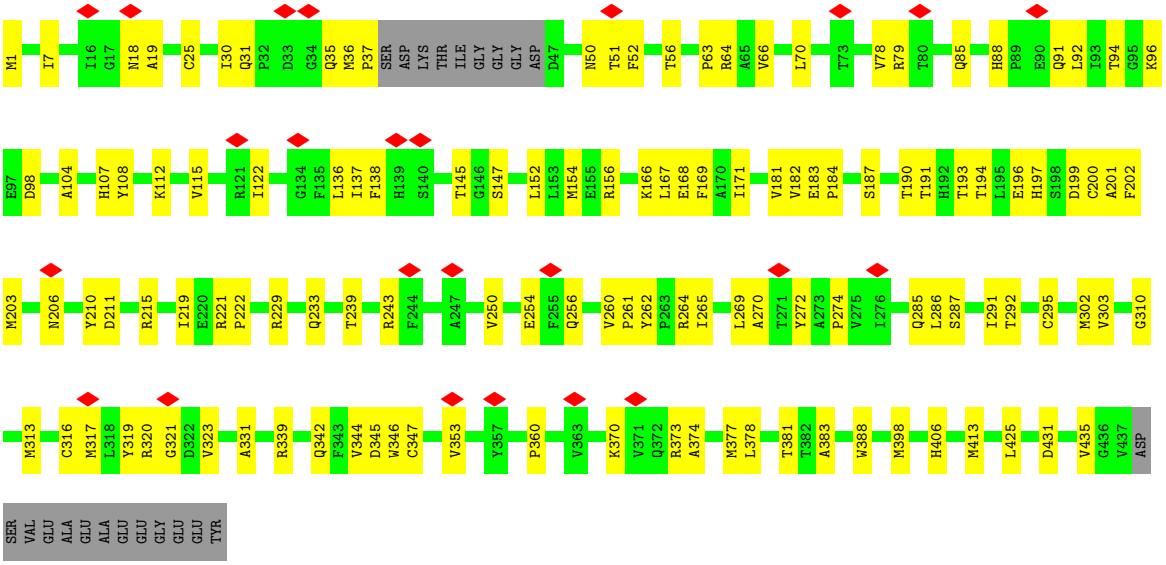
• Molecule 8: Tubulin alpha-3 chain

Chain QE:



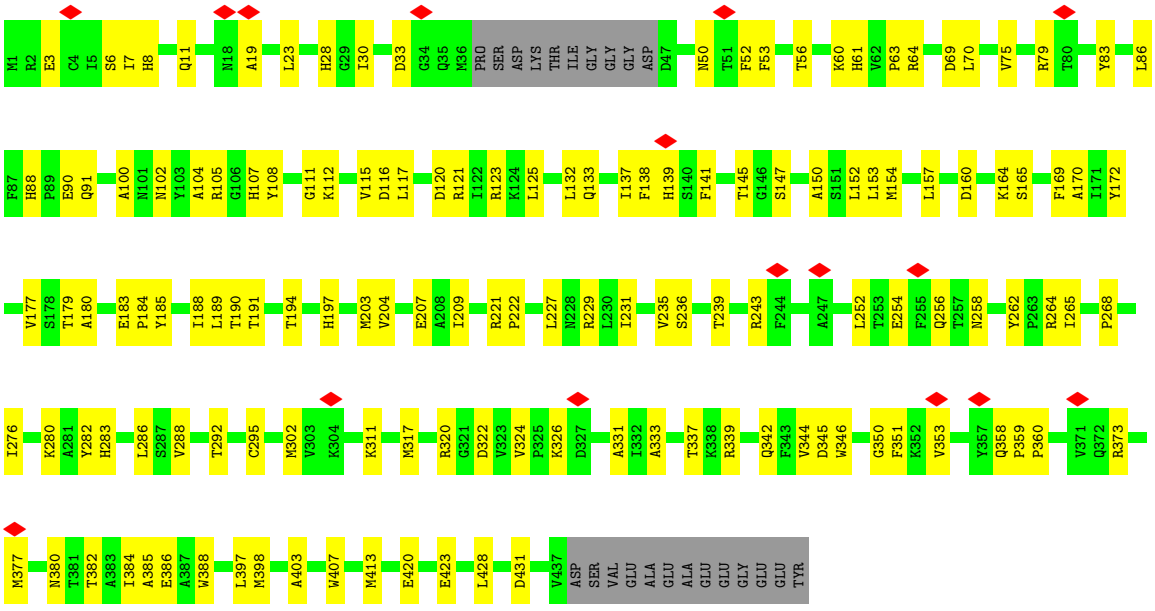
• Molecule 8: Tubulin alpha-3 chain

Chain QG:



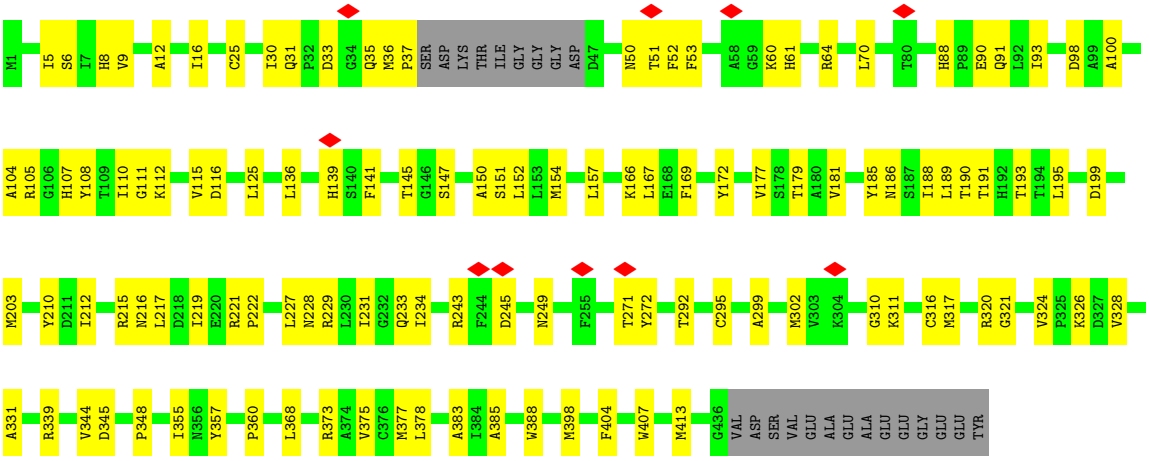
• Molecule 8: Tubulin alpha-3 chain

Chain QI:



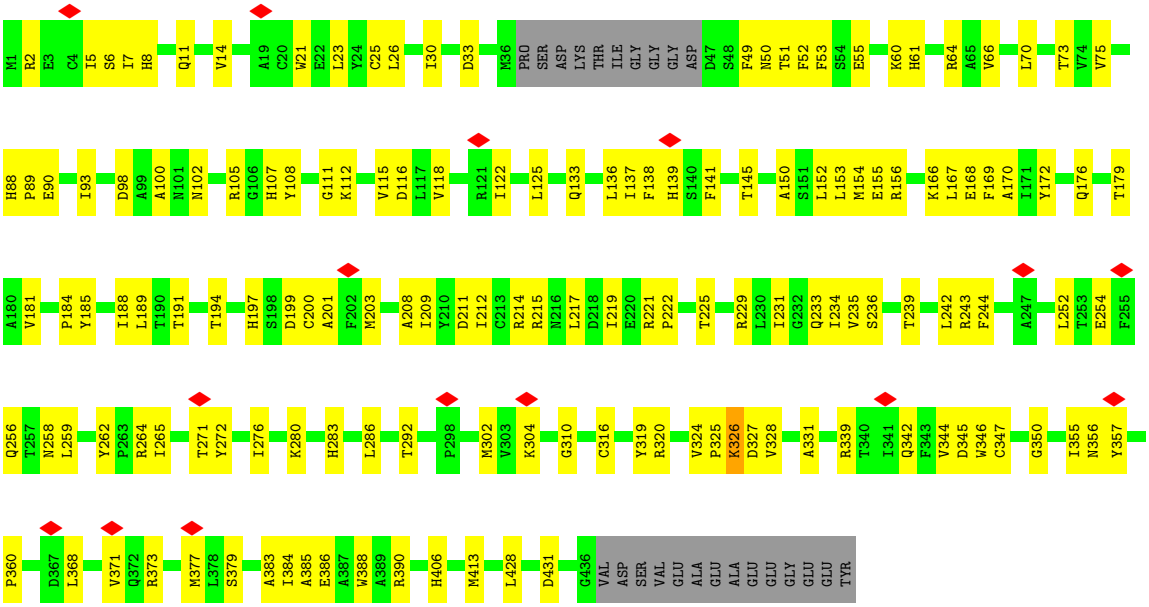
• Molecule 8: Tubulin alpha-3 chain

Chain QK:



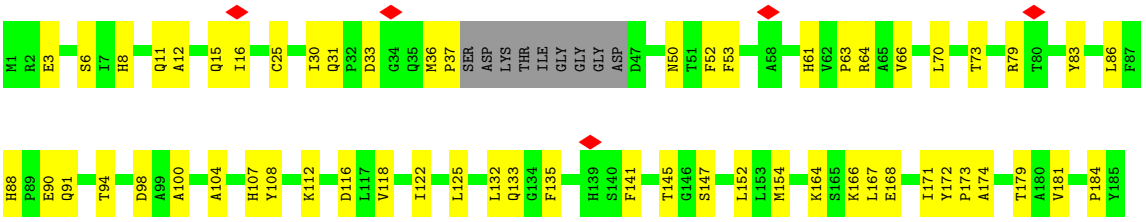
• Molecule 8: Tubulin alpha-3 chain

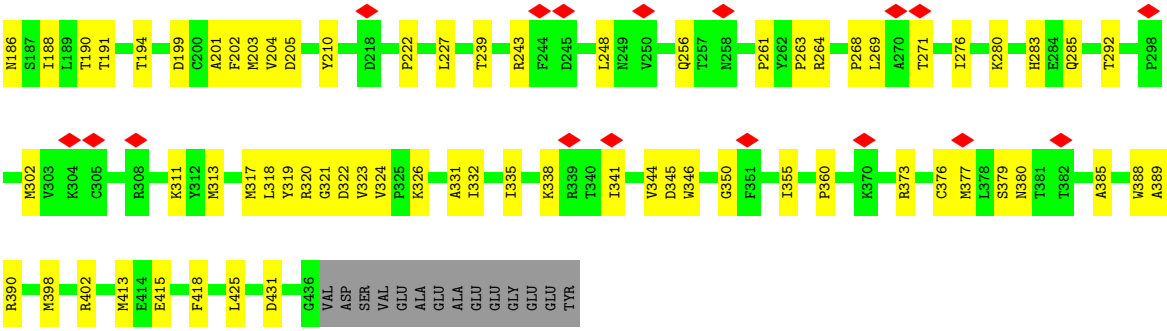
Chain QM:



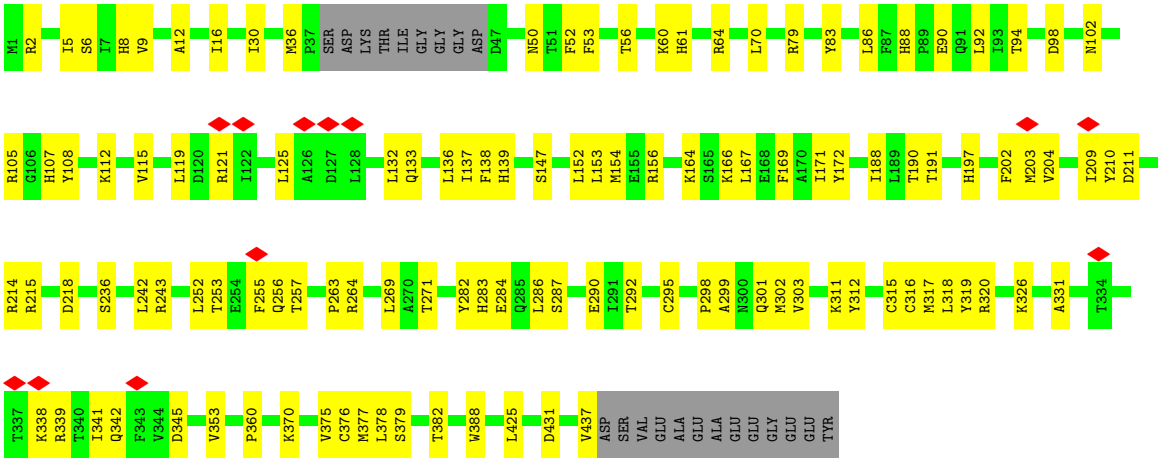
• Molecule 8: Tubulin alpha-3 chain

Chain QO:

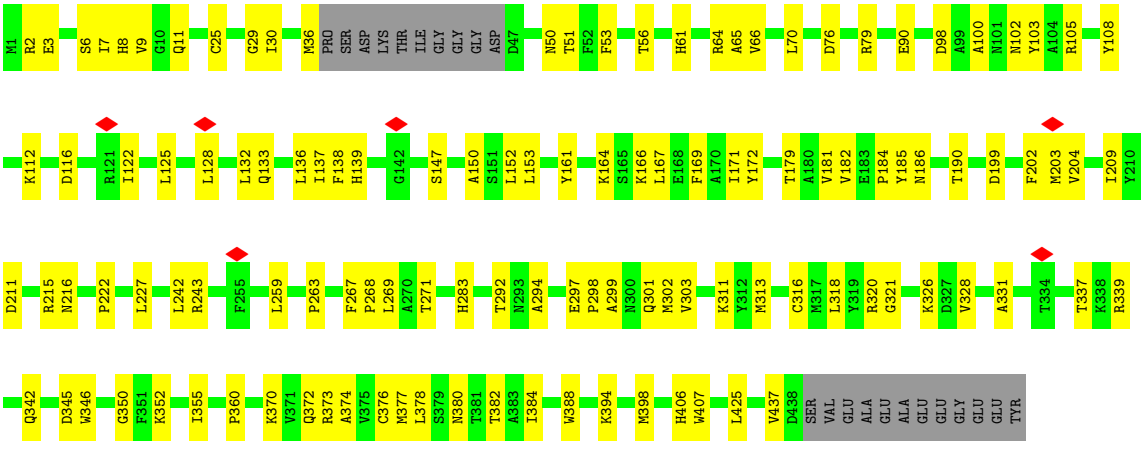




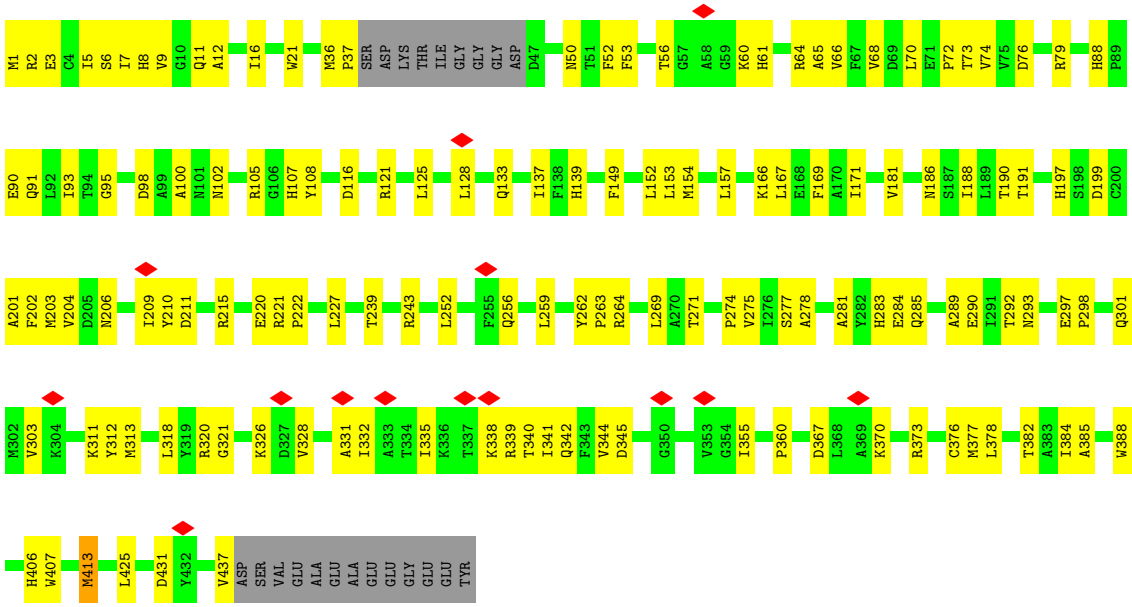
• Molecule 8: Tubulin alpha-3 chain



• Molecule 8: Tubulin alpha-3 chain

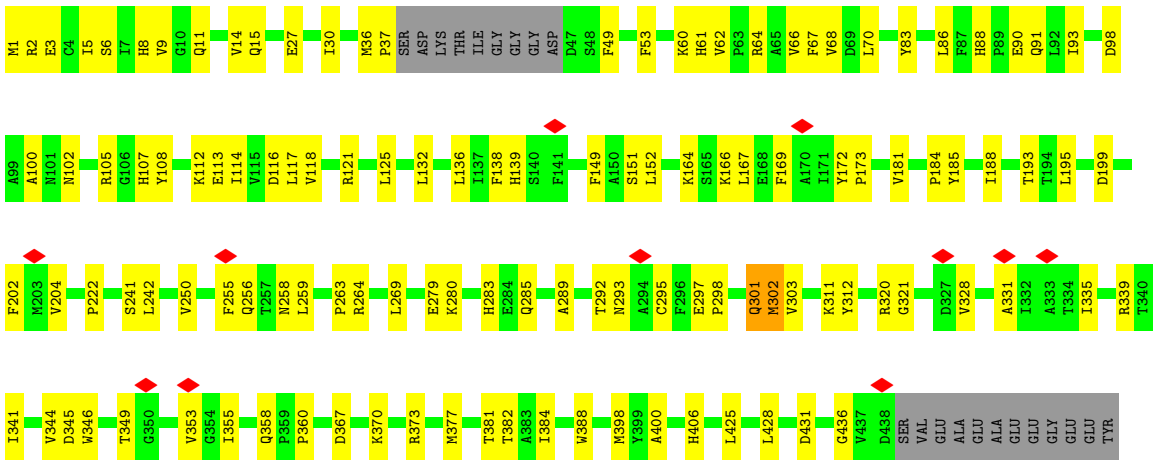


• Molecule 8: Tubulin alpha-3 chain



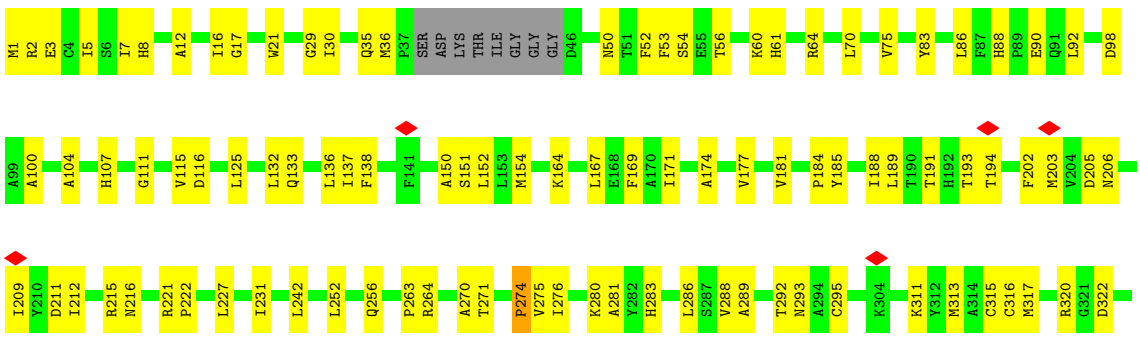
• Molecule 8: Tubulin alpha-3 chain

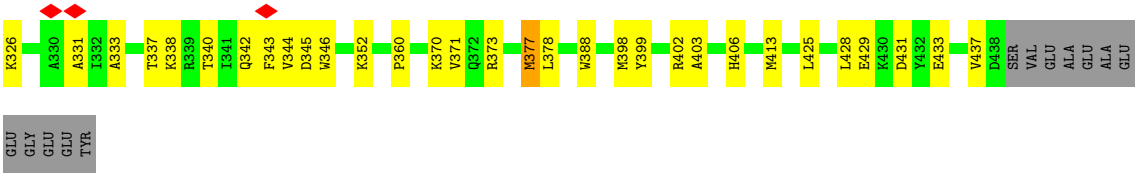
Chain RI:



• Molecule 8: Tubulin alpha-3 chain

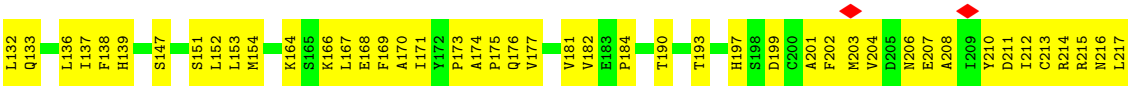
Chain RK:

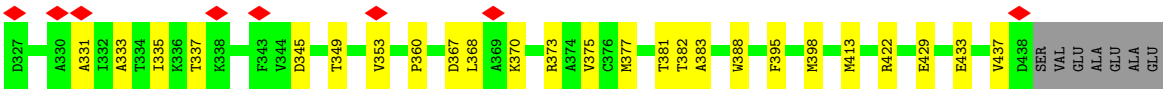




• Molecule 8: Tubulin alpha-3 chain

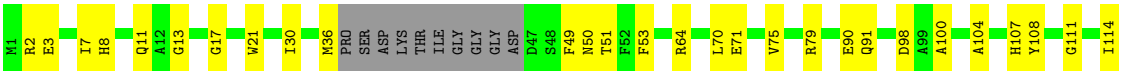
Chain RM:

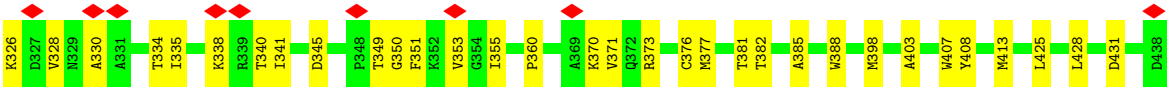




• Molecule 8: Tubulin alpha-3 chain

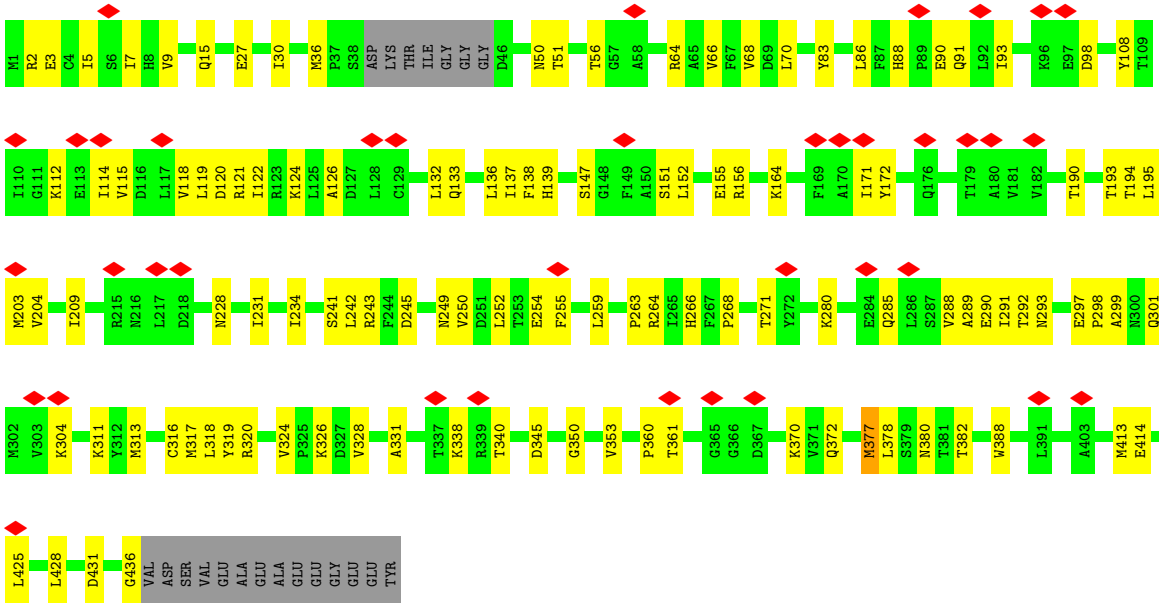
Chain RO:





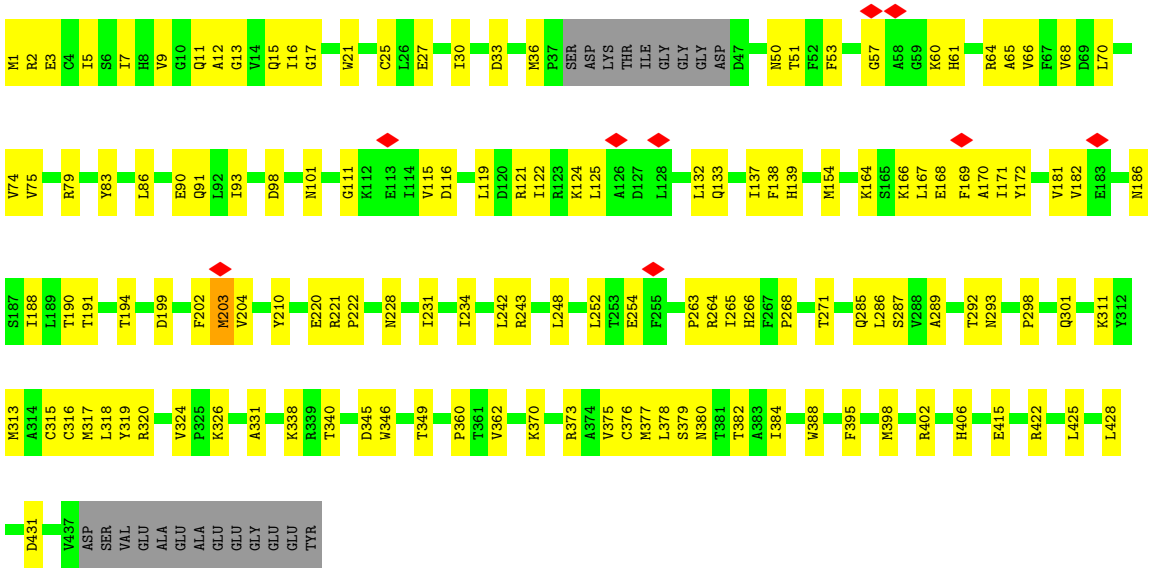
• Molecule 8: Tubulin alpha-3 chain

Chain SA:



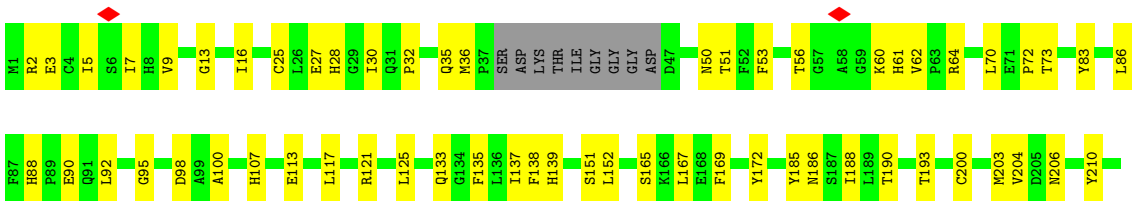
• Molecule 8: Tubulin alpha-3 chain

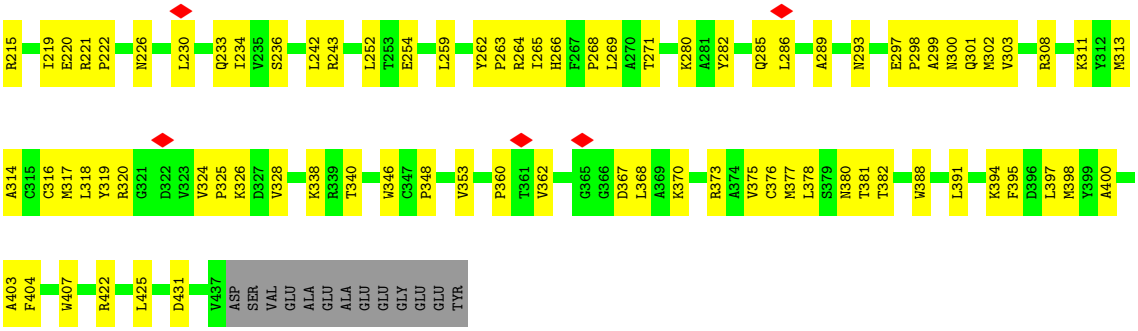
Chain SC:



• Molecule 8: Tubulin alpha-3 chain

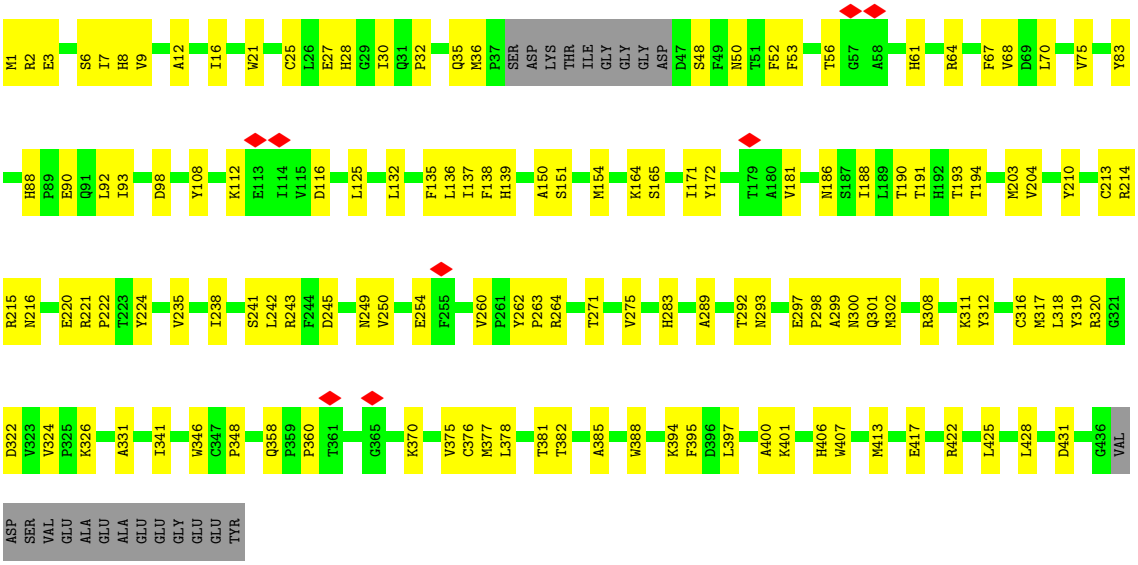
Chain SE:





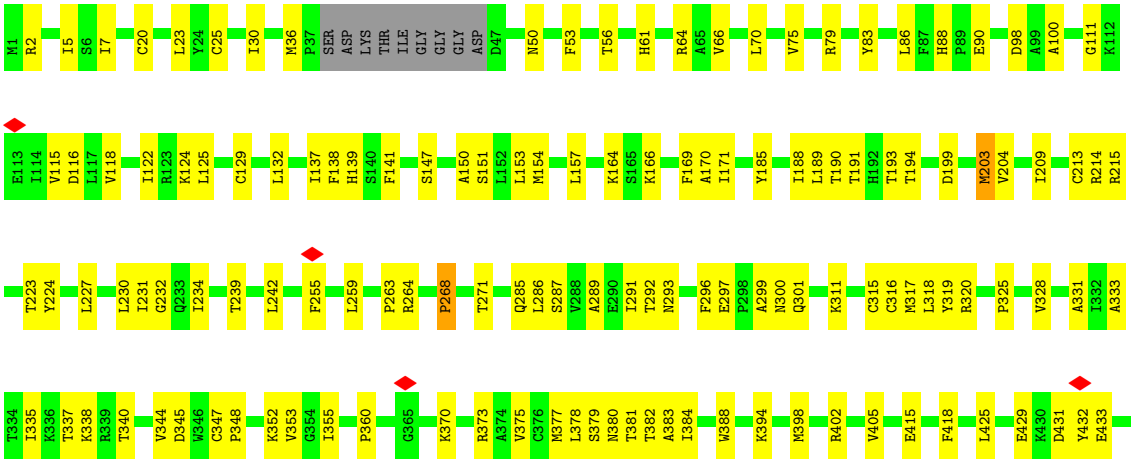
• Molecule 8: Tubulin alpha-3 chain

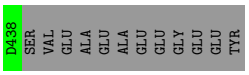
Chain SG:



• Molecule 8: Tubulin alpha-3 chain

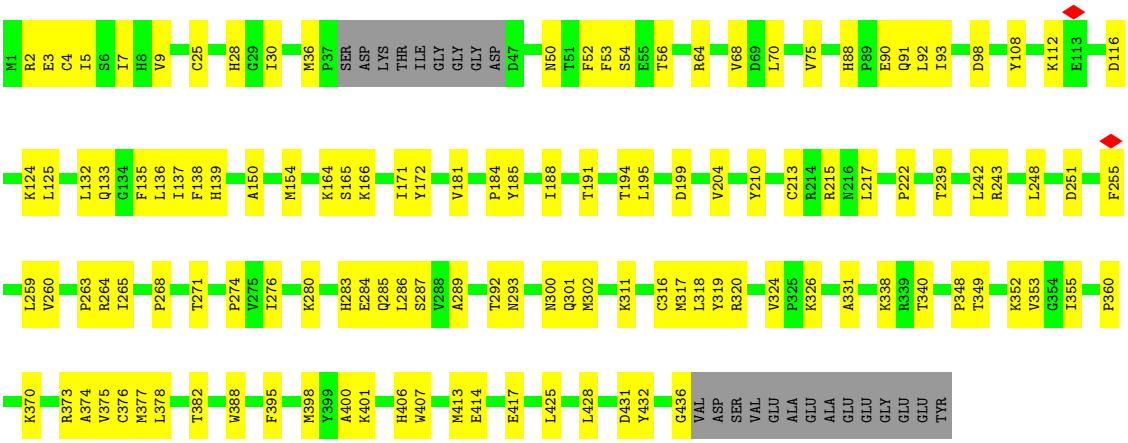
Chain SI:





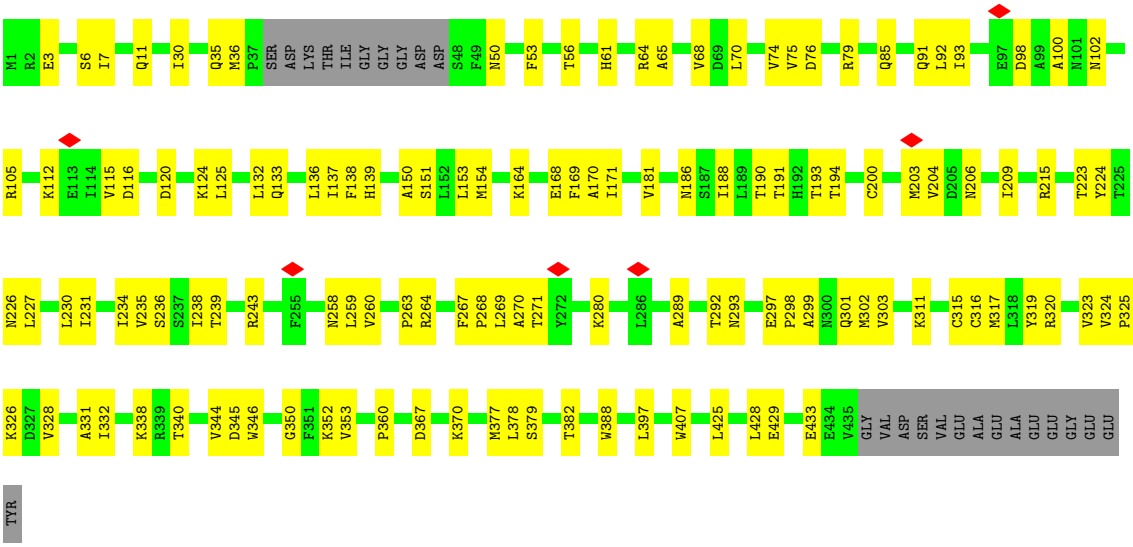
• Molecule 8: Tubulin alpha-3 chain

Chain SK:



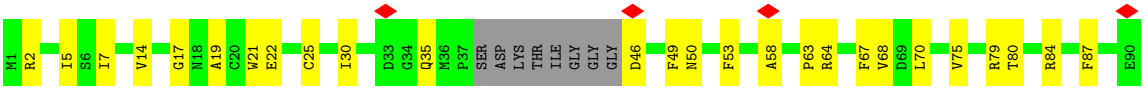
• Molecule 8: Tubulin alpha-3 chain

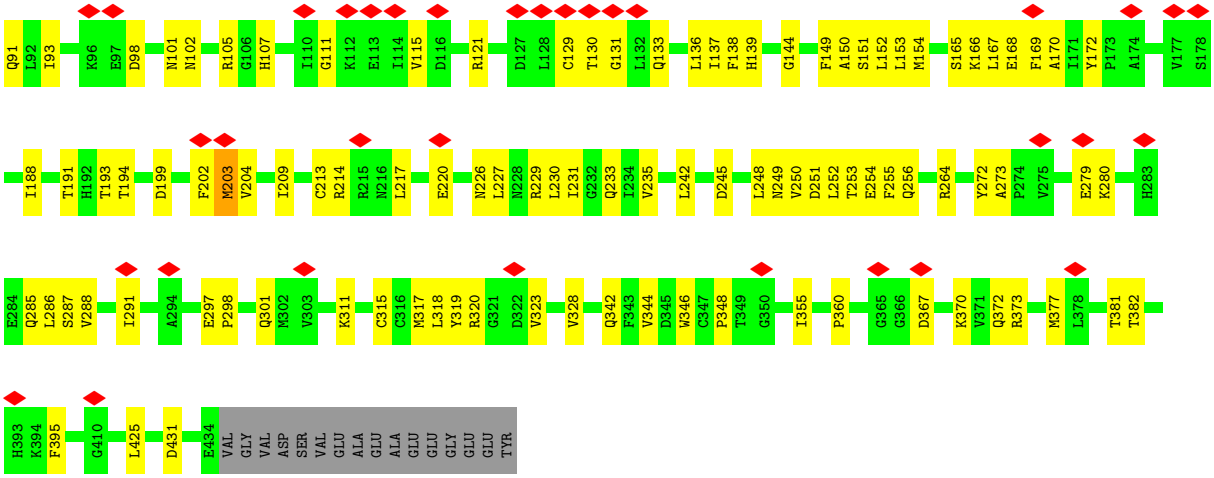
Chain SM:



• Molecule 8: Tubulin alpha-3 chain

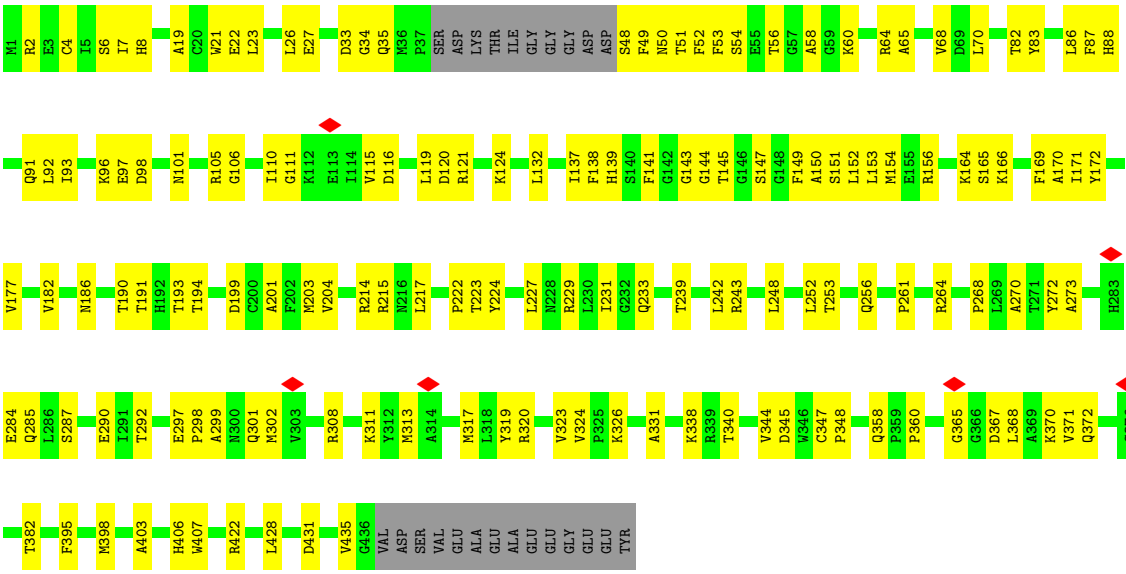
Chain TA:





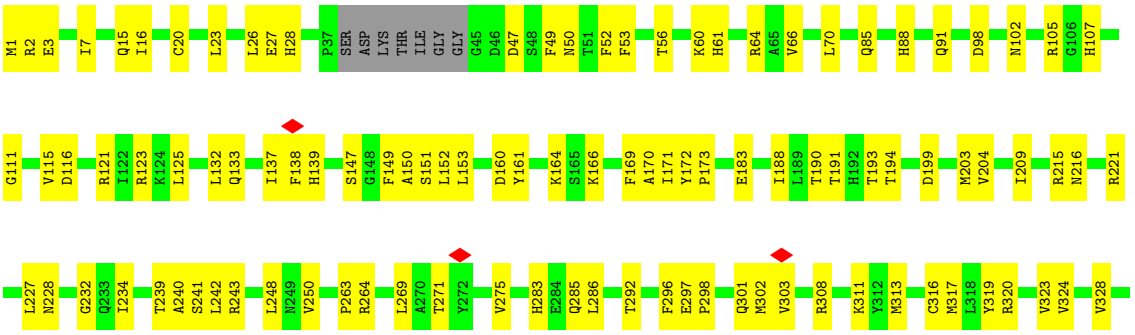
• Molecule 8: Tubulin alpha-3 chain

Chain TC:

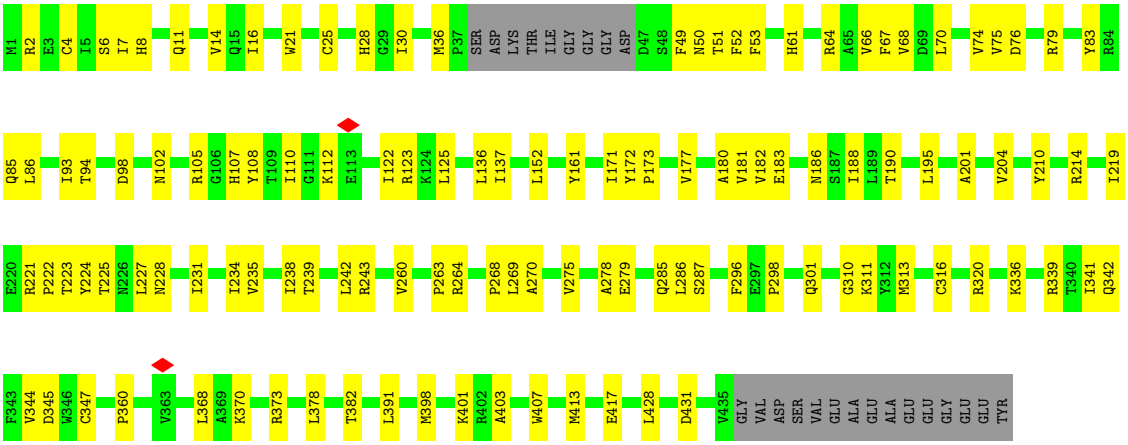


• Molecule 8: Tubulin alpha-3 chain

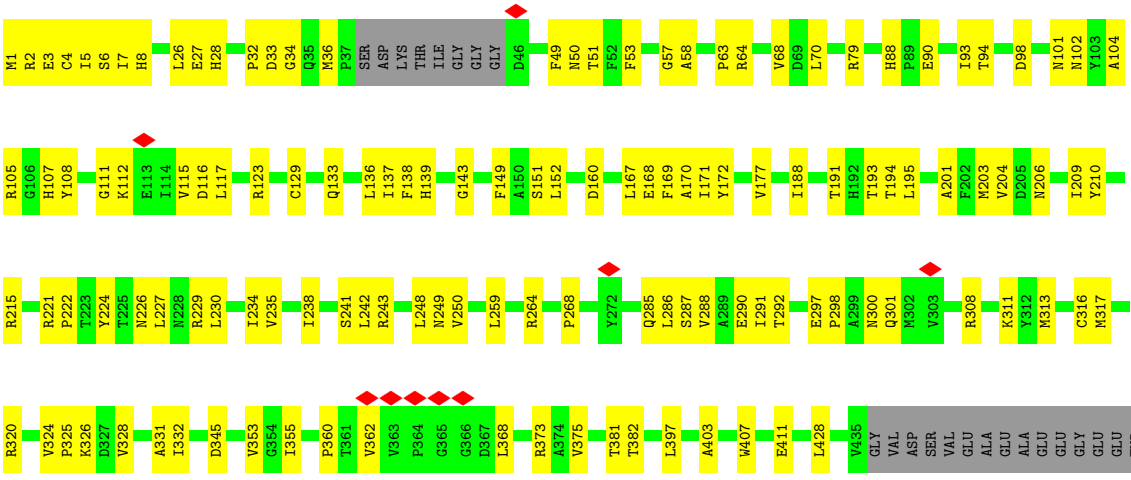
Chain TE:



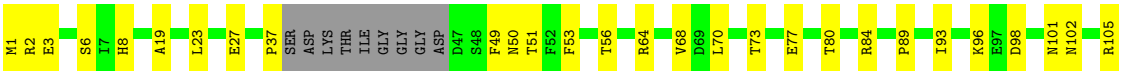
• Molecule 8: Tubulin alpha-3 chain

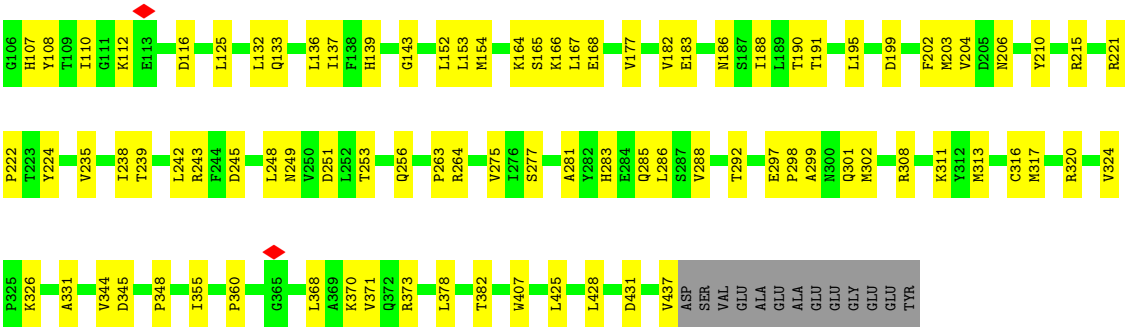


• Molecule 8: Tubulin alpha-3 chain

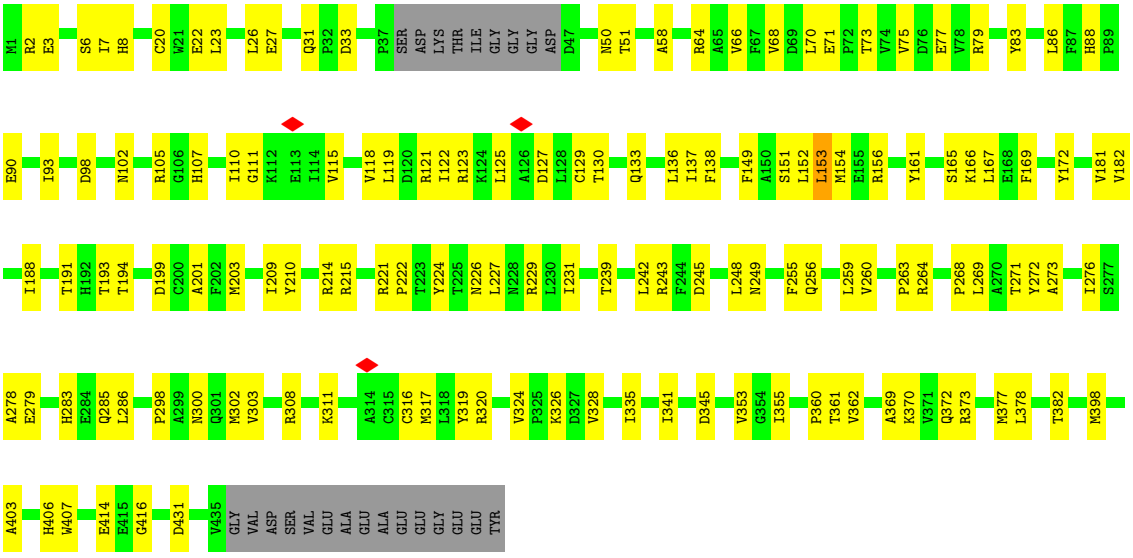


• Molecule 8: Tubulin alpha-3 chain

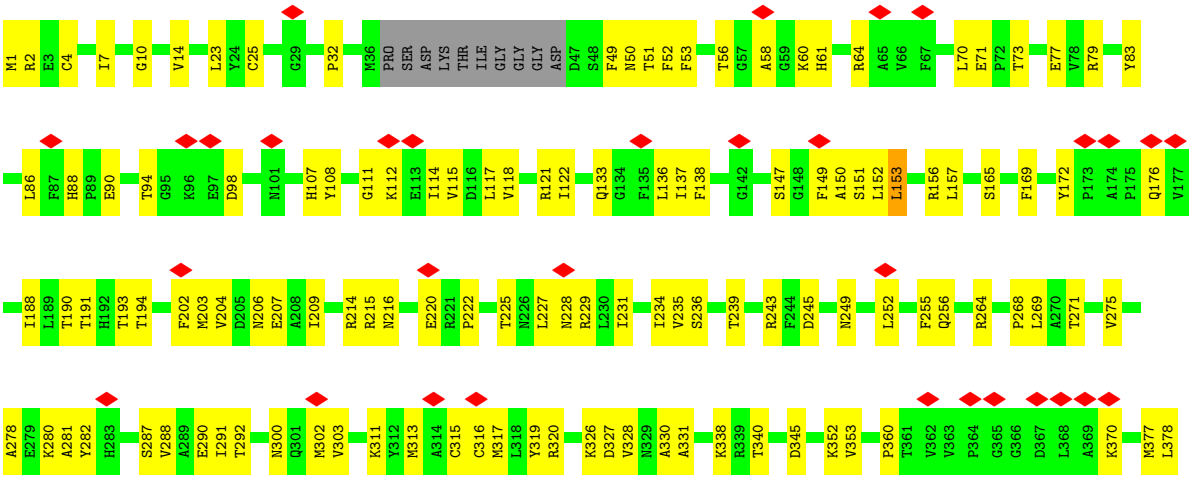




• Molecule 8: Tubulin alpha-3 chain

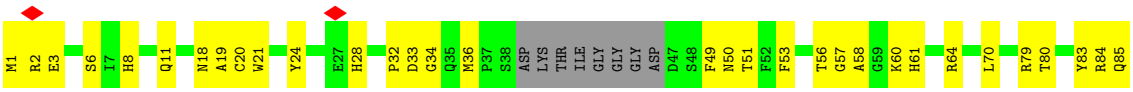


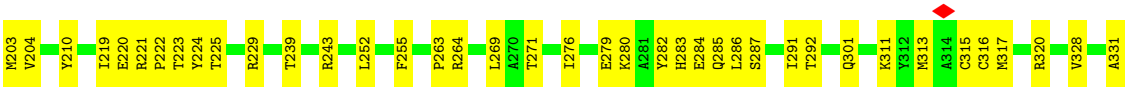
• Molecule 8: Tubulin alpha-3 chain

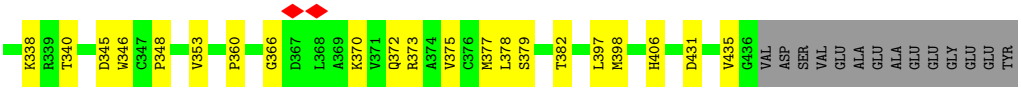


• Molecule 8: Tubulin alpha-3 chain

Chain UC:

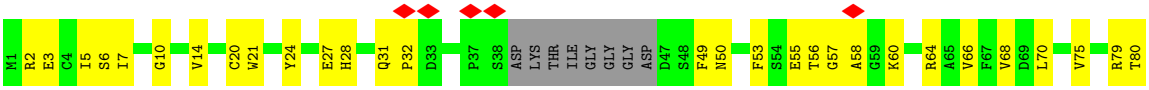


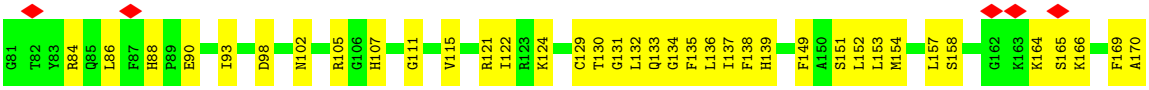


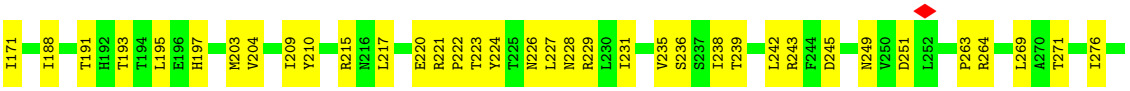


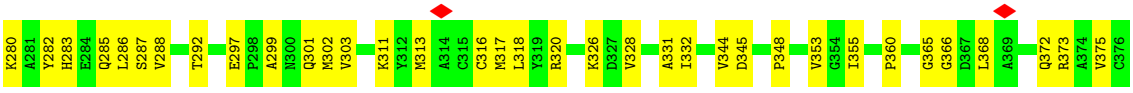
• Molecule 8: Tubulin alpha-3 chain

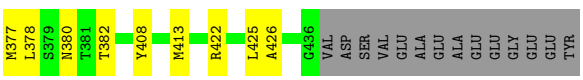
Chain UE:





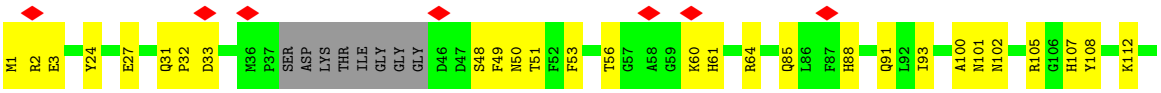


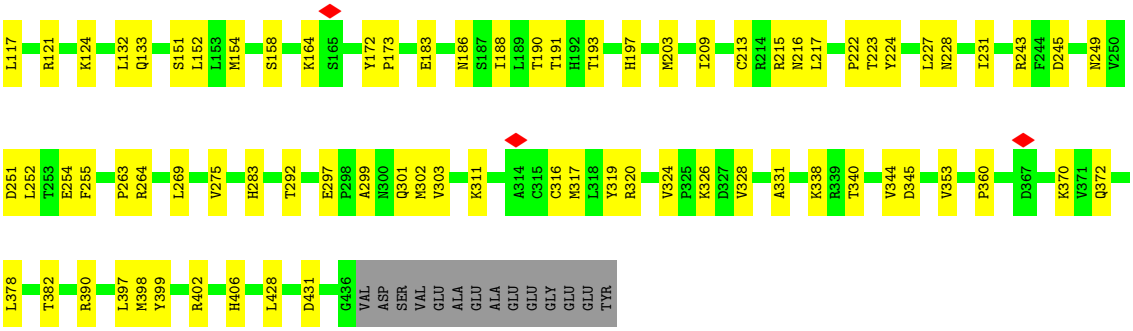




• Molecule 8: Tubulin alpha-3 chain

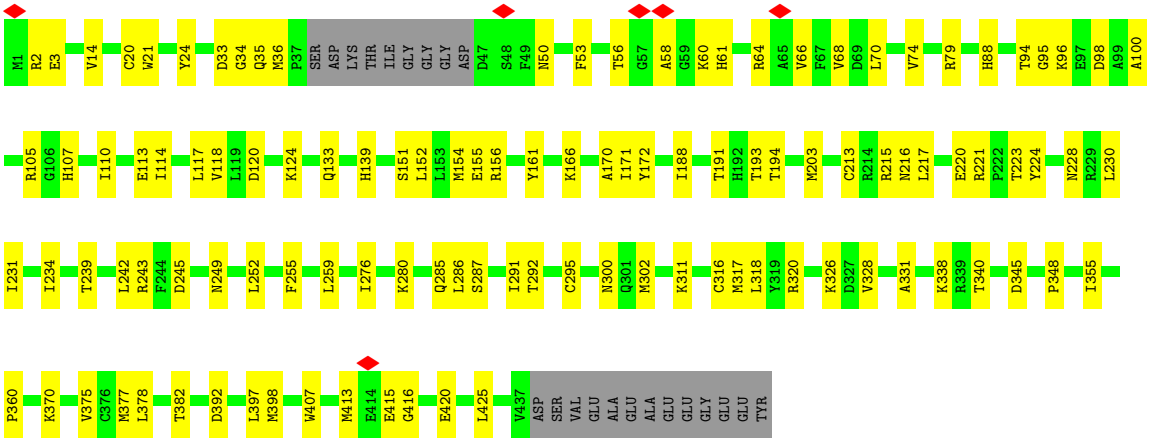
Chain UG:





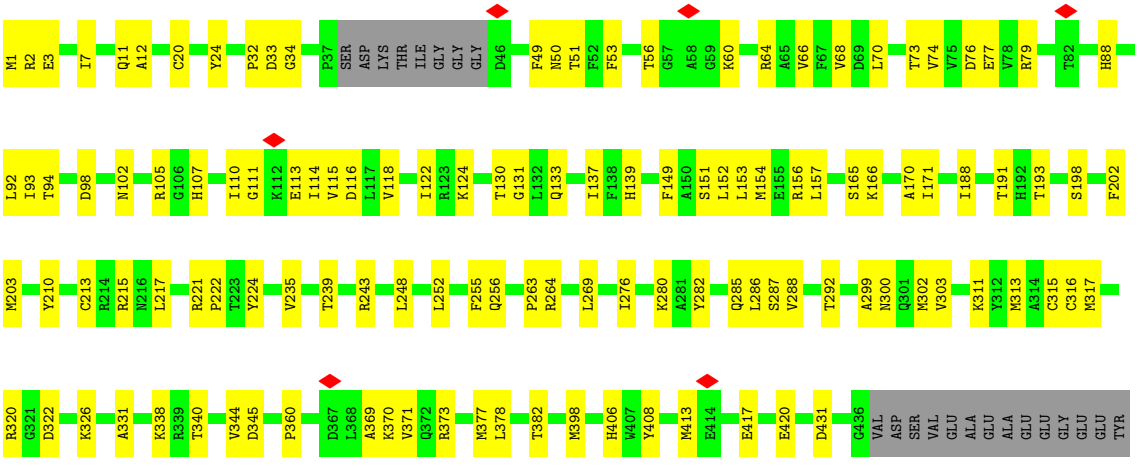
• Molecule 8: Tubulin alpha-3 chain

Chain UI:



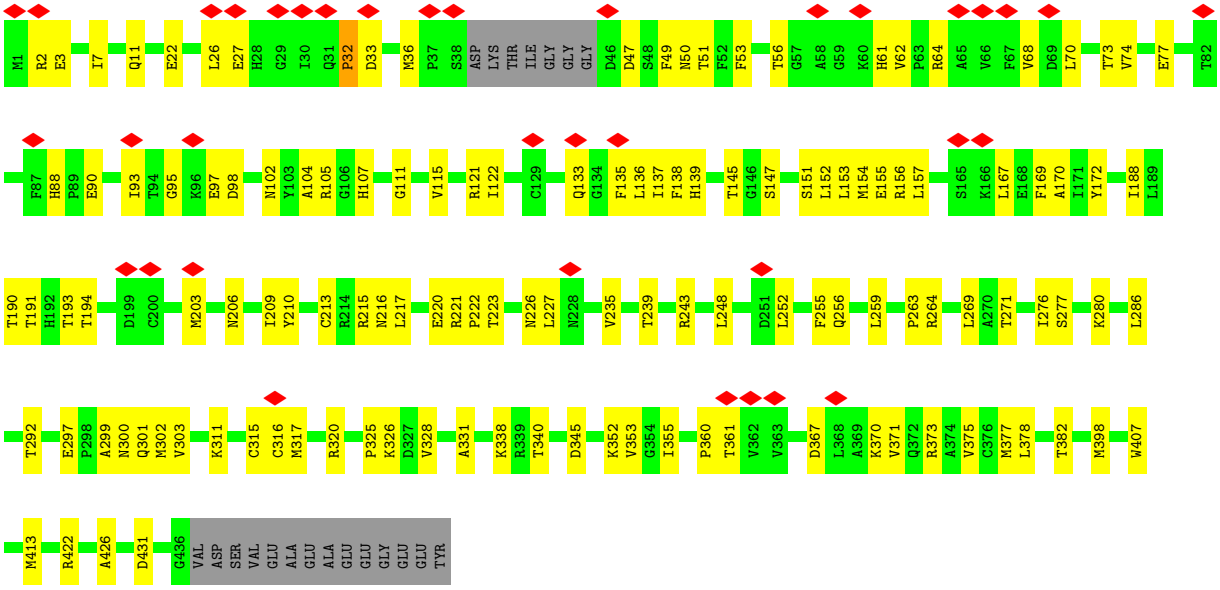
• Molecule 8: Tubulin alpha-3 chain

Chain UK:



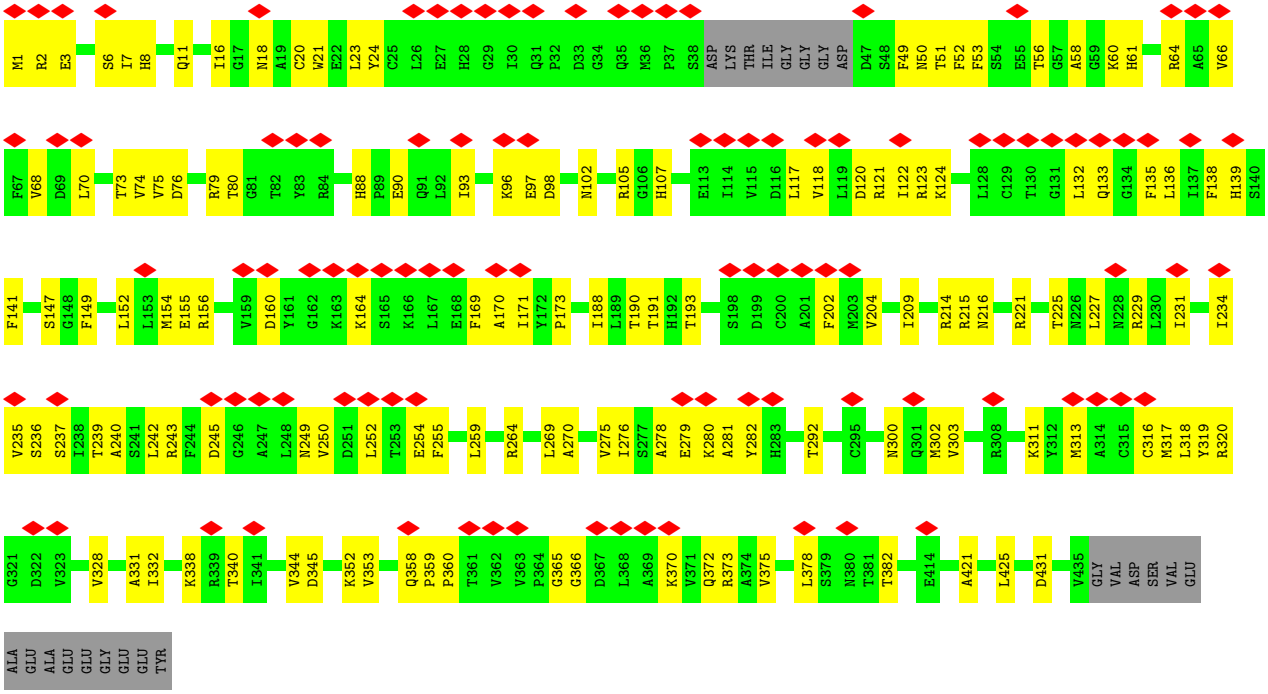
• Molecule 8: Tubulin alpha-3 chain

Chain UM:



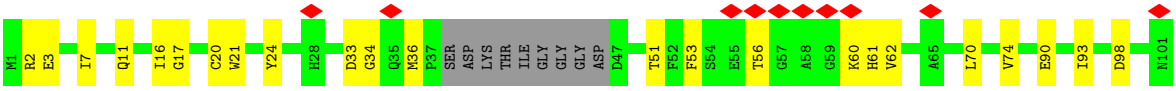
• Molecule 8: Tubulin alpha-3 chain

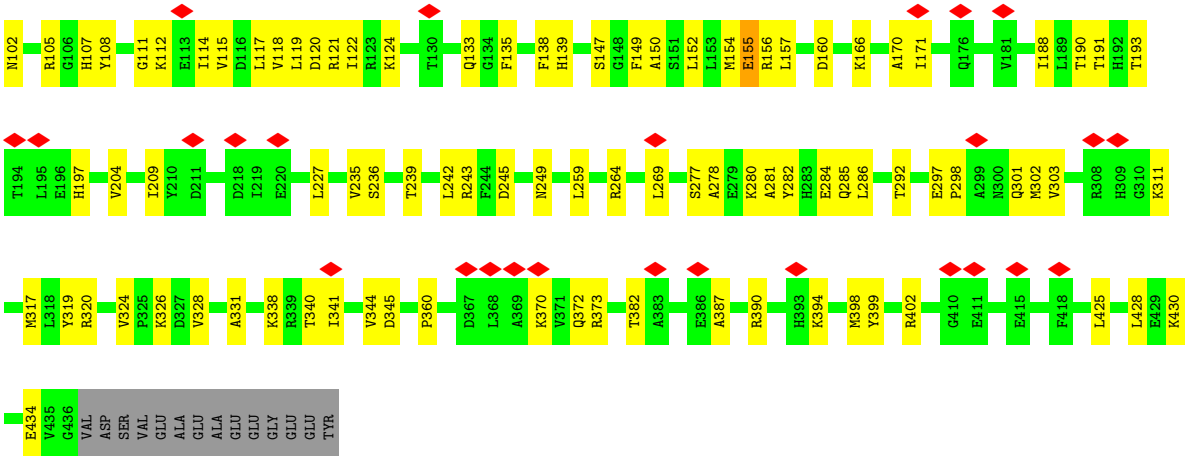
Chain UO:



• Molecule 8: Tubulin alpha-3 chain

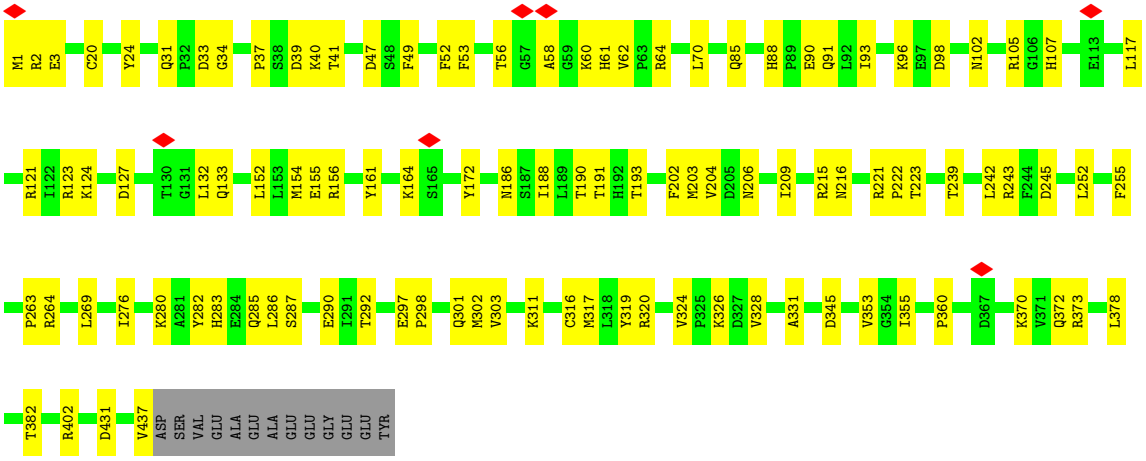
Chain VA:





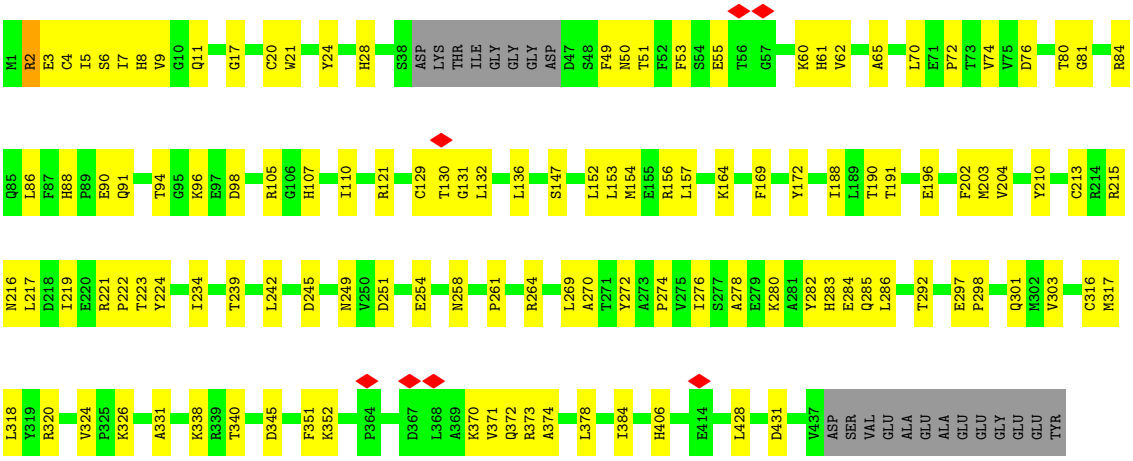
• Molecule 8: Tubulin alpha-3 chain

Chain VC:



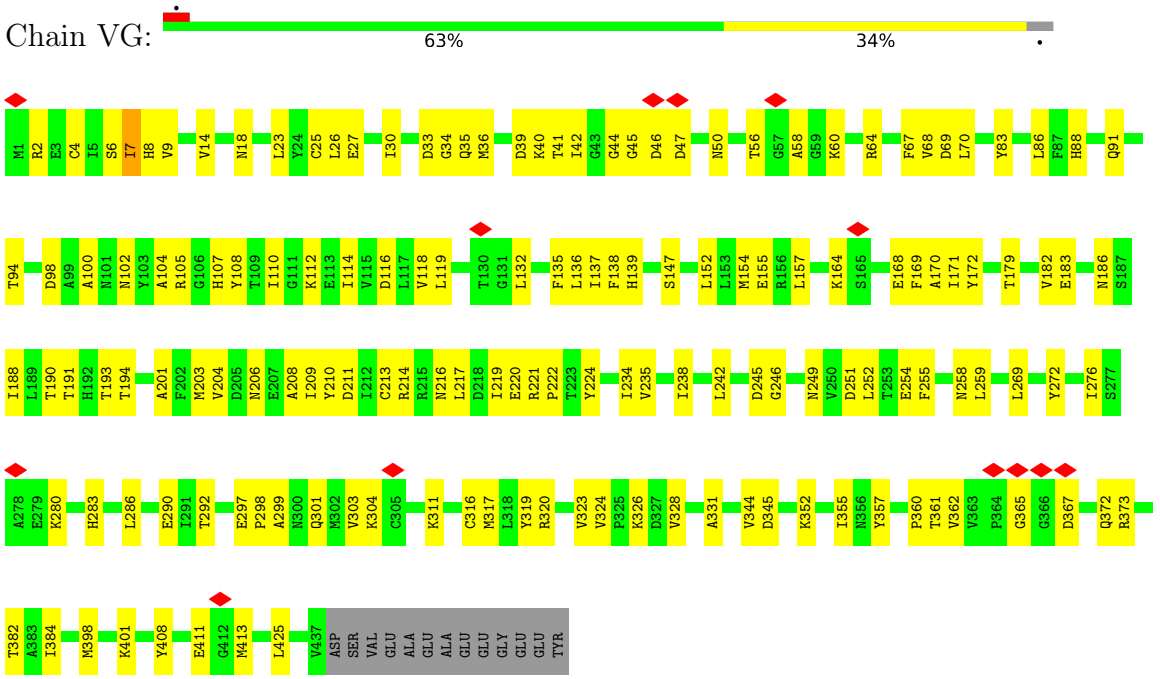
• Molecule 8: Tubulin alpha-3 chain

Chain VE:



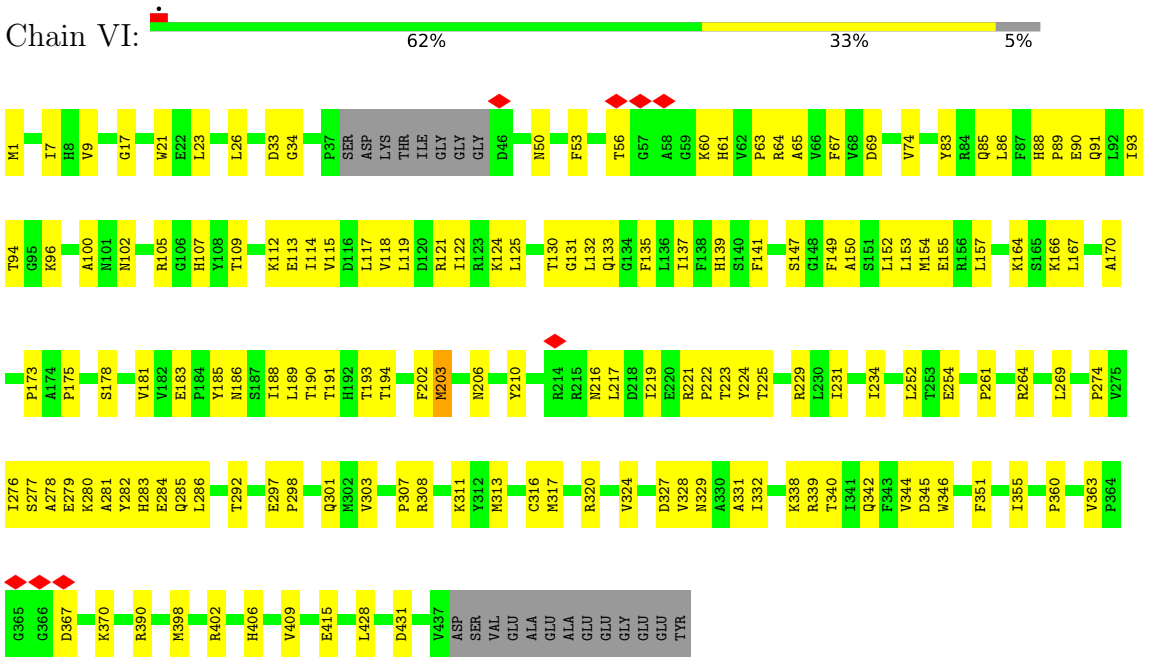
• Molecule 8: Tubulin alpha-3 chain

Chain VG:



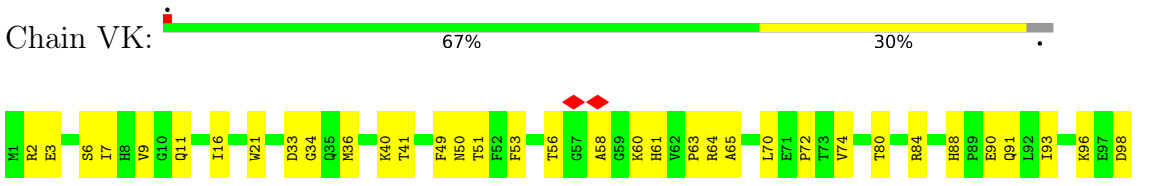
• Molecule 8: Tubulin alpha-3 chain

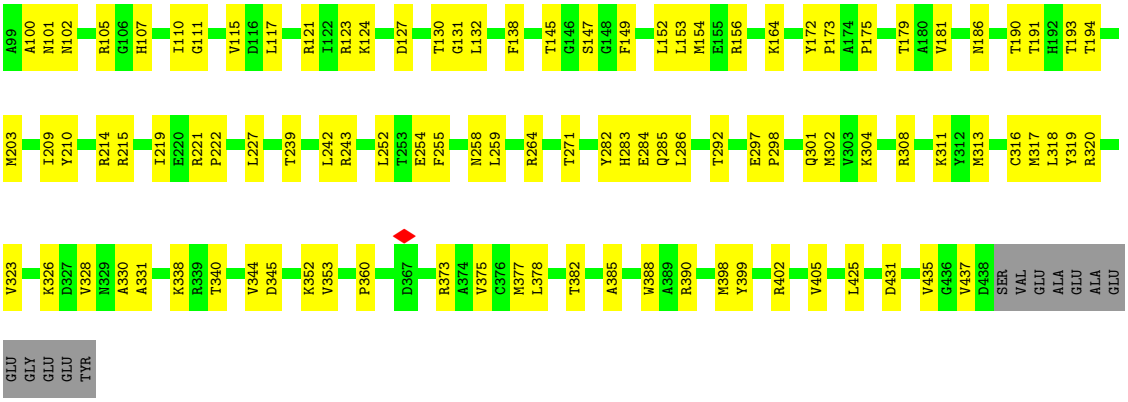
Chain VI:



• Molecule 8: Tubulin alpha-3 chain

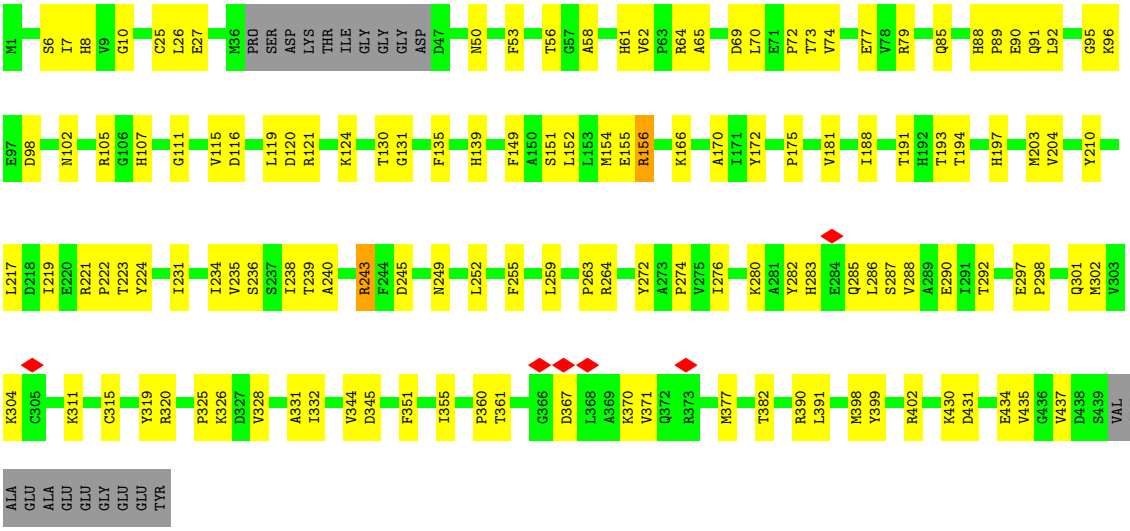
Chain VK:





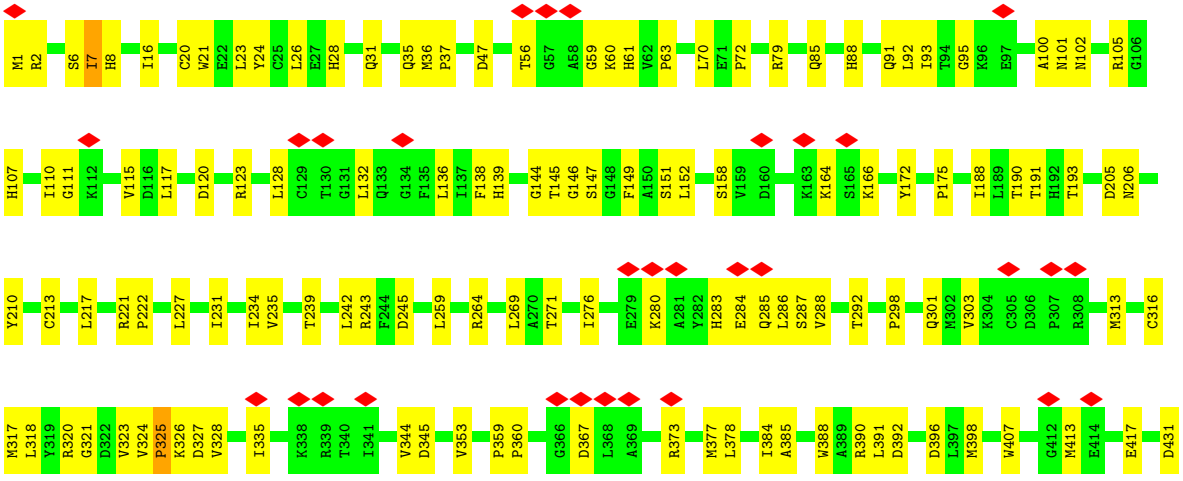
• Molecule 8: Tubulin alpha-3 chain

Chain VM:



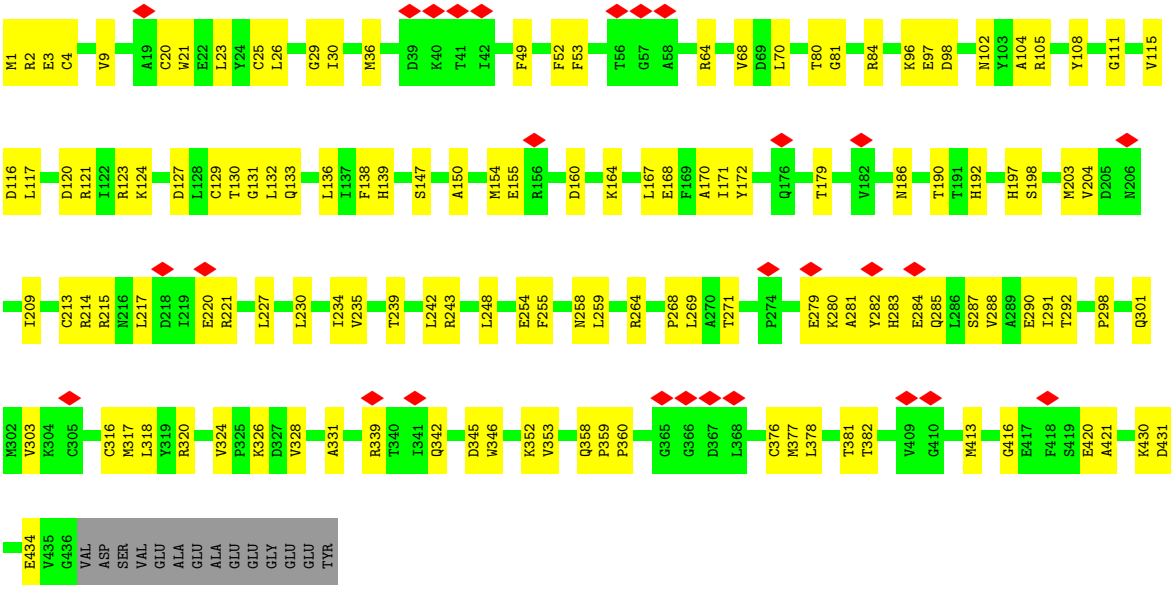
• Molecule 8: Tubulin alpha-3 chain

Chain VO:



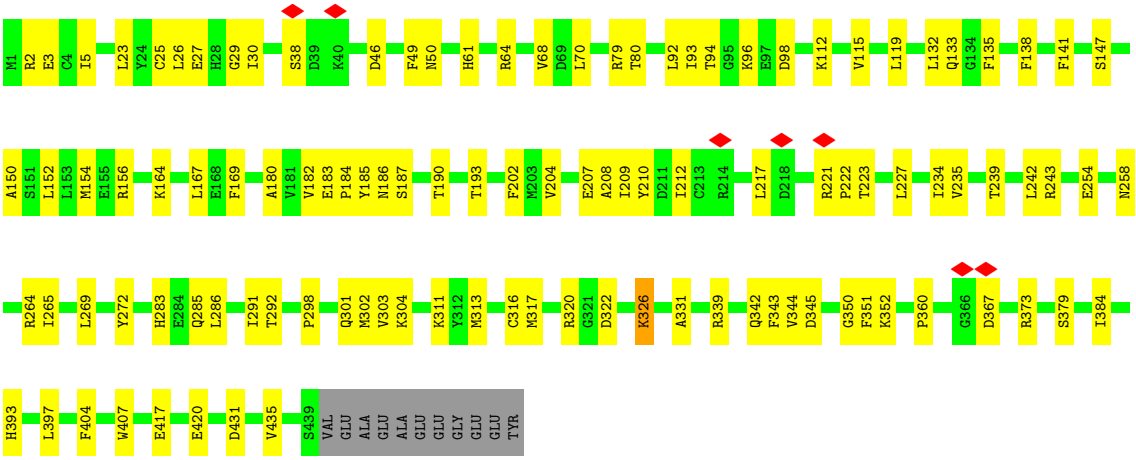
• Molecule 8: Tubulin alpha-3 chain

Chain WA:



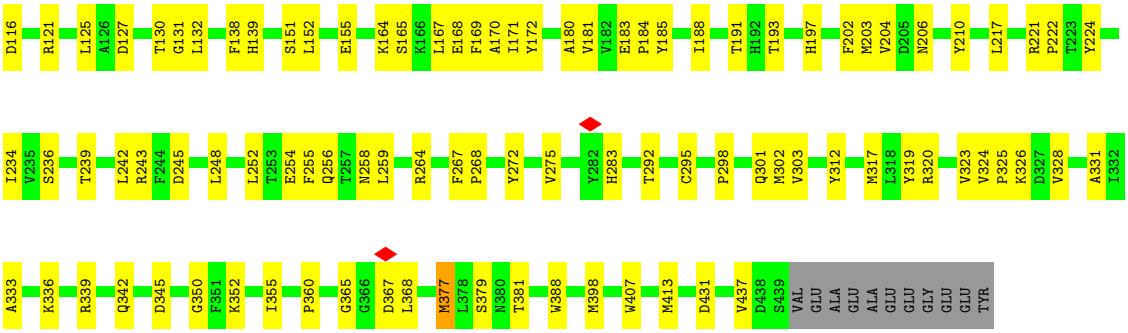
• Molecule 8: Tubulin alpha-3 chain

Chain WC:



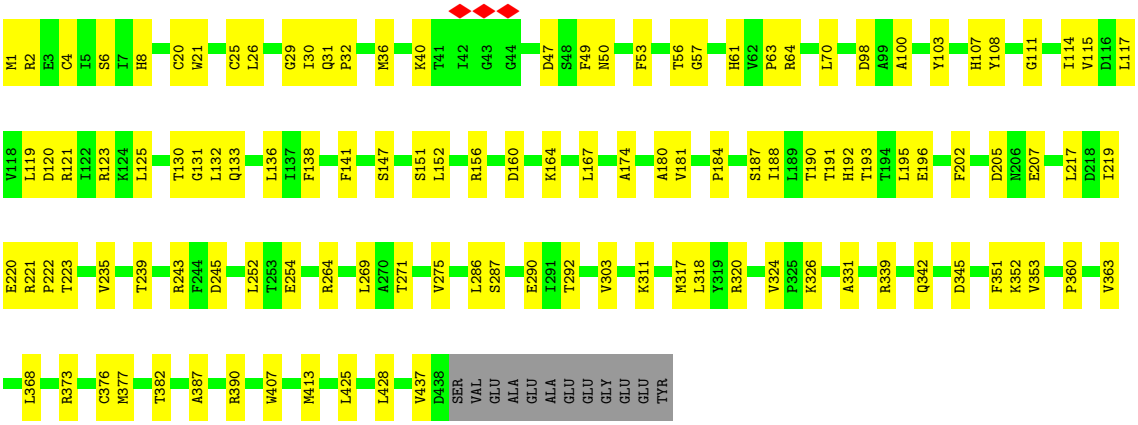
• Molecule 8: Tubulin alpha-3 chain

Chain WE:



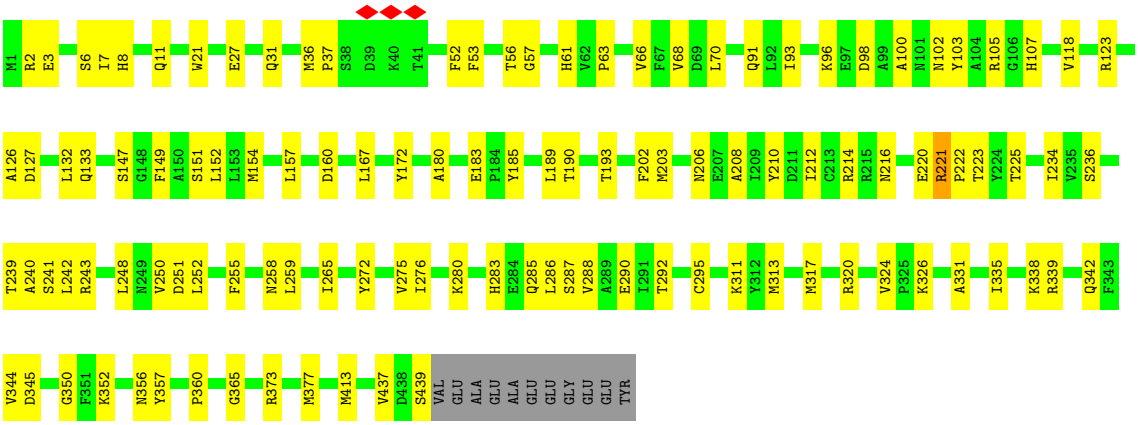
• Molecule 8: Tubulin alpha-3 chain

Chain WG:



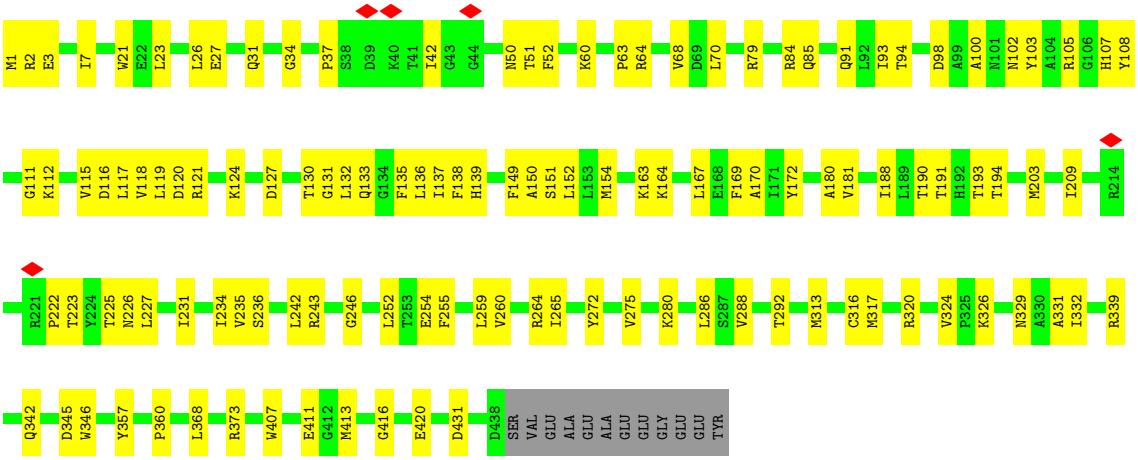
• Molecule 8: Tubulin alpha-3 chain

Chain WI:



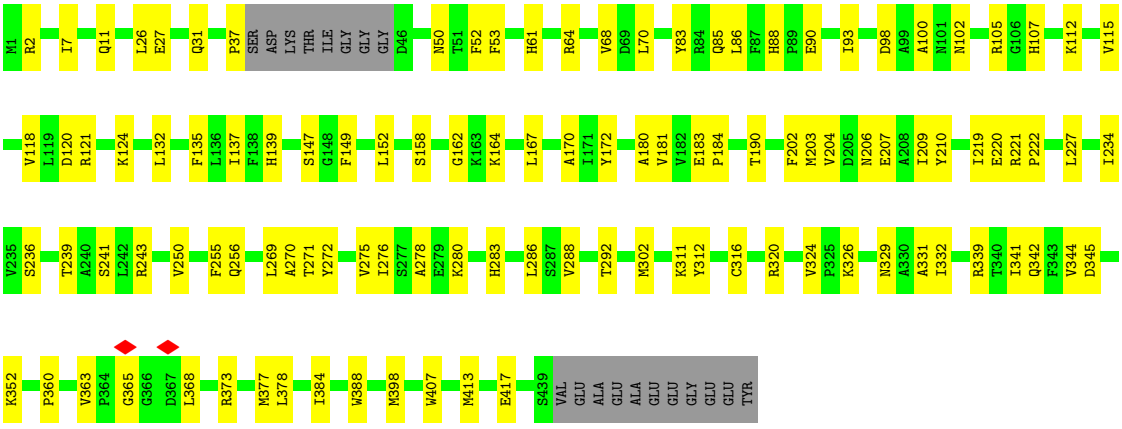
• Molecule 8: Tubulin alpha-3 chain

Chain WK:



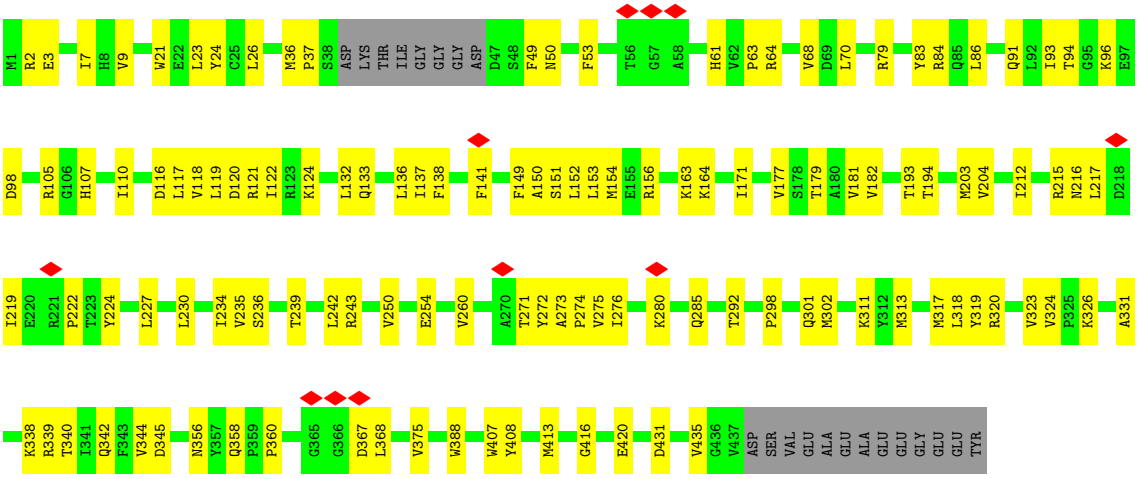
• Molecule 8: Tubulin alpha-3 chain

Chain WM:



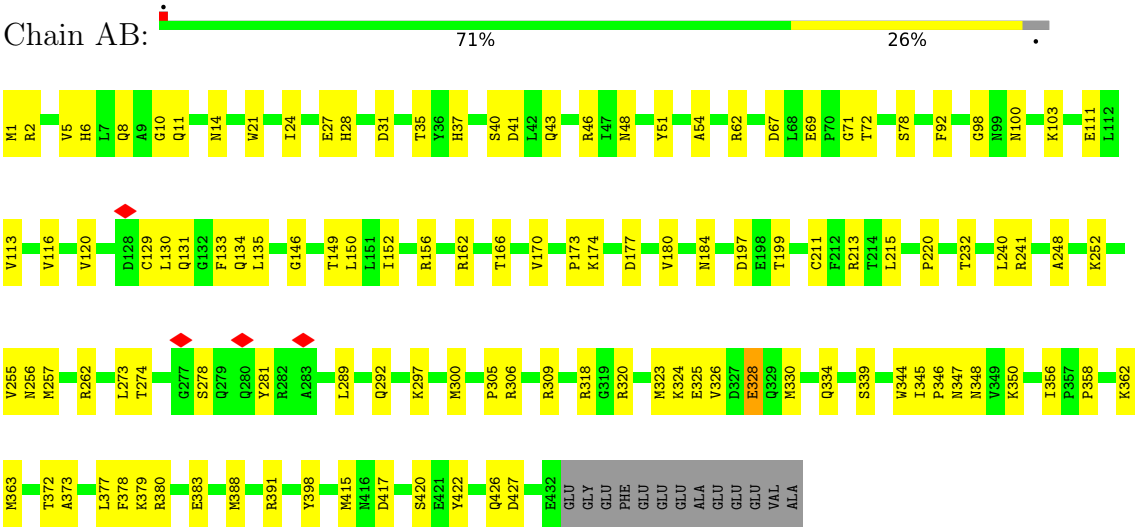
• Molecule 8: Tubulin alpha-3 chain

Chain WO:



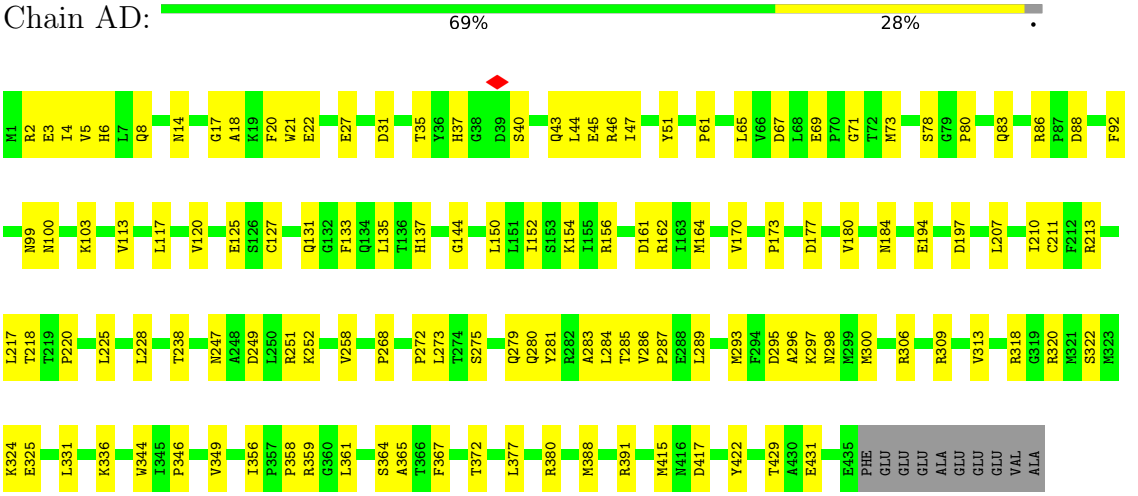
• Molecule 9: Tubulin beta-4B chain

Chain AB:



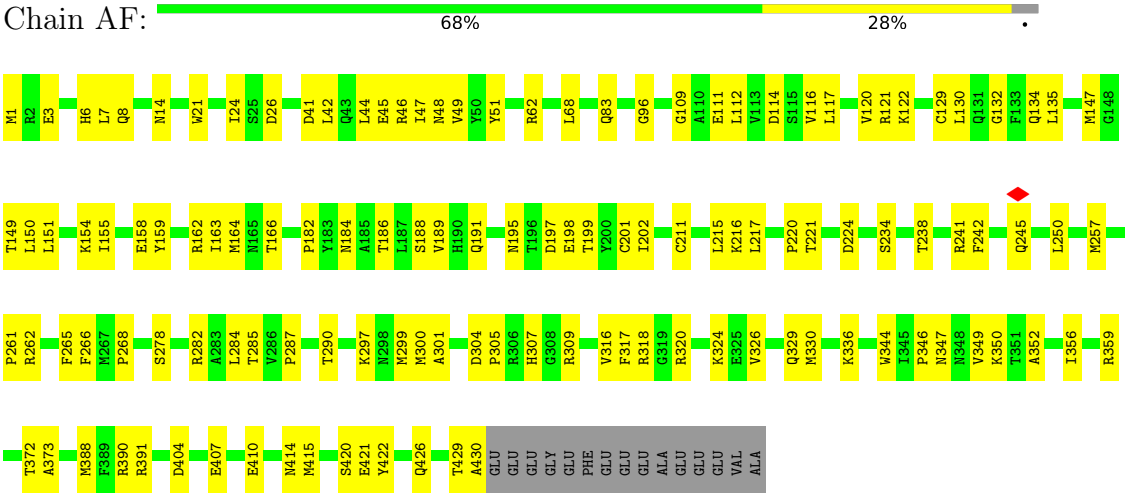
• Molecule 9: Tubulin beta-4B chain

Chain AD:



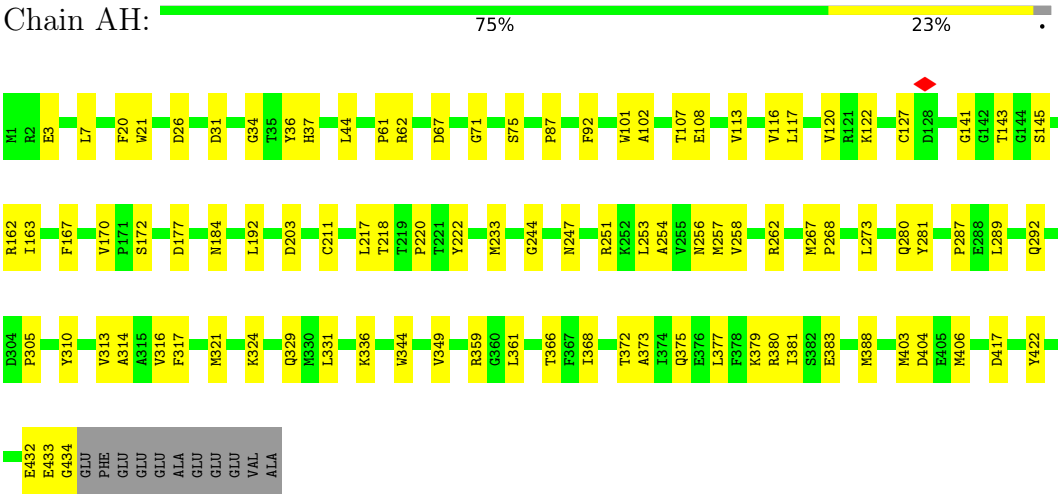
• Molecule 9: Tubulin beta-4B chain

Chain AF:



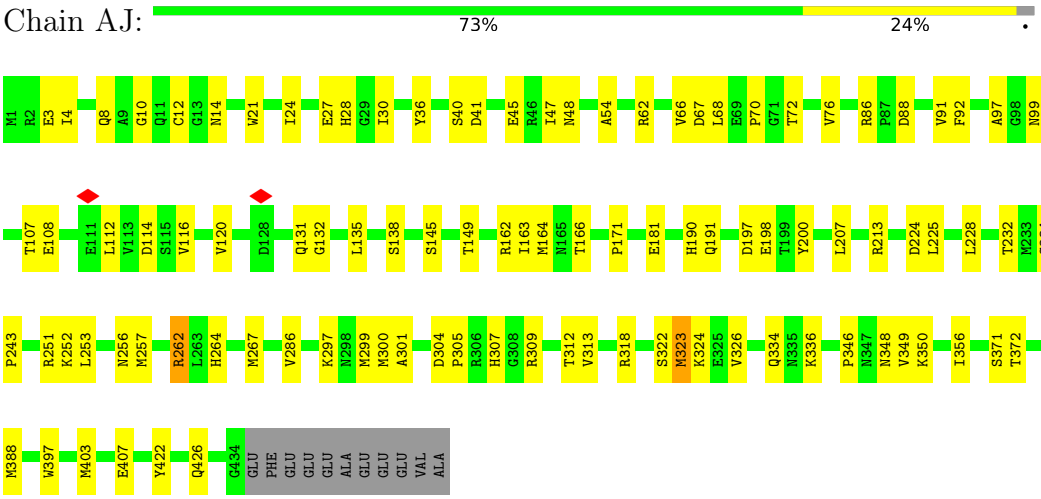
• Molecule 9: Tubulin beta-4B chain

Chain AH:



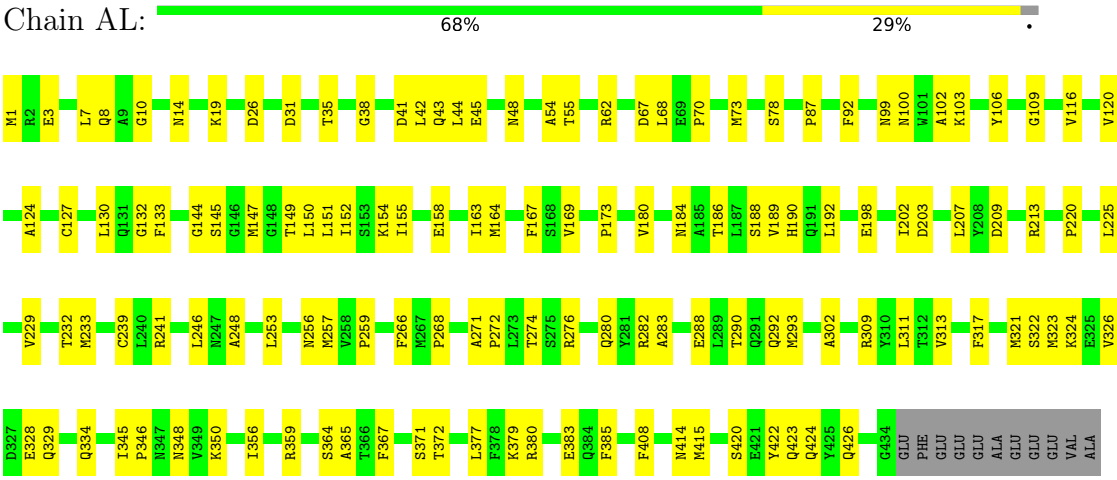
• Molecule 9: Tubulin beta-4B chain

Chain AJ:



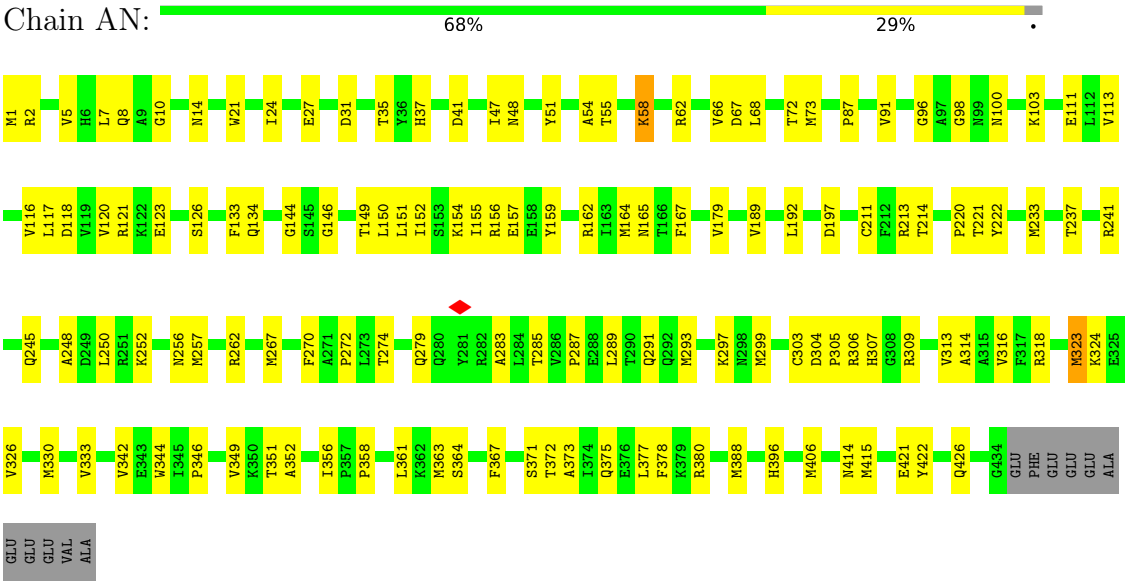
• Molecule 9: Tubulin beta-4B chain

Chain AL:



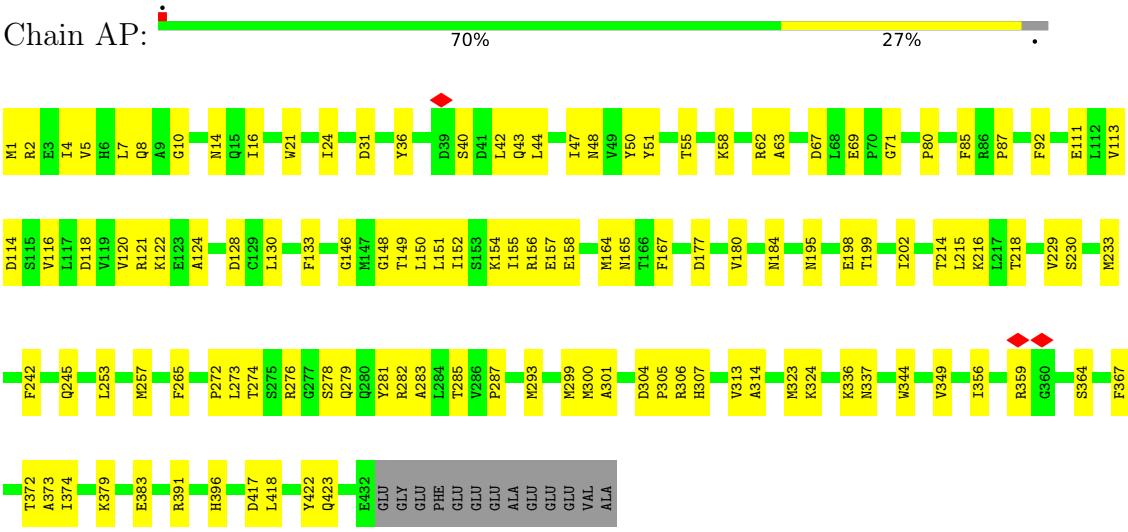
• Molecule 9: Tubulin beta-4B chain

Chain AN:



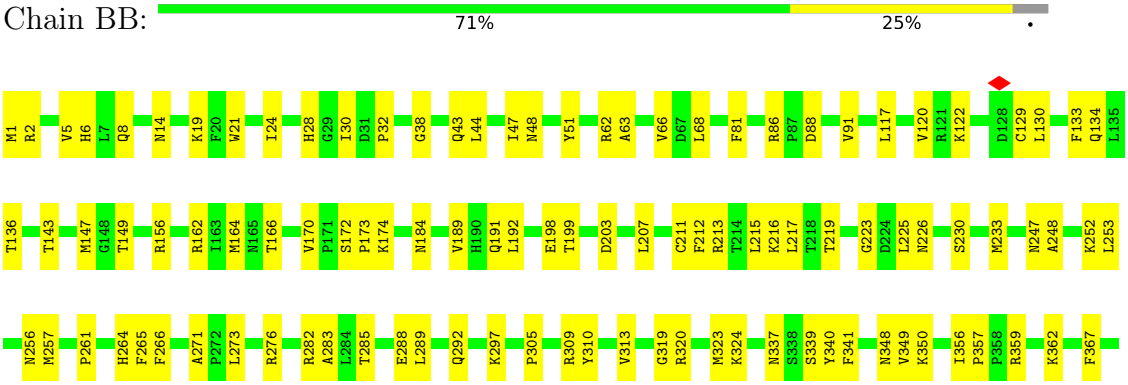
• Molecule 9: Tubulin beta-4B chain

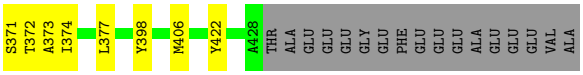
Chain AP:



• Molecule 9: Tubulin beta-4B chain

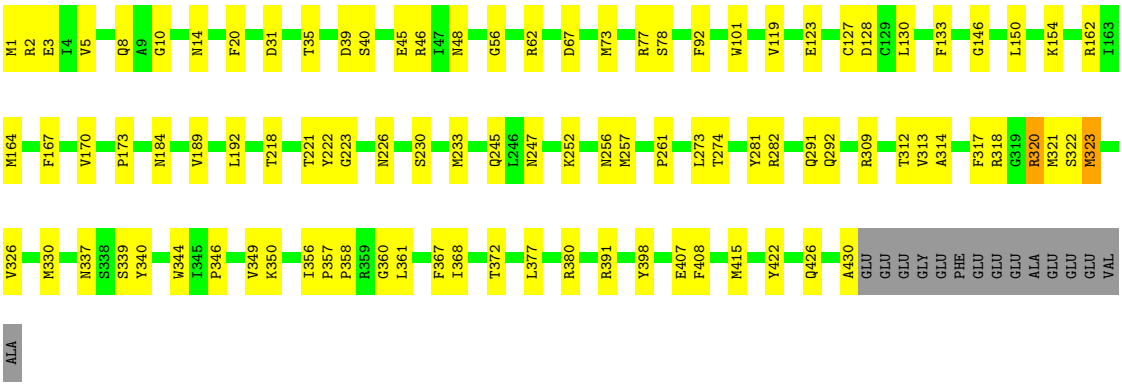
Chain BB:





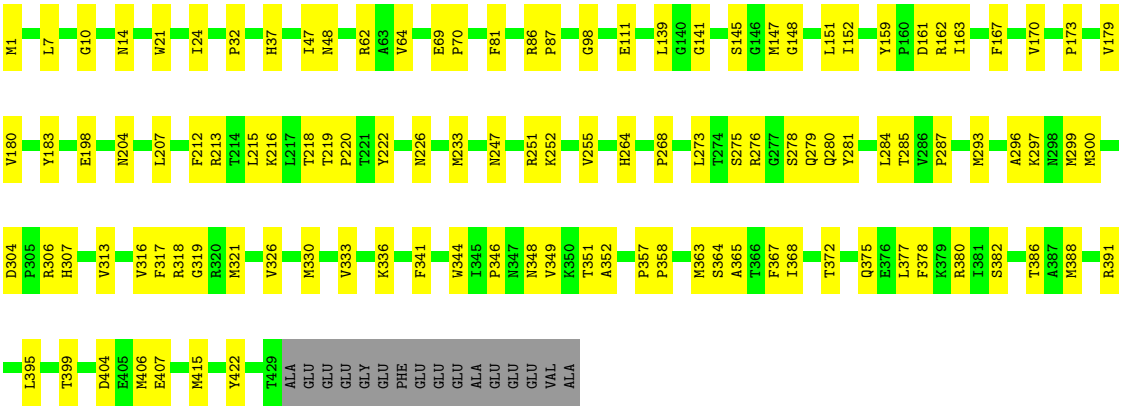
• Molecule 9: Tubulin beta-4B chain

Chain BD:



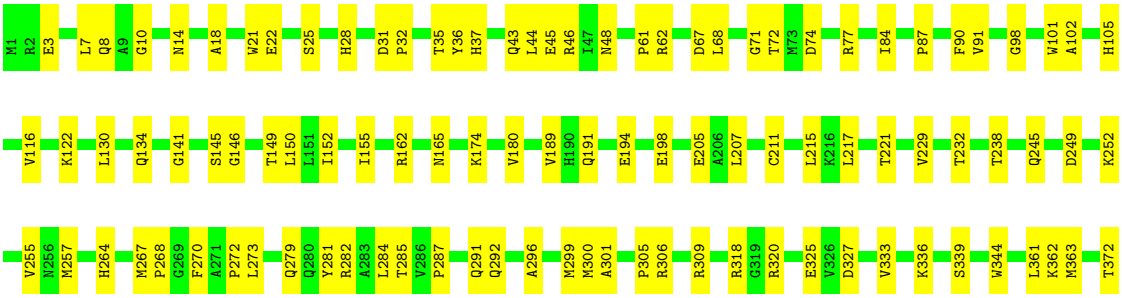
• Molecule 9: Tubulin beta-4B chain

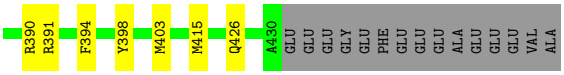
Chain BF:



• Molecule 9: Tubulin beta-4B chain

Chain BH:



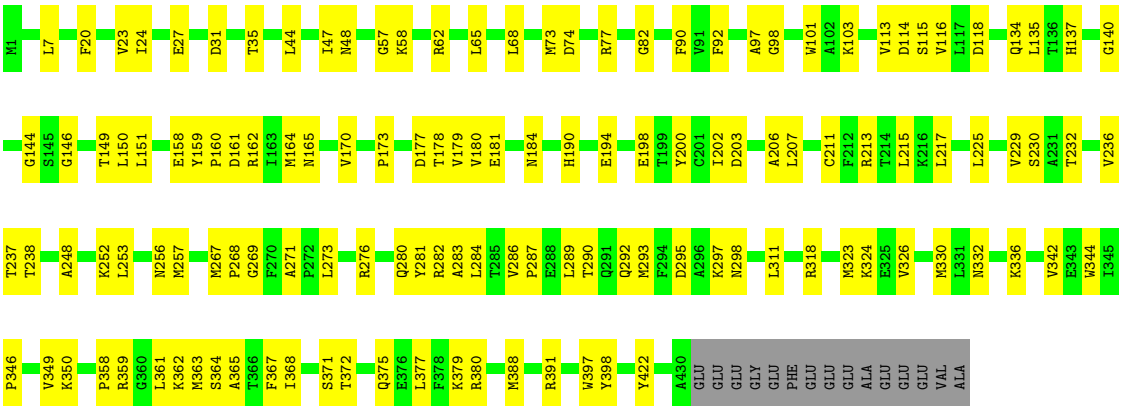


• Molecule 9: Tubulin beta-4B chain

Chain BJ:

• Molecule 9: Tubulin beta-4B chain

Chain BL:

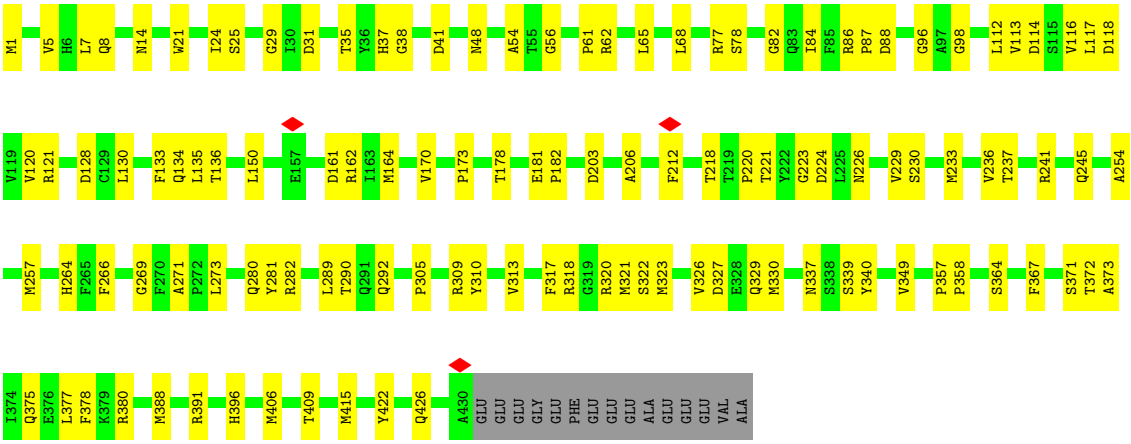


• Molecule 9: Tubulin beta-4B chain

Chain BN:

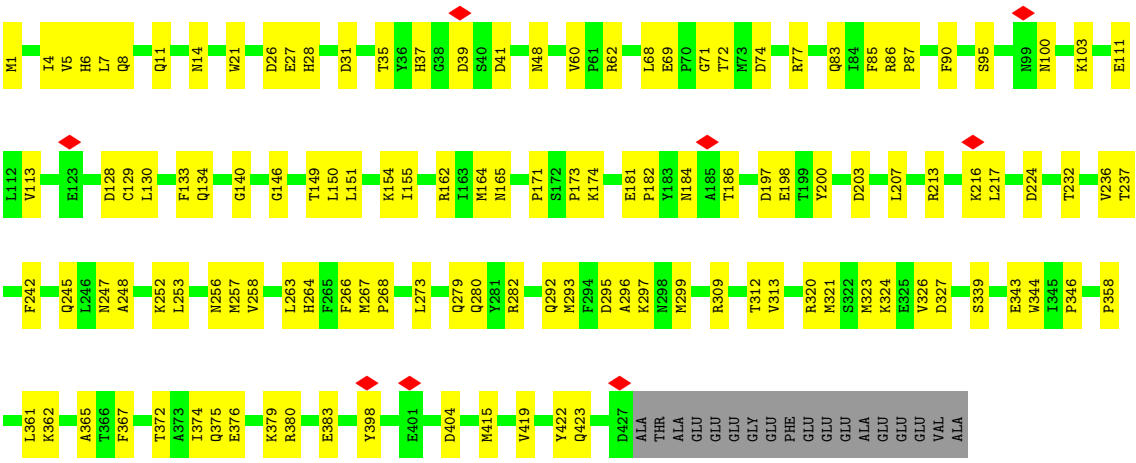
• Molecule 9: Tubulin beta-4B chain

Chain BP:



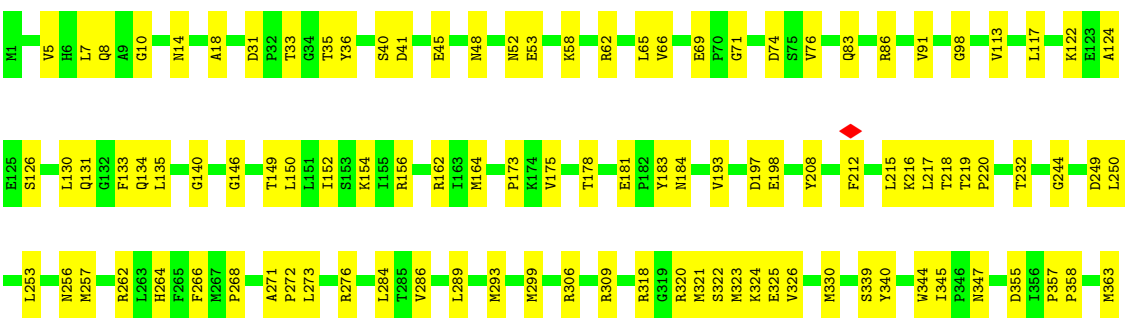
• Molecule 9: Tubulin beta-4B chain

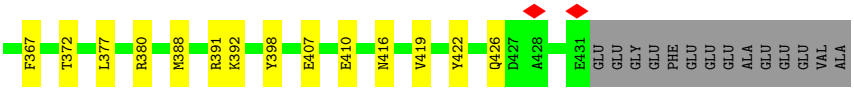
Chain CB:



• Molecule 9: Tubulin beta-4B chain

Chain CD:



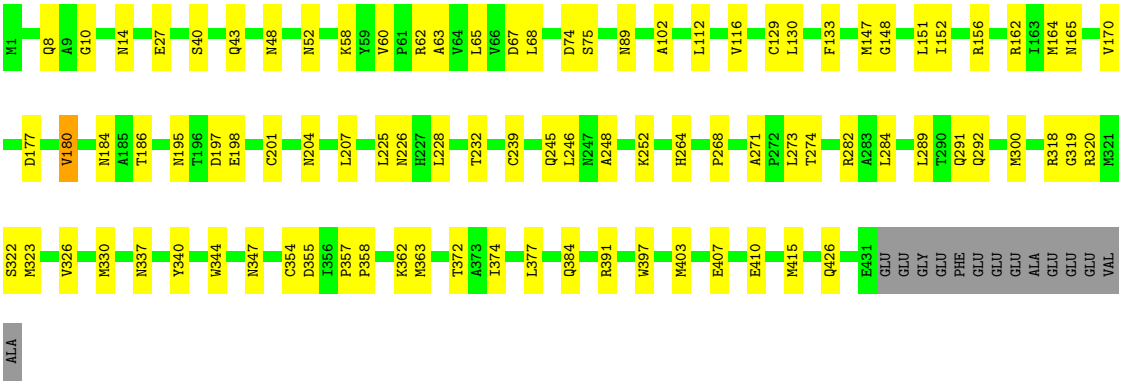


• Molecule 9: Tubulin beta-4B chain

Chain CF:

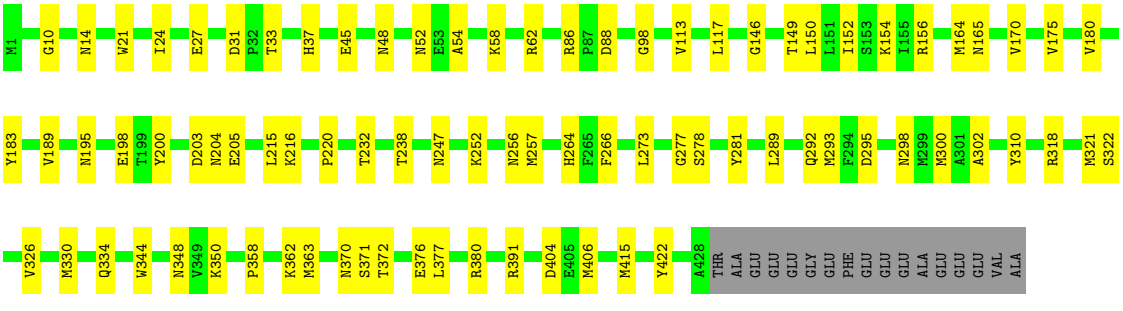
• Molecule 9: Tubulin beta-4B chain

Chain CH:



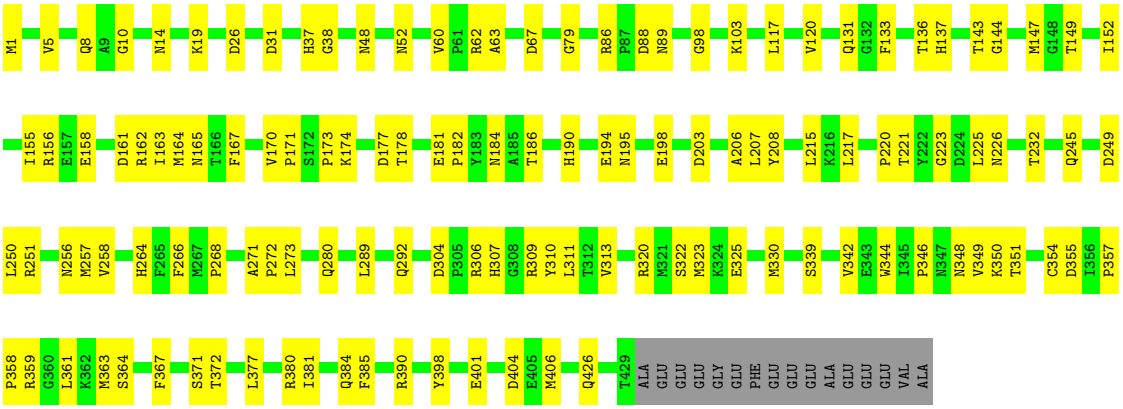
• Molecule 9: Tubulin beta-4B chain

Chain CJ:



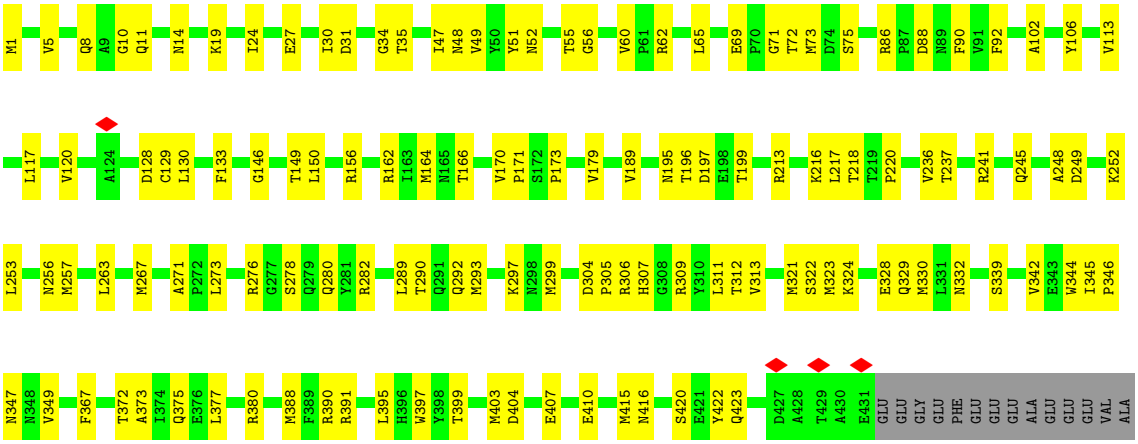
• Molecule 9: Tubulin beta-4B chain

Chain CL:



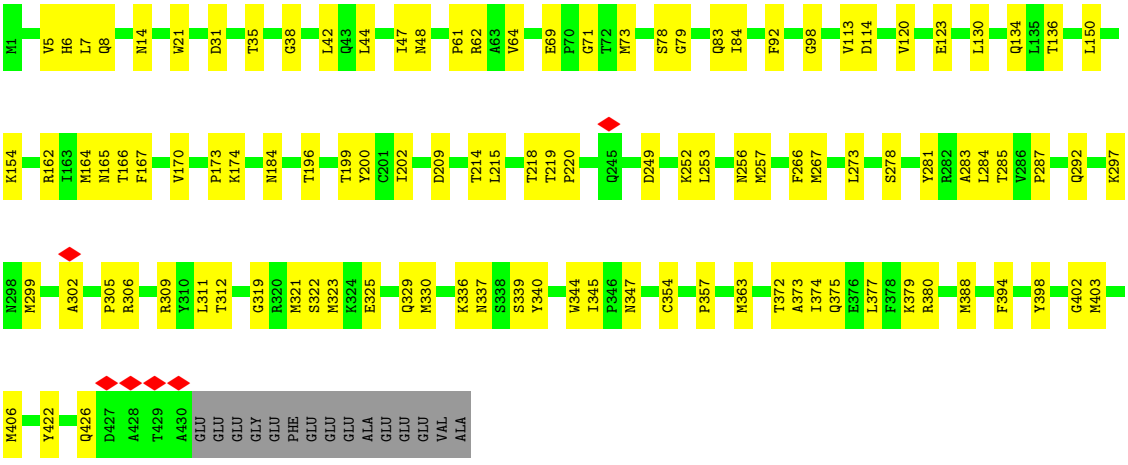
• Molecule 9: Tubulin beta-4B chain

Chain CN:



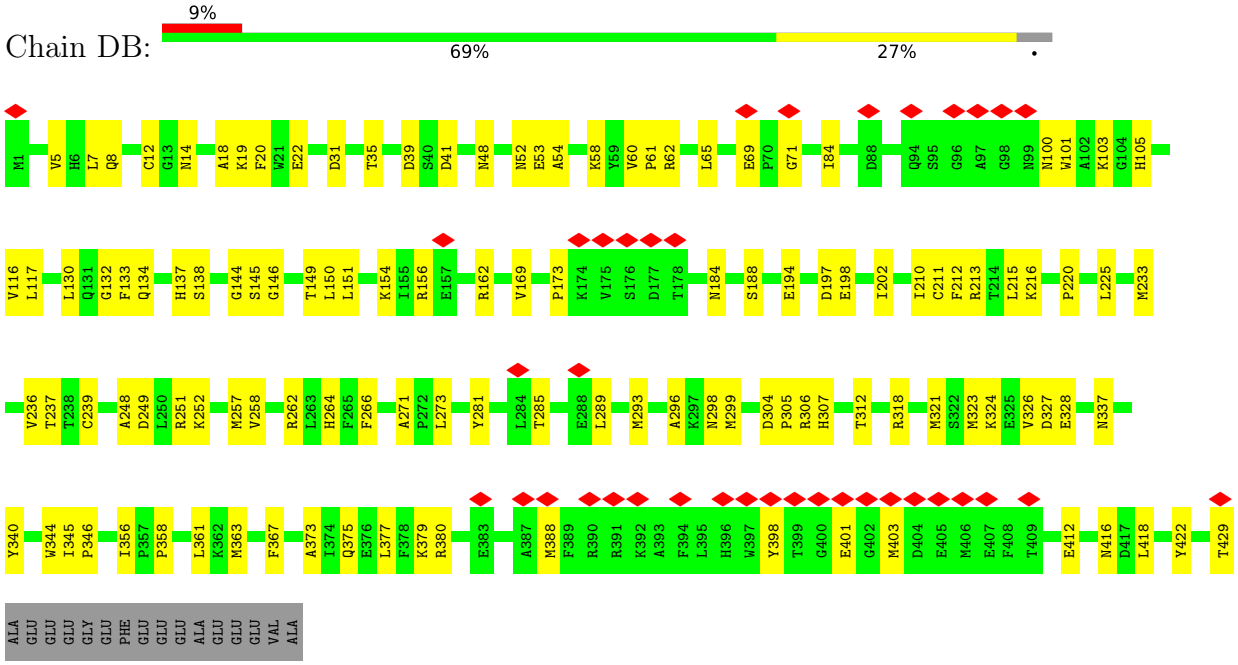
• Molecule 9: Tubulin beta-4B chain

Chain CP:



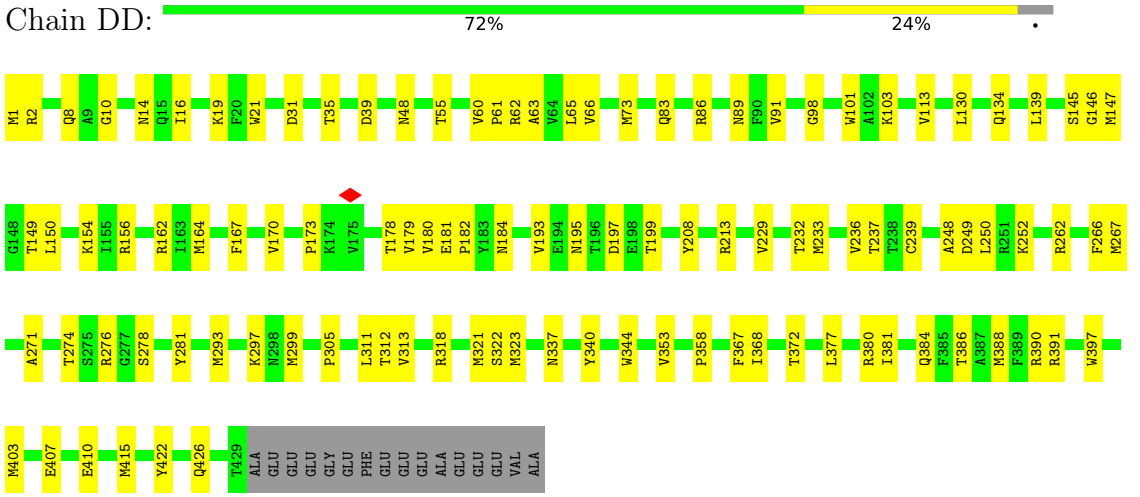
• Molecule 9: Tubulin beta-4B chain

Chain DB:



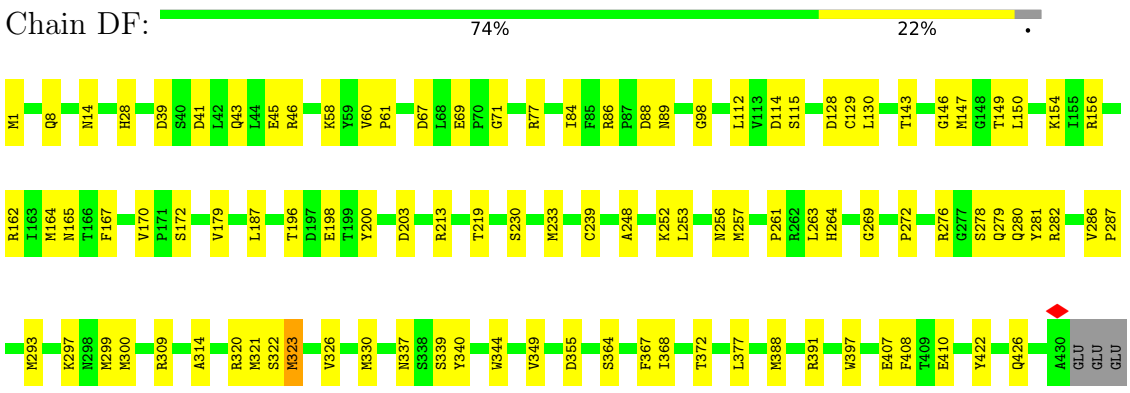
• Molecule 9: Tubulin beta-4B chain

Chain DD:



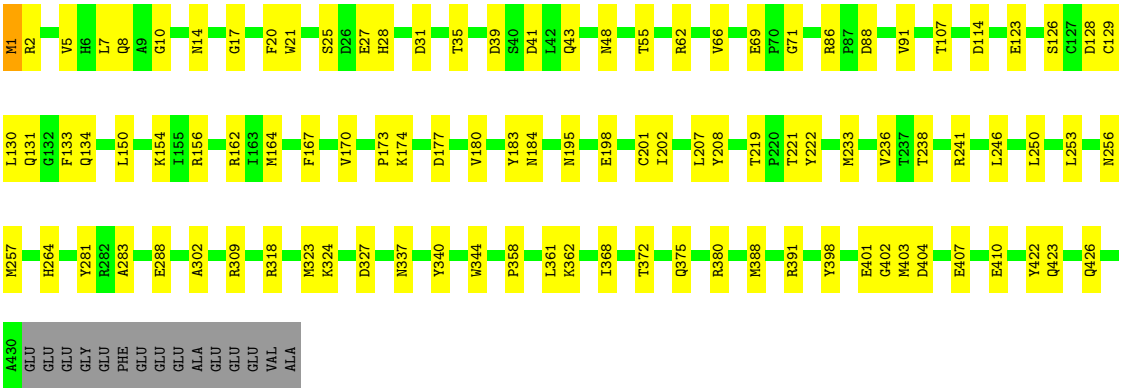
• Molecule 9: Tubulin beta-4B chain

Chain DF:



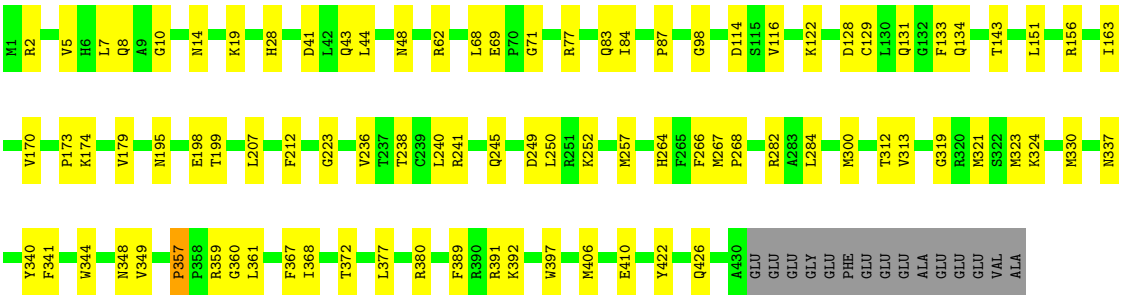
• Molecule 9: Tubulin beta-4B chain

Chain DH:



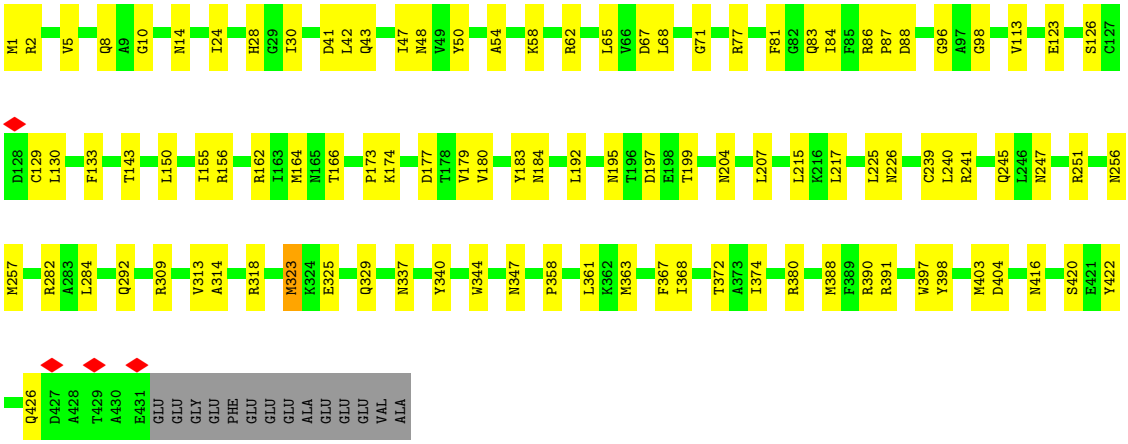
• Molecule 9: Tubulin beta-4B chain

Chain DJ:



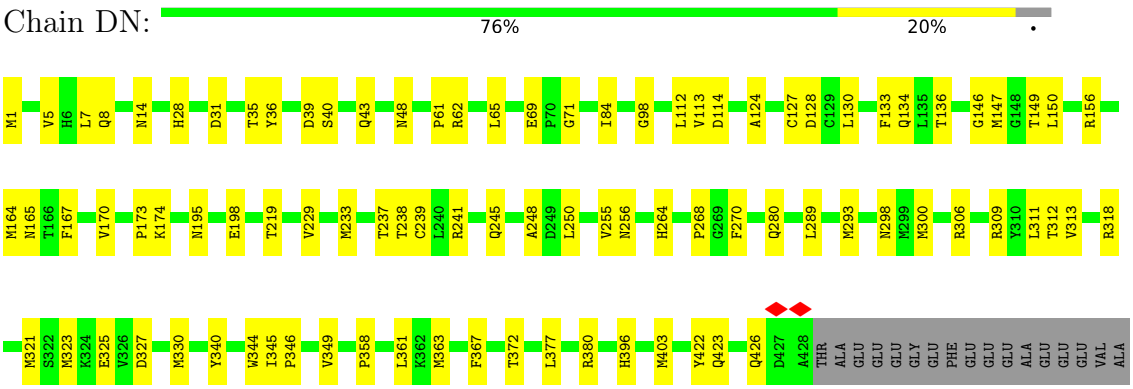
• Molecule 9: Tubulin beta-4B chain

Chain DL:



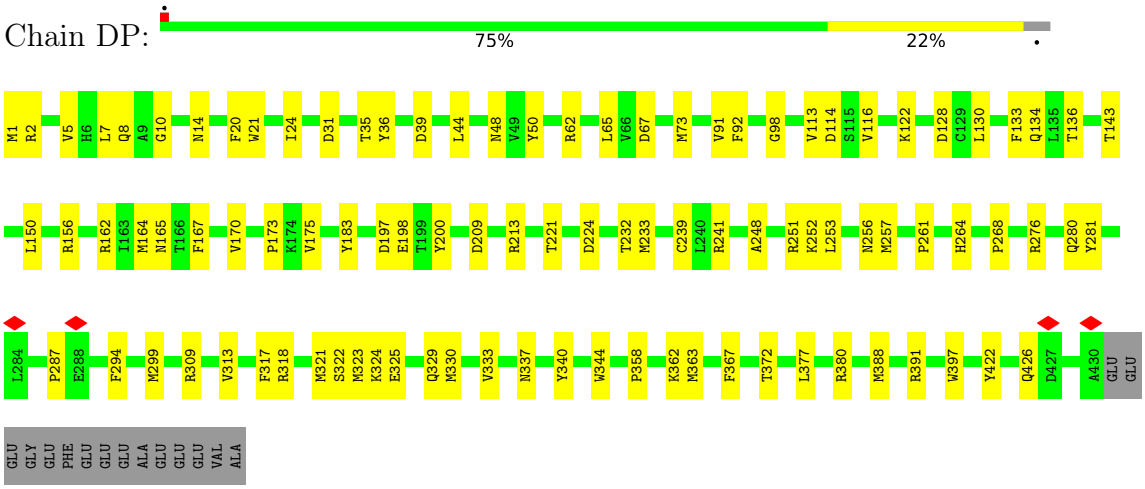
• Molecule 9: Tubulin beta-4B chain

Chain DN:



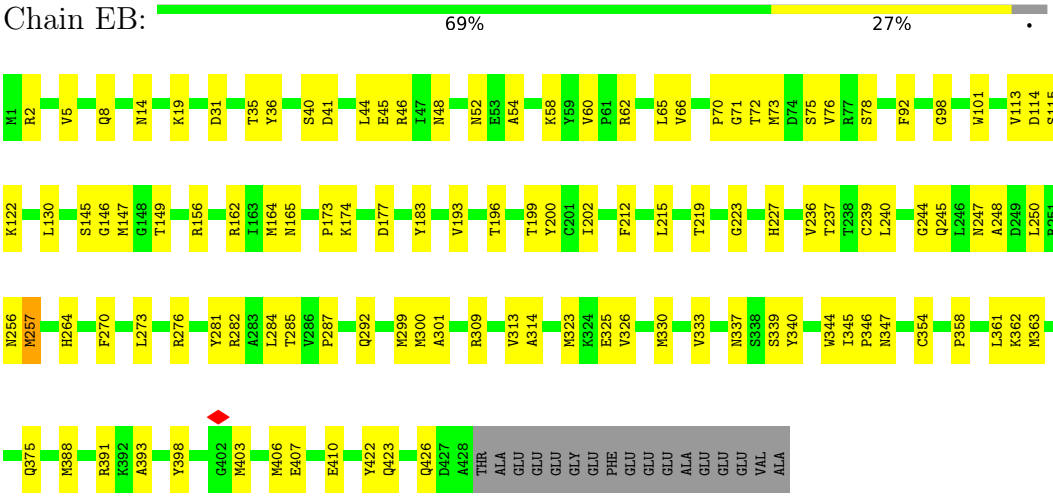
• Molecule 9: Tubulin beta-4B chain

Chain DP:



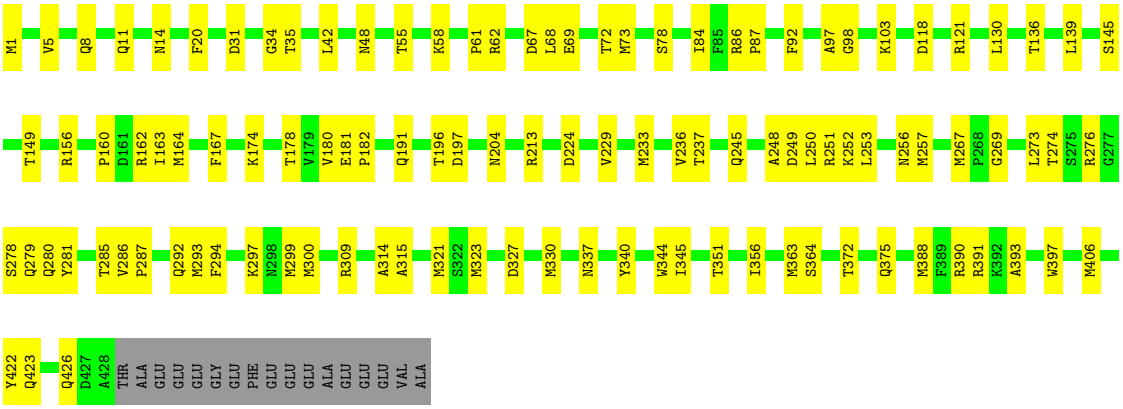
• Molecule 9: Tubulin beta-4B chain

Chain EB:



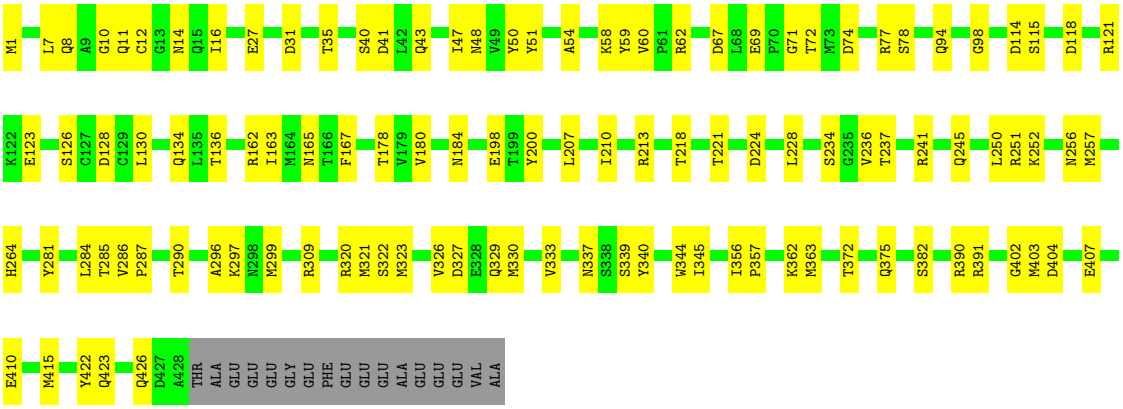
• Molecule 9: Tubulin beta-4B chain

Chain ED:



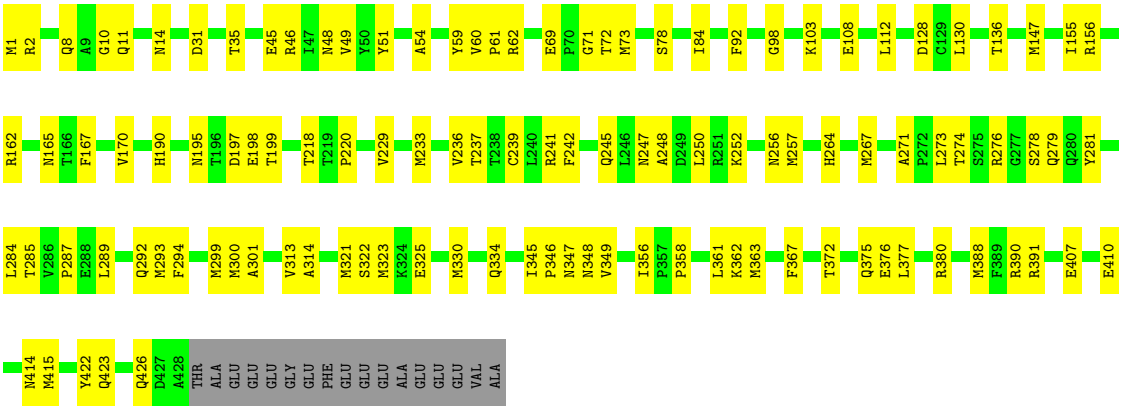
• Molecule 9: Tubulin beta-4B chain

Chain EF:



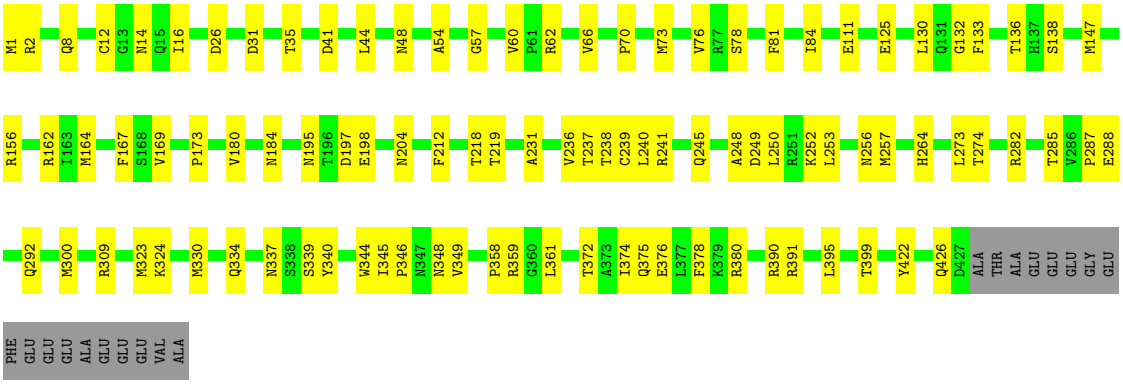
• Molecule 9: Tubulin beta-4B chain

Chain EH:



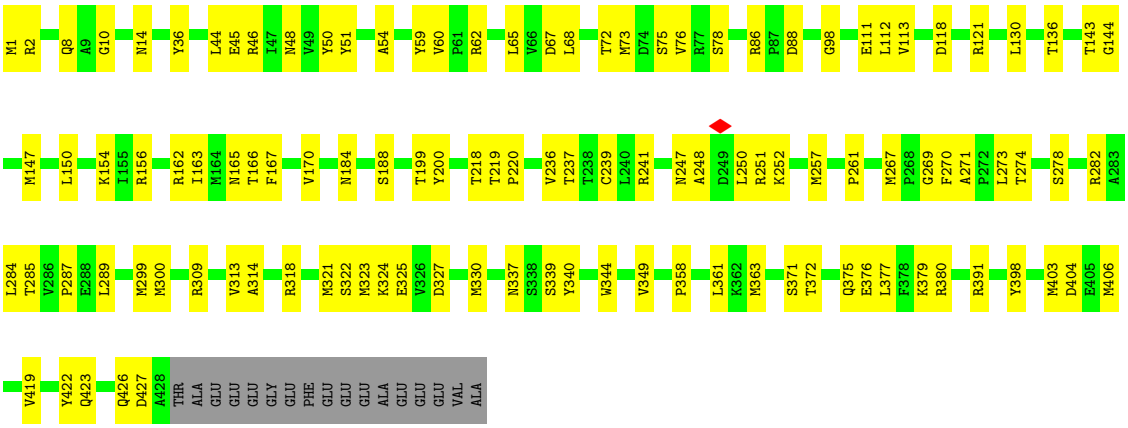
• Molecule 9: Tubulin beta-4B chain

Chain EJ:



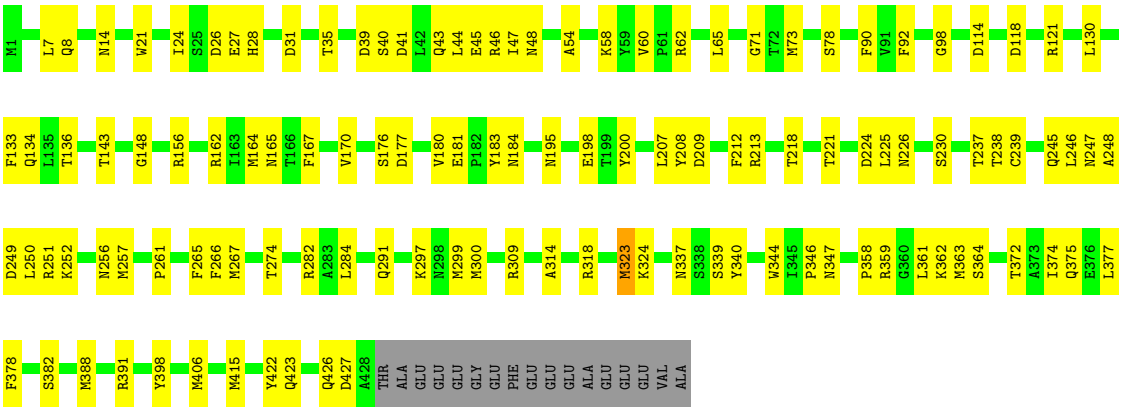
• Molecule 9: Tubulin beta-4B chain

Chain EL:



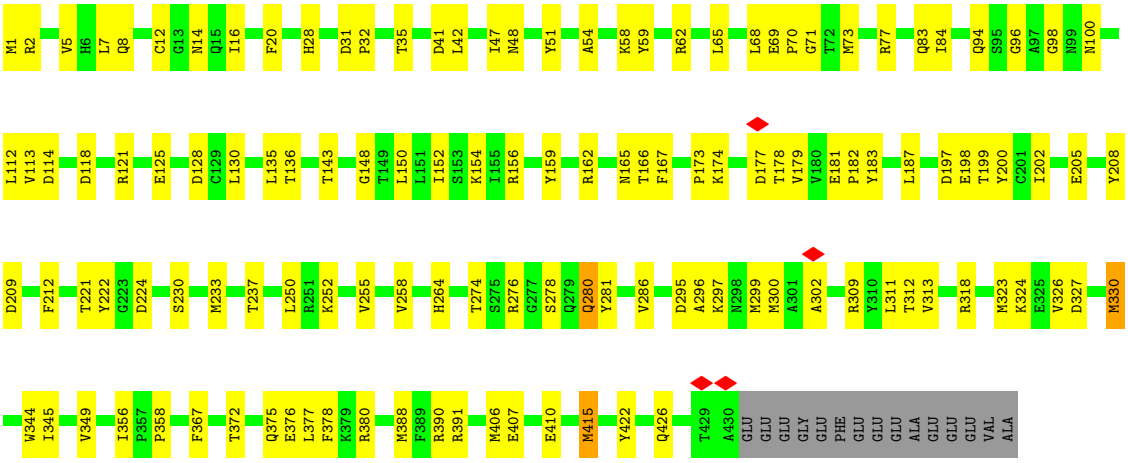
• Molecule 9: Tubulin beta-4B chain

Chain EN:



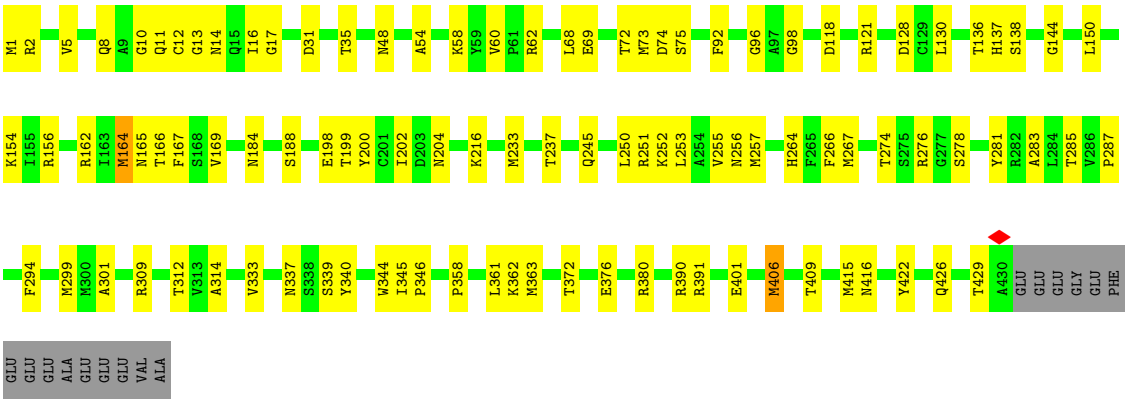
• Molecule 9: Tubulin beta-4B chain

Chain FB:



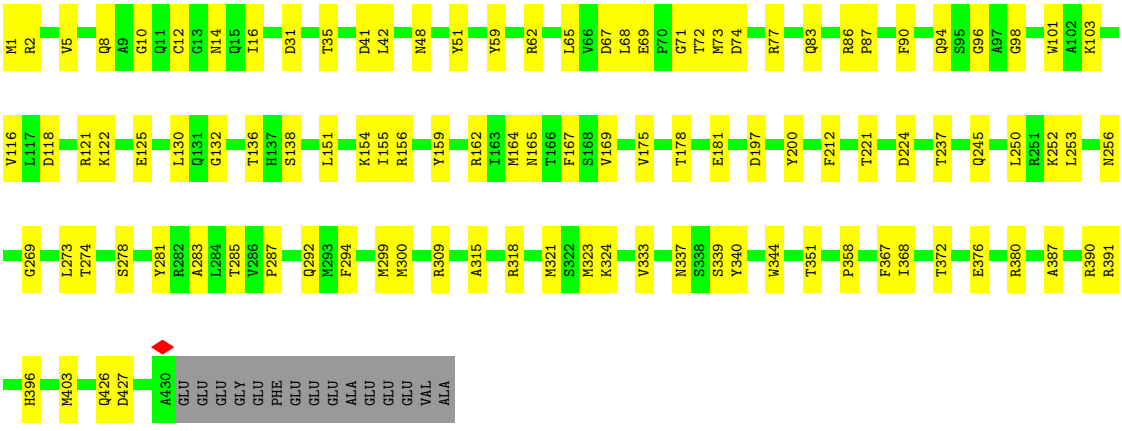
• Molecule 9: Tubulin beta-4B chain

Chain FD:



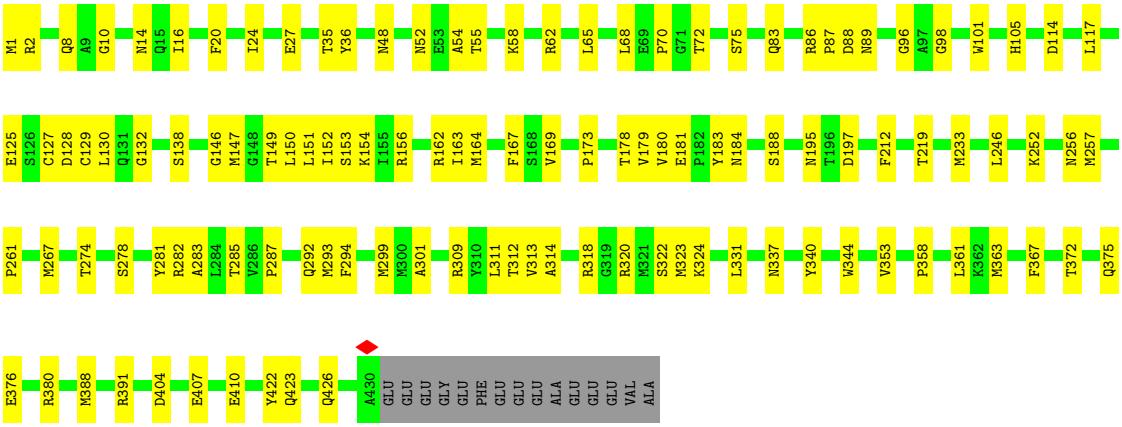
• Molecule 9: Tubulin beta-4B chain

Chain FF:



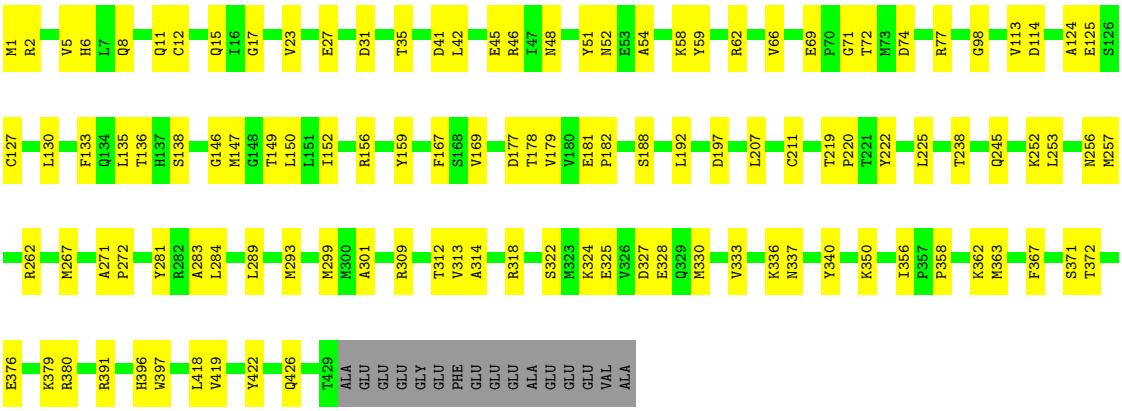
• Molecule 9: Tubulin beta-4B chain

Chain FH:



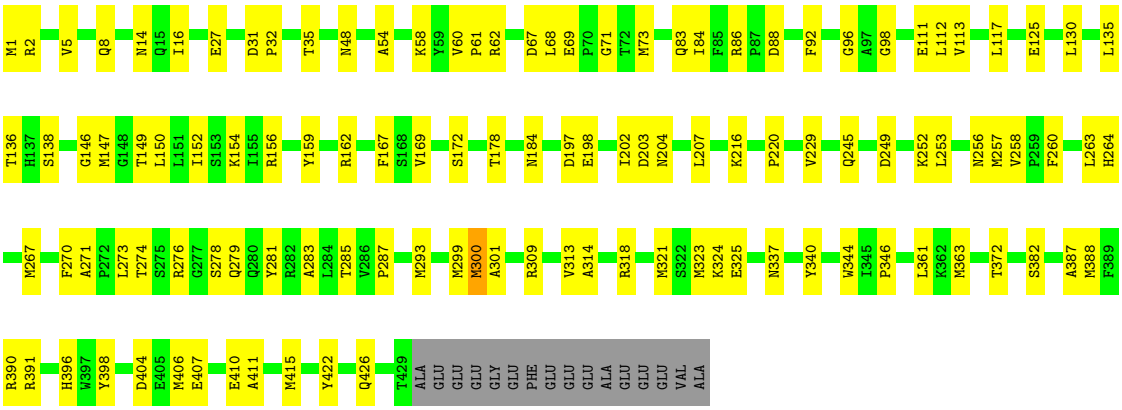
• Molecule 9: Tubulin beta-4B chain

Chain FJ:



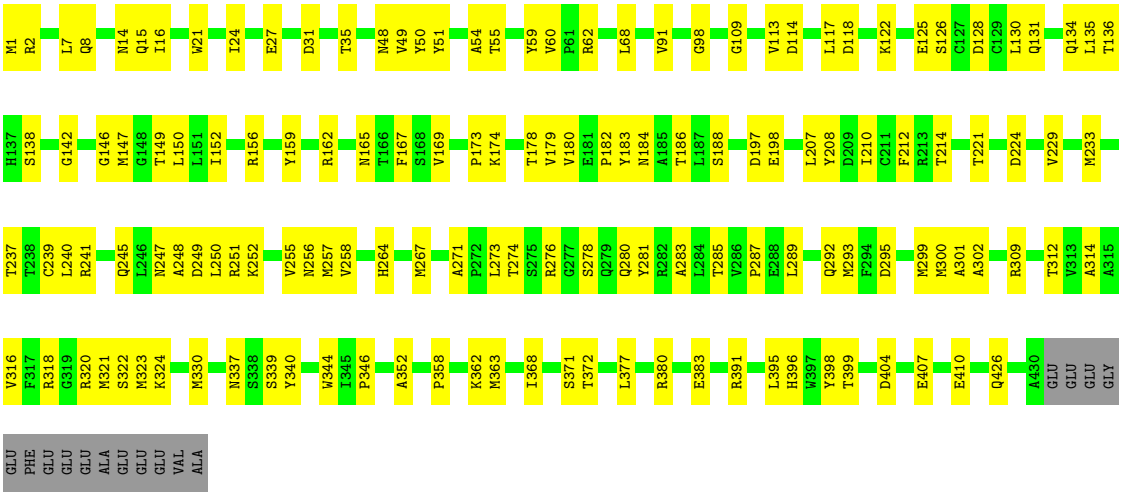
• Molecule 9: Tubulin beta-4B chain

Chain FL:



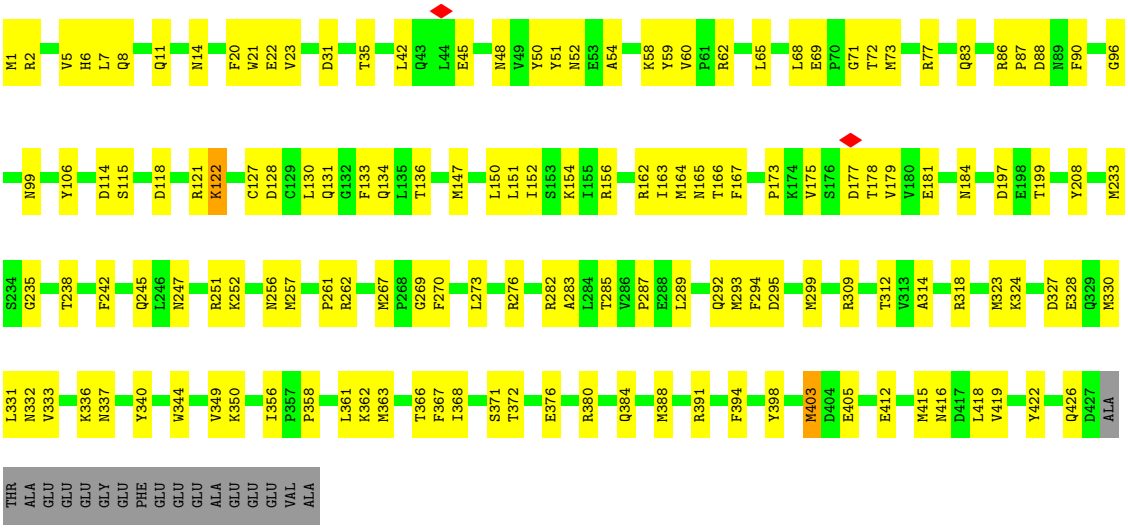
• Molecule 9: Tubulin beta-4B chain

Chain FN:



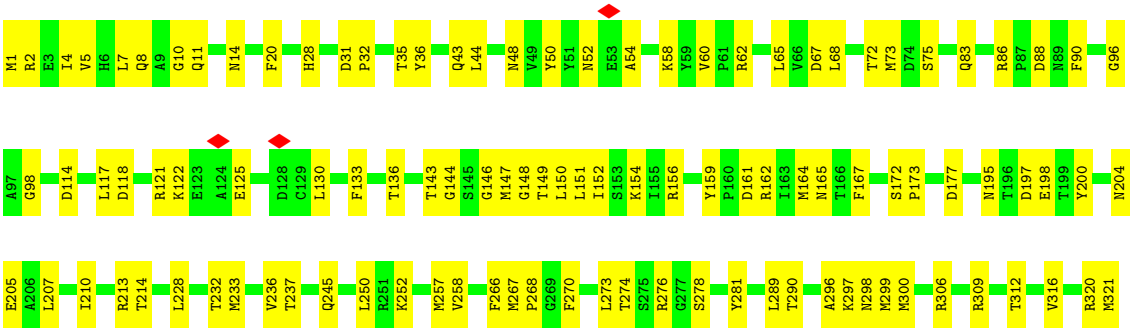
• Molecule 9: Tubulin beta-4B chain

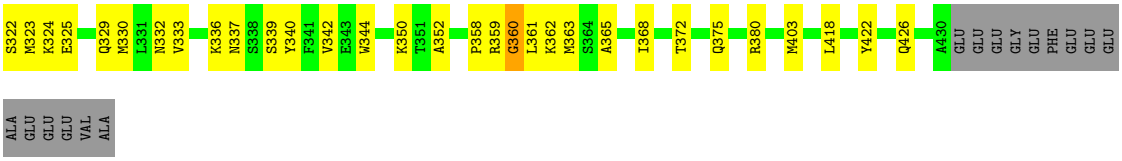
Chain GB:



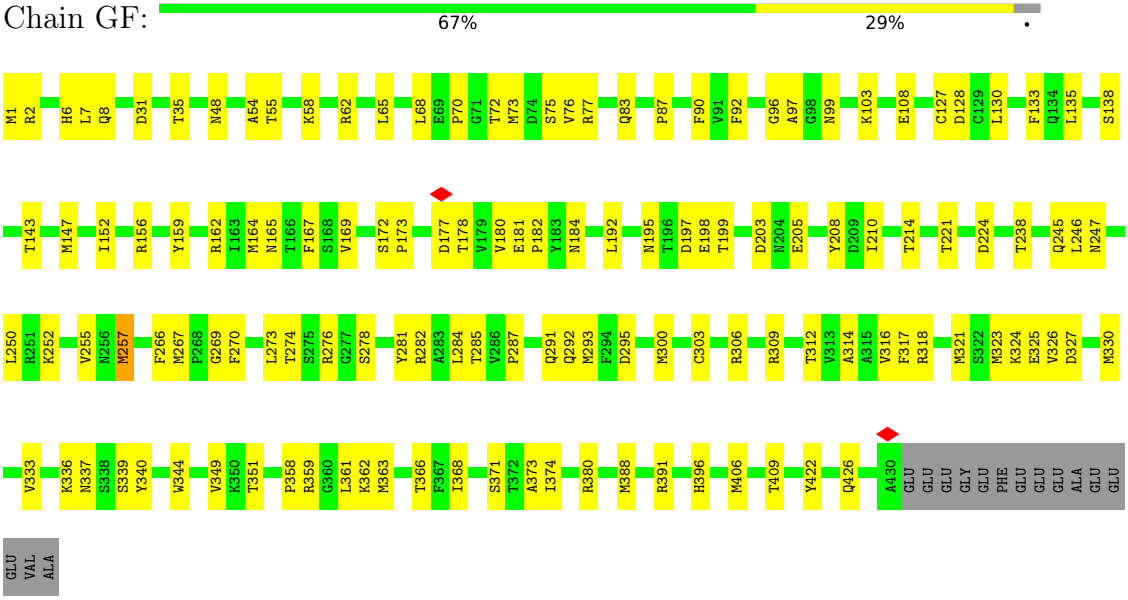
• Molecule 9: Tubulin beta-4B chain

Chain GD:

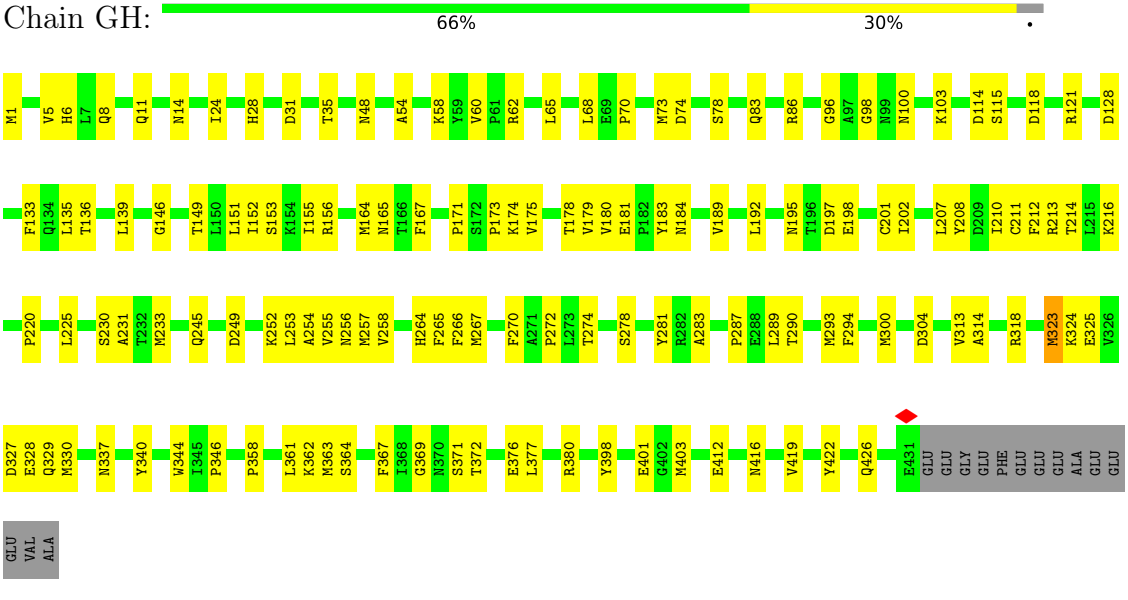




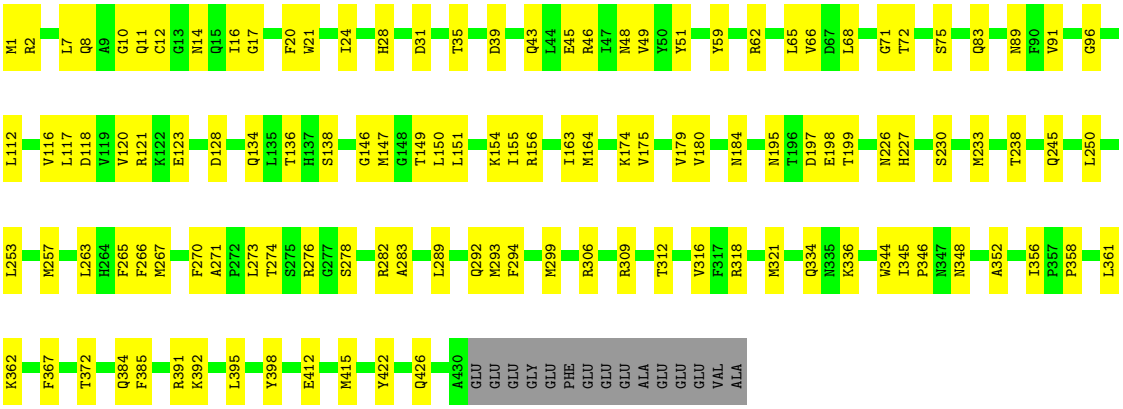
• Molecule 9: Tubulin beta-4B chain



• Molecule 9: Tubulin beta-4B chain

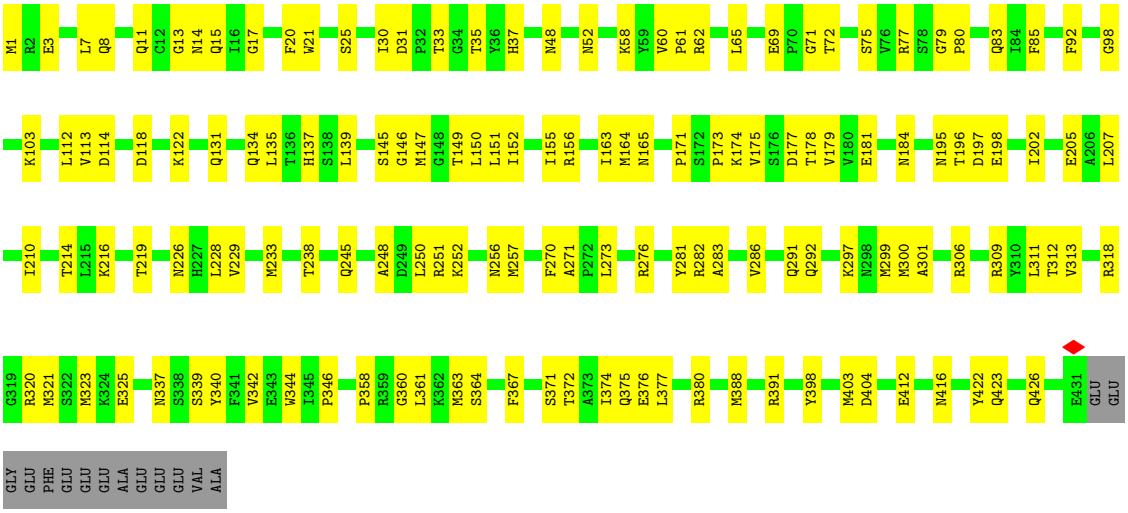


• Molecule 9: Tubulin beta-4B chain



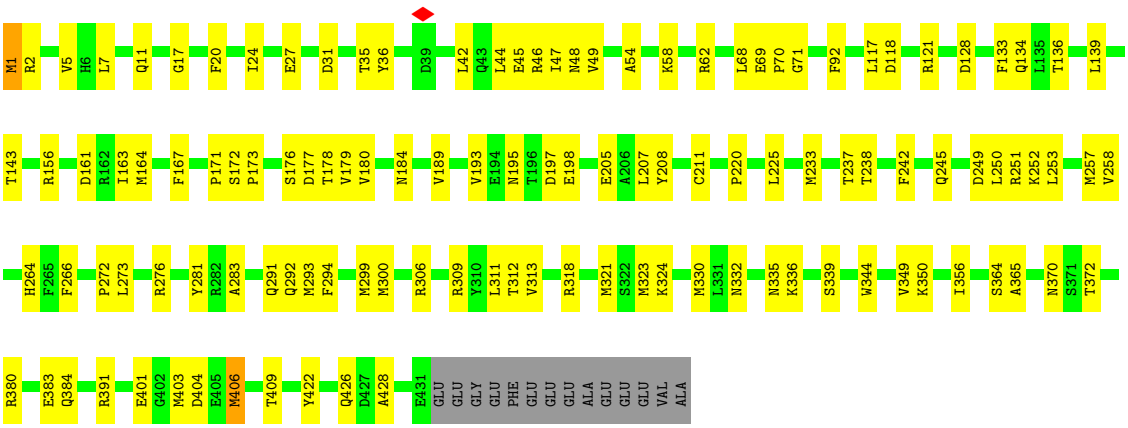
• Molecule 9: Tubulin beta-4B chain

Chain GL:



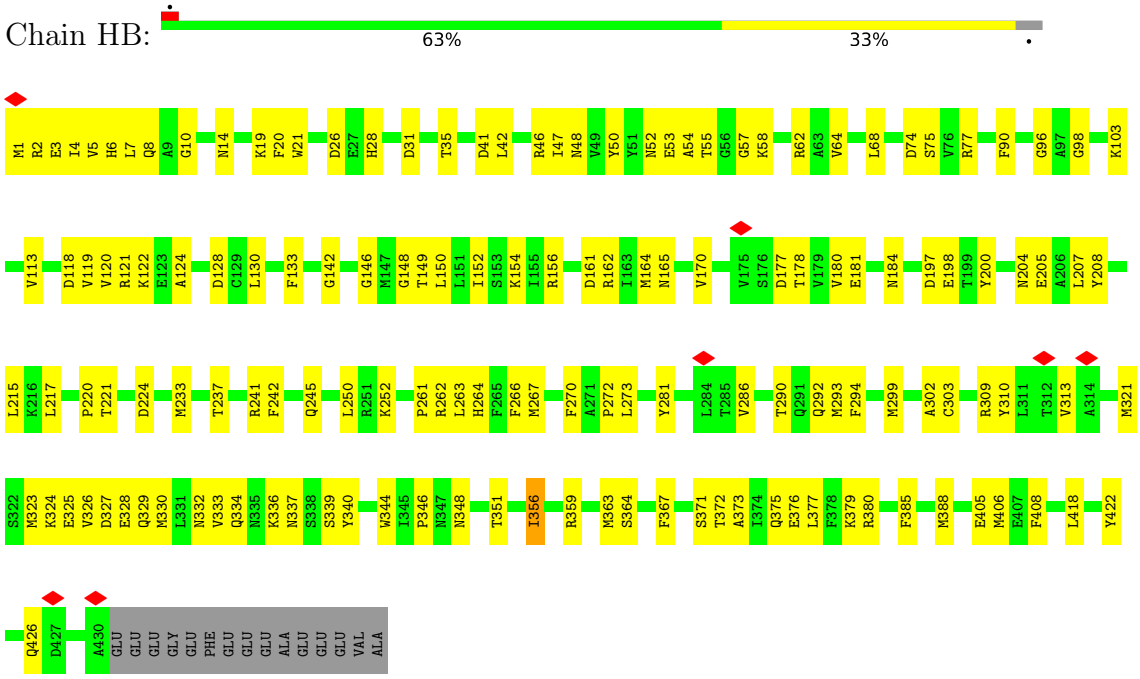
• Molecule 9: Tubulin beta-4B chain

Chain GN:



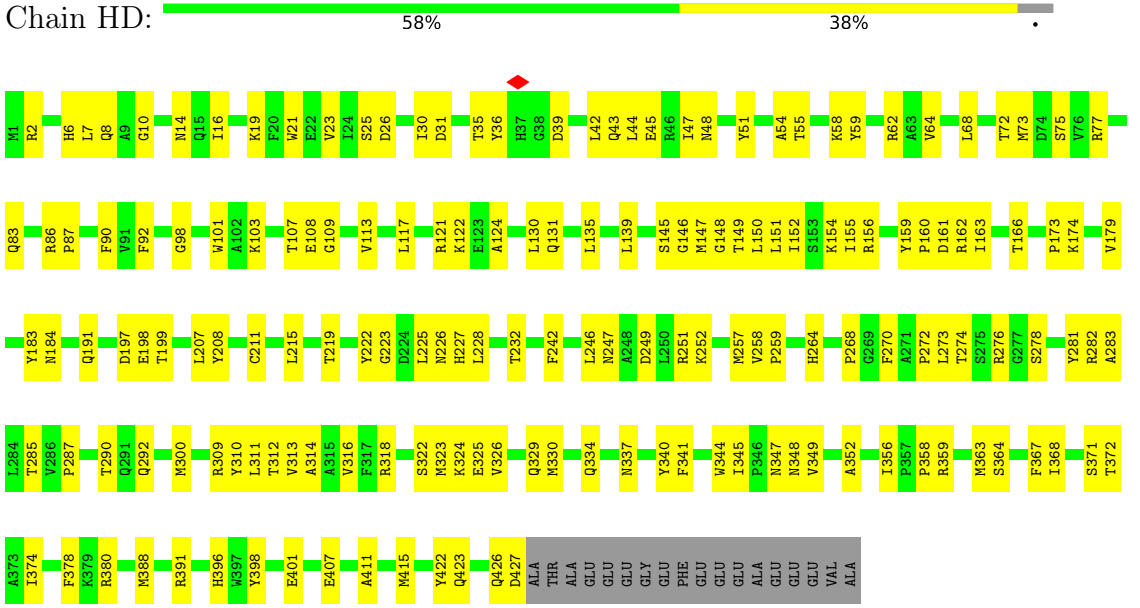
• Molecule 9: Tubulin beta-4B chain

Chain HB:



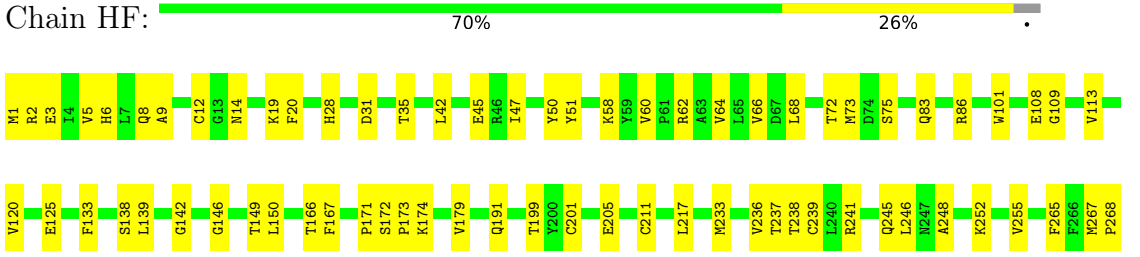
• Molecule 9: Tubulin beta-4B chain

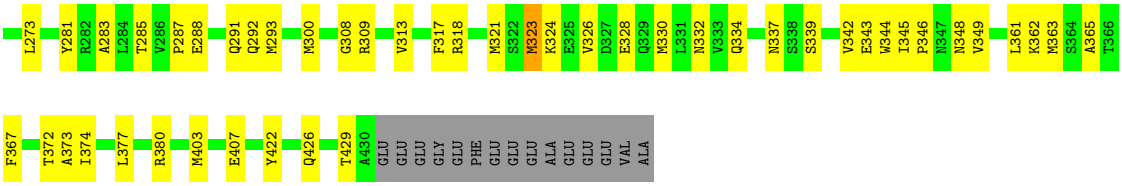
Chain HD:



• Molecule 9: Tubulin beta-4B chain

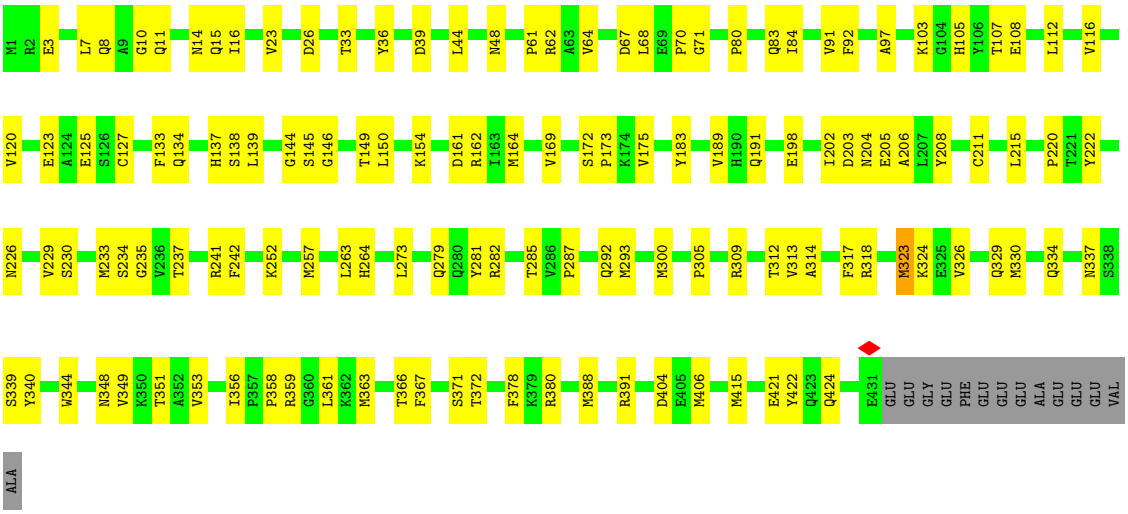
Chain HF:





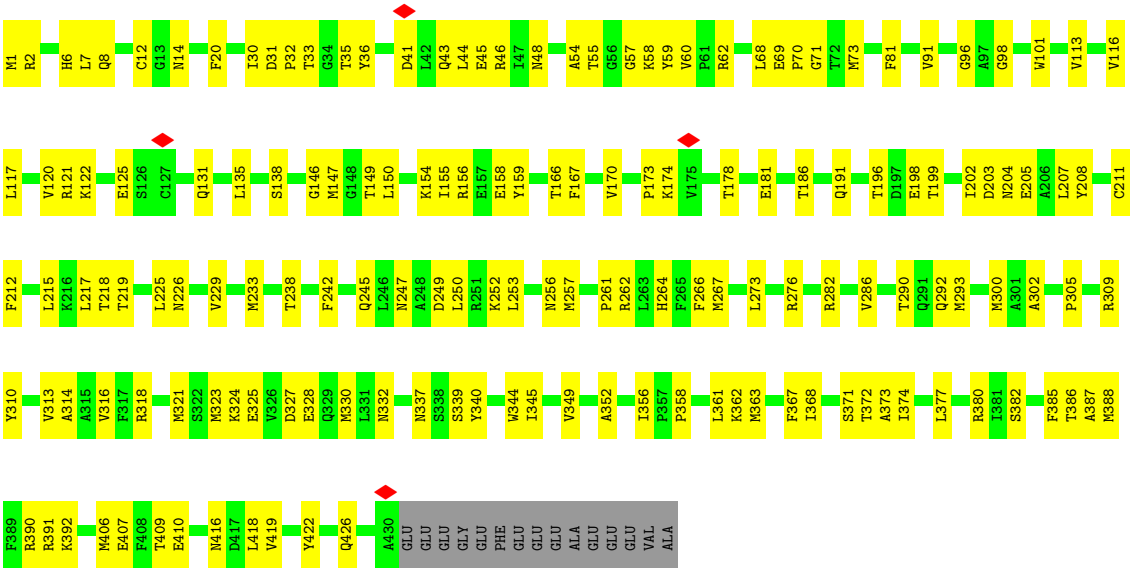
• Molecule 9: Tubulin beta-4B chain

Chain HH:



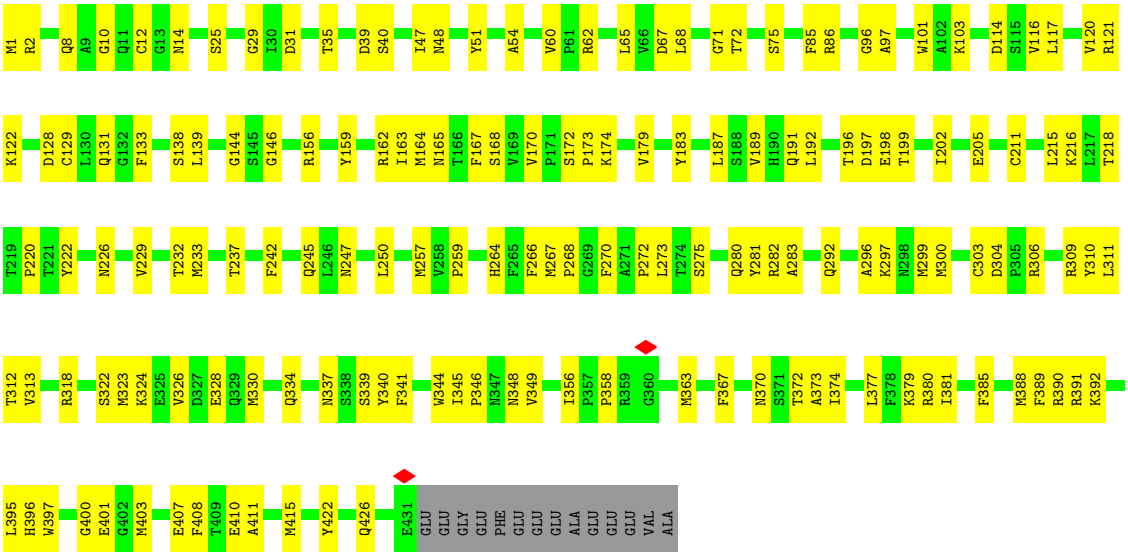
• Molecule 9: Tubulin beta-4B chain

Chain HJ:



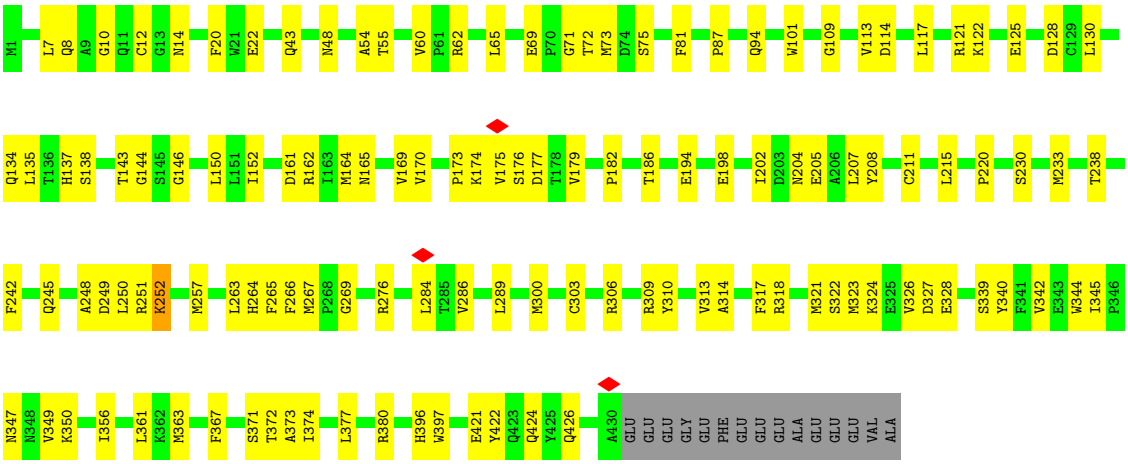
• Molecule 9: Tubulin beta-4B chain

Chain HL:



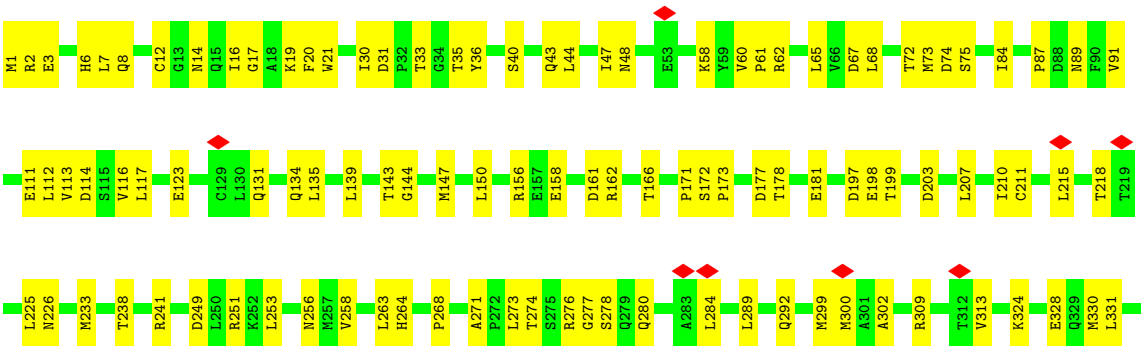
• Molecule 9: Tubulin beta-4B chain

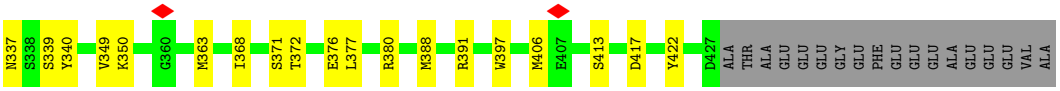
Chain HN:



• Molecule 9: Tubulin beta-4B chain

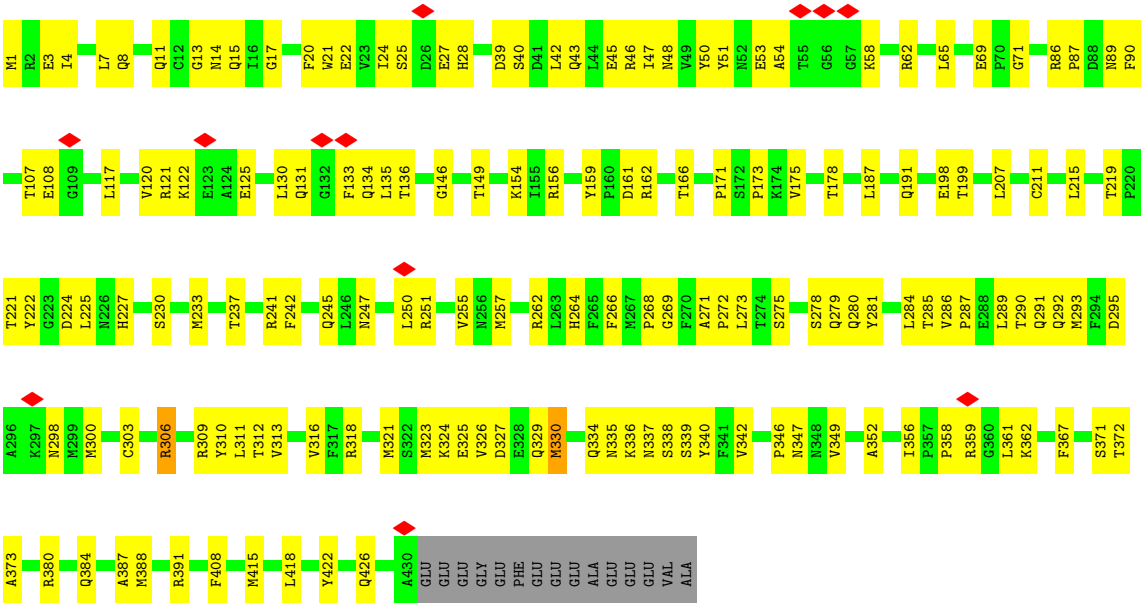
Chain HP:





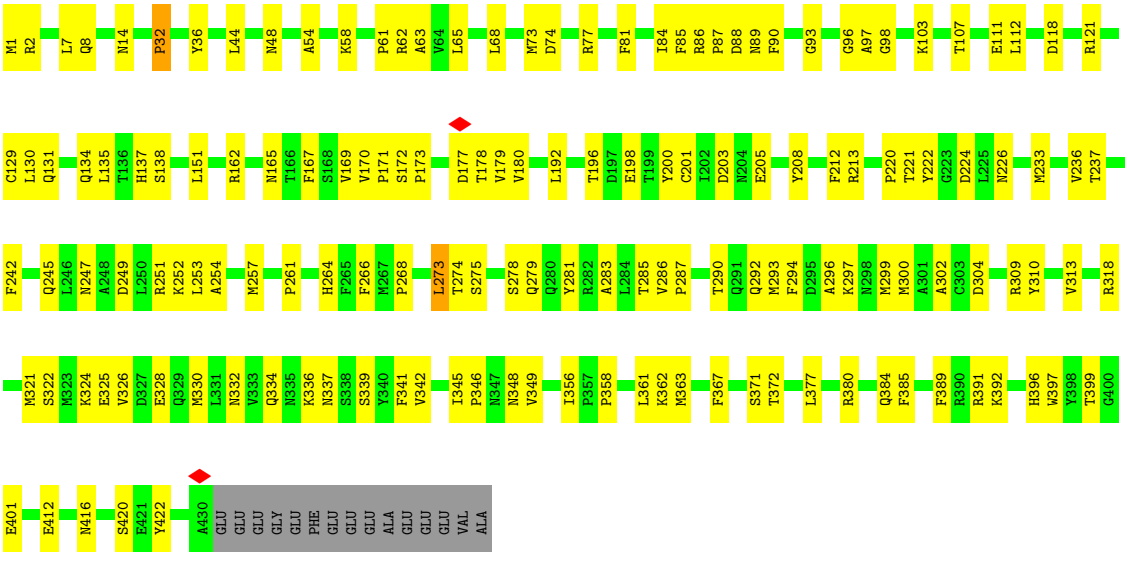
• Molecule 9: Tubulin beta-4B chain

Chain IB:



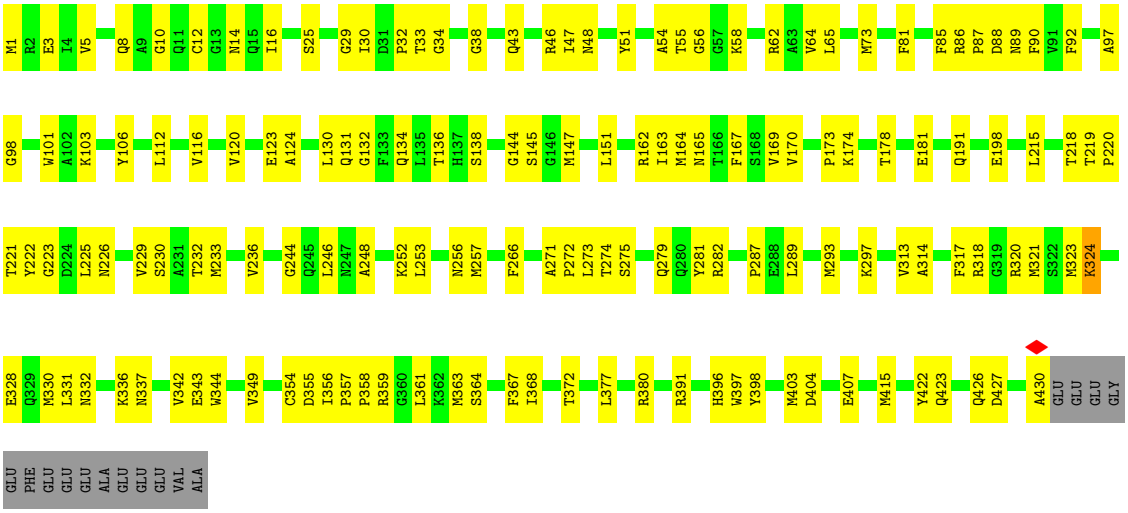
• Molecule 9: Tubulin beta-4B chain

Chain ID:



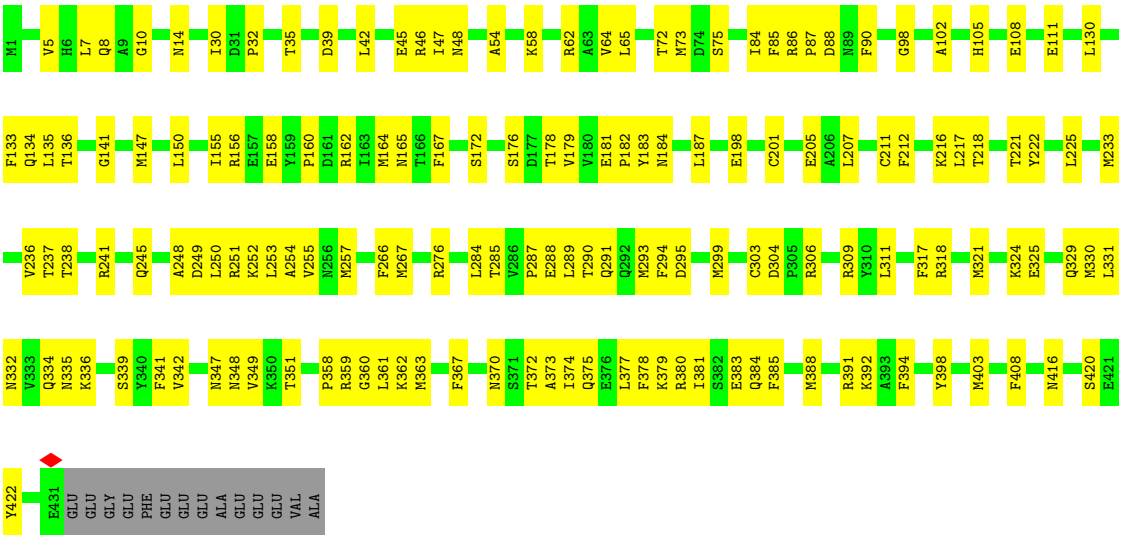
• Molecule 9: Tubulin beta-4B chain

Chain IF:



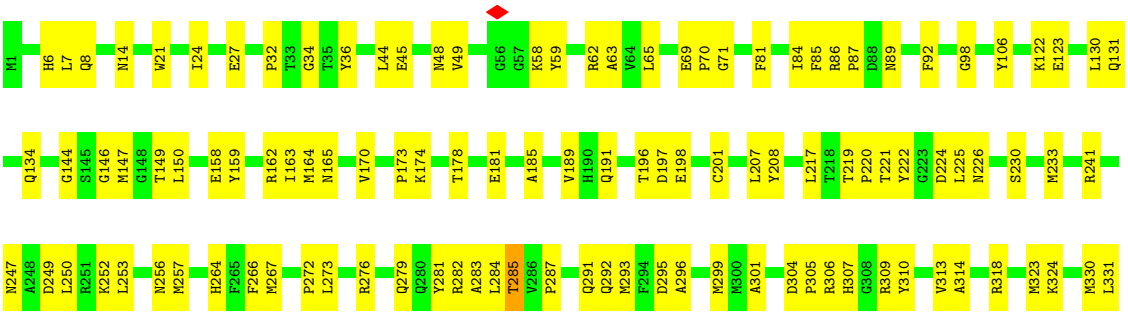
• Molecule 9: Tubulin beta-4B chain

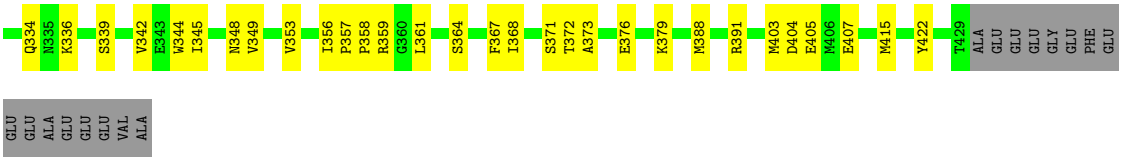
Chain IH:



• Molecule 9: Tubulin beta-4B chain

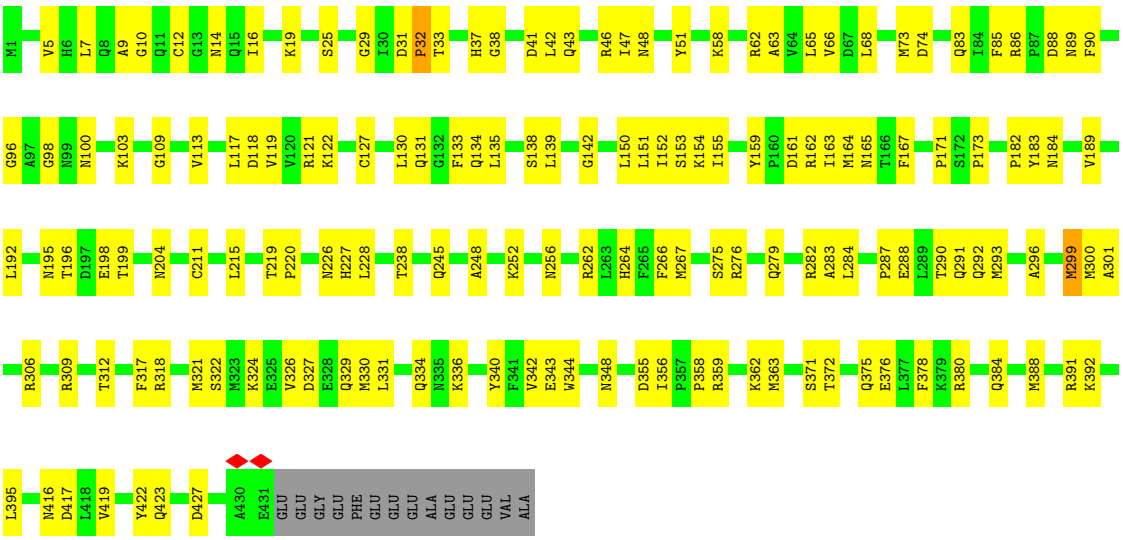
Chain IJ:





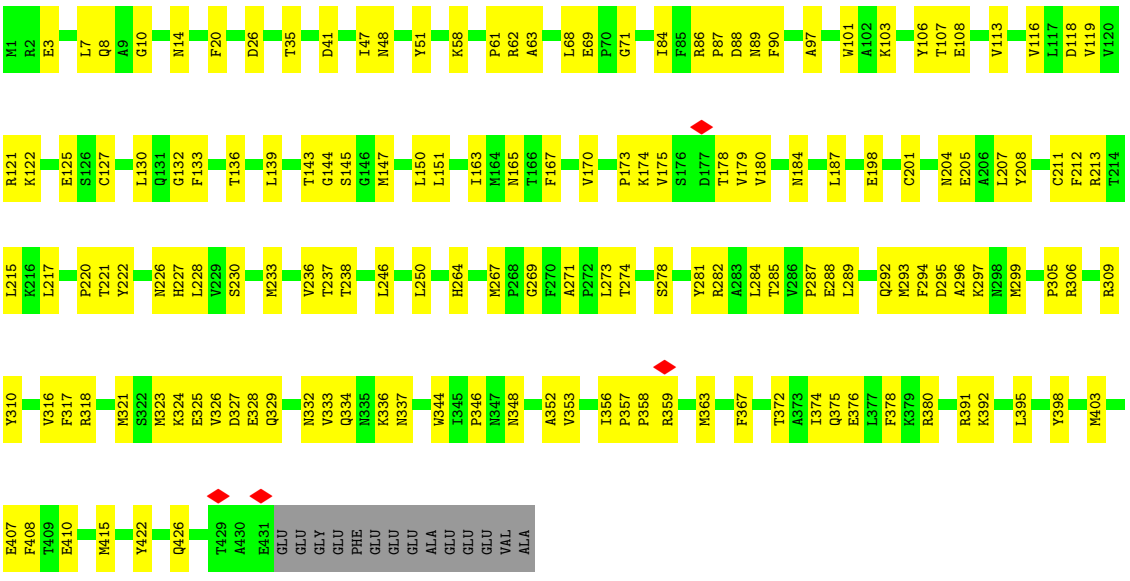
• Molecule 9: Tubulin beta-4B chain

Chain IL:



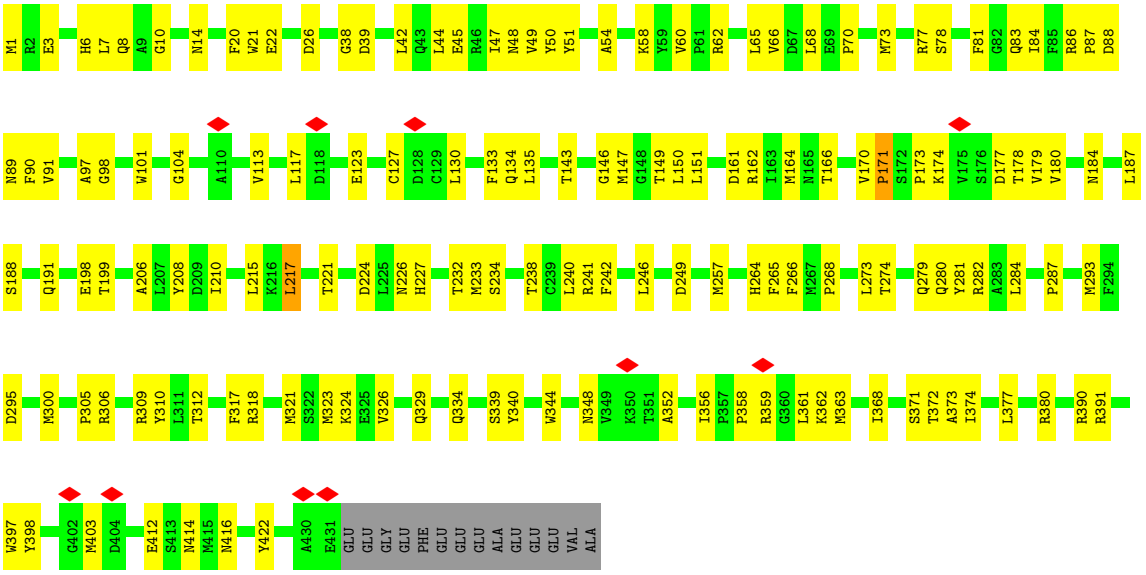
• Molecule 9: Tubulin beta-4B chain

Chain IN:



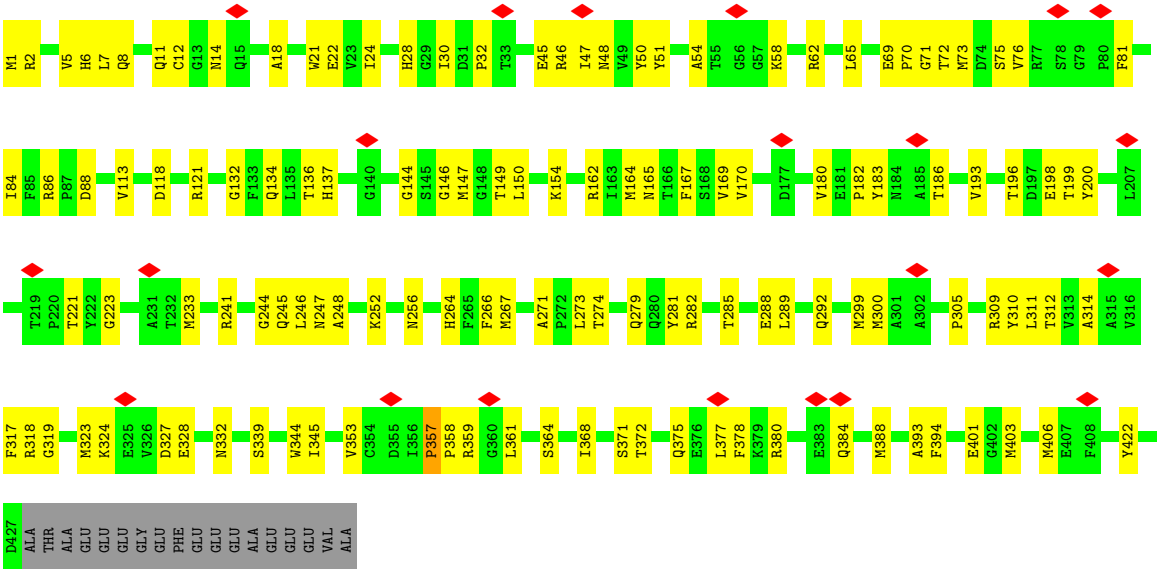
• Molecule 9: Tubulin beta-4B chain

Chain IP:



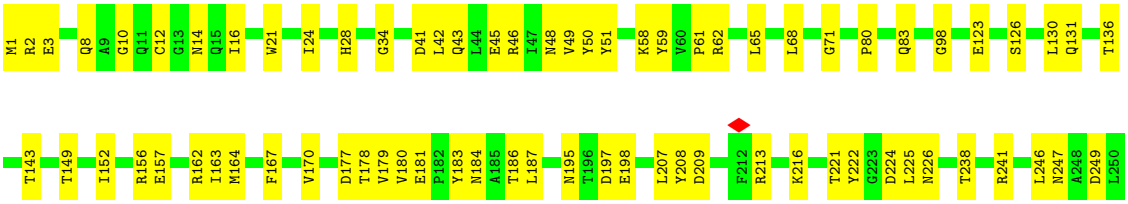
• Molecule 9: Tubulin beta-4B chain

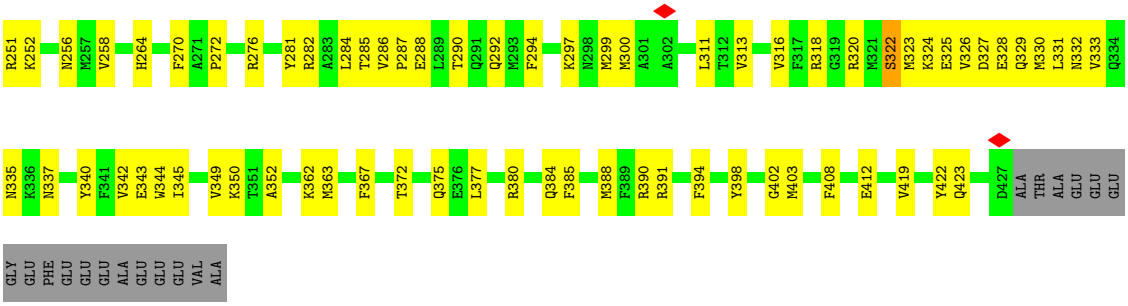
Chain JB:



• Molecule 9: Tubulin beta-4B chain

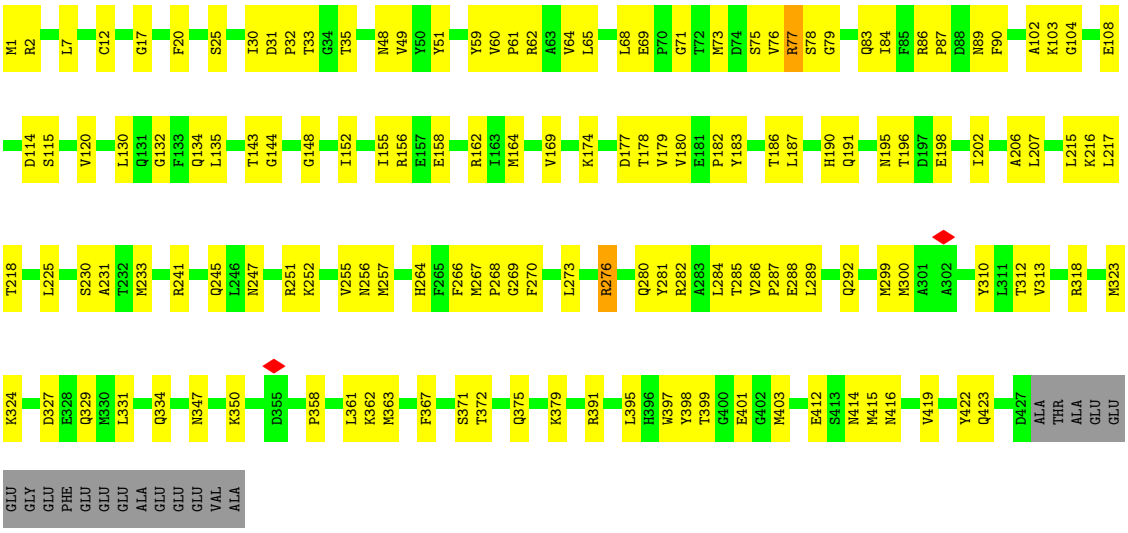
Chain JD:





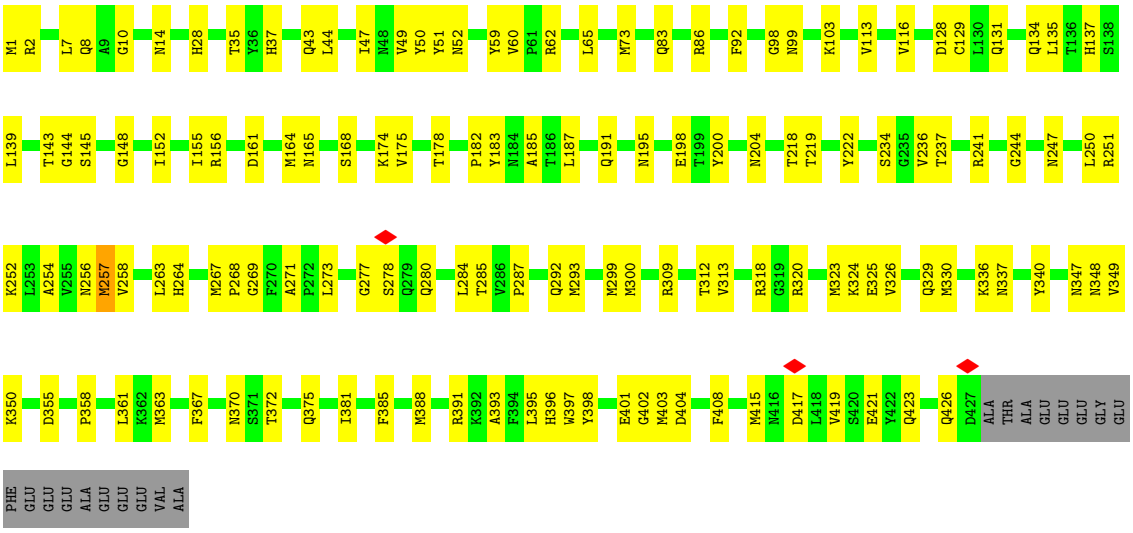
• Molecule 9: Tubulin beta-4B chain

Chain JF:



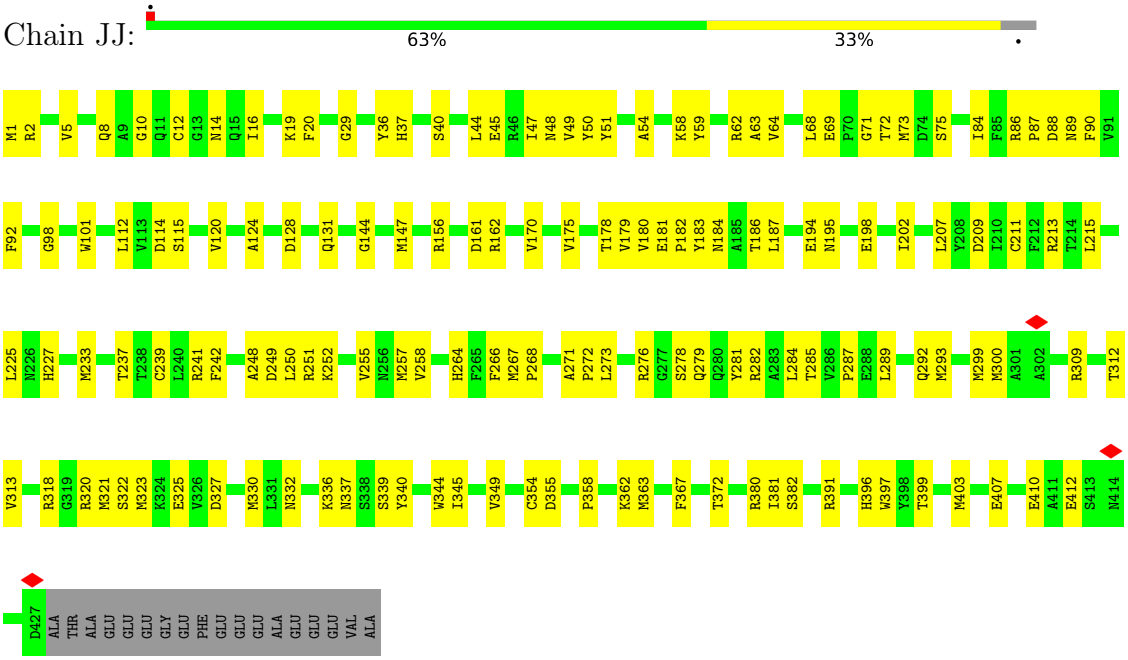
• Molecule 9: Tubulin beta-4B chain

Chain JH:



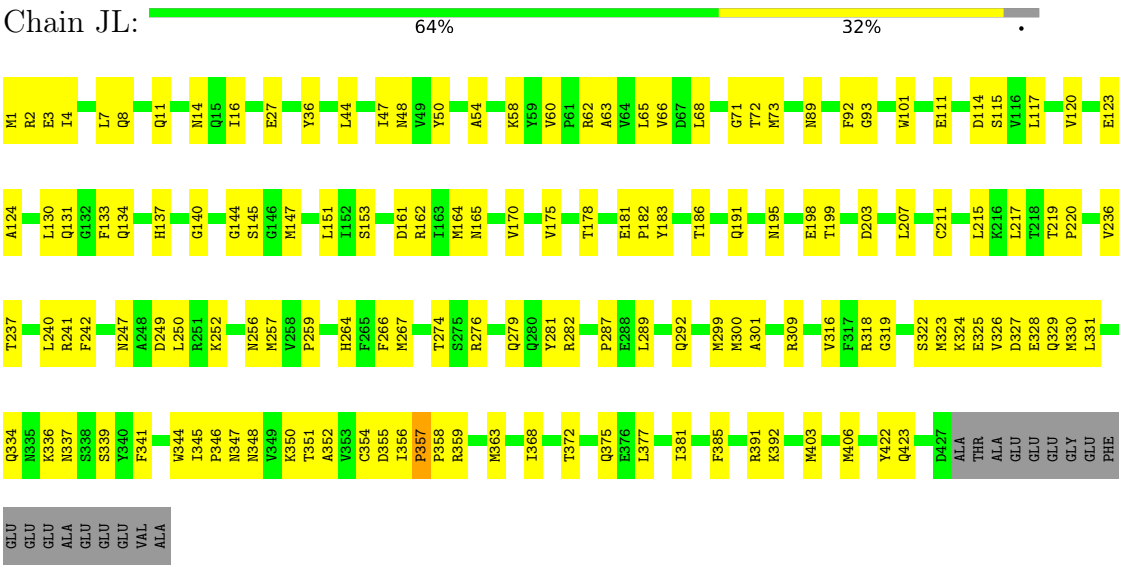
• Molecule 9: Tubulin beta-4B chain

Chain JJ:



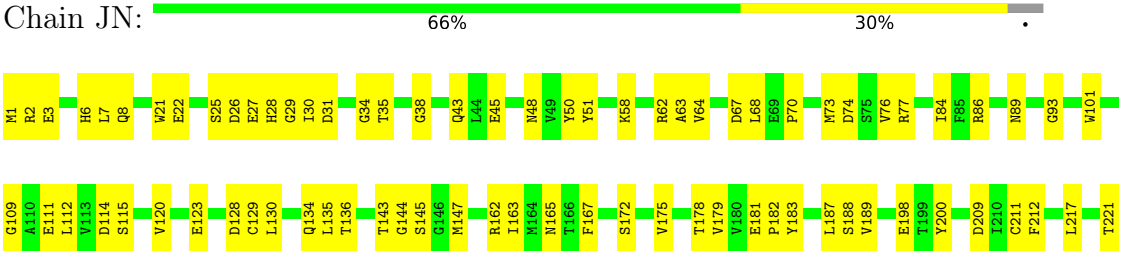
• Molecule 9: Tubulin beta-4B chain

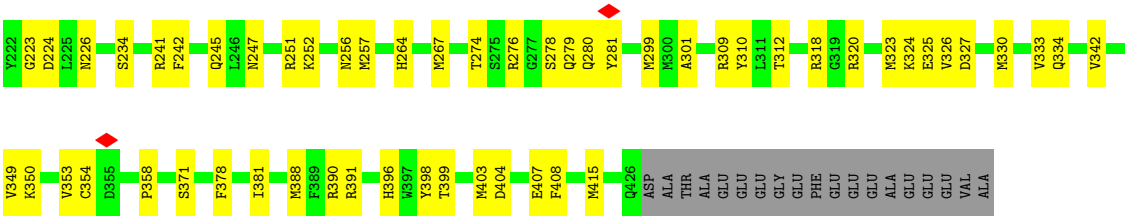
Chain JL:



• Molecule 9: Tubulin beta-4B chain

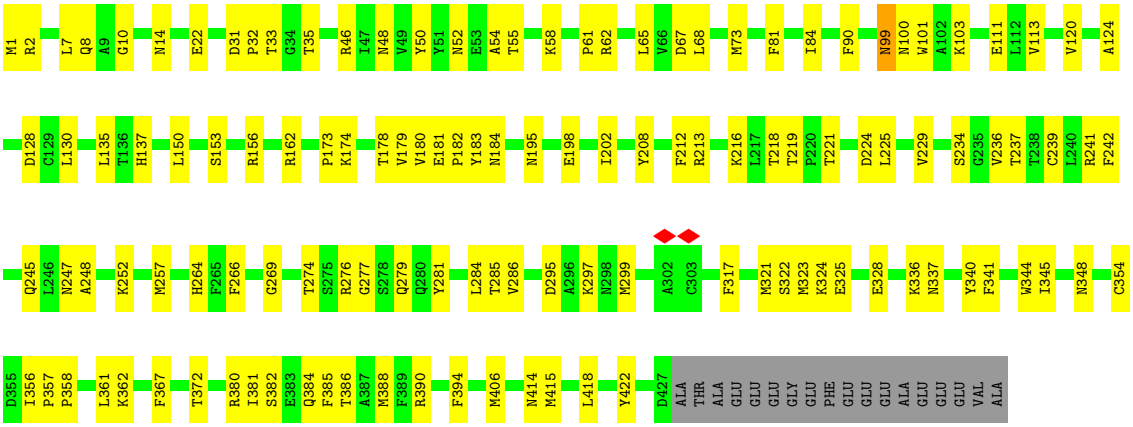
Chain JN:





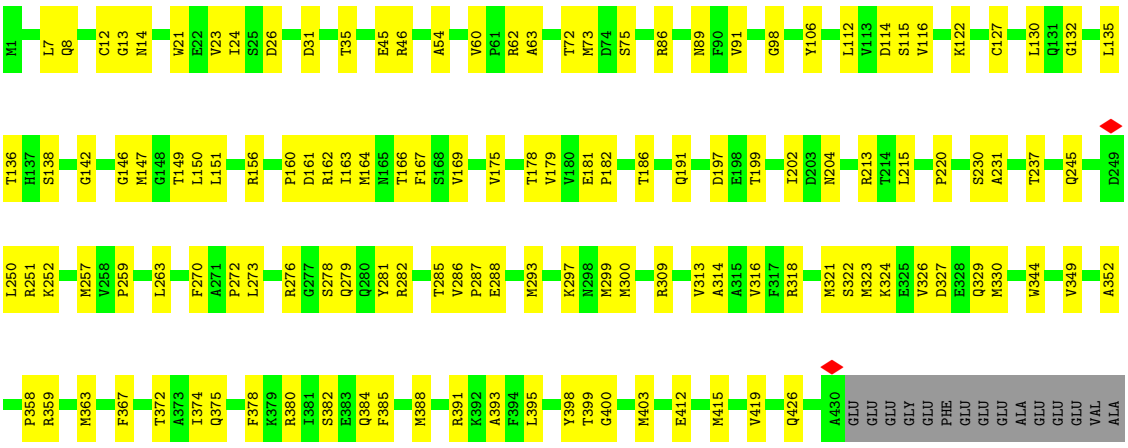
• Molecule 9: Tubulin beta-4B chain

Chain JP:



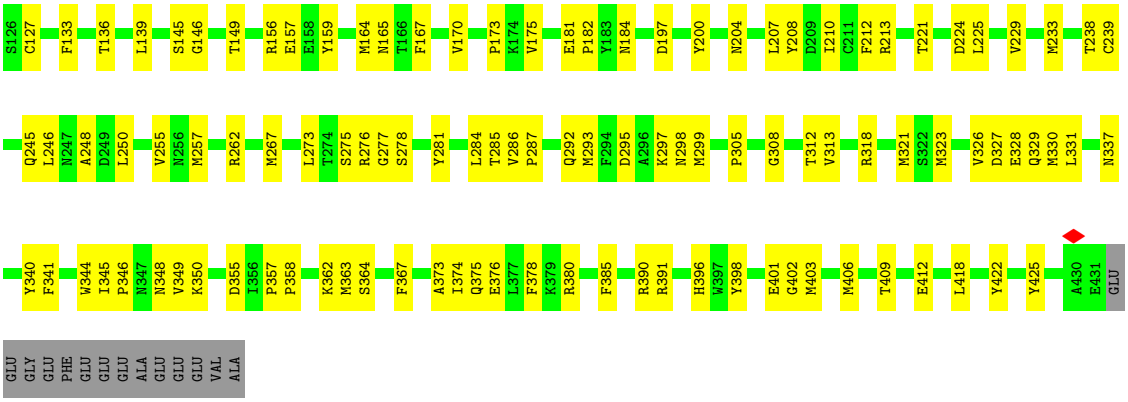
• Molecule 9: Tubulin beta-4B chain

Chain KB:



• Molecule 9: Tubulin beta-4B chain

Chain KD:

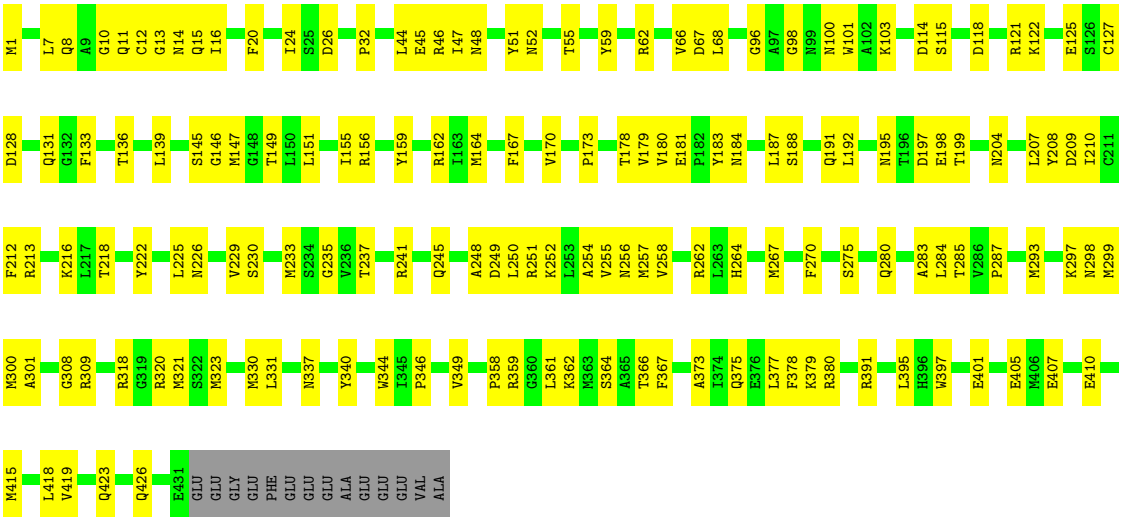


• Molecule 9: Tubulin beta-4B chain

Chain KF:

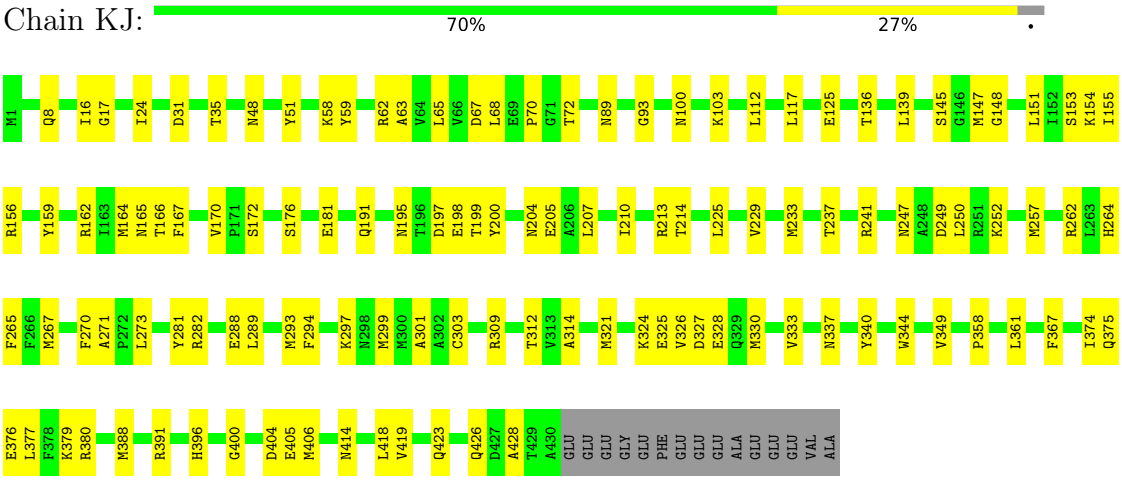
• Molecule 9: Tubulin beta-4B chain

Chain KH:



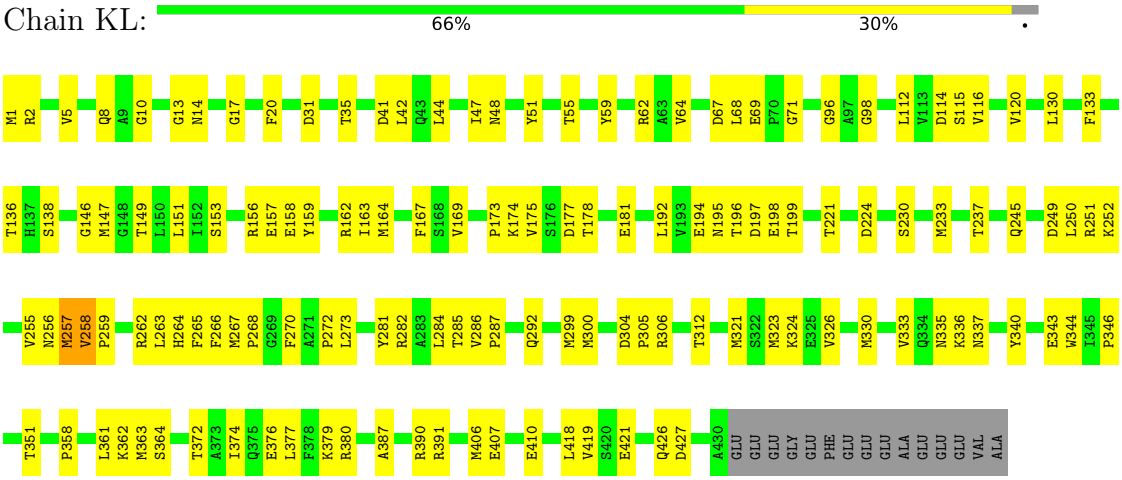
• Molecule 9: Tubulin beta-4B chain

Chain KJ:



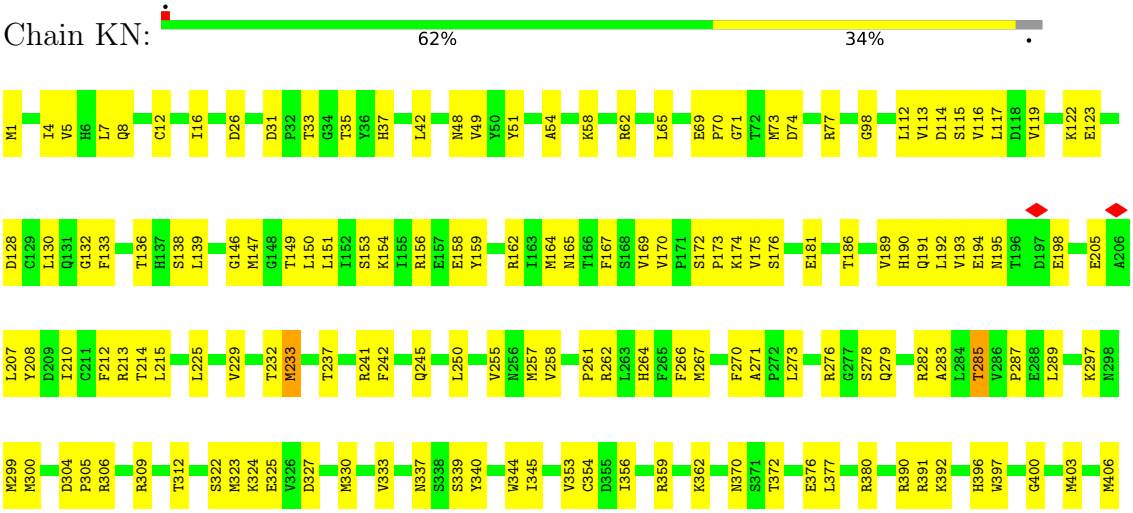
• Molecule 9: Tubulin beta-4B chain

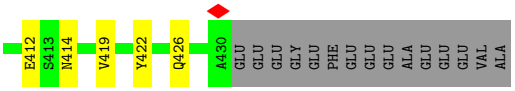
Chain KL:



• Molecule 9: Tubulin beta-4B chain

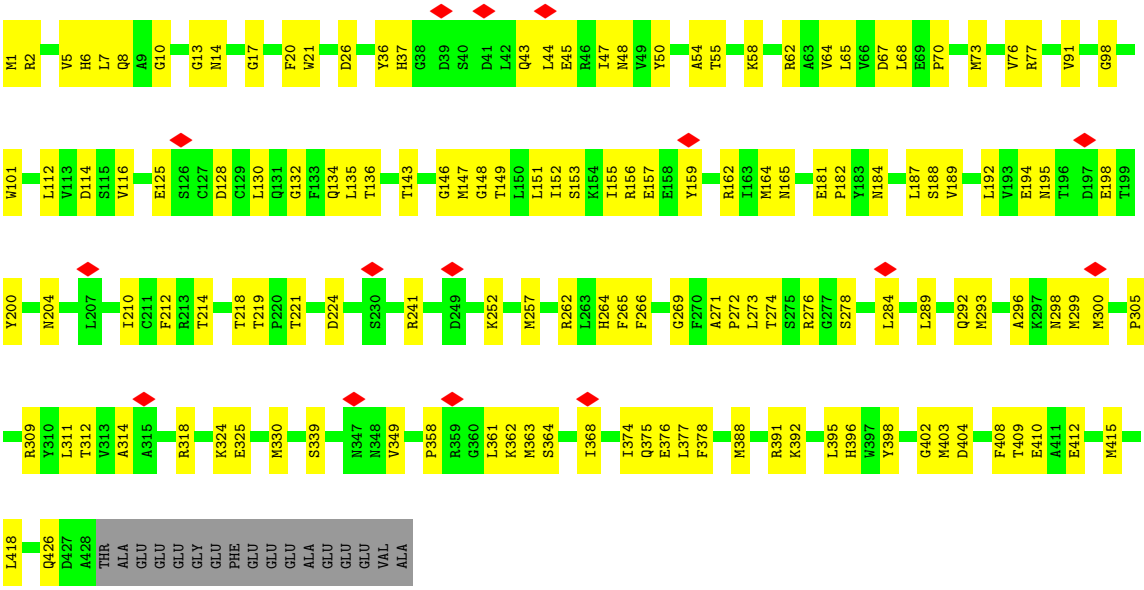
Chain KN:





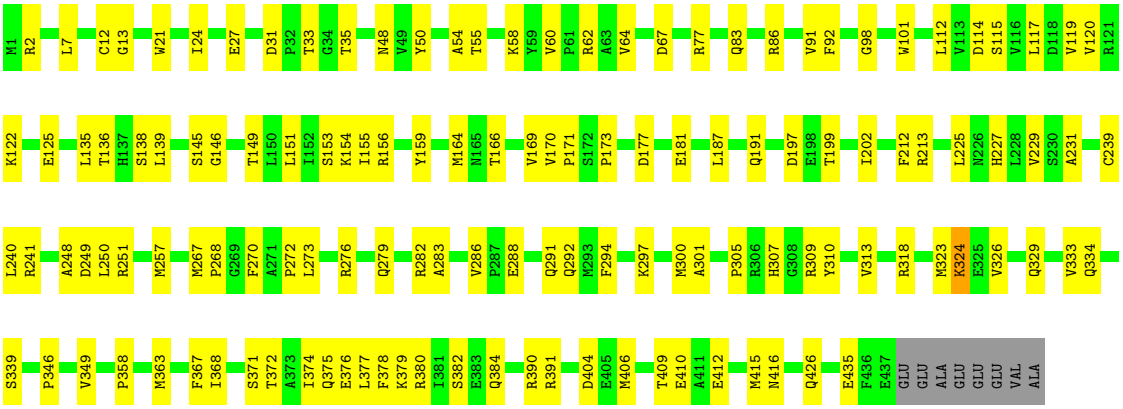
• Molecule 9: Tubulin beta-4B chain

Chain KP:



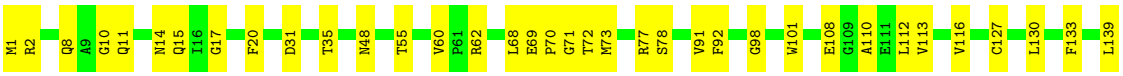
• Molecule 9: Tubulin beta-4B chain

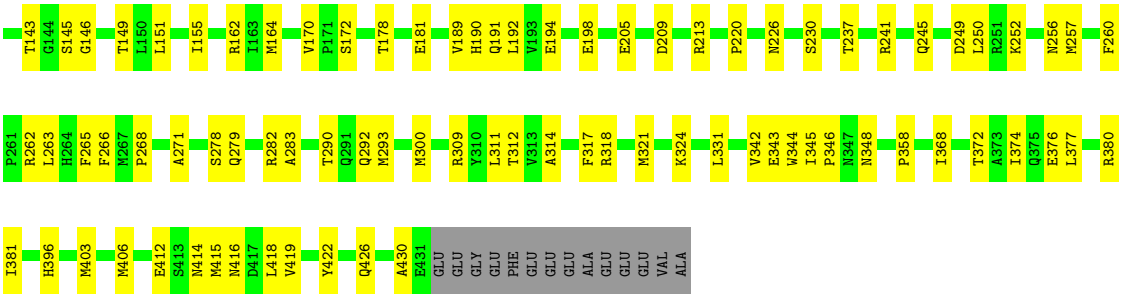
Chain LB:



• Molecule 9: Tubulin beta-4B chain

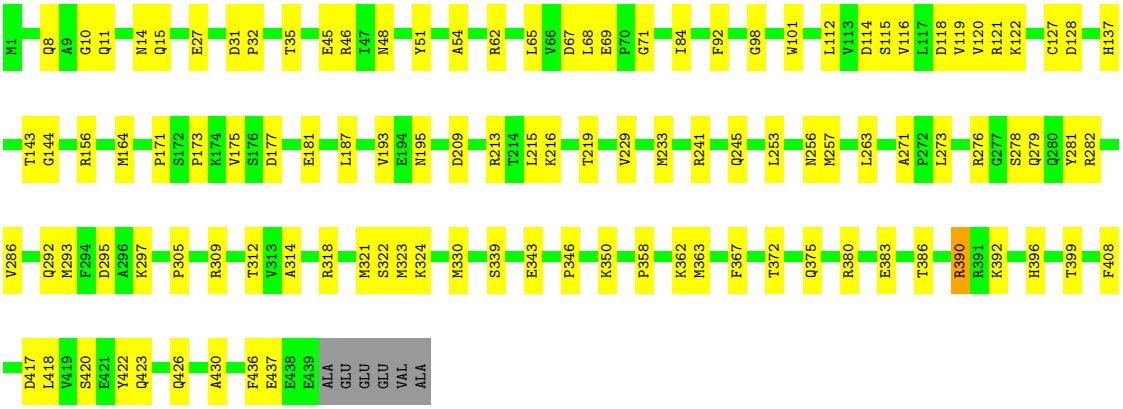
Chain LD:





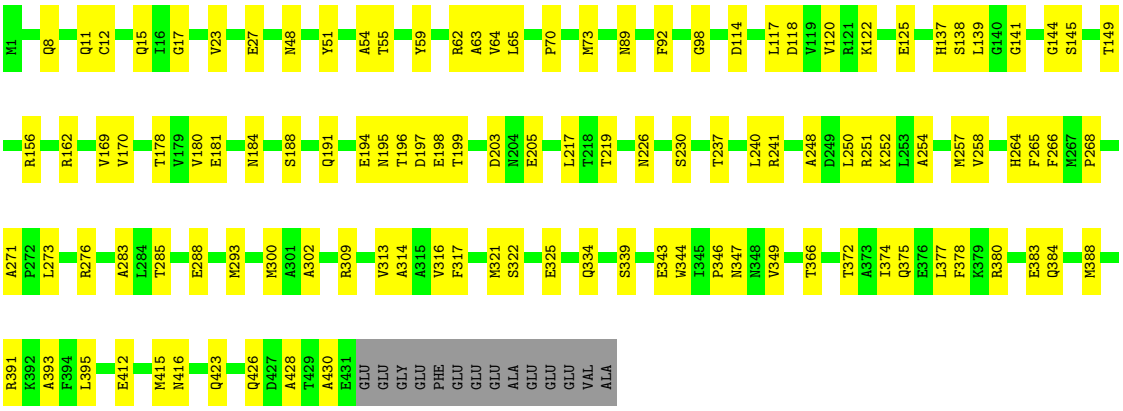
• Molecule 9: Tubulin beta-4B chain

Chain LF:



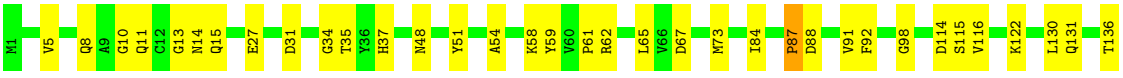
• Molecule 9: Tubulin beta-4B chain

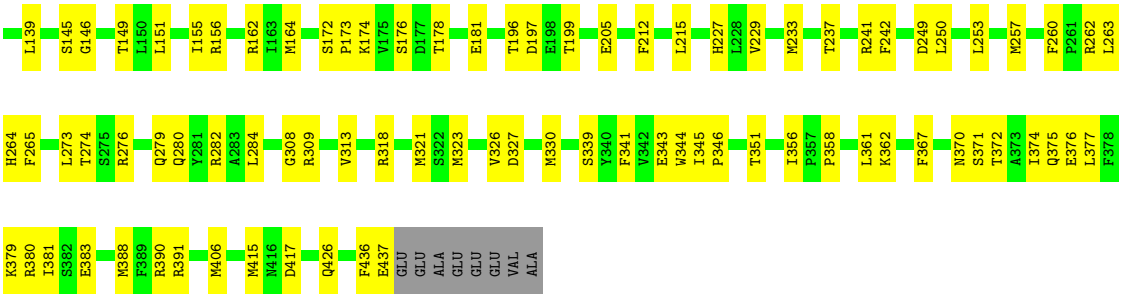
Chain LH:



• Molecule 9: Tubulin beta-4B chain

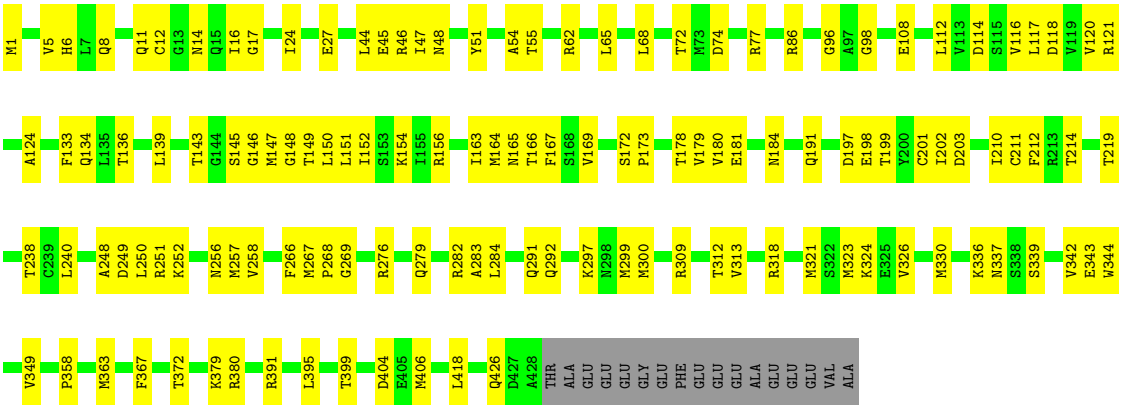
Chain LJ:





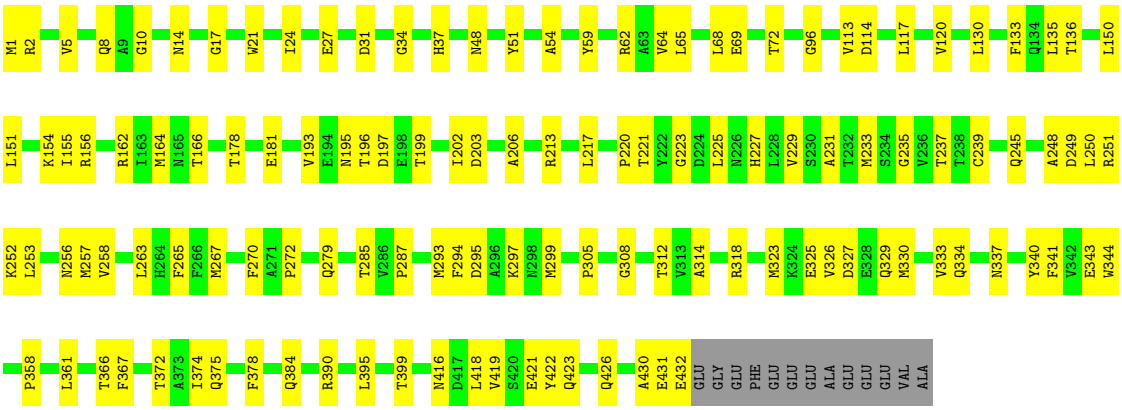
• Molecule 9: Tubulin beta-4B chain

Chain LL:



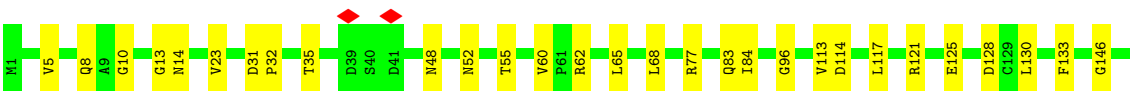
• Molecule 9: Tubulin beta-4B chain

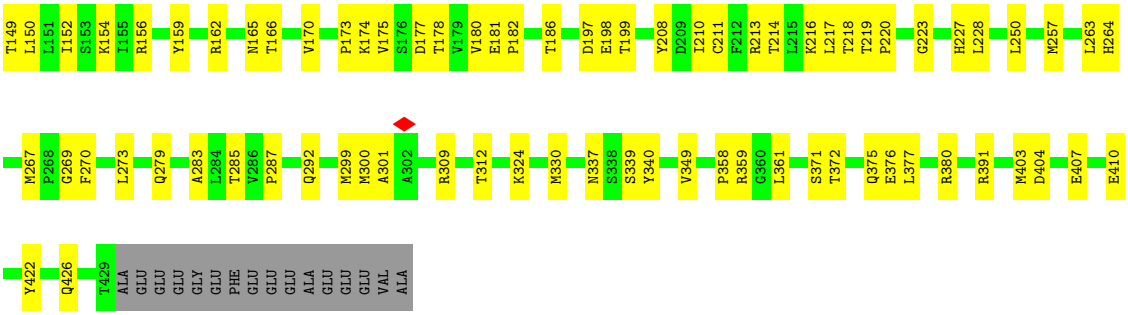
Chain LN:



• Molecule 9: Tubulin beta-4B chain

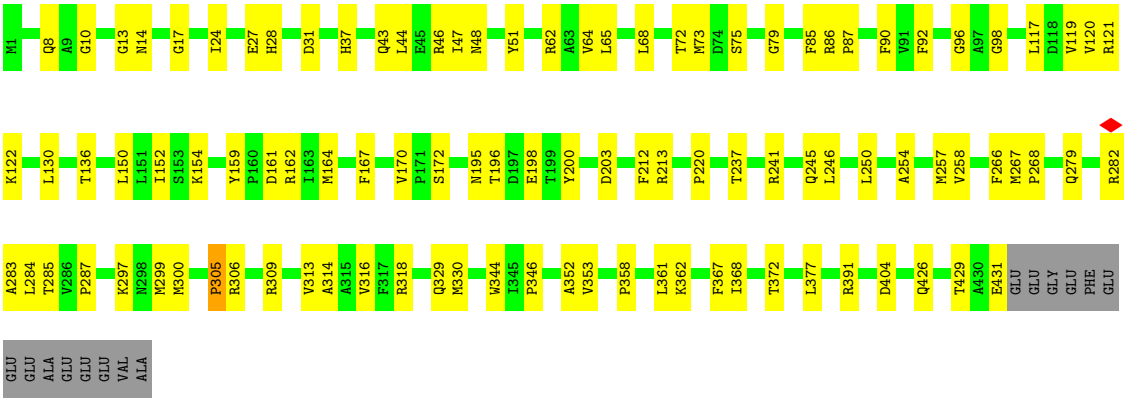
Chain LP:





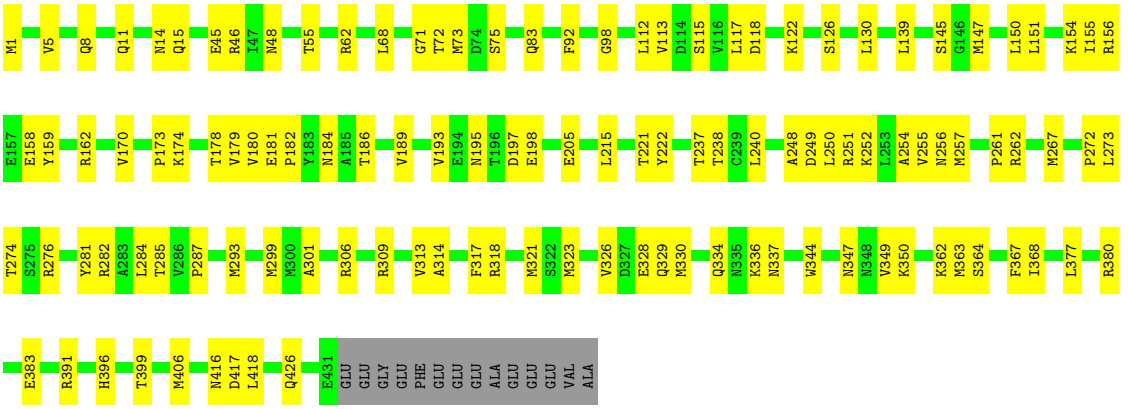
• Molecule 9: Tubulin beta-4B chain

Chain MB:



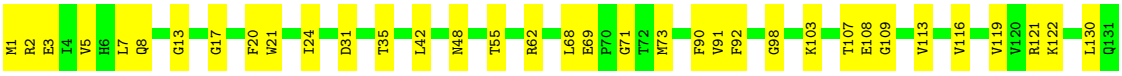
• Molecule 9: Tubulin beta-4B chain

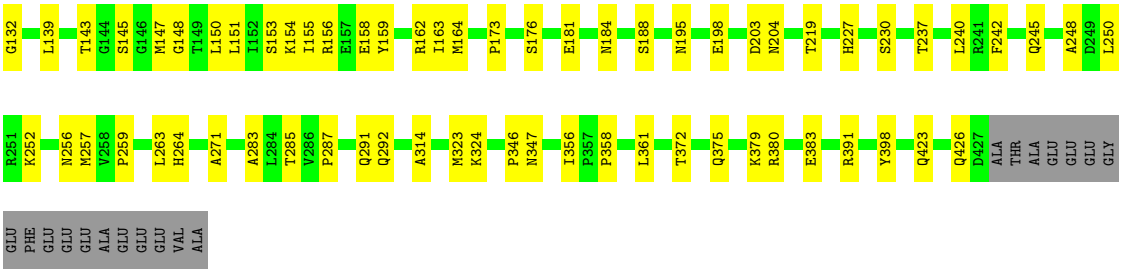
Chain MD:



• Molecule 9: Tubulin beta-4B chain

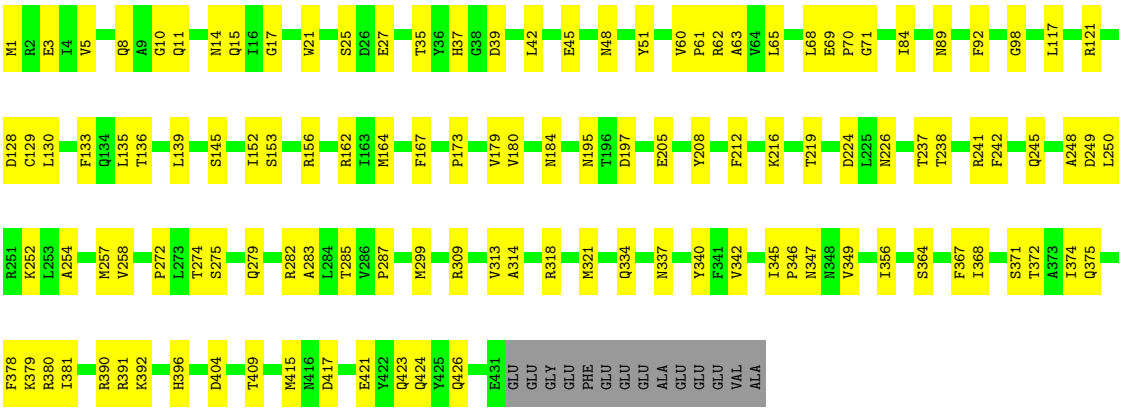
Chain MF:





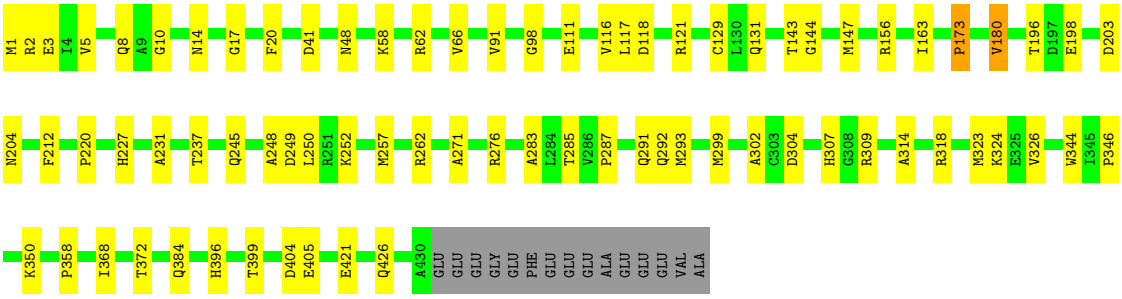
• Molecule 9: Tubulin beta-4B chain

Chain MH:



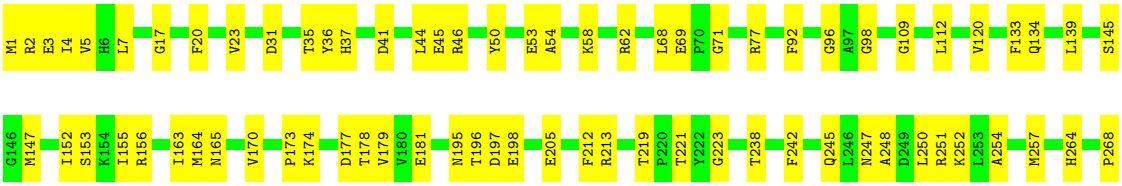
• Molecule 9: Tubulin beta-4B chain

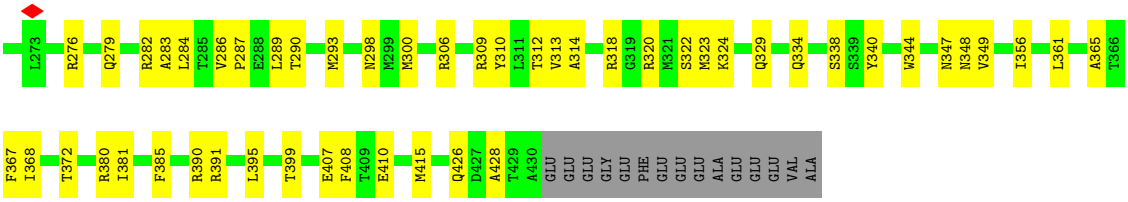
Chain MJ:



• Molecule 9: Tubulin beta-4B chain

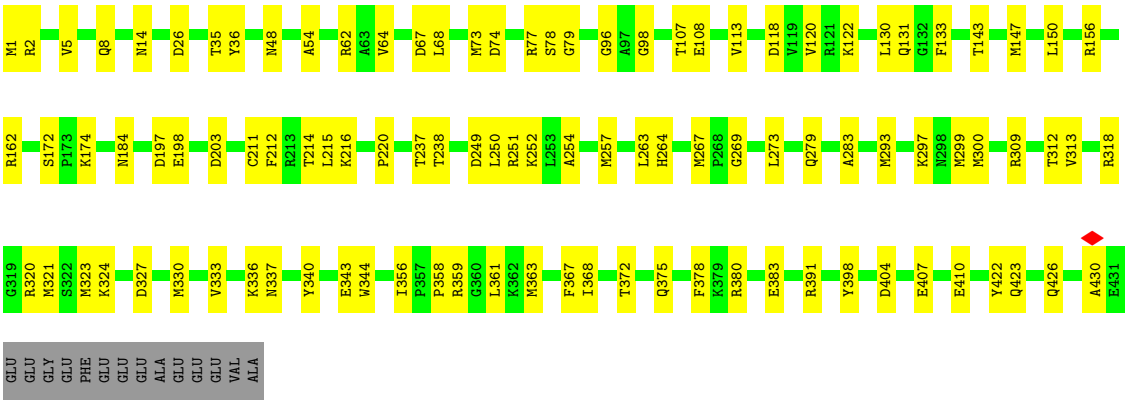
Chain ML:





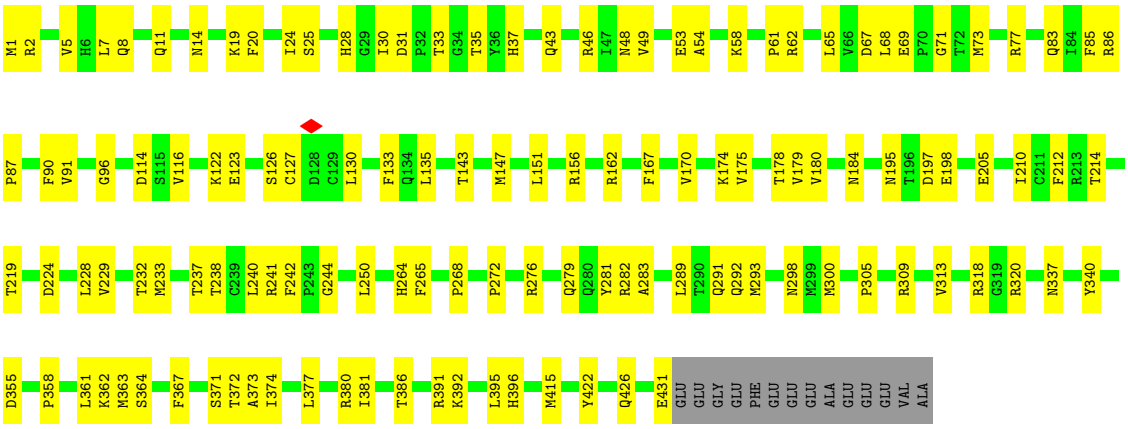
• Molecule 9: Tubulin beta-4B chain

Chain MN:



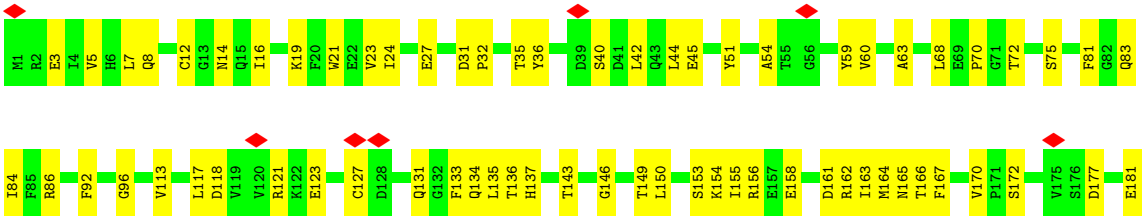
• Molecule 9: Tubulin beta-4B chain

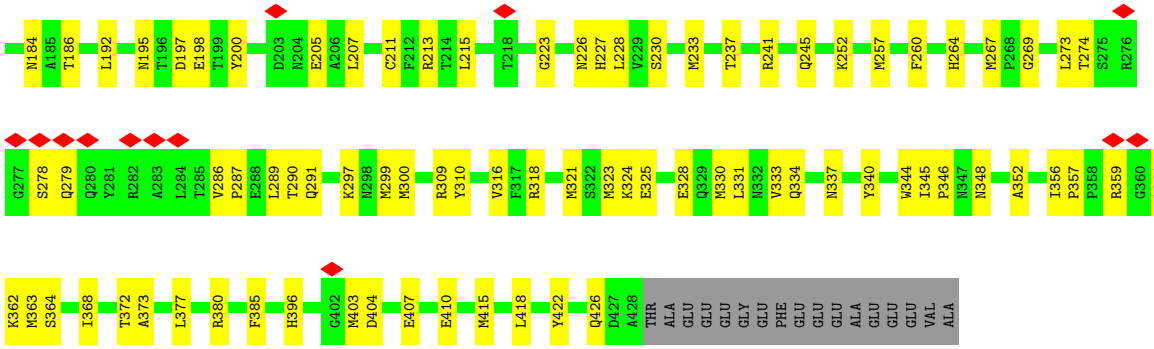
Chain MP:



• Molecule 9: Tubulin beta-4B chain

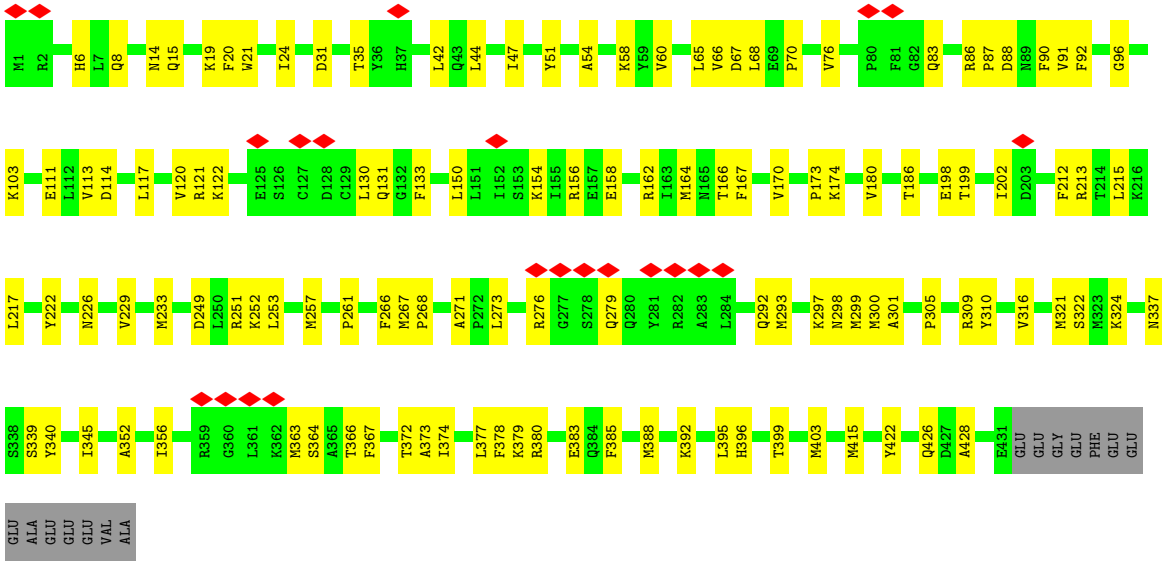
Chain NB:





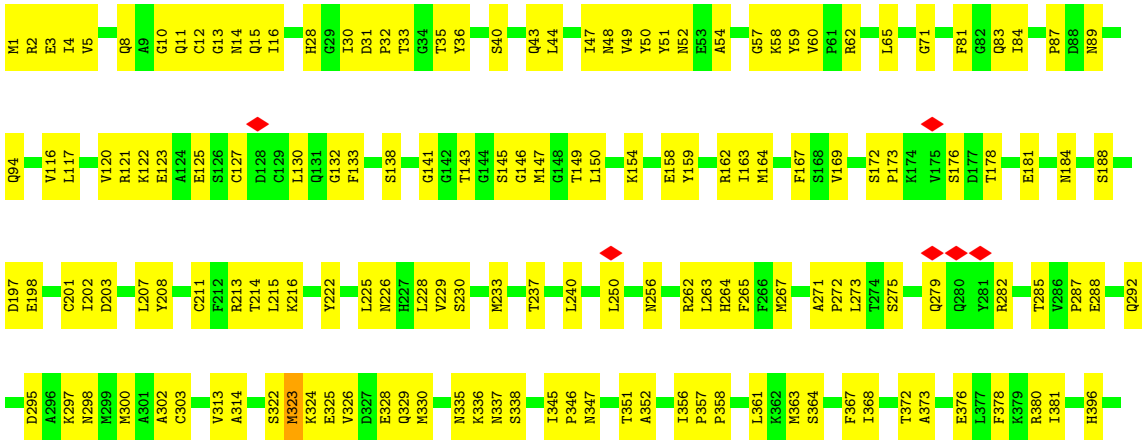
• Molecule 9: Tubulin beta-4B chain

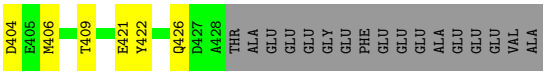
Chain ND:



• Molecule 9: Tubulin beta-4B chain

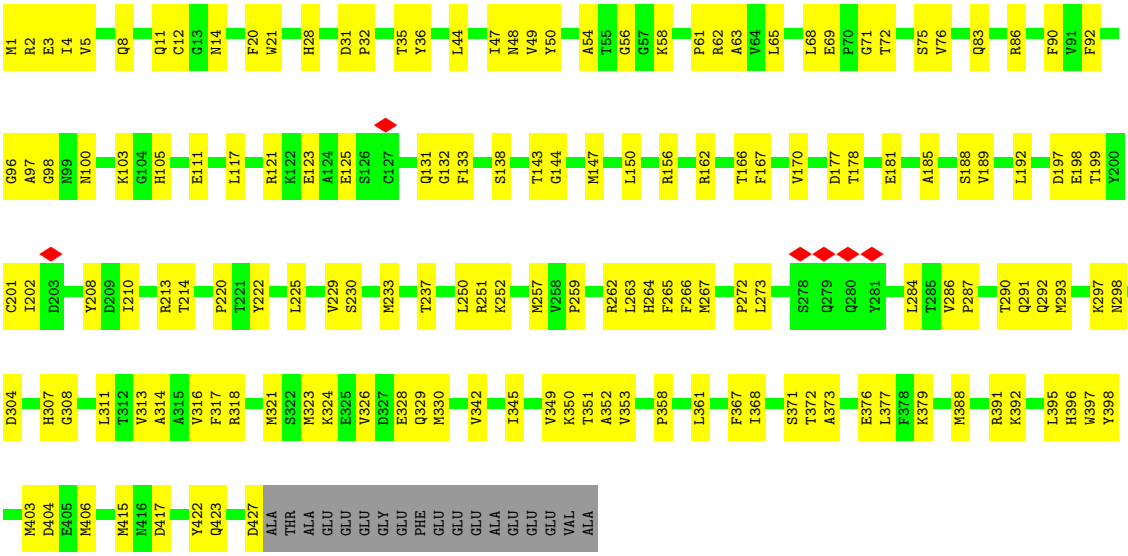
Chain NF:





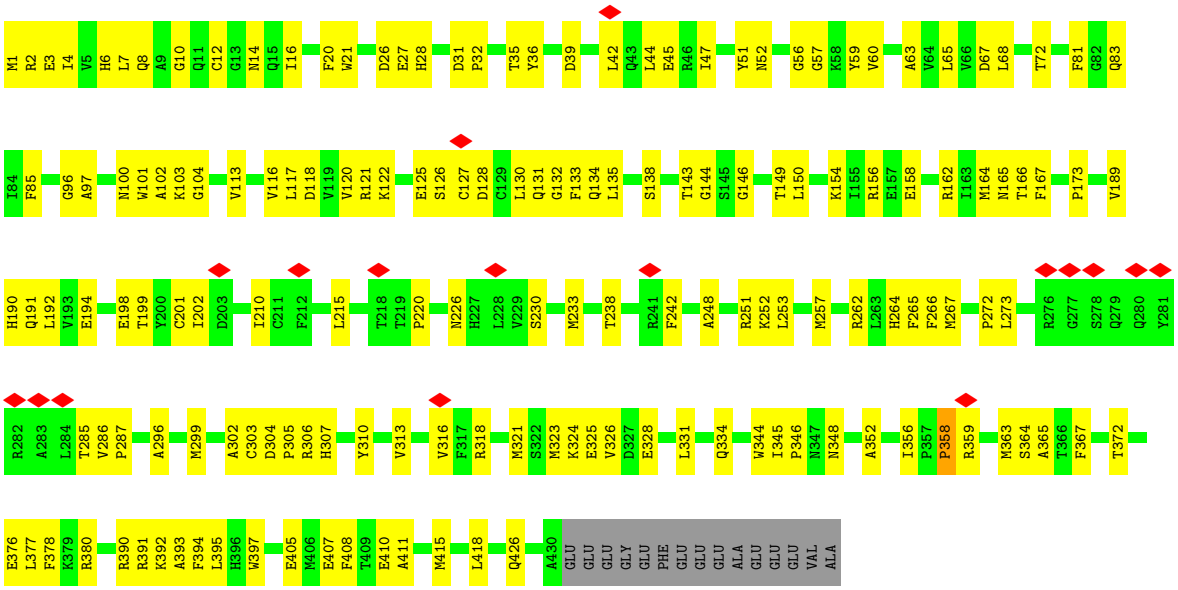
• Molecule 9: Tubulin beta-4B chain

Chain NH:



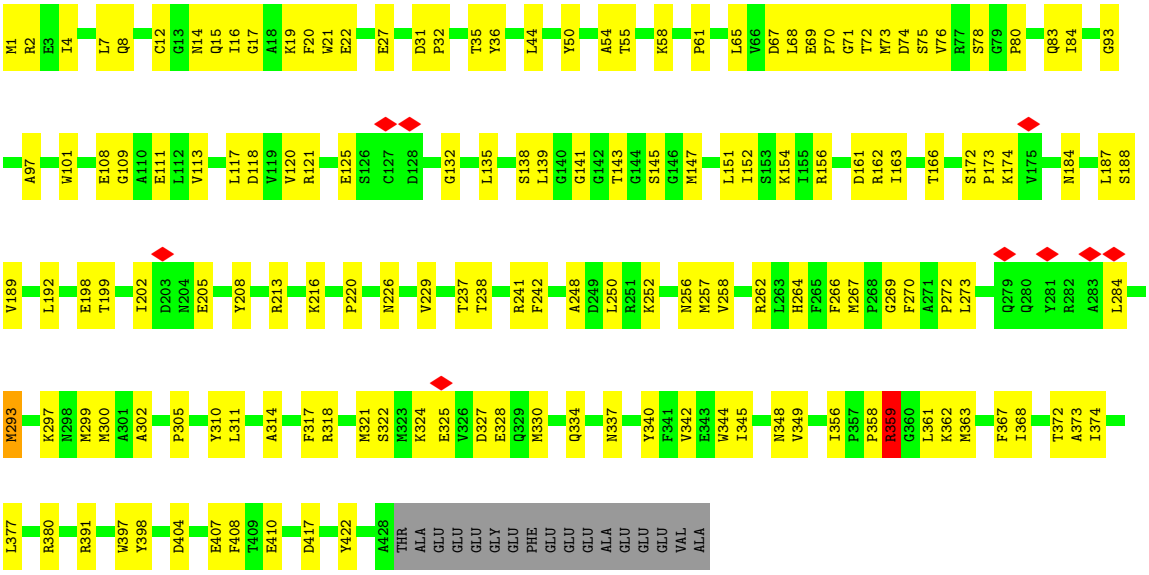
• Molecule 9: Tubulin beta-4B chain

Chain NJ:



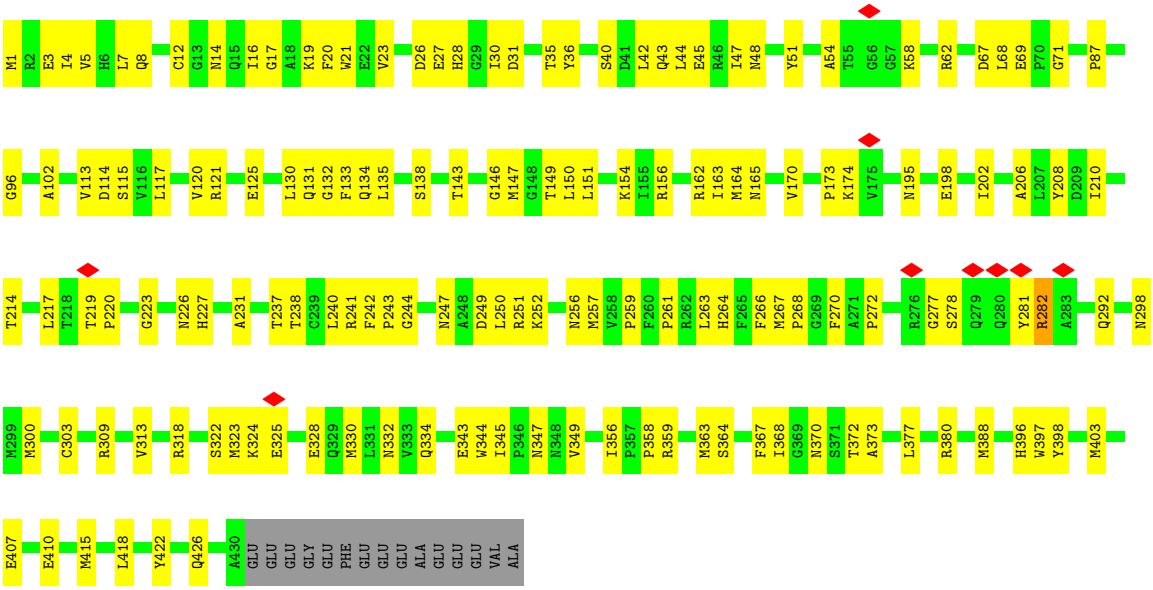
• Molecule 9: Tubulin beta-4B chain

Chain NL:



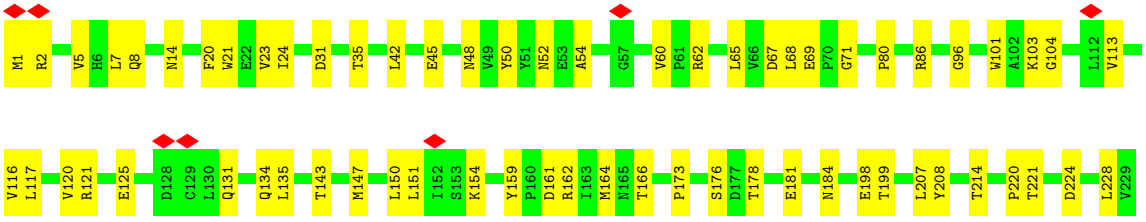
• Molecule 9: Tubulin beta-4B chain

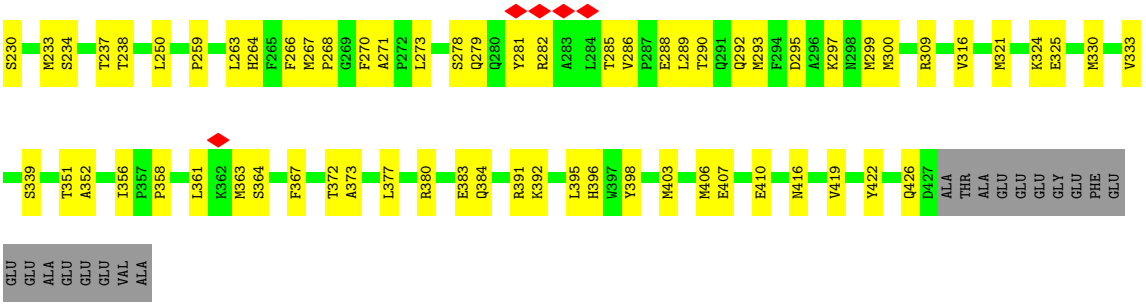
Chain NN:



• Molecule 9: Tubulin beta-4B chain

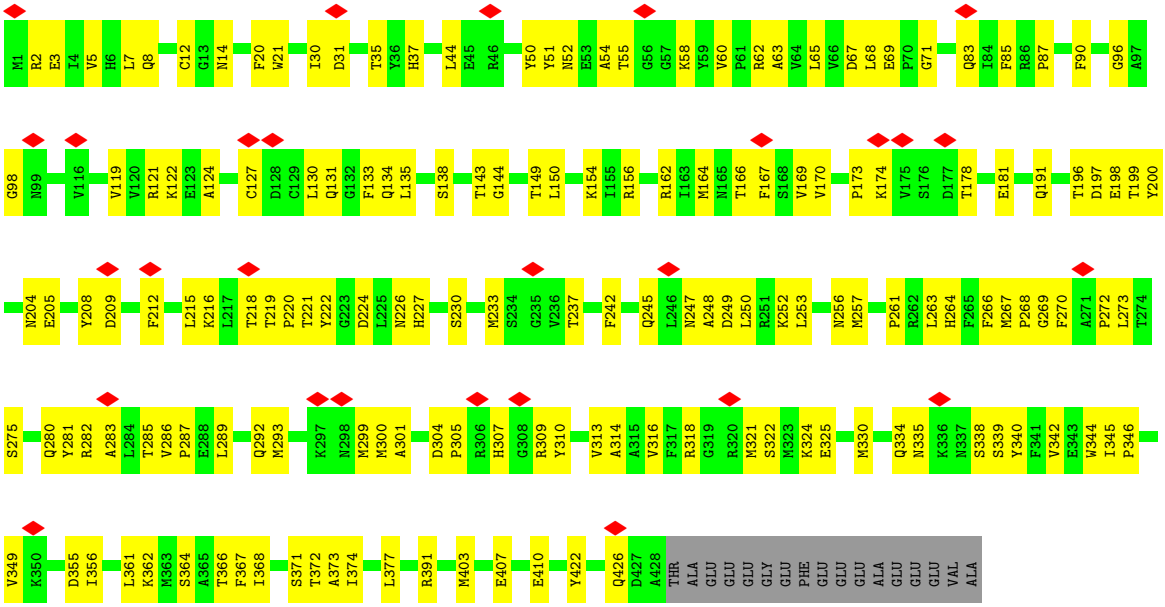
Chain NP:





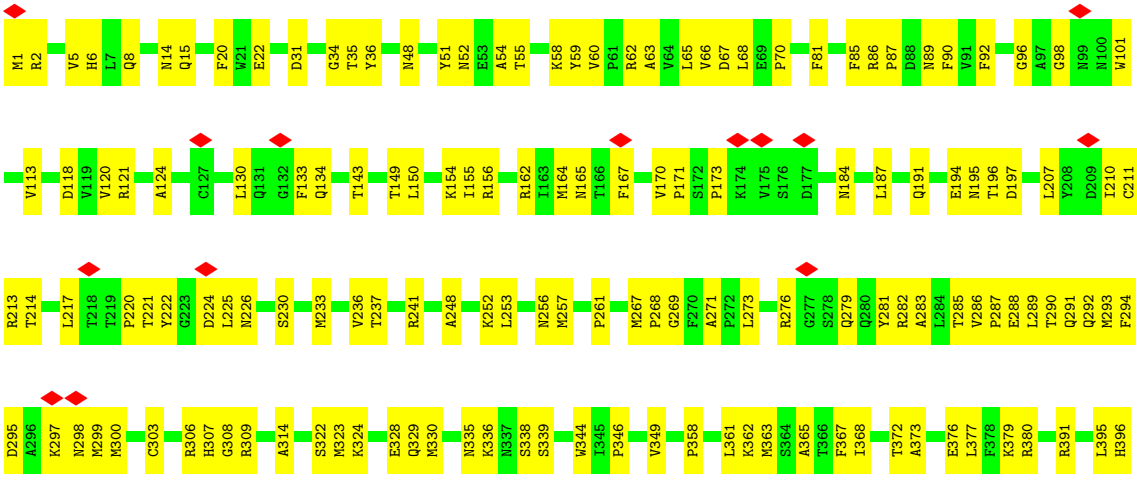
• Molecule 9: Tubulin beta-4B chain

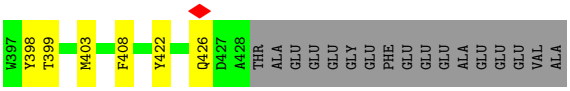
Chain OB:



• Molecule 9: Tubulin beta-4B chain

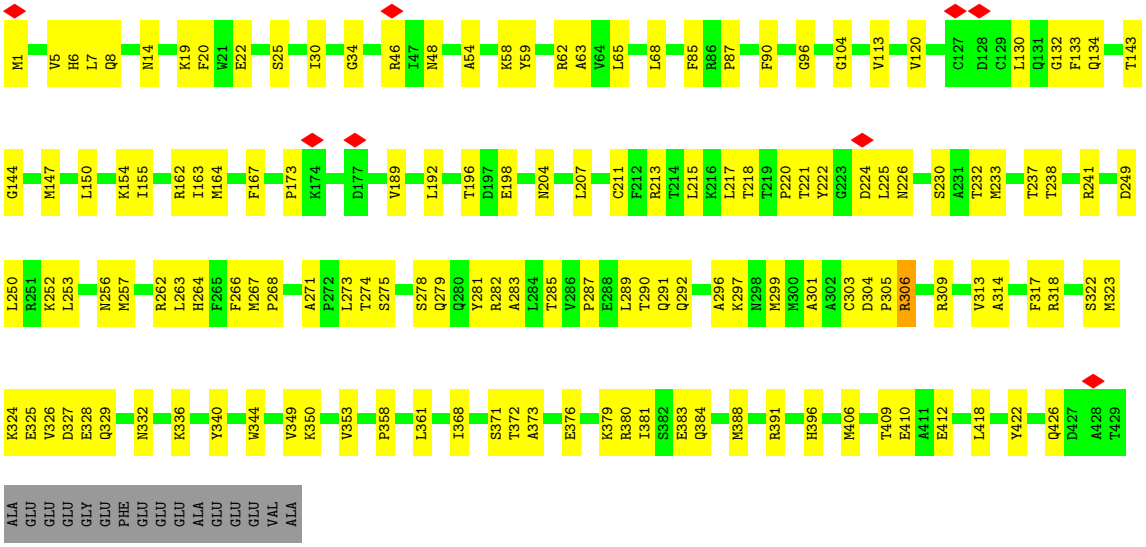
Chain OD:





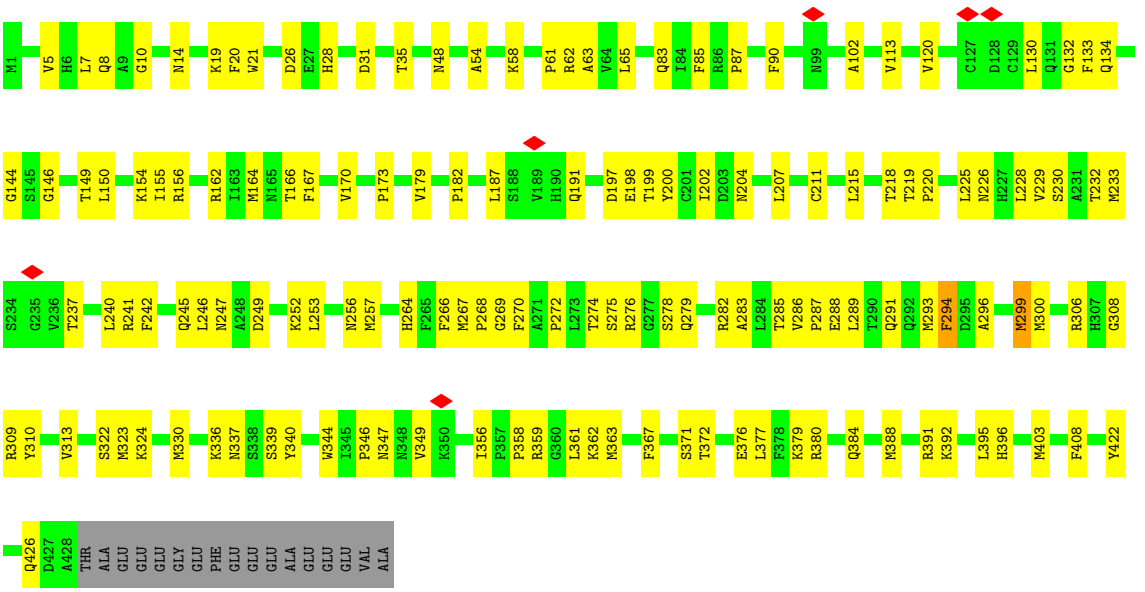
• Molecule 9: Tubulin beta-4B chain

Chain OF:



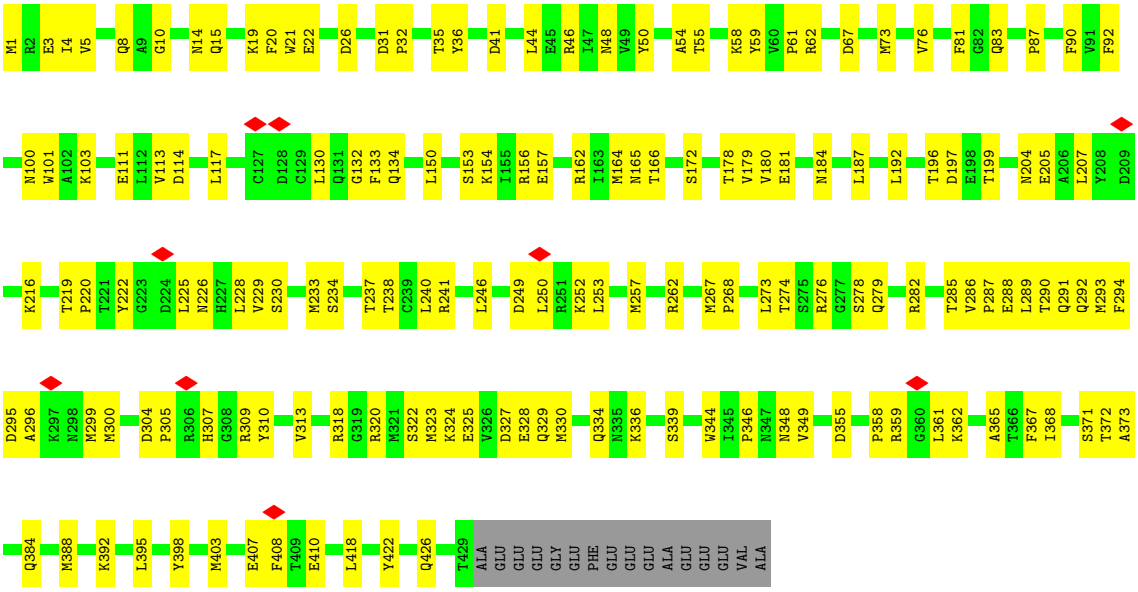
• Molecule 9: Tubulin beta-4B chain

Chain OH:



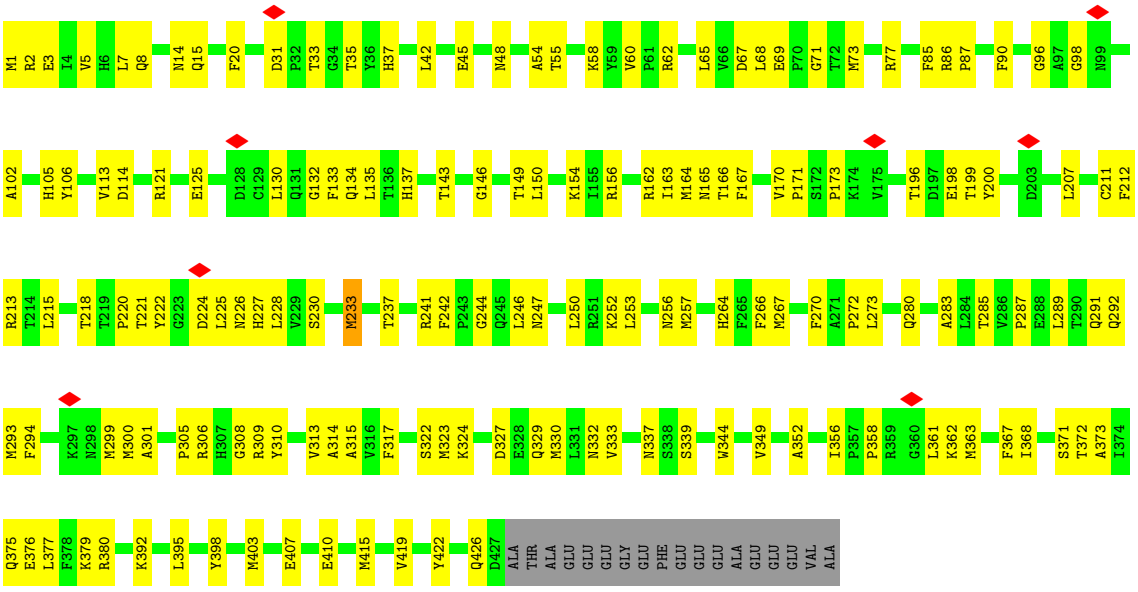
• Molecule 9: Tubulin beta-4B chain

Chain OJ:



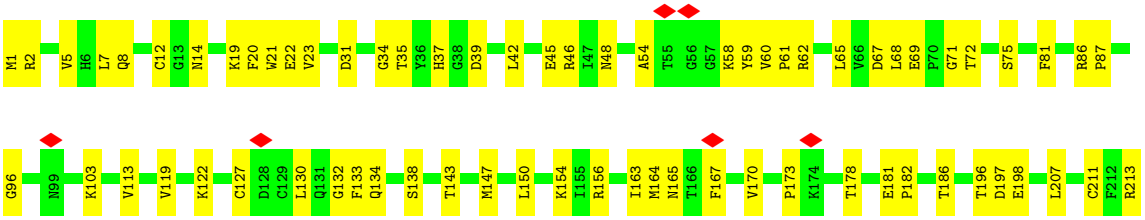
• Molecule 9: Tubulin beta-4B chain

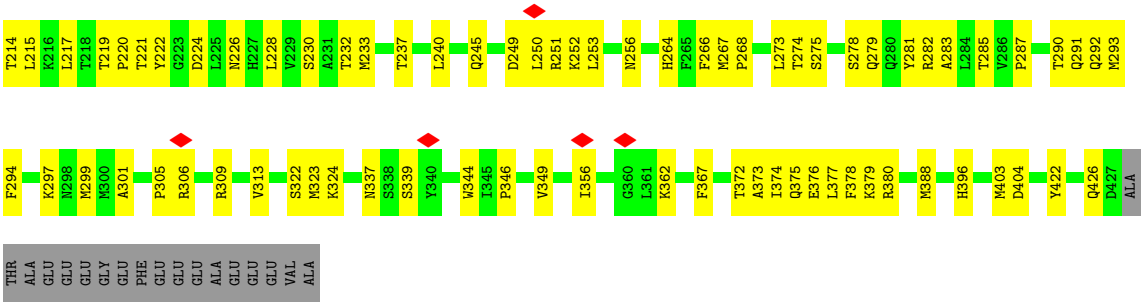
Chain OL:



• Molecule 9: Tubulin beta-4B chain

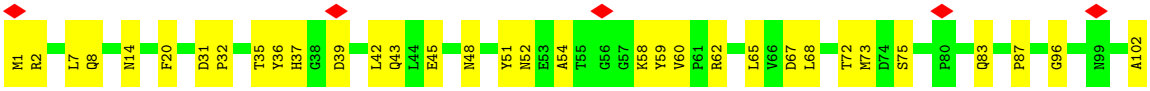
Chain ON:

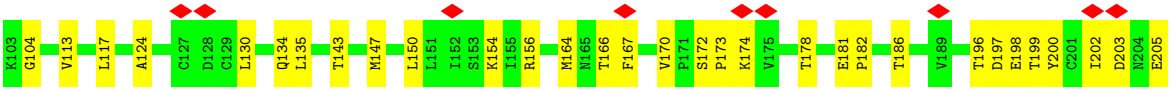


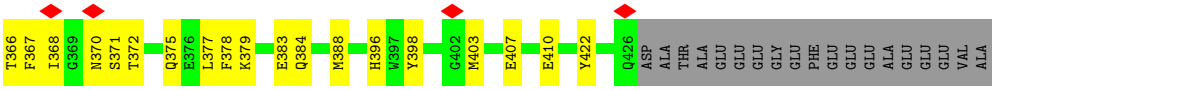


• Molecule 9: Tubulin beta-4B chain

Chain OP:

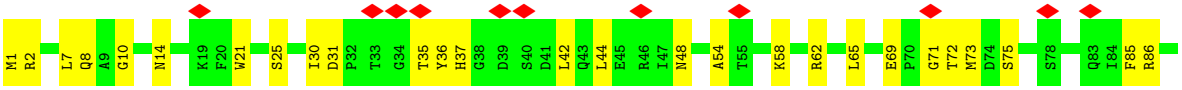


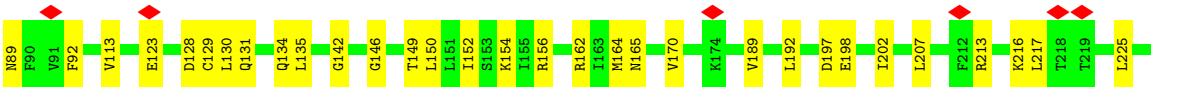


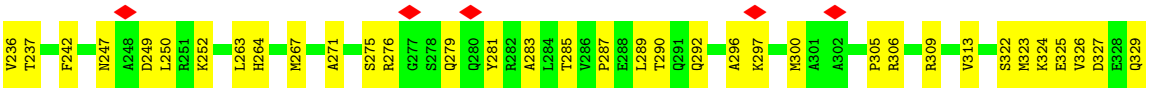


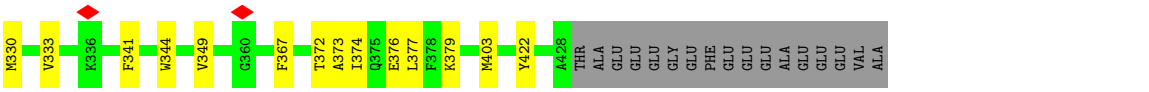
• Molecule 9: Tubulin beta-4B chain

Chain PB:



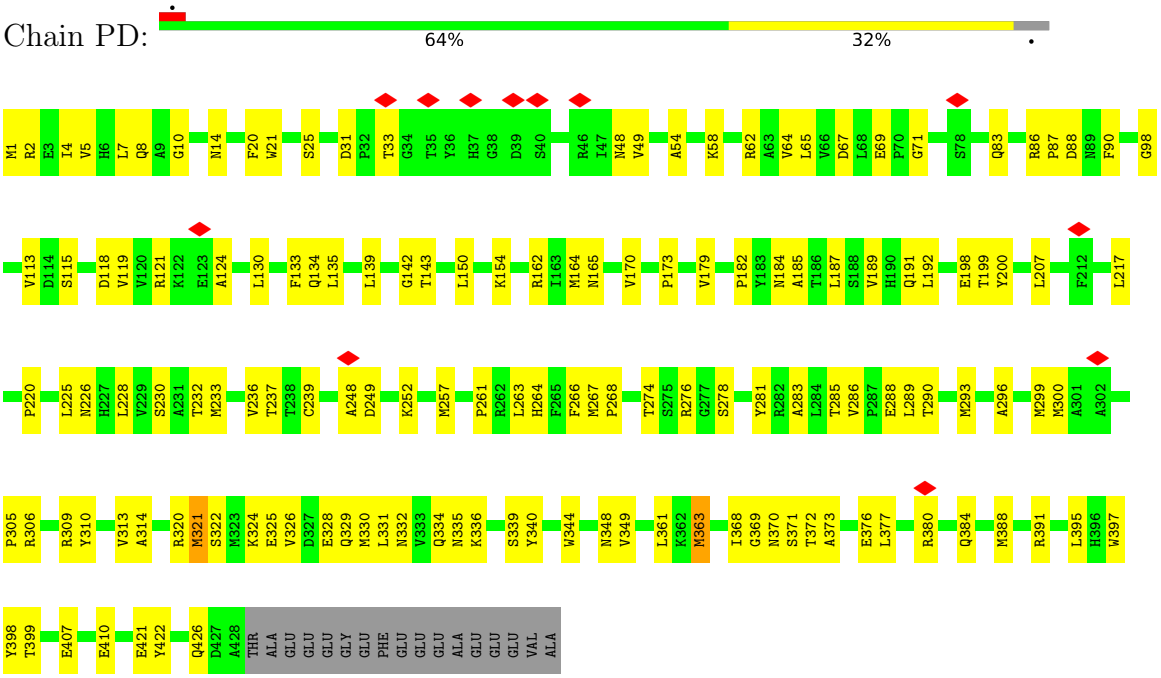






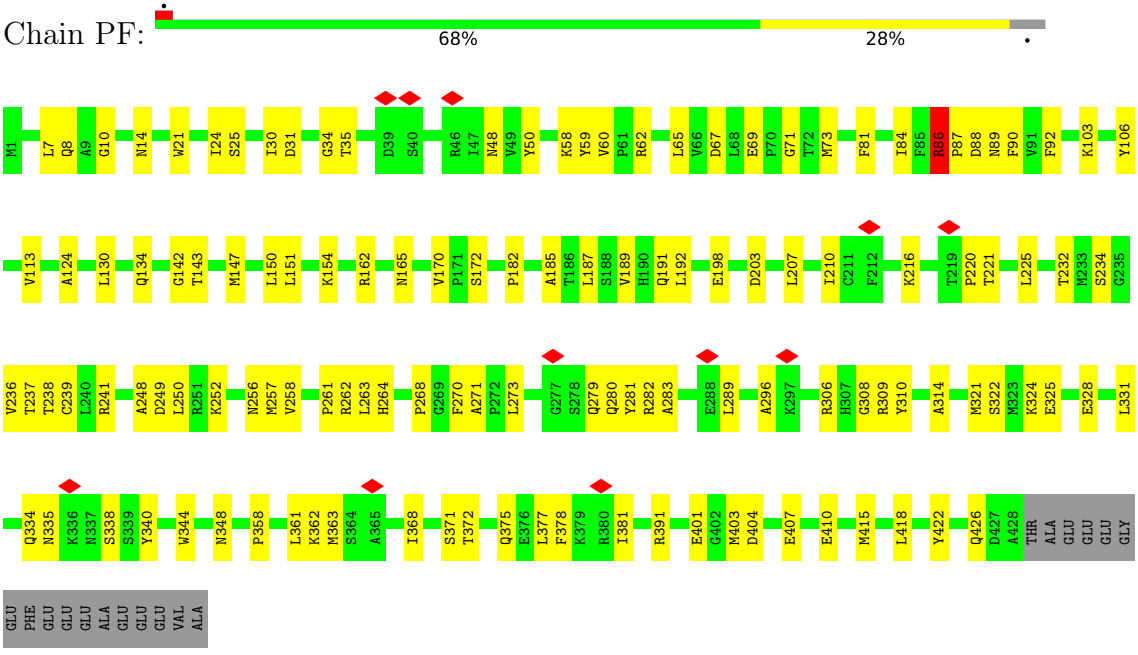
• Molecule 9: Tubulin beta-4B chain

Chain PD:



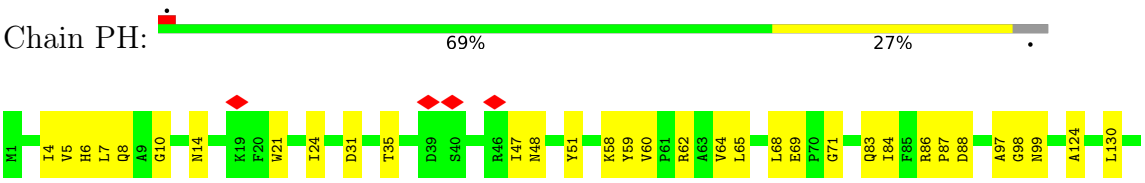
• Molecule 9: Tubulin beta-4B chain

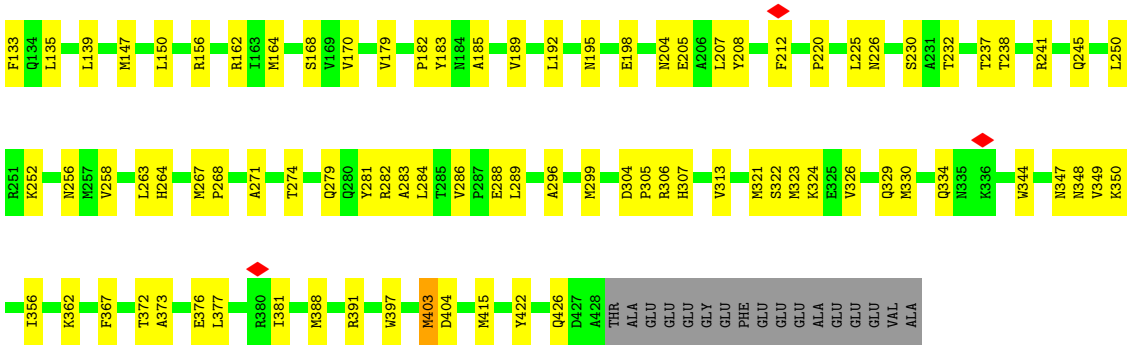
Chain PF:



• Molecule 9: Tubulin beta-4B chain

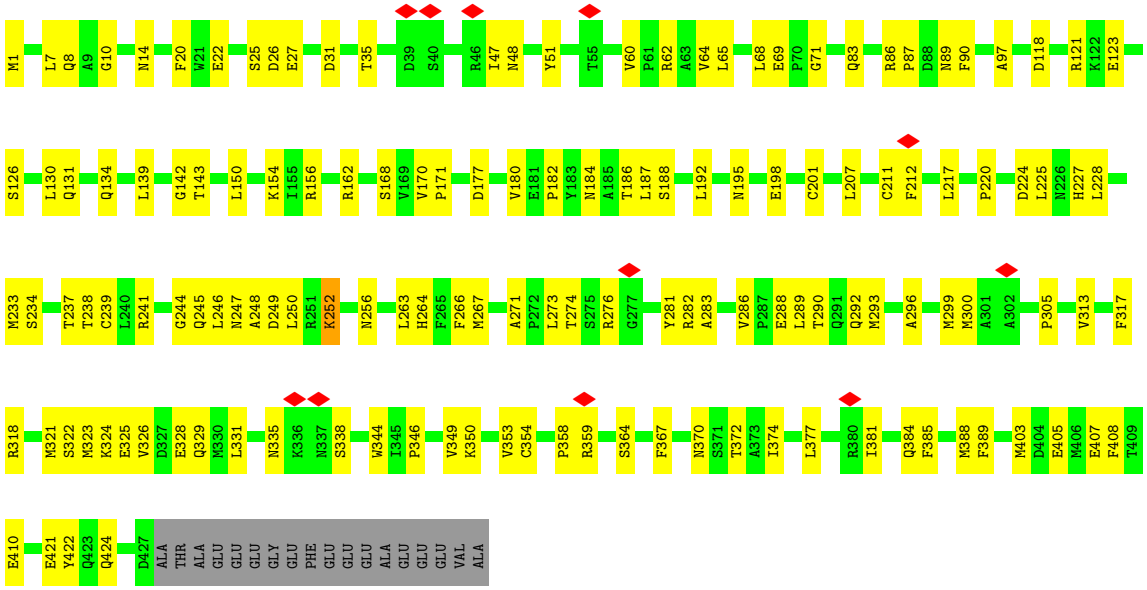
Chain PH:





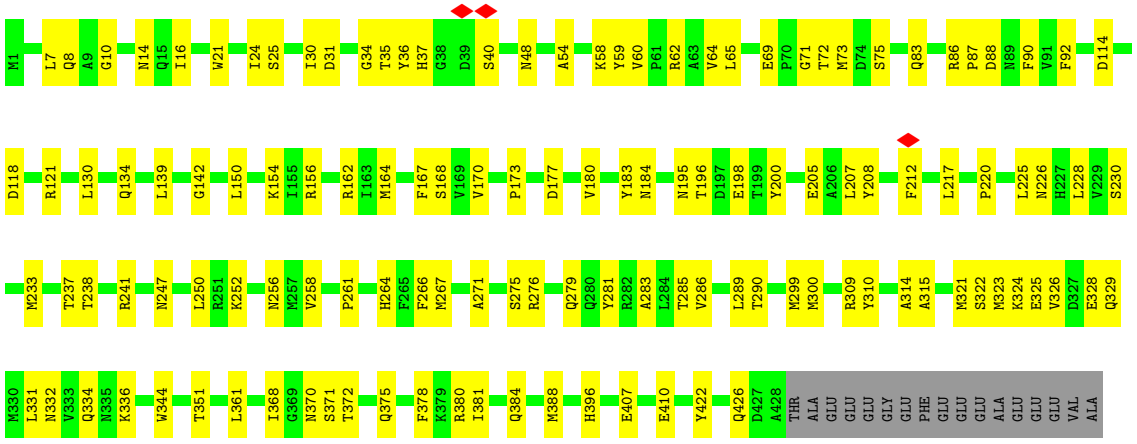
• Molecule 9: Tubulin beta-4B chain

Chain PJ:



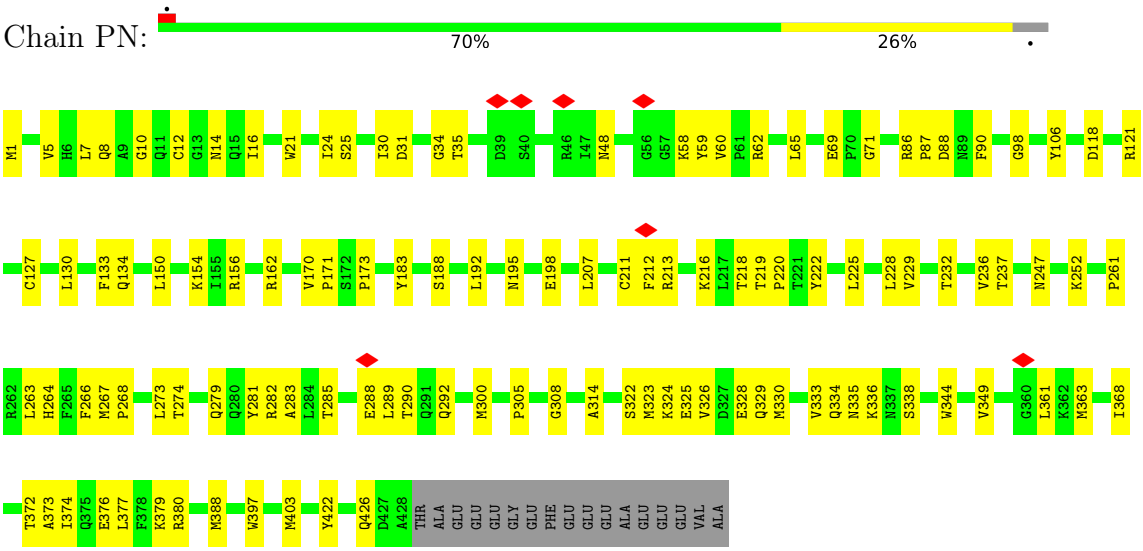
• Molecule 9: Tubulin beta-4B chain

Chain PL:



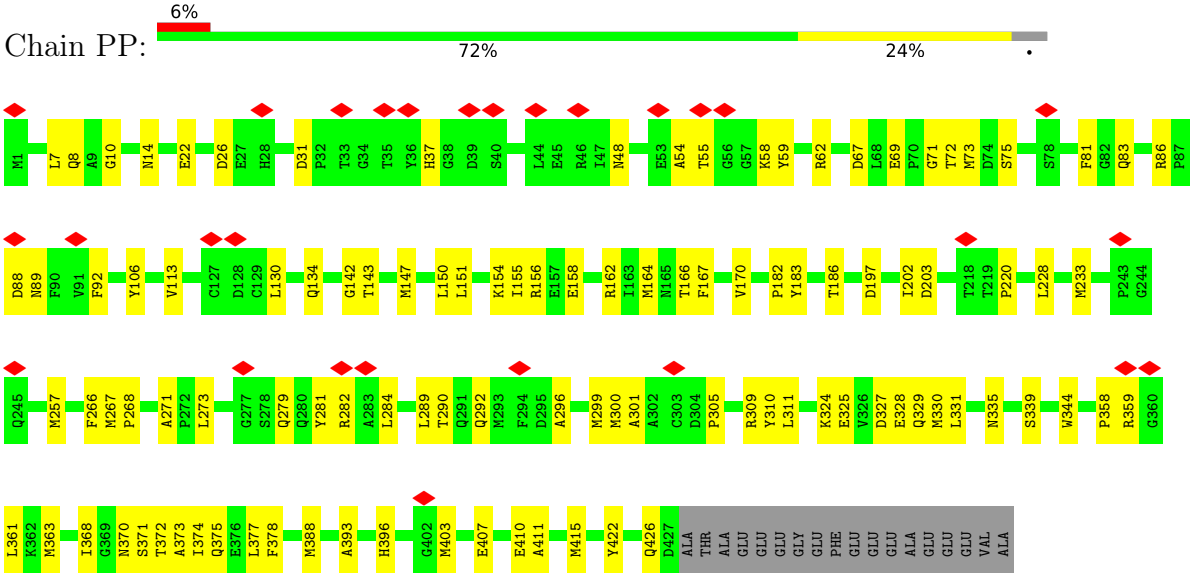
• Molecule 9: Tubulin beta-4B chain

Chain PN:



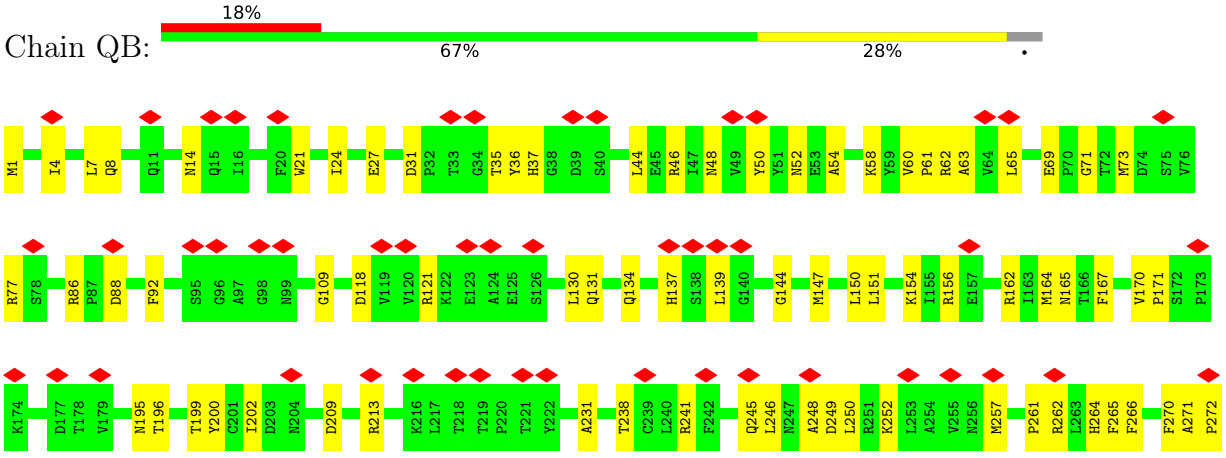
• Molecule 9: Tubulin beta-4B chain

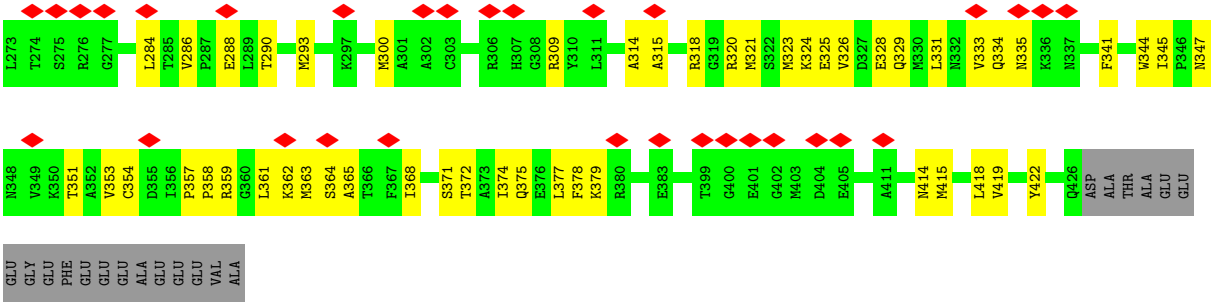
Chain PP:



• Molecule 9: Tubulin beta-4B chain

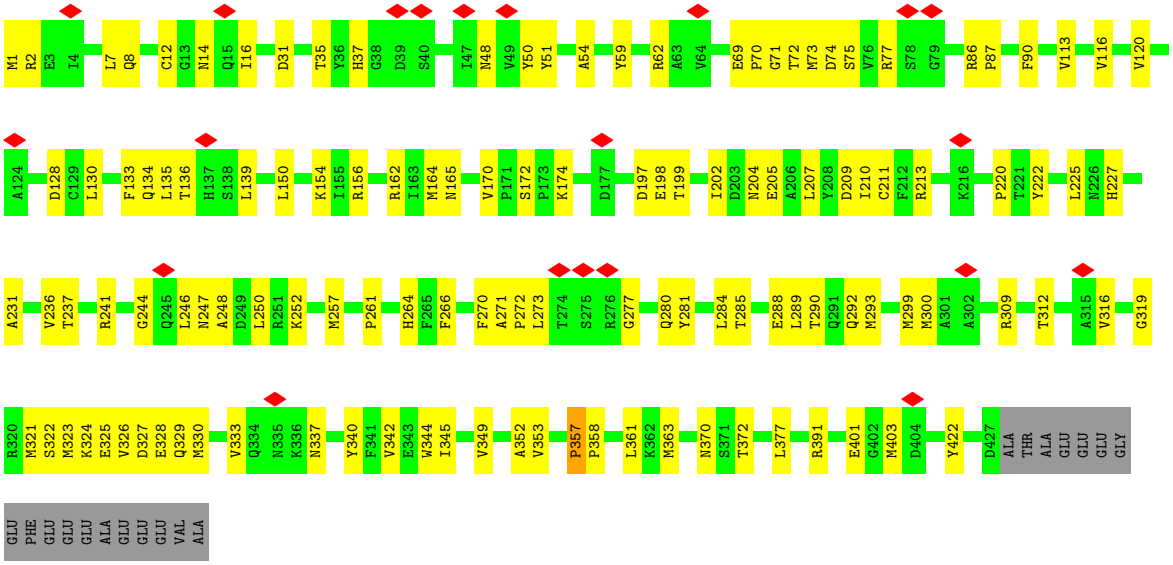
Chain QB:





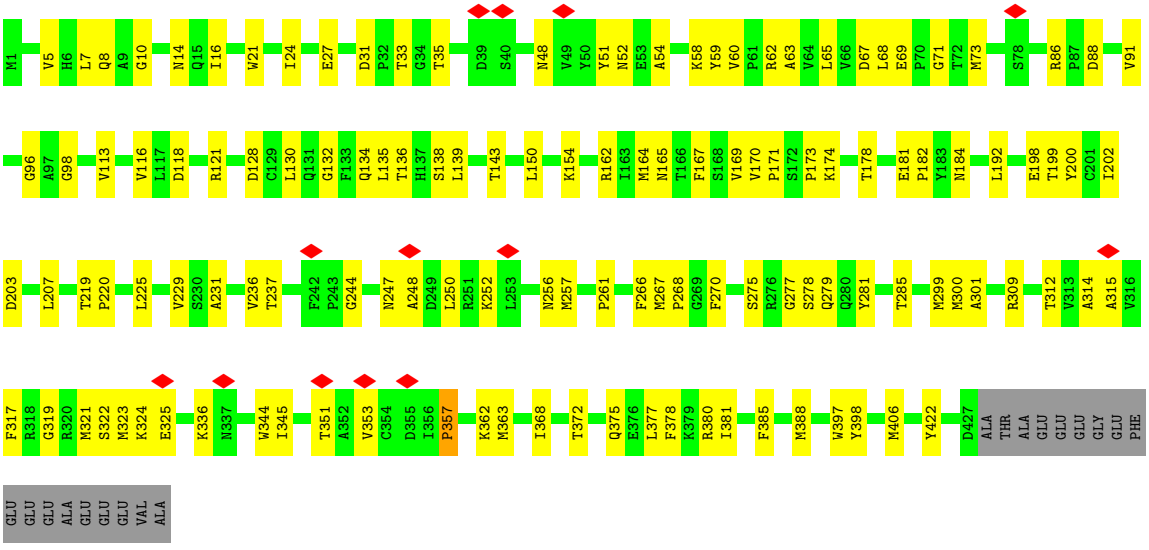
• Molecule 9: Tubulin beta-4B chain

Chain QD:



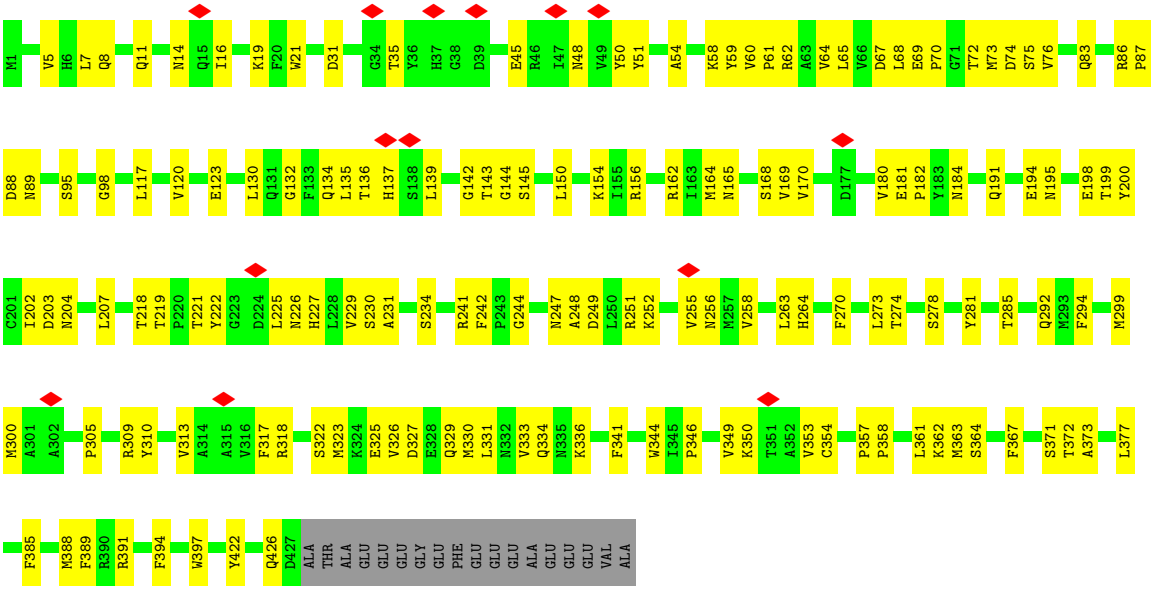
• Molecule 9: Tubulin beta-4B chain

Chain QF:



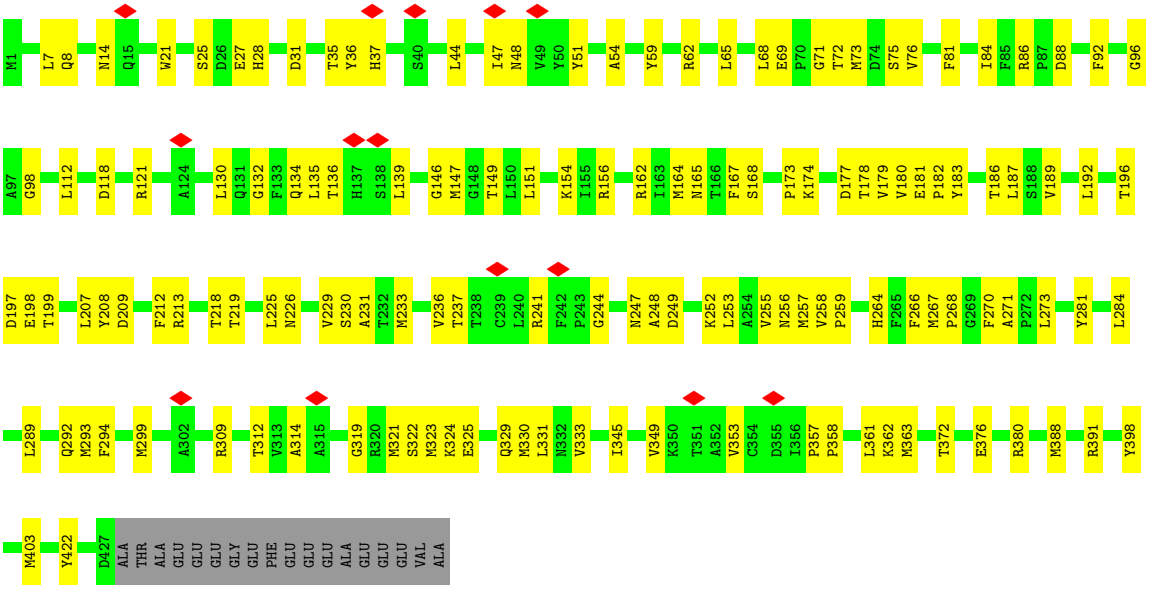
• Molecule 9: Tubulin beta-4B chain

Chain QH:



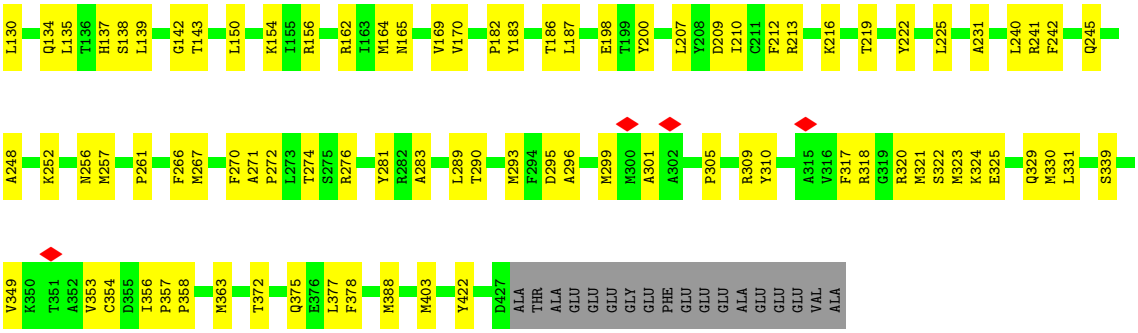
• Molecule 9: Tubulin beta-4B chain

Chain QJ:



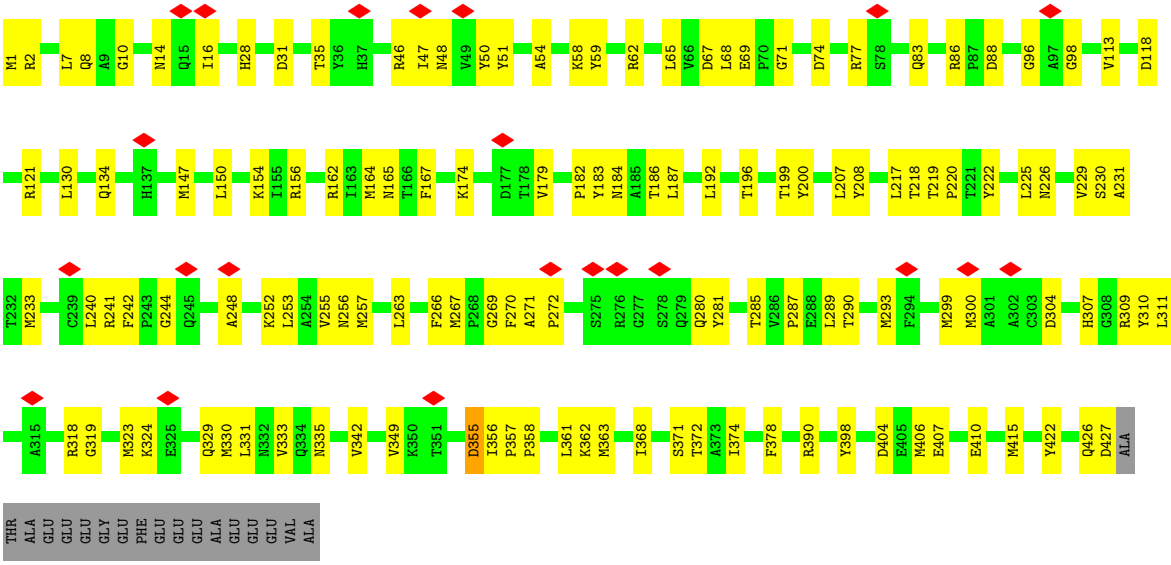
• Molecule 9: Tubulin beta-4B chain

Chain QL:



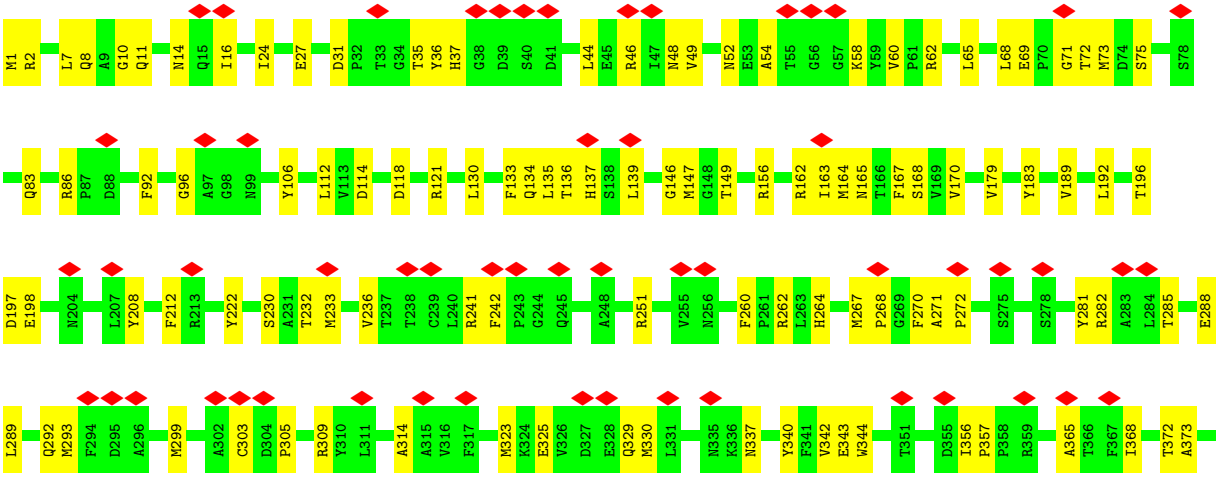
• Molecule 9: Tubulin beta-4B chain

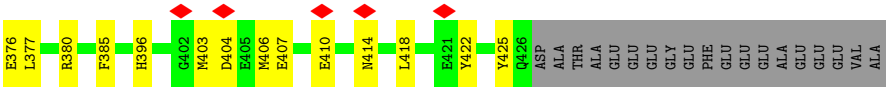
Chain QN:



• Molecule 9: Tubulin beta-4B chain

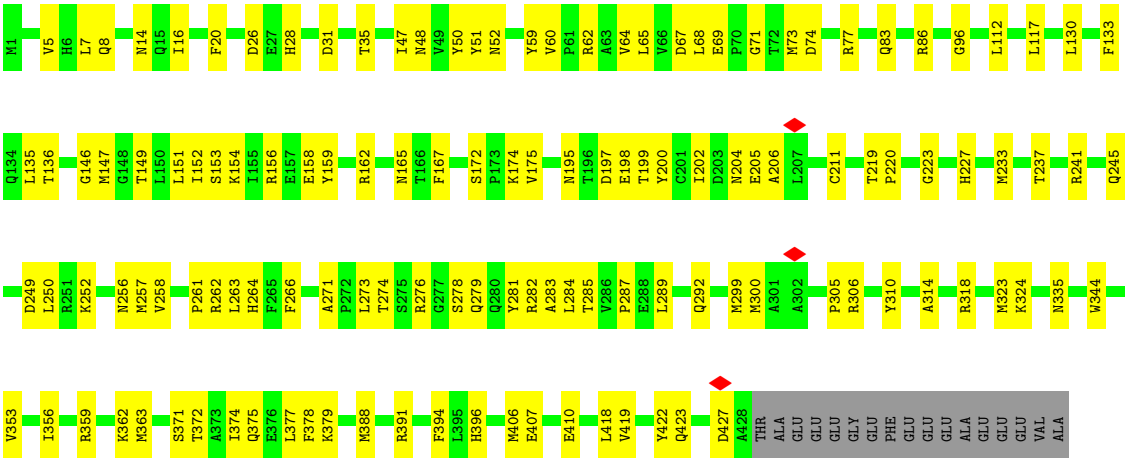
Chain QP:





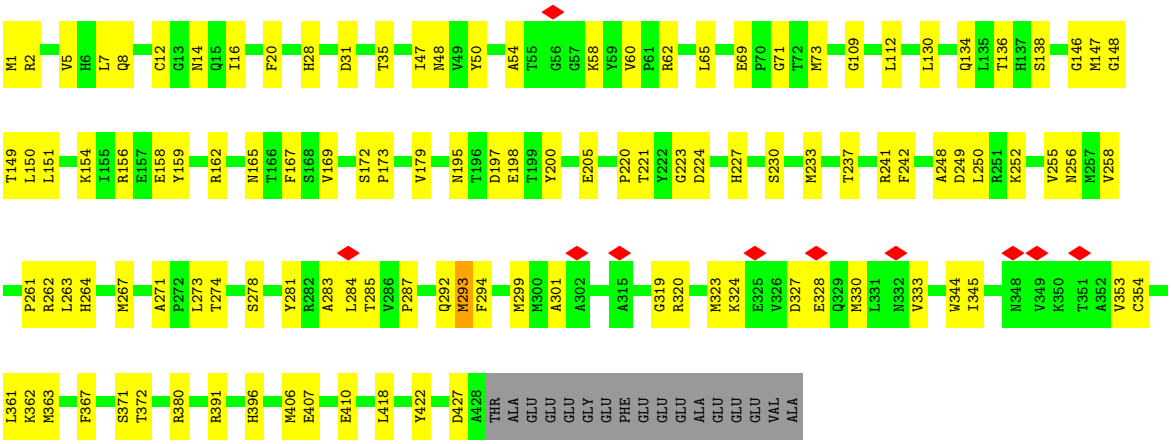
• Molecule 9: Tubulin beta-4B chain

Chain RD:



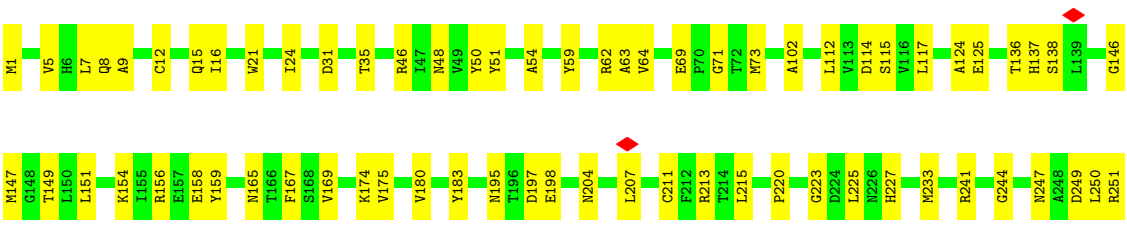
• Molecule 9: Tubulin beta-4B chain

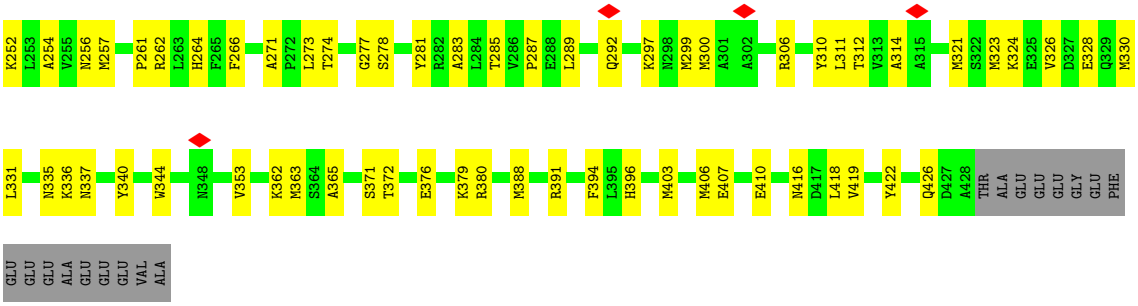
Chain RF:



• Molecule 9: Tubulin beta-4B chain

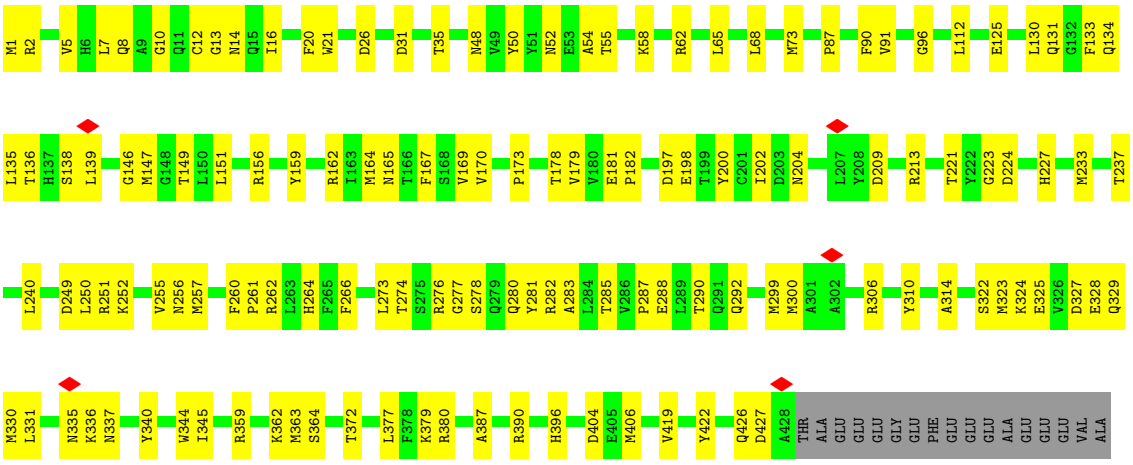
Chain RH:





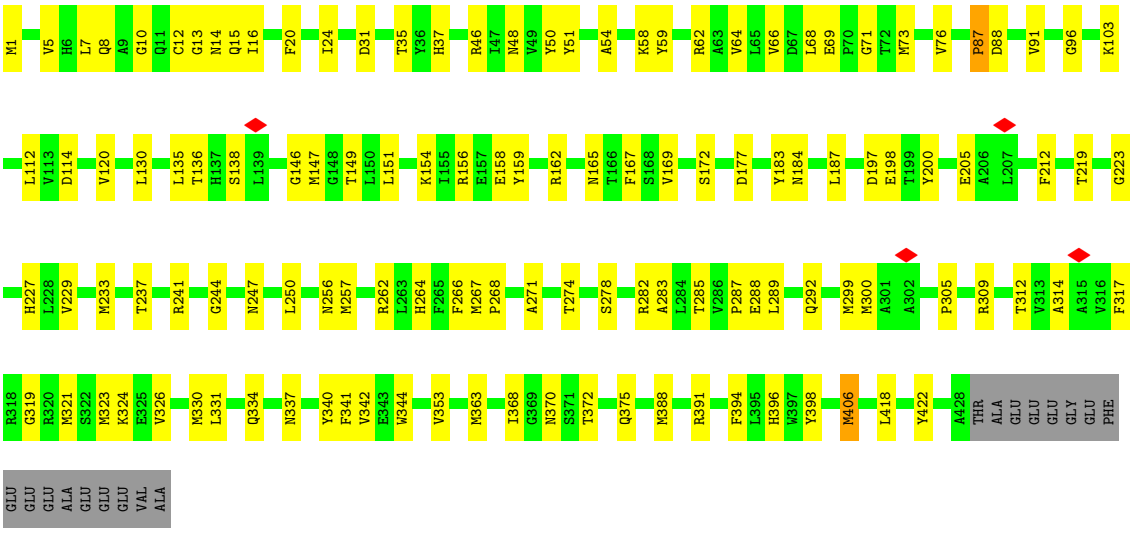
• Molecule 9: Tubulin beta-4B chain

Chain RJ:



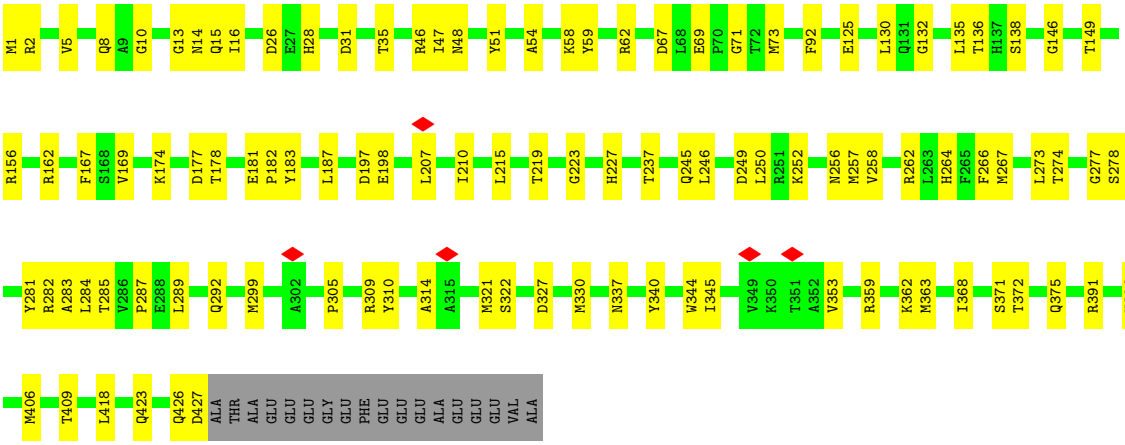
• Molecule 9: Tubulin beta-4B chain

Chain RL:



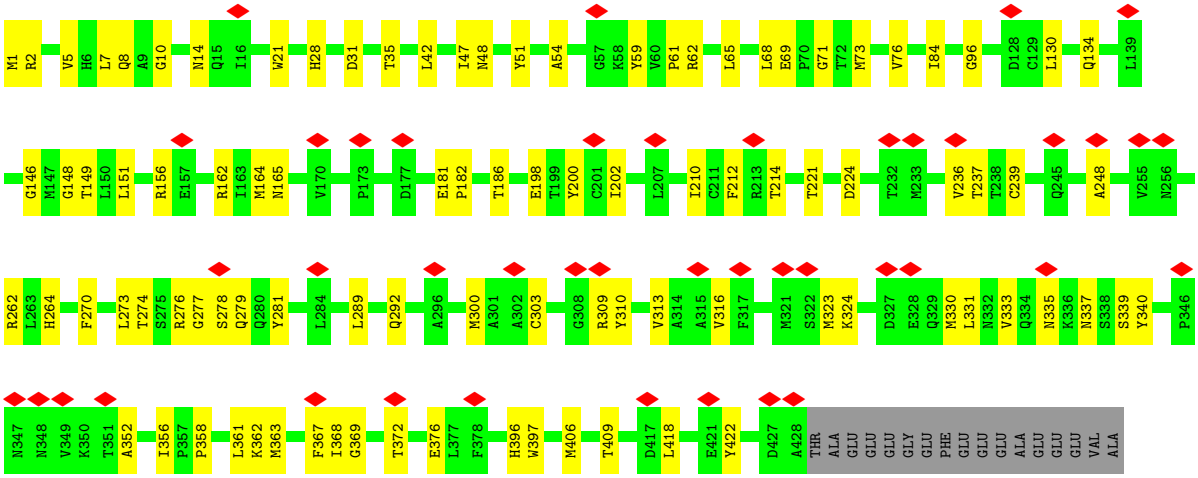
• Molecule 9: Tubulin beta-4B chain

Chain RN:



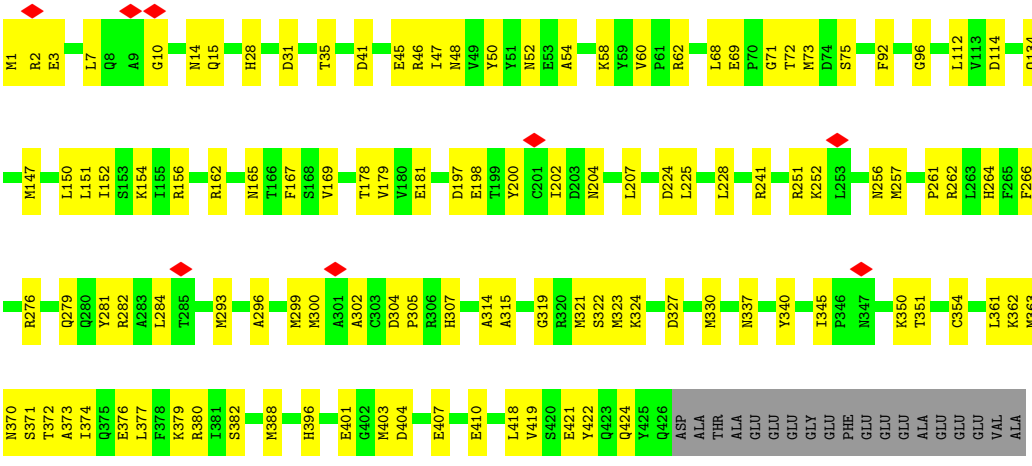
• Molecule 9: Tubulin beta-4B chain

Chain RP:



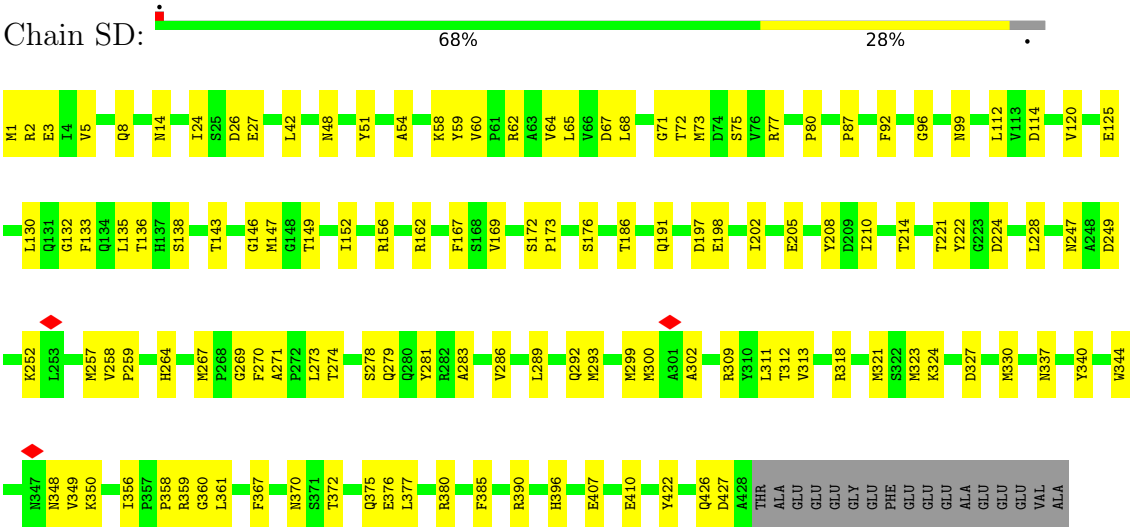
• Molecule 9: Tubulin beta-4B chain

Chain SB:



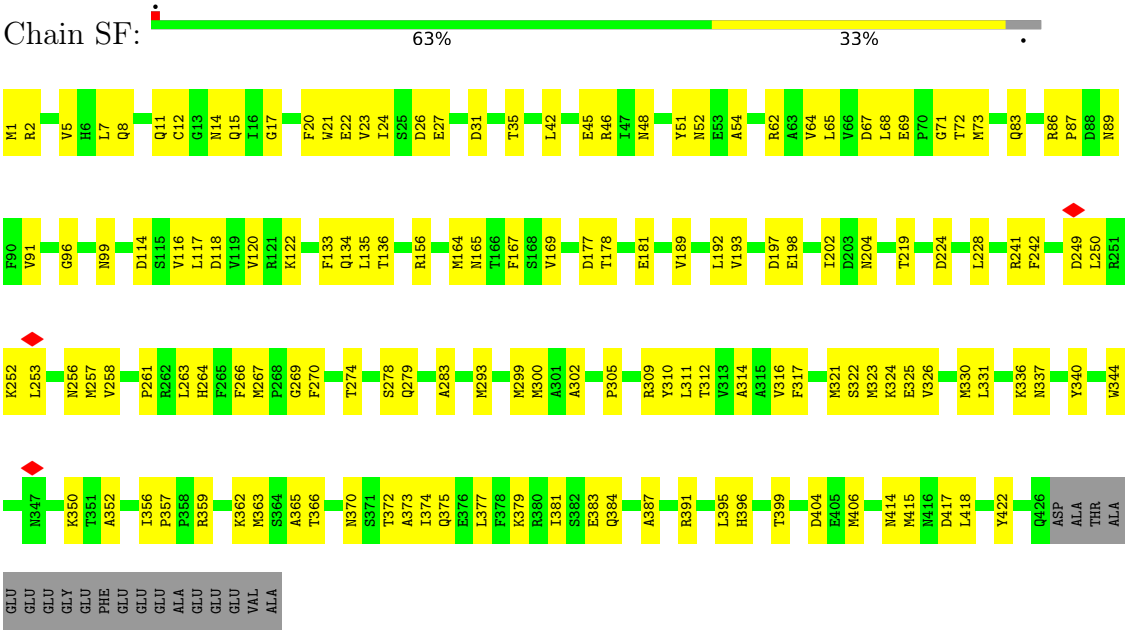
• Molecule 9: Tubulin beta-4B chain

Chain SD:



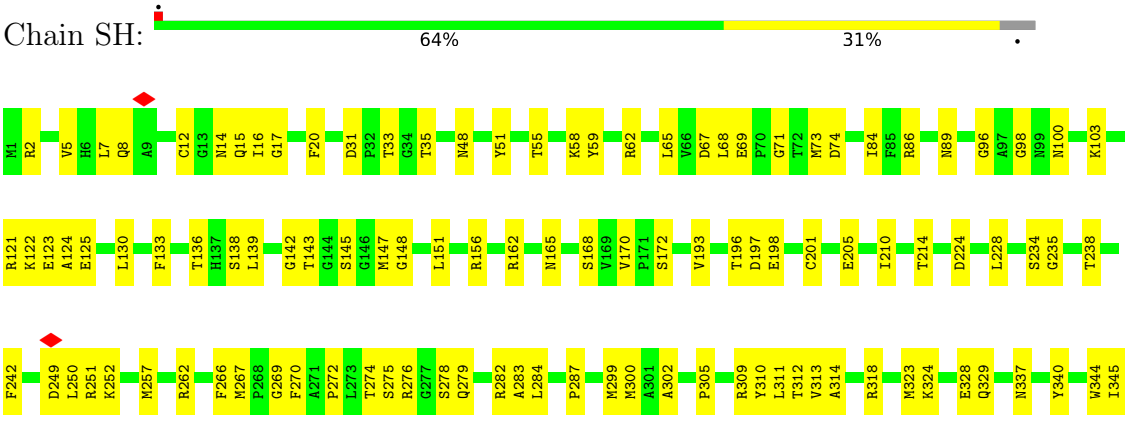
• Molecule 9: Tubulin beta-4B chain

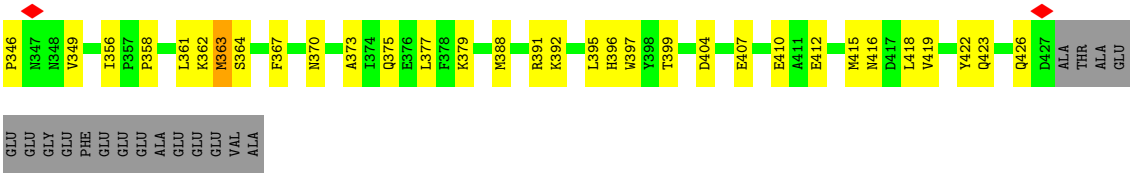
Chain SF:



• Molecule 9: Tubulin beta-4B chain

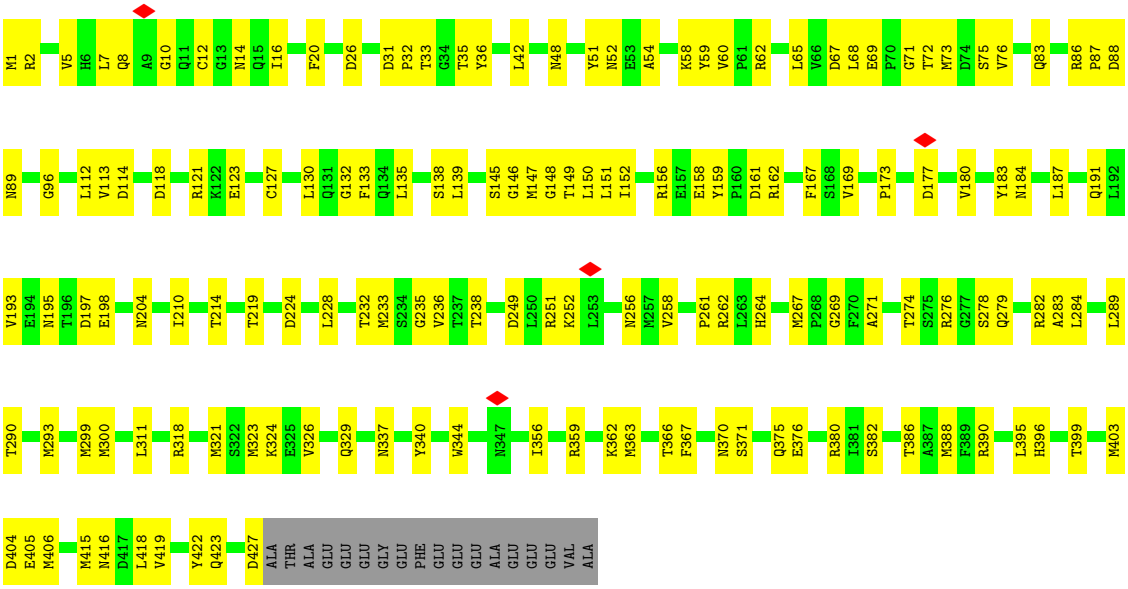
Chain SH:





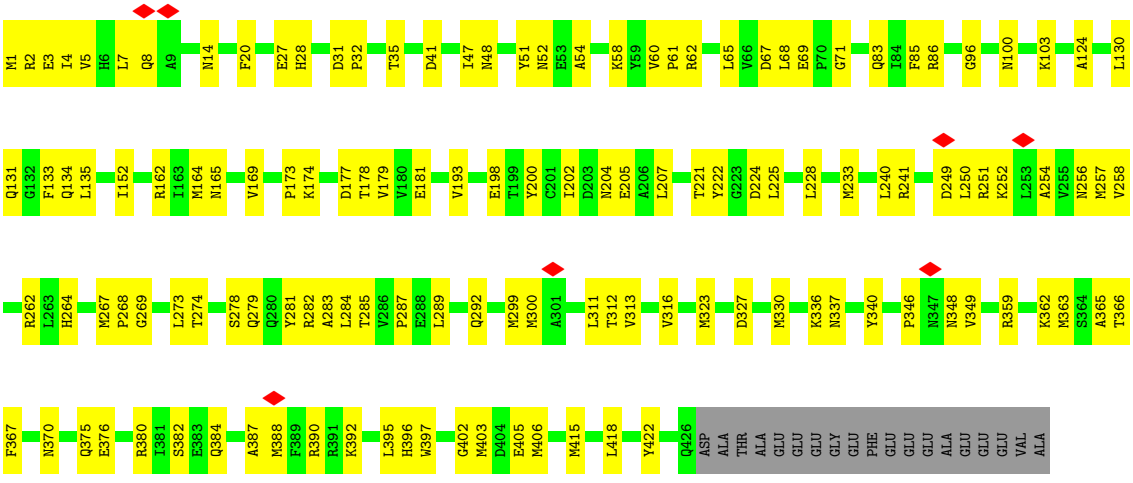
• Molecule 9: Tubulin beta-4B chain

Chain SJ:



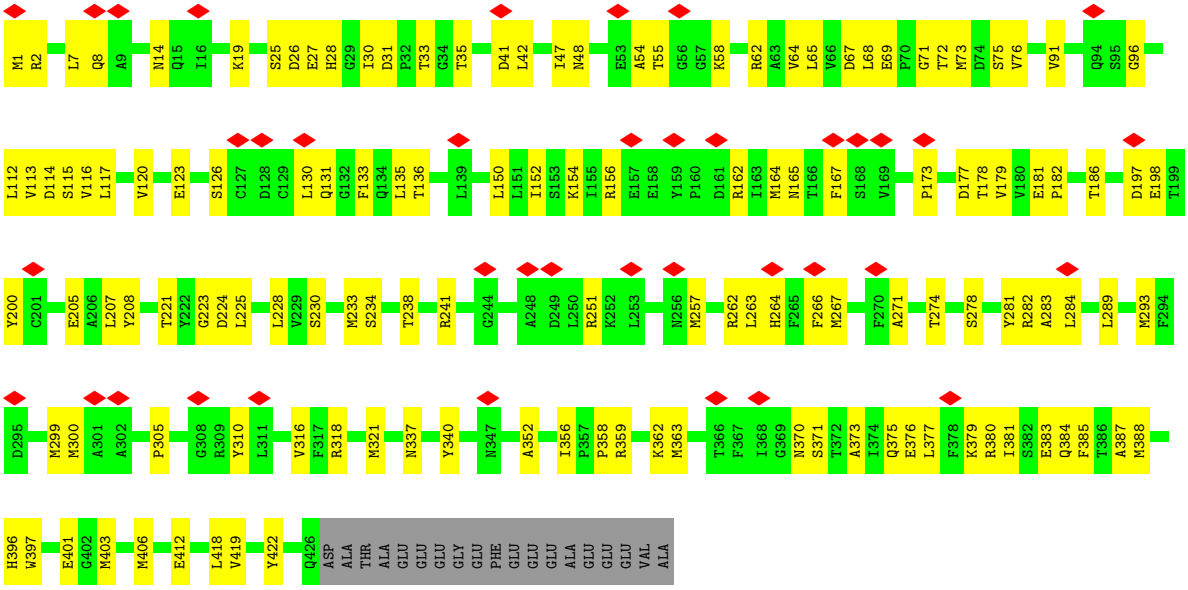
• Molecule 9: Tubulin beta-4B chain

Chain SL:



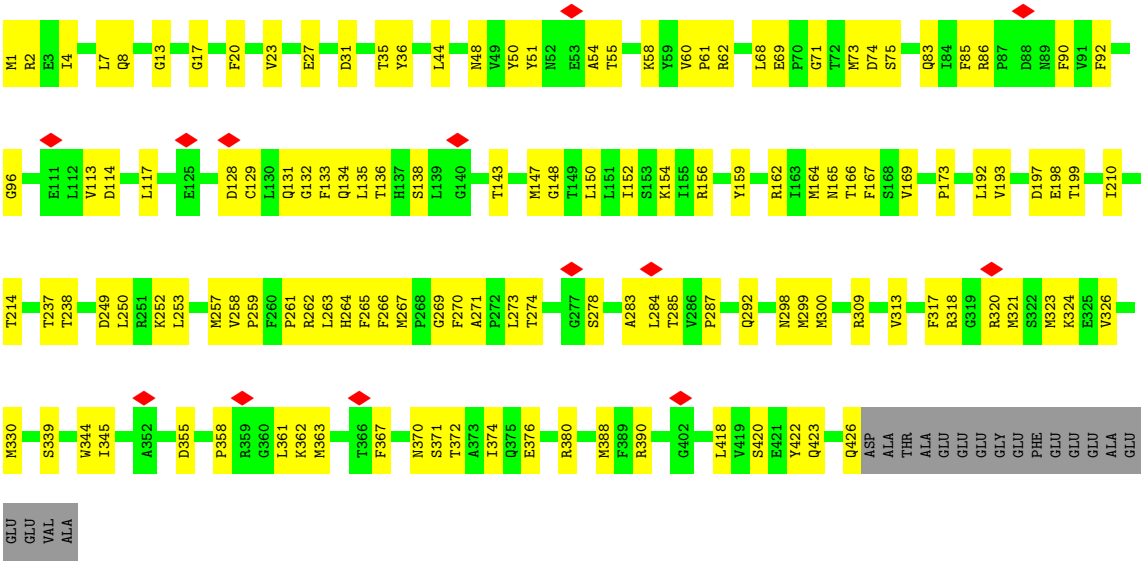
• Molecule 9: Tubulin beta-4B chain

Chain SN:



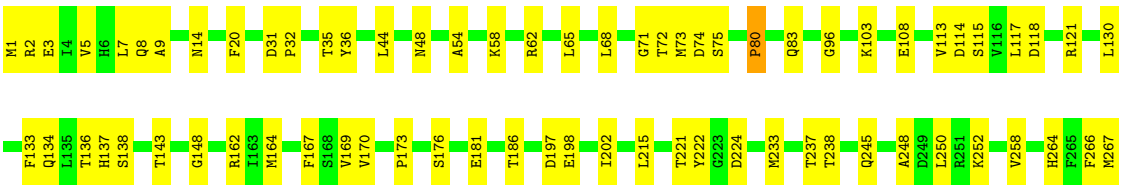
• Molecule 9: Tubulin beta-4B chain

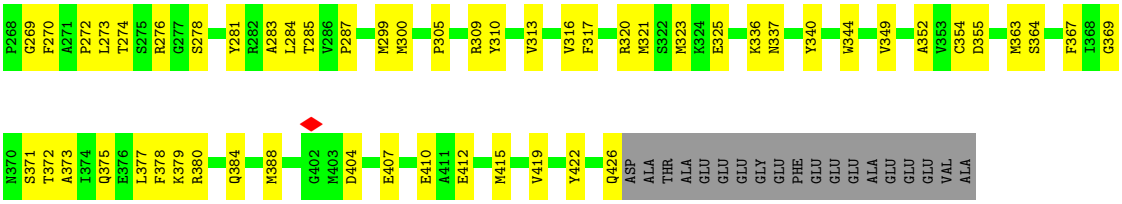
Chain TB:



• Molecule 9: Tubulin beta-4B chain

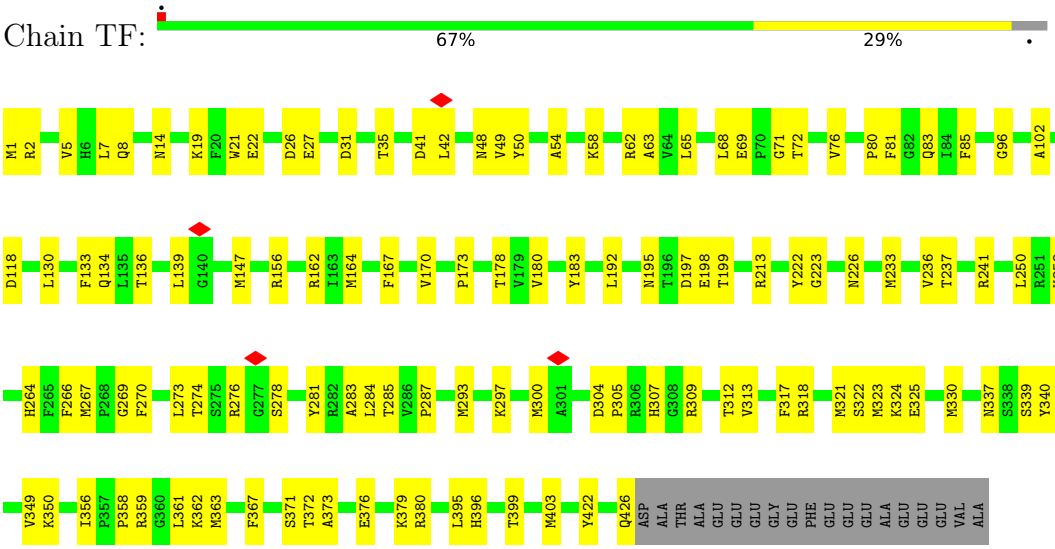
Chain TD:





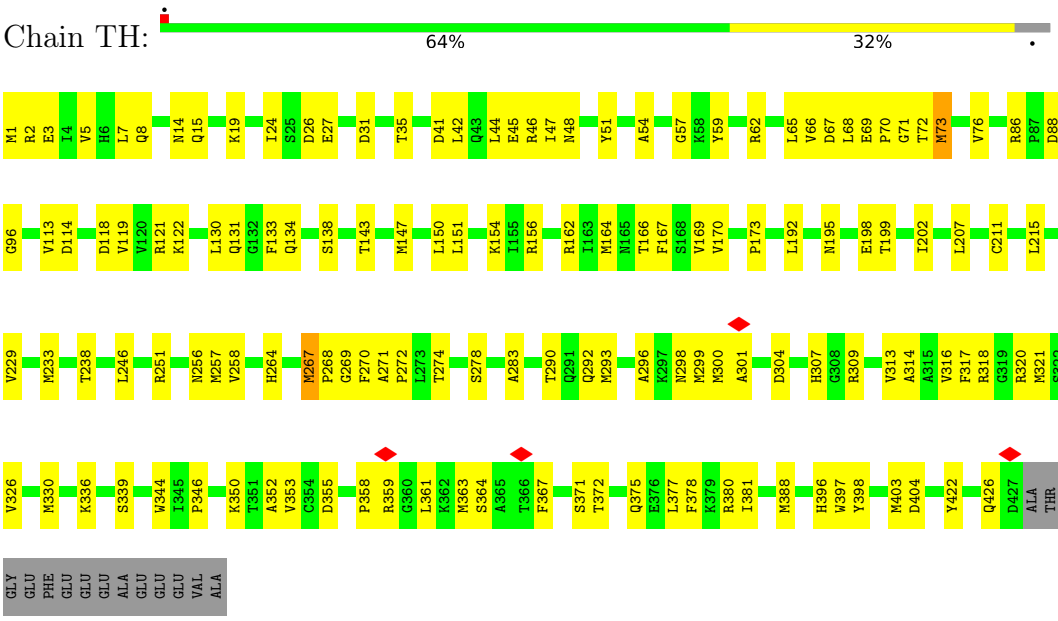
• Molecule 9: Tubulin beta-4B chain

Chain TF:



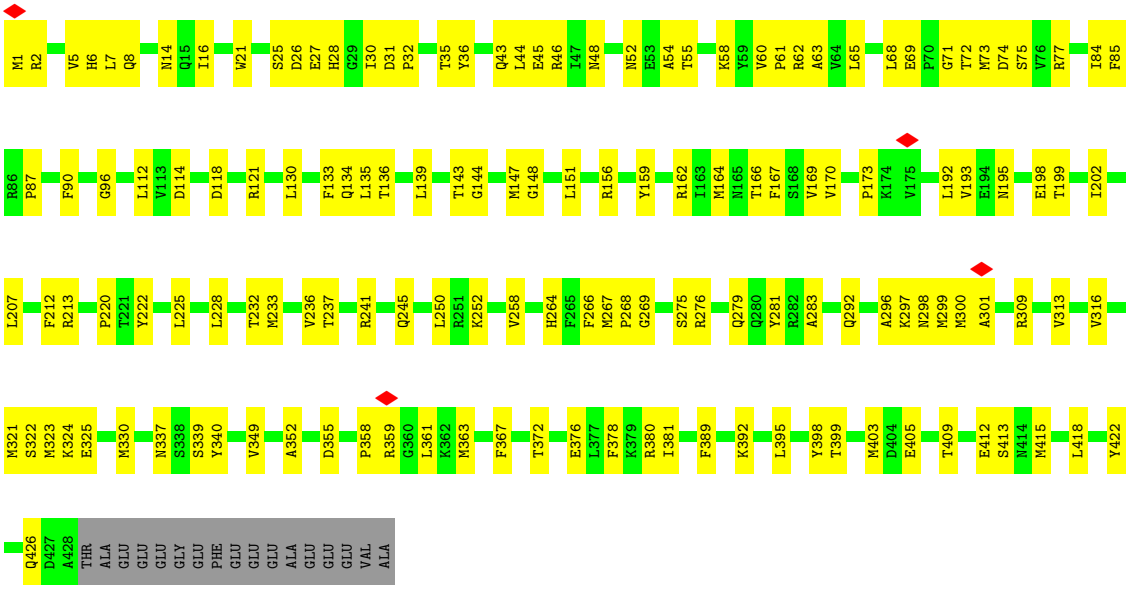
• Molecule 9: Tubulin beta-4B chain

Chain TH:



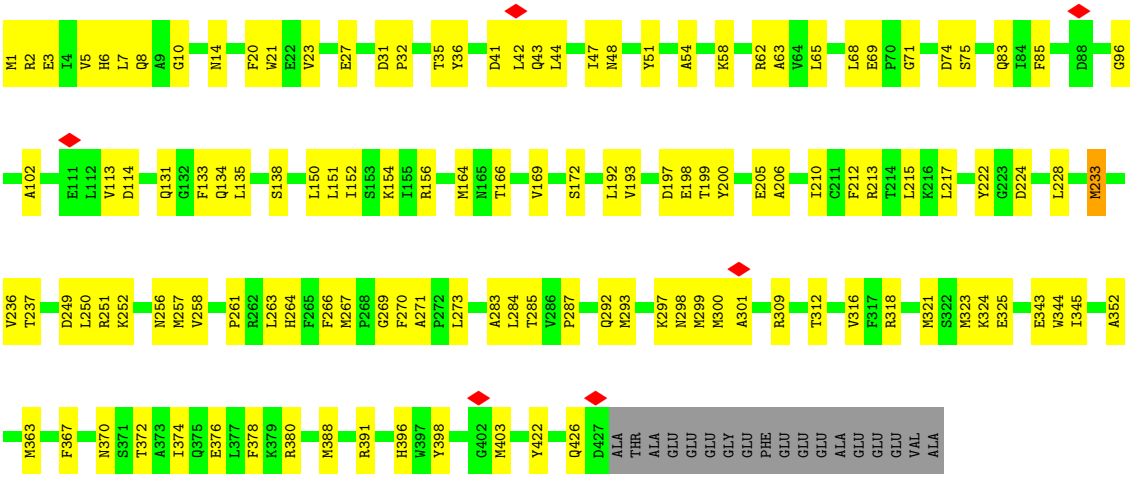
• Molecule 9: Tubulin beta-4B chain

Chain TJ:



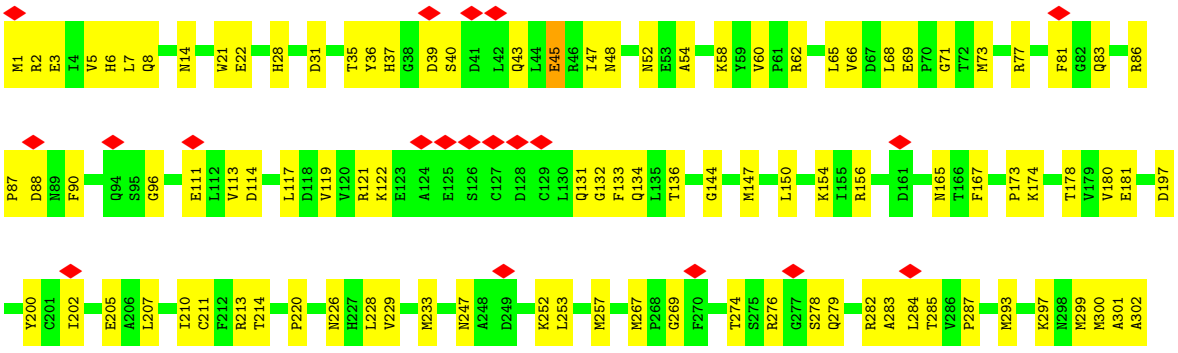
• Molecule 9: Tubulin beta-4B chain

Chain TL:



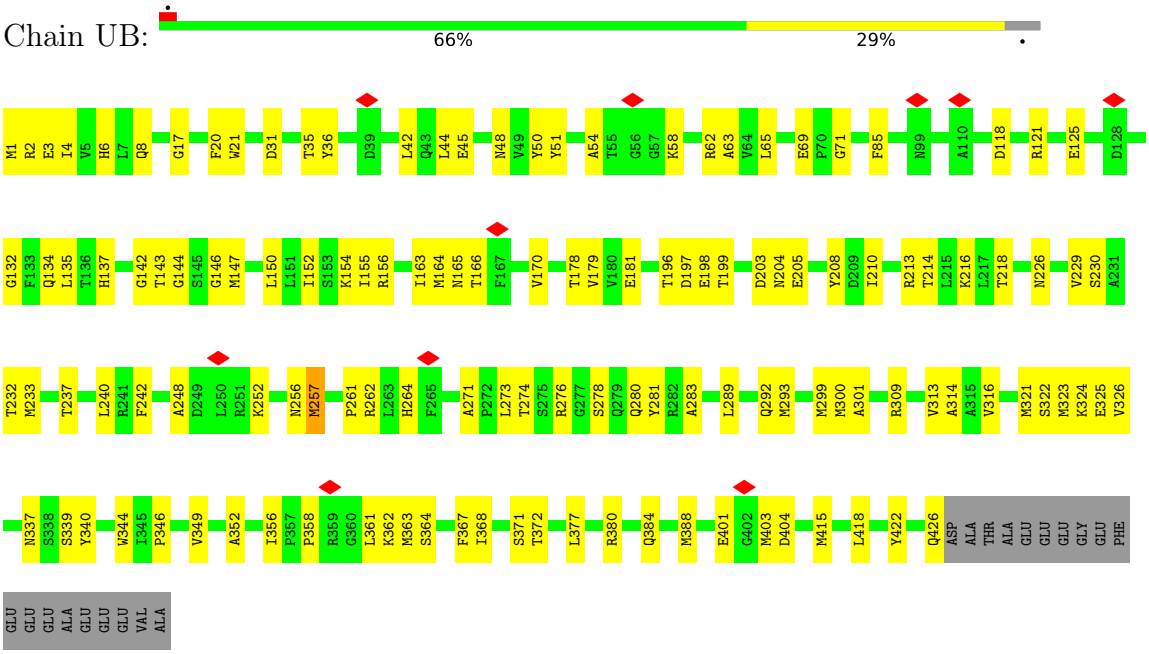
• Molecule 9: Tubulin beta-4B chain

Chain TN:



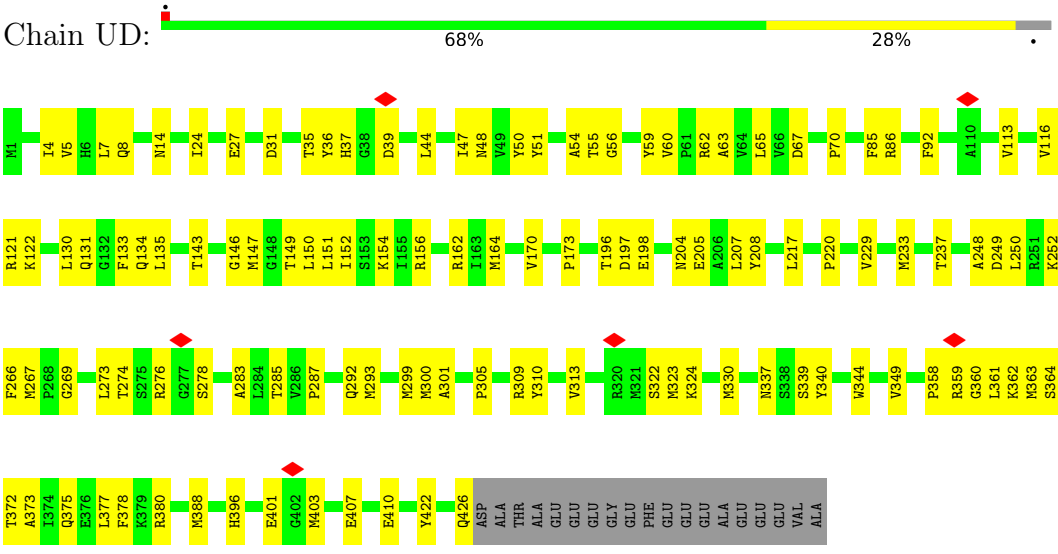
• Molecule 9: Tubulin beta-4B chain

Chain UB:



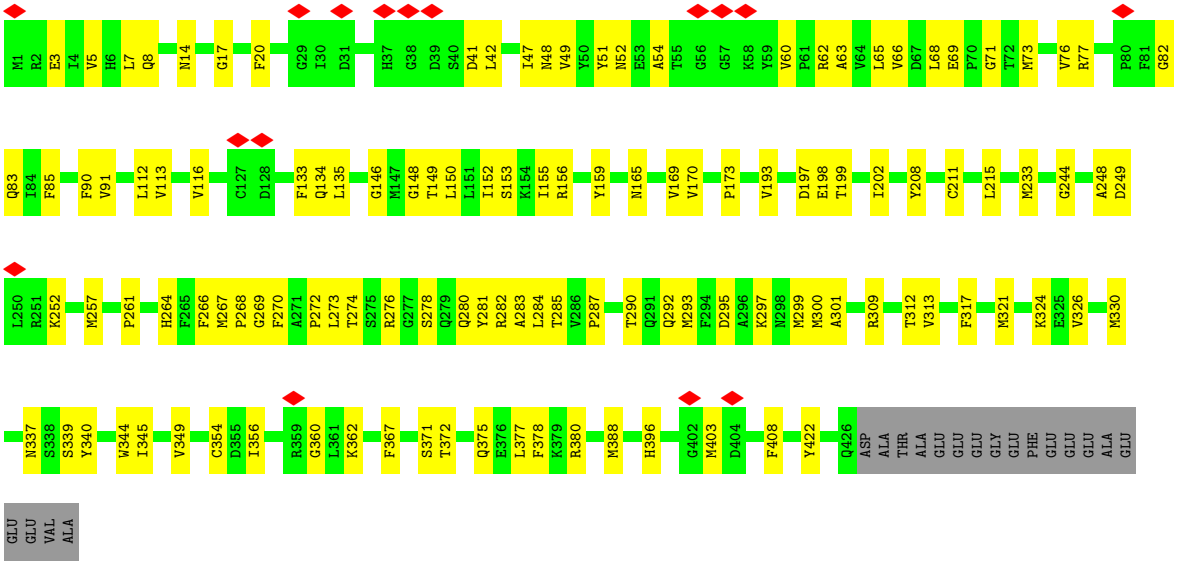
• Molecule 9: Tubulin beta-4B chain

Chain UD:



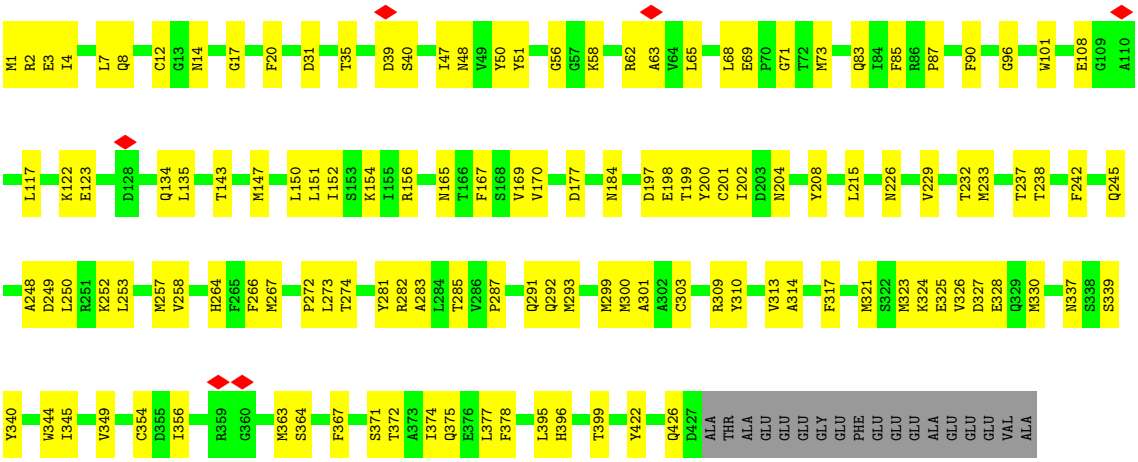
• Molecule 9: Tubulin beta-4B chain

Chain UF:



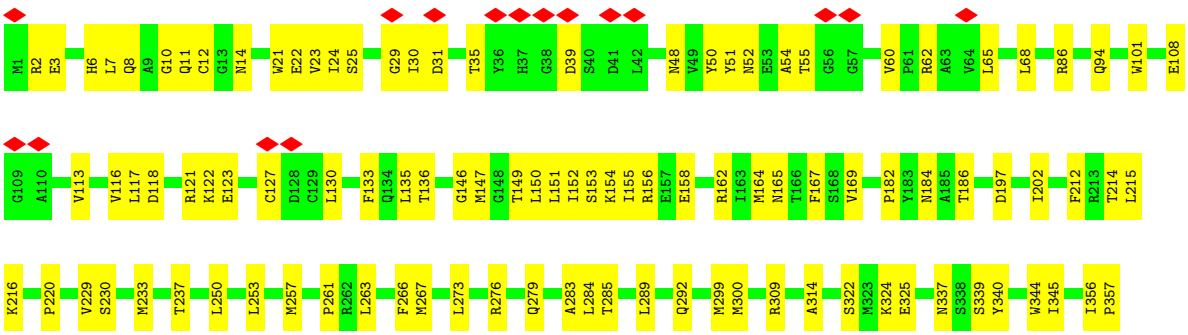
• Molecule 9: Tubulin beta-4B chain

Chain UH:



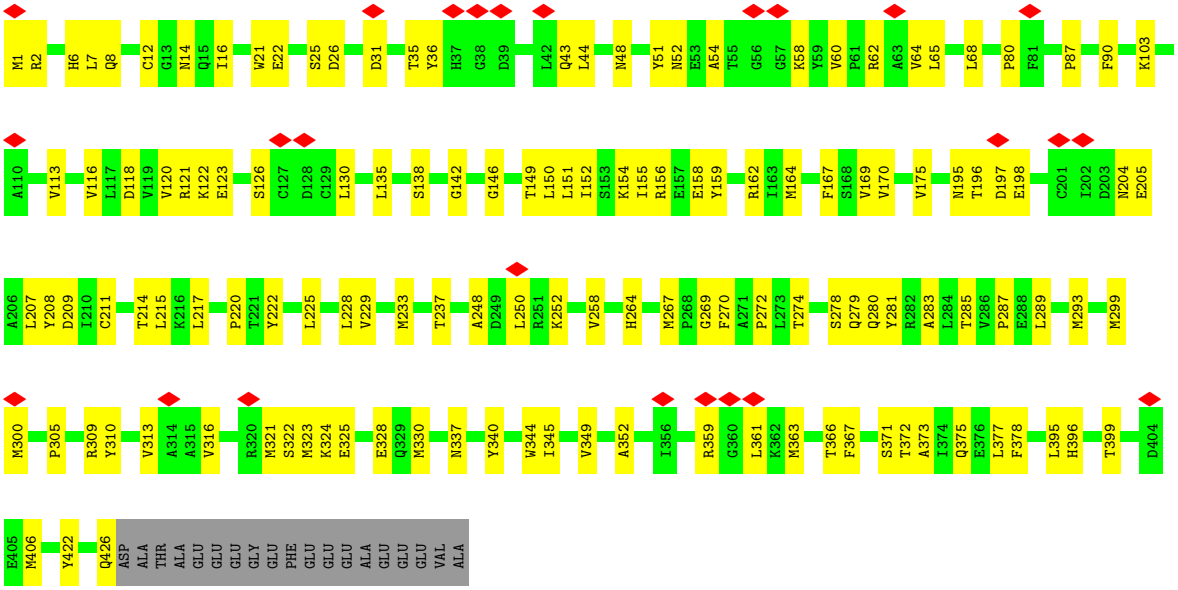
• Molecule 9: Tubulin beta-4B chain

Chain UJ:



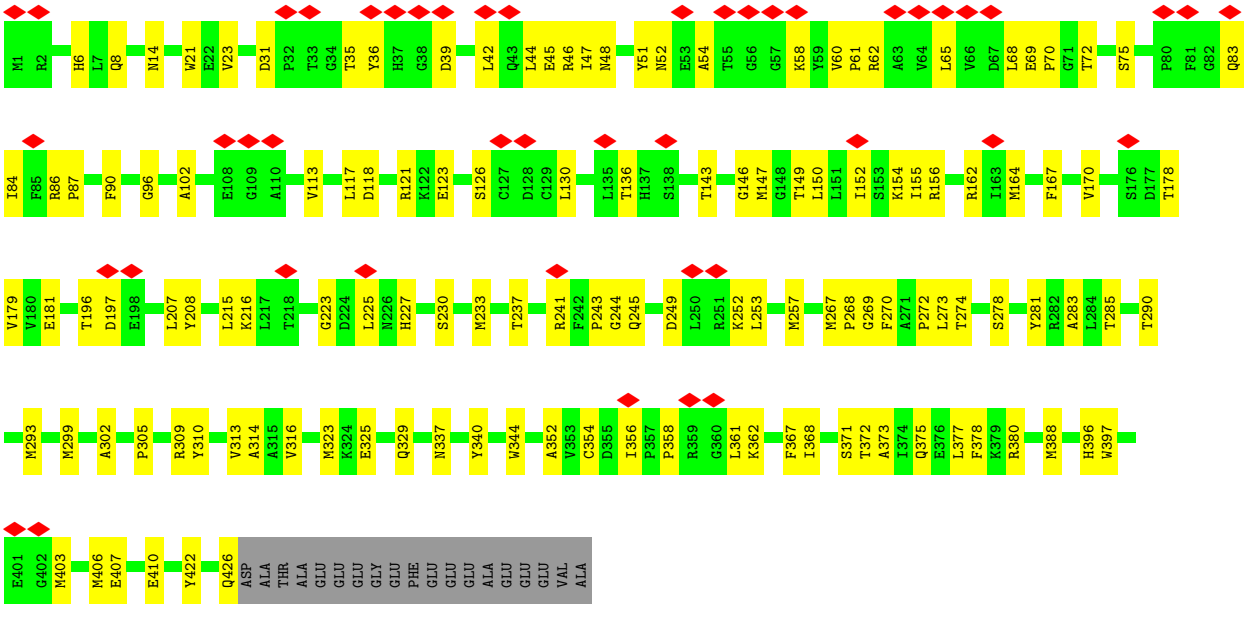
• Molecule 9: Tubulin beta-4B chain

Chain UL:



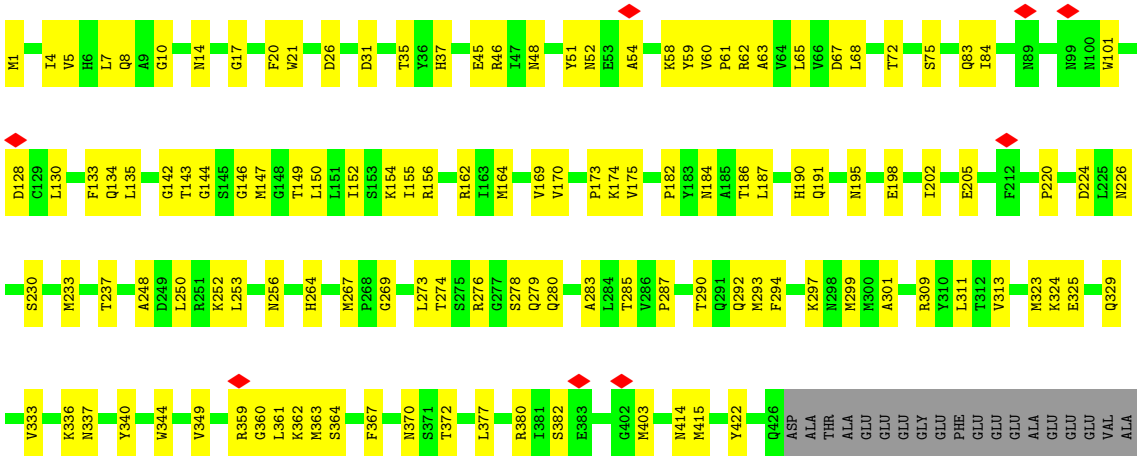
• Molecule 9: Tubulin beta-4B chain

Chain UN:



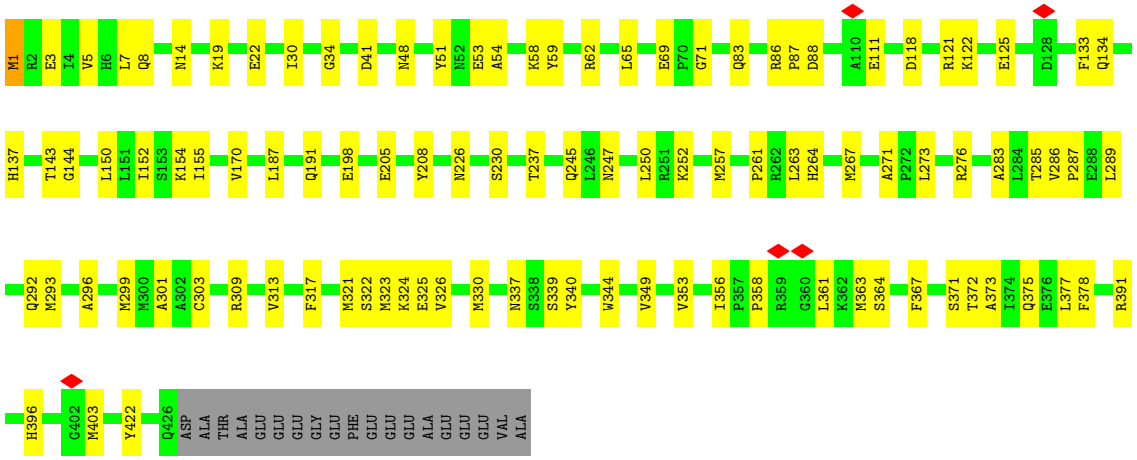
• Molecule 9: Tubulin beta-4B chain

Chain VB:



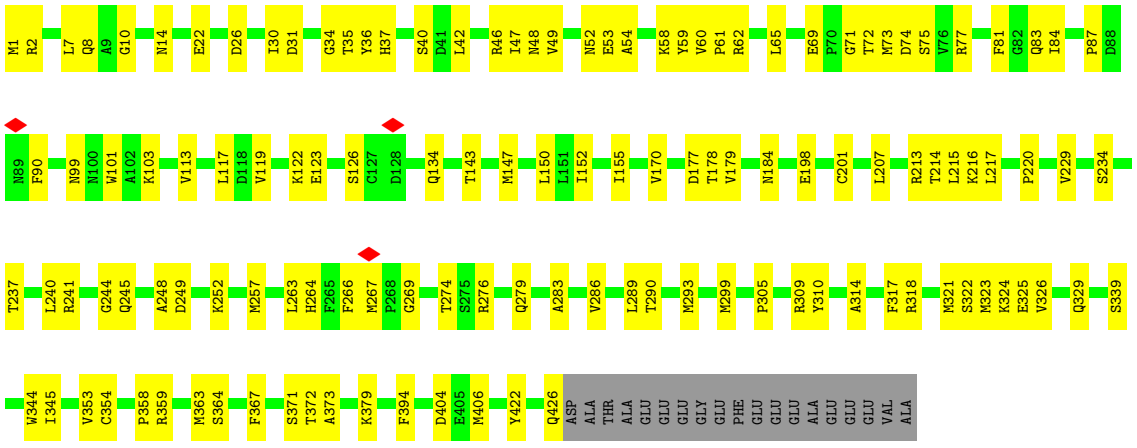
• Molecule 9: Tubulin beta-4B chain

Chain VD:



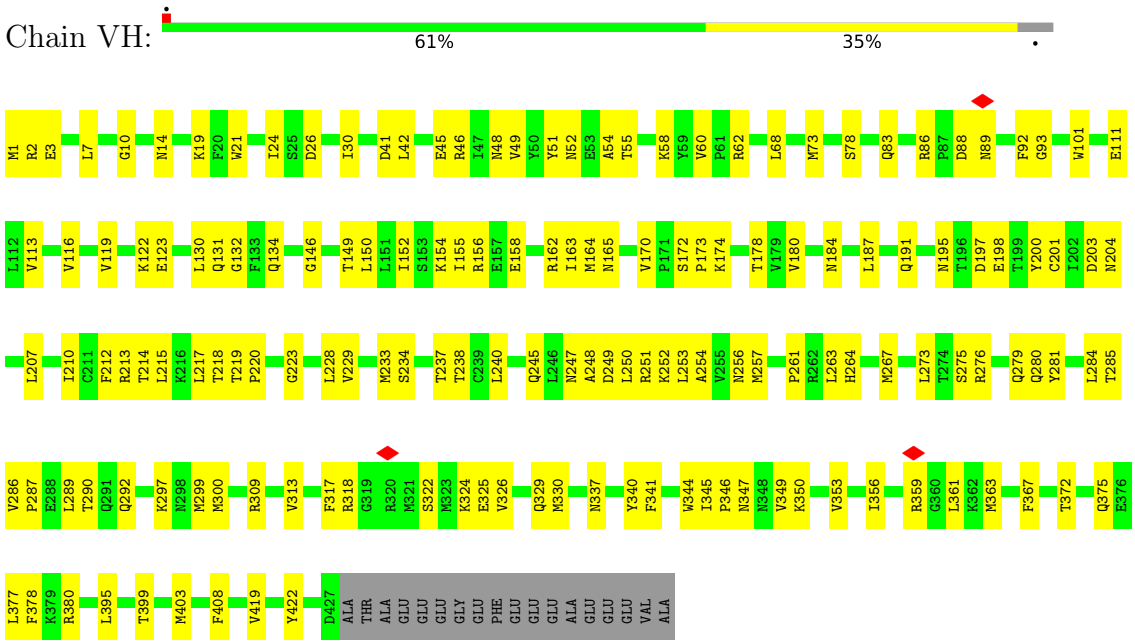
• Molecule 9: Tubulin beta-4B chain

Chain VF:



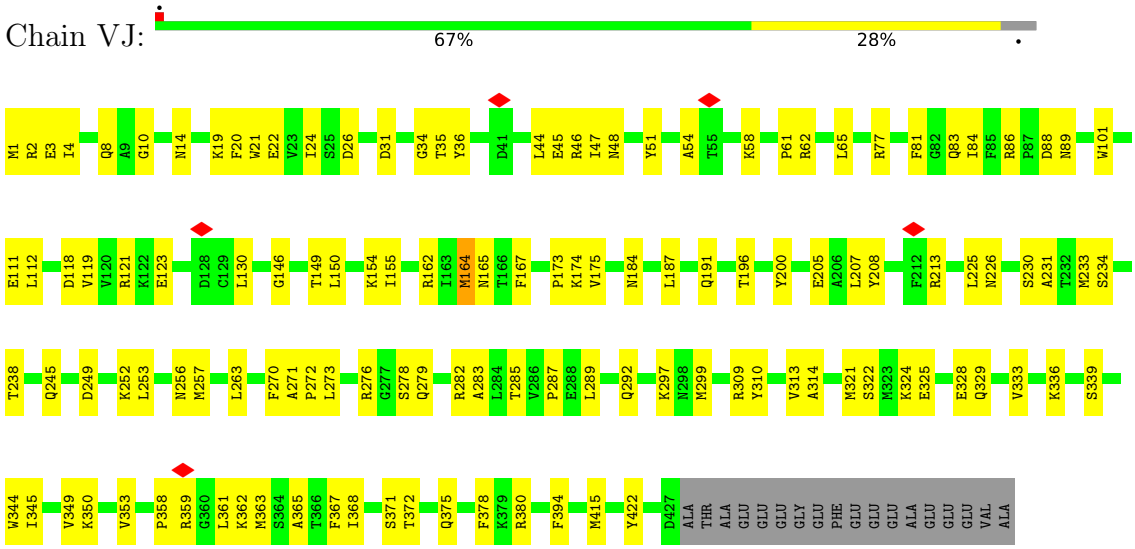
• Molecule 9: Tubulin beta-4B chain

Chain VH:



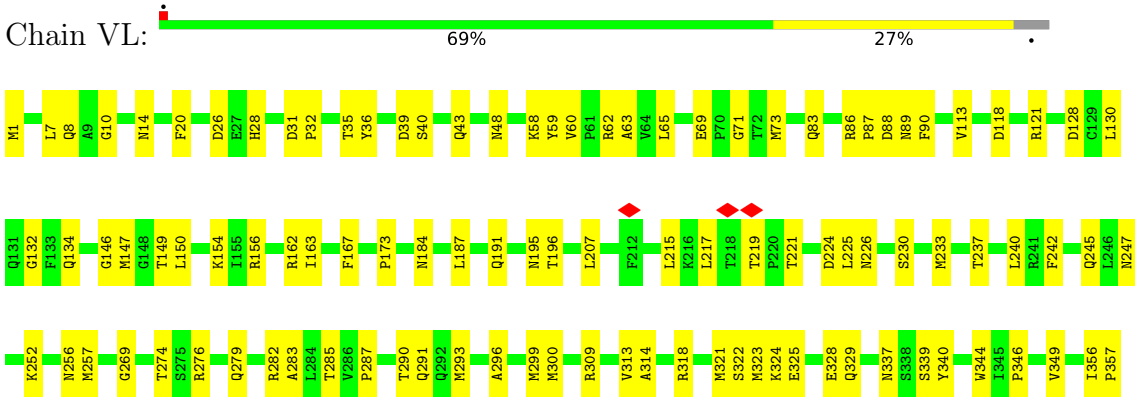
• Molecule 9: Tubulin beta-4B chain

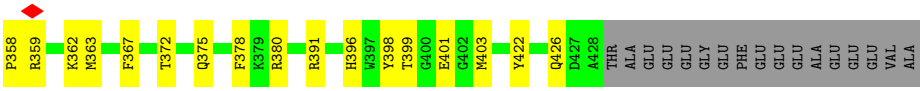
Chain VJ:



• Molecule 9: Tubulin beta-4B chain

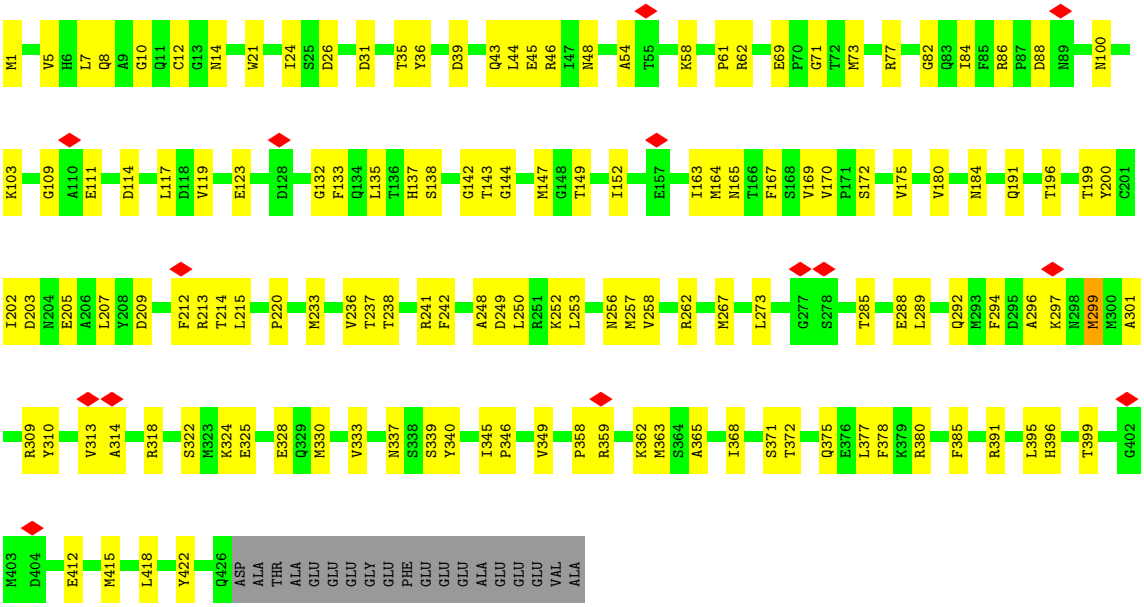
Chain VL:





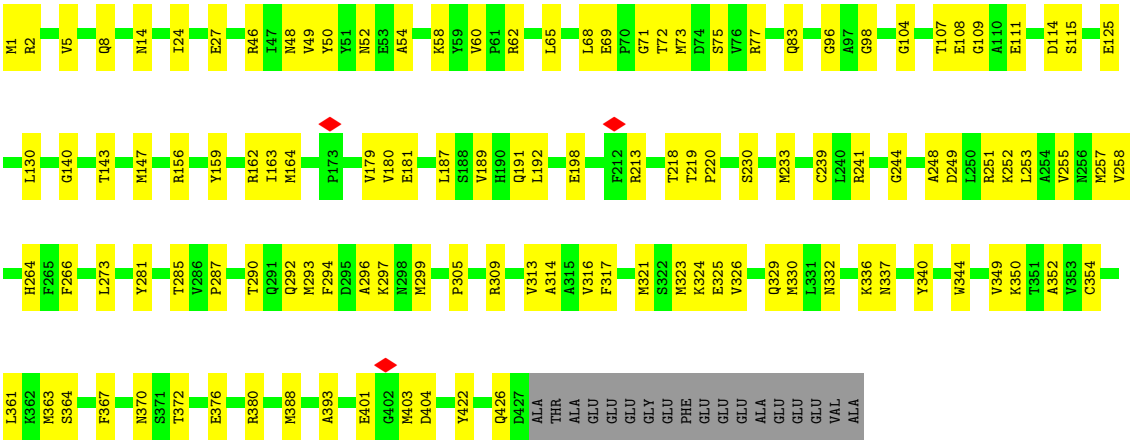
• Molecule 9: Tubulin beta-4B chain

Chain VN:



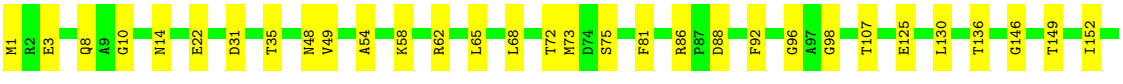
• Molecule 9: Tubulin beta-4B chain

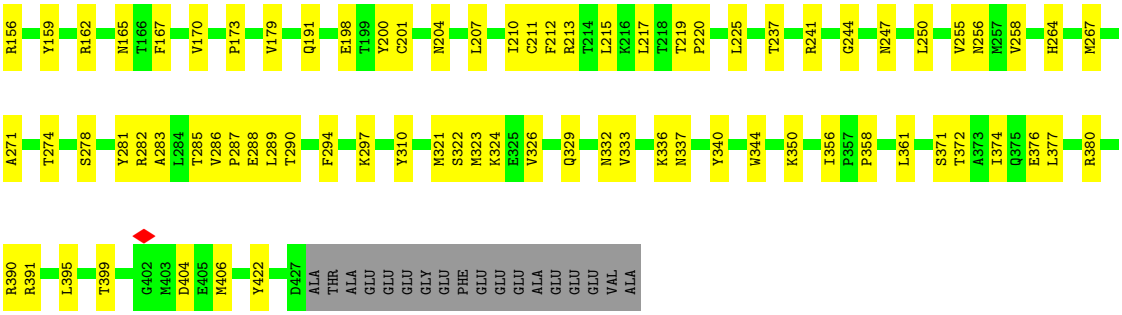
Chain WB:



• Molecule 9: Tubulin beta-4B chain

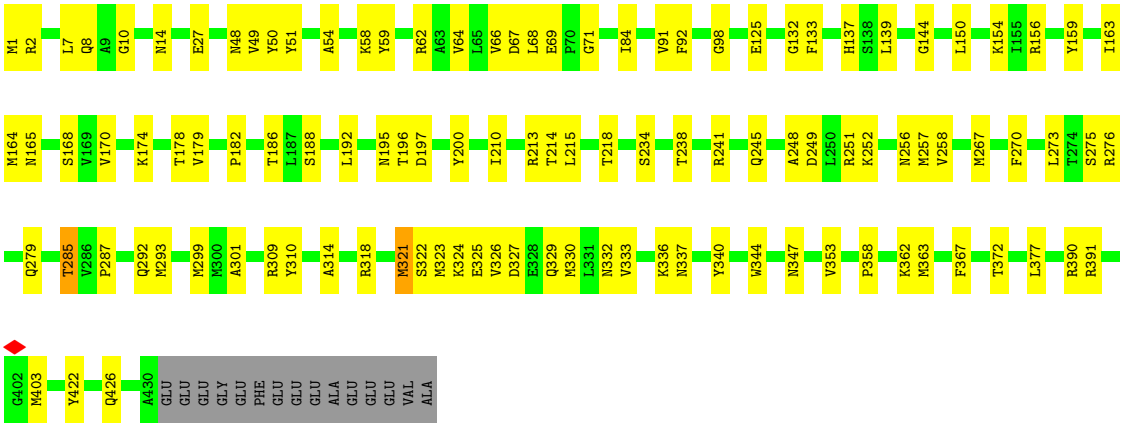
Chain WD:





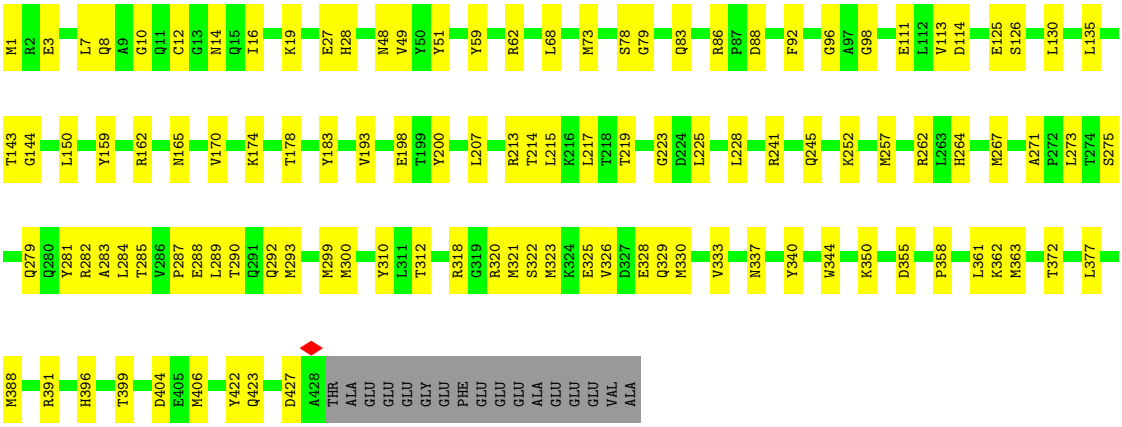
• Molecule 9: Tubulin beta-4B chain

Chain WF:



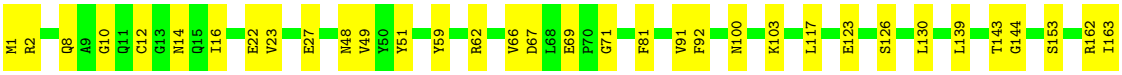
• Molecule 9: Tubulin beta-4B chain

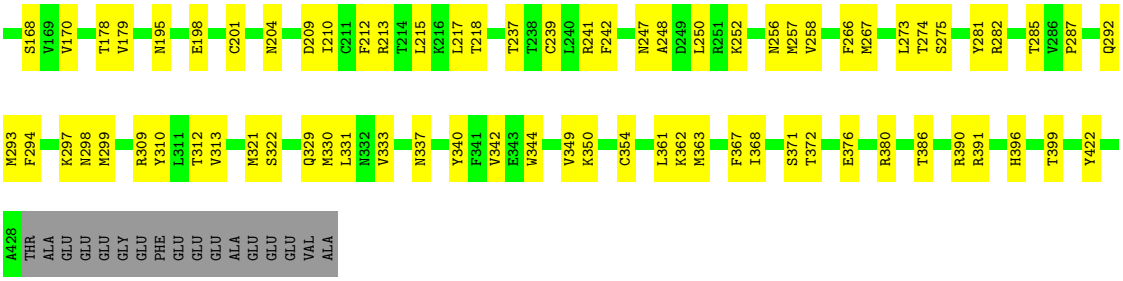
Chain WH:



• Molecule 9: Tubulin beta-4B chain

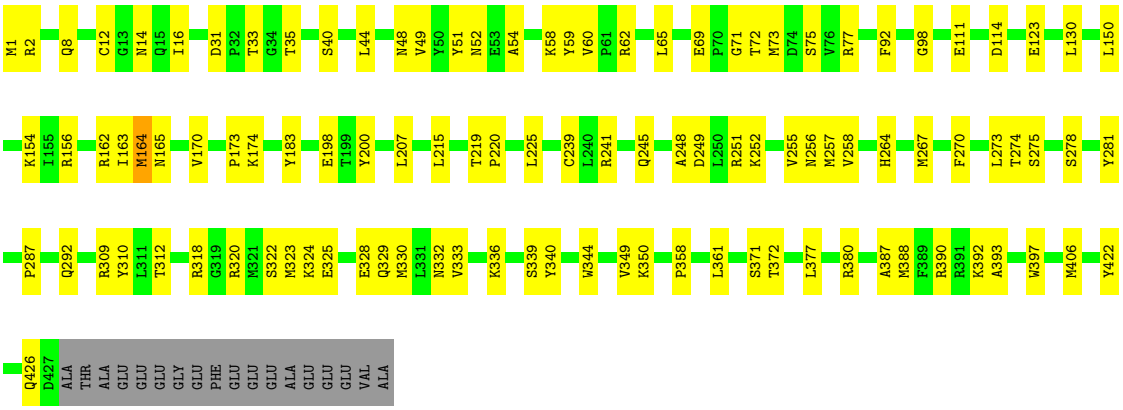
Chain WJ:





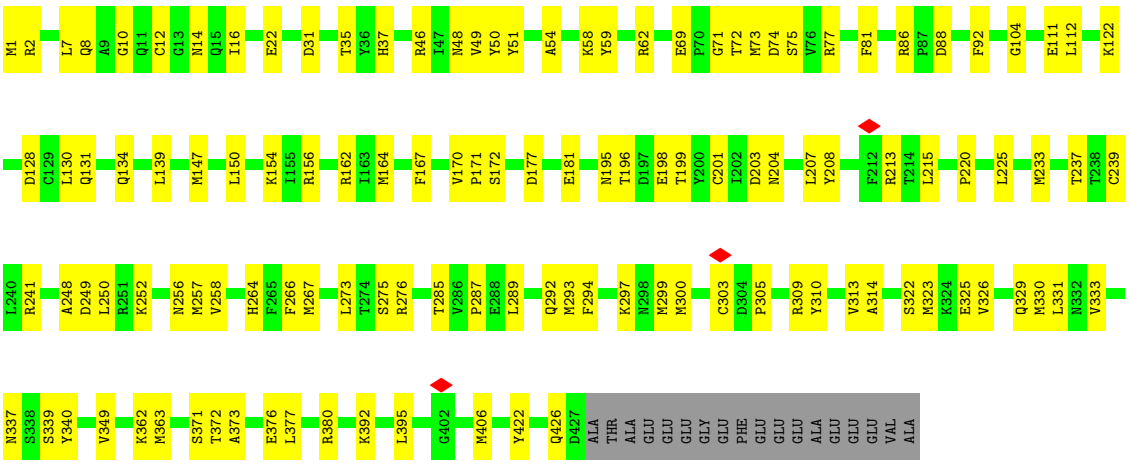
• Molecule 9: Tubulin beta-4B chain

Chain WL:



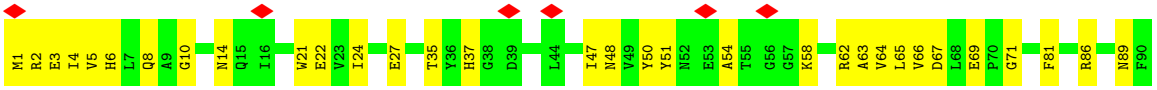
• Molecule 9: Tubulin beta-4B chain

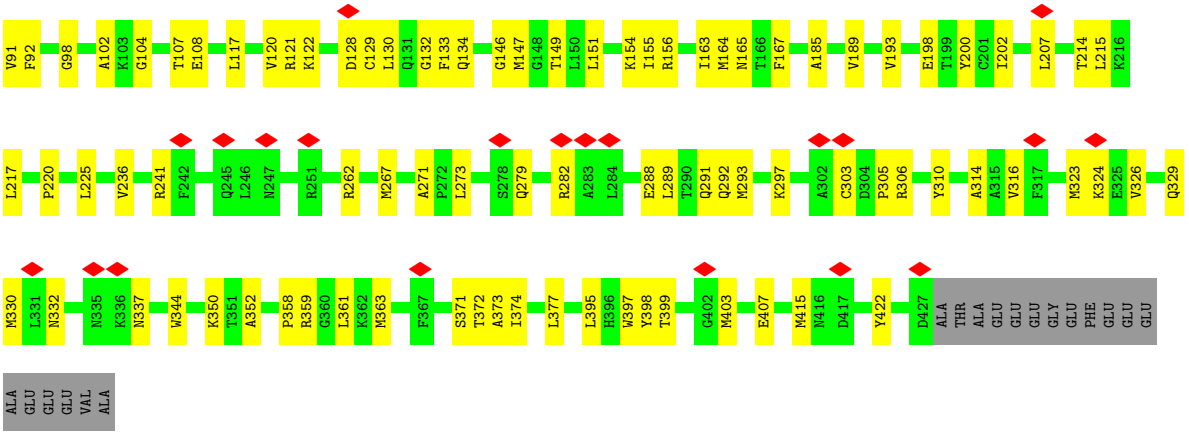
Chain WN:



• Molecule 9: Tubulin beta-4B chain

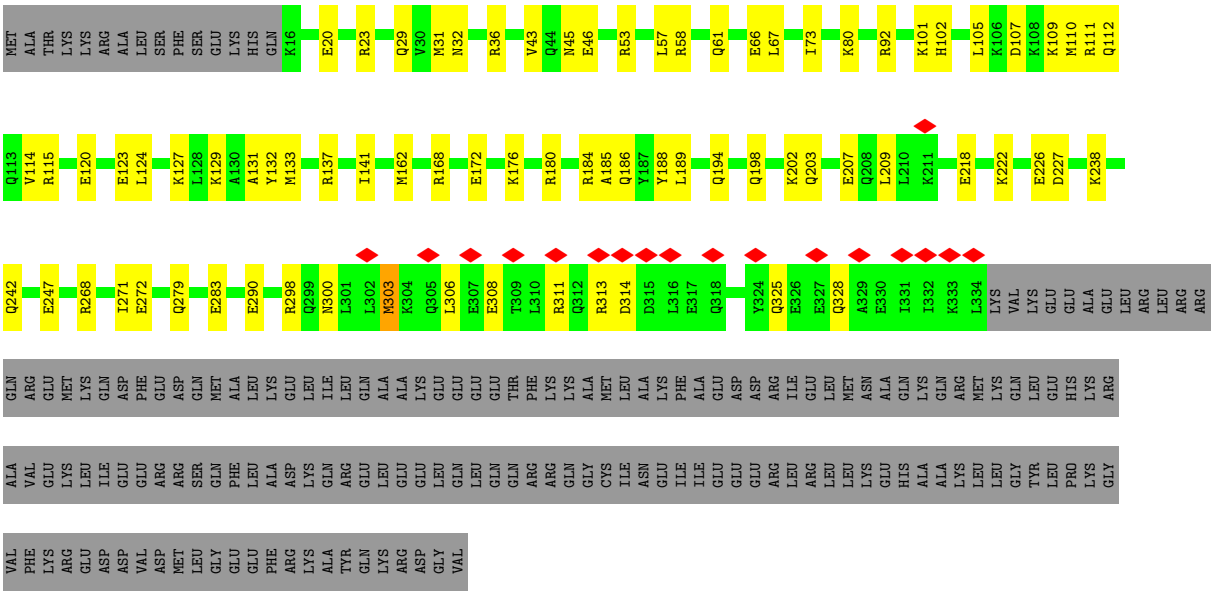
Chain WP:





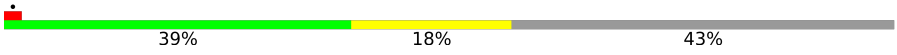
• Molecule 10: Meiosis-specific nuclear structural protein 1

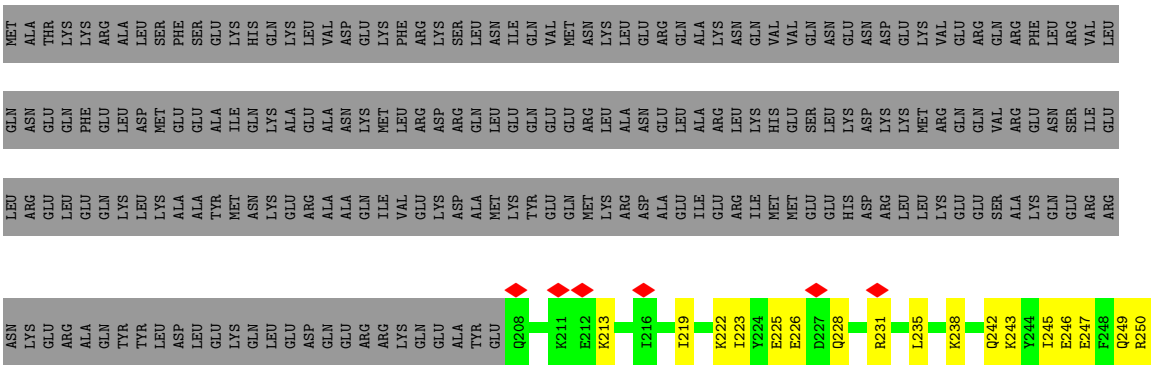
Chain B:

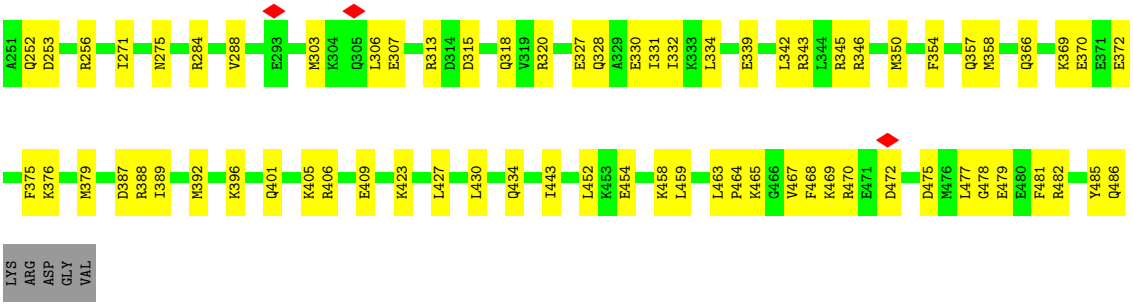


• Molecule 10: Meiosis-specific nuclear structural protein 1

Chain C:

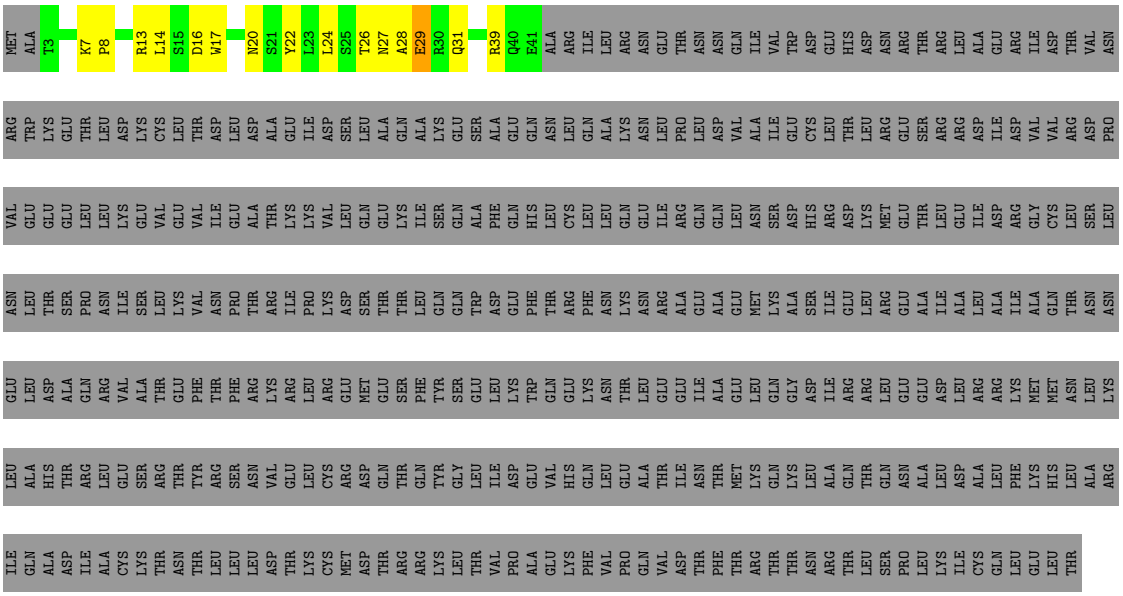






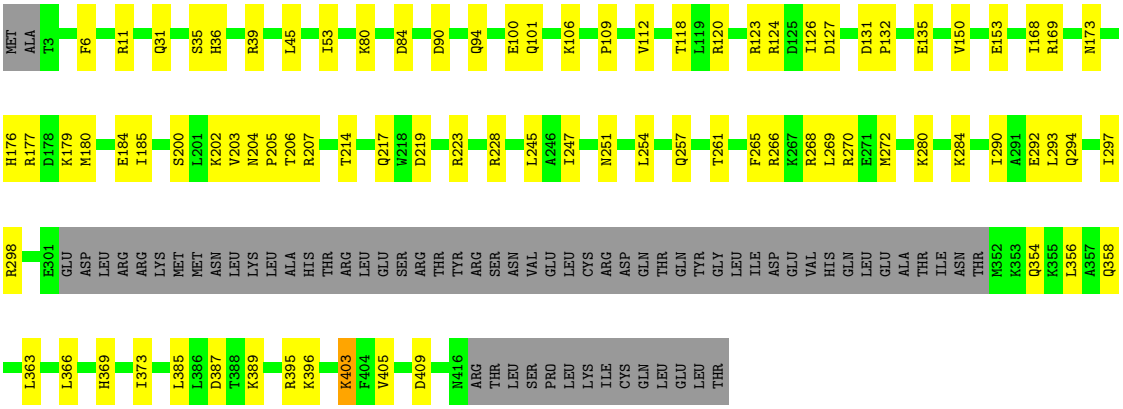
• Molecule 11: Tektin-2

Chain B0:



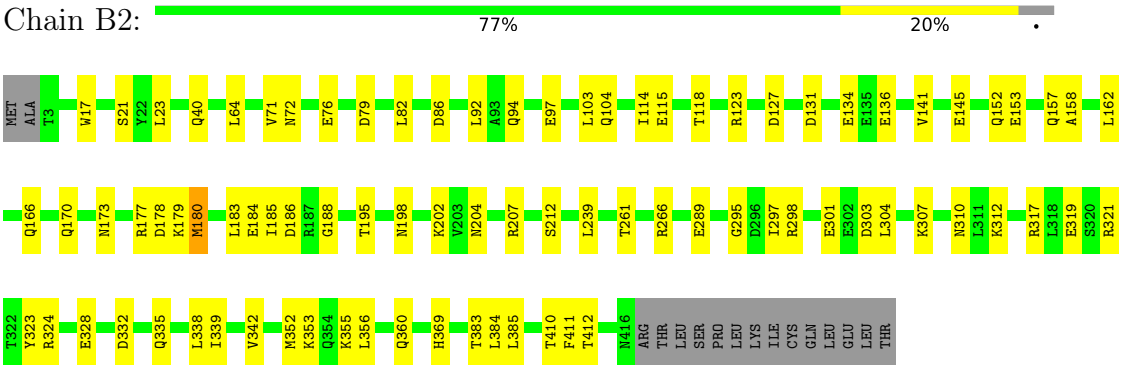
• Molecule 11: Tektin-2

Chain B1:



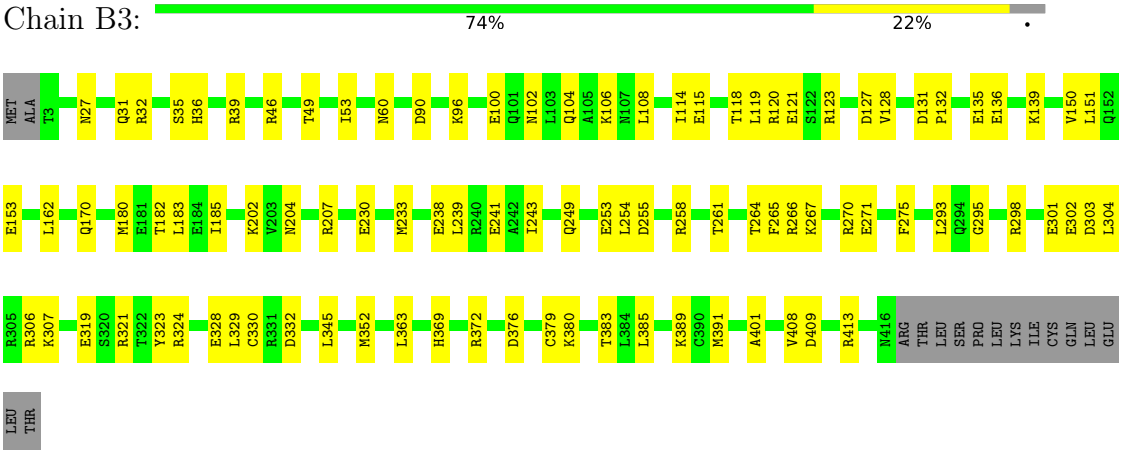
• Molecule 11: Tektin-2

Chain B2:



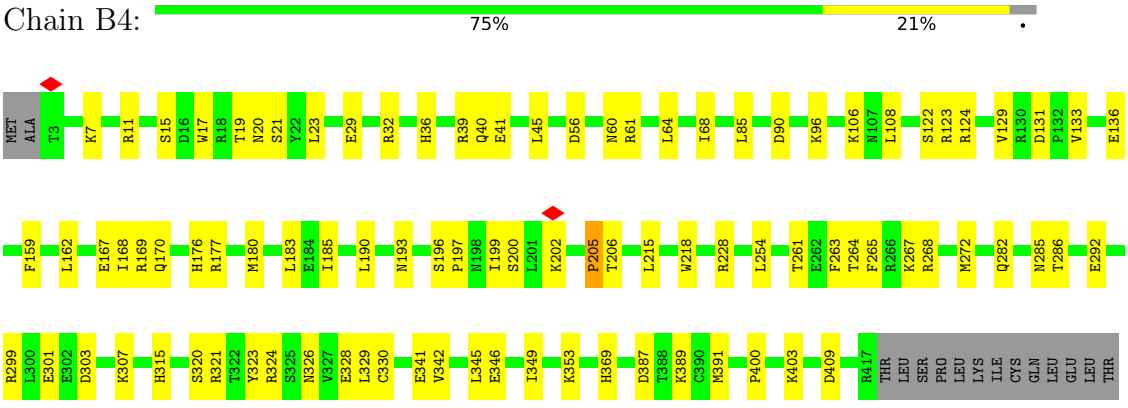
• Molecule 11: Tektin-2

Chain B3:



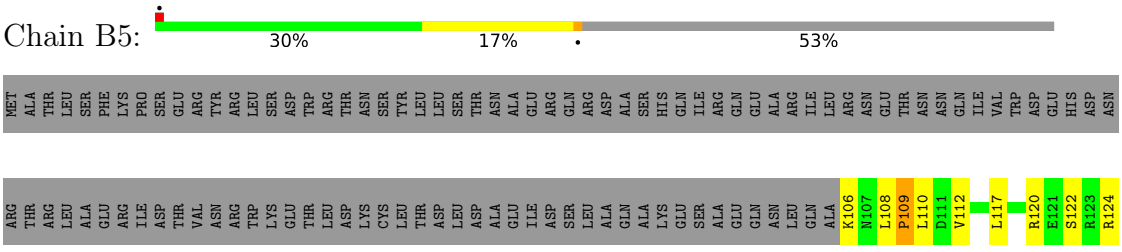
• Molecule 11: Tektin-2

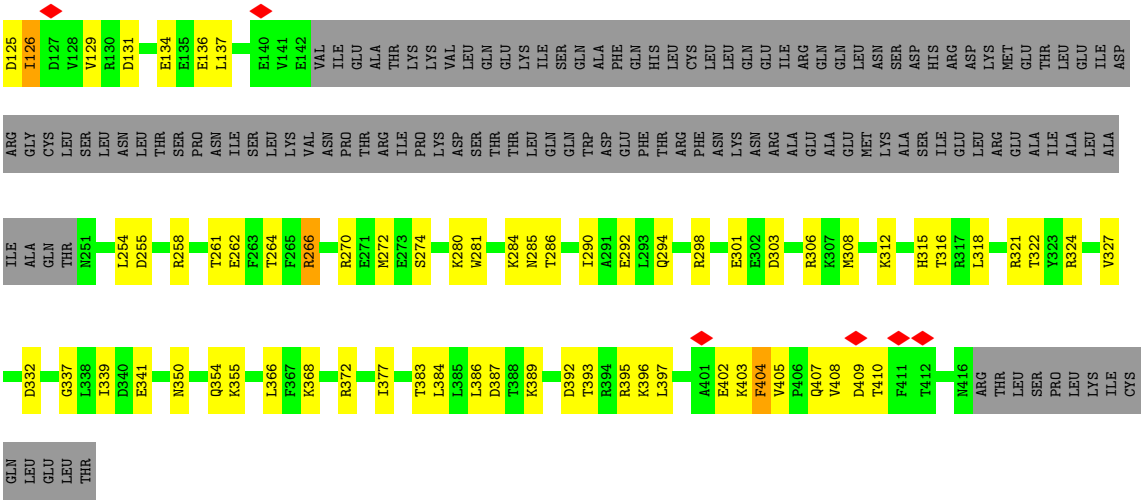
Chain B4:



• Molecule 11: Tektin-2

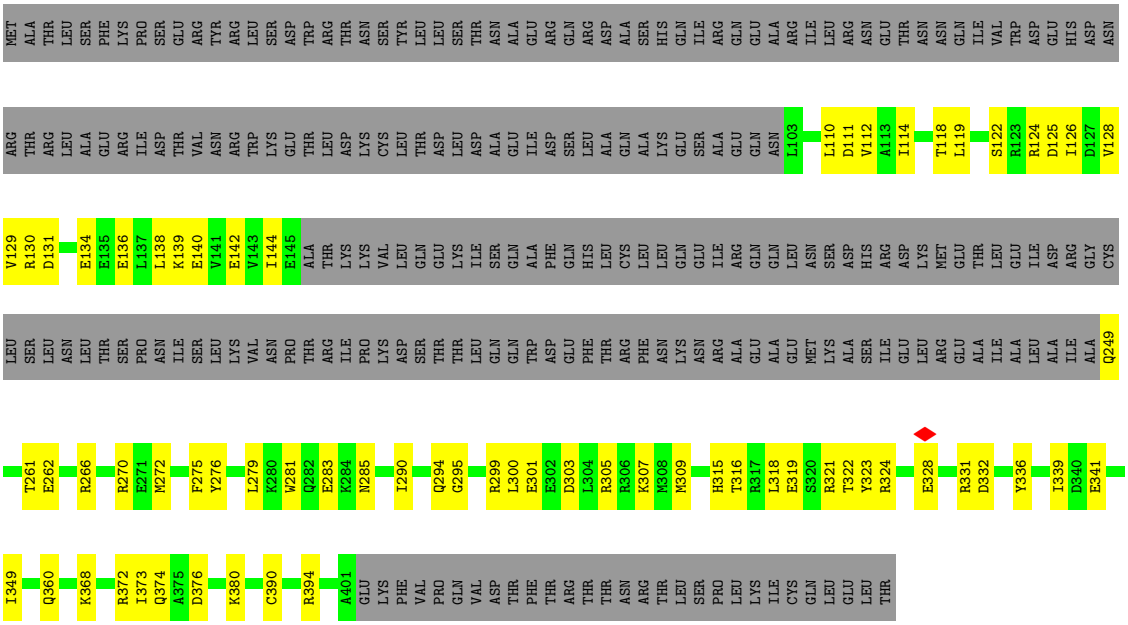
Chain B5:





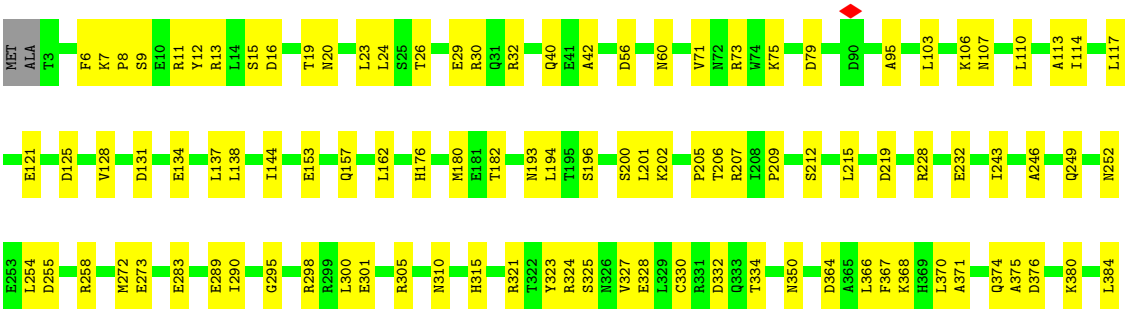
• Molecule 11: Tektin-2

Chain R0:



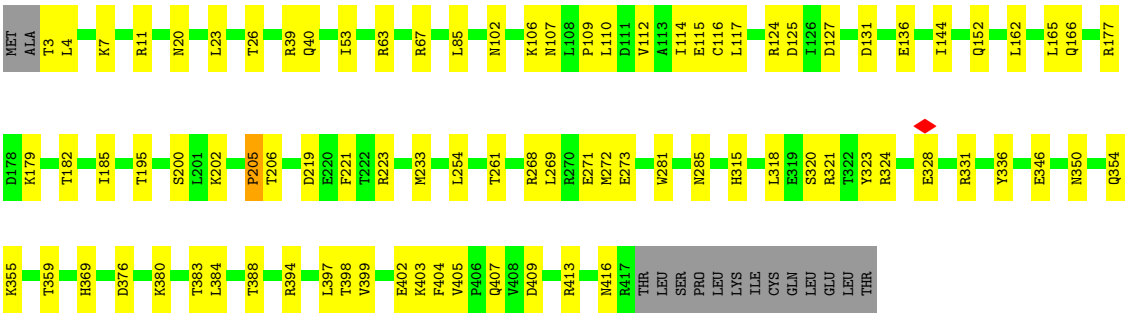
• Molecule 11: Tektin-2

Chain R1:



• Molecule 11: Tektin-2

Chain R2:

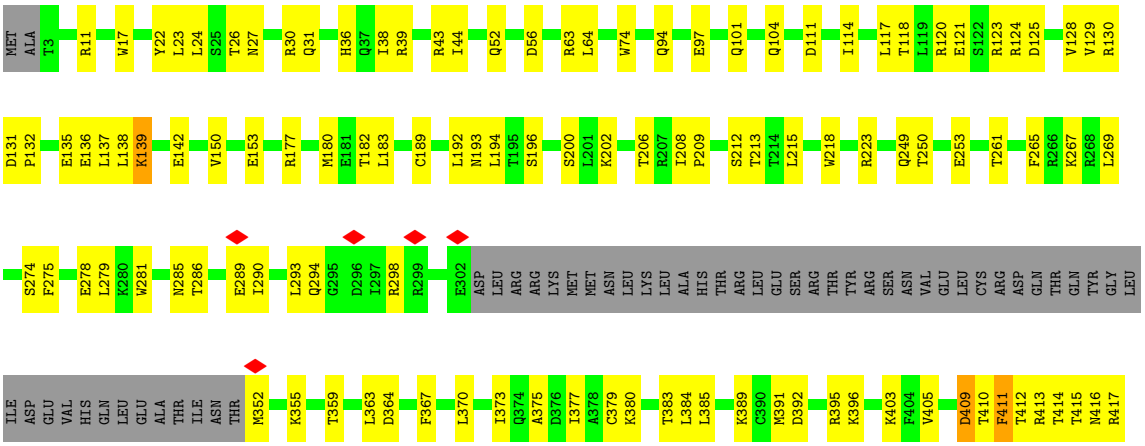


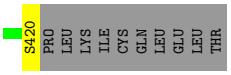
• Molecule 11: Tektin-2

Chain R3:

• Molecule 11: Tektin-2

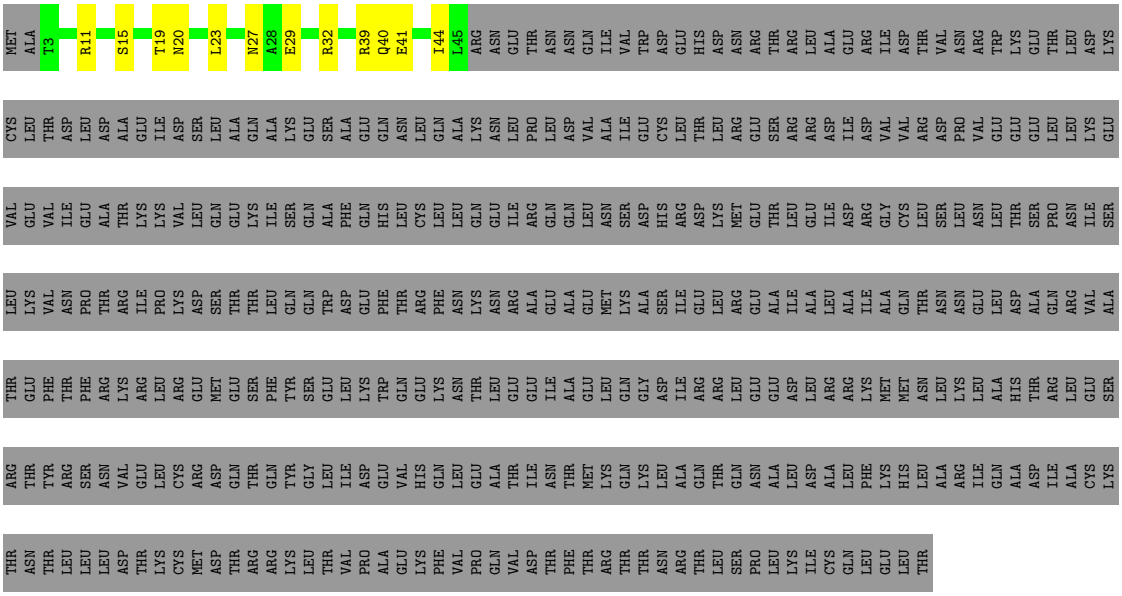
Chain R4:





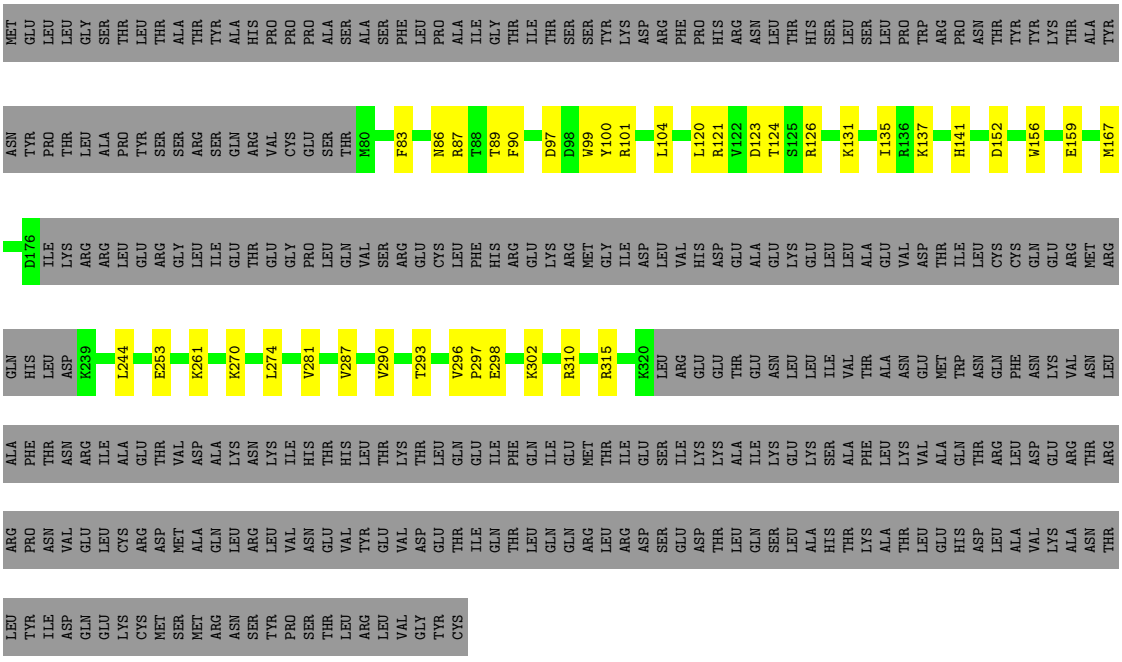
- Molecule 11: Tektin-2

Chain R5:



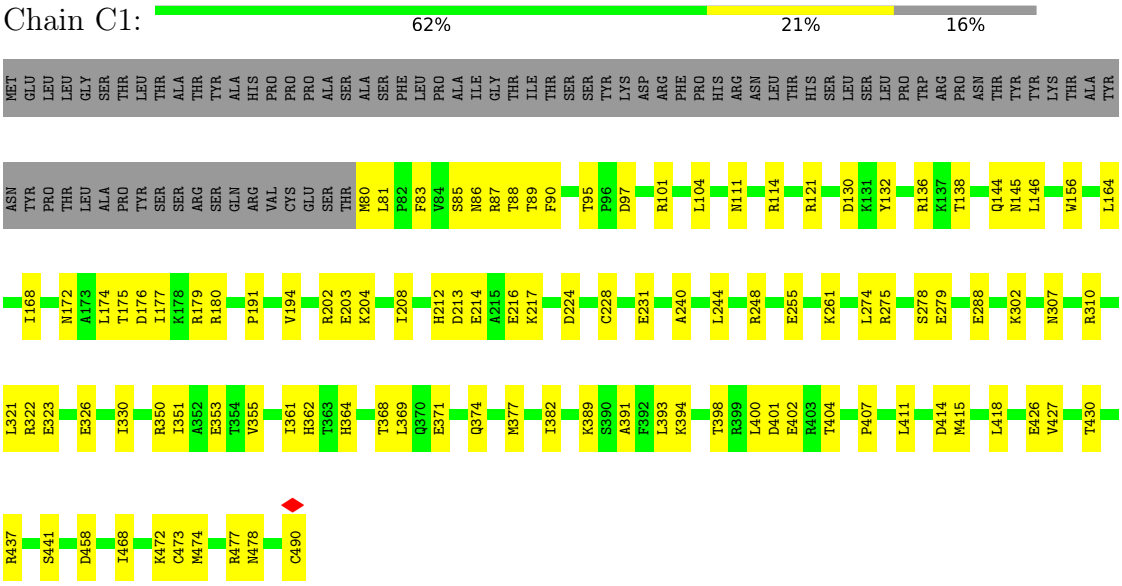
- Molecule 12: Tektin-3

Chain C0:



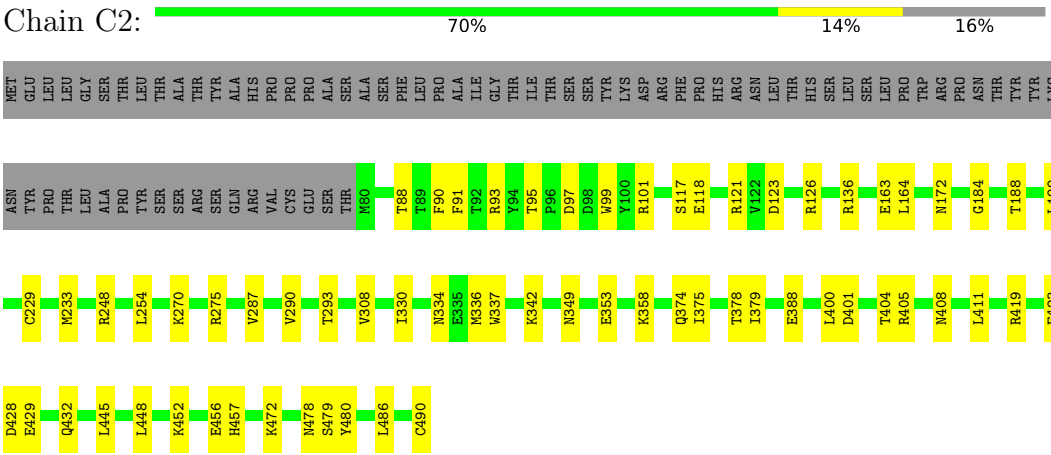
- Molecule 12: Tektin-3

Chain C1:



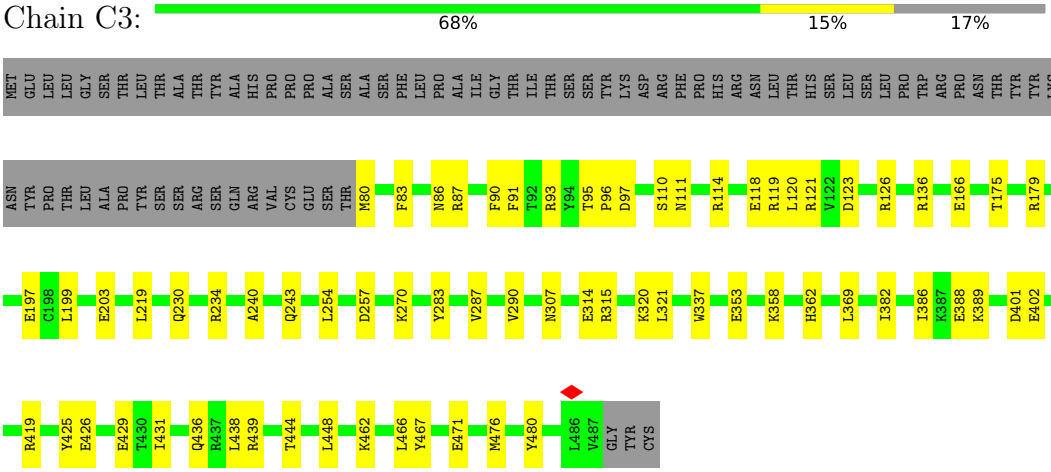
• Molecule 12: Tektin-3

Chain C2:



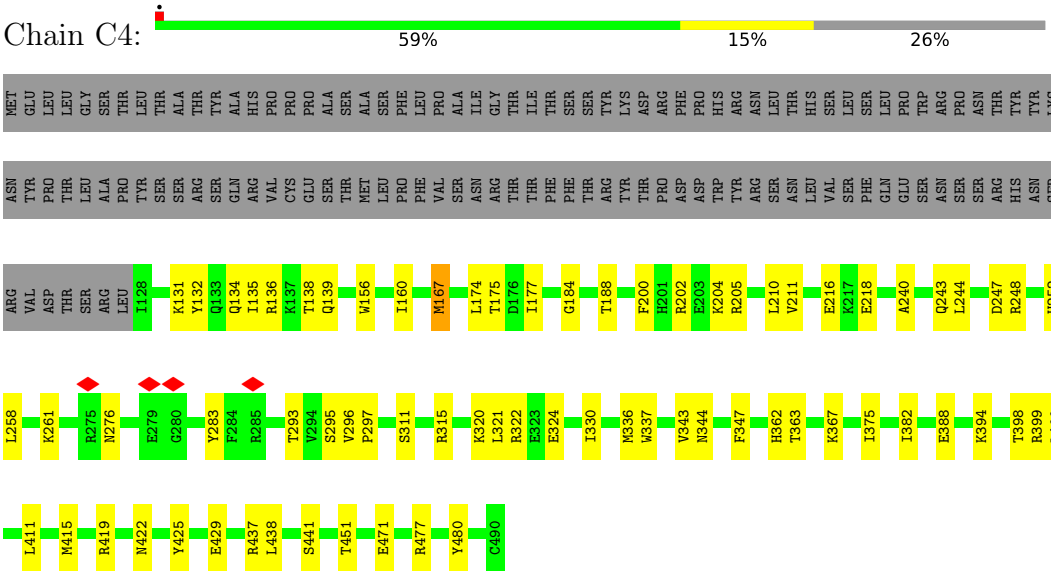
• Molecule 12: Tektin-3

Chain C3:



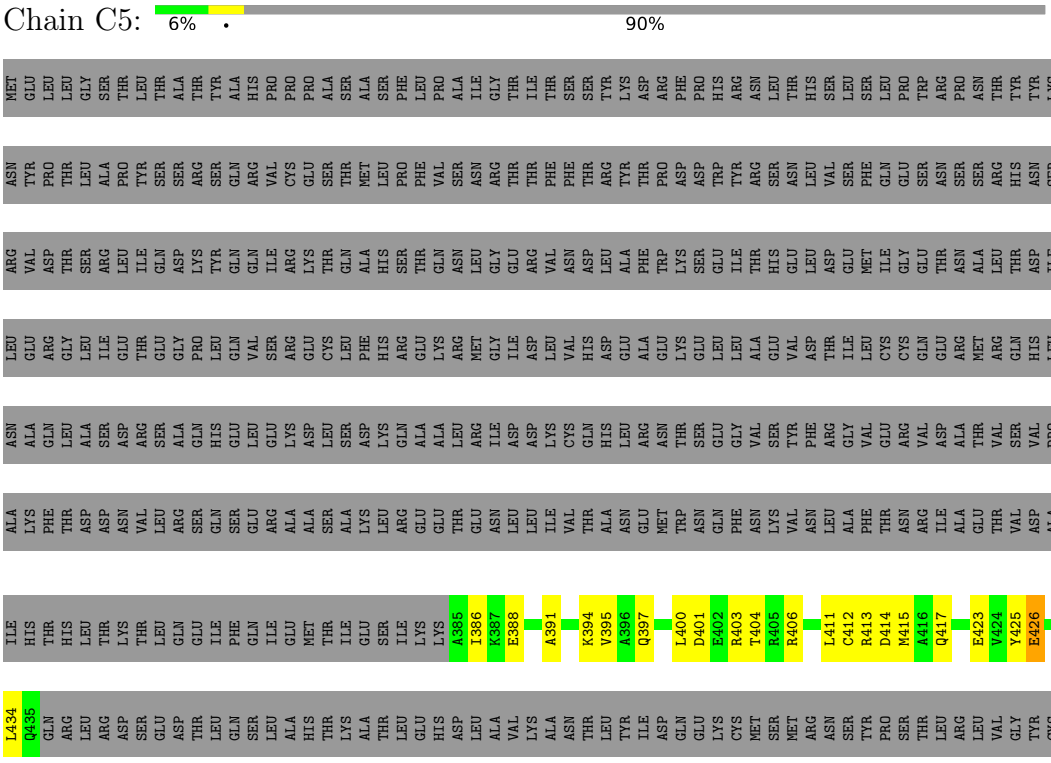
• Molecule 12: Tektin-3

Chain C4:



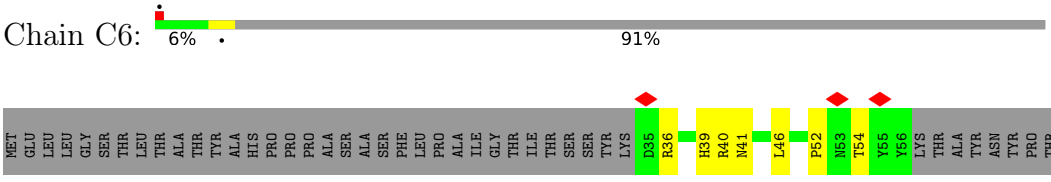
• Molecule 12: Tektin-3

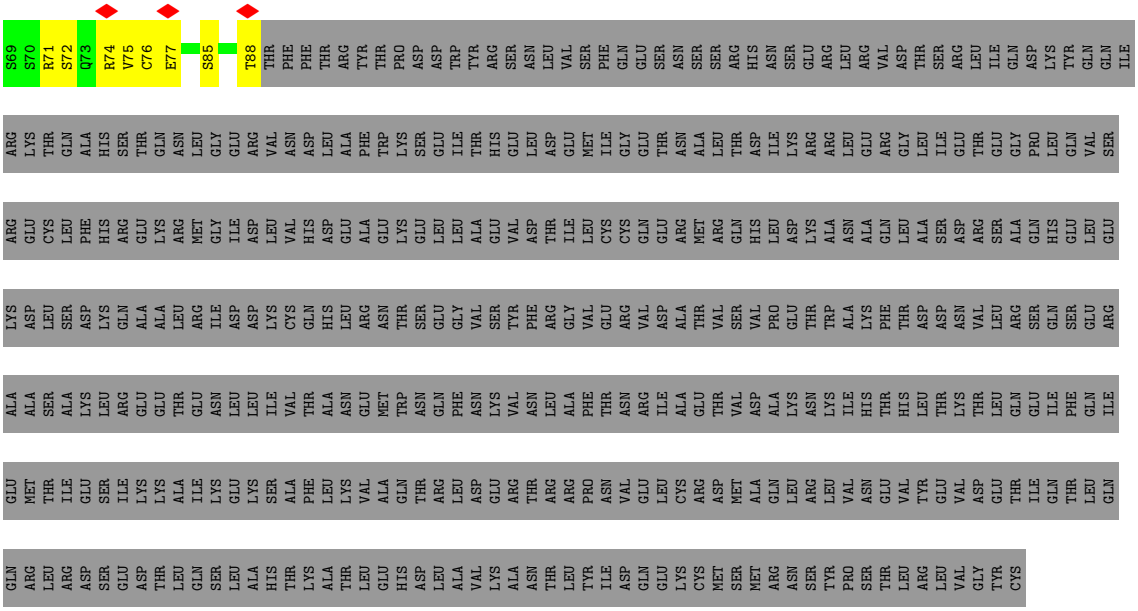
Chain C5:



• Molecule 12: Tektin-3

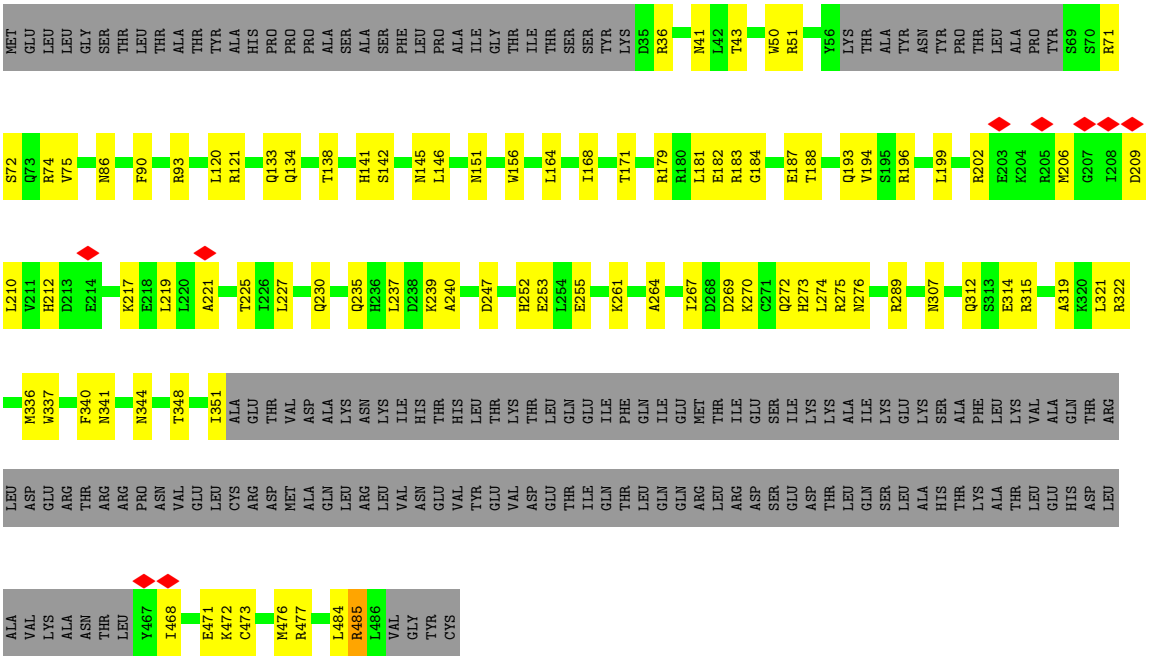
Chain C6:





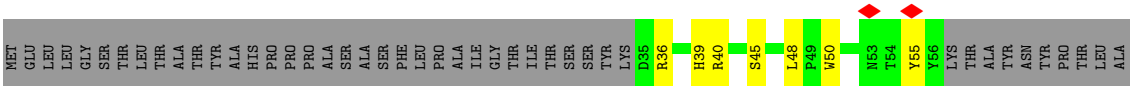
• Molecule 12: Tektin-3

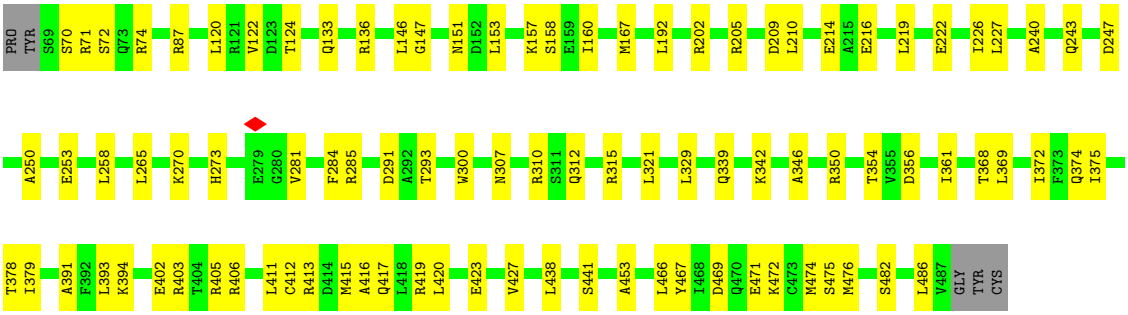
Chain S0:



• Molecule 12: Tektin-3

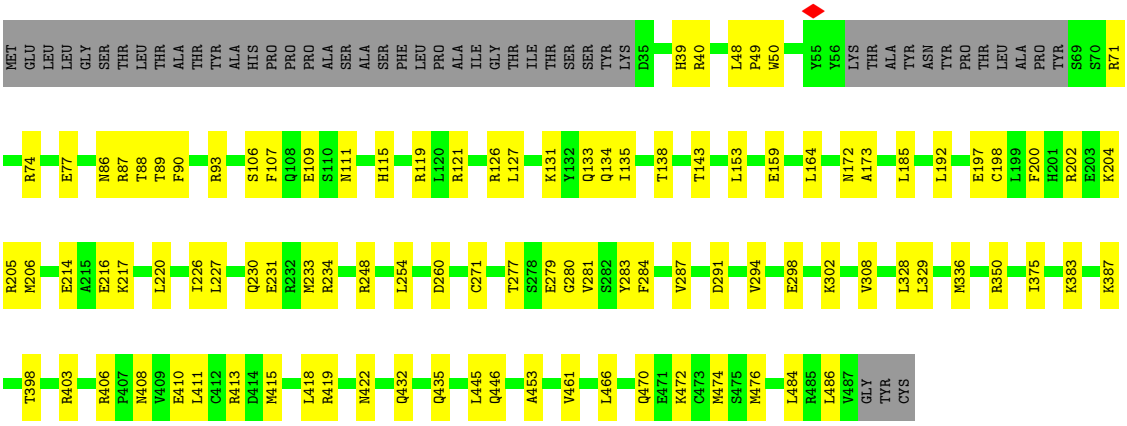
Chain S1:





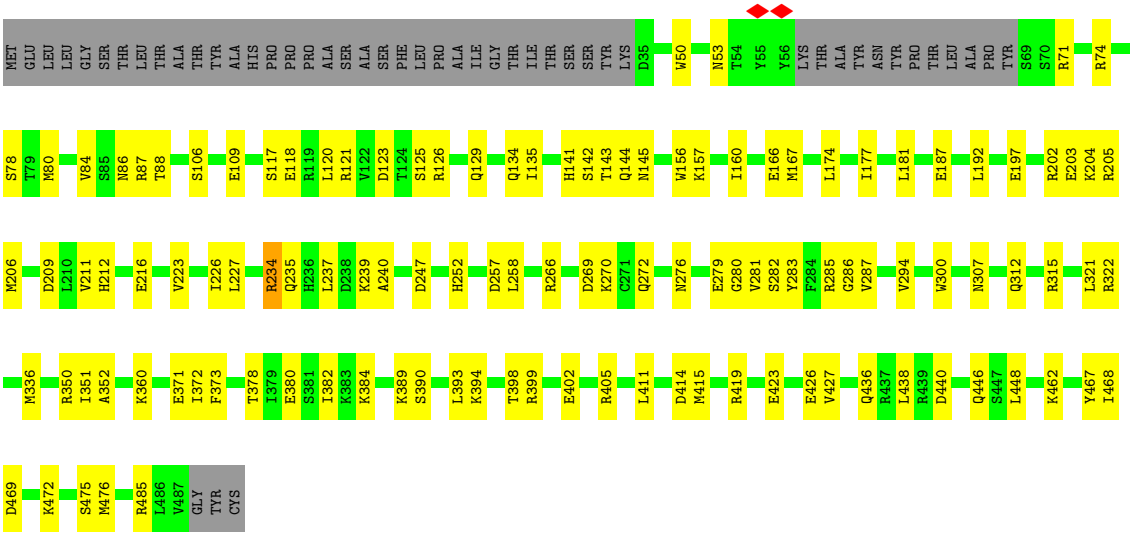
• Molecule 12: Tektin-3

Chain S2:



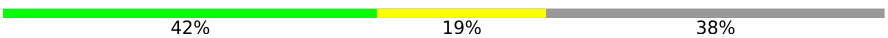
• Molecule 12: Tektin-3

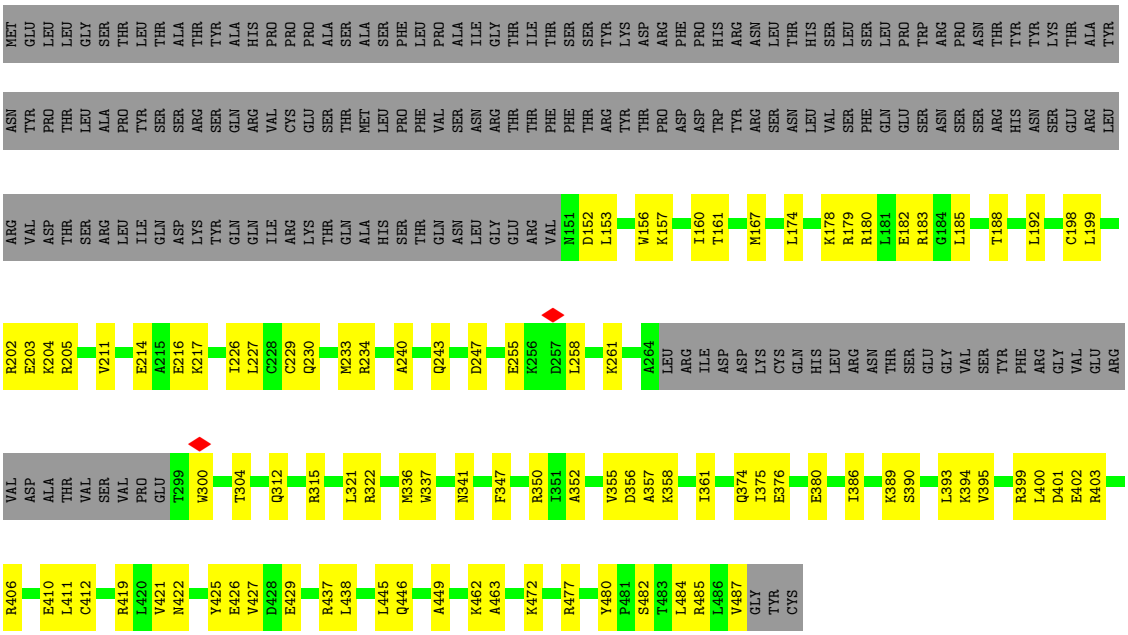
Chain S3:



• Molecule 12: Tektin-3

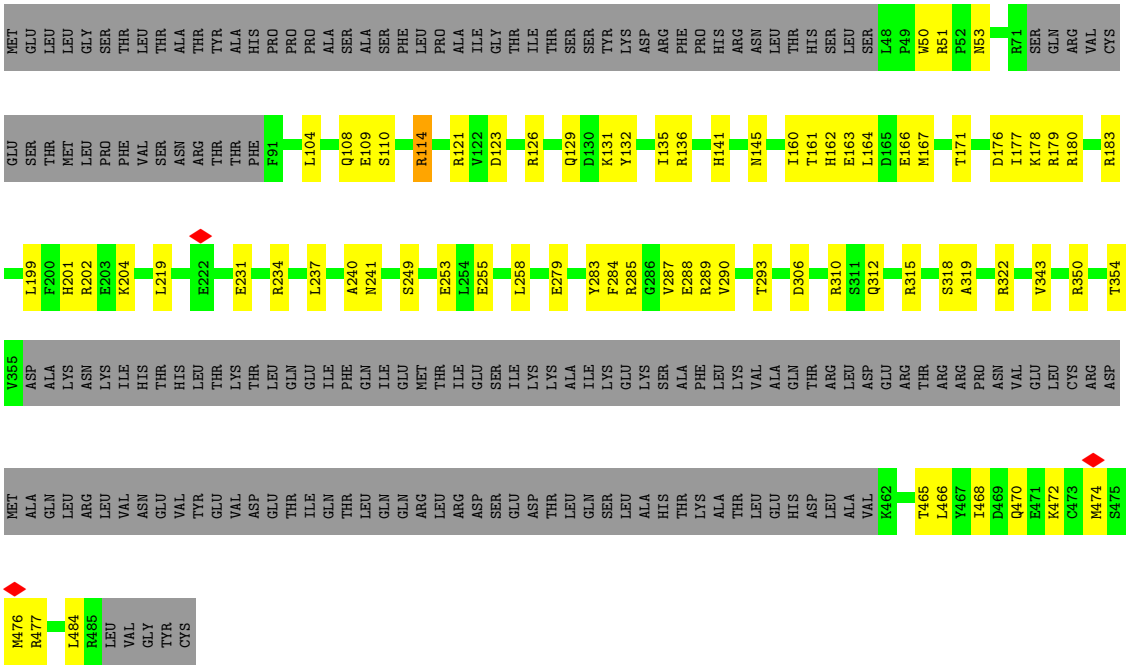
Chain S4:





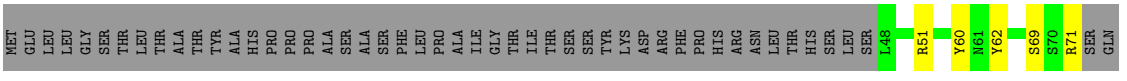
• Molecule 12: Tektin-3

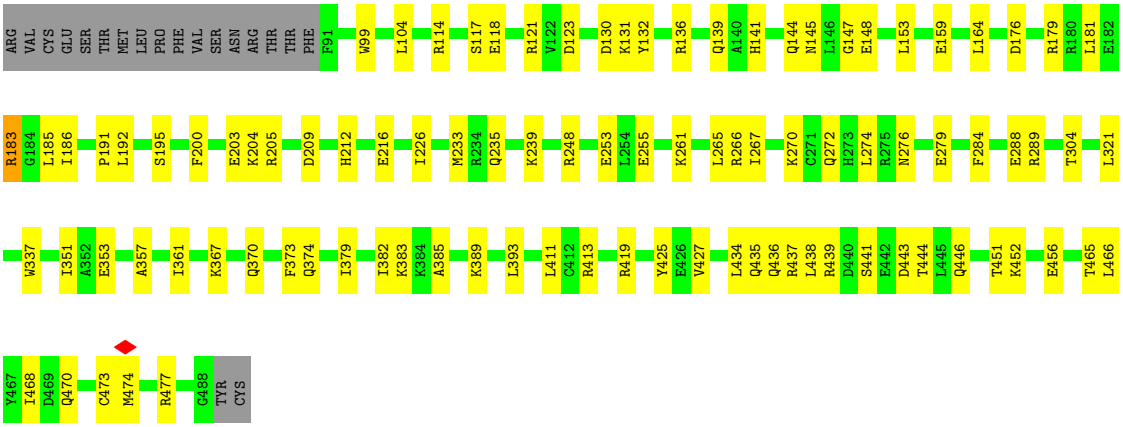
Chain S5:



• Molecule 12: Tektin-3

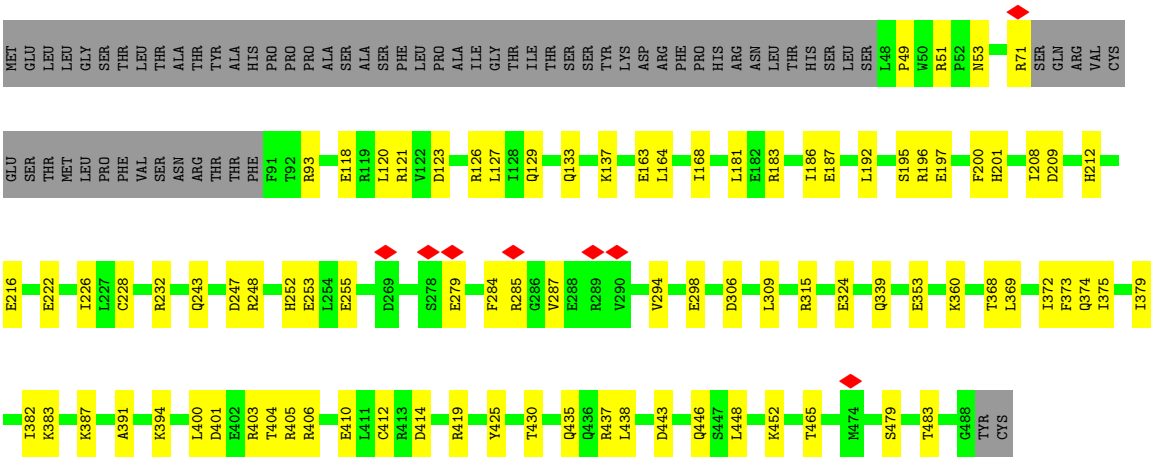
Chain S6:





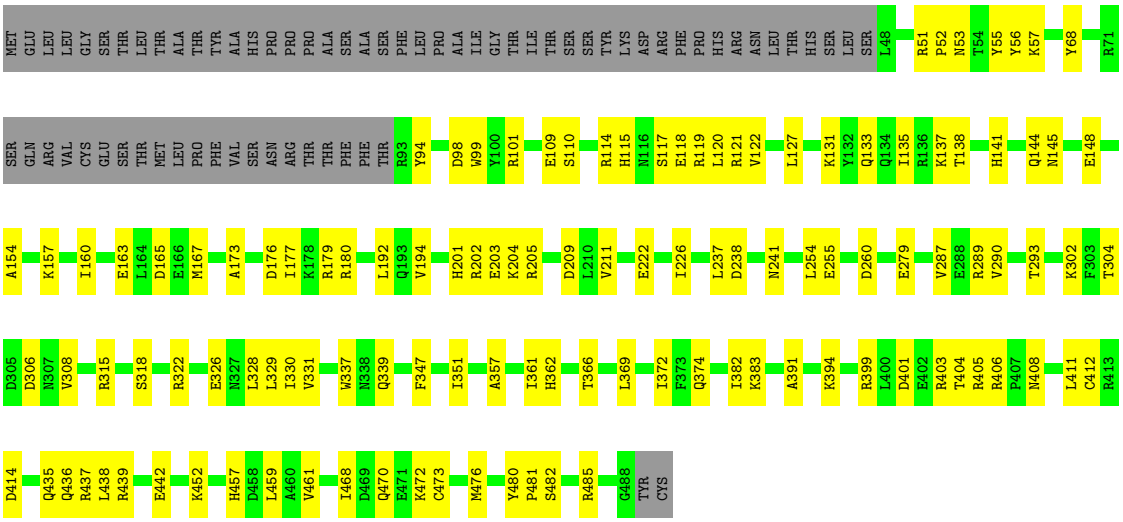
• Molecule 12: Tektin-3

Chain S7:



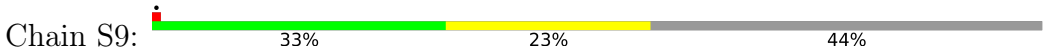
• Molecule 12: Tektin-3

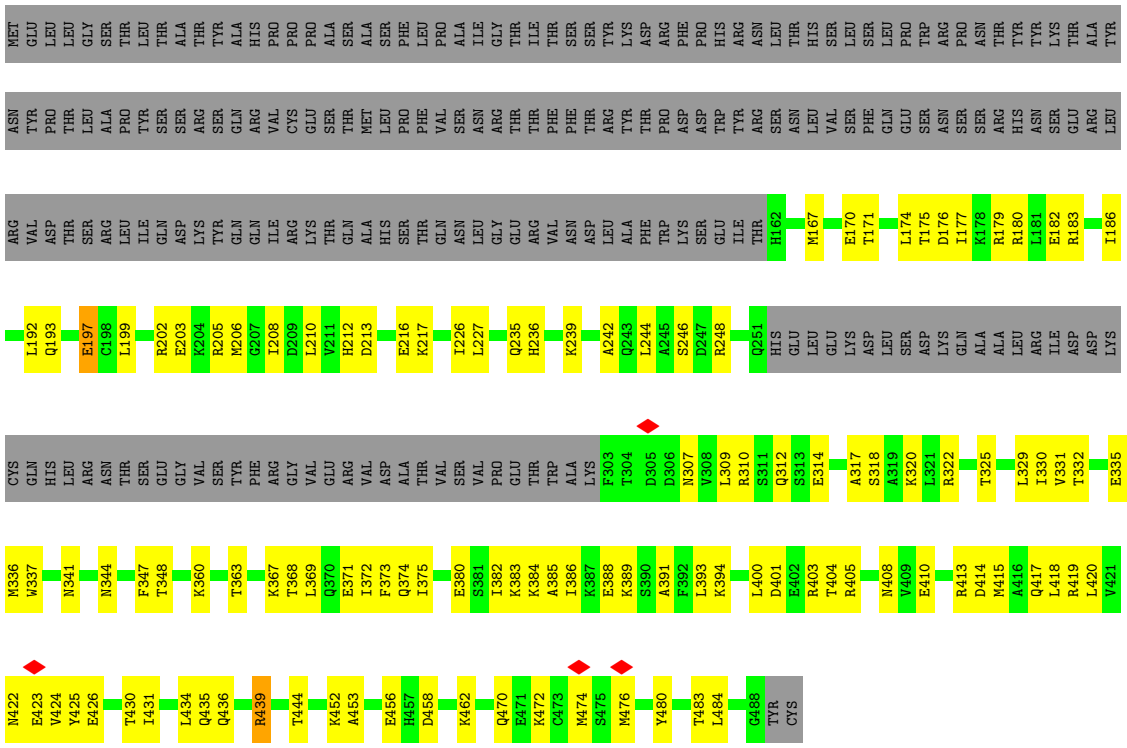
Chain S8:



• Molecule 12: Tektin-3

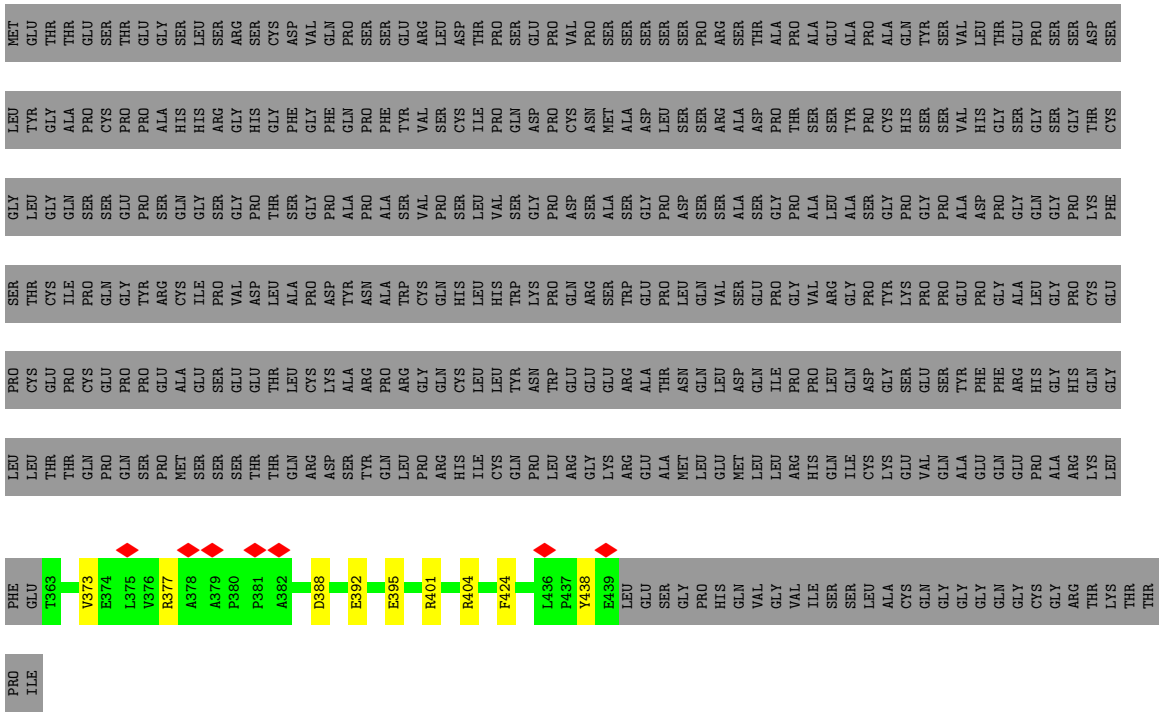
Chain S9:





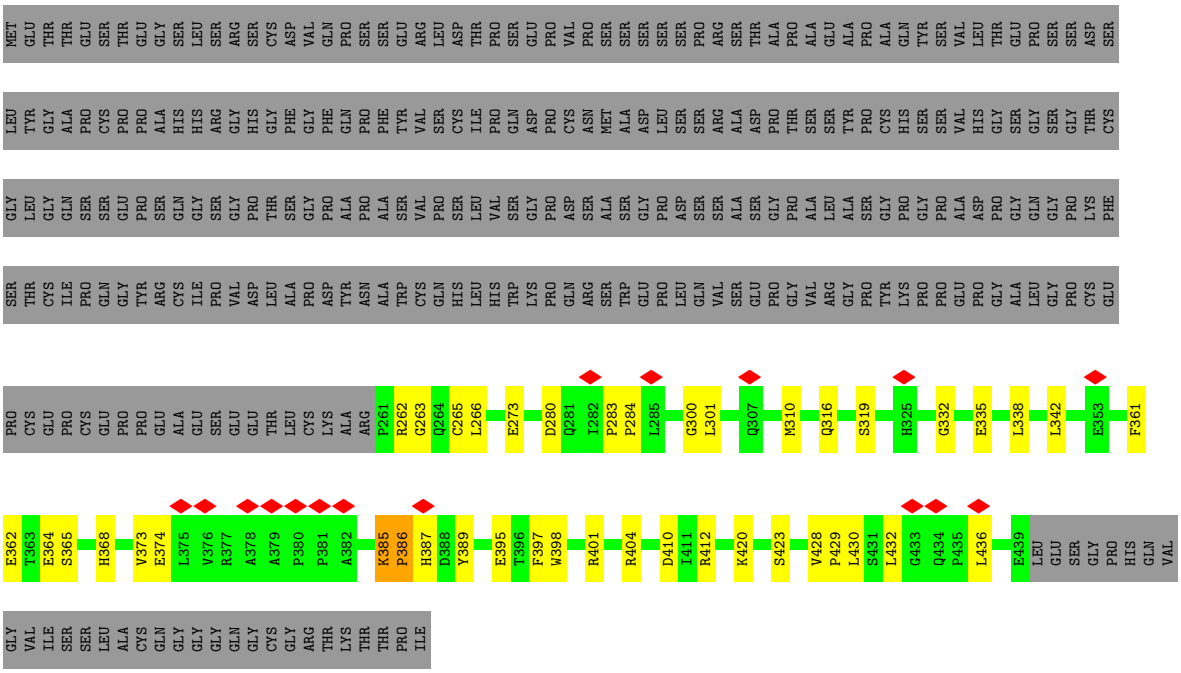
• Molecule 13: Sperm-associated antigen 8

Chain D:



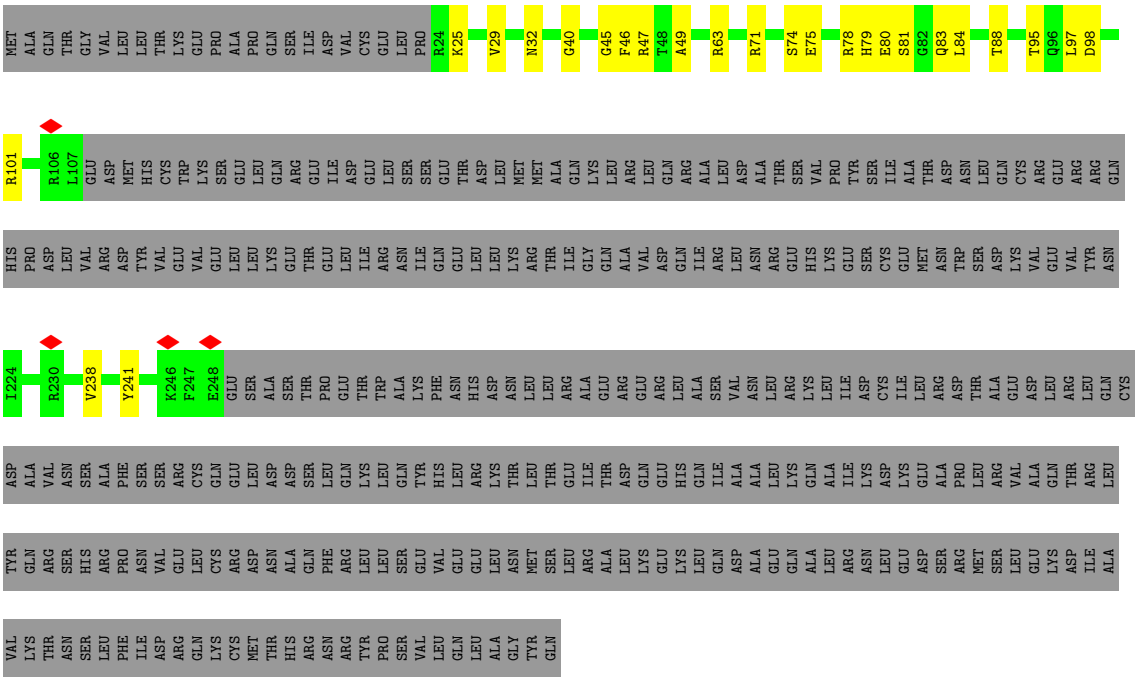
• Molecule 13: Sperm-associated antigen 8

Chain K3:



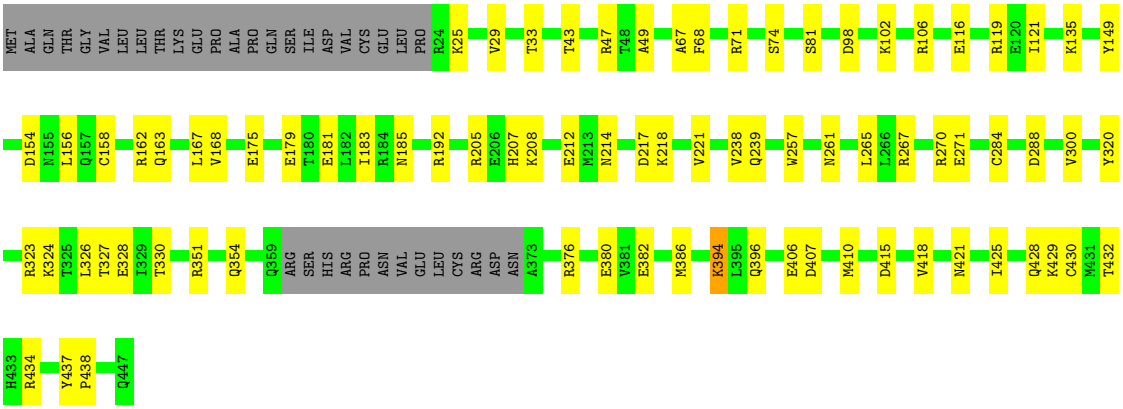
• Molecule 14: Tektin-4

Chain D0:



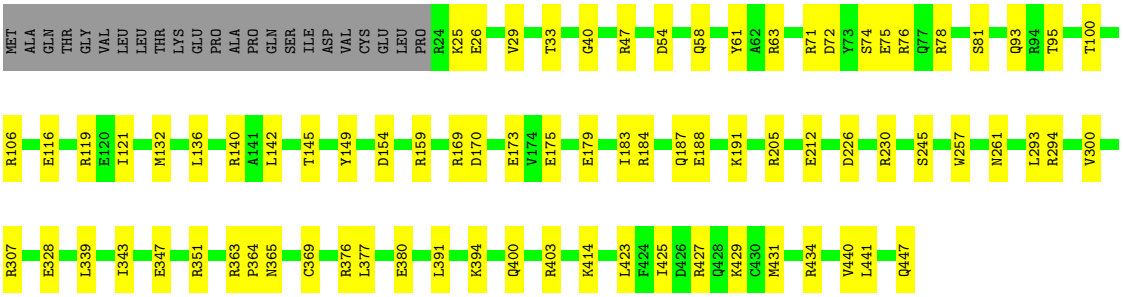
• Molecule 14: Tektin-4

Chain D1:



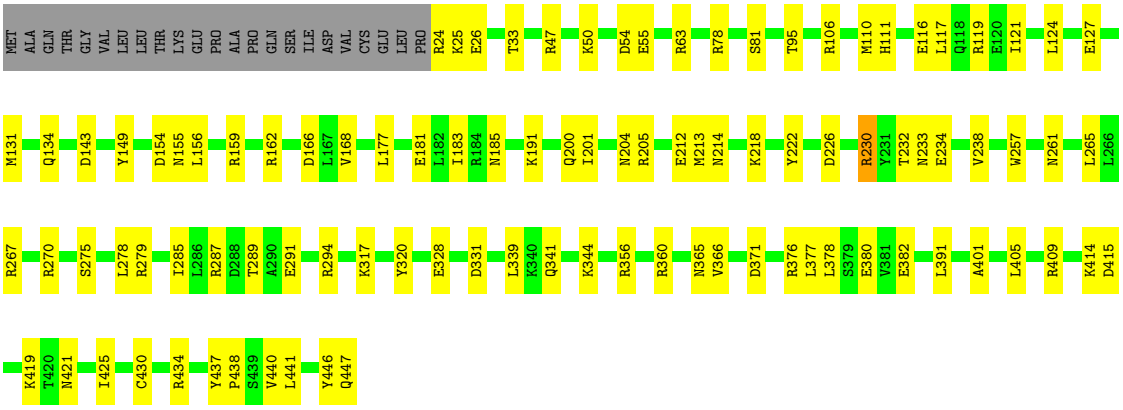
• Molecule 14: Tektin-4

Chain D2:



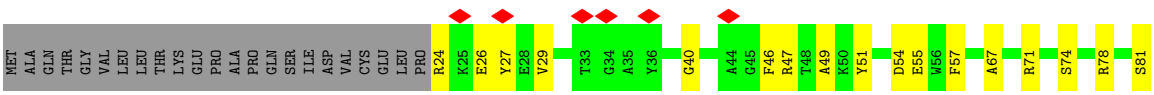
• Molecule 14: Tektin-4

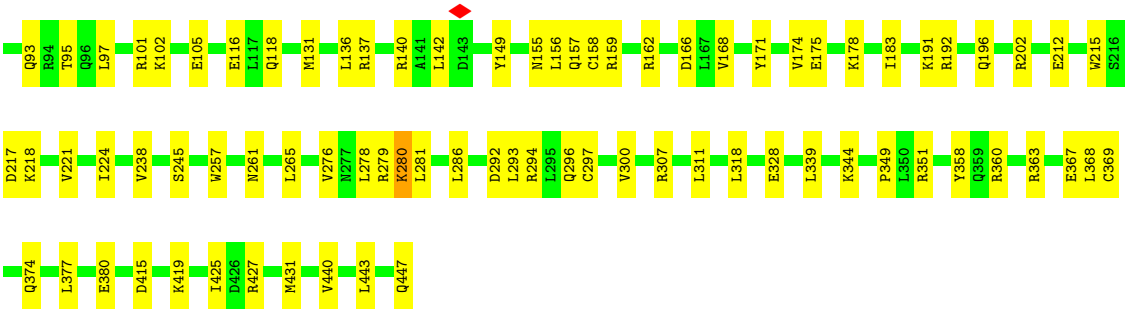
Chain D3:



• Molecule 14: Tektin-4

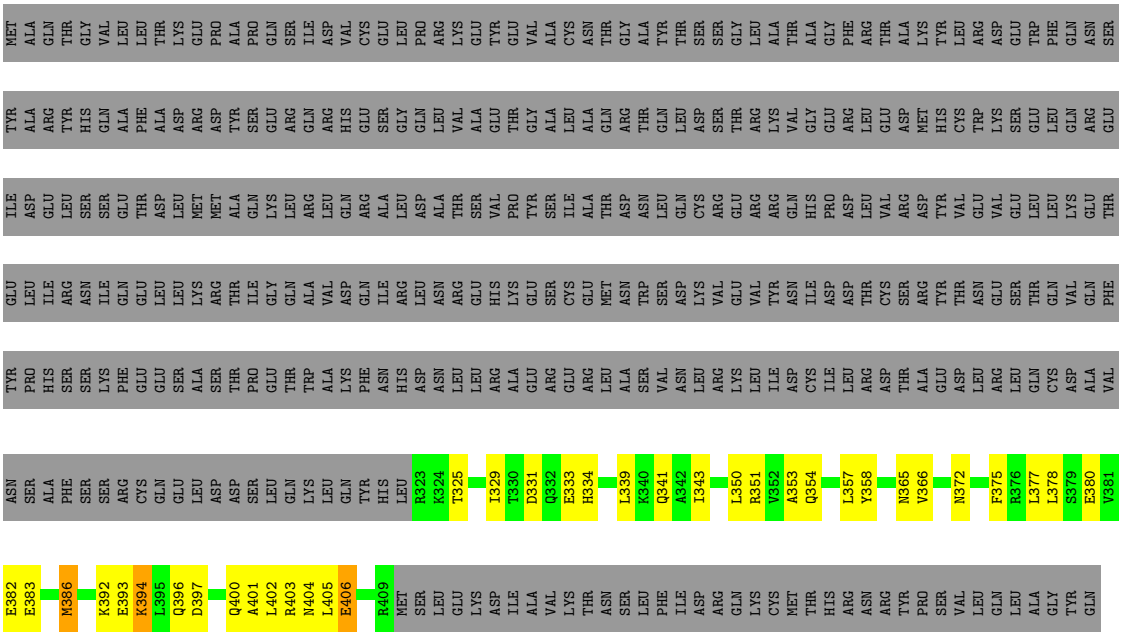
Chain D4:





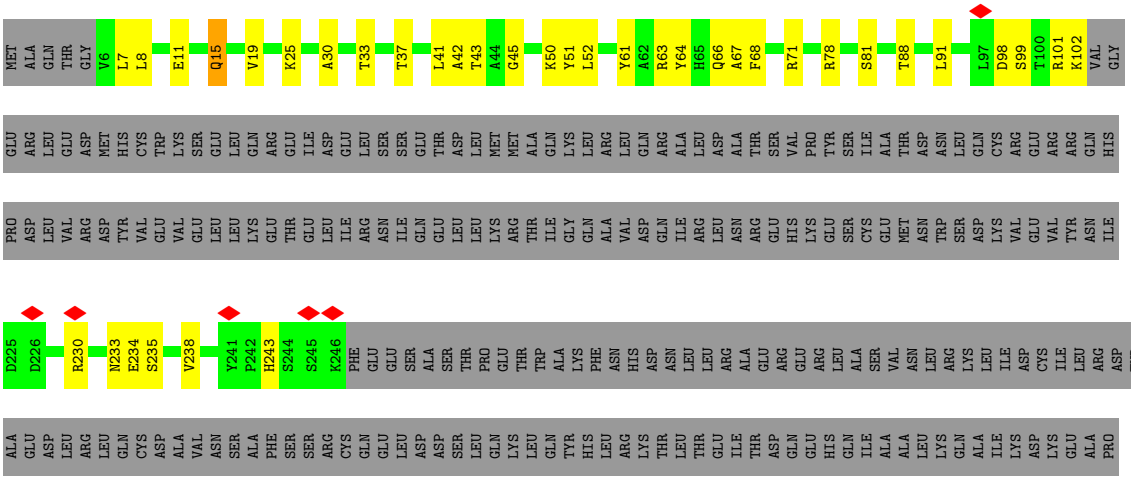
• Molecule 14: Tektin-4

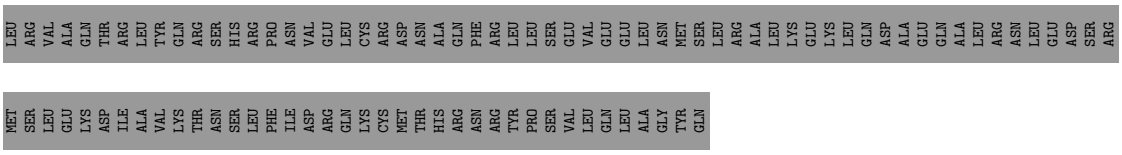
Chain D5:



• Molecule 14: Tektin-4

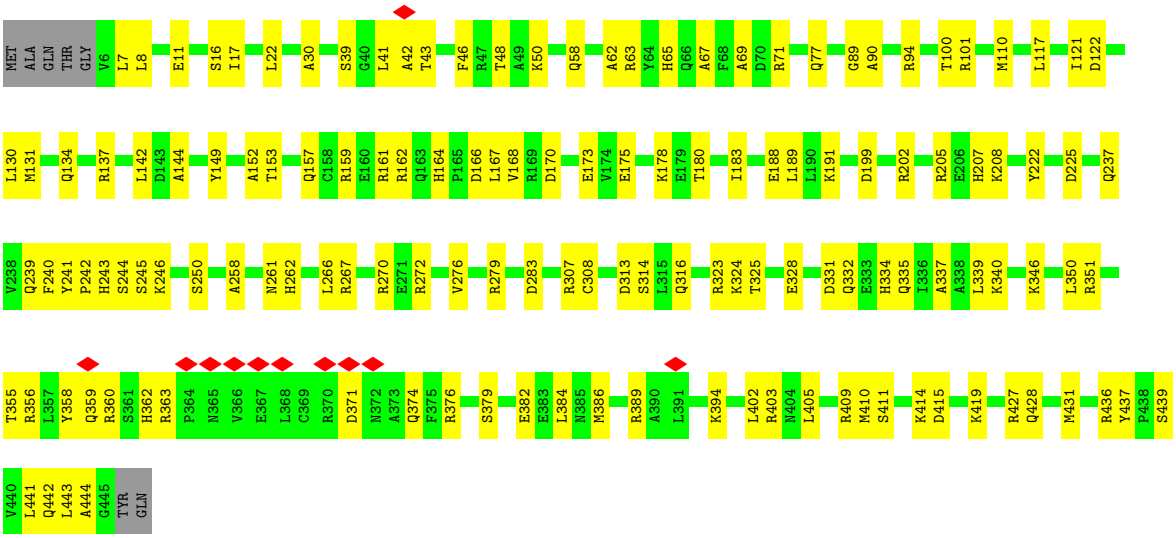
Chain T0:





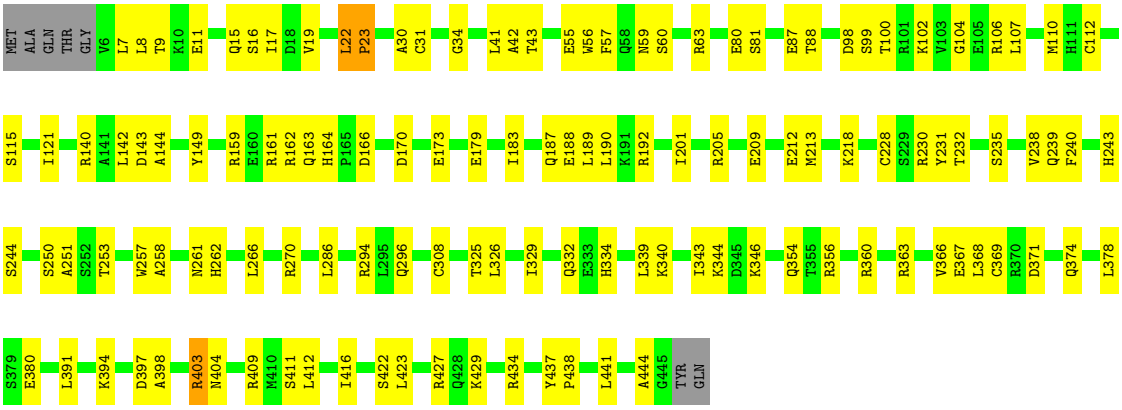
• Molecule 14: Tektin-4

Chain T1:



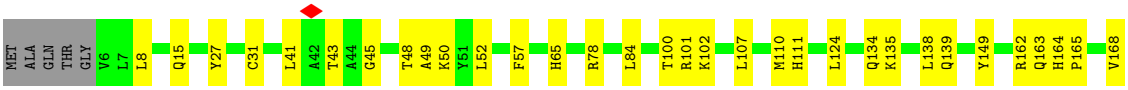
• Molecule 14: Tektin-4

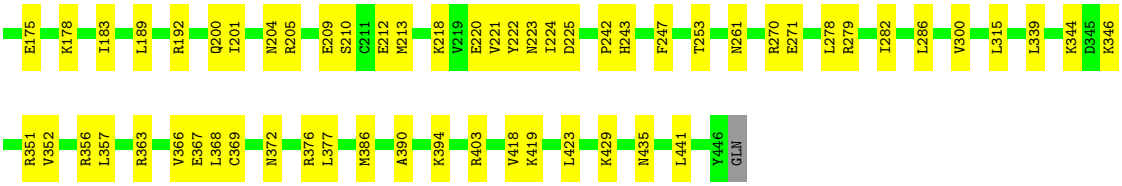
Chain T2:



• Molecule 14: Tektin-4

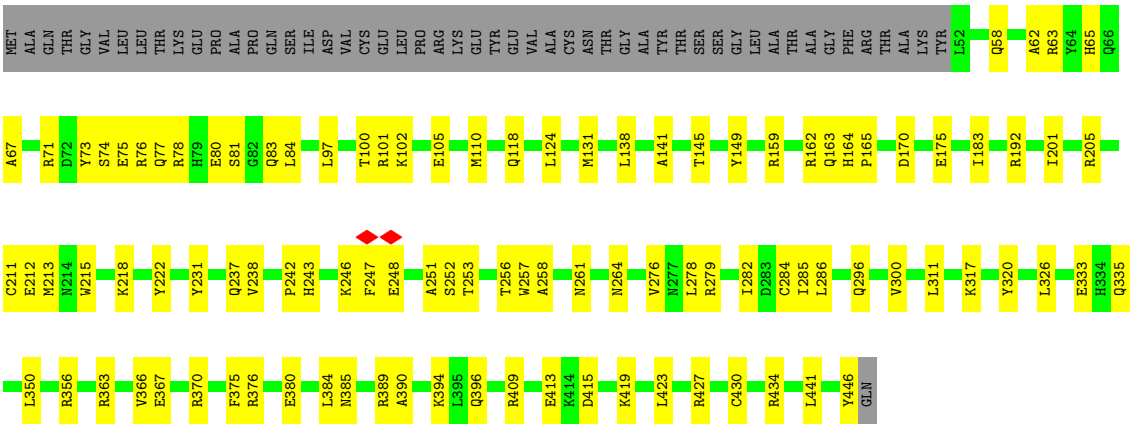
Chain T3:





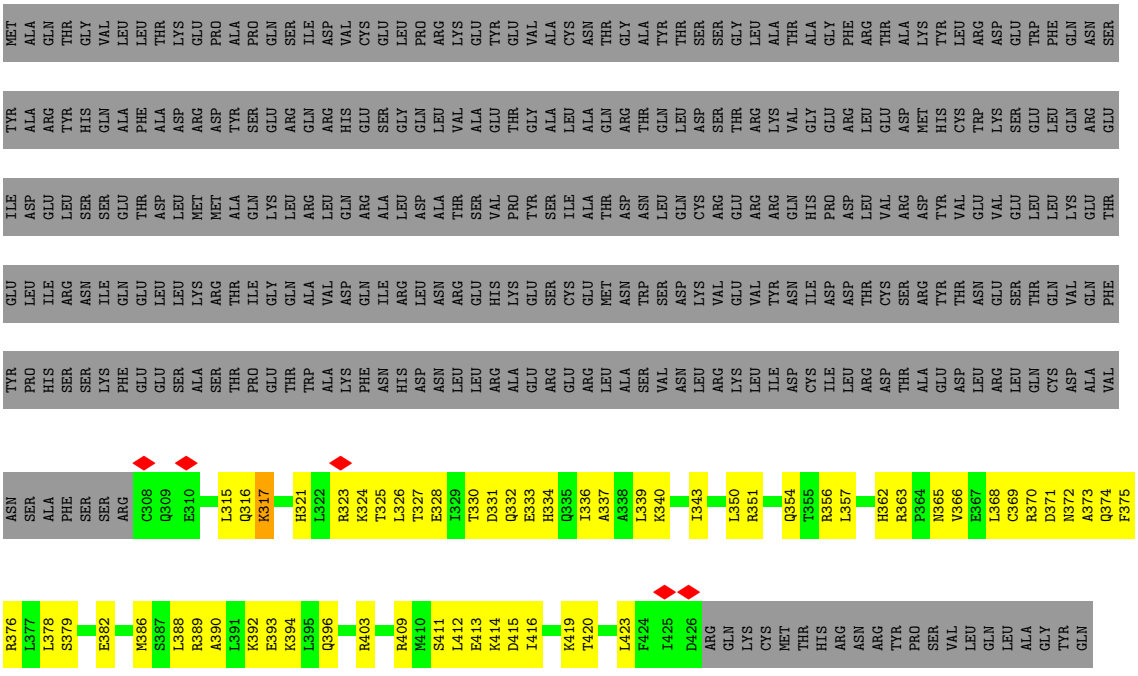
• Molecule 14: Tektin-4

Chain T4:



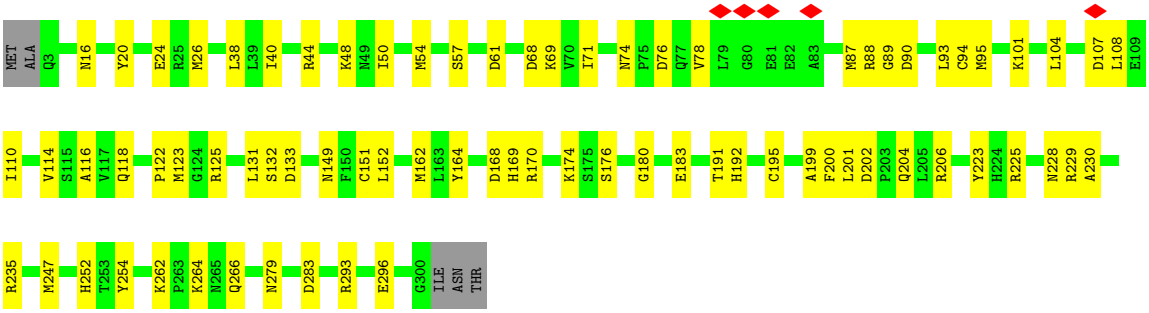
• Molecule 14: Tektin-4

Chain T5:



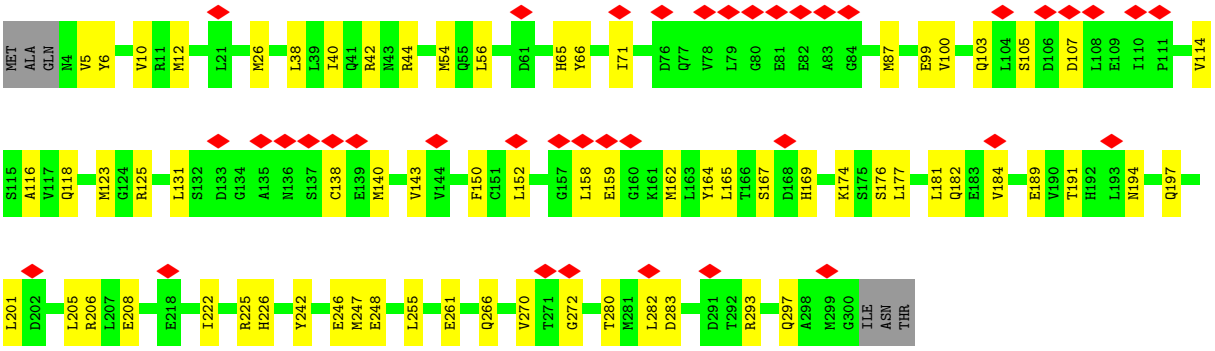
• Molecule 15: Cilia- and flagella-associated protein 161

Chain E:



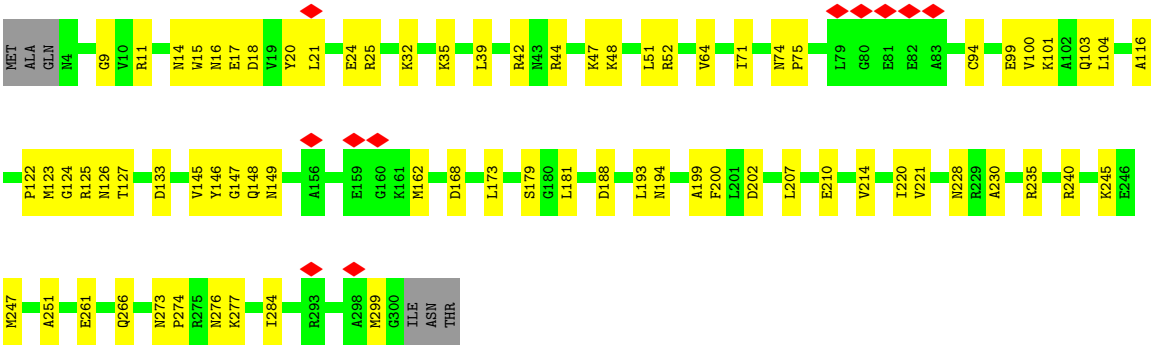
• Molecule 15: Cilia- and flagella-associated protein 161

Chain F:



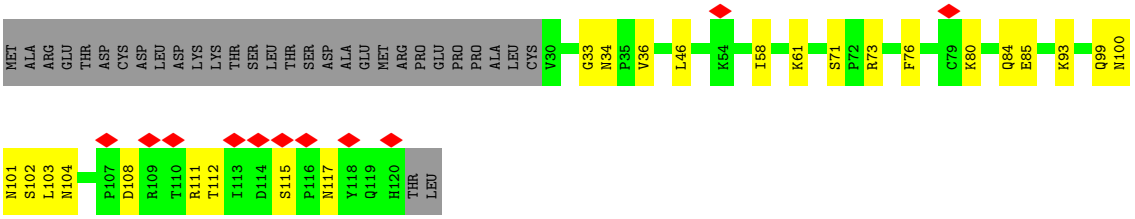
• Molecule 15: Cilia- and flagella-associated protein 161

Chain N2:



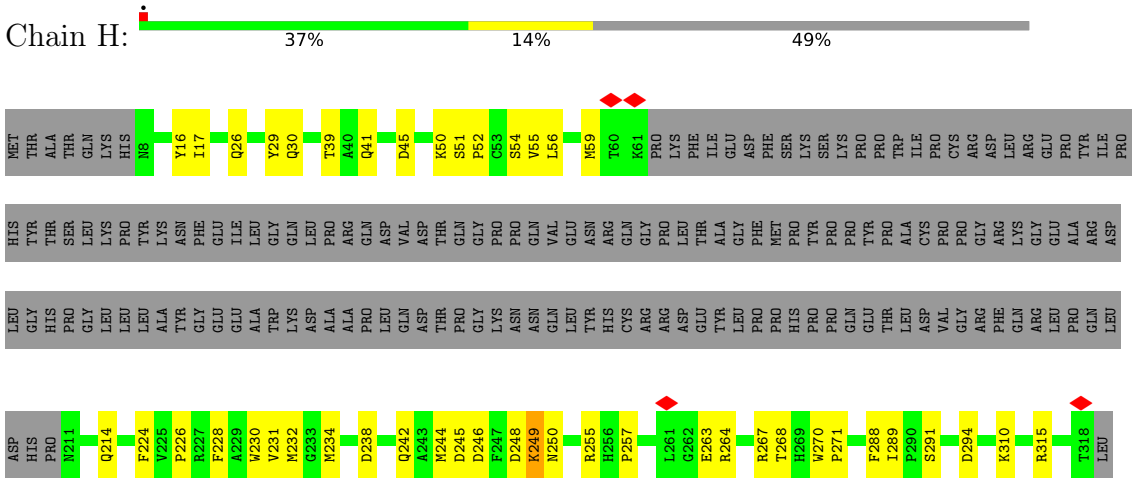
• Molecule 16: Piercer of microtubule wall 2 protein

Chain G:



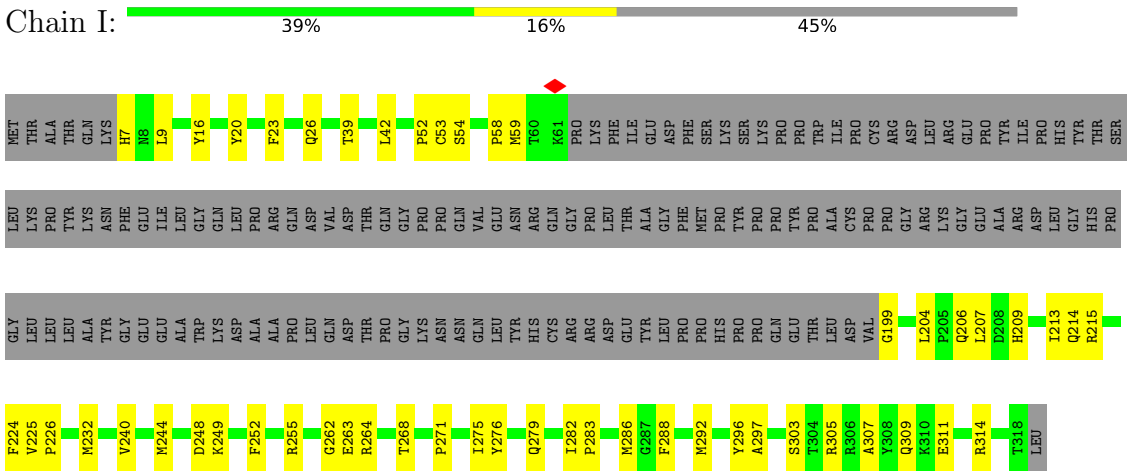
• Molecule 17: Protein FAM166A

Chain H:



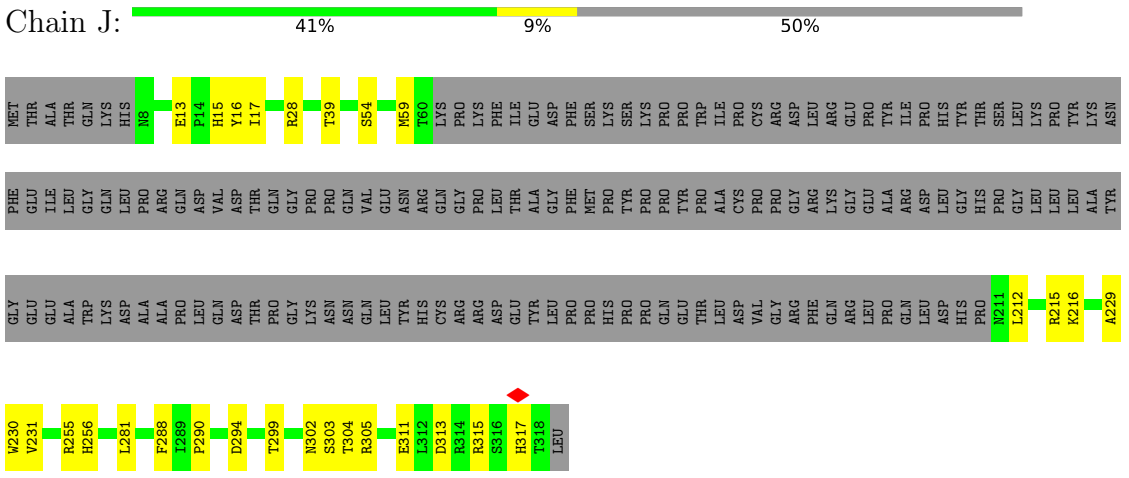
• Molecule 17: Protein FAM166A

Chain I:



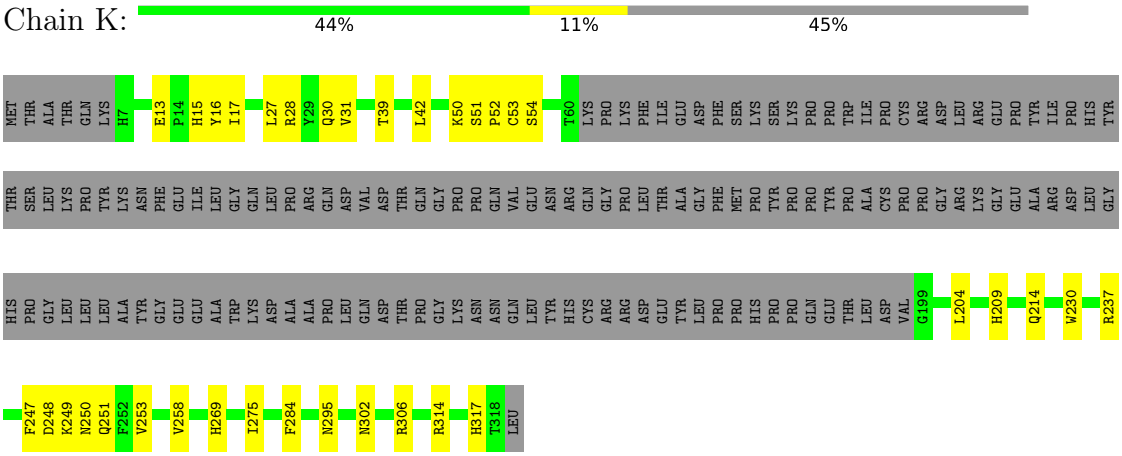
• Molecule 17: Protein FAM166A

Chain J:



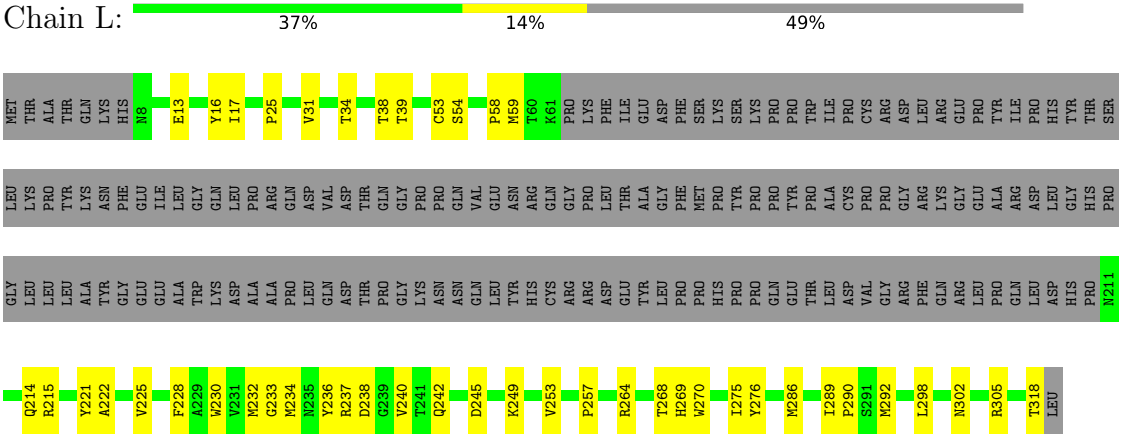
• Molecule 17: Protein FAM166A

Chain K:



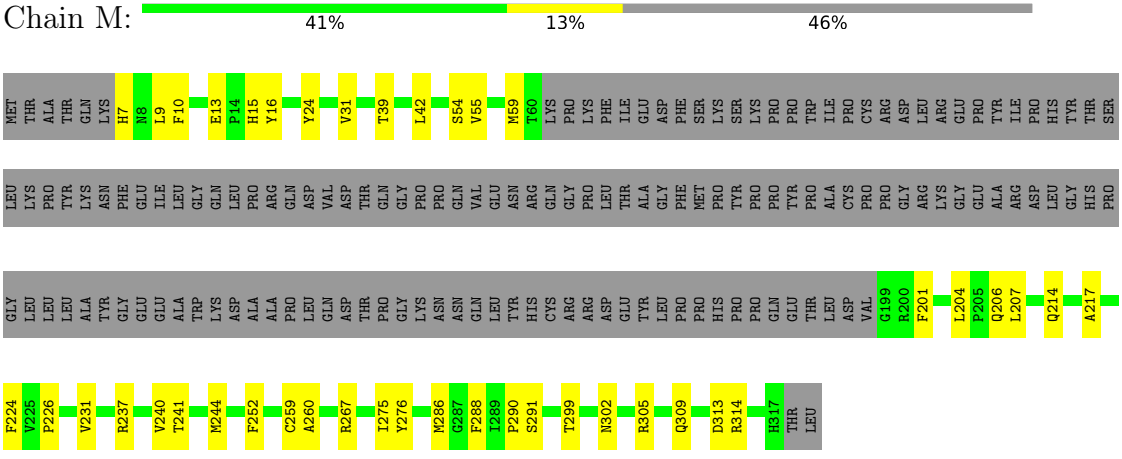
• Molecule 17: Protein FAM166A

Chain L:



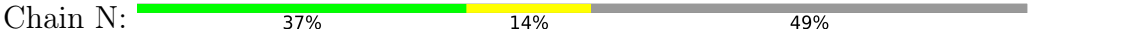
• Molecule 17: Protein FAM166A

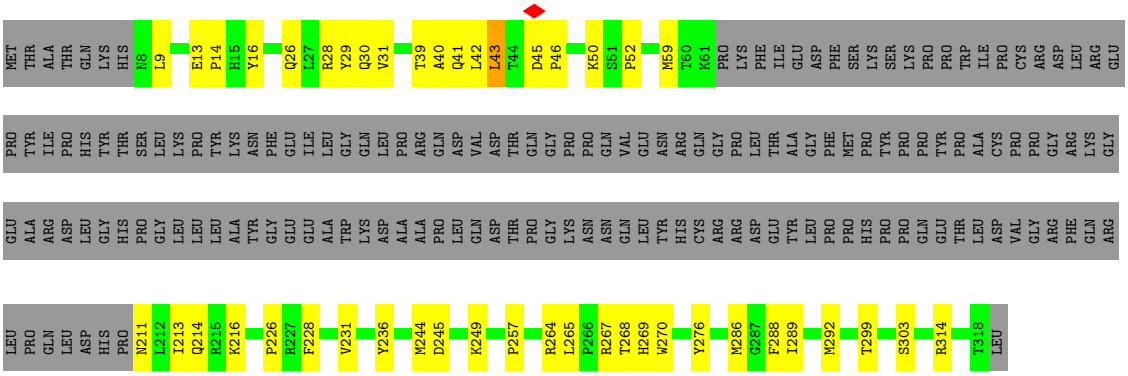
Chain M:



• Molecule 17: Protein FAM166A

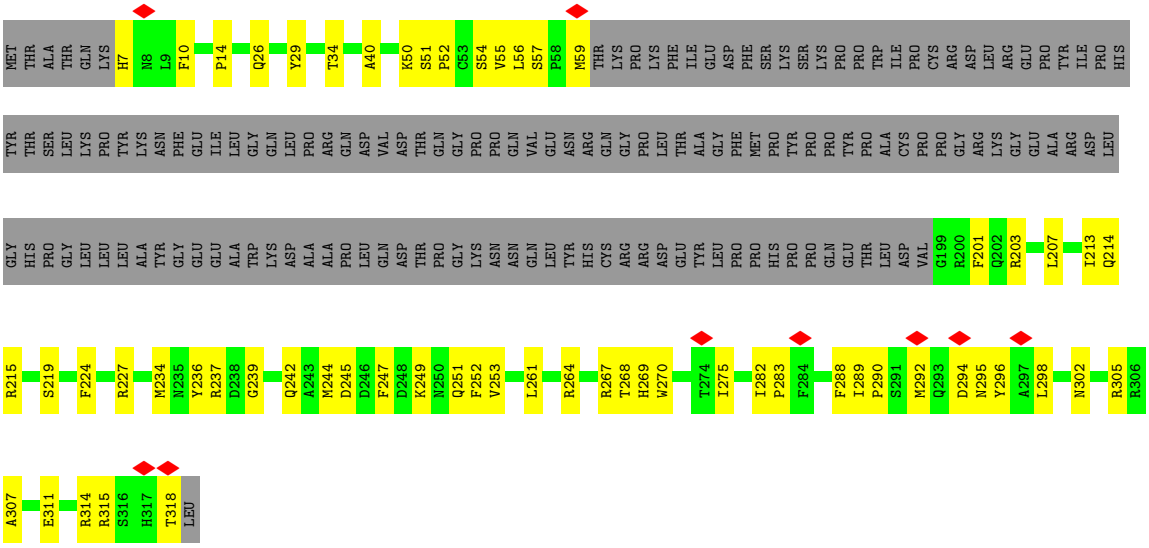
Chain N:





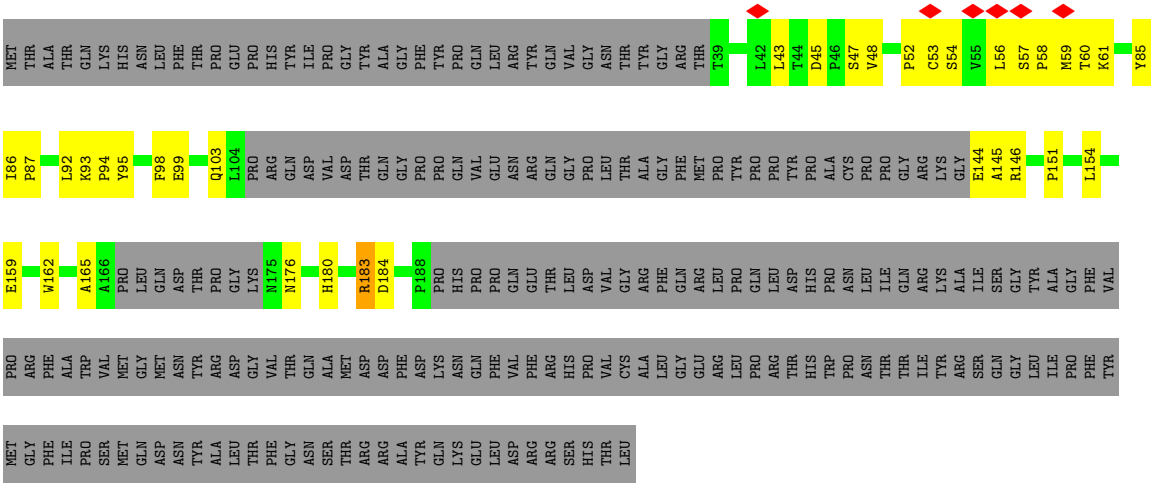
• Molecule 17: Protein FAM166A

Chain O7:



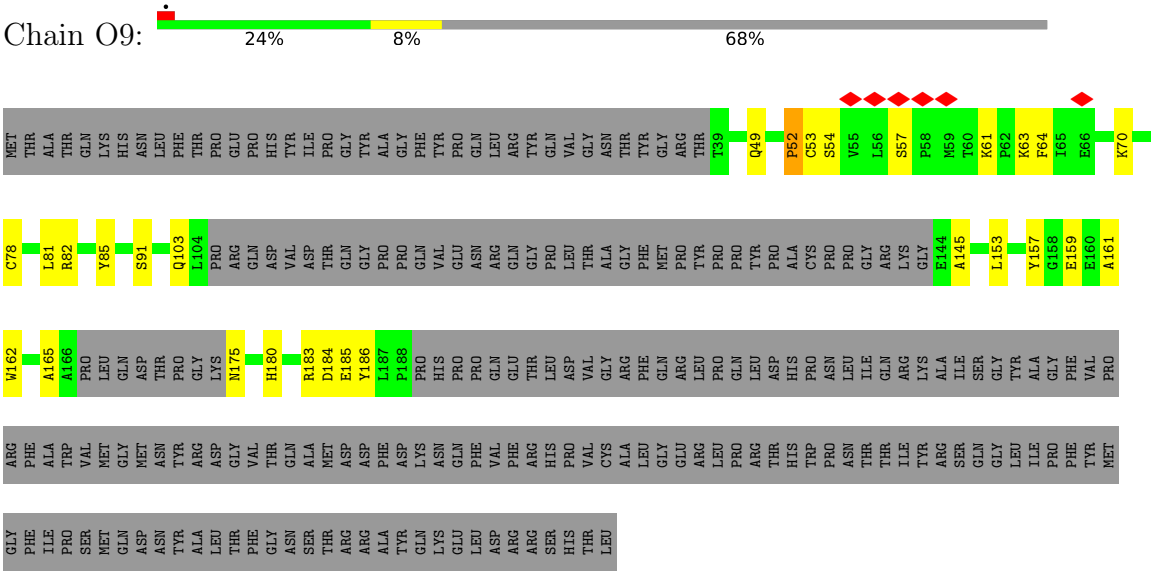
• Molecule 17: Protein FAM166A

Chain O8:



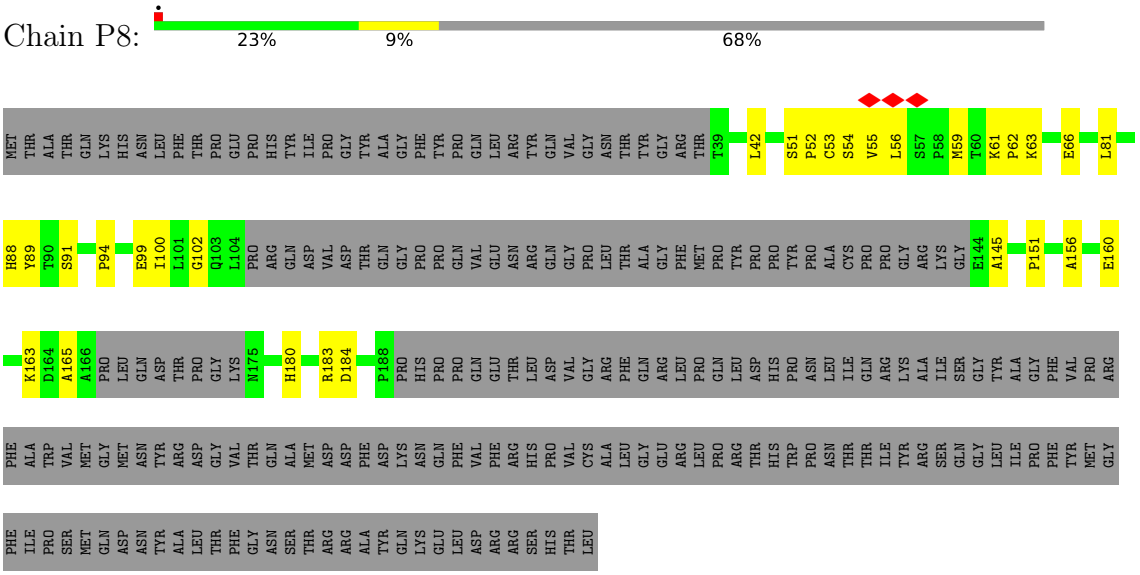
• Molecule 17: Protein FAM166A

Chain O9:



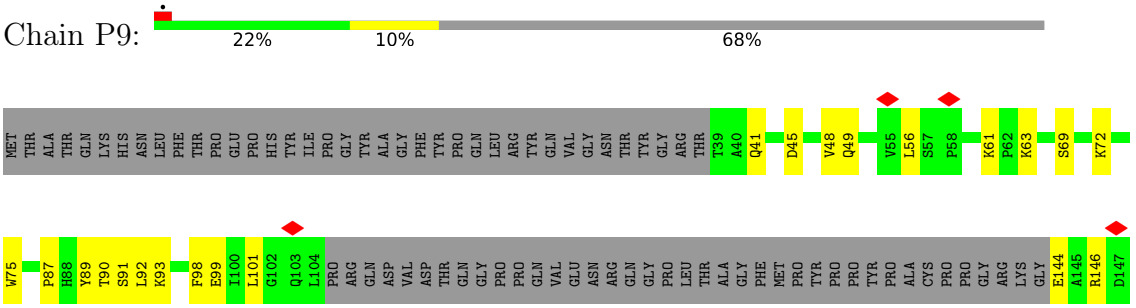
• Molecule 17: Protein FAM166A

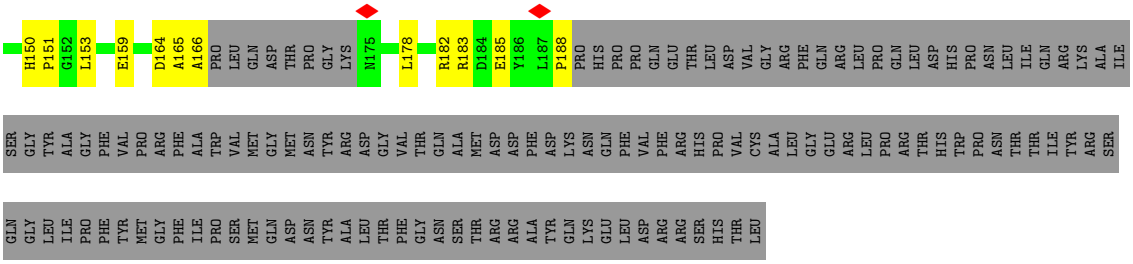
Chain P8:



• Molecule 17: Protein FAM166A

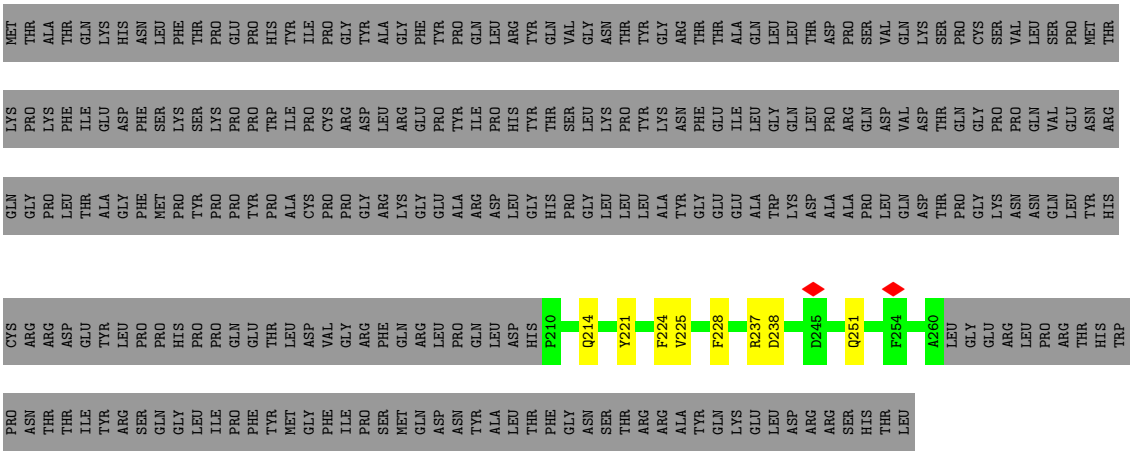
Chain P9:





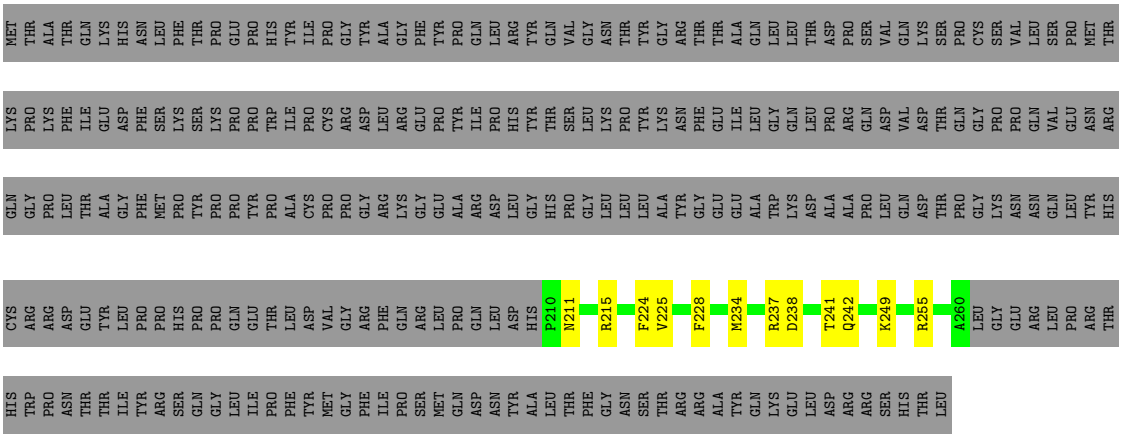
• Molecule 17: Protein FAM166A

Chain Z2:



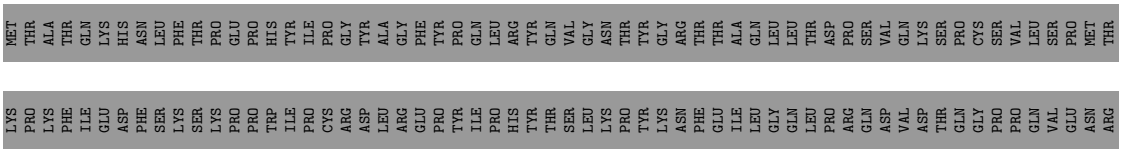
• Molecule 17: Protein FAM166A

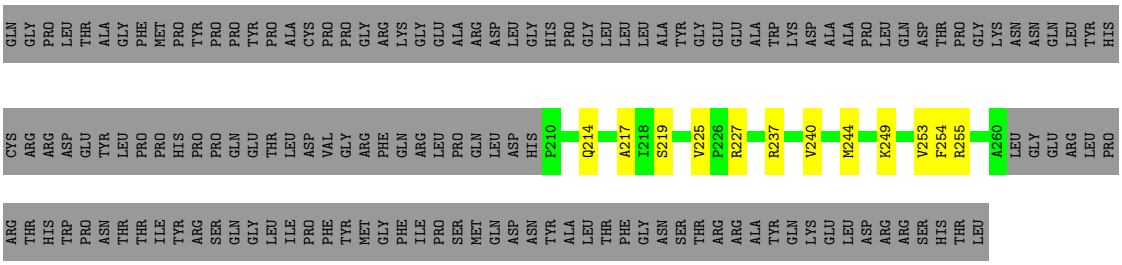
Chain Z3:



• Molecule 17: Protein FAM166A

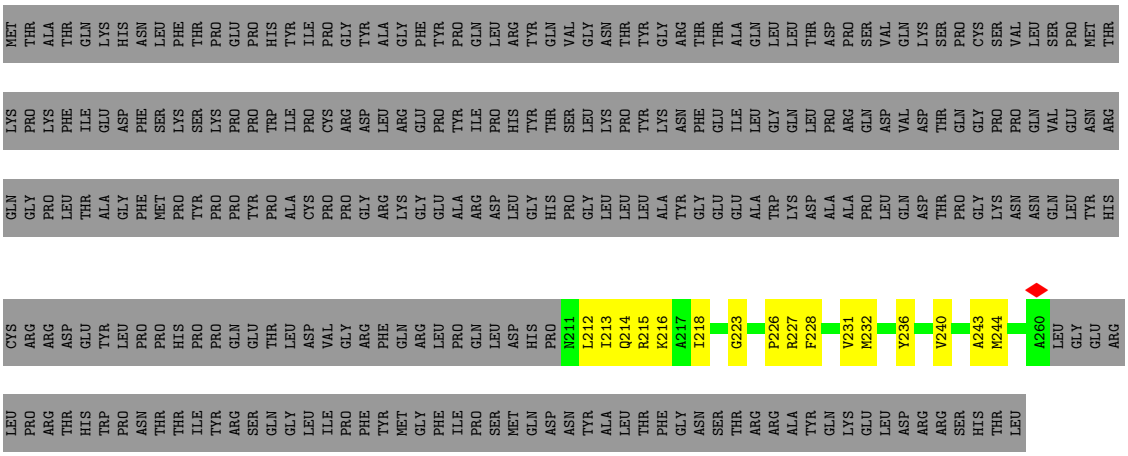
Chain Z4:





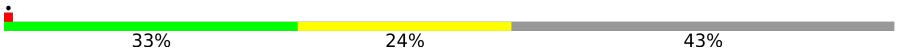
• Molecule 17: Protein FAM166A

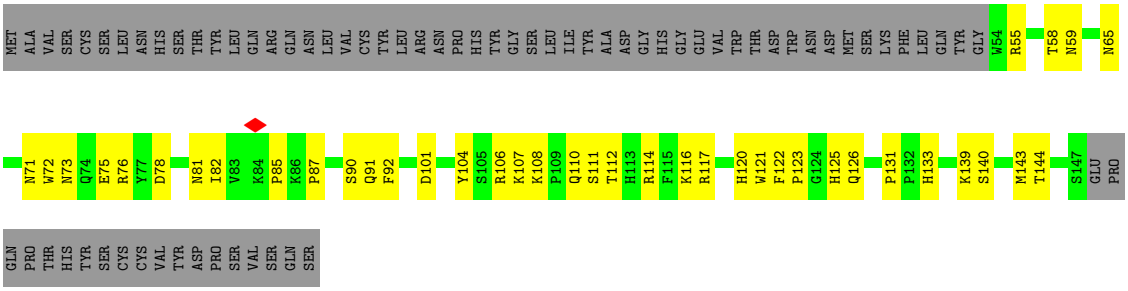
Chain Z5:



• Molecule 18: Cilia- and flagella-associated protein 68

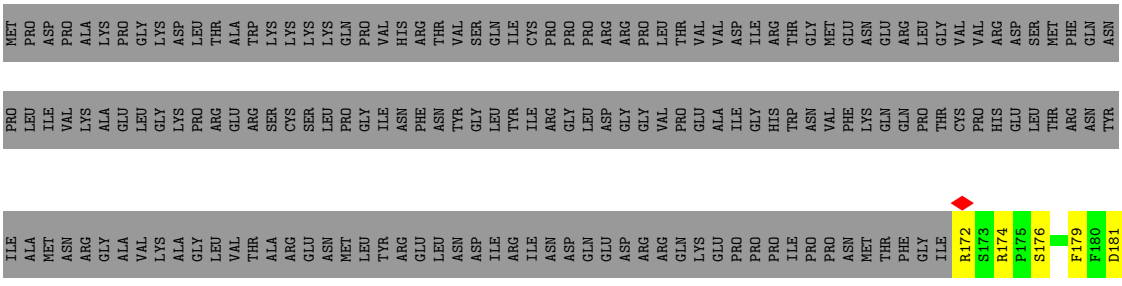
Chain I1:

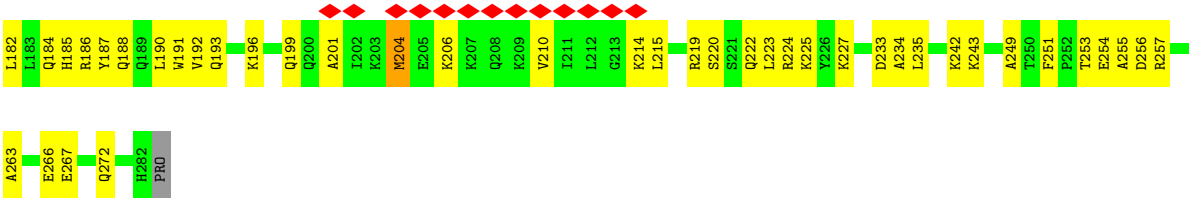




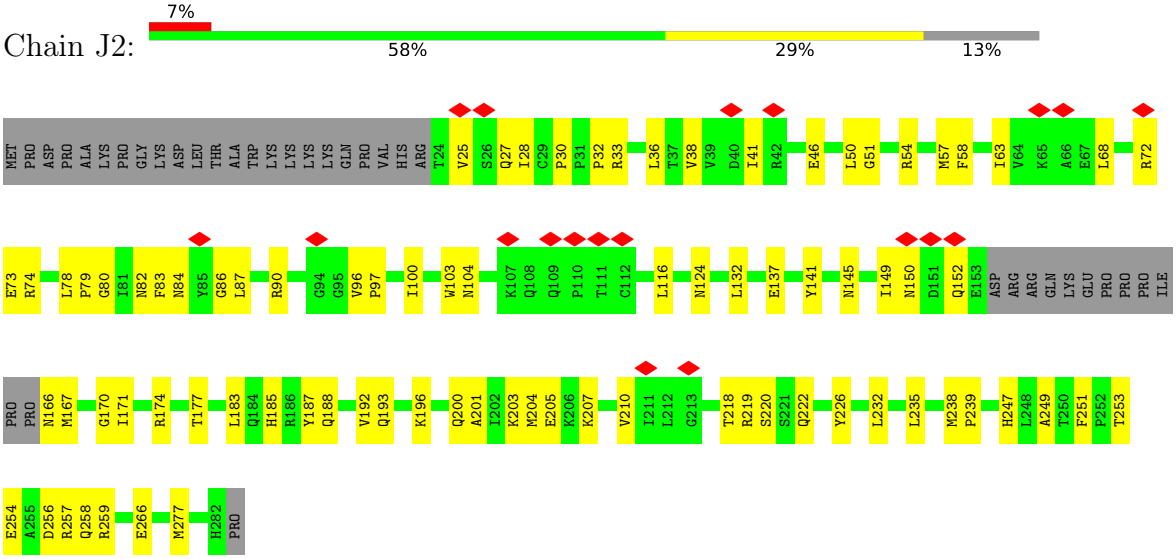
• Molecule 19: Cilia and flagella-associated protein 77

Chain J1:

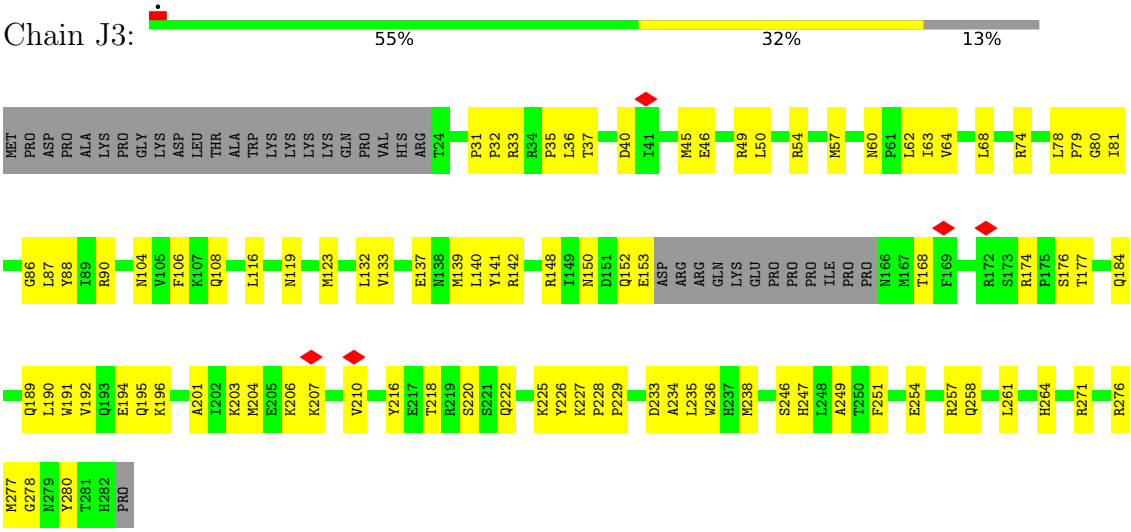




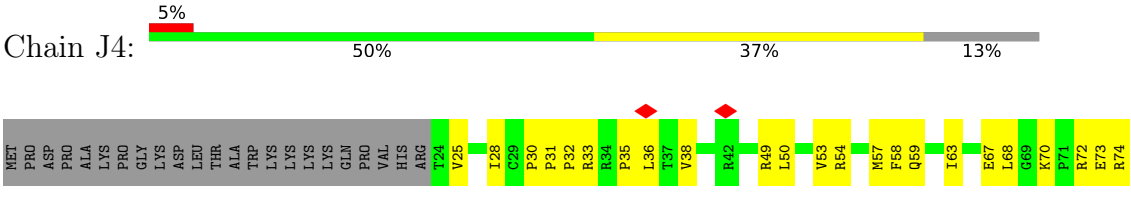
• Molecule 19: Cilia and flagella-associated protein 77

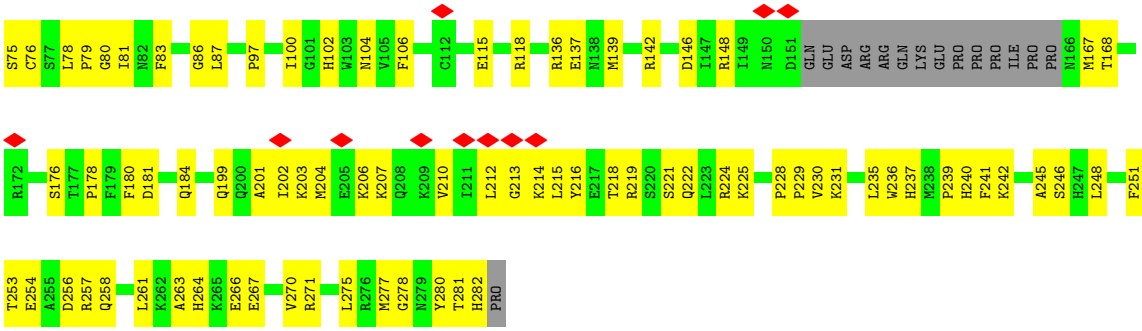


• Molecule 19: Cilia and flagella-associated protein 77



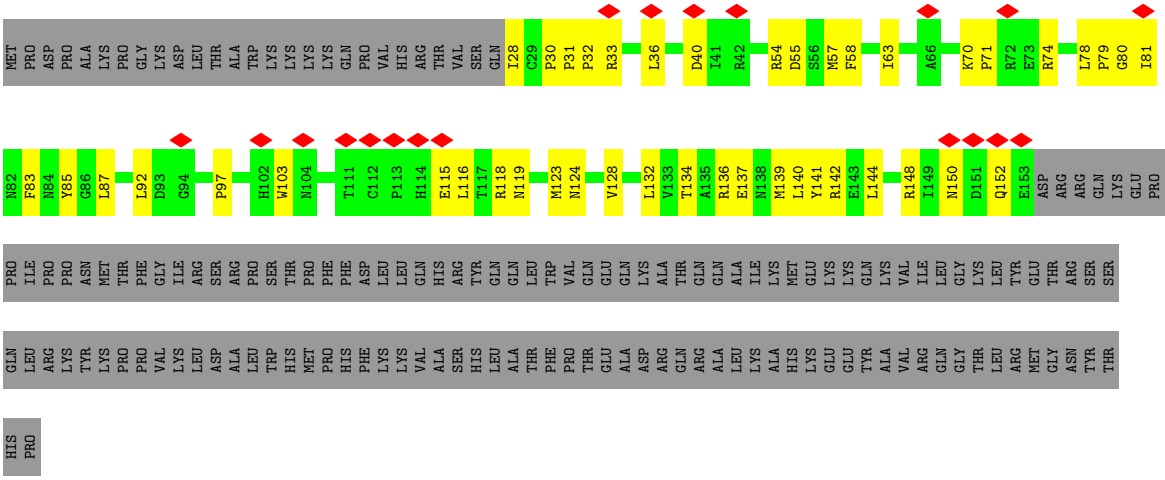
• Molecule 19: Cilia and flagella-associated protein 77





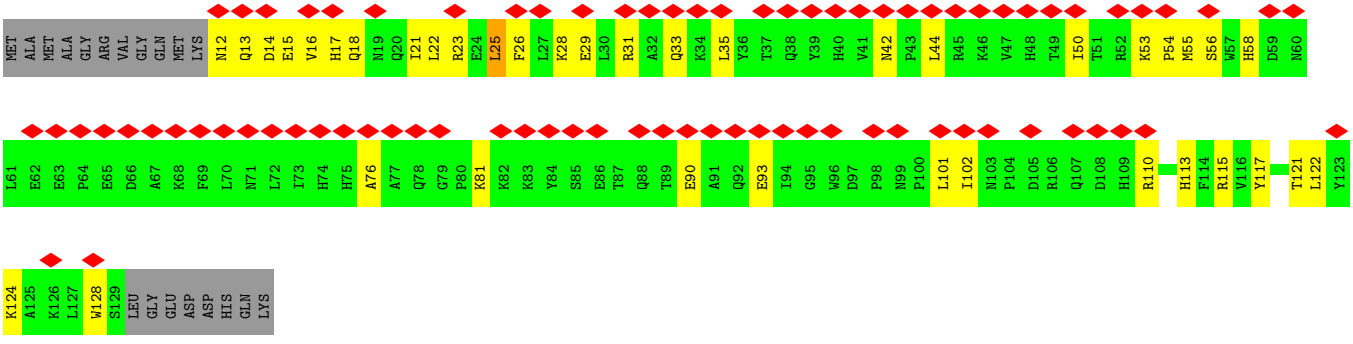
• Molecule 19: Cilia and flagella-associated protein 77

Chain J5:



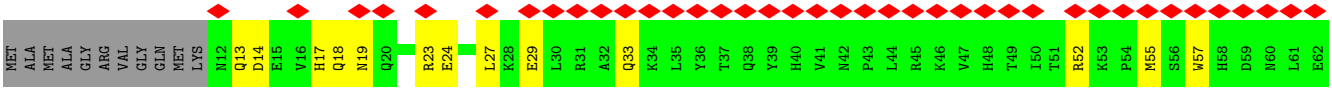
• Molecule 20: Family with sequence similarity 183, member B

Chain K1:



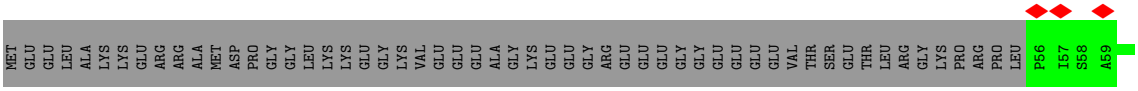
• Molecule 20: Family with sequence similarity 183, member B

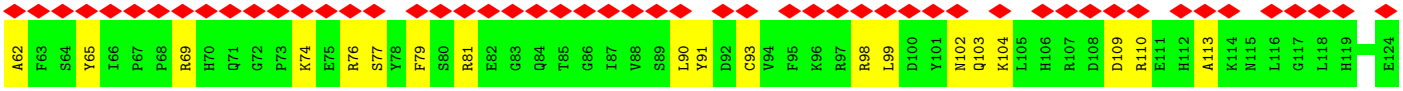
Chain K2:

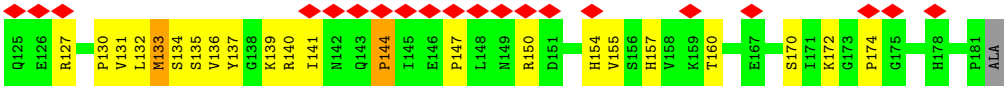


• Molecule 21: Cilia- and flagella-associated protein 90

Chain L1:

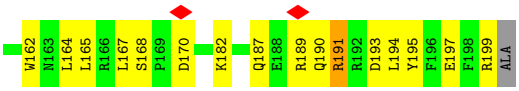






• Molecule 22: Protein FAM166C

Chain M1:

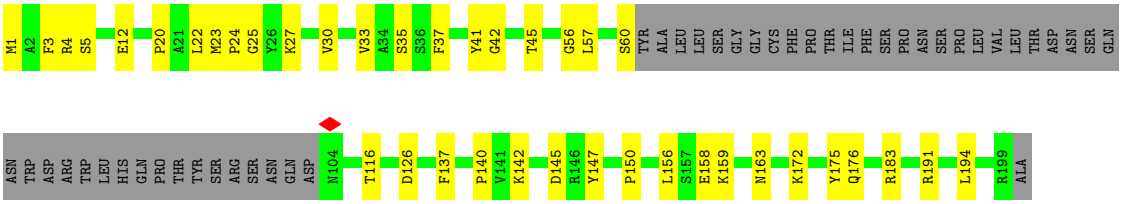


• Molecule 22: Protein FAM166C

Chain M2:

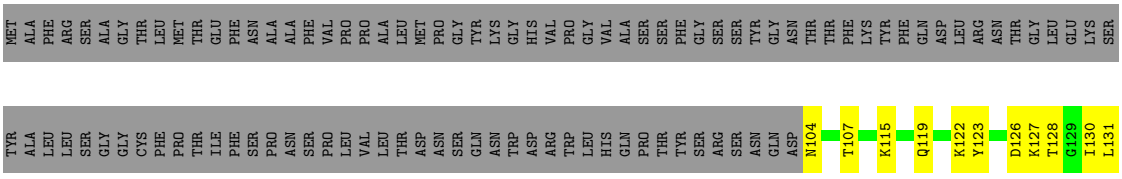
• Molecule 22: Protein FAM166C

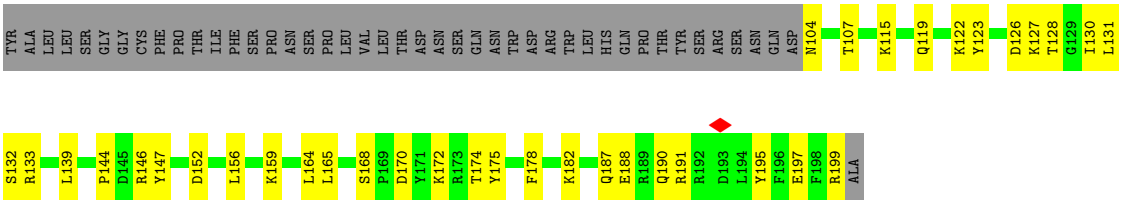
Chain M3:



• Molecule 22: Protein FAM166C

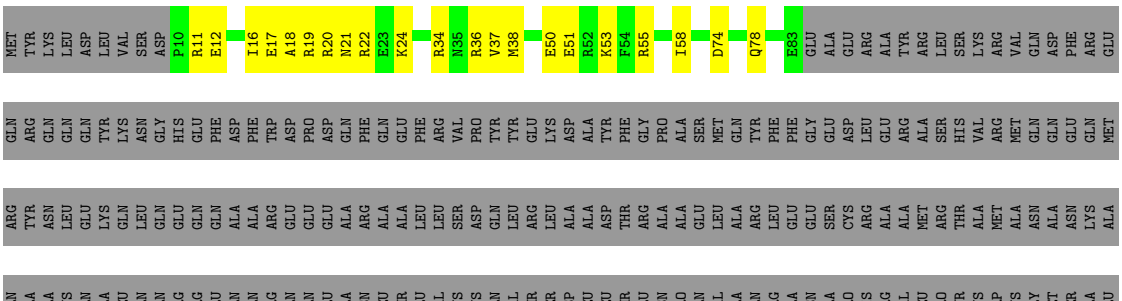
Chain M4:

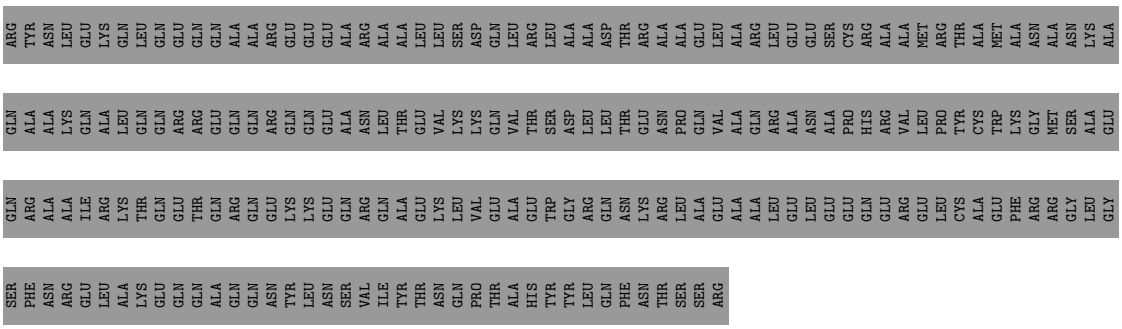




• Molecule 23: RIB43A-like with coiled-coils protein 1

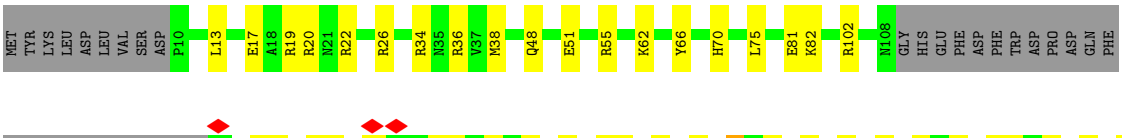
Chain O:

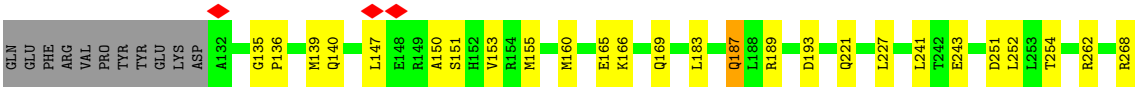


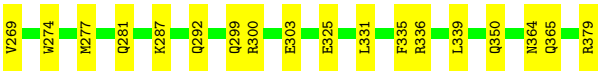


• Molecule 23: RIB43A-like with coiled-coils protein 1

Chain P:

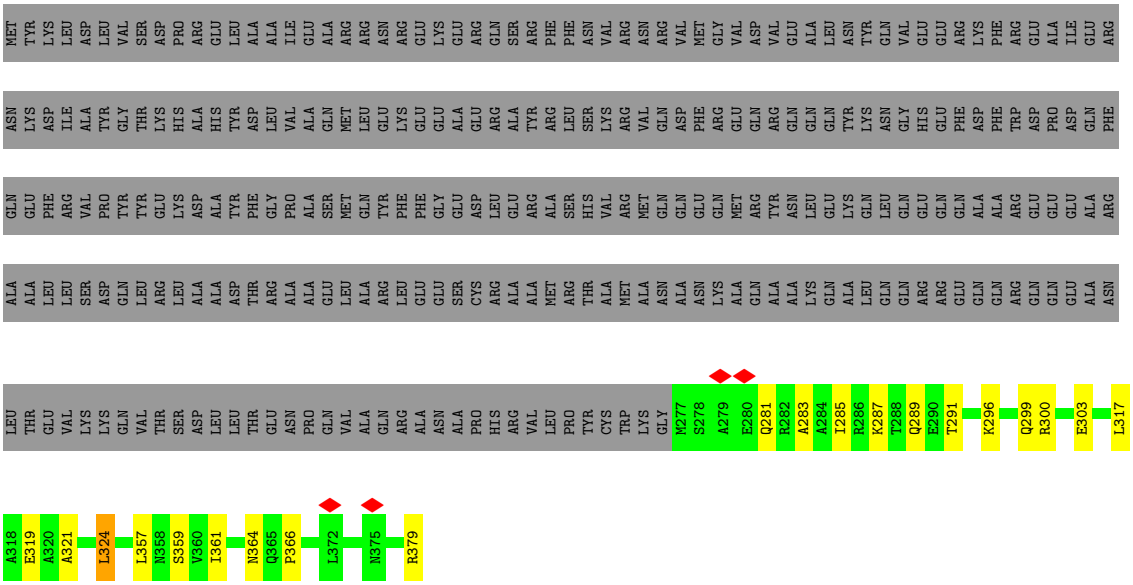






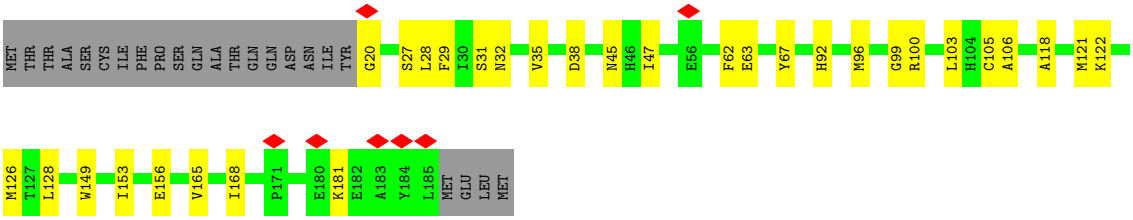
• Molecule 23: RIB43A-like with coiled-coils protein 1

Chain Q:



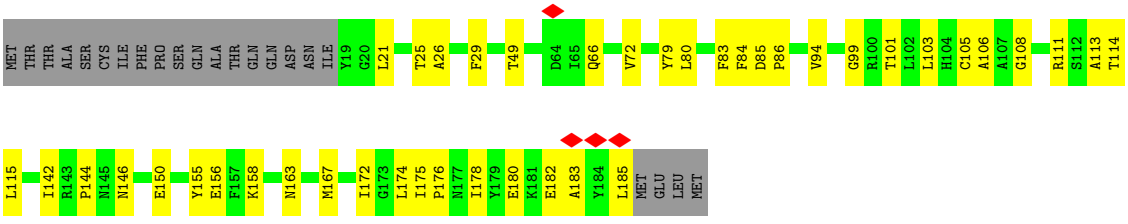
• Molecule 24: Dual specificity phosphatase 21

Chain O1:



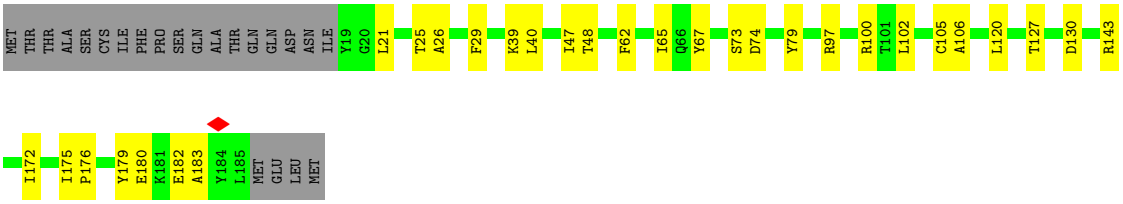
• Molecule 24: Dual specificity phosphatase 21

Chain O2:



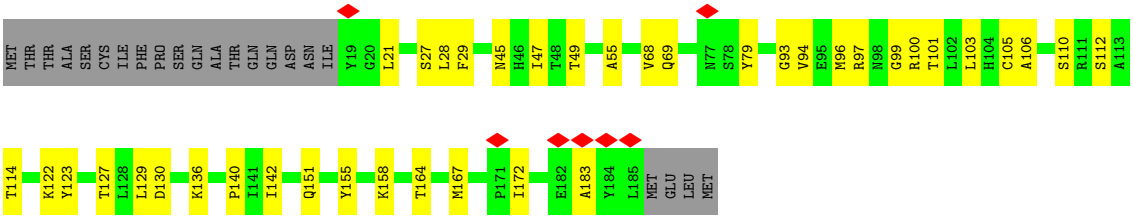
• Molecule 24: Dual specificity phosphatase 21

Chain O3:



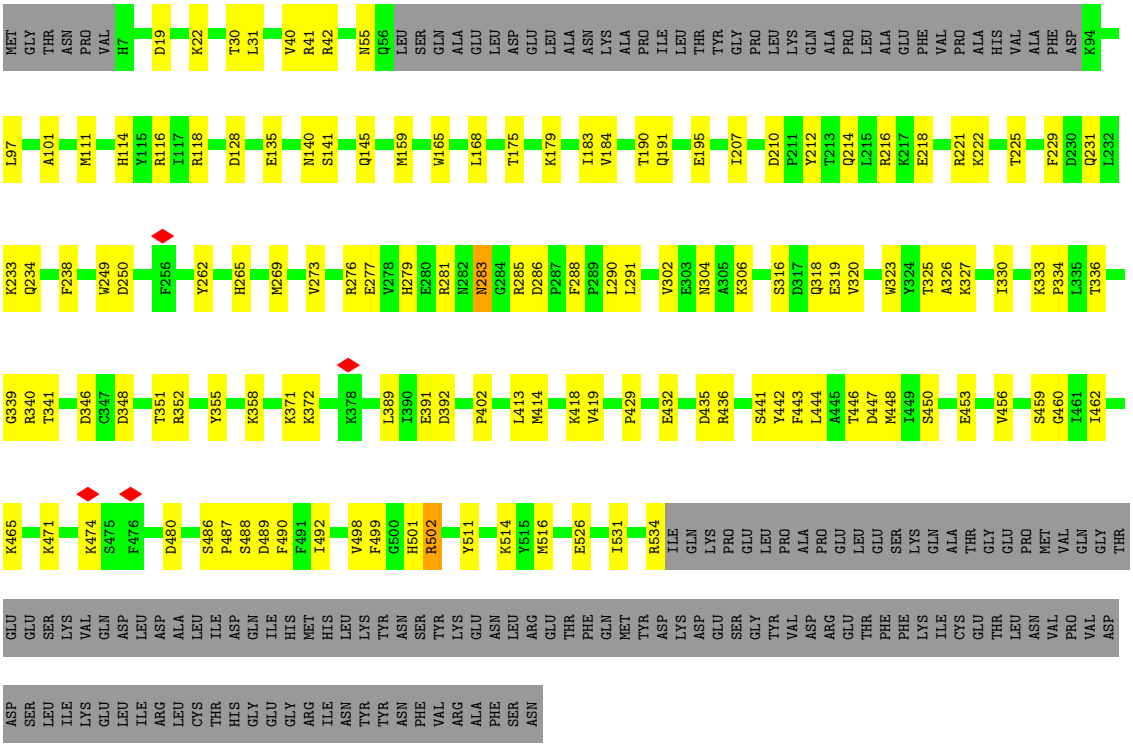
• Molecule 24: Dual specificity phosphatase 21

Chain O4:



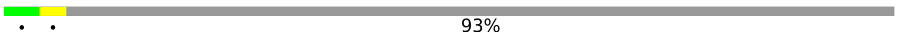
• Molecule 25: EF-hand domain-containing protein 1

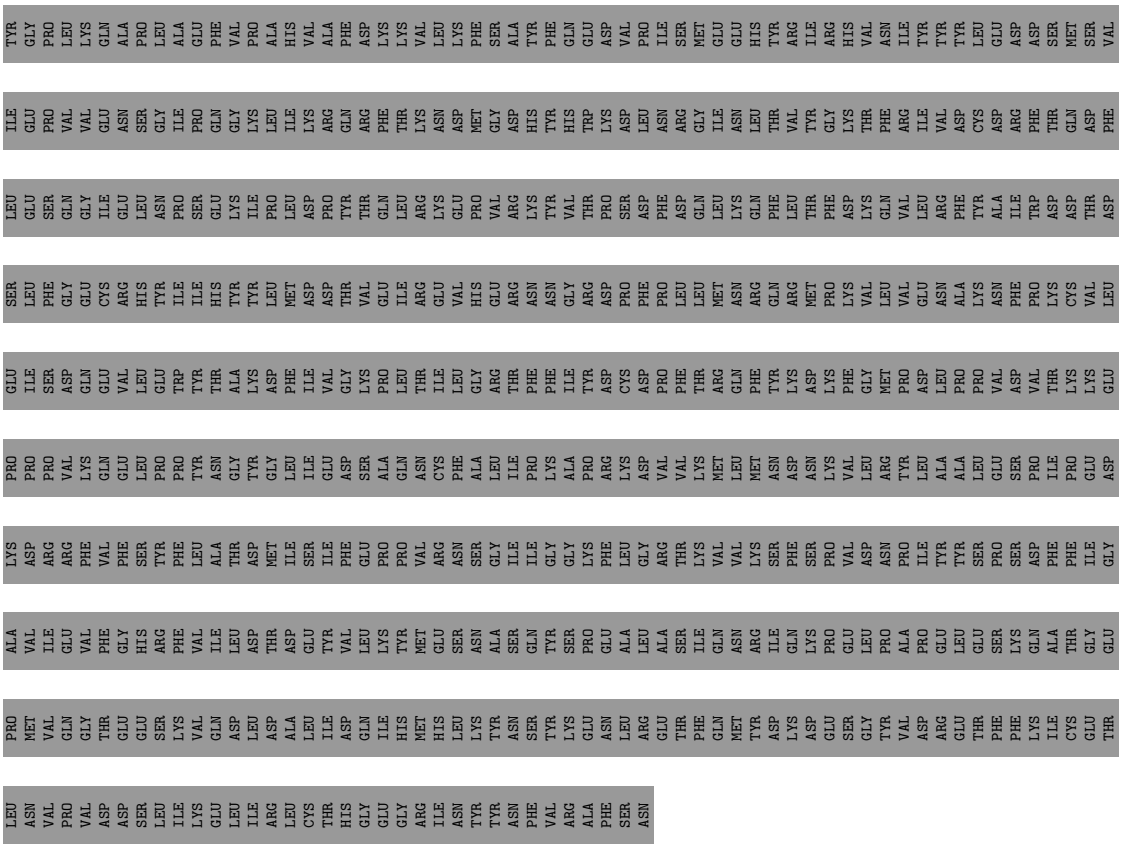
Chain O5:



• Molecule 25: EF-hand domain-containing protein 1

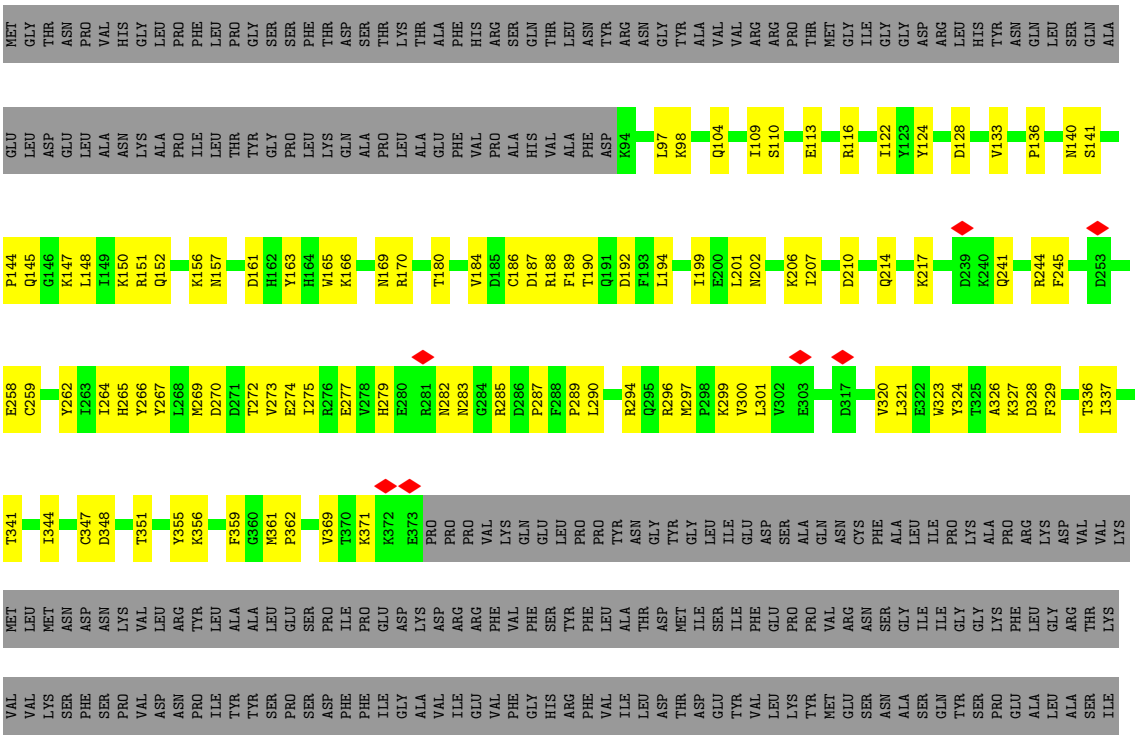
Chain O6:

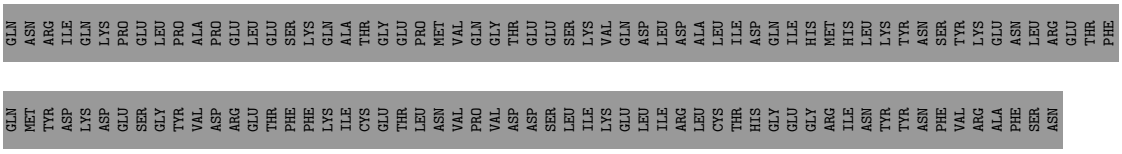




• Molecule 25: EF-hand domain-containing protein 1

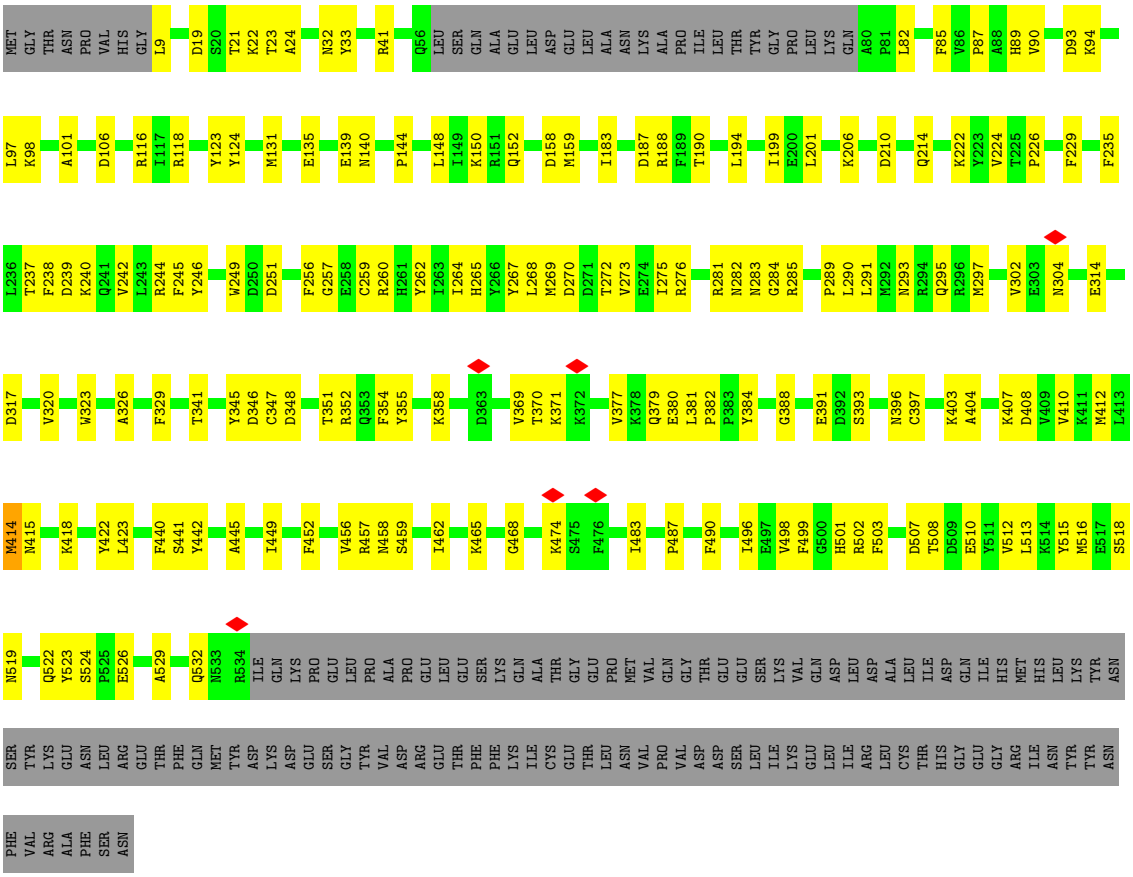
Chain T:





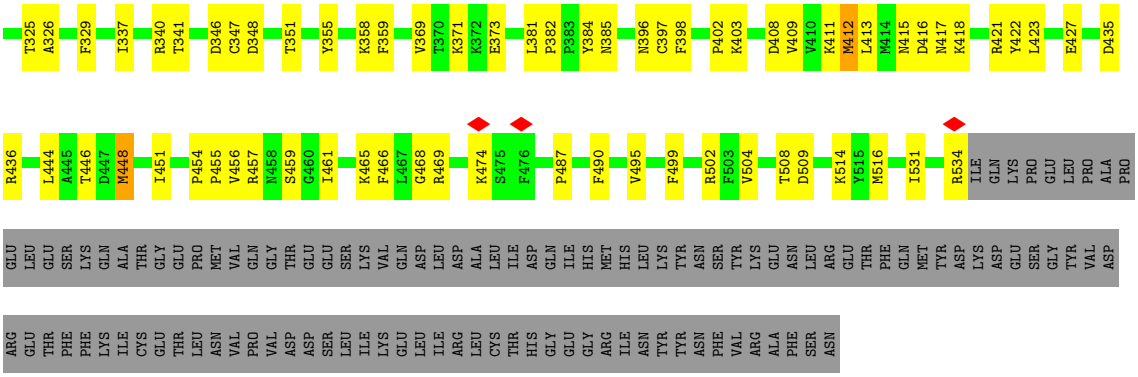
• Molecule 25: EF-hand domain-containing protein 1

Chain U:



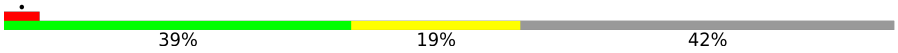
• Molecule 25: EF-hand domain-containing protein 1

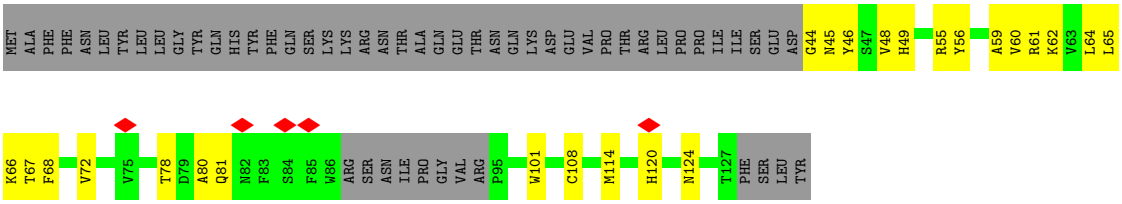
Chain V:



• Molecule 26: Testis expressed 49

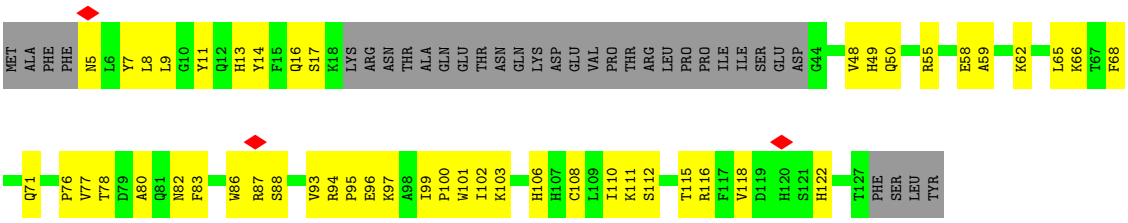
Chain P1:





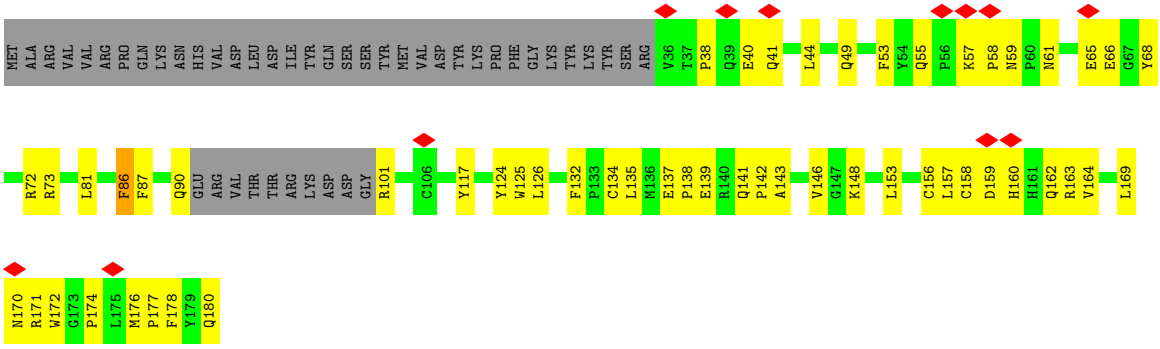
• Molecule 26: Testis expressed 49

Chain P2:



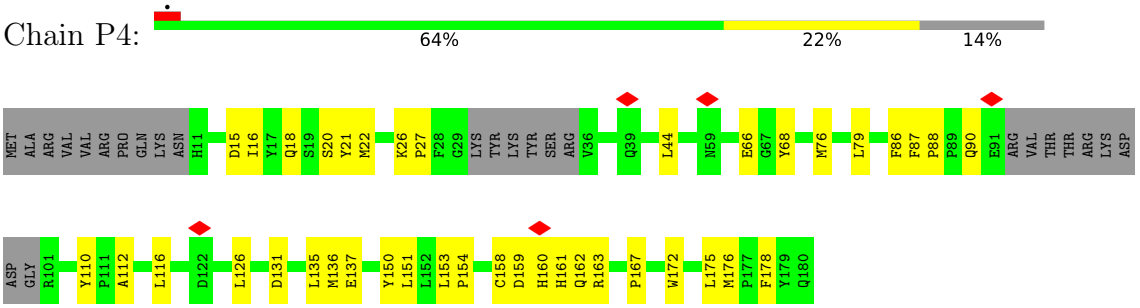
• Molecule 27: Testis-expressed sequence 37 protein

Chain P3:



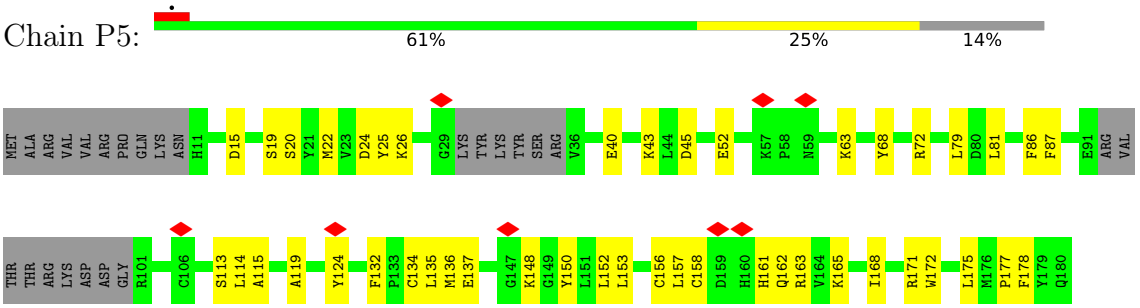
• Molecule 27: Testis-expressed sequence 37 protein

Chain P4:



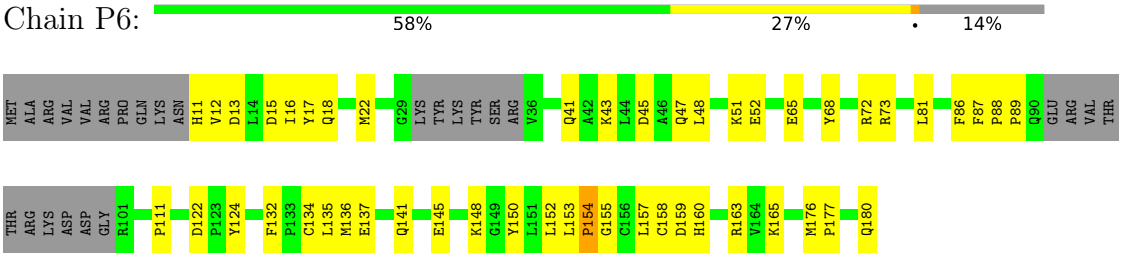
• Molecule 27: Testis-expressed sequence 37 protein

Chain P5:



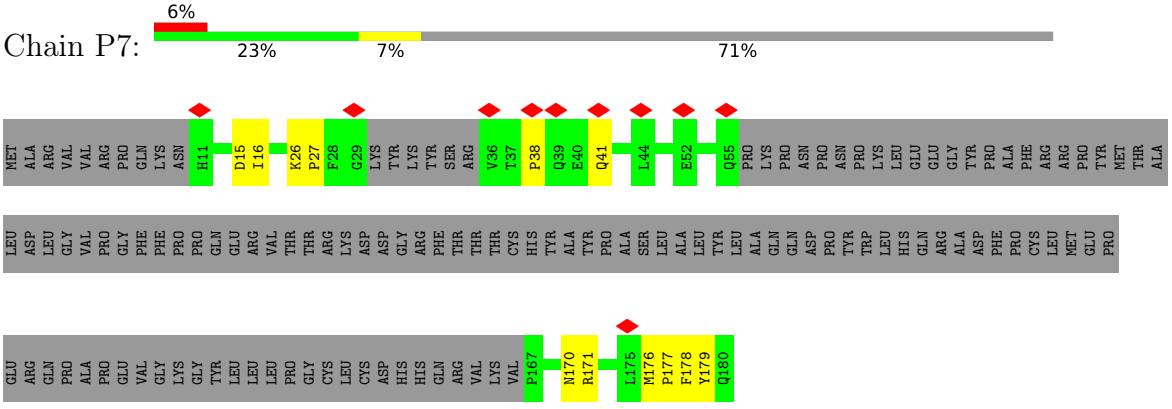
• Molecule 27: Testis-expressed sequence 37 protein

Chain P6:



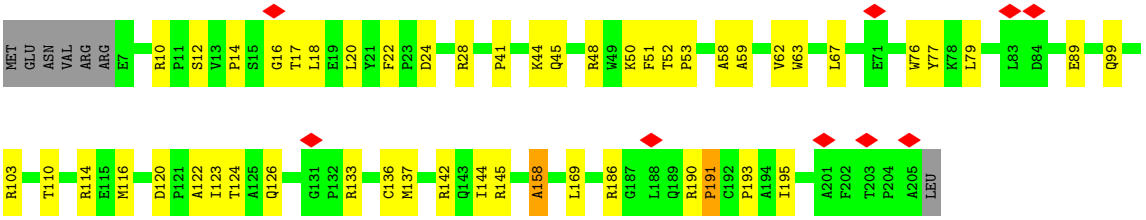
• Molecule 27: Testis-expressed sequence 37 protein

Chain P7:



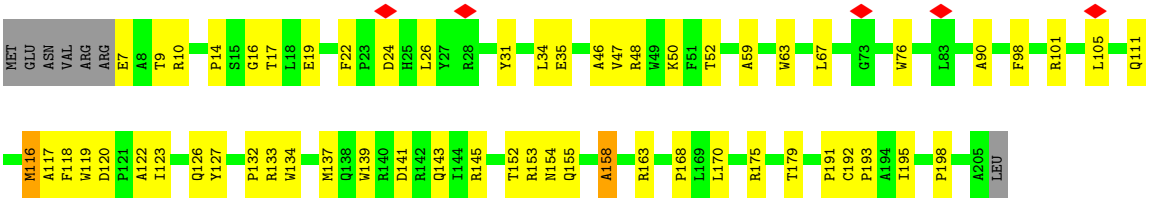
• Molecule 28: Tektin bundle-interacting protein 1

Chain Q1:



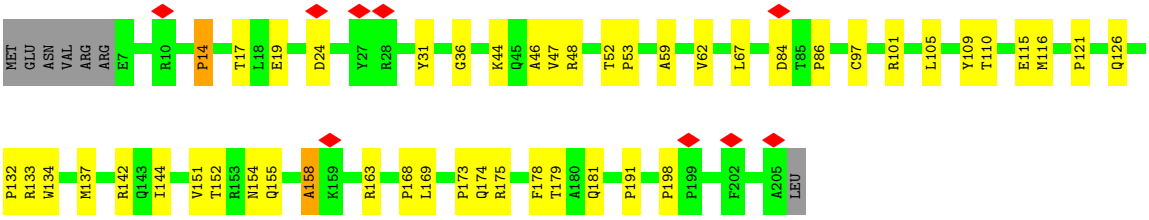
• Molecule 28: Tektin bundle-interacting protein 1

Chain Q2:



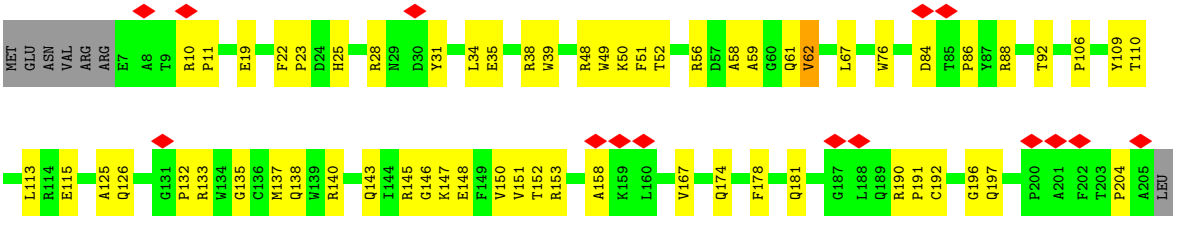
• Molecule 28: Tektin bundle-interacting protein 1

Chain Q3:



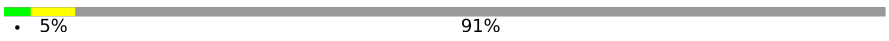
• Molecule 28: Tektin bundle-interacting protein 1

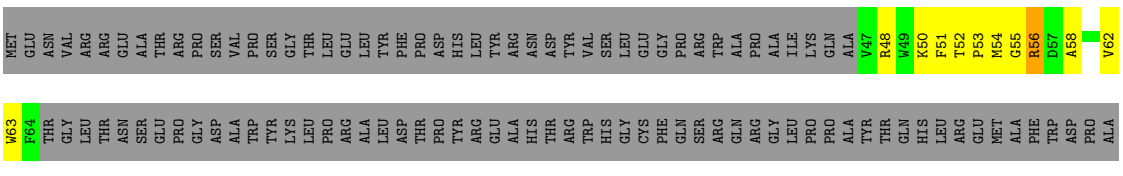
Chain Q4:



• Molecule 28: Tektin bundle-interacting protein 1

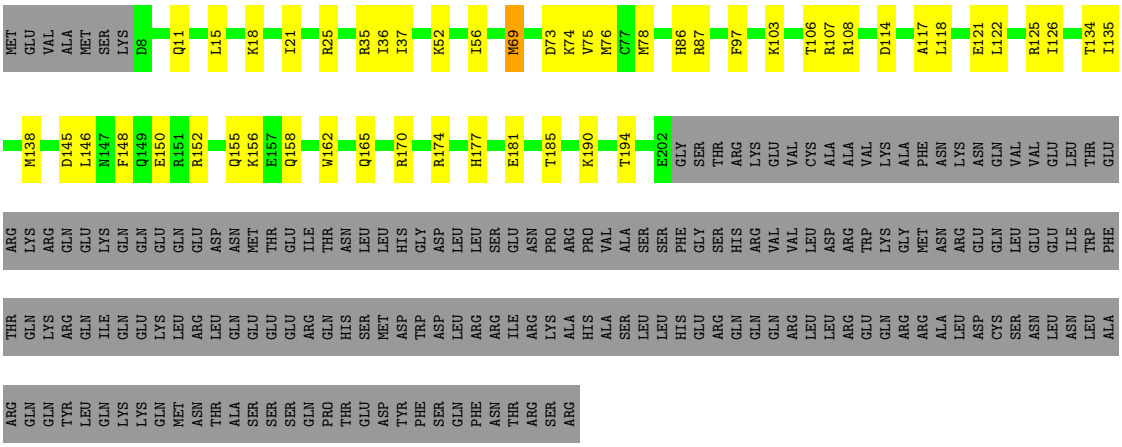
Chain Q5:





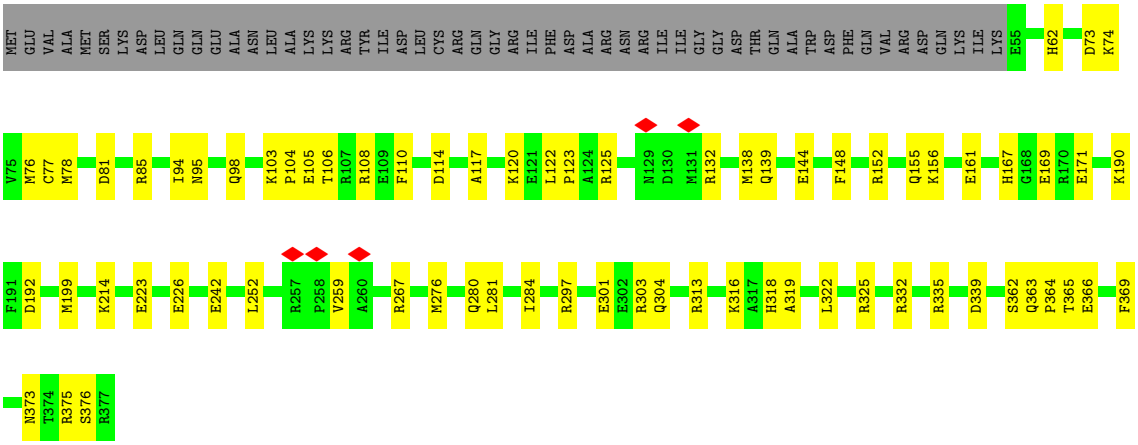
• Molecule 29: RIB43A-like with coiled-coils protein 2

Chain R:



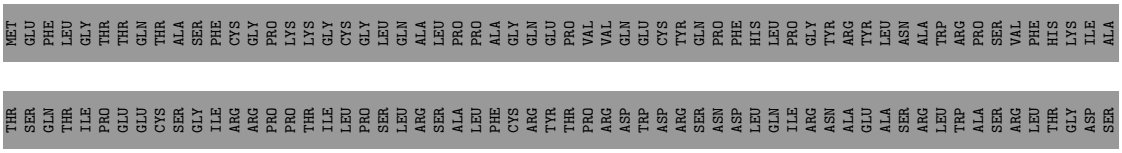
• Molecule 29: RIB43A-like with coiled-coils protein 2

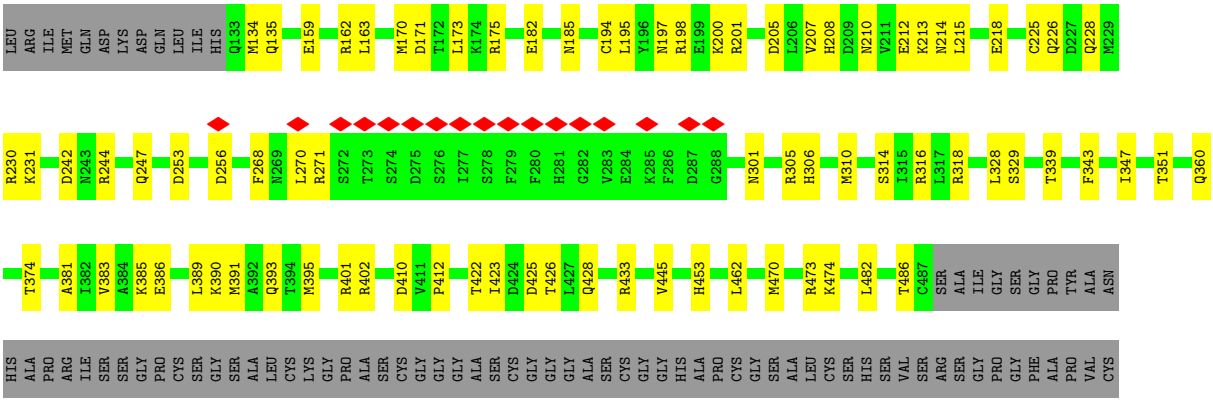
Chain S:



• Molecule 30: Tektin-5

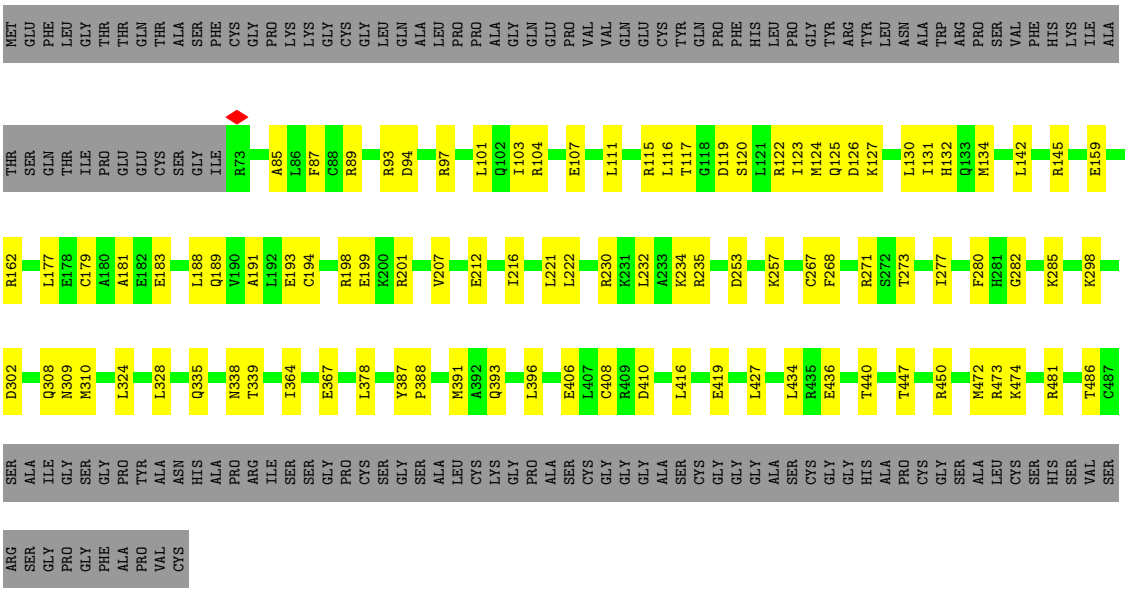
Chain U0:





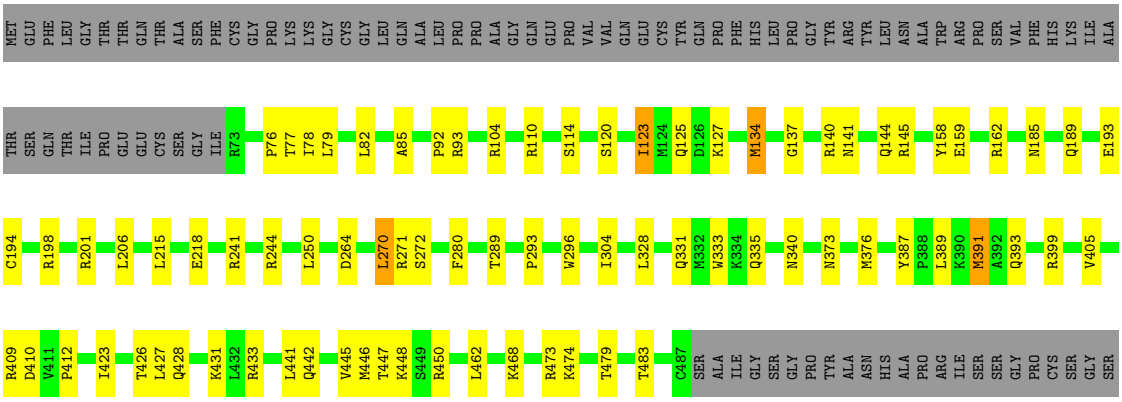
• Molecule 30: Tektin-5

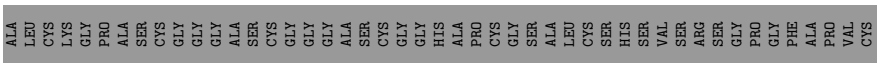
Chain U1:



• Molecule 30: Tektin-5

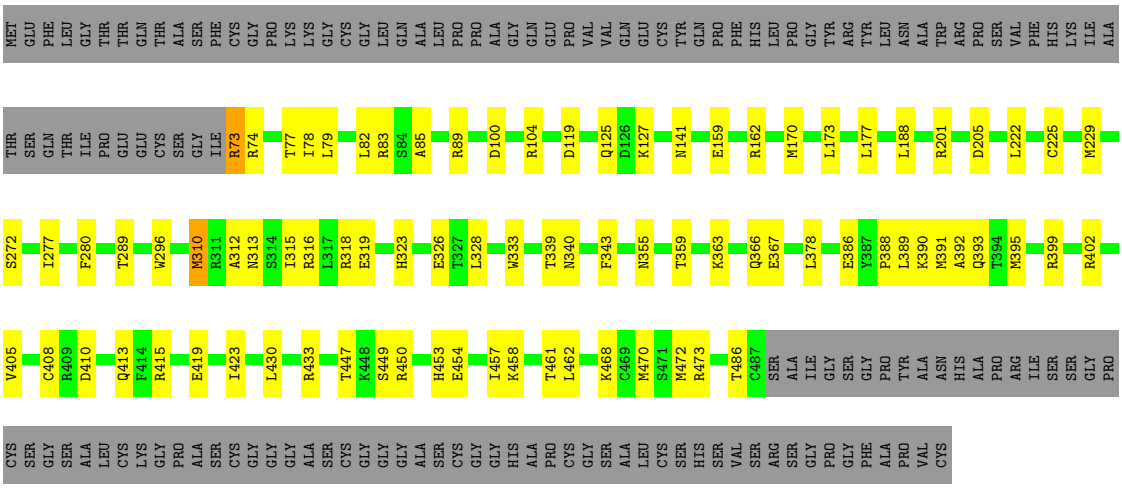
Chain U2:





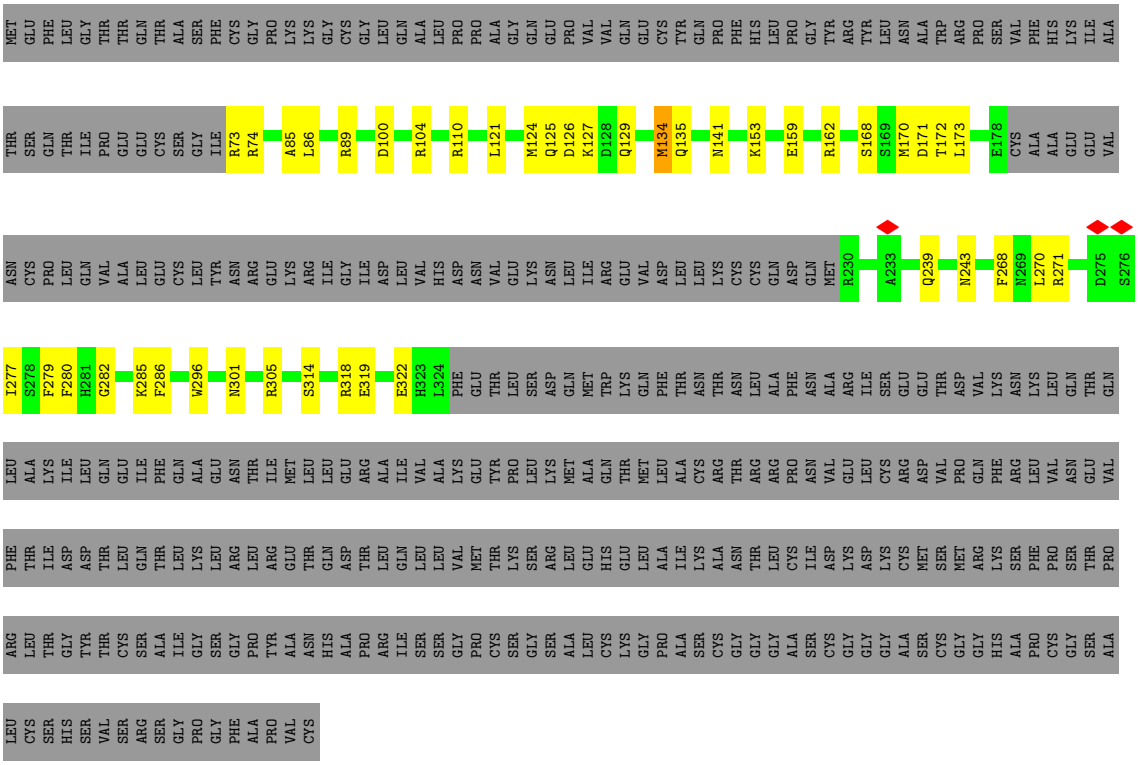
• Molecule 30: Tektin-5

Chain U3:



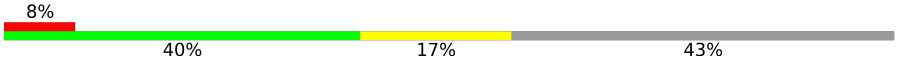
• Molecule 30: Tektin-5

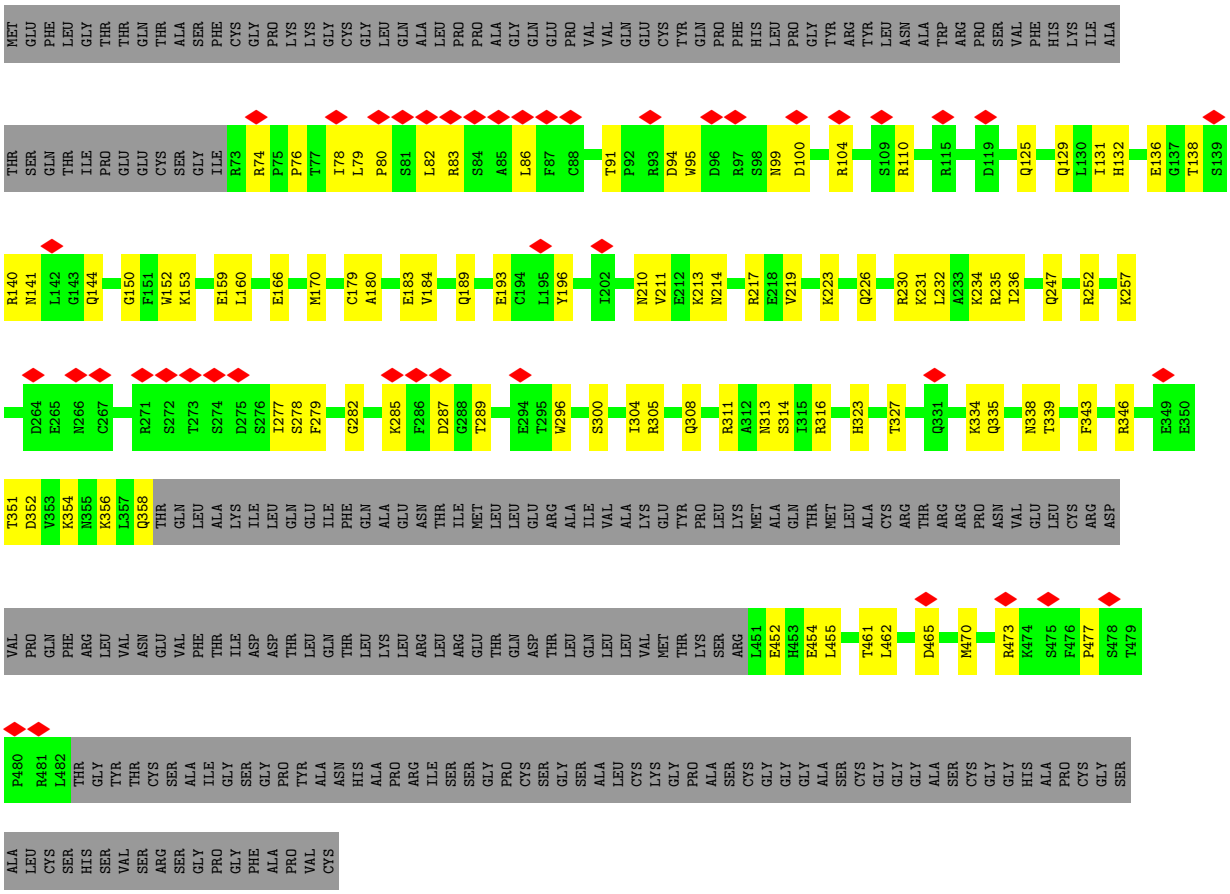
Chain U4:



• Molecule 30: Tektin-5

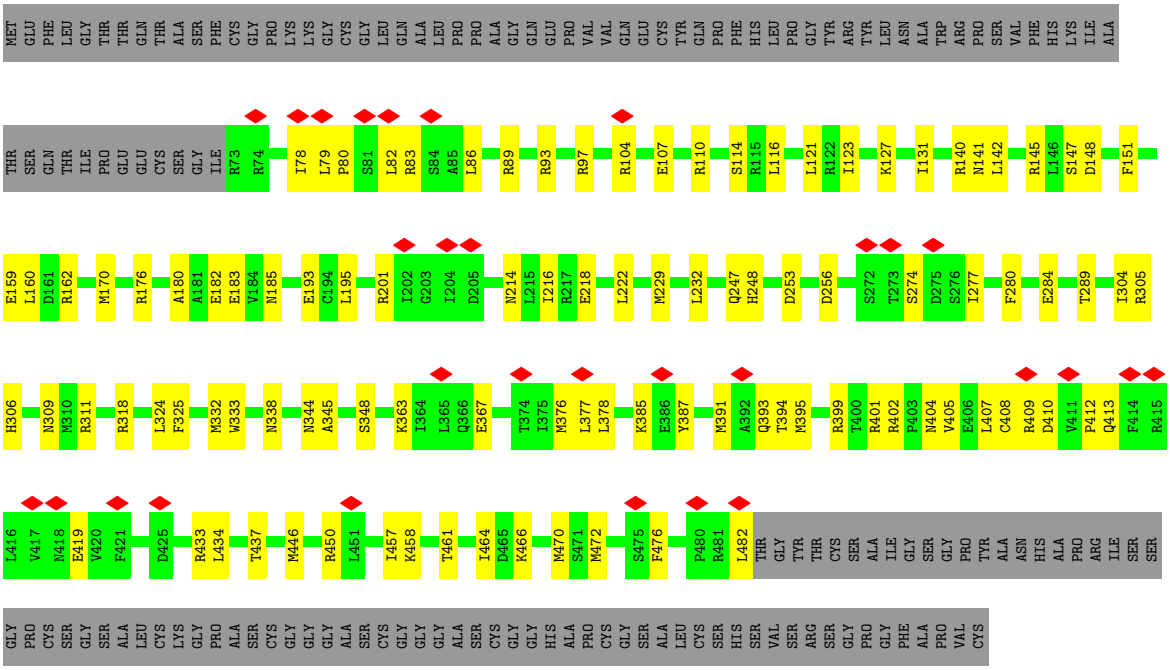
Chain U5:





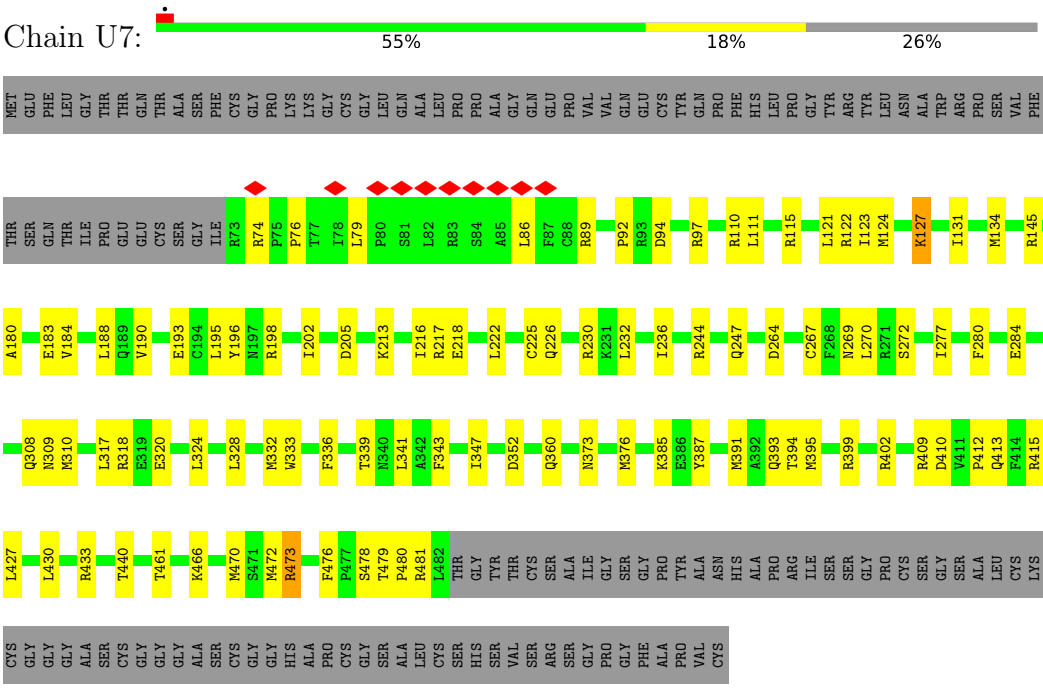
• Molecule 30: Tektin-5

Chain U6:



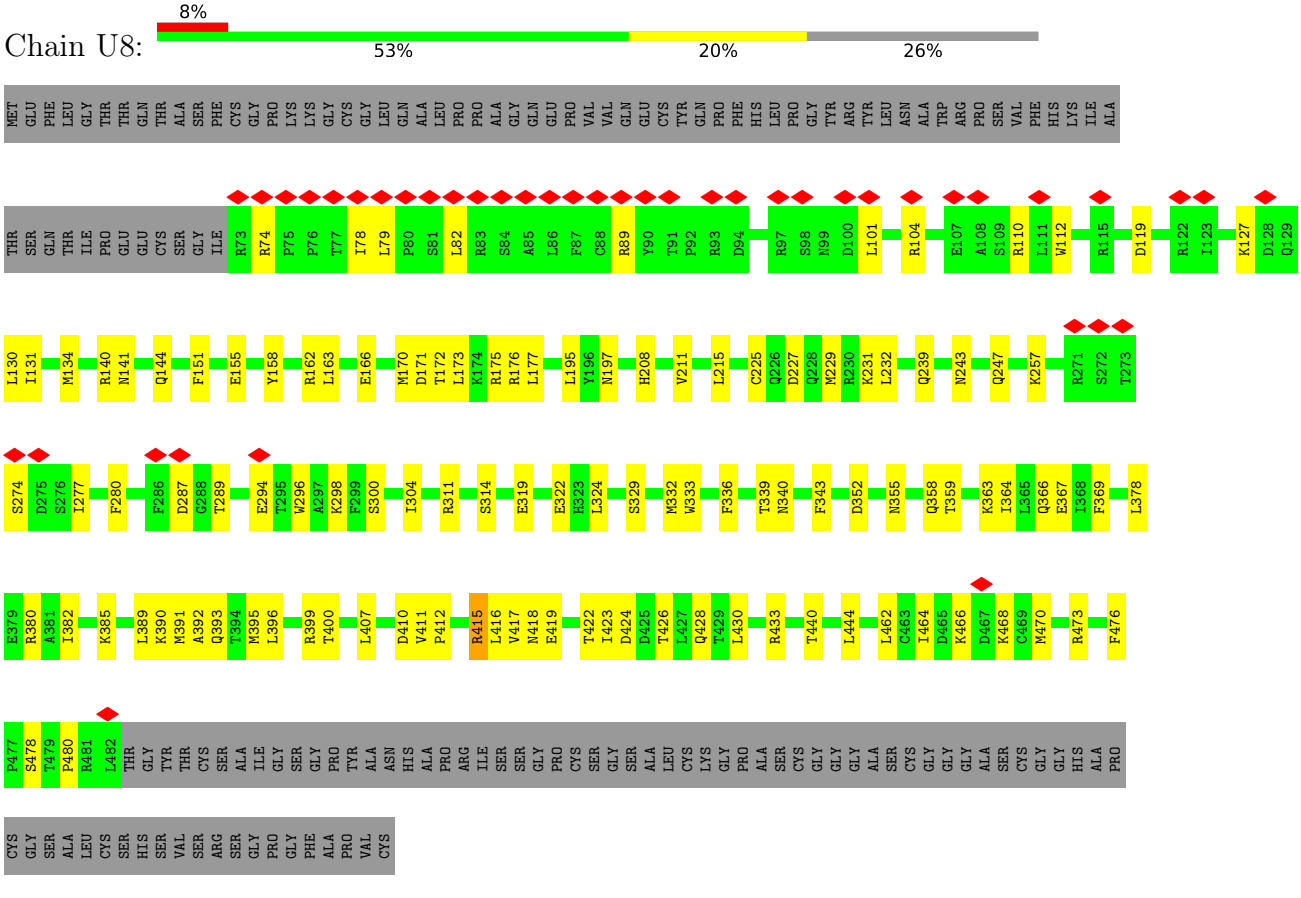
• Molecule 30: Tektin-5

Chain U7:



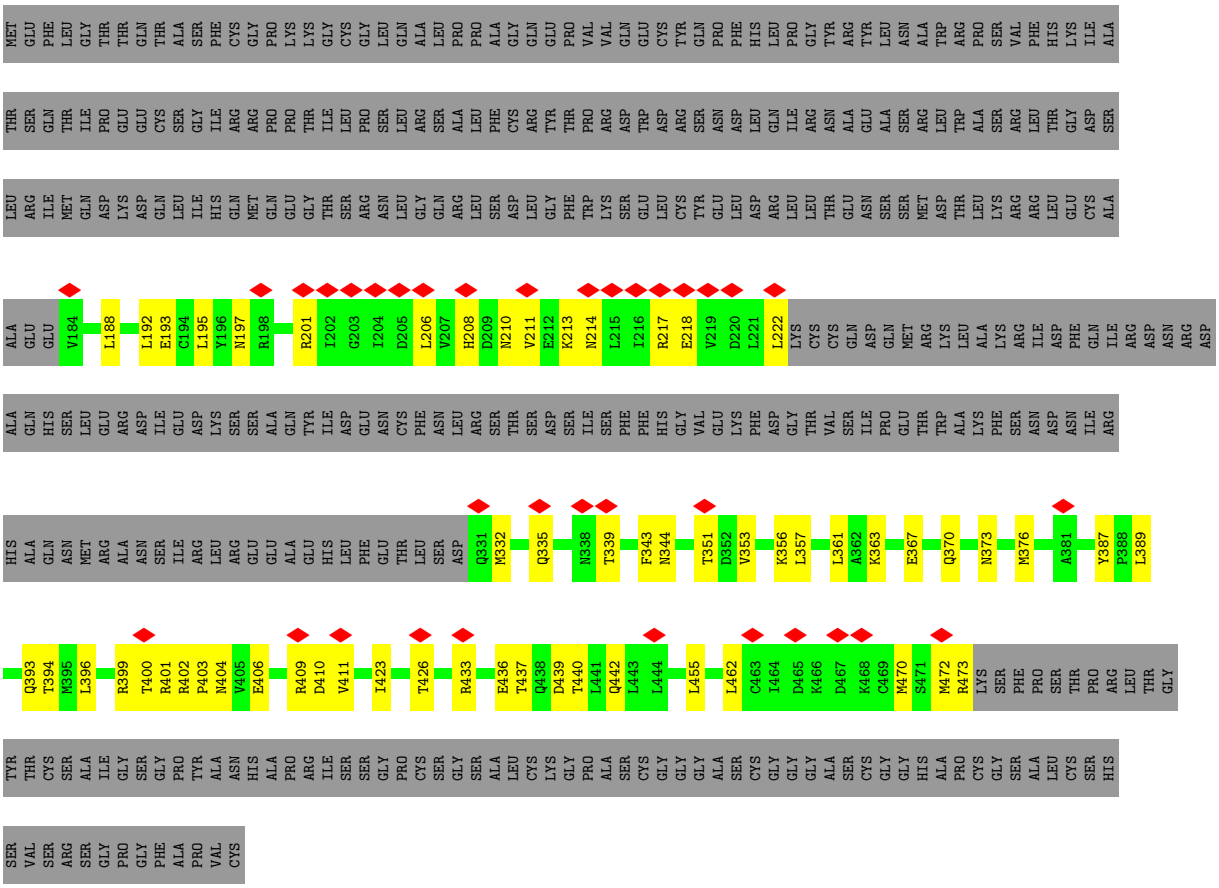
• Molecule 30: Tektin-5

Chain U8:



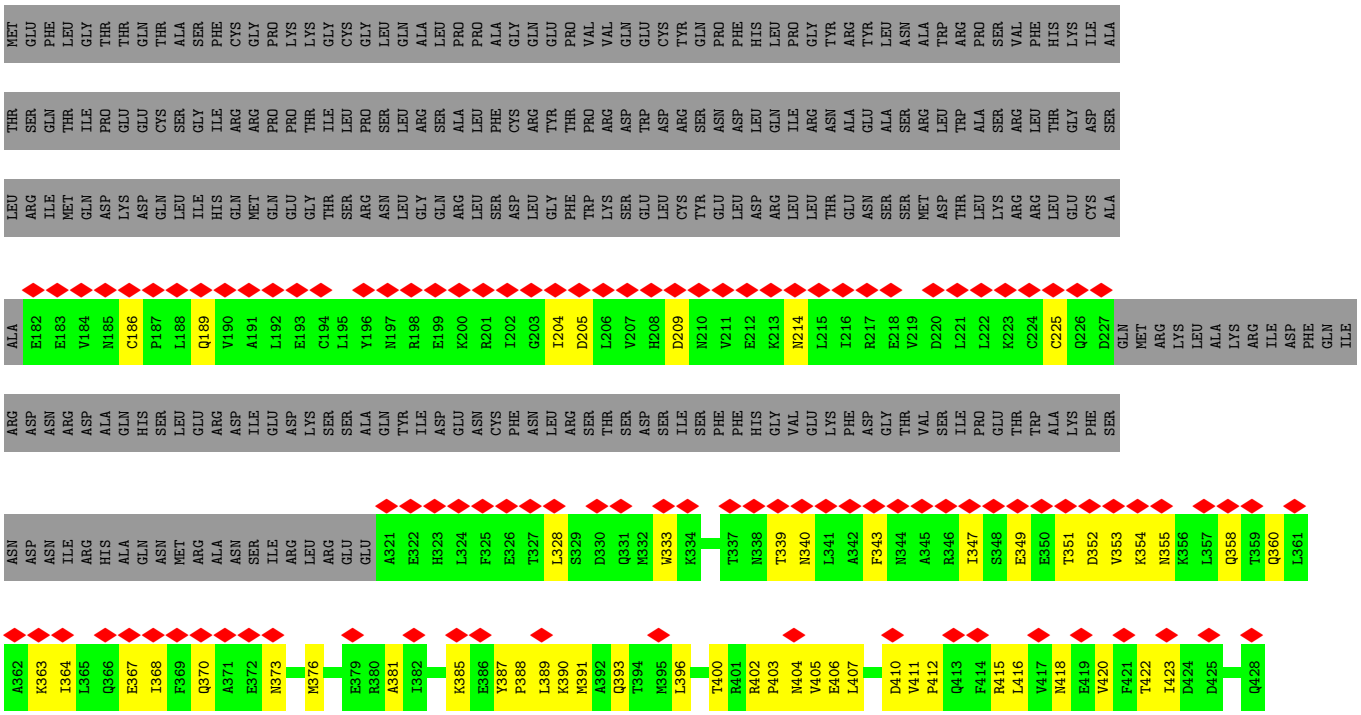
• Molecule 30: Tektin-5

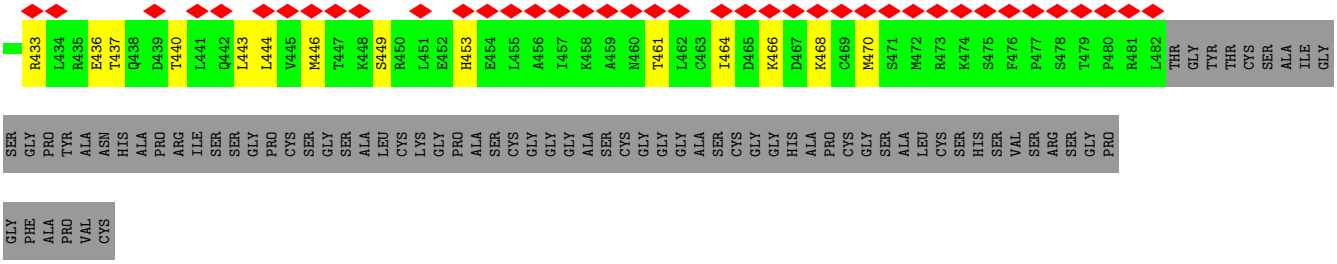
Chain U9:



• Molecule 30: Tektin-5

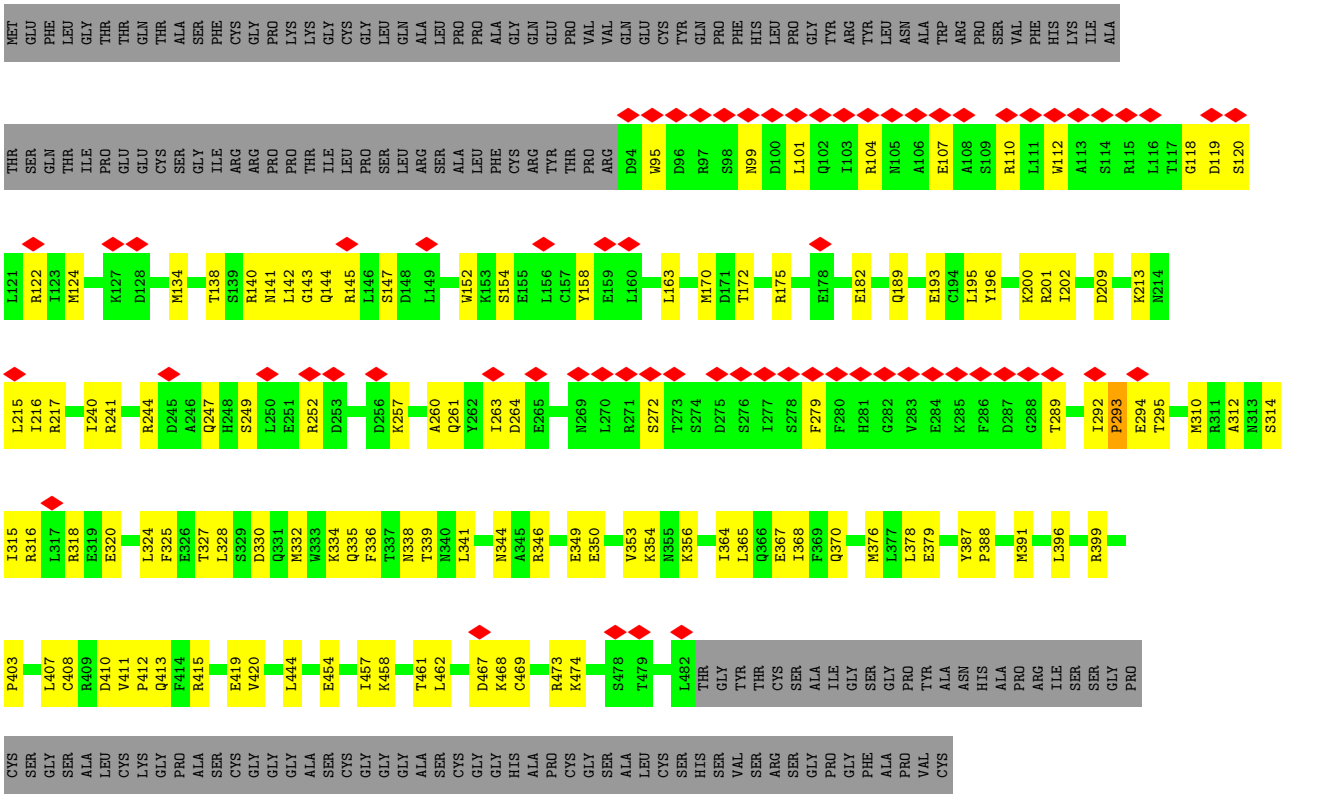
Chain V0:





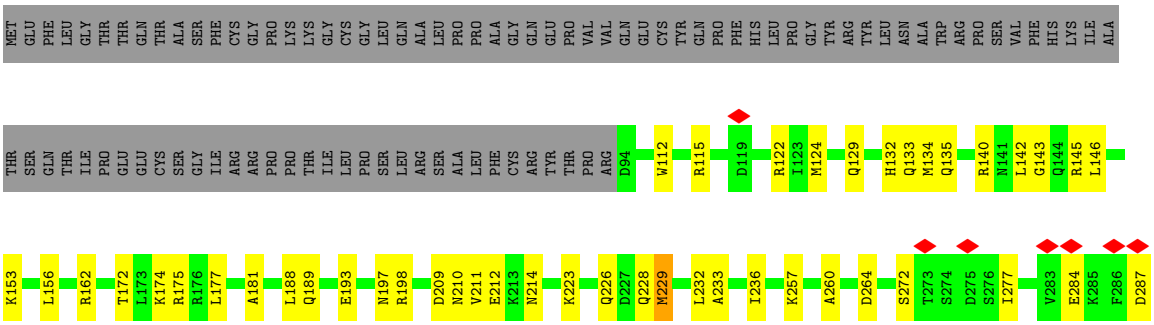
• Molecule 30: Tektin-5

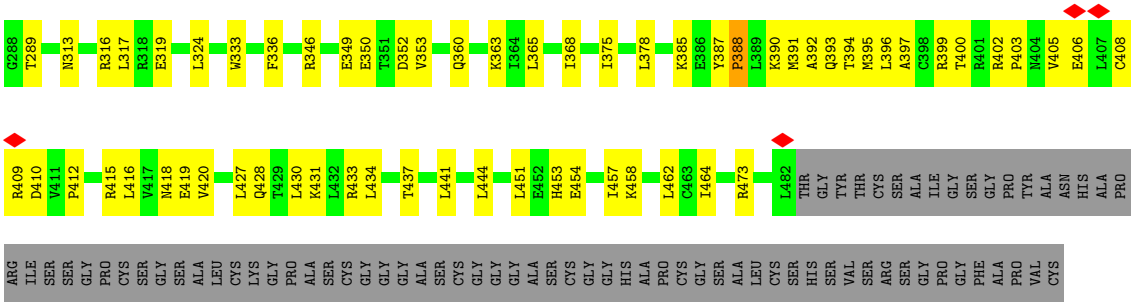
Chain V1:



• Molecule 30: Tektin-5

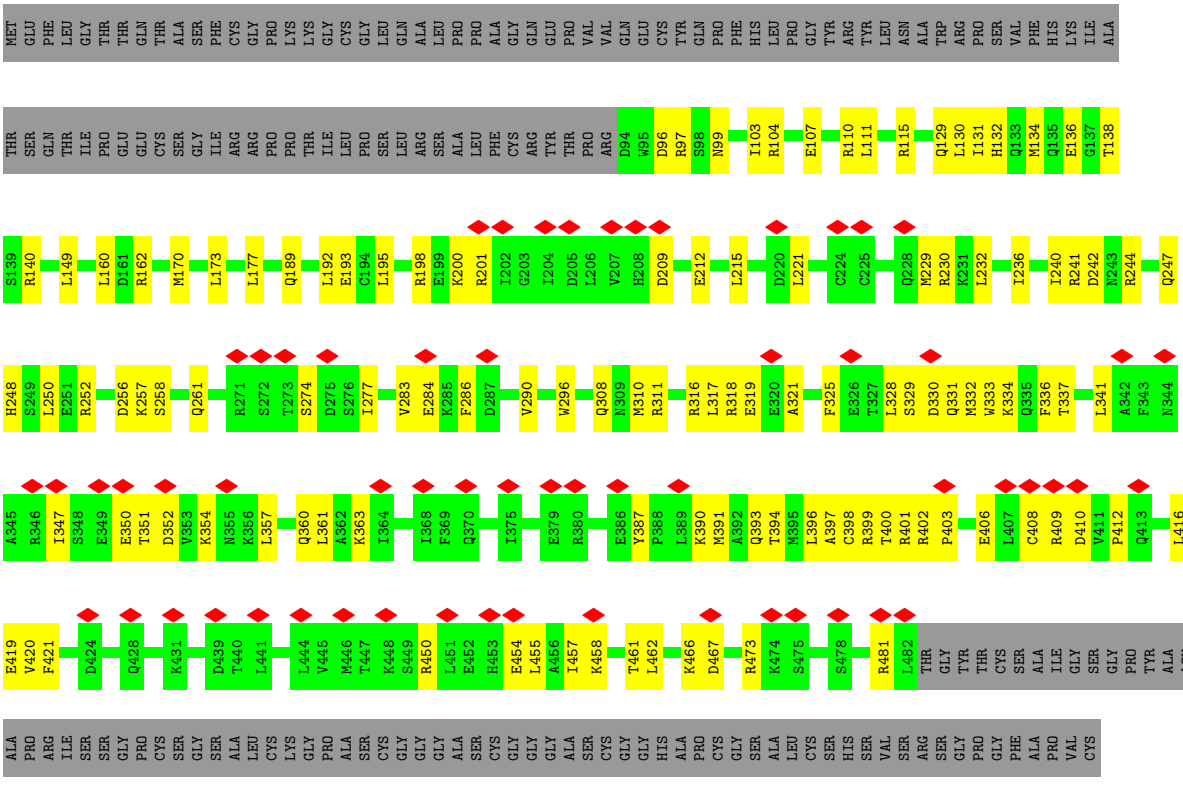
Chain V2:





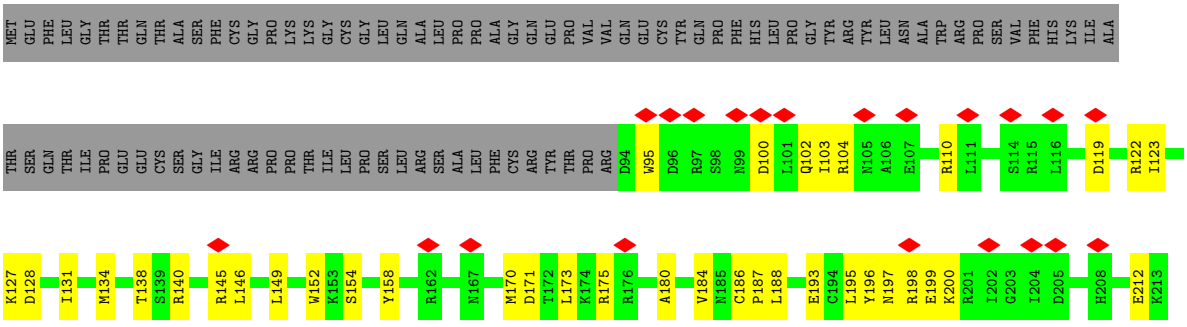
• Molecule 30: Tektin-5

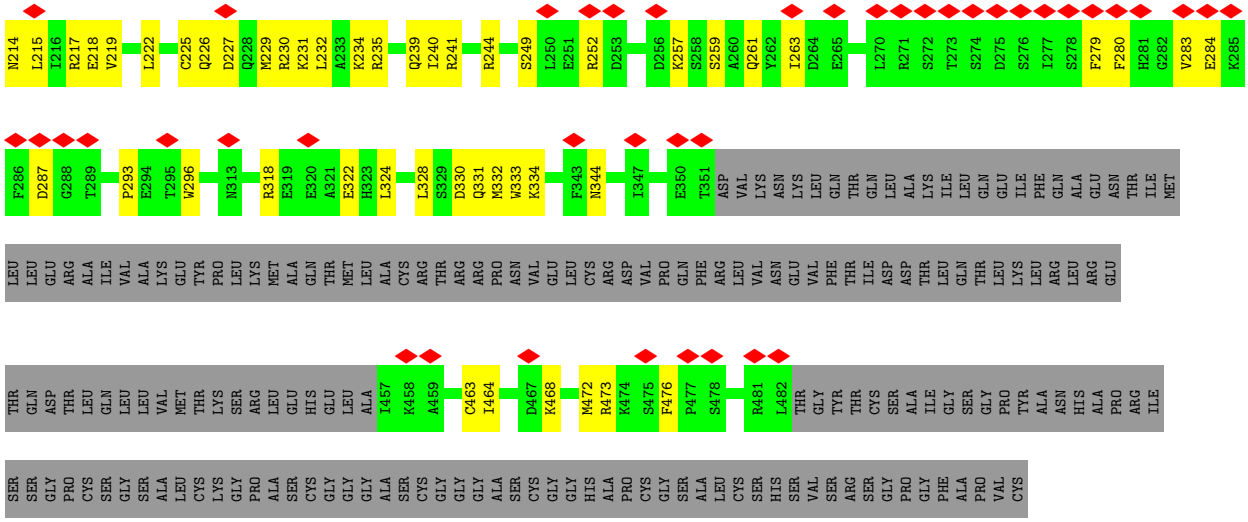
Chain V3:



• Molecule 30: Tektin-5

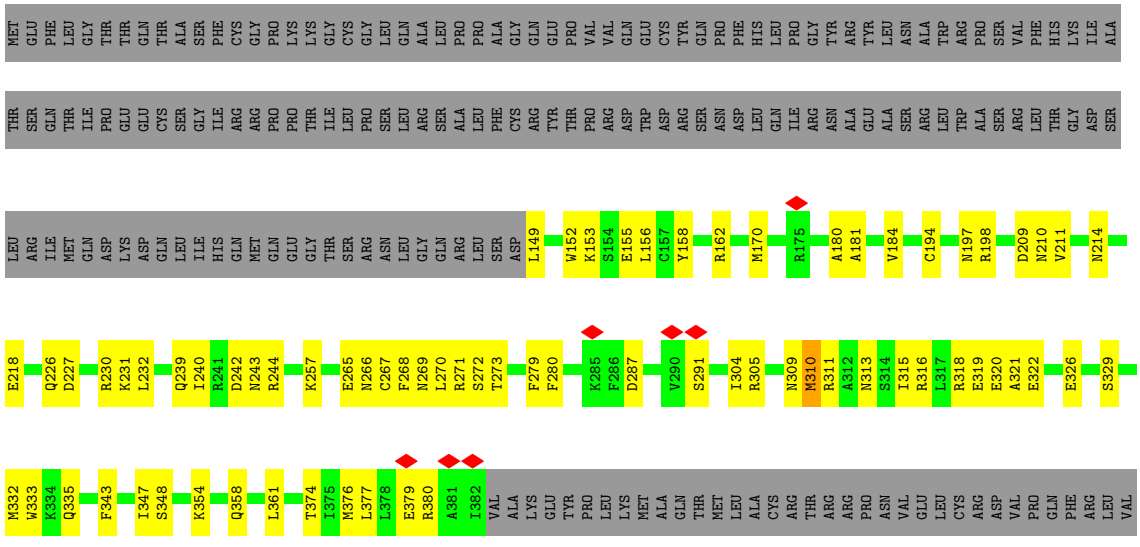
Chain V4:





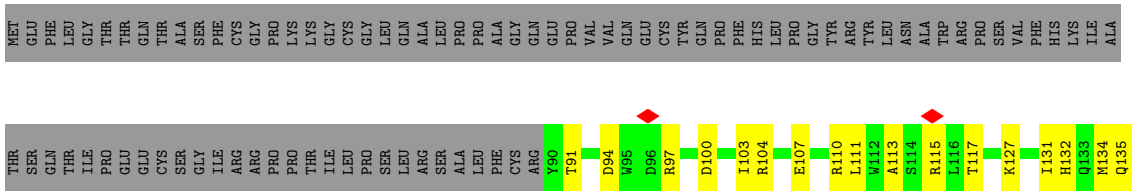
• Molecule 30: Tektin-5

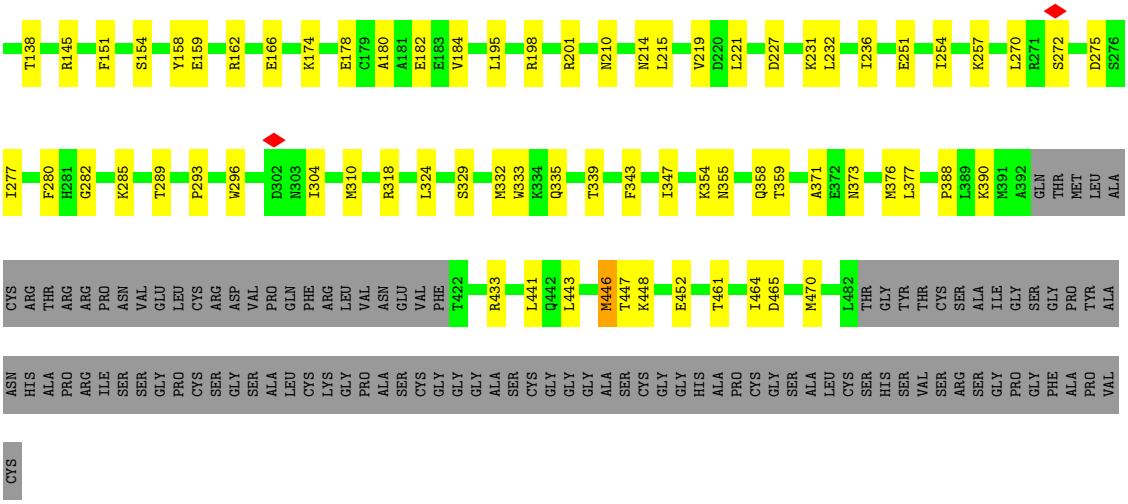
Chain V5:



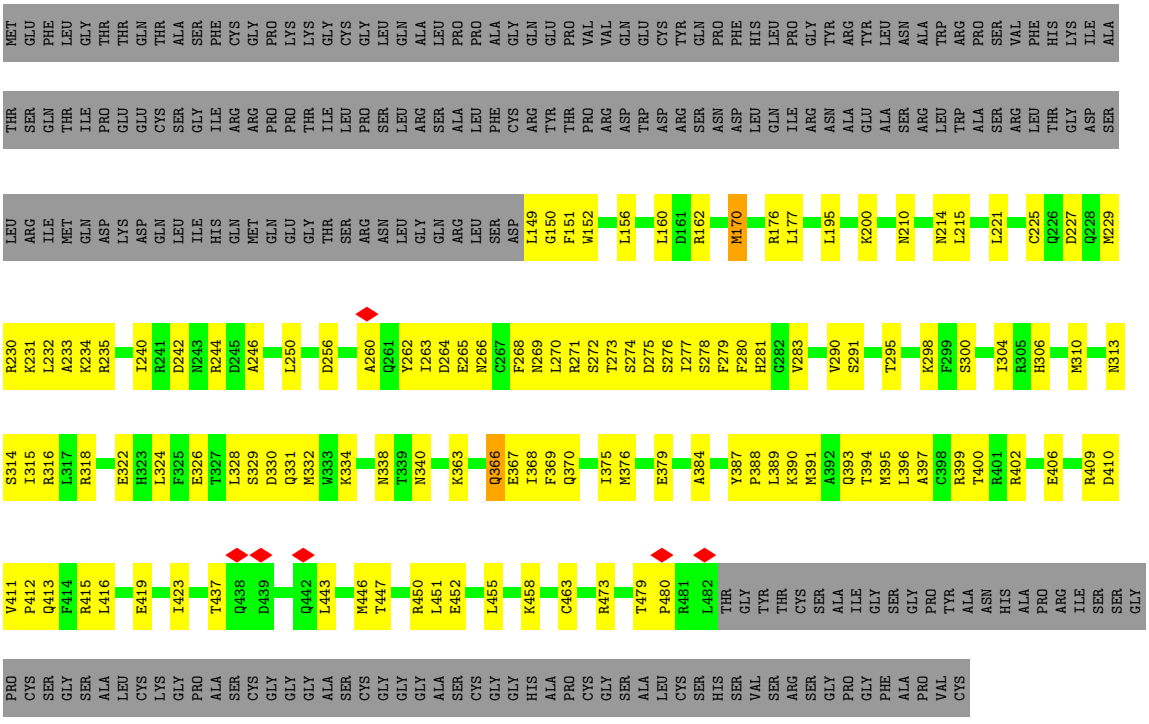
• Molecule 30: Tektin-5

Chain V6:

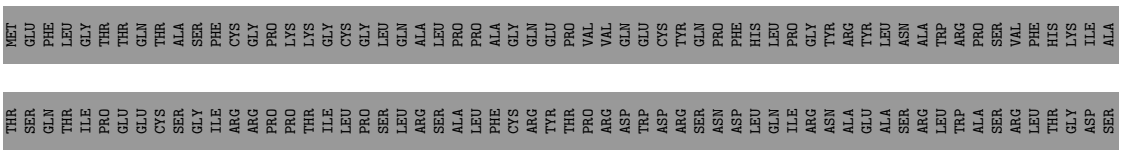


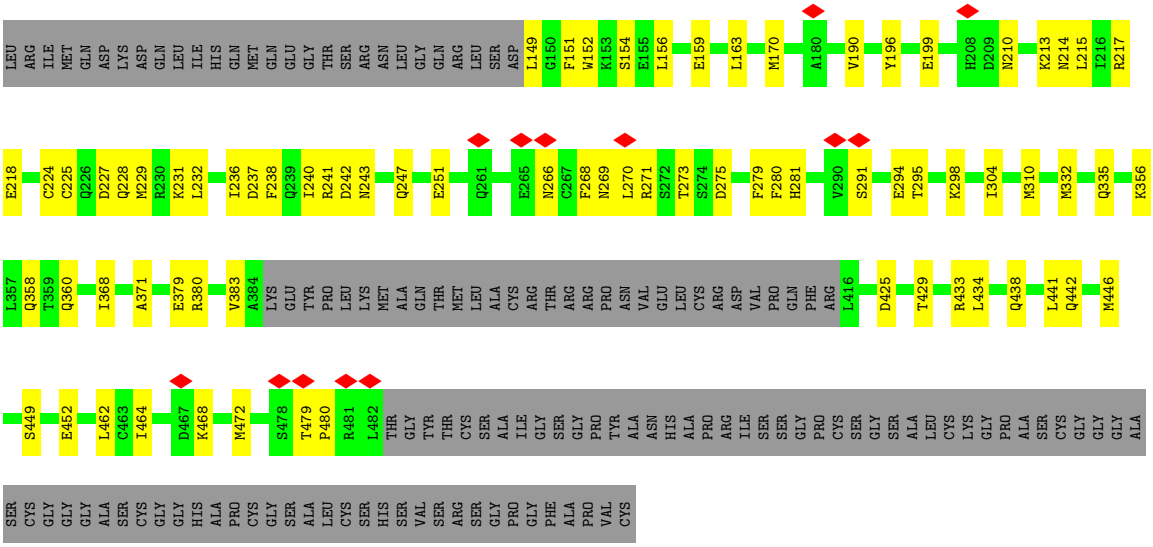


• Molecule 30: Tektin-5



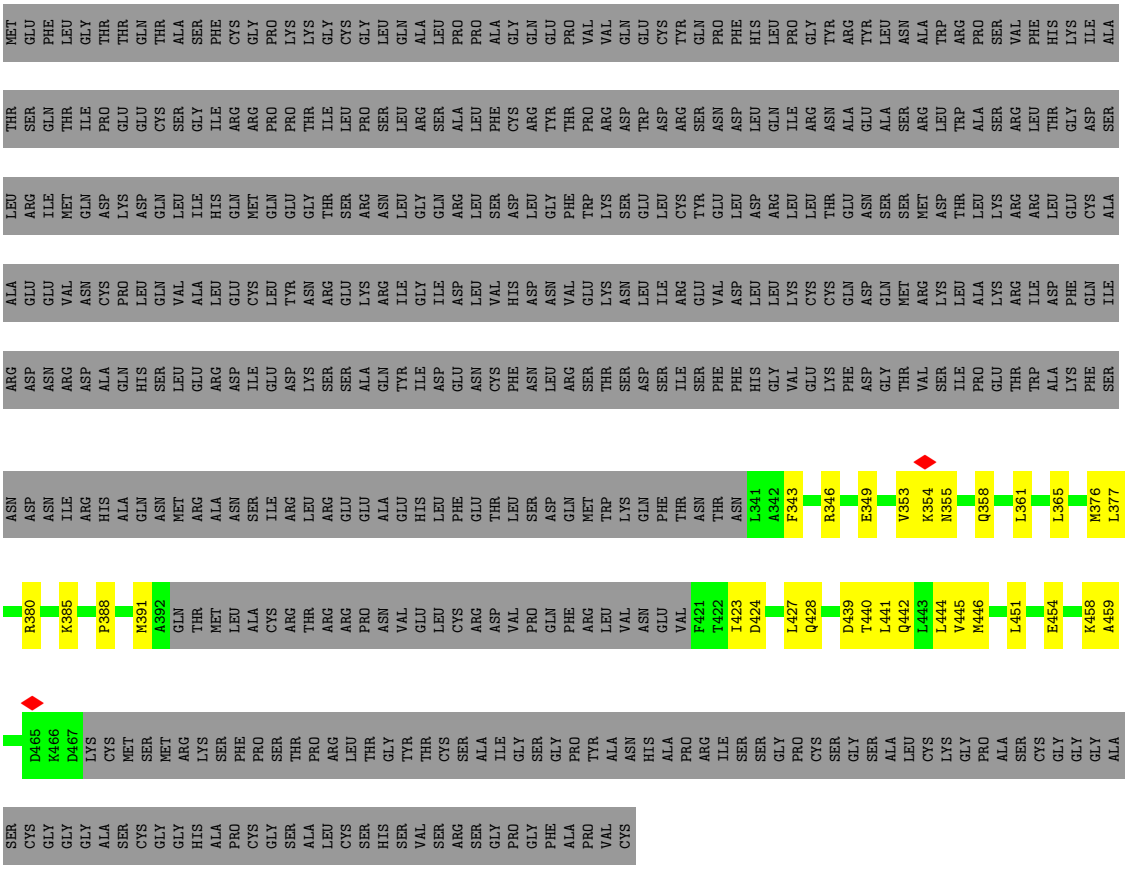
• Molecule 30: Tektin-5





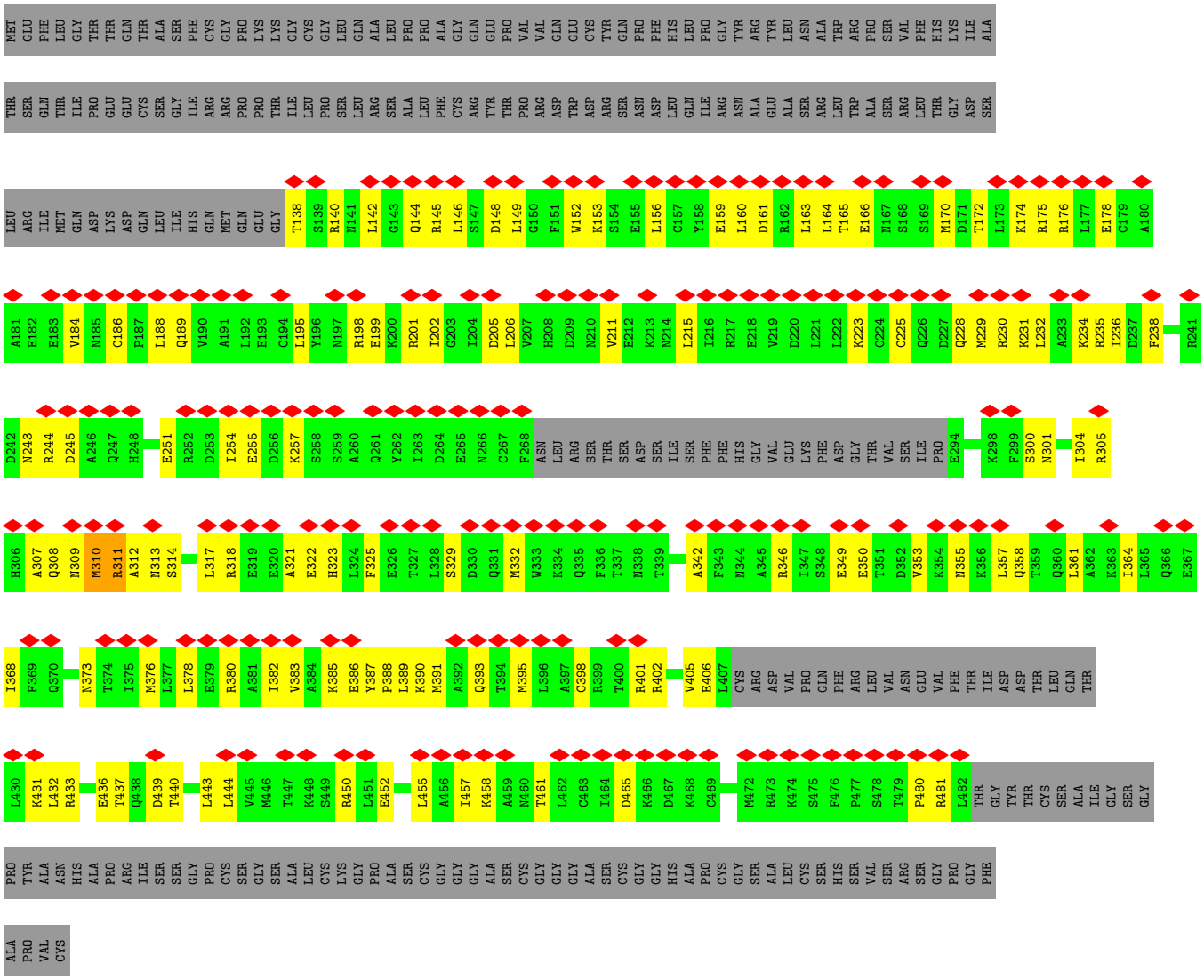
• Molecule 30: Tektin-5

Chain V9:



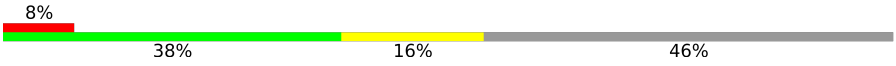
• Molecule 30: Tektin-5

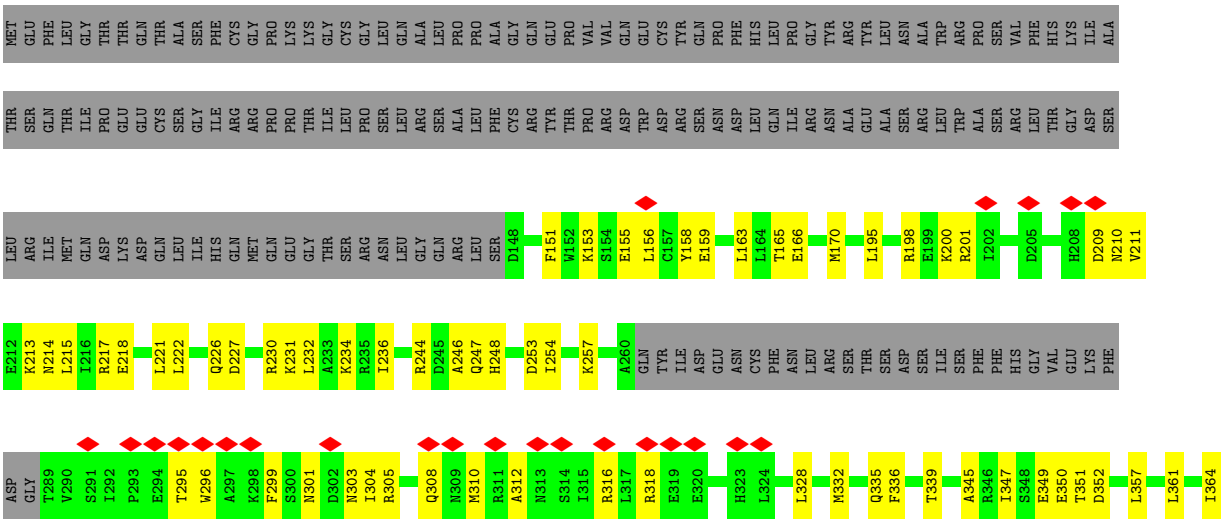
Chain W0:

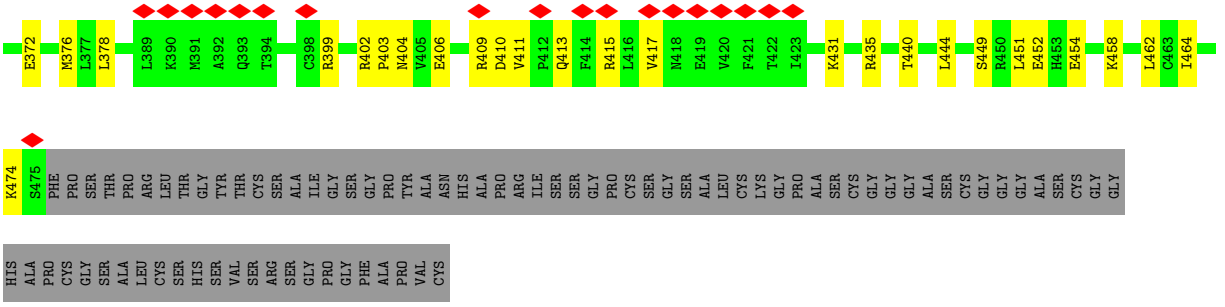


• Molecule 30: Tektin-5

Chain W2:

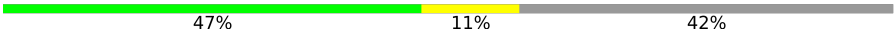


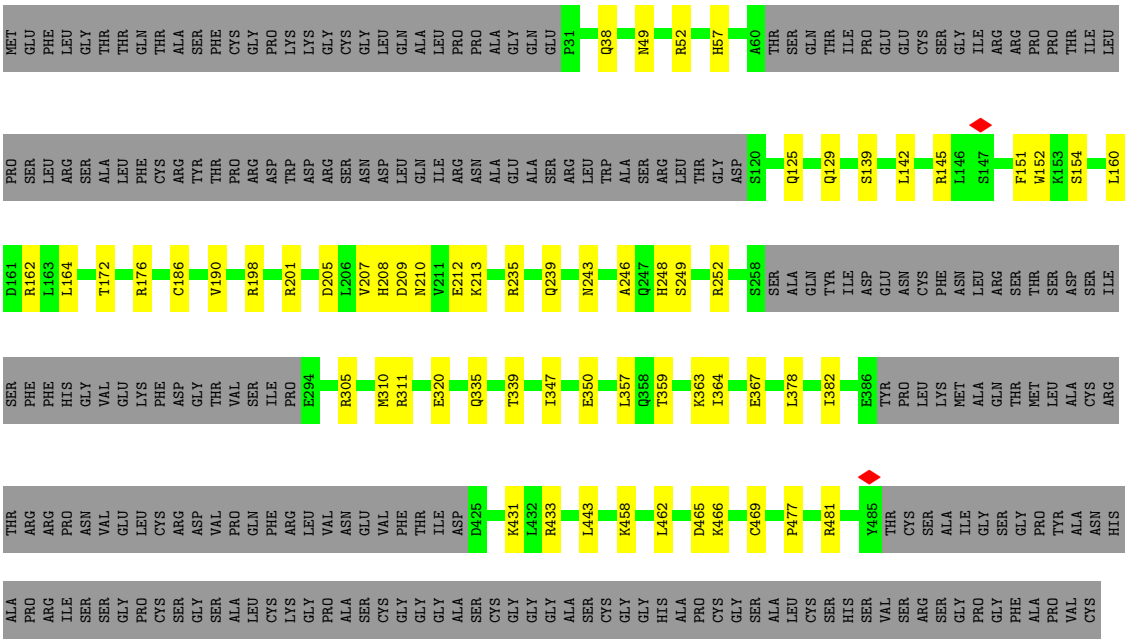




• Molecule 30: Tektin-5

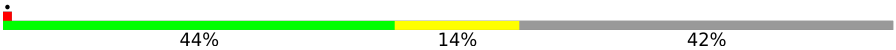
Chain W4:

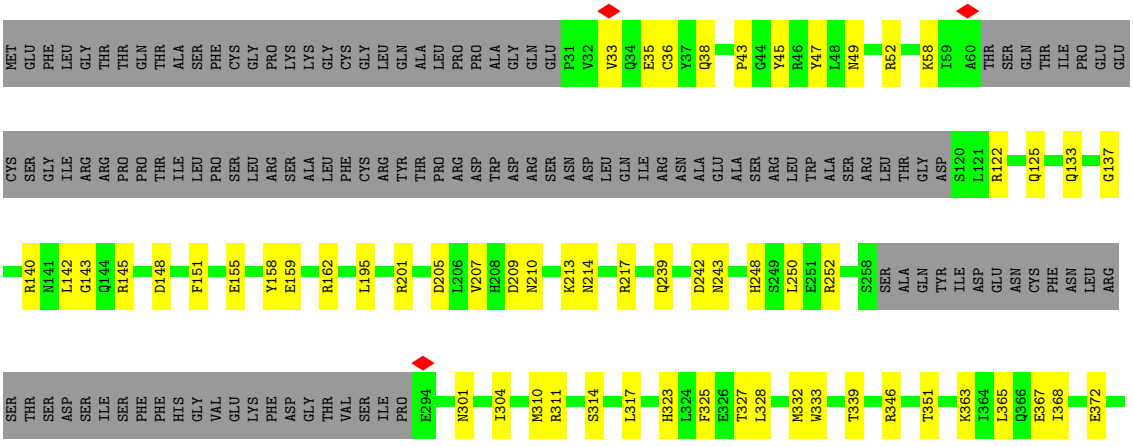


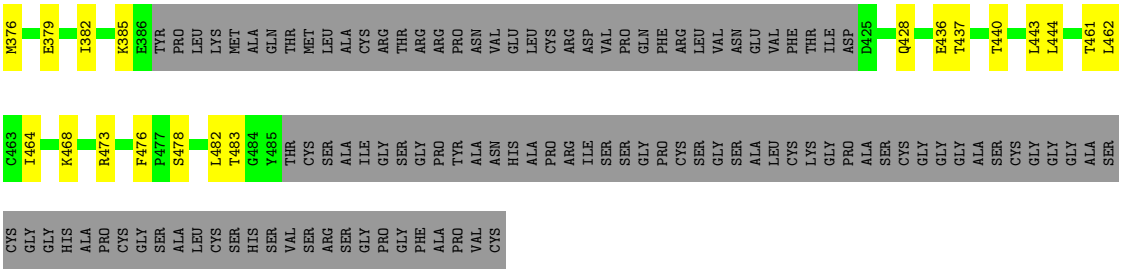


• Molecule 30: Tektin-5

Chain W5:

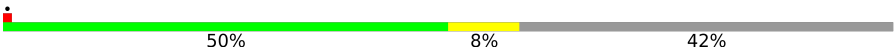


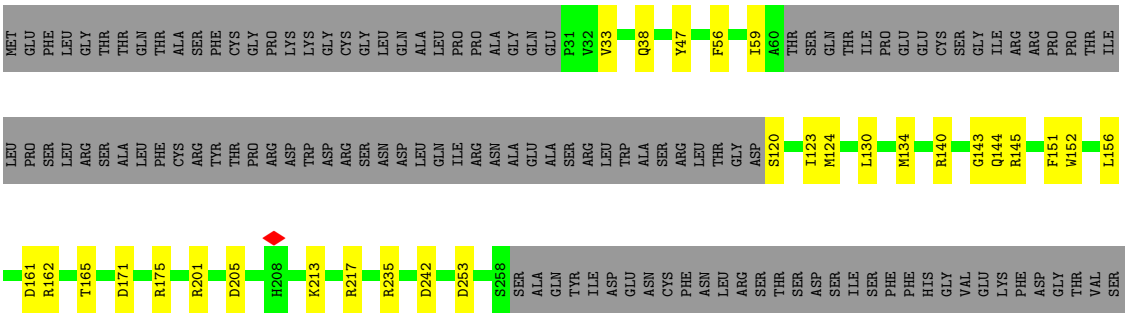




• Molecule 30: Tektin-5

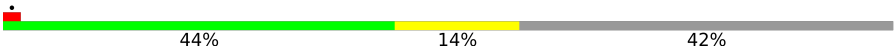
Chain W6:

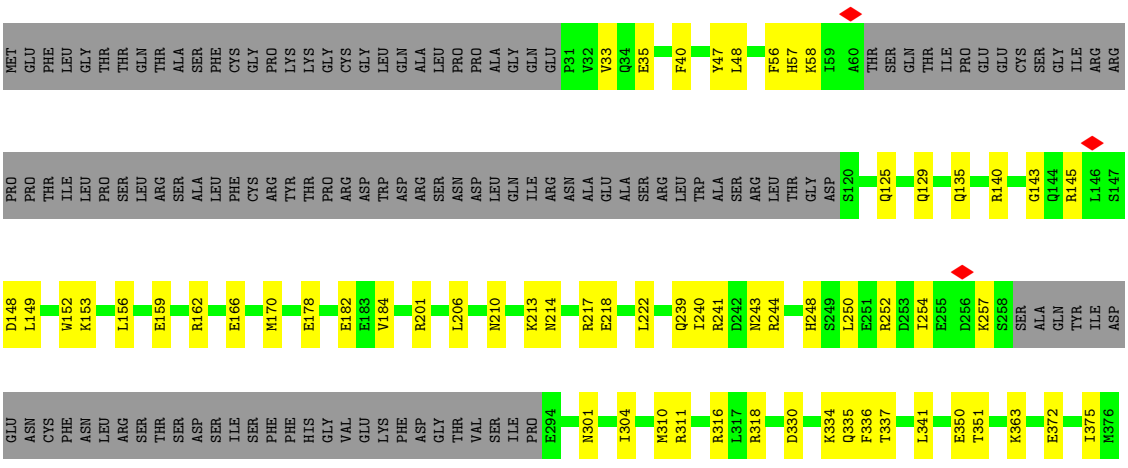


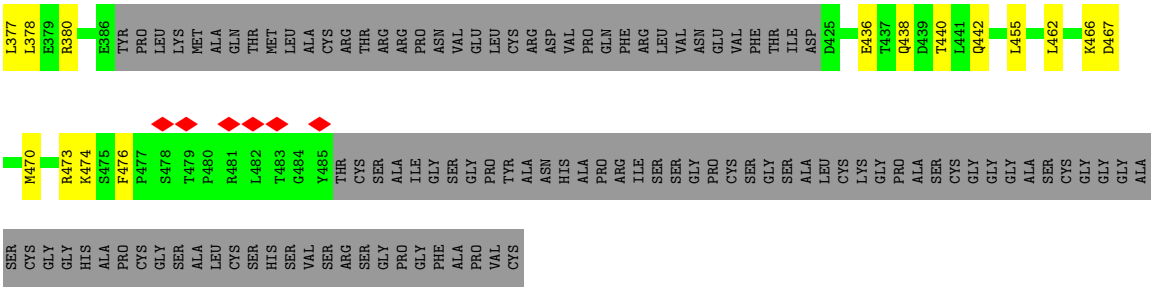


• Molecule 30: Tektin-5

Chain W7:

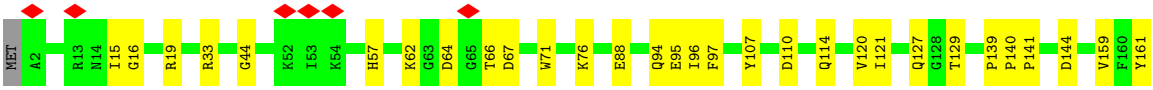


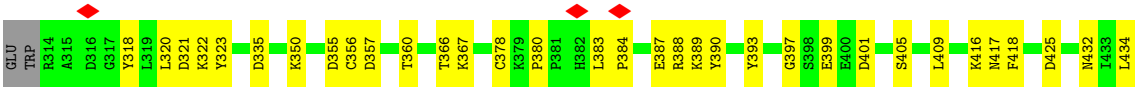


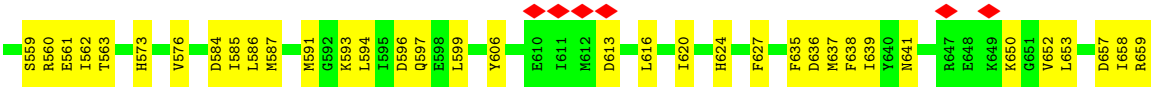


• Molecule 31: EF-hand domain-containing family member C2

Chain W:

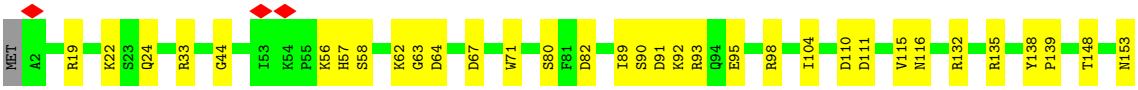


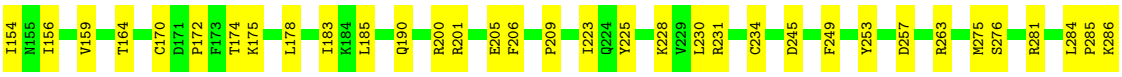


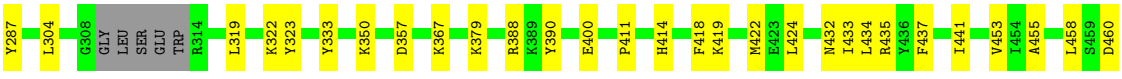


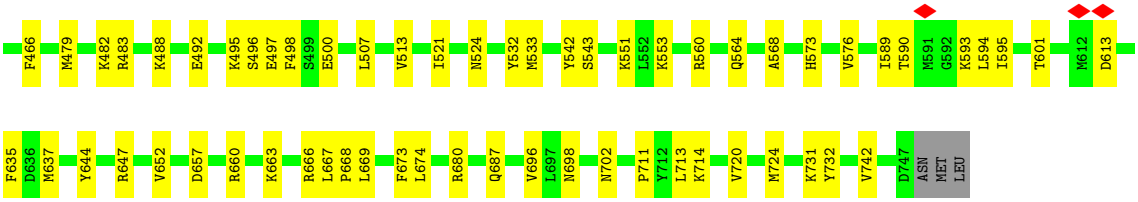
• Molecule 31: EF-hand domain-containing family member C2

Chain X:



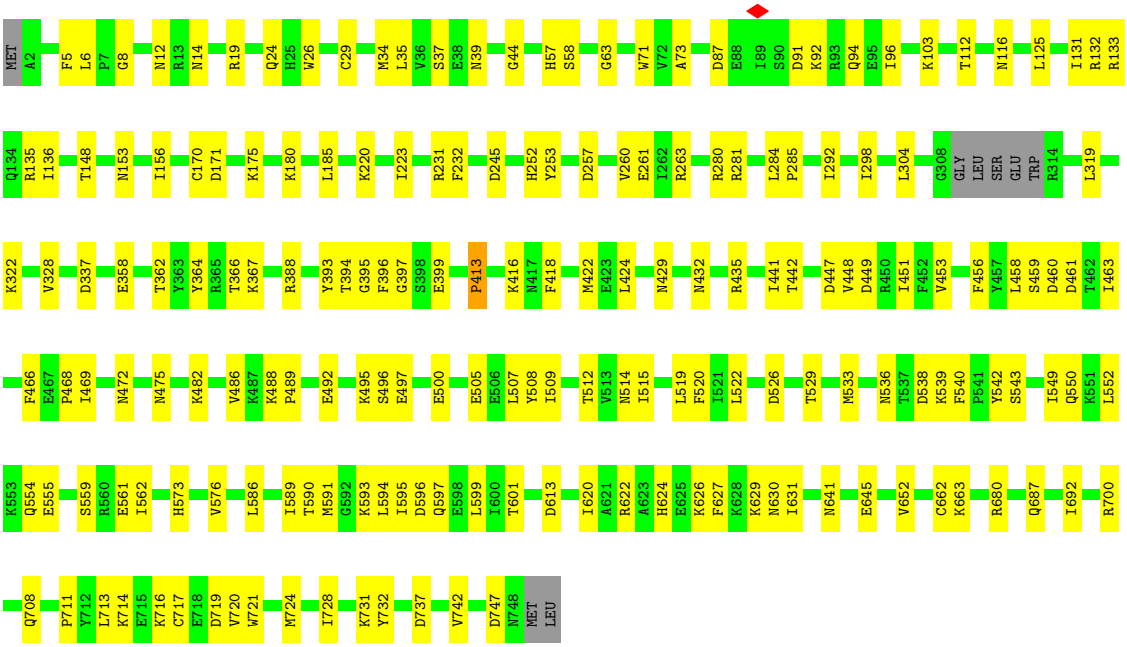






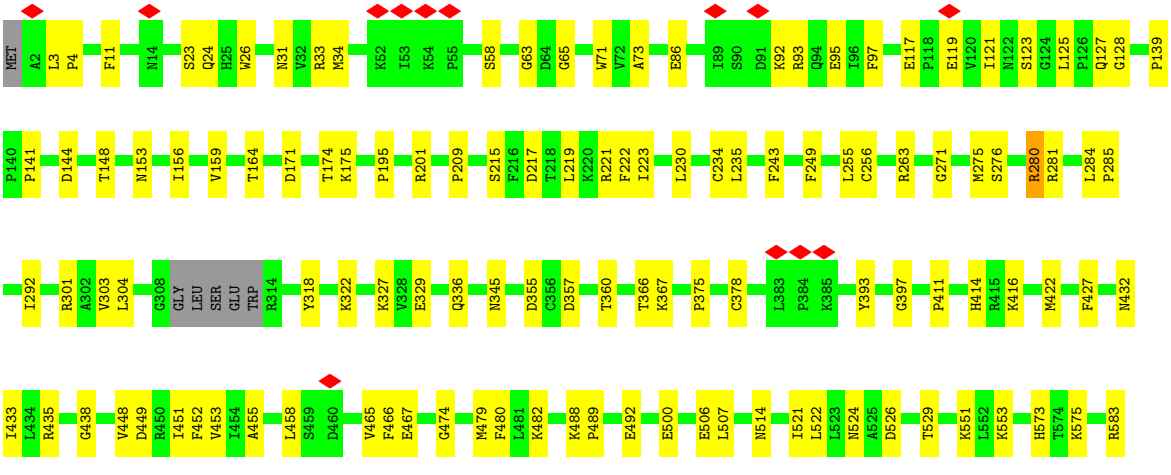
• Molecule 31: EF-hand domain-containing family member C2

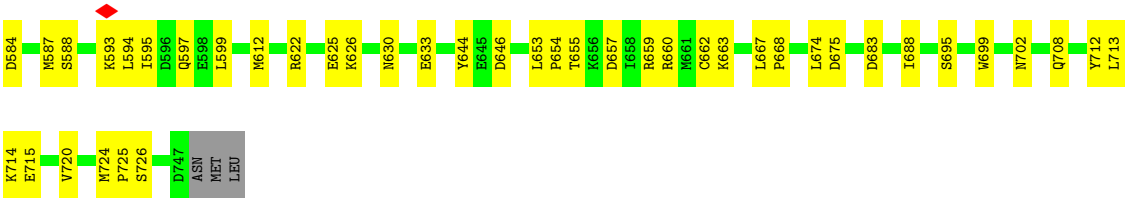
Chain Y:



• Molecule 31: EF-hand domain-containing family member C2

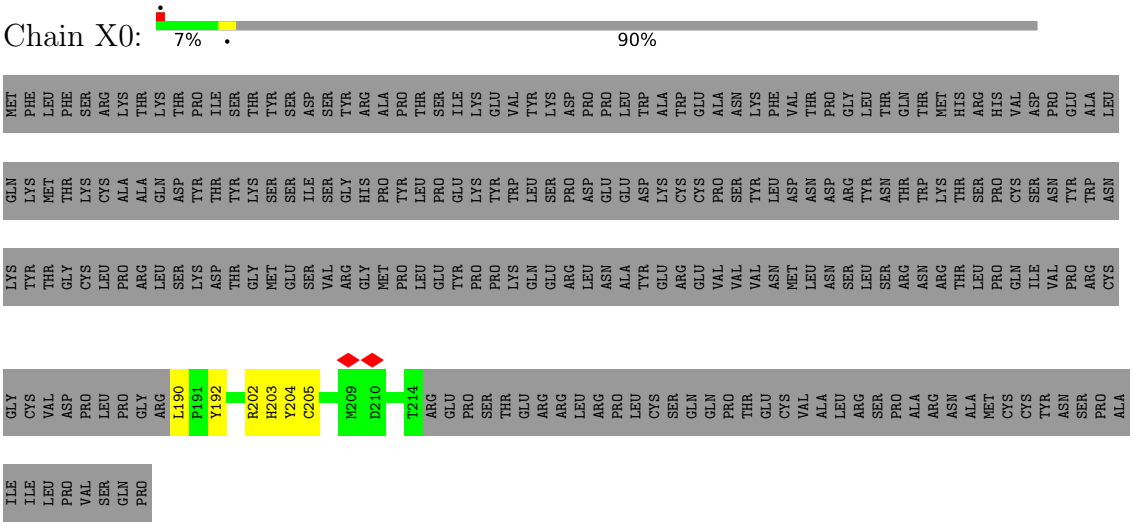
Chain Z:





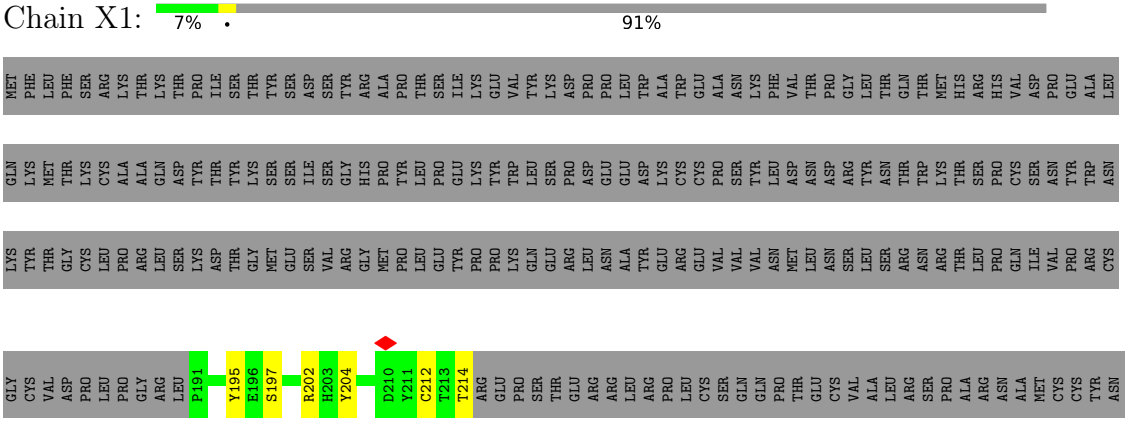
• Molecule 32: Spermatid-specific manchette-related protein 1

Chain X0:



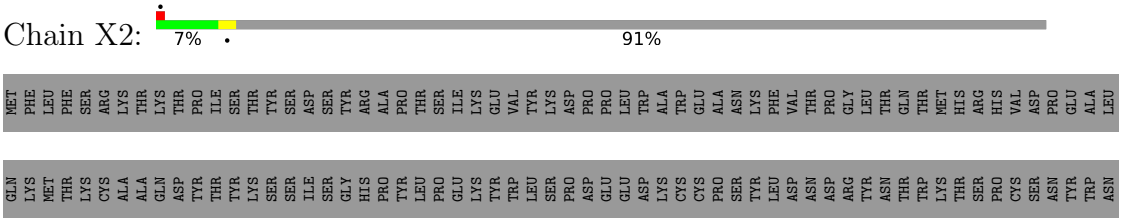
• Molecule 32: Spermatid-specific manchette-related protein 1

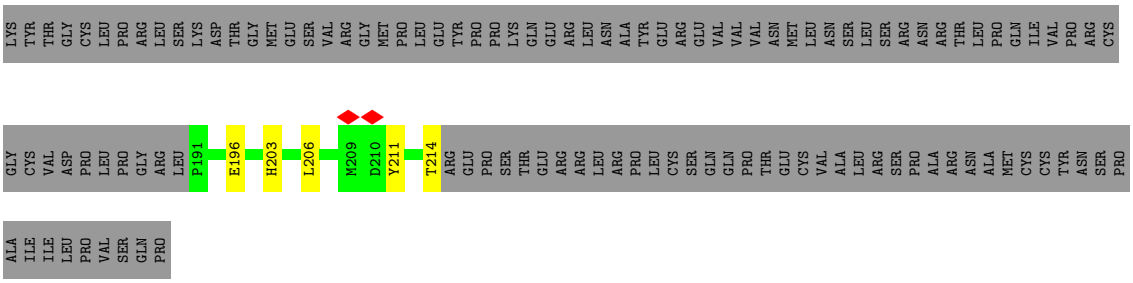
Chain X1:



• Molecule 32: Spermatid-specific manchette-related protein 1

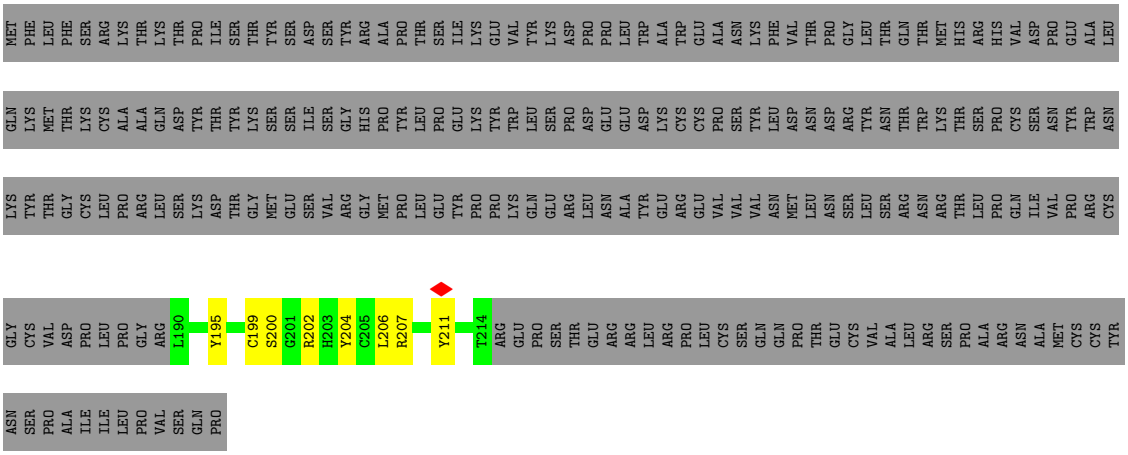
Chain X2:





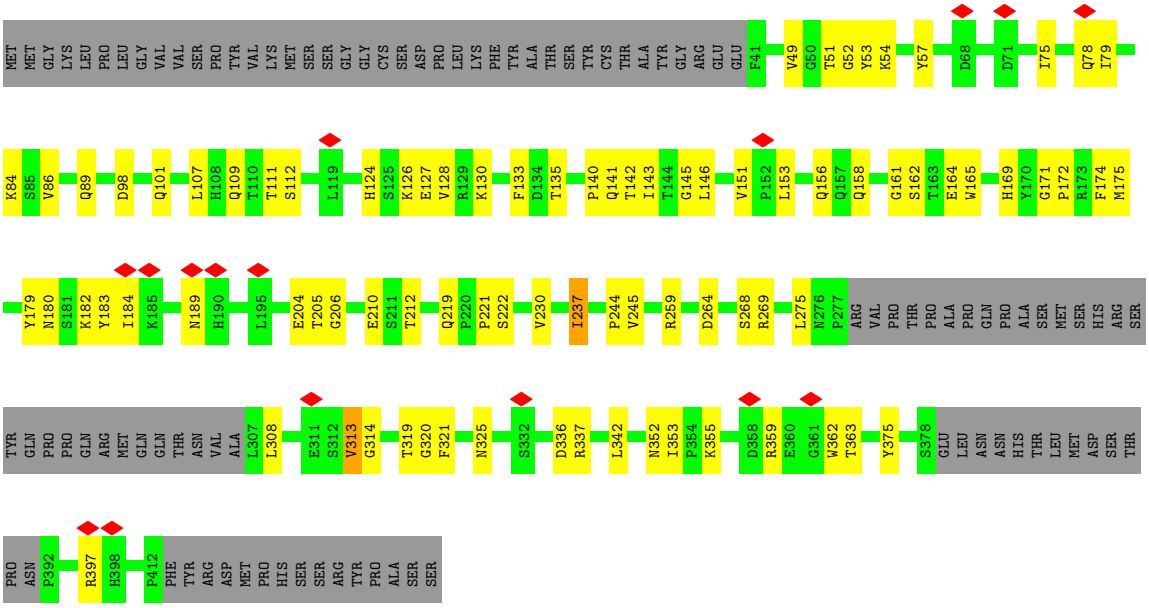
• Molecule 32: Spermatid-specific manchette-related protein 1

Chain X3:



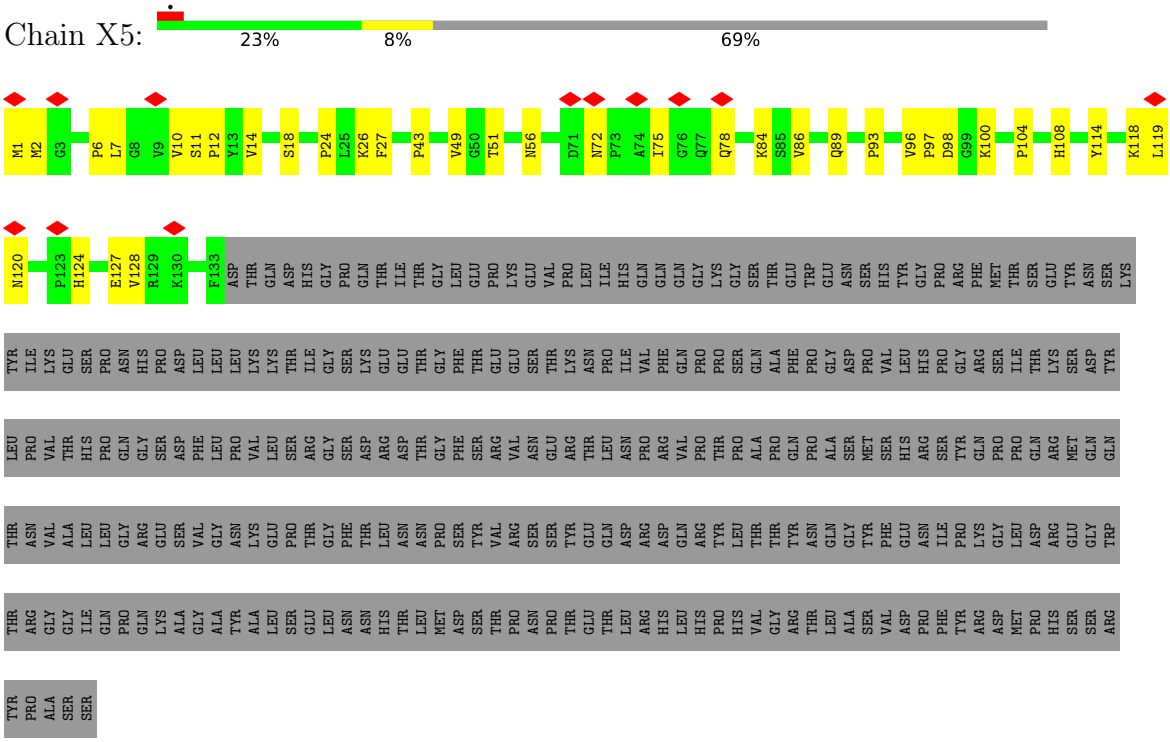
• Molecule 33: Protein phosphatase 1 regulatory subunit 32

Chain X4:



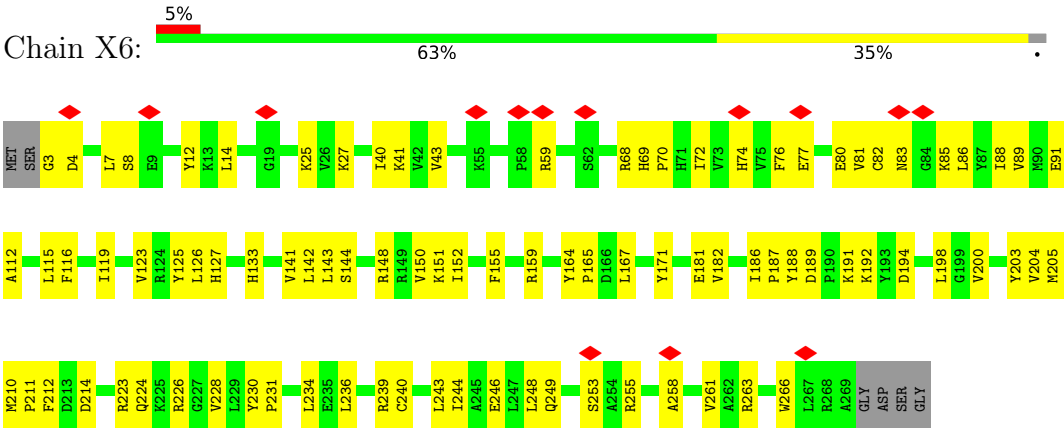
• Molecule 33: Protein phosphatase 1 regulatory subunit 32

Chain X5:



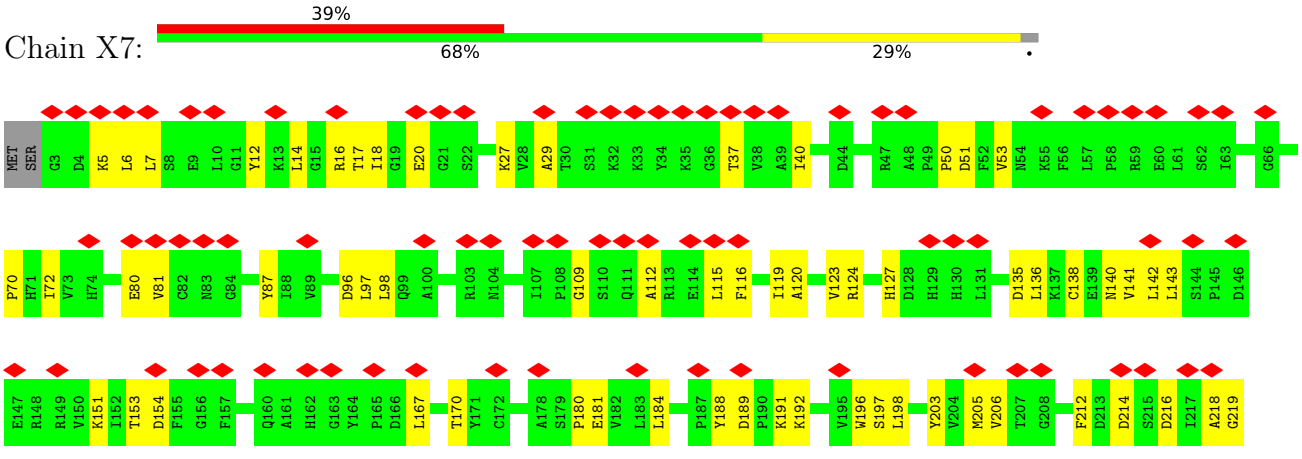
• Molecule 34: Testis-specific serine/threonine-protein kinase 6

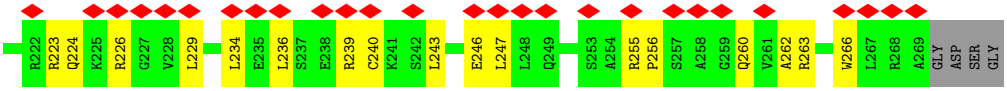
Chain X6:



• Molecule 34: Testis-specific serine/threonine-protein kinase 6

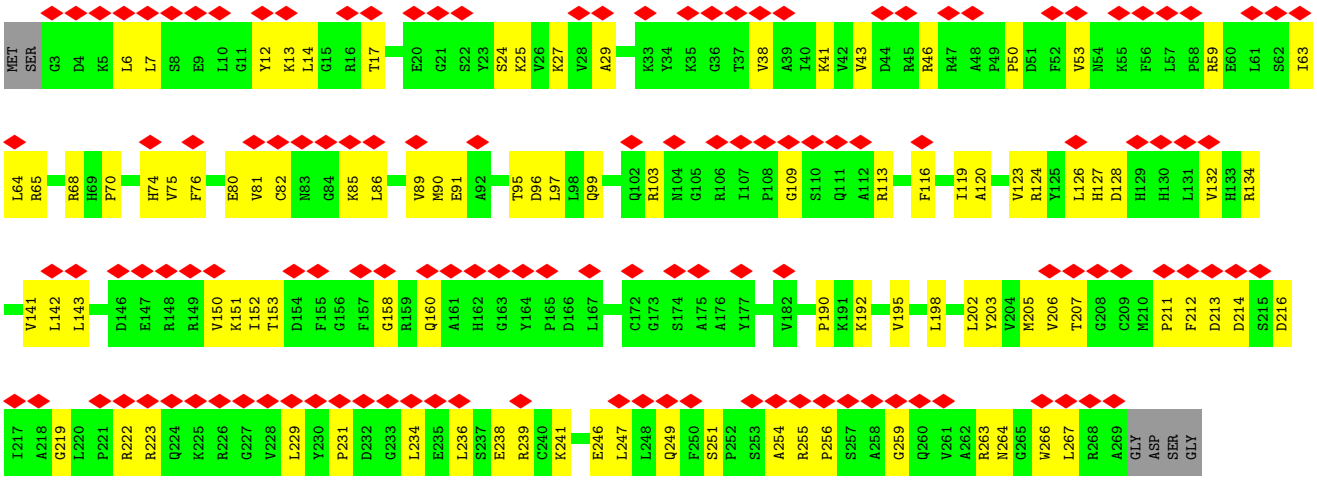
Chain X7:





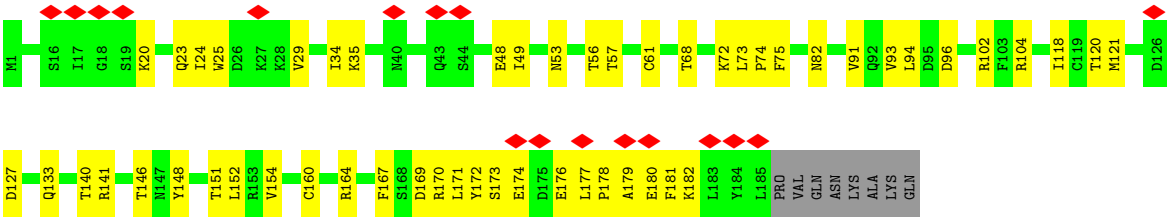
• Molecule 34: Testis-specific serine/threonine-protein kinase 6

Chain X8:



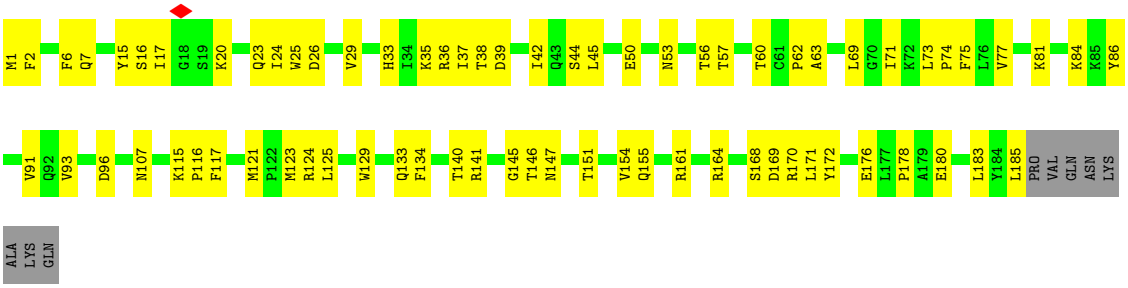
• Molecule 35: Cilia- and flagella-associated protein 20

Chain XA:



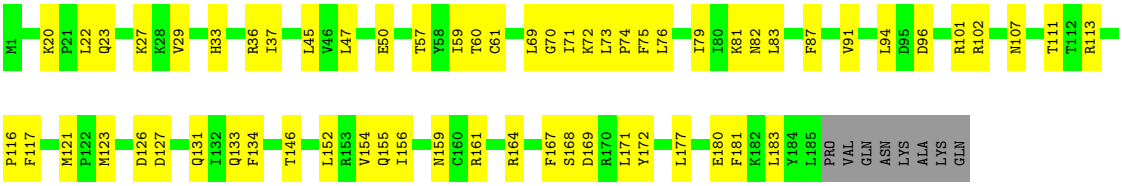
• Molecule 35: Cilia- and flagella-associated protein 20

Chain XB:



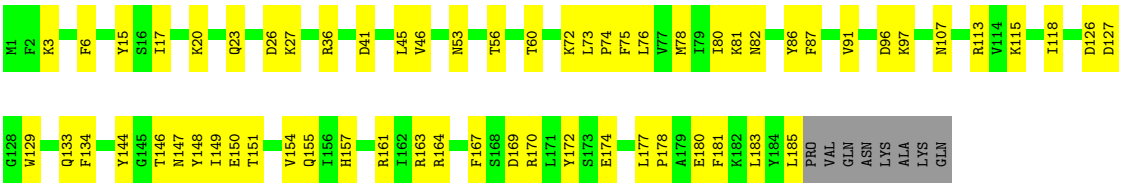
• Molecule 35: Cilia- and flagella-associated protein 20

Chain XC:



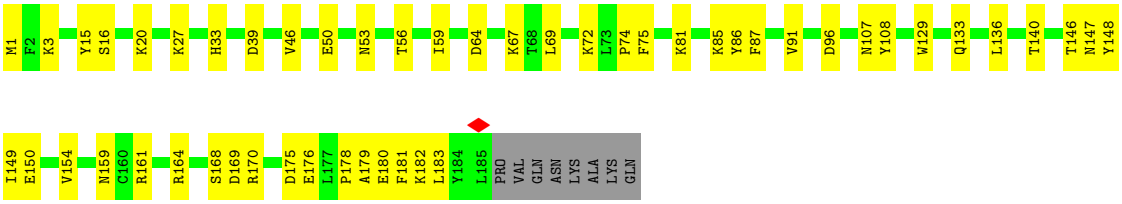
• Molecule 35: Cilia- and flagella-associated protein 20

Chain XD:



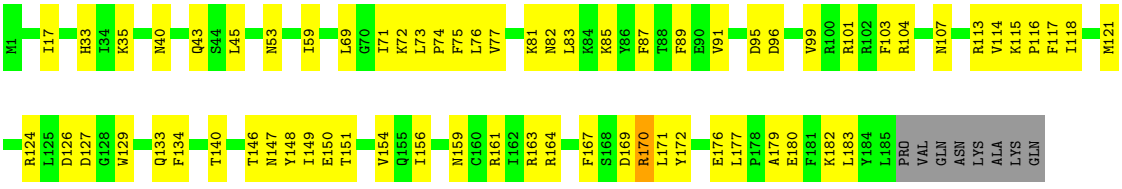
• Molecule 35: Cilia- and flagella-associated protein 20

Chain XE:



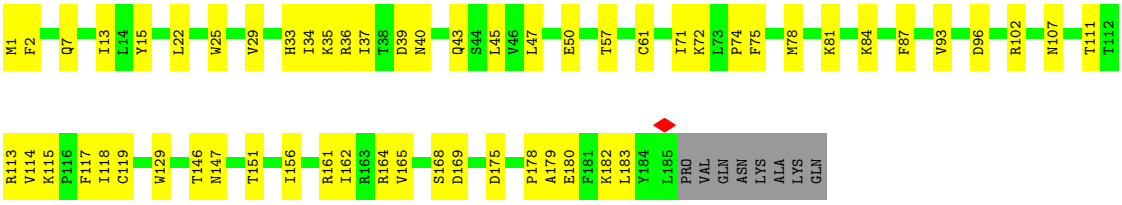
• Molecule 35: Cilia- and flagella-associated protein 20

Chain XF:



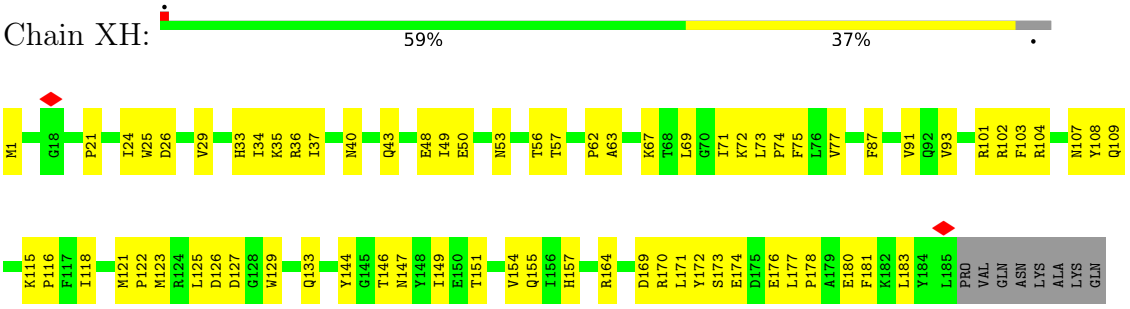
• Molecule 35: Cilia- and flagella-associated protein 20

Chain XG:



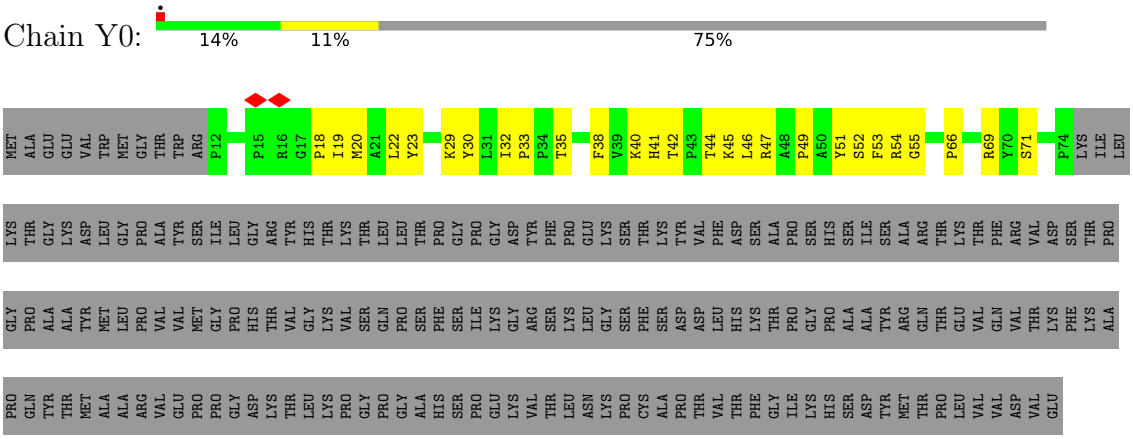
• Molecule 35: Cilia- and flagella-associated protein 20

Chain XH:



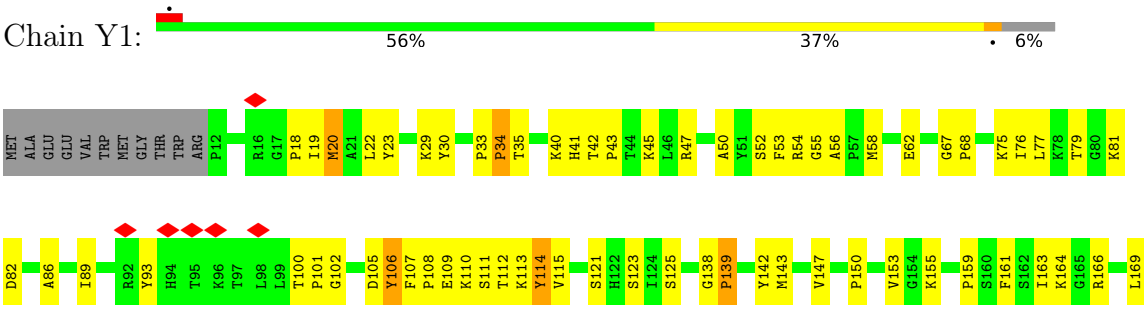
• Molecule 36: Outer dense fiber protein 3

Chain Y0:



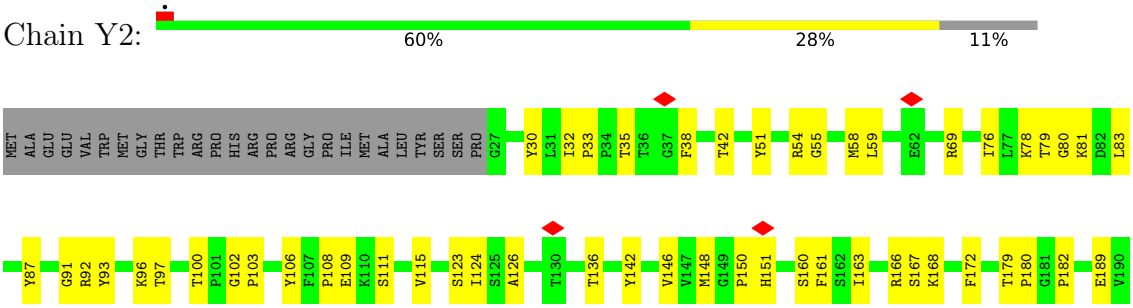
• Molecule 36: Outer dense fiber protein 3

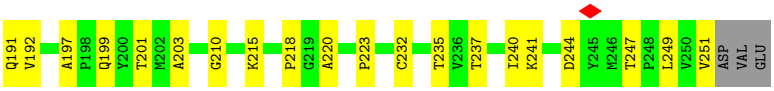
Chain Y1:



• Molecule 36: Outer dense fiber protein 3

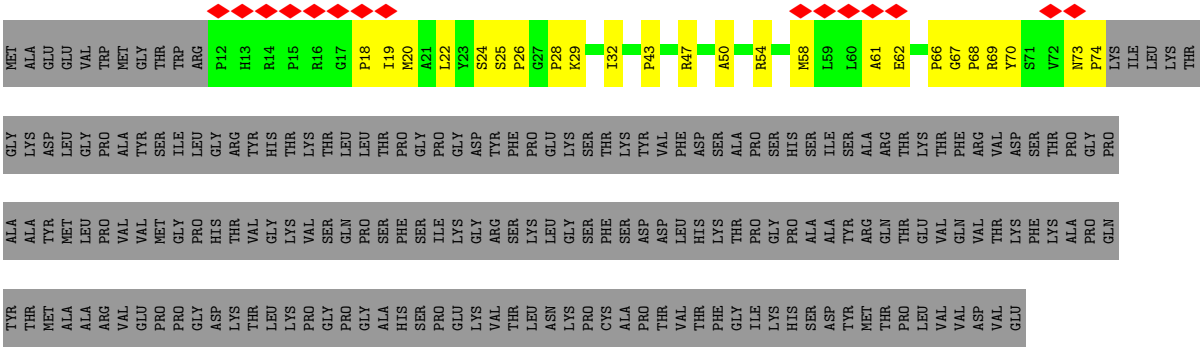
Chain Y2:





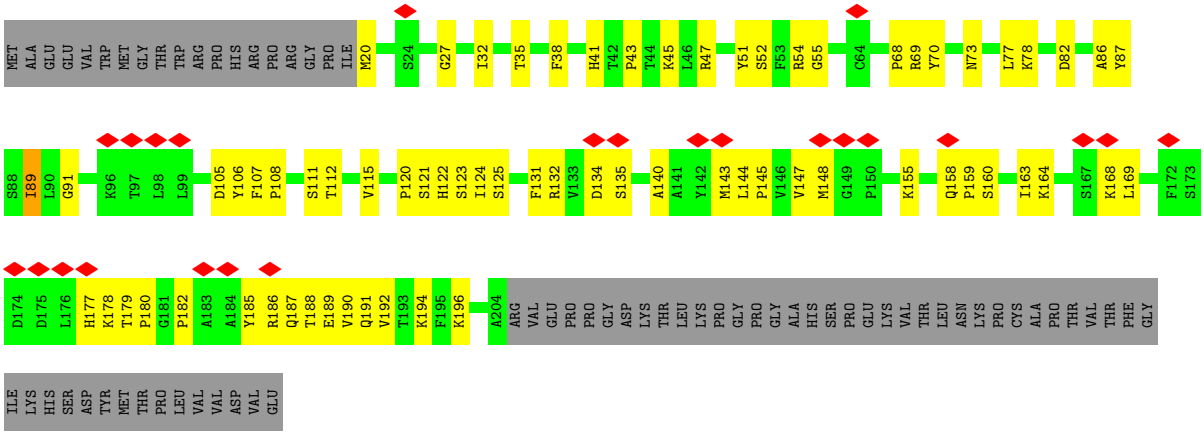
• Molecule 36: Outer dense fiber protein 3

Chain Y3:



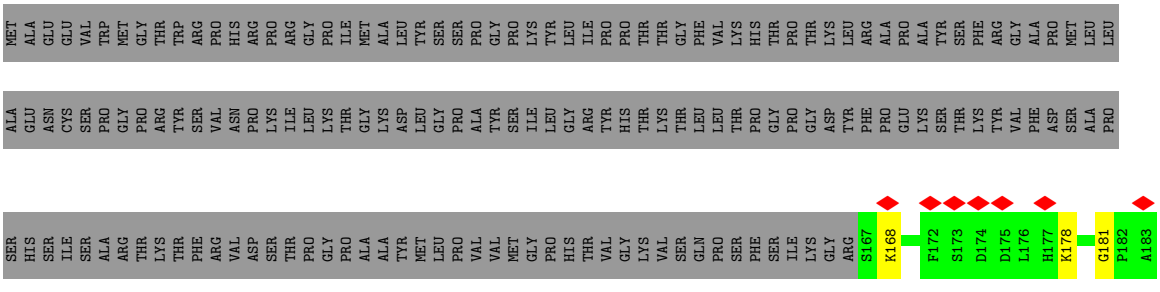
• Molecule 36: Outer dense fiber protein 3

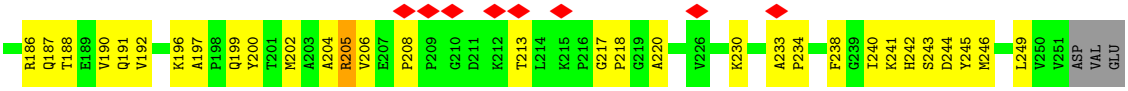
Chain Y4:



• Molecule 36: Outer dense fiber protein 3

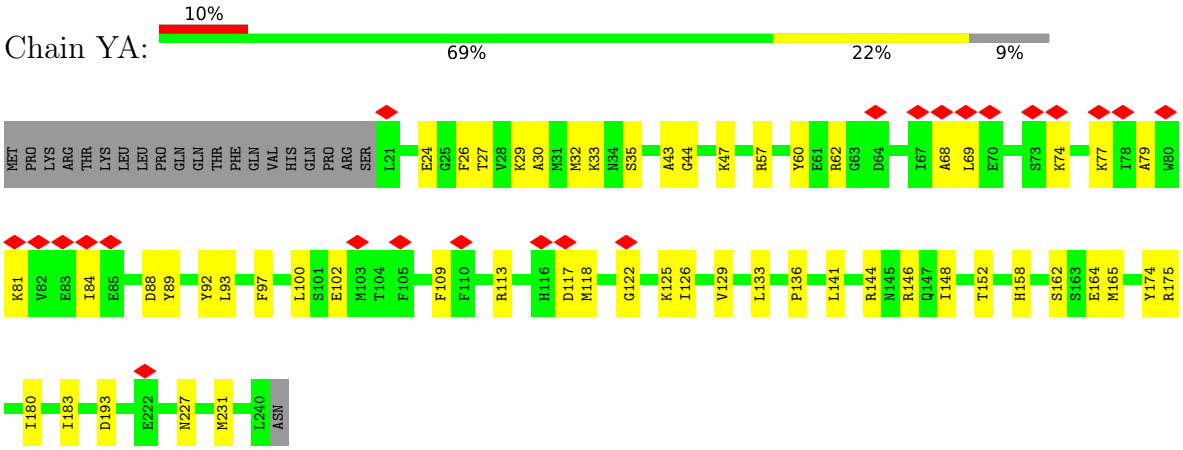
Chain Y5:





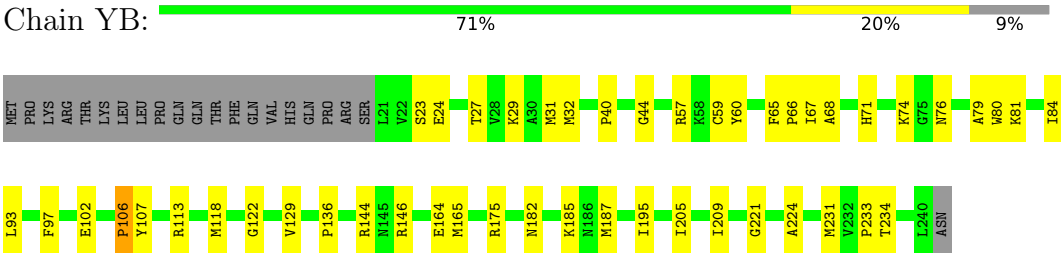
• Molecule 37: Parkin coregulated gene protein homolog

Chain YA:



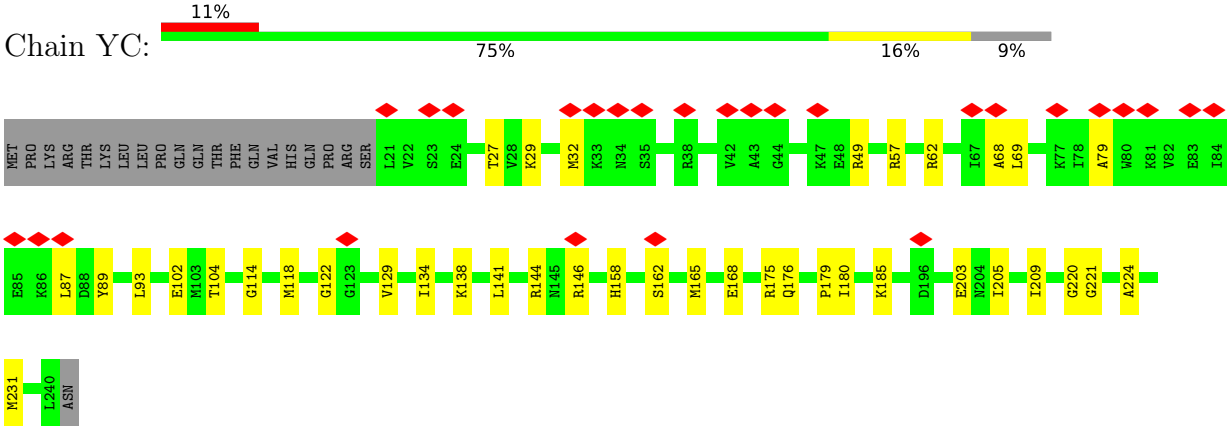
• Molecule 37: Parkin coregulated gene protein homolog

Chain YB:



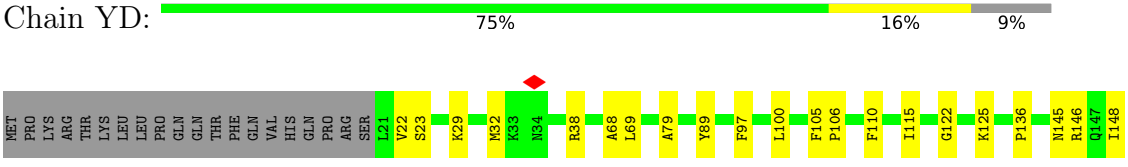
• Molecule 37: Parkin coregulated gene protein homolog

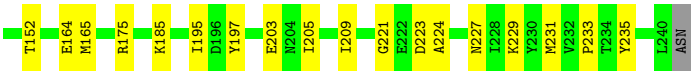
Chain YC:



• Molecule 37: Parkin coregulated gene protein homolog

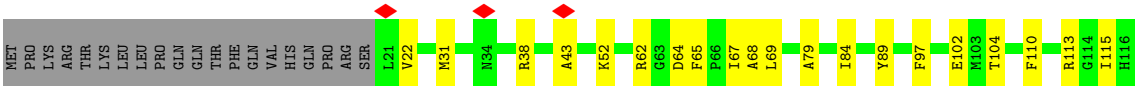
Chain YD:





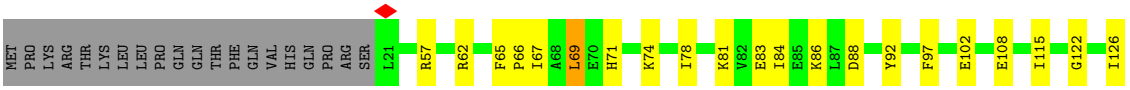
• Molecule 37: Parkin coregulated gene protein homolog

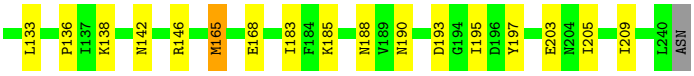
Chain YE:



• Molecule 37: Parkin coregulated gene protein homolog

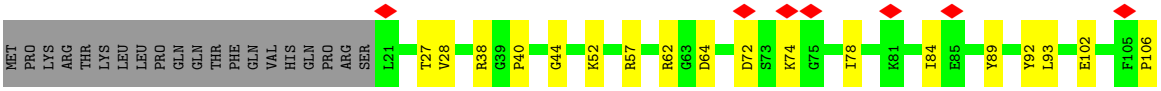
Chain YF:





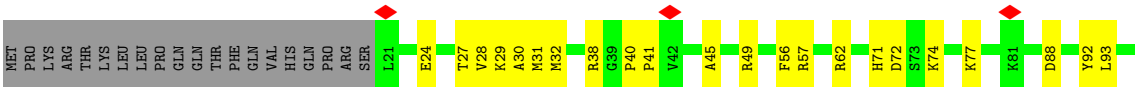
• Molecule 37: Parkin coregulated gene protein homolog

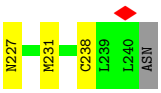
Chain YG:



• Molecule 37: Parkin coregulated gene protein homolog

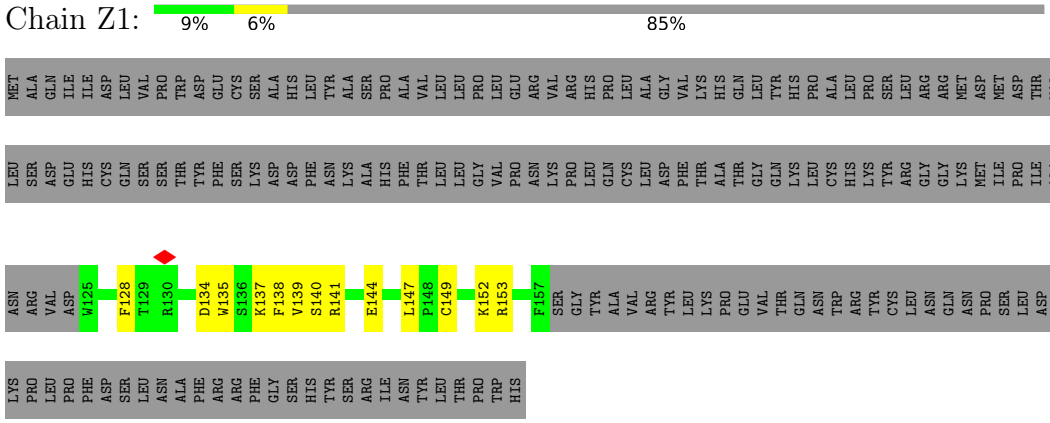
Chain YH:





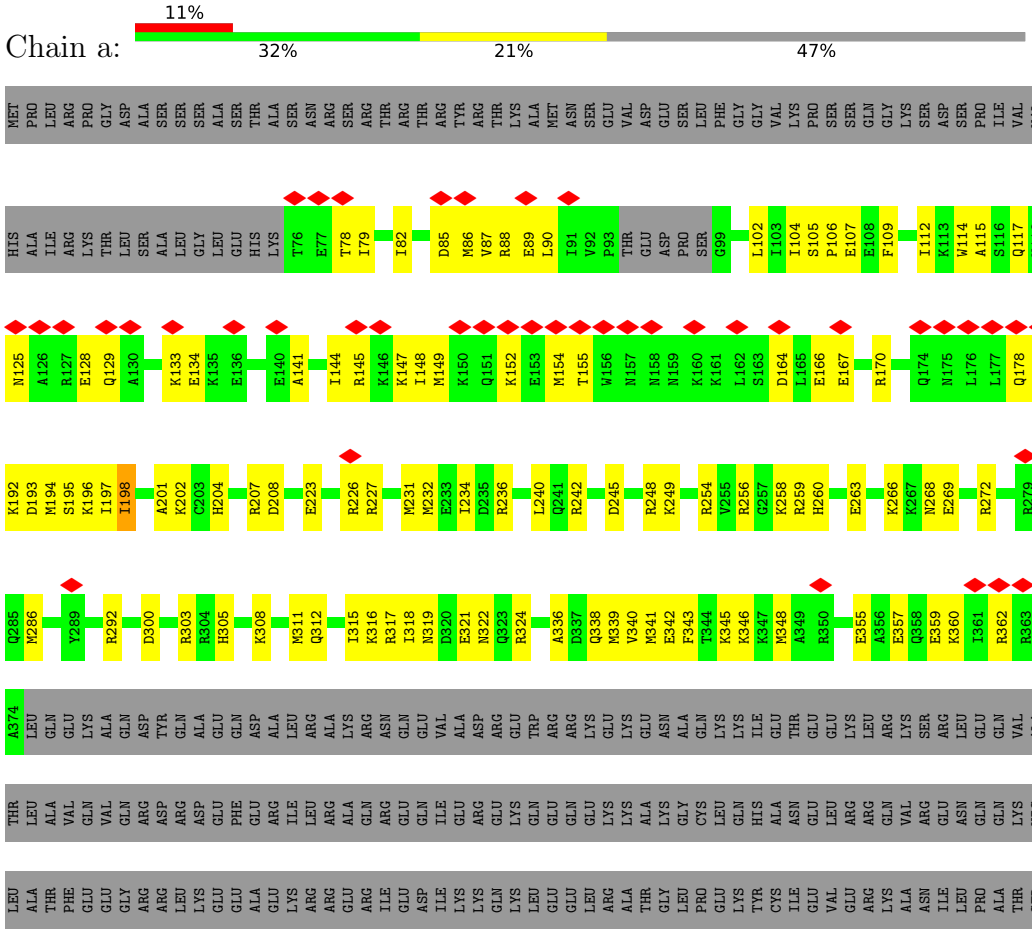
• Molecule 38: Testis, prostate and placenta-expressed protein

Chain Z1:



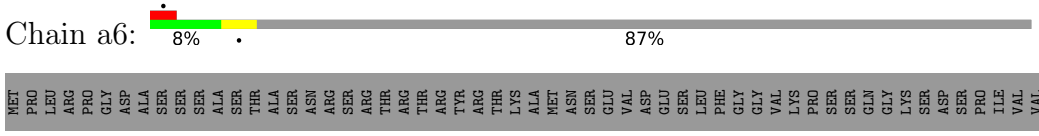
• Molecule 39: Cilia- and flagella-associated protein 45

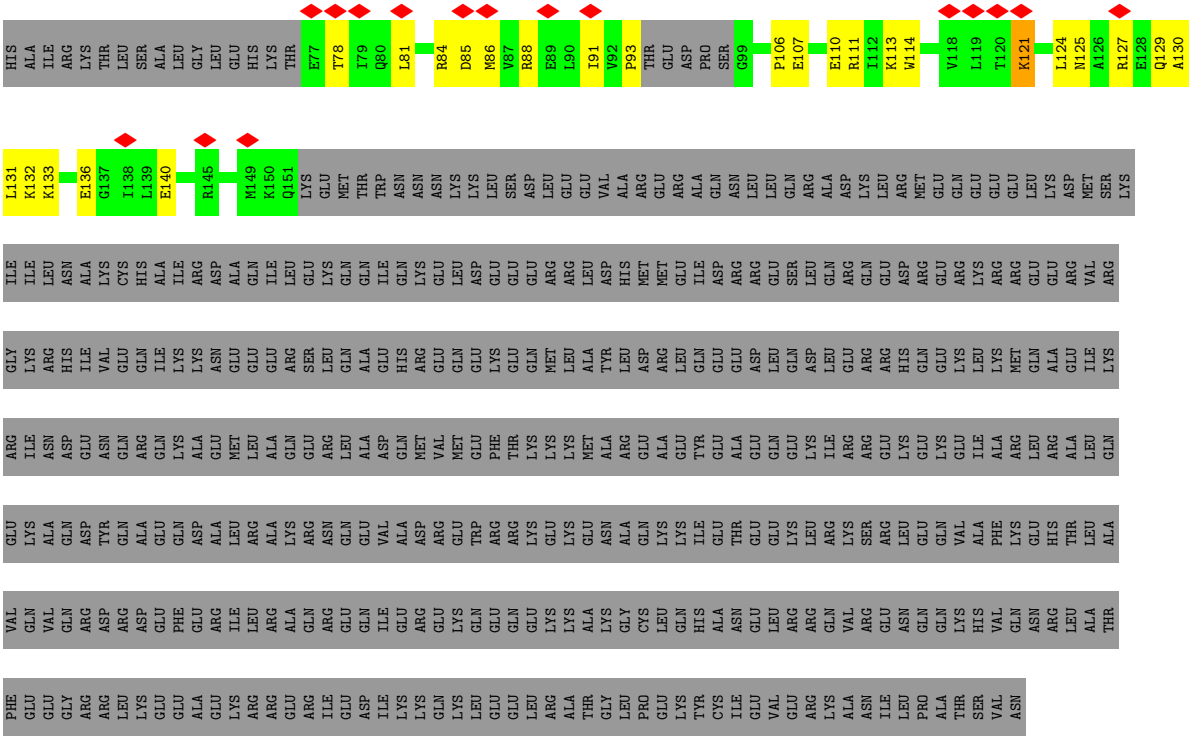
Chain a:



• Molecule 39: Cilia- and flagella-associated protein 45

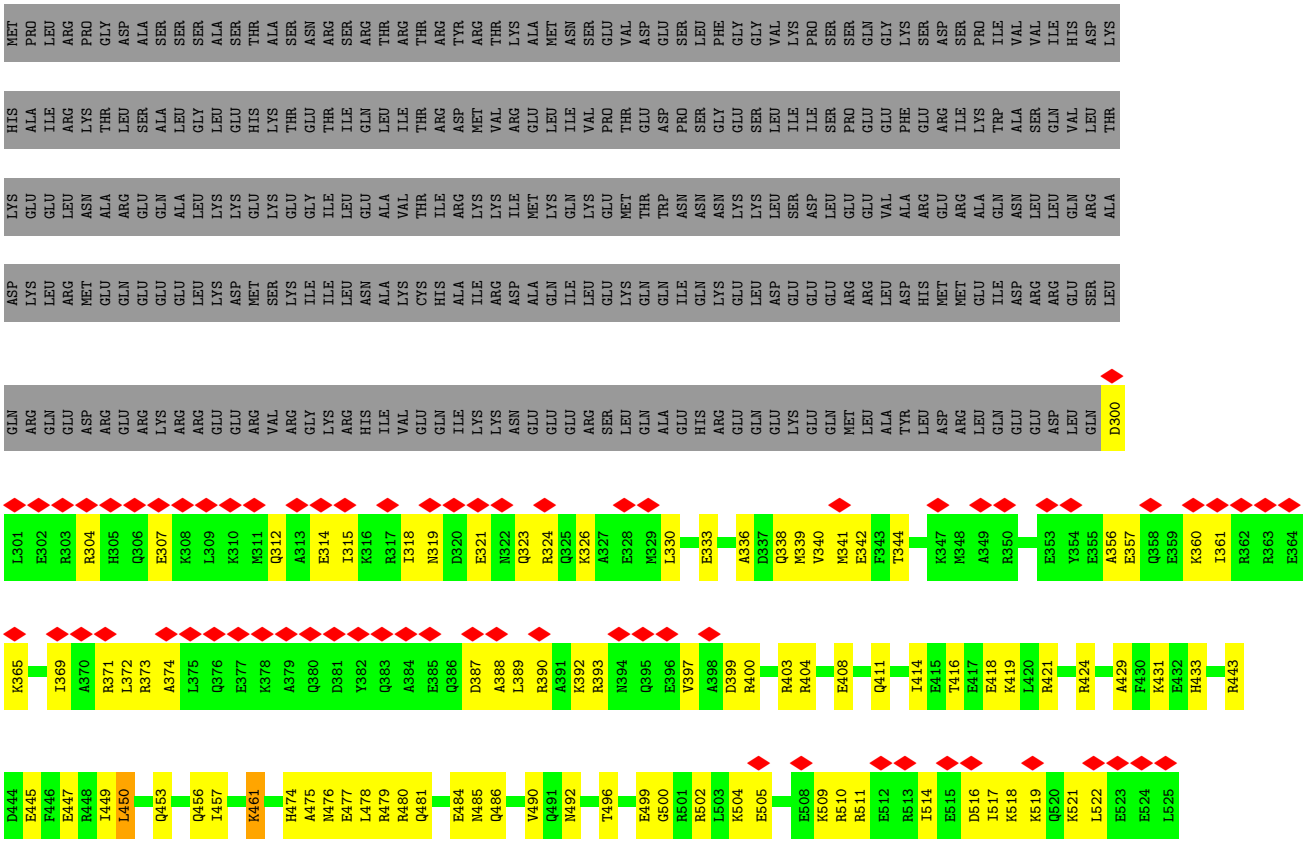
Chain a6:

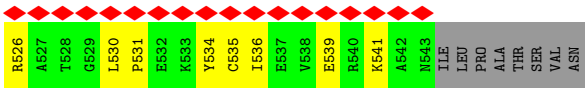




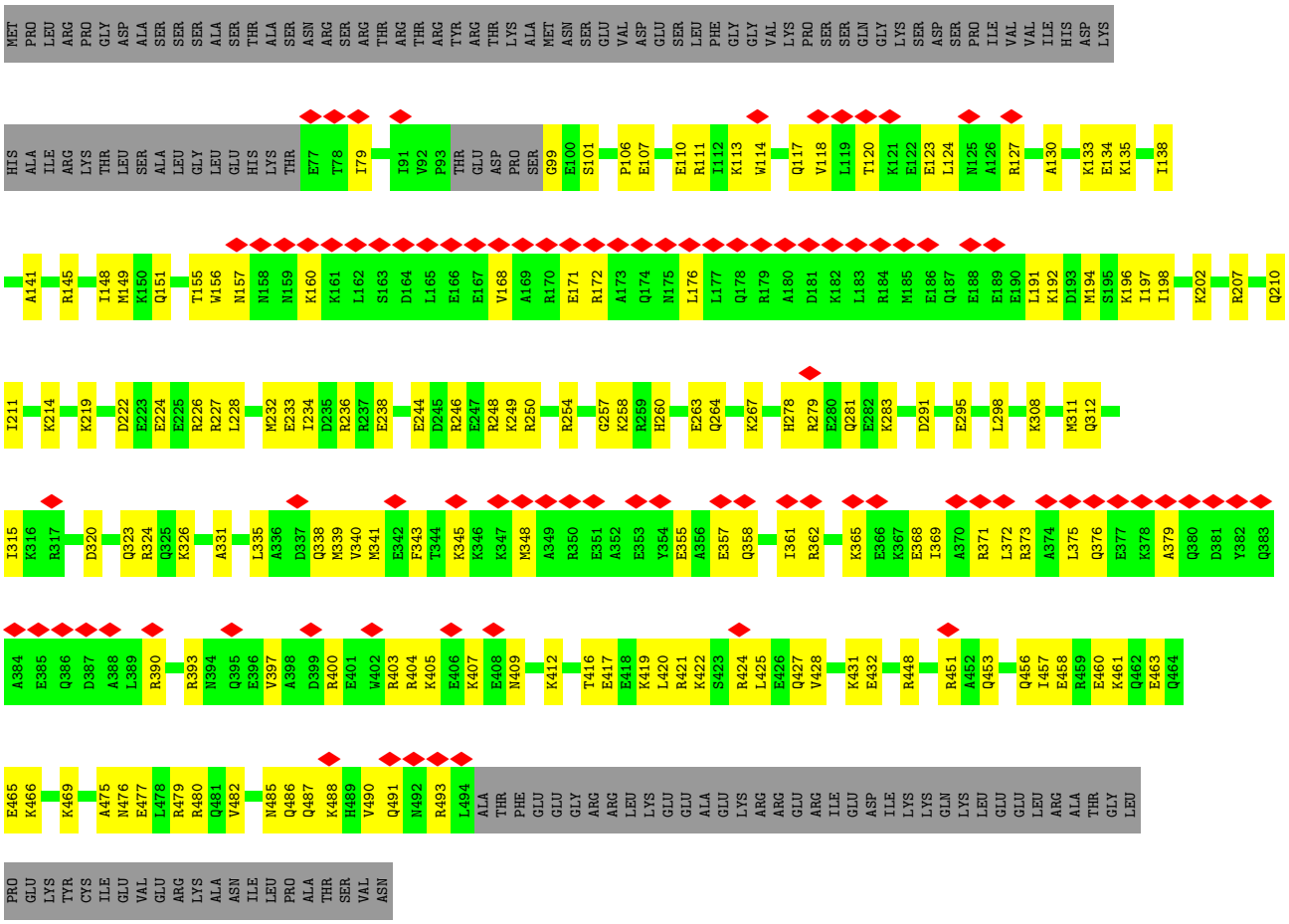
• Molecule 39: Cilia- and flagella-associated protein 45

Chain b:

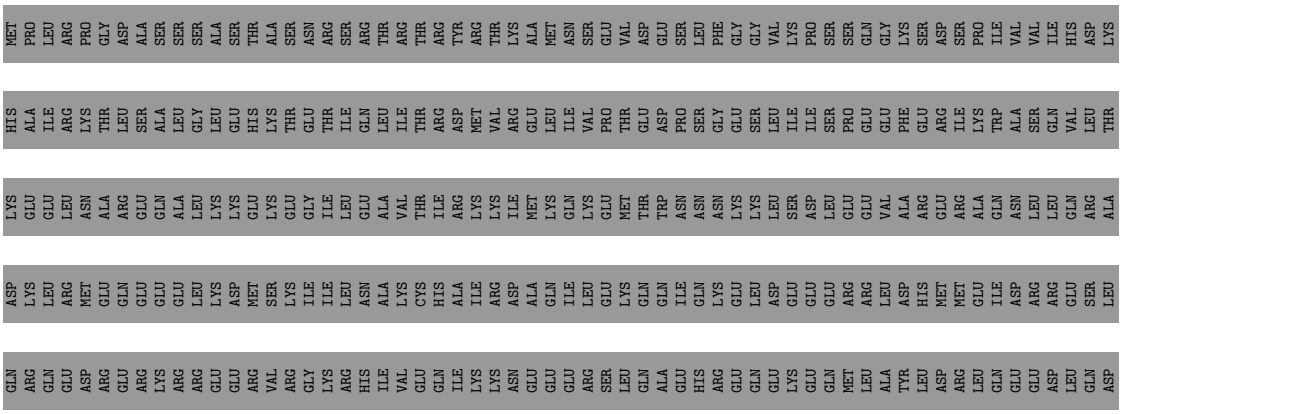


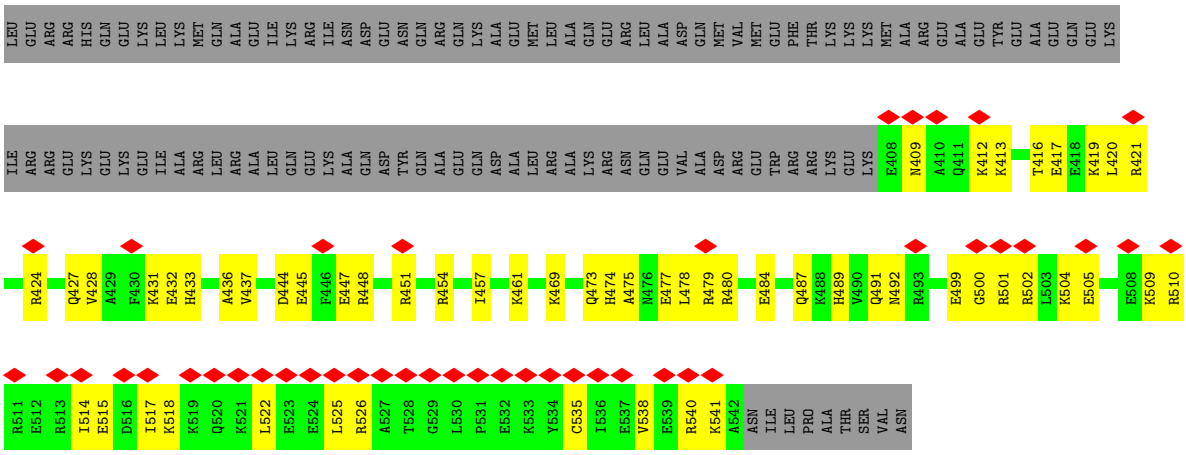


• Molecule 39: Cilia- and flagella-associated protein 45



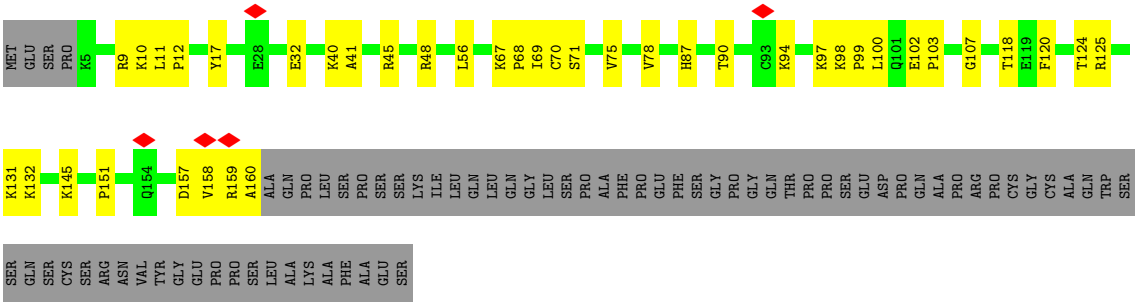
• Molecule 39: Cilia- and flagella-associated protein 45





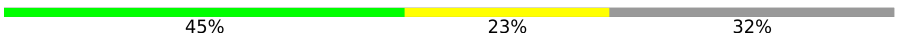
• Molecule 40: Uncharacterized protein C10orf82 homolog

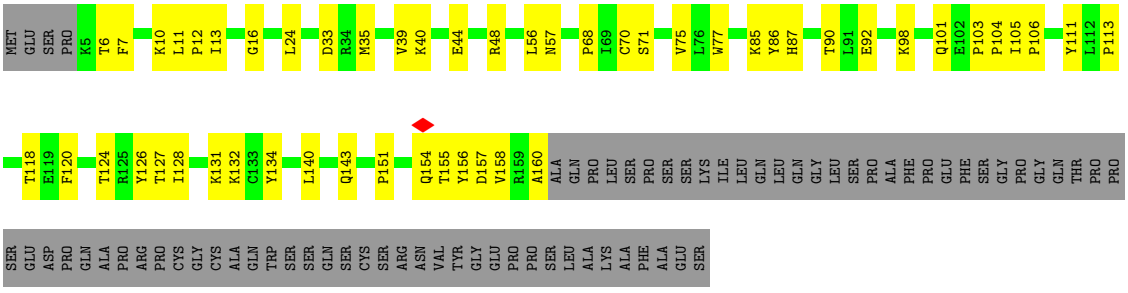
Chain a1:



• Molecule 40: Uncharacterized protein C10orf82 homolog

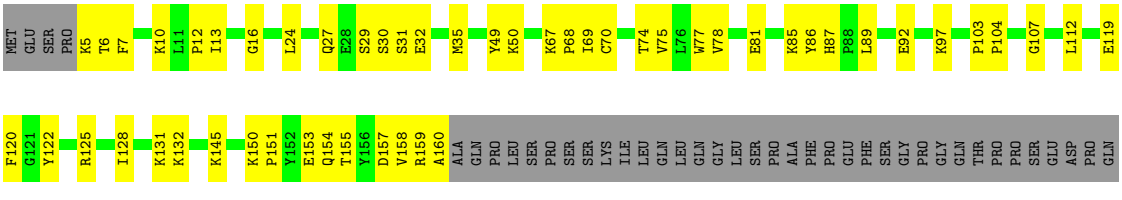
Chain a2:





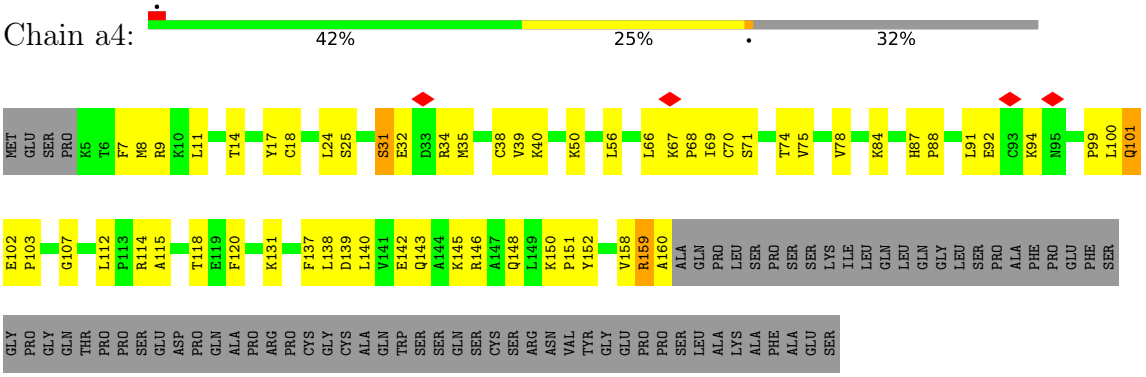
• Molecule 40: Uncharacterized protein C10orf82 homolog

Chain a3:



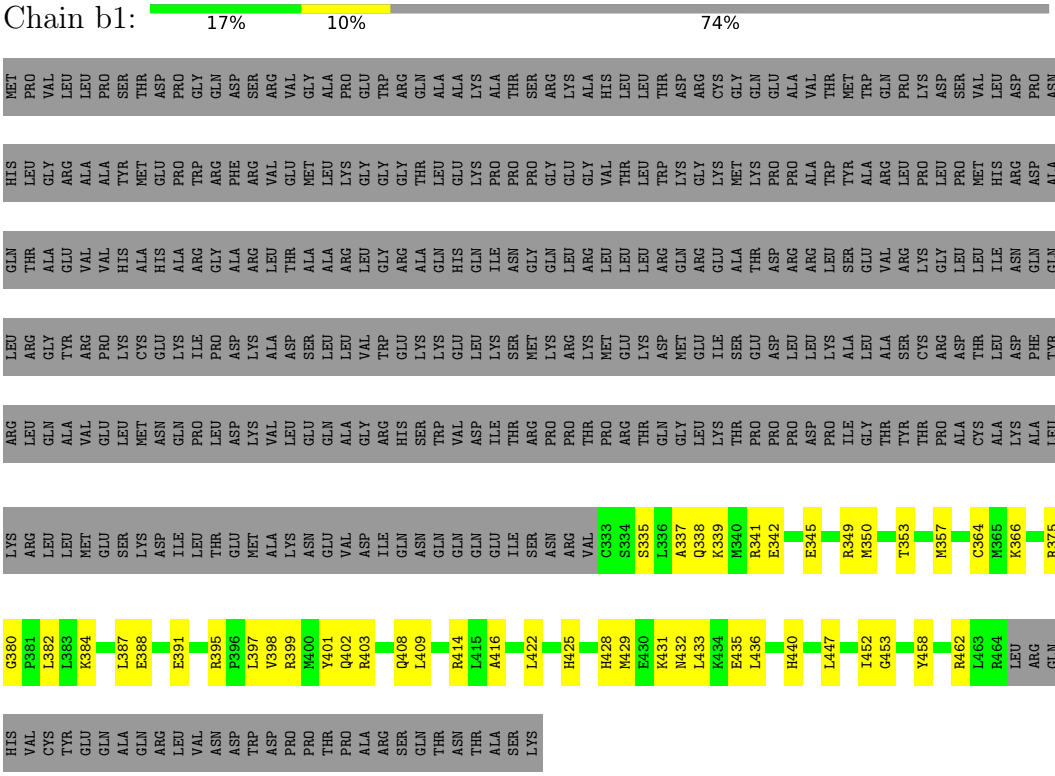
• Molecule 40: Uncharacterized protein C10orf82 homolog

Chain a4:



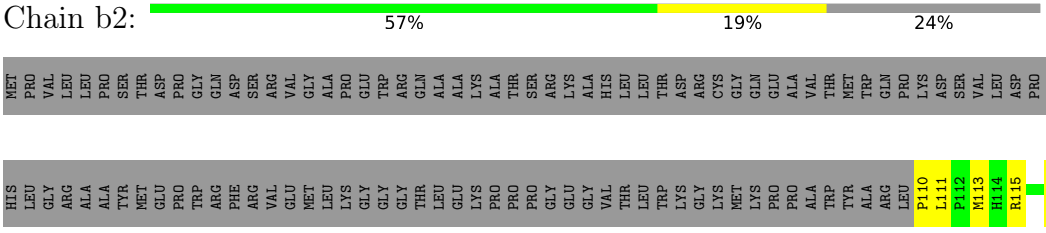
• Molecule 41: Coiled-coil domain-containing protein 105

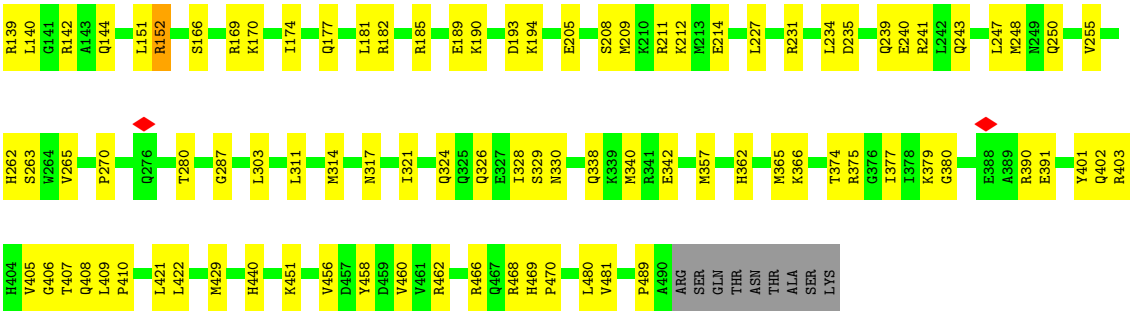
Chain b1:



• Molecule 41: Coiled-coil domain-containing protein 105

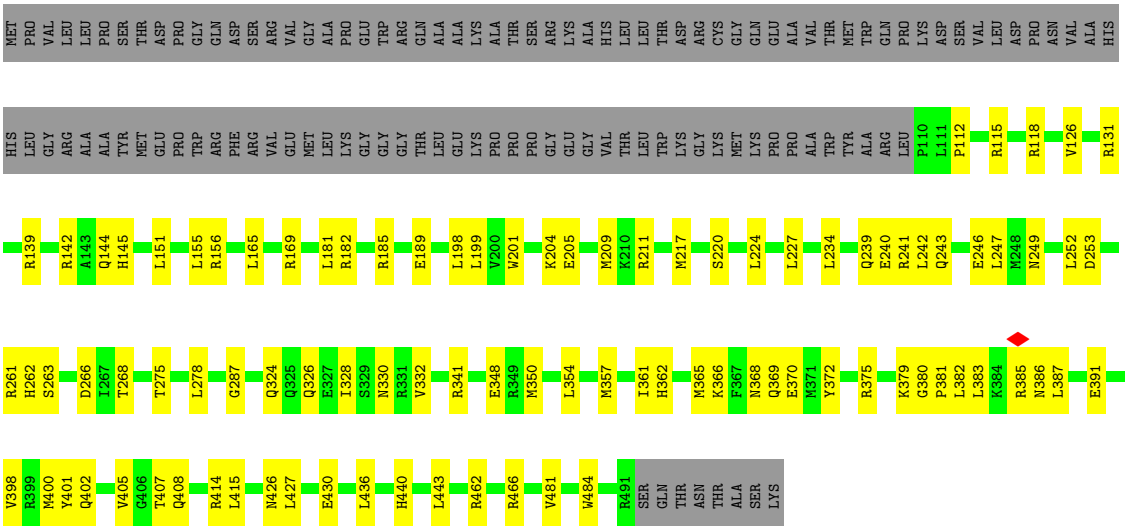
Chain b2:





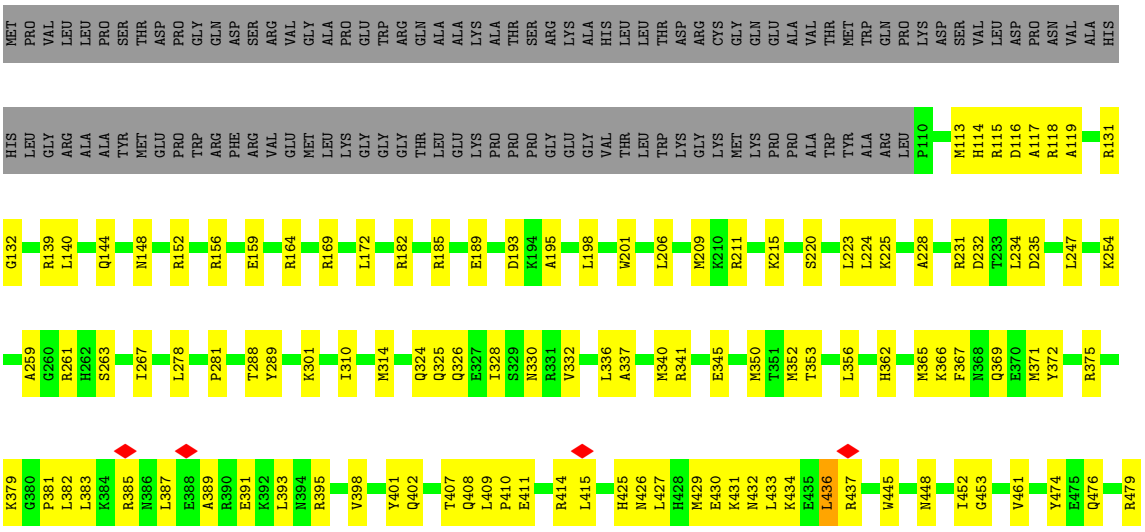
• Molecule 41: Coiled-coil domain-containing protein 105

Chain b3:



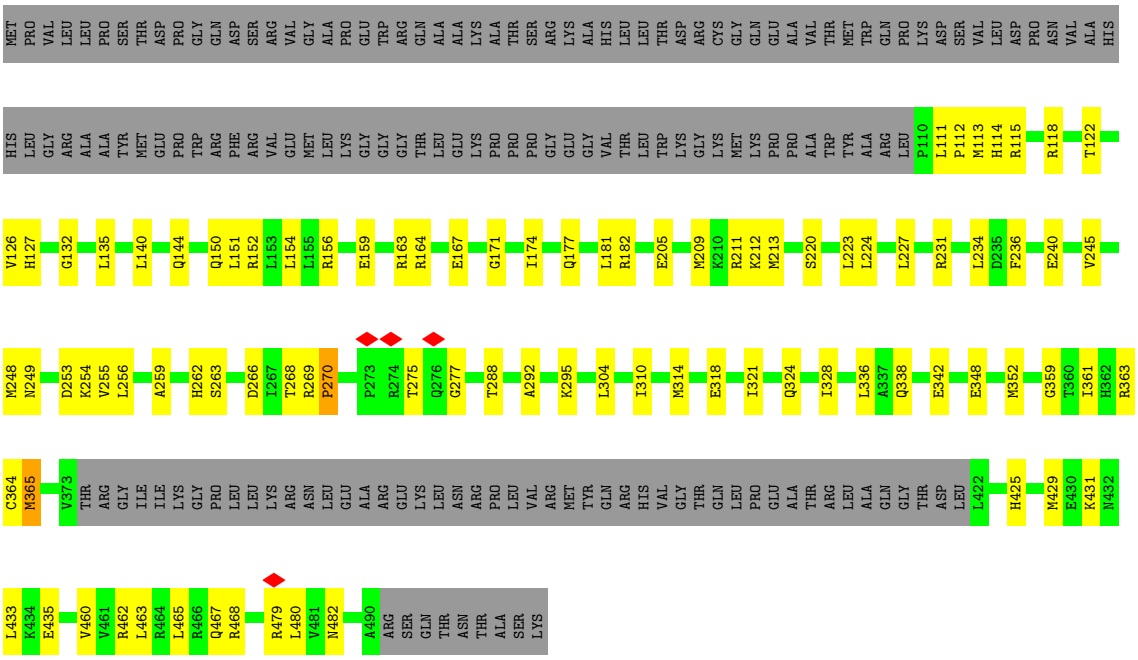
• Molecule 41: Coiled-coil domain-containing protein 105

Chain b4:



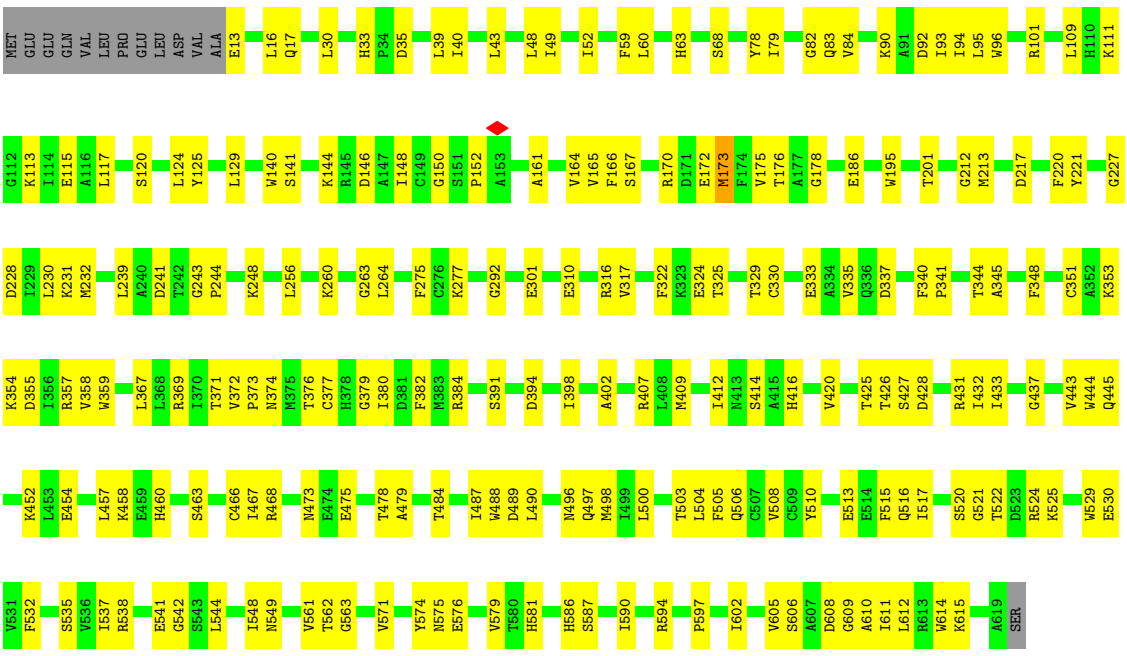
• Molecule 41: Coiled-coil domain-containing protein 105

Chain b5:



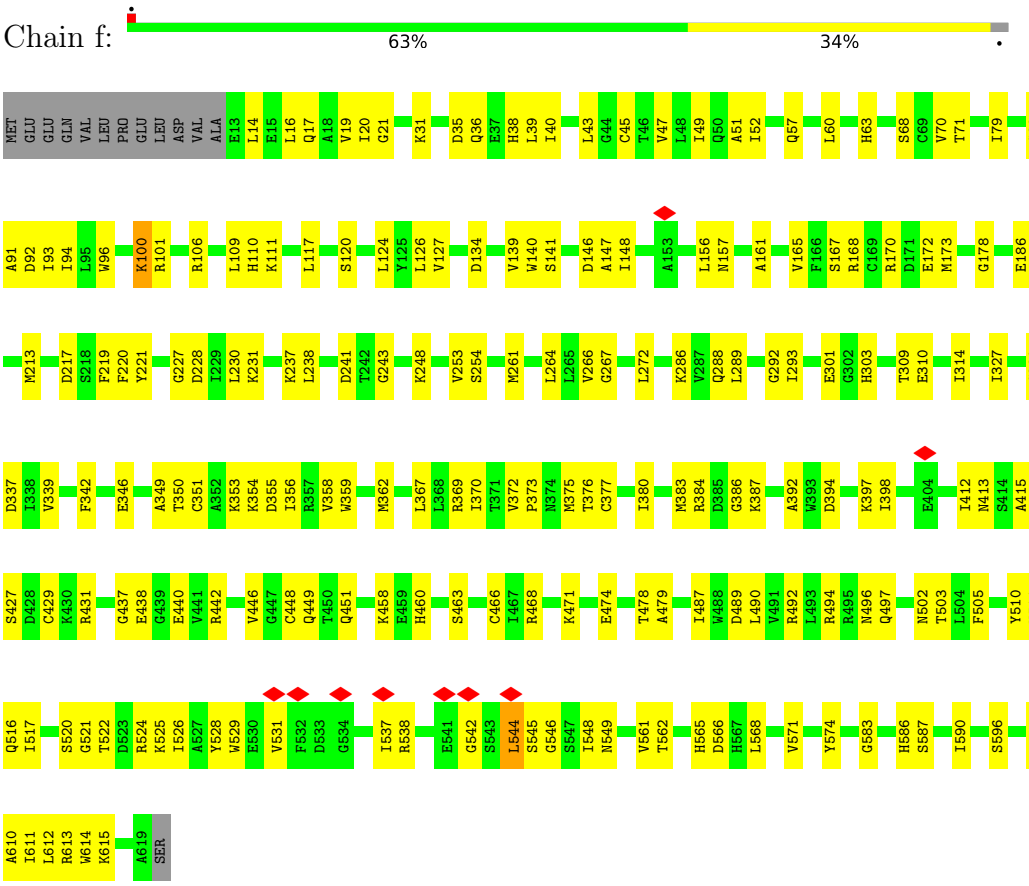
• Molecule 42: Cilia- and flagella-associated protein 52

Chain e:



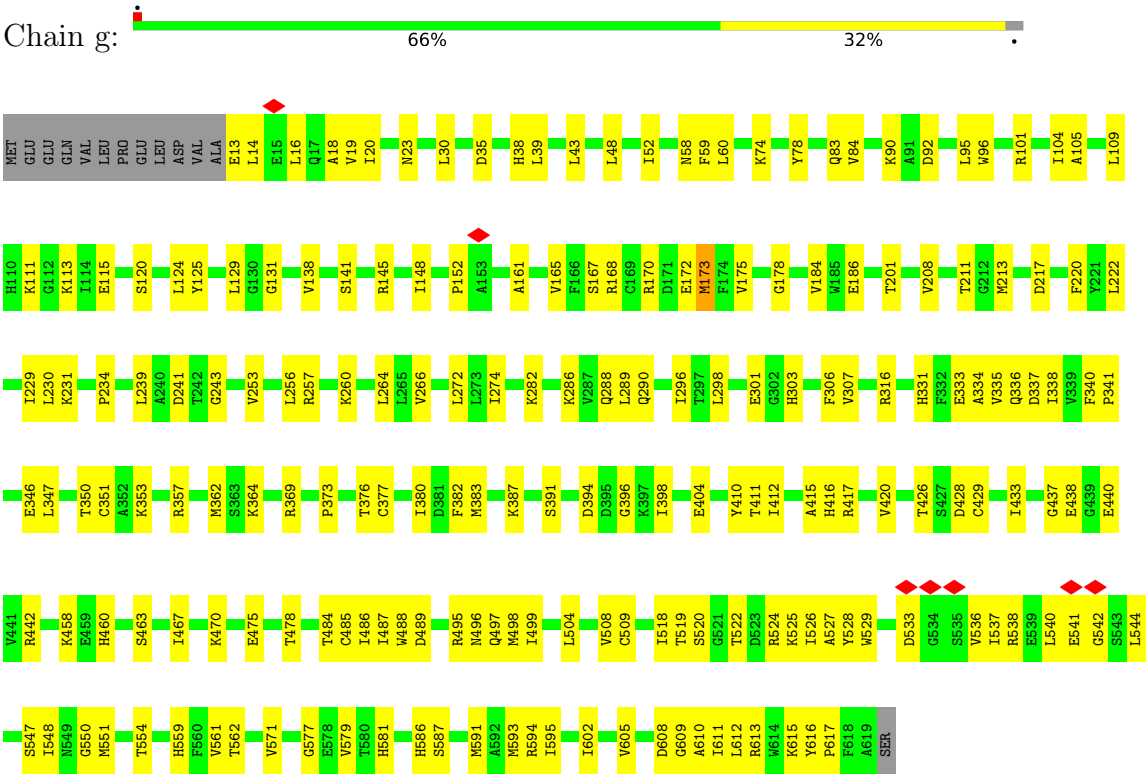
• Molecule 42: Cilia- and flagella-associated protein 52

Chain f:



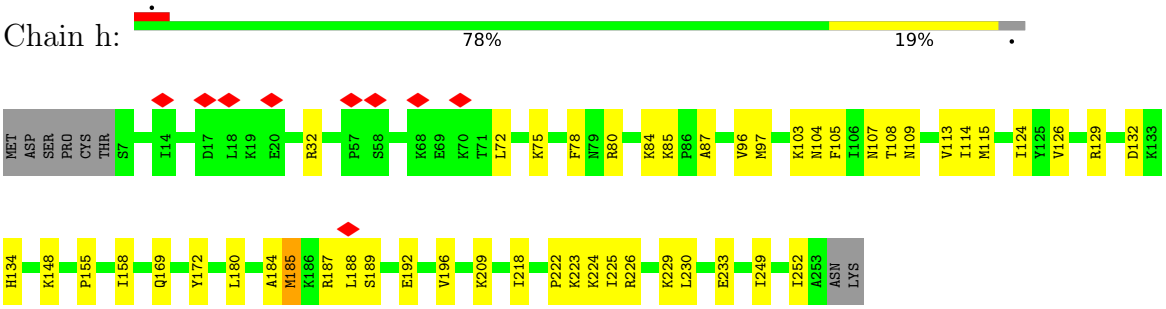
• Molecule 42: Cilia- and flagella-associated protein 52

Chain g:



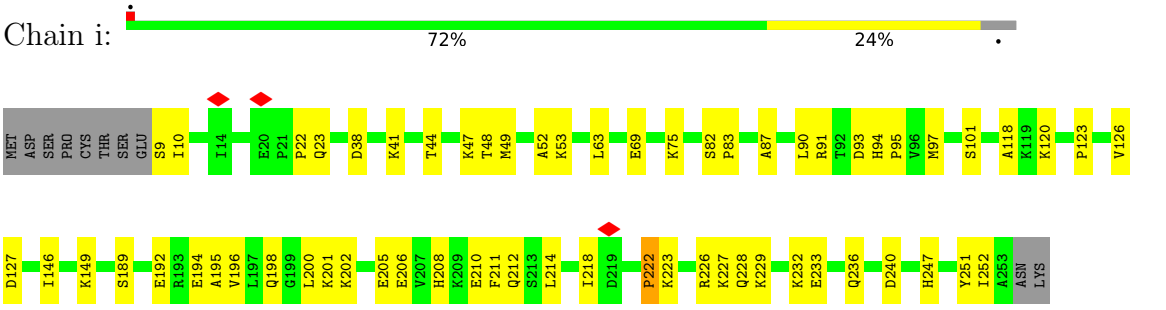
• Molecule 43: Enkurin

Chain h:



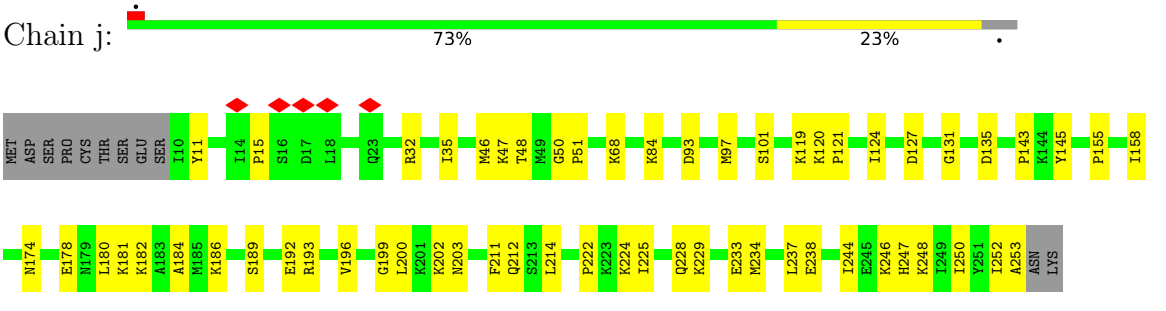
• Molecule 43: Enkurin

Chain i:



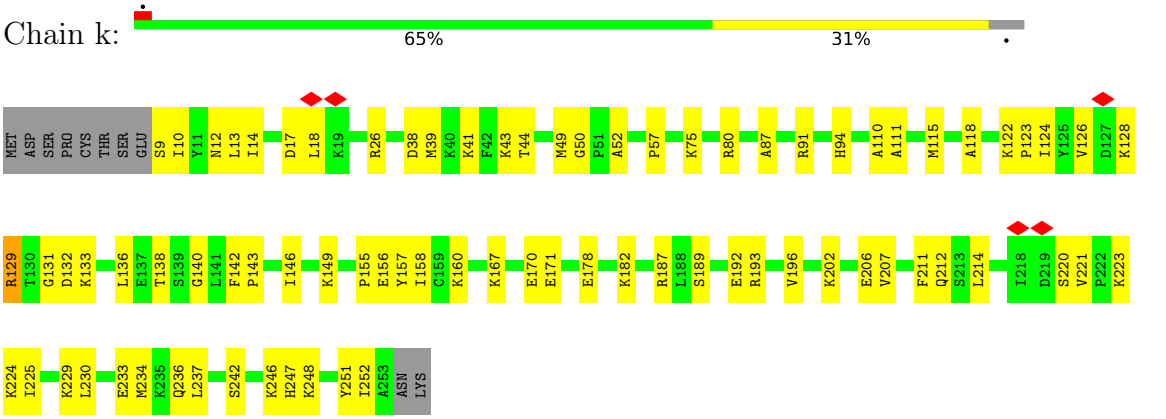
• Molecule 43: Enkurin

Chain j:



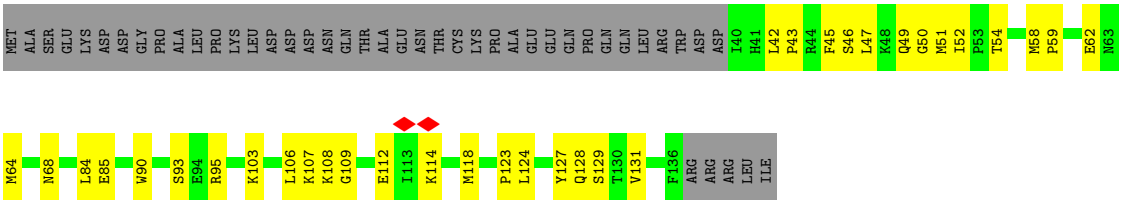
• Molecule 43: Enkurin

Chain k:



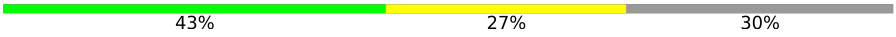
• Molecule 44: Testis-expressed protein 43

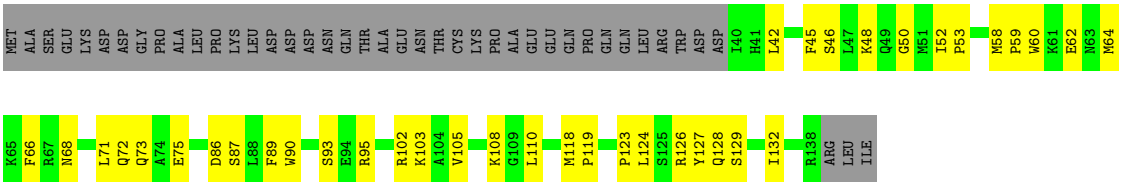
Chain h1:



• Molecule 44: Testis-expressed protein 43

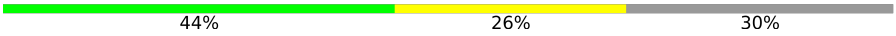
Chain h2:

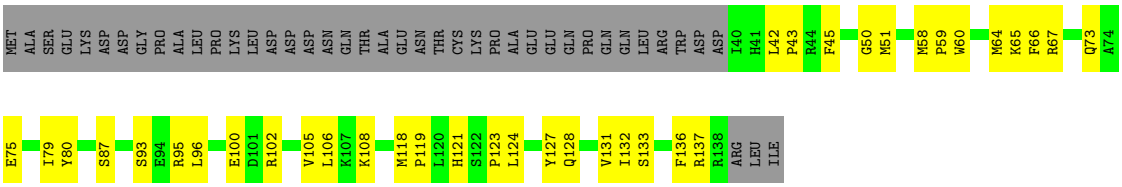




• Molecule 44: Testis-expressed protein 43

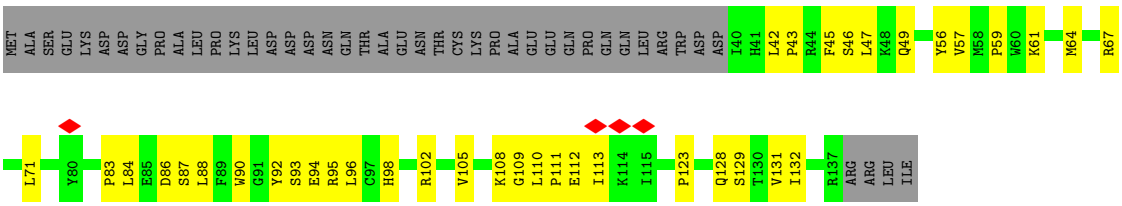
Chain h3:





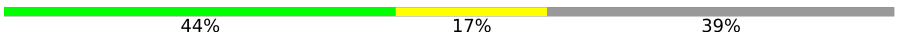
• Molecule 44: Testis-expressed protein 43

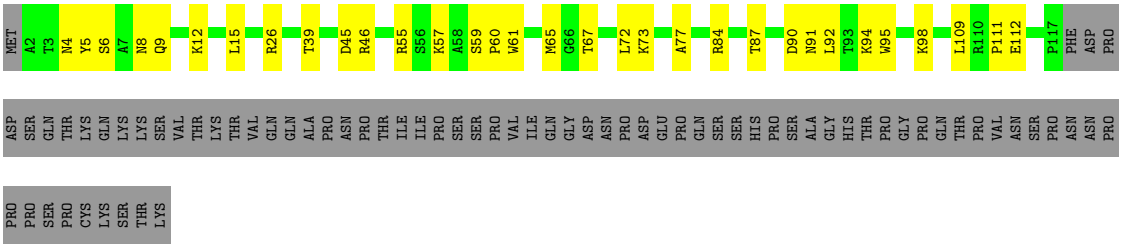
Chain h4:



• Molecule 45: Protein Flattop

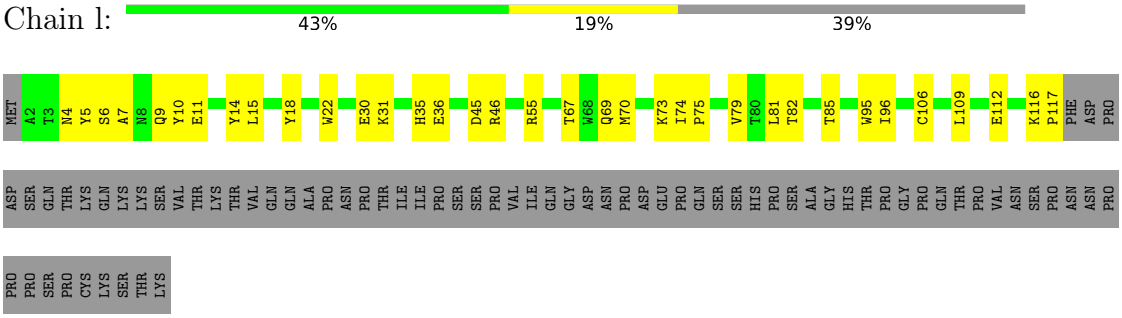
Chain i1:





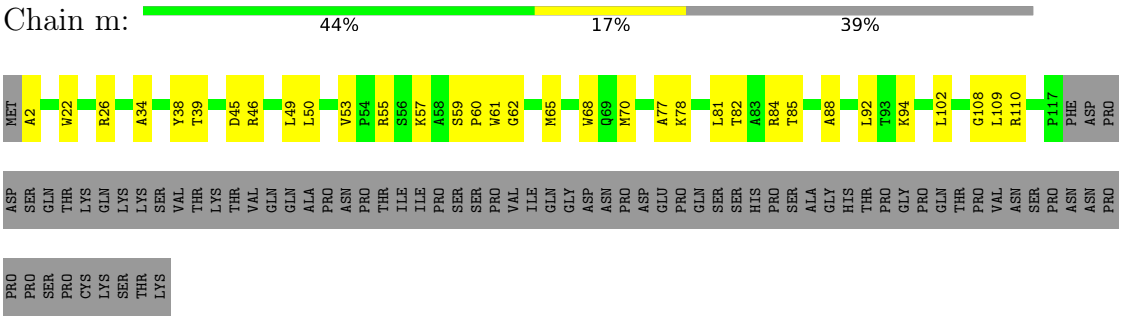
• Molecule 45: Protein Flattop

Chain l:



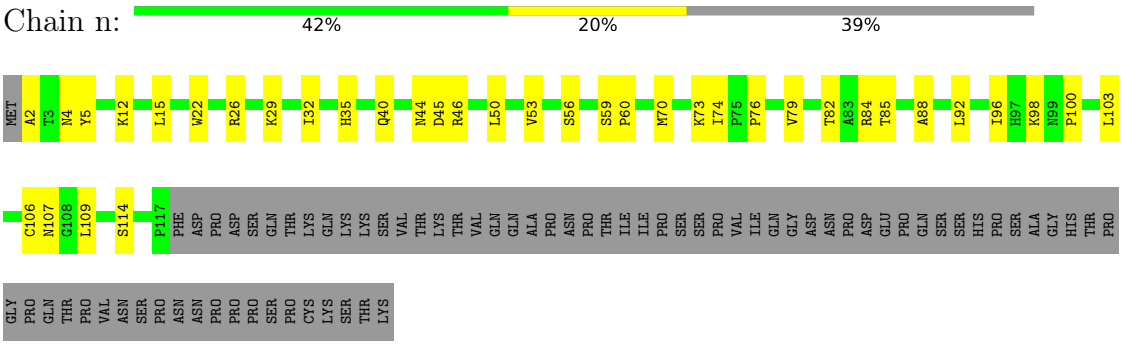
• Molecule 45: Protein Flattop

Chain m:



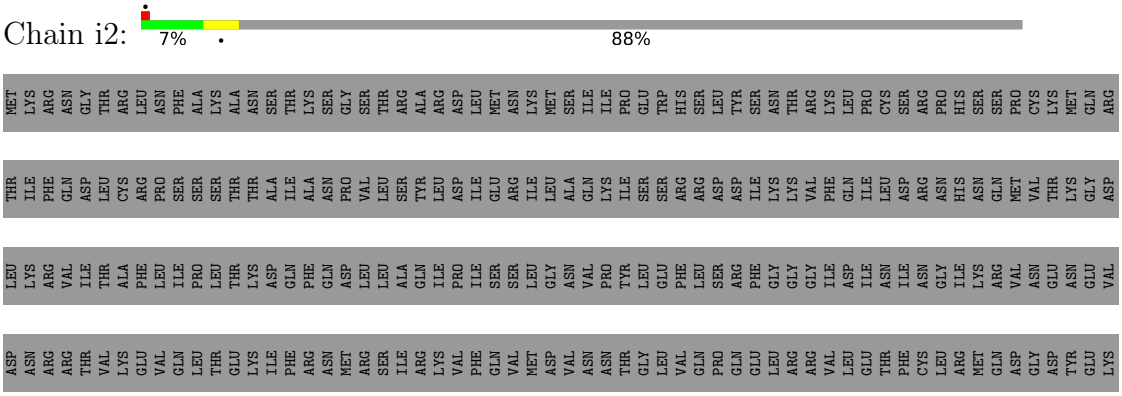
• Molecule 45: Protein Flattop

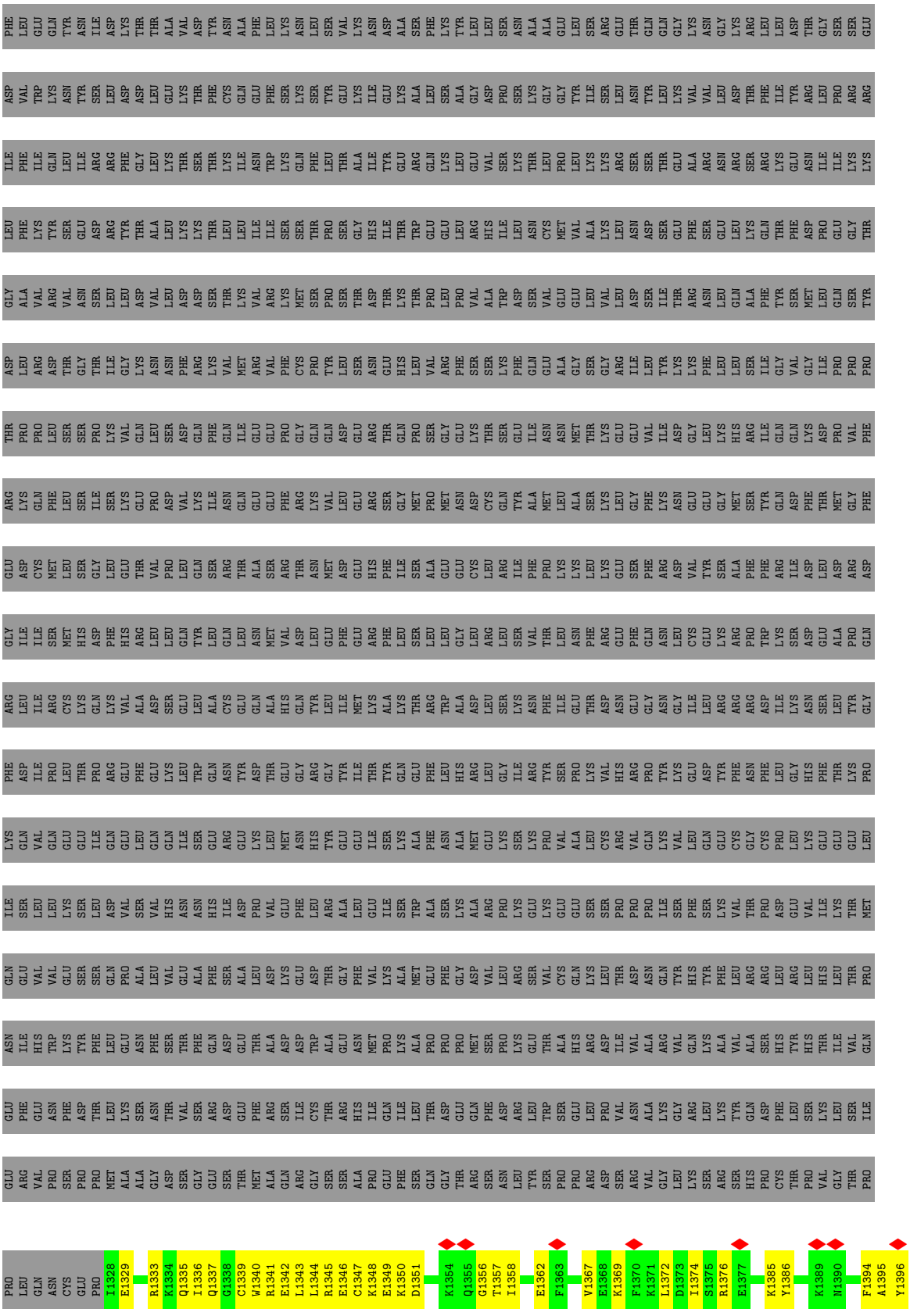
Chain n:

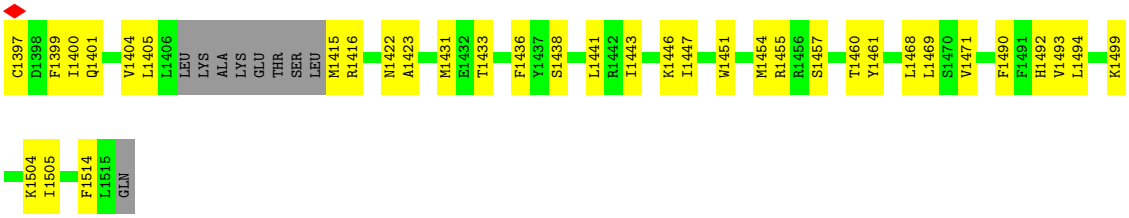


• Molecule 46: EF-hand calcium-binding domain-containing protein 6

Chain i2:

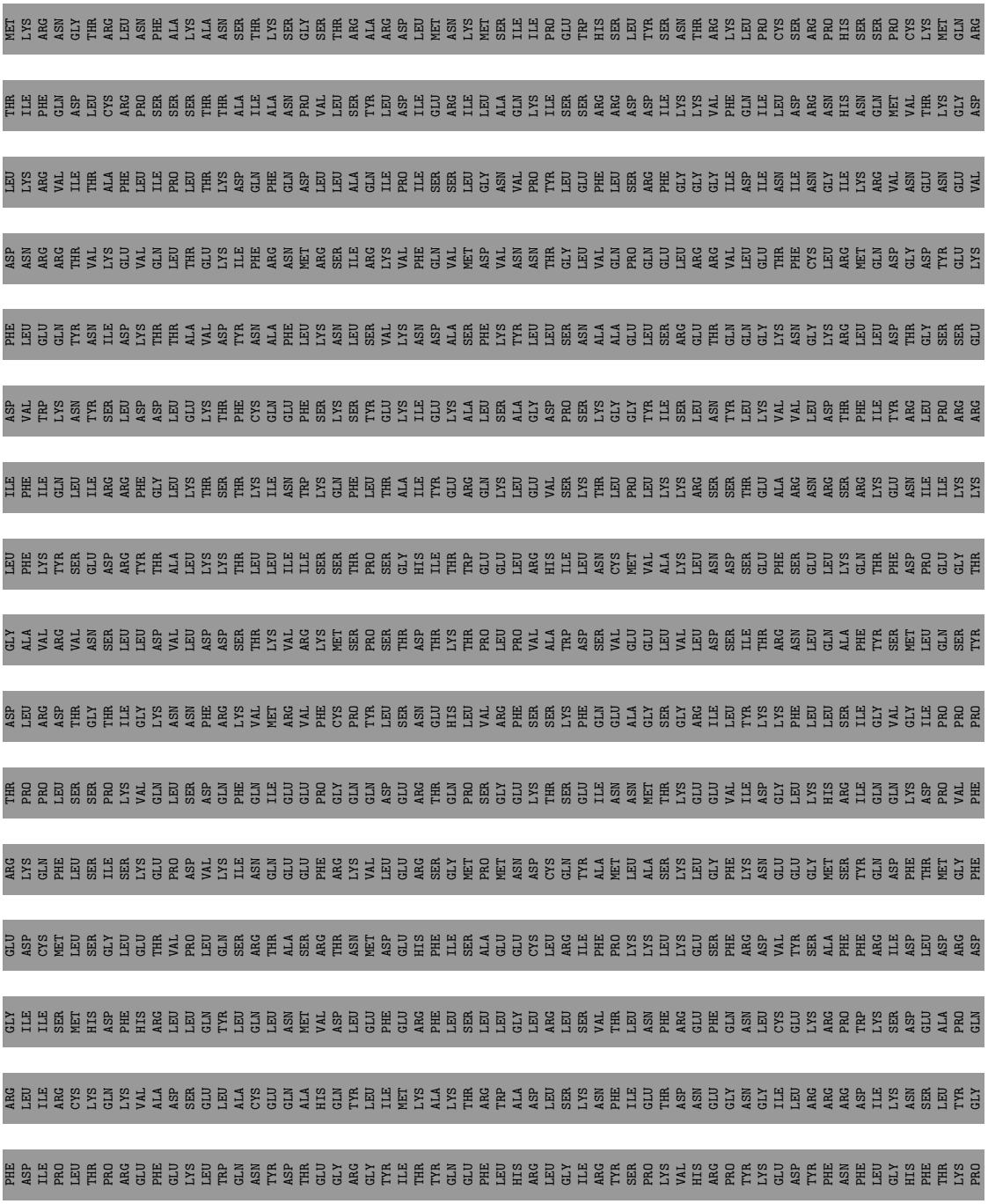


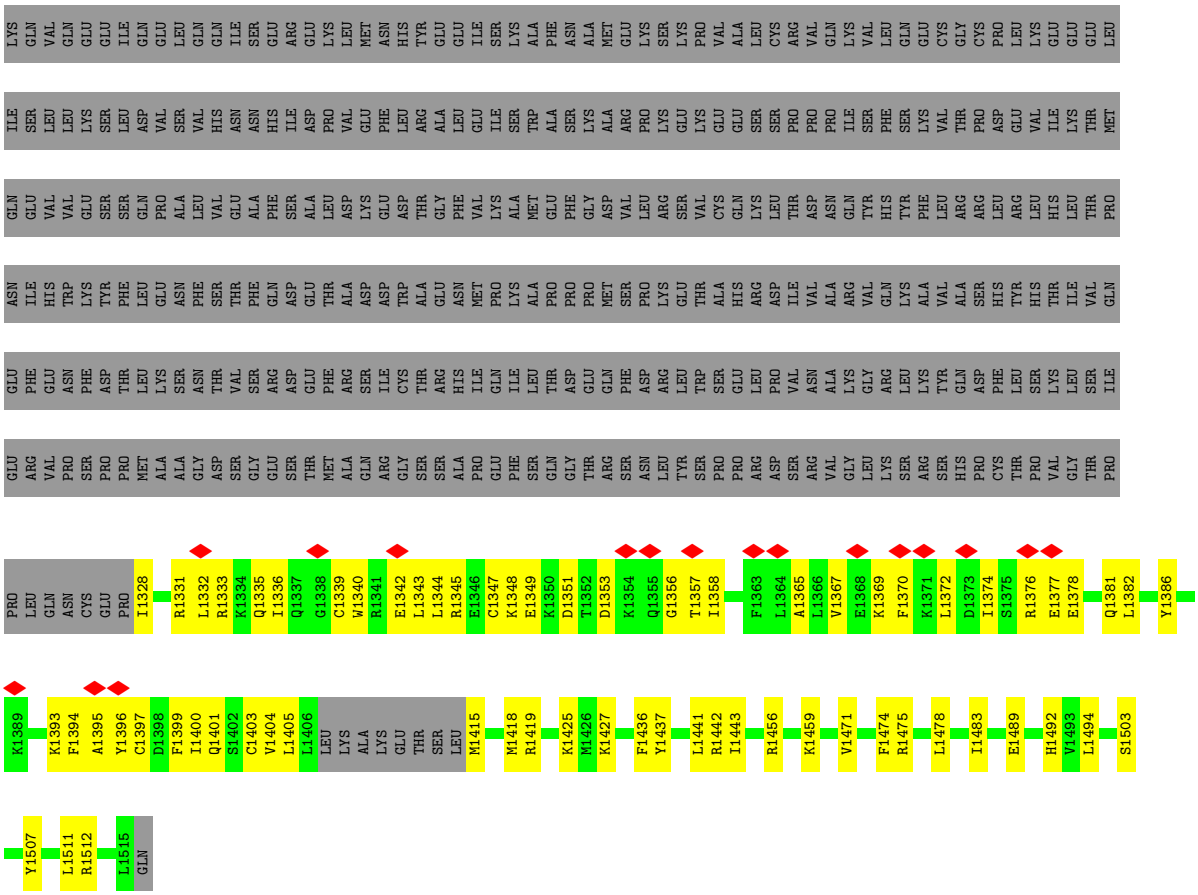

PHE LEU GLU GLN TYR ASN ILE ASP LYS THR THR ALA VAL ASP TYR ASN ALA PHE LEU LYS ASN LEU SER VAL LYS ASN ASP ALA SER PHE LYS TYR LEU LEU SER ASN ALA ALA GLU LEU SER ARG GLU THR GLN GLN GLY LYS ASN GLY LYS ARG LEU LEU ASP THR GLY SER SER GLU
ASP VAL TRP LYS ASN TYR SER LEU GLU ASP ASP LEU GLU LYS THR PHE CYS GLN GLU PHE SER LYS SER TYR GLU LYS LEU ASP ALA LEU SER ALA GLY ASP PRO SER LYS SER GLY GLY TYR ILE SER LEU ASN TYR LEU LYS VAL VAL LEU ASP THR PHE ILE TYR ARG LEU PRO ARG ARG
ILE PHE ILE GLN LEU ILE ARG ARG PHE GLY LEU LYS THR SER THR LYS ILE ASN TRP LYS LYS GLN PHE LEU THR ALA ILE TYR GLU ARG GLN LYS LEU GLU LEU ASN ARG SER SER THR GLU ALA ARG ASN ARG SER ARG ARG LYS GLU ASN ILE ILE LYS LYS
LEU PHE LYS TYR SER GLU ASP ARG TYR THR ALA LEU LYS LYS THR LEU LEU ILE ILE SER SER THR PRO SER GLY HIS ILE THR TRP GLU GLU LEU ARG HIS ILE LEU ASN CYS MET VAL ALA LYS LEU ASN ASP SER GLU PHE GLY LEU GLN LYS GLN THR PHE ASP PRO GLU GLY THR
GLY ALA VAL ARG VAL ASN SER LEU ASP VAL LEU ASP ASP SER THR LYS VAL ARG LYS MET SER PRO SER THR ASP LEU THR TRP ASP SER VAL GLU GLU LEU VAL LEU ASP SER ILE THR ARG ASN LEU GLN ALA PHE TYR SER MET LEU GLN SER TYR
ASP LEU ARG ASP THR ILE GLY LYS ASN ASN PHE ARG LYS VAL MET ARG VAL PHE CYS PRO TYR LEU SER ASN GLU HIS LEU VAL ARG PHE SER SER LYS PHE GLN GLU ILE LEU TYR LYS LYS PHE LEU LEU SER ILE GLY VAL GLY ILE PRO PRO PRO
THR PRO PRO LEU SER SER PRO LYS VAL GLN LEU SER ASP GLN PHE GLN ILE GLU GLU PRO GLY GLN GLN ASP GLU ARG THR GLN PRO SER GLY GLU LYS THR SER GLU ILE ASN ASN MET THR LYS GLU GLU VAL ILE LEU ASP GLY LEU LYS HIS ARG ILE GLN GLN LYS ASP PRO VAL PHE
ARG LYS GLN PHE LEU SER ILE ASN GLN GLU GLU PHE ARG LYS VAL LEU GLU ARG SER GLY MET PRO MET ASN ASP CYS GLN TYR ALA MET LEU ALA SER LYS LEU GLY PHE LYS ASN GLU GLU GLY MET SER TYR GLN ASP PHE THR MET GLY PHE
GLU ASP CYS MET LEU SER GLY LEU GLU HIS PHE ILE SER ALA GLU GLU CYS LEU GLN ARG ILE PHE PRO LYS LYS LEU LYS GLU SER PHE ARG ASP VAL ASP ARG PHE PHE ARG GLN ILE ASP LEU ASP ARG ASP
GLY ILE ILE SER MET HIS ASP PHE HIS ARG LEU LEU GLN TYR LEU GLN LEU ASN MET VAL ASP LEU GLU PHE GLU ARG PHE LEU SER LEU LEU GLY LEU ARG LEU SER VAL THR LEU ASN PHE ARG GLU PHE GLN ASN LEU CYS GLU LYS ARG PRO TRP LYS SER ASP GLU ALA PRO GLN
ARG LEU ILE ARG CYS LYS GLN LYS VAL ALA CYS GLU GLN LEU ASN MET LYS ALA HIS GLN TYR LEU ILE MET LYS ALA LYS THR ARG TRP ALA ASP LEU SER LYS ASN PHE ILE GLU THR ASP ASN GLU GLY ASN GLY ILE LEU LEU ARG ARG PRO ASP PHE ILE LYS ASN SER LEU TYR GLY
PHE ASP ILE PRO LEU THR PRO ARG GLU PHE GLU GLU LYS LEU THR GLN ASN TYR ASP THR GLU GLY GLY TYR ILE THR TYR GLN GLU PHE LEU HIS ARG LEU GLY ILE ARG TYR SER PRO LYS VAL HIS ARG PRO TYR LYS GLU ASP TYR PHE ASN PHE LEU GLY HIS PHE THR LYS PRO
LYS GLN VAL GLN GLU LEU GLN GLN ILE SER GLU ARG GLU LYS LEU MET ASN HIS TYR GLU GLU ILE SER LYS ALA PHE ASN ALA MET GLU LYS SER LYS PRO VAL ALA LEU CYS ARG VAL GLN LYS VAL LEU GLN GLU GLU CYS GLY CYS PRO LEU LYS GLU VAL ILE LYS GLU GLU LEU
ILE SER LEU LEU LYS SER LEU ASP VAL SER VAL HIS ASN ASN HIS ILE ASP PRO VAL GLU PHE LEU ARG ALA LEU ILE SER TRP ALA GLU ASP ALA ARG PRO LYS GLU LYS GLU GLU SER SER PRO PRO ILE SER SER PHE SER LYS VAL THR PRO ASP GLU VAL LYS THR MET
GLN GLU VAL VAL GLU SER SER GLN PRO ALA LEU VAL ASP LEU ALA LEU ASP THR GLY PHE VAL LYS ALA MET GLU PHE GLY ASP VAL LEU ARG SER GLU VAL CYS GLN LYS LEU THR ASP ASN GLN TYR HIS TYR PHE LEU ARG ARG LEU ARG LEU ARG HIS HIS LEU THR PRO
ASN ILE HIS TRP LYS TYR PHE LEU GLU ASN PHE SER THR PHE GLN ASP GLU THR ALA ASP ASP TRP ALA GLU ASN MET PRO LYS ALA PRO PRO MET SER PRO LYS GLU THR ALA HIS ARG ASP ILE ASP ARG VAL GLN LYS ALA VAL ALA ALA SER HIS TYR HIS THR ILE VAL GLN
GLU PHE GLU ASN PHE ASP THR LEU LYS ILE ASP PHE GLN ILE ILE LEU THR ASP GLU GLN GLN PHE GLU LEU PRO ASN MET ALA ASN ARG SER ILE CYS THR ARG HIS ILE GLN ILE LEU THR ASP GLU GLU PHE ARG LEU TRP SER GLU LEU PRO ARG ASP ILE VAL ASN ALA LYS GLY LEU LYS SER ARG TYR GLN SER PHE ILE
GLU ARG VAL PRO SER PRO PRO MET ALA GLN ARG GLY SER ALA PRO GLU PHE SER GLN GLY THR ARG SER ASN LEU TYR SER PRO PRO ARG ASP SER ARG VAL GLY LEU LYS SER ARG SER HIS PRO CYS THR PRO VAL GLY THR PRO
PRO LEU GLN ASN CYS PRO I1328 E1329 R1333 K1334 Q1335 I1336 Q1337 G1338 C1339 W1340 R1341 E1342 L1343 L1344 R1345 E1346 C1347 K1348 E1349 K1350 D1351 K1354 Q1355 G1356 T1357 I1358 E1362 F1363 V1367 E1368 K1369 F1370 K1371 L1372 D1373 I1374 S1375 R1376 E1377 K1385 Y1386 K1389 N1390 F1394 A1395 Y1396

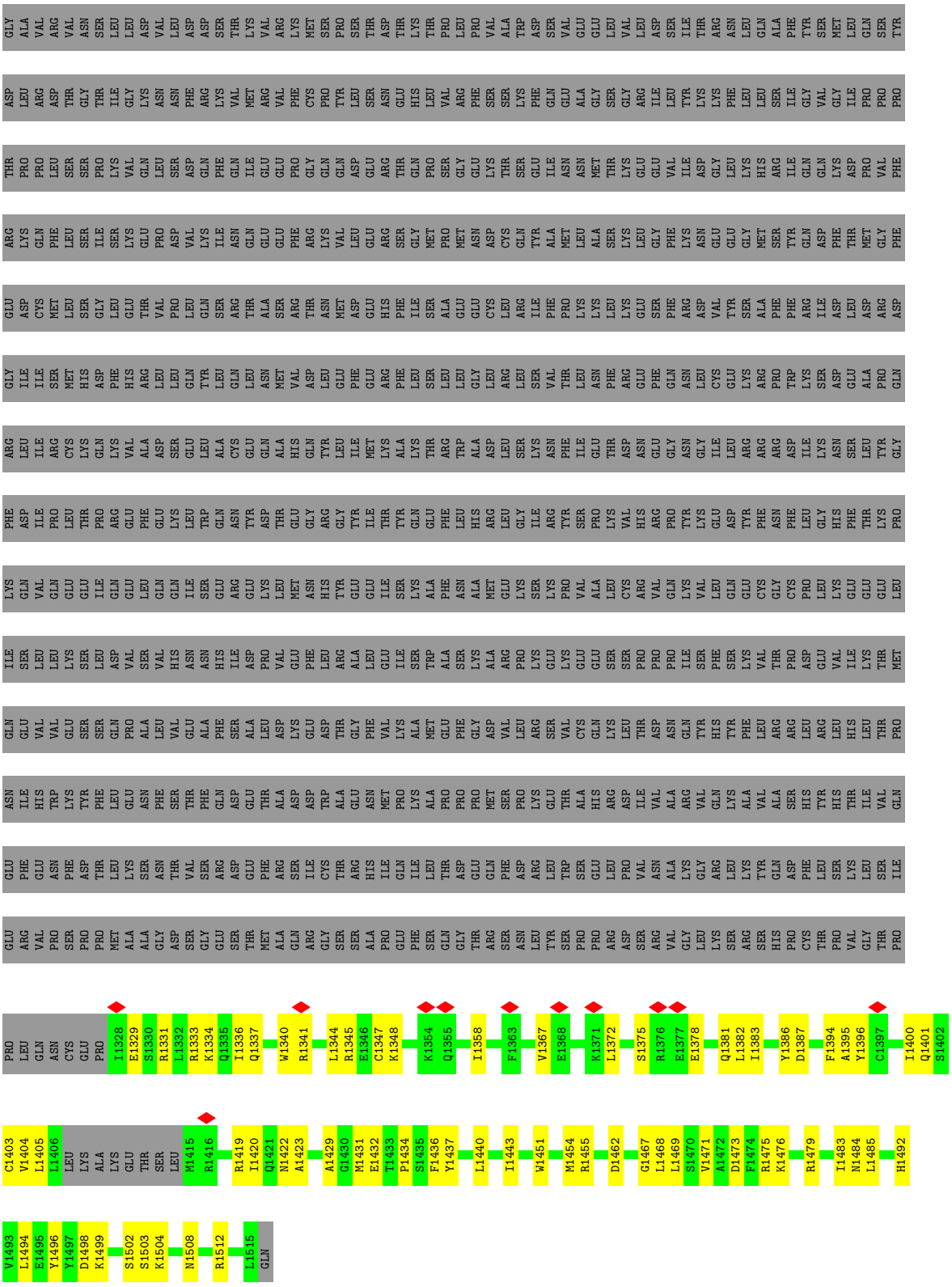


• Molecule 46: EF-hand calcium-binding domain-containing protein 6

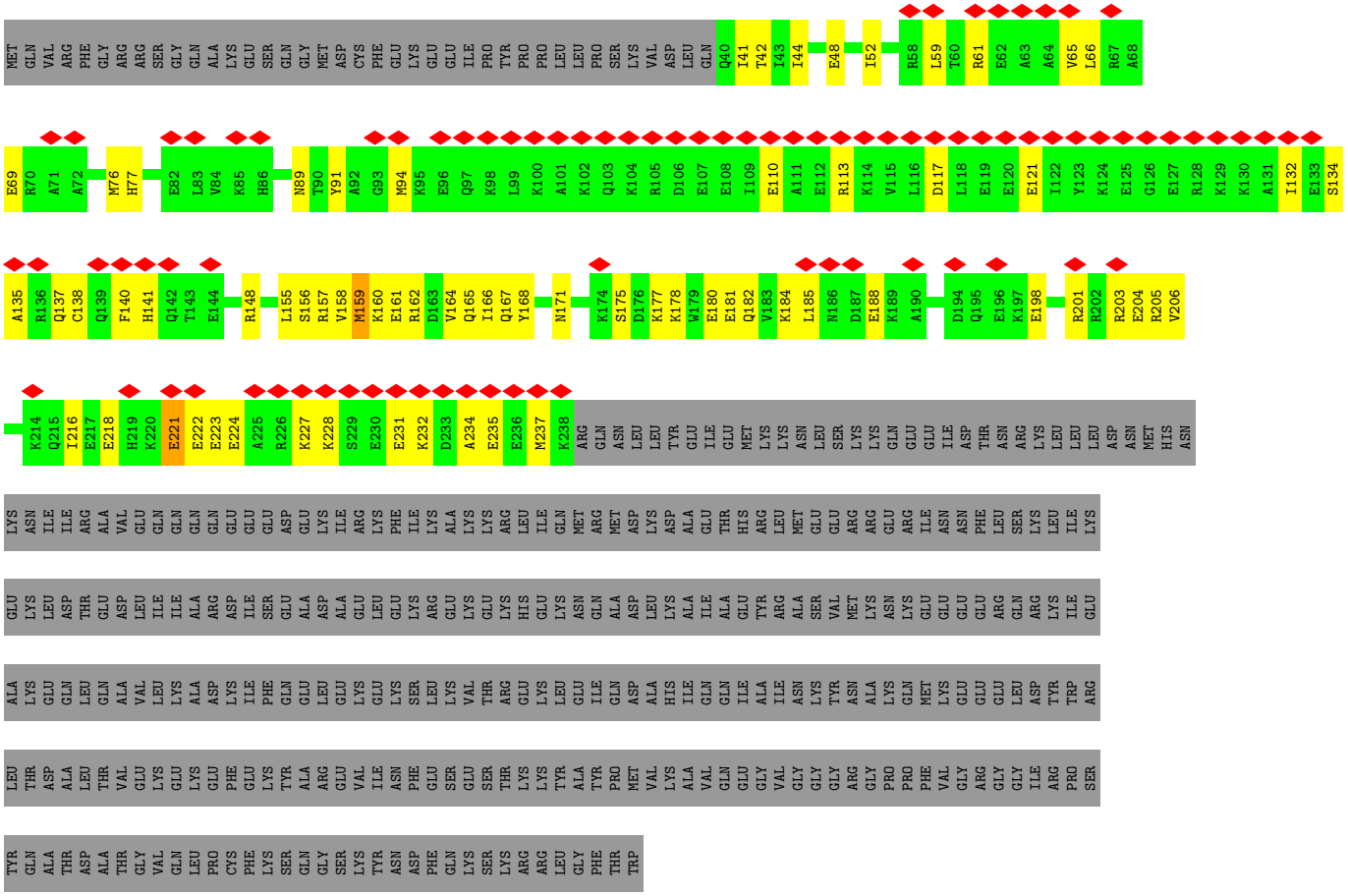
Chain i3:





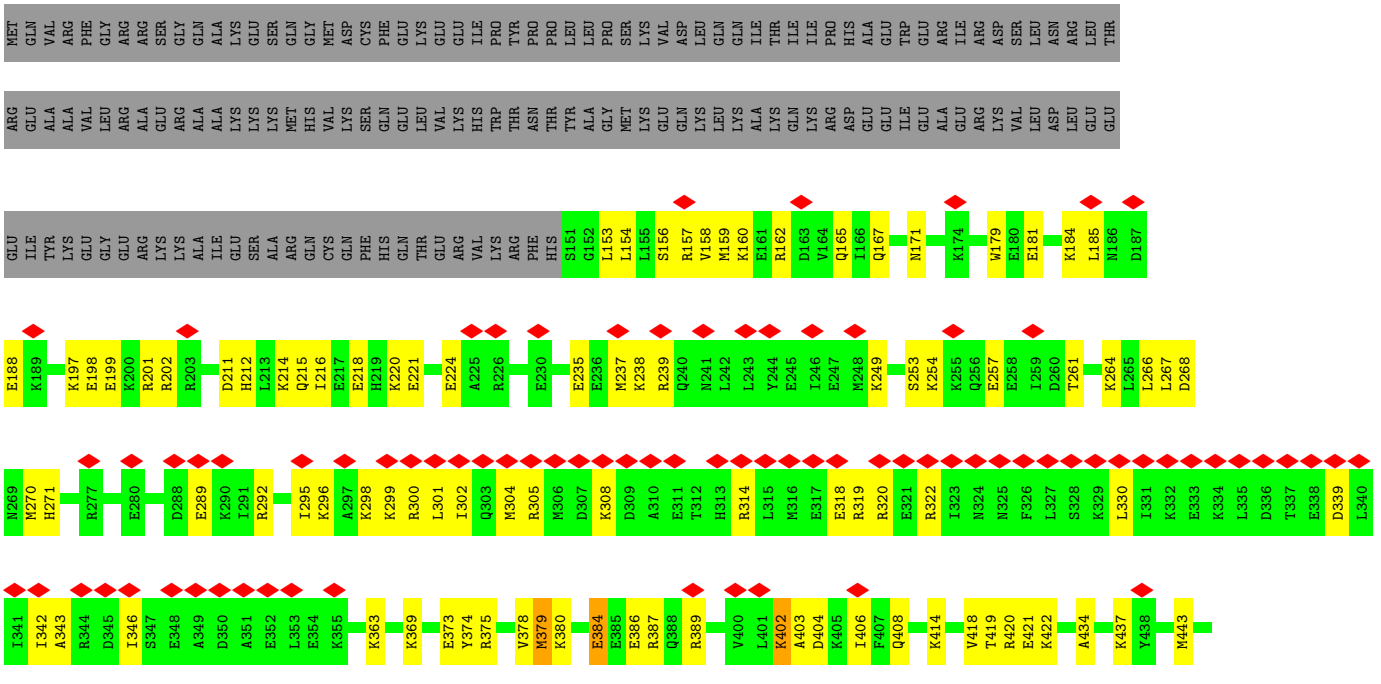


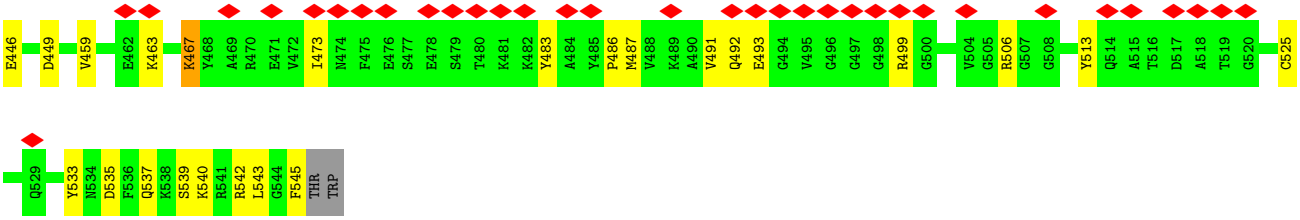
• Molecule 47: Cilia- and flagella-associated protein 210



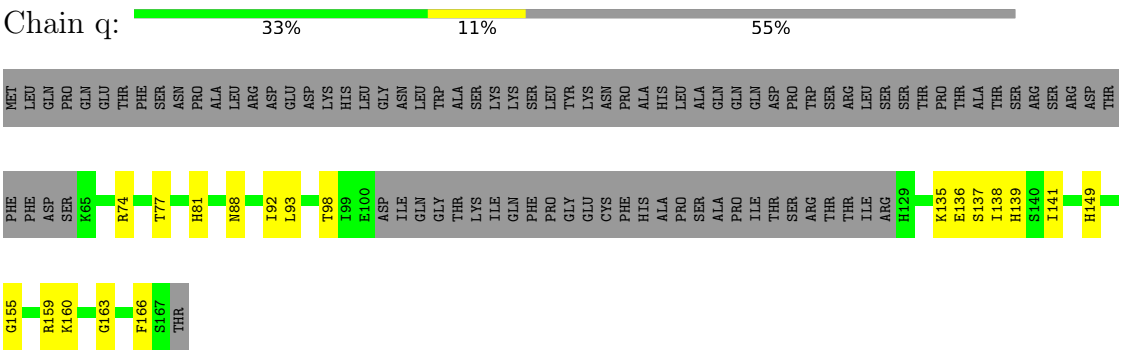
• Molecule 47: Cilia- and flagella-associated protein 210

Chain p:

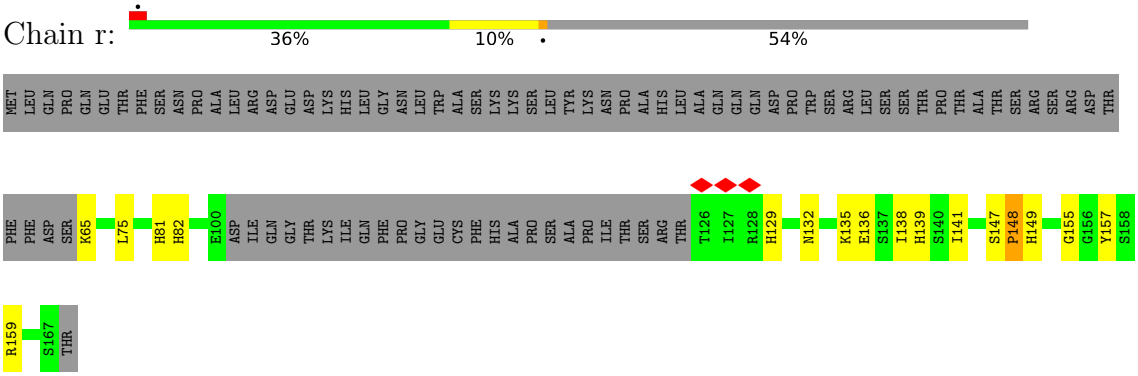




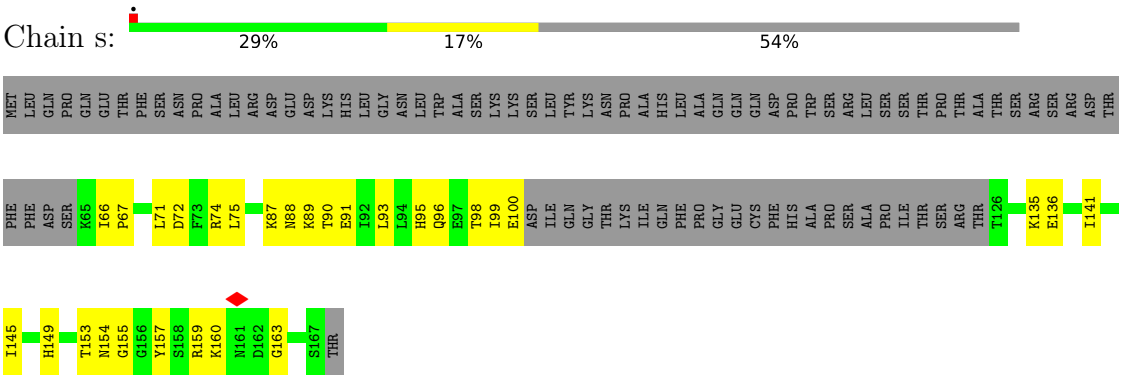
• Molecule 48: Cilia- and flagella-associated protein 276



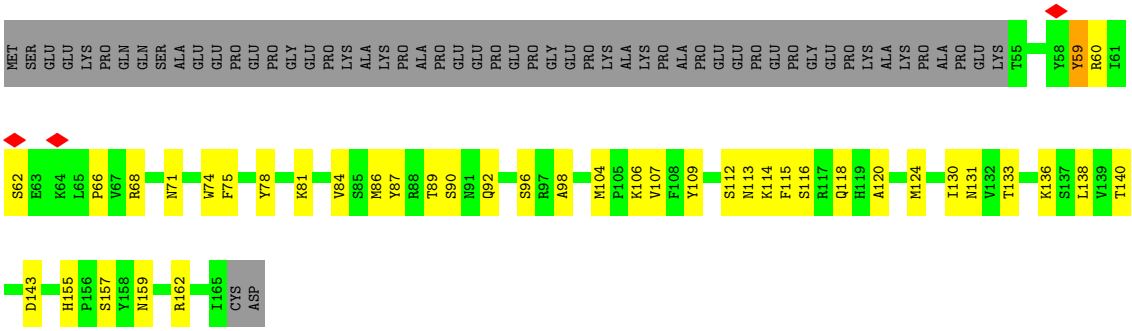
• Molecule 48: Cilia- and flagella-associated protein 276



• Molecule 48: Cilia- and flagella-associated protein 276



• Molecule 49: Piercer of microtubule wall 1 protein


MET SER GLU GLU LYS PRO GLN GLN SER ALA GLU GLU PRO GLU PRO GLY GLU PRO LYS ALA LYS PRO ALA PRO GLU GLU PRO GLU PRO GLY GLU PRO LYS ALA LYS PRO ALA PRO GLU GLU PRO GLU PRO GLY GLU GLU PRO GLU PRO LYS ALA LYS PRO ALA PRO GLU LYS T55 Y58 Y59 R60 I61
S62 E63 K64 L65 P66 W67 R68 N71 W74 F75 Y78 K81 V84 S85 M86 Y87 R88 T89 S90 N91 Q92 S96 R97 A98 M104 P105 K106 V107 F108 Y109 S112 N113 K114 F115 S116 R117 Q118 H119 A120 M124 I130 N131 V132 T133 K136 S137 L138 V139 T140
D143 H155 P156 S157 Y158 N159 R162 T165 CYS ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95290	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.821	Depositor
Minimum map value	0.000	Depositor
Average map value	0.073	Depositor
Map value standard deviation	0.176	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	576.11, 463.062, 869.60004	wwPDB
Map dimensions	530, 426, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.40	0/685	0.76	2/918 (0.2%)
1	7	0.29	0/1206	0.64	0/1629
2	1	0.22	0/3827	0.50	0/5169
2	2	0.30	0/2224	0.59	0/3010
3	3	0.34	0/4056	0.53	3/5386 (0.1%)
3	4	0.28	0/1237	0.56	0/1646
4	5	0.22	0/3038	0.46	0/4102
4	6	0.18	0/3038	0.44	0/4102
4	j1	0.25	0/3038	0.59	0/4102
5	8	0.29	0/1523	0.70	5/2073 (0.2%)
6	A	0.27	0/819	0.61	0/1097
6	N1	0.38	0/819	0.64	1/1097 (0.1%)
7	A0	0.35	0/449	0.59	0/605
7	A1	0.26	0/2965	0.42	0/3994
7	A2	0.25	0/3327	0.42	0/4483
7	A3	0.29	0/3327	0.46	0/4483
7	A4	0.25	0/3313	0.44	0/4465
7	A5	0.31	0/1419	0.54	0/1910
8	AA	0.16	0/3502	0.41	1/4755 (0.0%)
8	AC	0.19	0/3502	0.41	0/4755
8	AE	0.26	0/3509	0.57	1/4765 (0.0%)
8	AG	0.28	0/3518	0.52	0/4777
8	AI	0.25	0/3509	0.52	0/4765
8	AK	0.23	0/3496	0.44	0/4747
8	AM	0.24	0/3509	0.51	0/4765
8	AO	0.22	0/3509	0.49	0/4765
8	BC	0.18	0/3451	0.38	0/4686
8	BE	0.25	0/3518	0.55	3/4777 (0.1%)
8	BG	0.22	0/3473	0.47	0/4716
8	BI	0.25	0/3518	0.54	1/4777 (0.0%)
8	BK	0.24	0/3467	0.50	2/4708 (0.0%)
8	BM	0.24	0/3502	0.51	0/4755

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	BO	0.23	0/3473	0.52	1/4716 (0.0%)
8	CC	0.21	0/3502	0.43	1/4755 (0.0%)
8	CE	0.19	0/3502	0.47	1/4755 (0.0%)
8	CG	0.20	0/3502	0.43	0/4755
8	CI	0.22	0/3502	0.46	0/4755
8	CK	0.21	0/3502	0.42	0/4755
8	CM	0.25	0/3509	0.55	2/4765 (0.0%)
8	CO	0.18	0/3502	0.42	0/4755
8	CQ	0.21	0/3488	0.47	0/4736
8	DC	0.22	0/3459	0.45	1/4697 (0.0%)
8	DE	0.18	0/3443	0.42	0/4675
8	DG	0.23	0/3443	0.45	1/4675 (0.0%)
8	DI	0.21	0/3451	0.46	0/4686
8	DK	0.18	0/3450	0.36	0/4685
8	DM	0.16	0/3457	0.39	0/4694
8	DO	0.18	0/3449	0.41	0/4683
8	DQ	0.18	0/3437	0.40	0/4667
8	EA	0.21	0/3502	0.44	1/4755 (0.0%)
8	EC	0.17	0/3496	0.40	0/4747
8	EE	0.16	0/3502	0.37	0/4755
8	EG	0.16	0/3502	0.39	0/4755
8	EI	0.18	0/3502	0.42	1/4755 (0.0%)
8	EK	0.17	0/3502	0.38	0/4755
8	EM	0.15	0/3502	0.38	0/4755
8	EO	0.16	0/3488	0.42	0/4736
8	FA	0.21	0/3443	0.52	1/4675 (0.0%)
8	FC	0.20	0/3443	0.43	0/4675
8	FE	0.15	0/3443	0.38	0/4675
8	FG	0.20	0/3427	0.51	2/4652 (0.0%)
8	FI	0.22	0/3443	0.44	1/4675 (0.0%)
8	FK	0.16	0/3450	0.40	1/4685 (0.0%)
8	FM	0.17	0/3443	0.40	0/4675
8	FO	0.18	0/3432	0.47	1/4660 (0.0%)
8	GA	0.15	0/3445	0.38	0/4678
8	GC	0.19	0/3450	0.45	0/4685
8	GE	0.22	0/3450	0.48	0/4685
8	GG	0.25	0/3509	0.51	0/4765
8	GI	0.20	0/3464	0.46	0/4704
8	GK	0.22	0/3464	0.50	1/4704 (0.0%)
8	GM	0.22	0/3472	0.52	0/4715
8	GO	0.20	0/3472	0.51	0/4715
8	HA	0.21	0/3448	0.51	0/4682
8	HC	0.25	0/3466	0.56	0/4706

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	HE	0.23	0/3509	0.56	2/4765 (0.0%)
8	HG	0.27	1/3509 (0.0%)	0.51	0/4765
8	HI	0.21	0/3509	0.51	1/4765 (0.0%)
8	HK	0.23	0/3443	0.53	1/4675 (0.0%)
8	HM	0.27	0/3466	0.57	0/4706
8	HO	0.26	0/3458	0.57	0/4696
8	IA	0.21	0/3457	0.48	0/4694
8	IC	0.26	0/3509	0.57	0/4765
8	IE	0.25	0/3518	0.57	0/4777
8	IG	0.34	1/3464 (0.0%)	0.63	1/4704 (0.0%)
8	II	0.29	0/3476	0.58	2/4720 (0.0%)
8	IK	0.31	0/3488	0.58	1/4736 (0.0%)
8	IM	0.30	0/3468	0.61	4/4709 (0.1%)
8	IO	0.28	0/3509	0.59	0/4765
8	JC	0.21	0/3465	0.47	0/4704
8	JE	0.25	0/3502	0.55	1/4755 (0.0%)
8	JG	0.24	0/3437	0.51	1/4667 (0.0%)
8	JI	0.28	0/3467	0.60	1/4708 (0.0%)
8	JK	0.23	0/3458	0.50	1/4696 (0.0%)
8	JM	0.20	0/3443	0.45	0/4675
8	JO	0.26	0/3456	0.57	1/4693 (0.0%)
8	JQ	0.23	0/3480	0.55	0/4725
8	KA	0.20	0/3457	0.45	2/4694 (0.0%)
8	KC	0.23	0/3466	0.48	0/4705
8	KE	0.25	0/3474	0.52	1/4716 (0.0%)
8	KG	0.23	0/3457	0.47	1/4694 (0.0%)
8	KI	0.23	0/3451	0.47	0/4686
8	KK	0.22	0/3449	0.45	0/4683
8	KM	0.22	0/3457	0.52	1/4694 (0.0%)
8	KO	0.24	0/3466	0.50	0/4705
8	LA	0.21	0/3473	0.50	1/4716 (0.0%)
8	LC	0.24	0/3451	0.47	2/4686 (0.0%)
8	LE	0.28	1/3465 (0.0%)	0.51	2/4705 (0.0%)
8	LG	0.23	0/3518	0.46	0/4777
8	LI	0.23	0/3518	0.46	0/4777
8	LK	0.24	0/3518	0.48	1/4777 (0.0%)
8	LM	0.20	0/3481	0.45	0/4727
8	LO	0.21	0/3443	0.43	0/4675
8	MA	0.16	0/3451	0.39	0/4686
8	MC	0.21	0/3451	0.42	0/4686
8	ME	0.23	0/3502	0.45	0/4755
8	MG	0.22	0/3457	0.42	1/4694 (0.0%)
8	MI	0.24	0/3455	0.47	0/4691

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	MK	0.27	0/3467	0.49	1/4708 (0.0%)
8	MM	0.21	0/3457	0.43	0/4694
8	MO	0.19	0/3429	0.45	0/4656
8	NA	0.18	0/3430	0.44	0/4657
8	NC	0.15	0/3429	0.39	0/4656
8	NE	0.21	0/3471	0.46	0/4713
8	NG	0.23	0/3459	0.49	0/4697
8	NI	0.24	0/3450	0.50	0/4685
8	NK	0.25	0/3450	0.60	1/4685 (0.0%)
8	NM	0.30	0/3459	0.55	2/4697 (0.0%)
8	NO	0.20	0/3459	0.51	0/4697
8	OA	0.17	0/3451	0.44	0/4686
8	OC	0.17	0/3443	0.46	0/4675
8	OE	0.21	0/3449	0.49	0/4683
8	OG	0.20	0/3443	0.44	1/4675 (0.0%)
8	OI	0.22	0/3437	0.46	0/4667
8	OK	0.22	0/3451	0.53	1/4686 (0.0%)
8	OM	0.19	0/3429	0.45	0/4656
8	OO	0.21	0/3406	0.51	0/4624
8	PC	0.22	0/3429	0.51	1/4656 (0.0%)
8	PE	0.18	0/3406	0.47	1/4625 (0.0%)
8	PG	0.17	0/3443	0.42	1/4675 (0.0%)
8	PI	0.22	0/3443	0.47	1/4675 (0.0%)
8	PK	0.23	0/3443	0.52	0/4674
8	PM	0.21	0/3457	0.49	0/4694
8	PO	0.19	0/3443	0.47	0/4675
8	QC	0.19	0/3429	0.47	0/4656
8	QE	0.23	0/3443	0.48	0/4675
8	QG	0.19	0/3429	0.43	0/4656
8	QI	0.19	0/3421	0.47	0/4644
8	QK	0.17	0/3422	0.42	0/4646
8	QM	0.23	0/3414	0.52	1/4634 (0.0%)
8	QO	0.20	0/3422	0.45	0/4646
8	RC	0.16	0/3429	0.40	0/4656
8	RE	0.17	0/3429	0.42	1/4655 (0.0%)
8	RG	0.16	0/3429	0.43	2/4656 (0.0%)
8	RI	0.18	0/3437	0.46	4/4667 (0.1%)
8	RK	0.21	0/3445	0.49	2/4678 (0.0%)
8	RM	0.30	0/3437	0.57	1/4666 (0.0%)
8	RO	0.22	0/3429	0.50	2/4655 (0.0%)
8	SA	0.15	0/3436	0.44	1/4665 (0.0%)
8	SC	0.26	1/3429 (0.0%)	0.51	3/4656 (0.1%)
8	SE	0.19	0/3429	0.44	0/4656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	SG	0.18	0/3422	0.45	0/4646
8	SI	0.30	1/3437 (0.0%)	0.57	3/4667 (0.1%)
8	SK	0.17	0/3422	0.42	0/4646
8	SM	0.21	0/3410	0.50	0/4630
8	TA	0.20	0/3419	0.52	1/4642 (0.0%)
8	TC	0.21	0/3414	0.52	0/4635
8	TE	0.21	0/3434	0.49	0/4662
8	TG	0.15	0/3418	0.38	0/4641
8	TI	0.20	0/3426	0.45	0/4652
8	TK	0.16	0/3429	0.43	0/4656
8	TM	0.20	0/3418	0.49	1/4641 (0.0%)
8	UA	0.20	0/3403	0.52	1/4619 (0.0%)
8	UC	0.19	0/3428	0.47	0/4654
8	UE	0.18	0/3428	0.45	0/4654
8	UG	0.16	0/3430	0.42	0/4657
8	UI	0.19	0/3429	0.43	0/4656
8	UK	0.18	0/3430	0.49	2/4657 (0.0%)
8	UM	0.22	0/3436	0.49	1/4665 (0.0%)
8	UO	0.18	0/3424	0.48	0/4649
8	VA	0.17	0/3422	0.44	1/4646 (0.0%)
8	VC	0.16	0/3488	0.41	0/4736
8	VE	0.20	0/3435	0.44	0/4664
8	VG	0.20	0/3488	0.51	1/4736 (0.0%)
8	VI	0.22	0/3437	0.54	1/4667 (0.0%)
8	VK	0.21	0/3496	0.47	1/4747 (0.0%)
8	VM	0.22	0/3435	0.50	1/4663 (0.0%)
8	VO	0.20	0/3481	0.45	2/4726 (0.0%)
8	WA	0.22	0/3481	0.50	0/4726
8	WC	0.18	0/3502	0.46	2/4755 (0.0%)
8	WE	0.18	0/3459	0.49	1/4696 (0.0%)
8	WG	0.16	0/3496	0.42	0/4747
8	WI	0.17	0/3502	0.42	0/4755
8	WK	0.19	0/3496	0.46	0/4747
8	WM	0.18	0/3451	0.47	0/4686
8	WO	0.18	0/3435	0.47	0/4664
9	AB	0.20	0/3466	0.45	1/4697 (0.0%)
9	AD	0.22	0/3488	0.47	0/4726
9	AF	0.22	0/3448	0.46	0/4673
9	AH	0.25	0/3479	0.49	0/4714
9	AJ	0.29	0/3479	0.55	2/4714 (0.0%)
9	AL	0.25	0/3479	0.50	0/4714
9	AN	0.22	0/3479	0.50	4/4714 (0.1%)
9	AP	0.20	0/3466	0.46	0/4697

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	BB	0.16	0/3436	0.39	0/4656
9	BD	0.18	0/3448	0.41	2/4673 (0.0%)
9	BF	0.24	0/3443	0.43	0/4666
9	BH	0.23	0/3448	0.44	0/4673
9	BJ	0.24	0/3457	0.45	1/4685 (0.0%)
9	BL	0.23	0/3448	0.46	0/4673
9	BN	0.20	0/3448	0.43	0/4673
9	BP	0.17	0/3448	0.43	0/4673
9	CB	0.22	0/3431	0.47	0/4649
9	CD	0.18	0/3457	0.43	0/4685
9	CF	0.20	0/3457	0.42	1/4685 (0.0%)
9	CH	0.20	0/3457	0.42	1/4685 (0.0%)
9	CJ	0.18	0/3436	0.41	0/4656
9	CL	0.25	0/3443	0.49	1/4666 (0.0%)
9	CN	0.19	0/3457	0.40	0/4685
9	CP	0.17	0/3448	0.42	0/4673
9	DB	0.17	0/3443	0.44	0/4666
9	DD	0.18	0/3443	0.42	0/4666
9	DF	0.17	0/3448	0.41	1/4673 (0.0%)
9	DH	0.17	0/3448	0.40	1/4673 (0.0%)
9	DJ	0.18	0/3448	0.39	1/4673 (0.0%)
9	DL	0.17	0/3457	0.40	1/4685 (0.0%)
9	DN	0.16	0/3436	0.40	0/4656
9	DP	0.15	0/3448	0.41	0/4673
9	EB	0.21	0/3436	0.43	1/4656 (0.0%)
9	ED	0.16	0/3436	0.40	0/4656
9	EF	0.18	0/3436	0.42	0/4656
9	EH	0.17	0/3436	0.41	1/4656 (0.0%)
9	EJ	0.18	0/3431	0.42	0/4649
9	EL	0.16	0/3436	0.42	0/4656
9	EN	0.17	0/3436	0.41	1/4656 (0.0%)
9	FB	0.23	0/3448	0.51	3/4673 (0.1%)
9	FD	0.18	0/3448	0.44	2/4673 (0.0%)
9	FF	0.17	0/3448	0.41	0/4673
9	FH	0.17	0/3448	0.44	0/4673
9	FJ	0.22	0/3443	0.44	1/4666 (0.0%)
9	FL	0.17	0/3443	0.40	1/4666 (0.0%)
9	FN	0.17	0/3448	0.43	0/4673
9	GB	0.19	0/3431	0.45	2/4649 (0.0%)
9	GD	0.22	1/3448 (0.0%)	0.49	2/4673 (0.0%)
9	GF	0.18	0/3448	0.41	2/4673 (0.0%)
9	GH	0.19	0/3457	0.43	1/4685 (0.0%)
9	GJ	0.20	0/3448	0.42	0/4673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	GL	0.25	0/3457	0.47	0/4685
9	GN	0.21	0/3457	0.47	2/4685 (0.0%)
9	HB	0.23	1/3448 (0.0%)	0.49	0/4673
9	HD	0.26	0/3431	0.52	0/4649
9	HF	0.24	1/3448 (0.0%)	0.46	2/4673 (0.0%)
9	HH	0.23	0/3457	0.48	3/4685 (0.1%)
9	HJ	0.26	0/3448	0.54	0/4673
9	HL	0.25	0/3457	0.52	0/4685
9	HN	0.24	0/3448	0.48	1/4673 (0.0%)
9	HP	0.24	0/3431	0.53	0/4649
9	IB	0.25	0/3448	0.54	2/4673 (0.0%)
9	ID	0.23	0/3448	0.53	2/4673 (0.0%)
9	IF	0.27	1/3448 (0.0%)	0.52	1/4673 (0.0%)
9	IH	0.29	0/3457	0.58	2/4685 (0.0%)
9	IJ	0.20	0/3443	0.45	2/4666 (0.0%)
9	IL	0.31	1/3457 (0.0%)	0.60	3/4685 (0.1%)
9	IN	0.26	0/3457	0.53	0/4685
9	IP	0.29	1/3457 (0.0%)	0.61	4/4685 (0.1%)
9	JB	0.22	0/3431	0.50	2/4649 (0.0%)
9	JD	0.25	0/3431	0.56	1/4649 (0.0%)
9	JF	0.29	0/3431	0.59	2/4649 (0.0%)
9	JH	0.29	0/3431	0.57	2/4649 (0.0%)
9	JJ	0.24	0/3431	0.53	1/4649 (0.0%)
9	JL	0.25	0/3431	0.57	2/4649 (0.0%)
9	JN	0.25	0/3423	0.50	2/4638 (0.0%)
9	JP	0.23	0/3431	0.51	1/4649 (0.0%)
9	KB	0.25	0/3448	0.49	1/4673 (0.0%)
9	KD	0.24	0/3457	0.51	0/4685
9	KF	0.22	0/3457	0.43	1/4685 (0.0%)
9	KH	0.21	0/3457	0.45	0/4685
9	KJ	0.22	0/3448	0.46	0/4673
9	KL	0.23	0/3448	0.52	3/4673 (0.1%)
9	KN	0.22	0/3448	0.49	3/4673 (0.1%)
9	KP	0.23	0/3436	0.52	1/4656 (0.0%)
9	LB	0.25	0/3509	0.52	2/4754 (0.0%)
9	LD	0.22	0/3457	0.40	0/4685
9	LF	0.25	0/3527	0.51	2/4778 (0.0%)
9	LH	0.24	0/3457	0.44	0/4685
9	LJ	0.24	0/3509	0.50	1/4754 (0.0%)
9	LL	0.22	0/3436	0.44	0/4656
9	LN	0.19	0/3466	0.44	0/4697
9	LP	0.16	0/3443	0.39	0/4666
9	MB	0.21	0/3457	0.46	1/4685 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	MD	0.24	0/3457	0.45	0/4685
9	MF	0.21	0/3431	0.44	0/4649
9	MH	0.23	0/3457	0.43	0/4685
9	MJ	0.24	0/3448	0.46	2/4673 (0.0%)
9	ML	0.23	0/3448	0.46	0/4673
9	MN	0.20	0/3457	0.44	0/4685
9	MP	0.21	0/3457	0.44	0/4685
9	NB	0.17	0/3436	0.44	0/4656
9	ND	0.19	0/3457	0.46	0/4685
9	NF	0.28	0/3436	0.55	1/4656 (0.0%)
9	NH	0.23	0/3431	0.49	0/4649
9	NJ	0.27	0/3448	0.58	2/4673 (0.0%)
9	NL	0.26	0/3436	0.54	2/4656 (0.0%)
9	NN	0.22	0/3448	0.50	0/4673
9	NP	0.16	0/3431	0.42	1/4649 (0.0%)
9	OB	0.22	0/3436	0.49	0/4656
9	OD	0.19	0/3436	0.48	0/4656
9	OF	0.26	0/3443	0.52	0/4666
9	OH	0.27	1/3436 (0.0%)	0.53	1/4656 (0.0%)
9	OJ	0.28	0/3443	0.62	2/4666 (0.0%)
9	OL	0.22	0/3431	0.47	2/4649 (0.0%)
9	ON	0.21	0/3431	0.46	0/4649
9	OP	0.22	0/3423	0.52	2/4638 (0.0%)
9	PB	0.19	0/3436	0.44	0/4656
9	PD	0.24	0/3436	0.55	5/4656 (0.1%)
9	PF	0.18	0/3436	0.47	1/4656 (0.0%)
9	PH	0.22	0/3436	0.51	1/4656 (0.0%)
9	PJ	0.21	0/3431	0.50	1/4649 (0.0%)
9	PL	0.18	0/3436	0.46	2/4656 (0.0%)
9	PN	0.18	0/3436	0.44	0/4656
9	PP	0.15	0/3431	0.41	0/4649
9	QB	0.25	0/3423	0.51	0/4638
9	QD	0.19	0/3431	0.48	1/4649 (0.0%)
9	QF	0.18	0/3431	0.45	1/4649 (0.0%)
9	QH	0.23	0/3431	0.51	0/4649
9	QJ	0.20	0/3431	0.49	1/4649 (0.0%)
9	QL	0.16	0/3431	0.43	0/4649
9	QN	0.22	0/3431	0.49	2/4649 (0.0%)
9	QP	0.20	0/3423	0.47	0/4638
9	RD	0.16	0/3436	0.44	1/4656 (0.0%)
9	RF	0.15	0/3436	0.41	1/4656 (0.0%)
9	RH	0.16	0/3436	0.39	0/4656
9	RJ	0.19	0/3436	0.43	0/4656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	RL	0.22	0/3436	0.48	2/4656 (0.0%)
9	RN	0.16	0/3431	0.41	0/4649
9	RP	0.15	0/3436	0.40	0/4656
9	SB	0.16	0/3423	0.42	0/4638
9	SD	0.19	0/3436	0.43	0/4656
9	SF	0.21	0/3423	0.46	0/4638
9	SH	0.19	0/3431	0.45	1/4649 (0.0%)
9	SJ	0.20	0/3431	0.49	0/4649
9	SL	0.17	0/3423	0.45	0/4638
9	SN	0.16	0/3423	0.43	0/4638
9	TB	0.20	0/3423	0.46	0/4638
9	TD	0.22	1/3423 (0.0%)	0.50	2/4638 (0.0%)
9	TF	0.17	0/3423	0.43	1/4638 (0.0%)
9	TH	0.20	0/3431	0.47	3/4649 (0.1%)
9	TJ	0.19	0/3436	0.44	0/4656
9	TL	0.24	0/3431	0.47	1/4649 (0.0%)
9	TN	0.19	0/3423	0.45	1/4638 (0.0%)
9	UB	0.18	0/3423	0.49	1/4638 (0.0%)
9	UD	0.16	0/3423	0.39	0/4638
9	UF	0.18	0/3423	0.43	0/4638
9	UH	0.19	0/3431	0.44	0/4649
9	UJ	0.21	0/3431	0.46	0/4649
9	UL	0.17	0/3423	0.40	0/4638
9	UN	0.16	0/3423	0.44	2/4638 (0.0%)
9	VB	0.16	0/3423	0.37	0/4638
9	VD	0.15	0/3423	0.42	1/4638 (0.0%)
9	VF	0.20	0/3423	0.47	0/4638
9	VH	0.18	0/3431	0.48	0/4649
9	VJ	0.20	0/3431	0.51	1/4649 (0.0%)
9	VL	0.18	0/3436	0.44	2/4656 (0.0%)
9	VN	0.19	0/3423	0.53	1/4638 (0.0%)
9	WB	0.19	0/3431	0.45	0/4649
9	WD	0.16	0/3431	0.40	0/4649
9	WF	0.21	0/3448	0.49	3/4673 (0.1%)
9	WH	0.19	0/3436	0.43	0/4656
9	WJ	0.18	0/3436	0.47	0/4656
9	WL	0.19	0/3431	0.43	2/4649 (0.0%)
9	WN	0.19	0/3431	0.46	1/4649 (0.0%)
9	WP	0.20	0/3431	0.48	0/4649
10	B	0.24	0/2787	0.53	2/3696 (0.1%)
10	C	0.31	0/2427	0.59	0/3218
11	B0	0.33	0/340	0.76	1/457 (0.2%)
11	B1	0.28	0/3018	0.53	1/4069 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	B2	0.31	0/3440	0.53	1/4638 (0.0%)
11	B3	0.32	0/3440	0.52	1/4638 (0.0%)
11	B4	0.25	0/3451	0.47	2/4652 (0.0%)
11	B5	0.34	0/1691	0.71	4/2274 (0.2%)
11	R0	0.27	0/1625	0.49	0/2184
11	R1	0.23	0/3451	0.49	1/4652 (0.0%)
11	R2	0.27	0/3451	0.49	1/4652 (0.0%)
11	R3	0.29	0/3451	0.49	0/4652
11	R4	0.32	0/3059	0.60	4/4124 (0.1%)
11	R5	0.33	0/372	0.63	0/500
12	C0	0.27	0/1476	0.45	0/1991
12	C1	0.30	0/3399	0.44	0/4581
12	C2	0.27	0/3399	0.40	0/4581
12	C3	0.27	0/3376	0.41	0/4550
12	C4	0.25	0/2978	0.40	1/4010 (0.0%)
12	C5	0.30	0/422	0.76	3/567 (0.5%)
12	C6	0.25	0/364	0.53	0/493
12	S0	0.28	0/2719	0.54	0/3665
12	S1	0.20	0/3666	0.39	0/4944
12	S2	0.23	0/3666	0.43	0/4944
12	S3	0.31	0/3666	0.55	2/4944 (0.0%)
12	S4	0.27	0/2485	0.48	0/3344
12	S5	0.25	0/2610	0.48	1/3522 (0.0%)
12	S6	0.24	0/3504	0.43	0/4728
12	S7	0.30	0/3504	0.48	0/4728
12	S8	0.32	0/3485	0.53	0/4702
12	S9	0.33	0/2252	0.61	1/3028 (0.0%)
13	D	0.22	0/642	0.57	0/879
13	K3	0.23	0/1500	0.61	2/2037 (0.1%)
14	D0	0.26	0/906	0.50	0/1219
14	D1	0.29	0/3416	0.47	1/4598 (0.0%)
14	D2	0.29	0/3529	0.49	0/4752
14	D3	0.28	0/3529	0.46	0/4752
14	D4	0.27	0/3529	0.47	1/4752 (0.0%)
14	D5	0.47	0/720	0.94	4/965 (0.4%)
14	T0	0.40	0/976	0.79	1/1319 (0.1%)
14	T1	0.20	0/3645	0.46	0/4913
14	T2	0.33	1/3645 (0.0%)	0.58	4/4913 (0.1%)
14	T3	0.29	0/3658	0.49	0/4931
14	T4	0.31	0/3305	0.51	0/4450
14	T5	0.38	0/983	0.80	2/1319 (0.2%)
15	E	0.23	0/2415	0.48	0/3259
15	F	0.20	0/2406	0.49	0/3247

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	N2	0.20	0/2406	0.46	0/3247
16	G	0.24	0/747	0.61	0/1015
17	H	0.27	0/1356	0.57	1/1840 (0.1%)
17	I	0.23	0/1474	0.55	0/2000
17	J	0.23	0/1347	0.44	0/1829
17	K	0.23	0/1465	0.53	0/1989
17	L	0.24	0/1356	0.53	0/1840
17	M	0.23	0/1458	0.50	0/1979
17	N	0.28	0/1356	0.58	1/1840 (0.1%)
17	O7	0.30	0/1458	0.63	0/1979
17	O8	0.28	0/862	0.59	0/1170
17	O9	0.29	0/862	0.61	1/1170 (0.1%)
17	P8	0.33	0/862	0.61	0/1170
17	P9	0.28	0/862	0.66	1/1170 (0.1%)
17	Z2	0.21	0/424	0.48	0/571
17	Z3	0.22	0/424	0.50	0/571
17	Z4	0.21	0/424	0.49	0/571
17	Z5	0.29	0/416	0.60	0/560
18	I1	0.42	1/826 (0.1%)	0.78	3/1123 (0.3%)
19	J1	0.26	0/958	0.69	1/1287 (0.1%)
19	J2	0.30	0/2055	0.64	1/2772 (0.0%)
19	J3	0.26	0/2055	0.60	0/2772
19	J4	0.37	0/2037	0.68	2/2748 (0.1%)
19	J5	0.28	0/1021	0.66	0/1382
20	K1	0.26	0/1038	0.58	1/1407 (0.1%)
20	K2	0.27	0/1038	0.46	0/1407
21	L1	0.33	1/1063 (0.1%)	0.75	3/1435 (0.2%)
22	M1	0.23	0/849	0.52	0/1148
22	M2	0.27	0/849	0.57	0/1148
22	M3	0.26	0/1316	0.60	0/1778
22	M4	0.30	0/849	0.60	0/1148
23	O	0.24	0/635	0.56	0/846
23	P	0.26	0/2911	0.46	1/3896 (0.0%)
23	Q	0.29	0/868	0.65	4/1161 (0.3%)
24	O1	0.19	0/1366	0.46	0/1862
24	O2	0.21	0/1379	0.46	0/1880
24	O3	0.19	0/1379	0.44	0/1880
24	O4	0.23	0/1379	0.51	0/1880
25	O5	0.21	0/4158	0.50	1/5631 (0.0%)
25	O6	0.22	0/393	0.58	0/531
25	T	0.20	0/2429	0.49	0/3285
25	U	0.28	0/4253	0.56	1/5764 (0.0%)
25	V	0.25	0/4417	0.54	3/5988 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	P1	0.23	0/658	0.50	0/892
26	P2	0.30	0/852	0.66	0/1155
27	P3	0.47	0/1145	0.80	2/1564 (0.1%)
27	P4	0.31	0/1319	0.62	0/1799
27	P5	0.38	0/1319	0.65	0/1799
27	P6	0.41	0/1310	0.68	2/1787 (0.1%)
27	P7	0.25	0/460	0.70	0/621
28	Q1	0.29	0/1696	0.67	2/2315 (0.1%)
28	Q2	0.34	0/1696	0.67	3/2315 (0.1%)
28	Q3	0.29	0/1696	0.60	2/2315 (0.1%)
28	Q4	0.29	0/1696	0.65	1/2315 (0.0%)
28	Q5	0.59	0/158	0.90	1/213 (0.5%)
29	R	0.21	0/1674	0.47	1/2232 (0.0%)
29	S	0.25	0/2770	0.53	1/3701 (0.0%)
30	U0	0.24	0/2934	0.41	0/3946
30	U1	0.21	0/3444	0.43	0/4637
30	U2	0.21	0/3444	0.47	4/4637 (0.1%)
30	U3	0.26	0/3444	0.43	1/4637 (0.0%)
30	U4	0.26	0/1691	0.46	1/2271 (0.0%)
30	U5	0.28	0/2646	0.53	2/3557 (0.1%)
30	U6	0.19	0/3407	0.43	0/4586
30	U7	0.28	1/3407 (0.0%)	0.48	2/4586 (0.0%)
30	U8	0.30	0/3407	0.55	0/4586
30	U9	0.28	0/1499	0.54	0/2018
30	V0	0.36	1/1713 (0.1%)	0.75	3/2307 (0.1%)
30	V1	0.19	0/3226	0.45	1/4339 (0.0%)
30	V2	0.21	0/3226	0.52	2/4339 (0.0%)
30	V3	0.32	0/3226	0.62	2/4339 (0.0%)
30	V4	0.34	0/2357	0.56	0/3165
30	V5	0.29	0/2437	0.58	3/3274 (0.1%)
30	V6	0.27	0/3018	0.52	2/4057 (0.0%)
30	V7	0.36	0/2772	0.63	2/3729 (0.1%)
30	V8	0.28	0/2507	0.60	0/3371
30	V9	0.35	0/804	0.78	0/1080
30	W0	0.35	0/2473	0.66	3/3317 (0.1%)
30	W2	0.31	0/2484	0.56	2/3338 (0.1%)
30	W4	0.16	0/2697	0.40	0/3621
30	W5	0.21	0/2697	0.46	0/3621
30	W6	0.17	0/2697	0.39	0/3621
30	W7	0.24	0/2697	0.51	0/3621
31	W	0.24	0/6283	0.51	1/8495 (0.0%)
31	X	0.26	1/6283 (0.0%)	0.49	0/8495
31	Y	0.22	0/6291	0.52	5/8506 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	Z	0.23	0/6283	0.48	0/8495
32	X0	0.20	0/206	0.56	0/278
32	X1	0.25	0/198	0.58	0/266
32	X2	0.21	0/198	0.59	0/266
32	X3	0.17	0/206	0.52	0/278
33	X4	0.26	1/2694 (0.0%)	0.58	1/3661 (0.0%)
33	X5	0.26	0/1072	0.54	0/1454
34	X6	0.38	0/2144	0.61	1/2899 (0.0%)
34	X7	0.30	0/2144	0.60	0/2899
34	X8	0.22	0/2144	0.53	0/2899
35	XA	0.23	0/1573	0.49	0/2122
35	XB	0.20	0/1573	0.46	0/2122
35	XC	0.16	0/1573	0.38	0/2122
35	XD	0.17	0/1573	0.44	0/2122
35	XE	0.20	0/1573	0.42	0/2122
35	XF	0.22	0/1573	0.48	0/2122
35	XG	0.24	0/1573	0.49	0/2122
35	XH	0.20	0/1573	0.49	0/2122
36	Y0	0.31	0/503	0.69	0/688
36	Y1	0.38	0/1890	0.84	6/2576 (0.2%)
36	Y2	0.25	0/1767	0.58	0/2408
36	Y3	0.25	0/503	0.63	0/688
36	Y4	0.29	0/1458	0.76	3/1984 (0.2%)
36	Y5	0.35	0/663	0.67	0/903
37	YA	0.22	0/1817	0.55	0/2455
37	YB	0.23	0/1817	0.50	1/2455 (0.0%)
37	YC	0.18	0/1817	0.39	0/2455
37	YD	0.20	0/1817	0.43	0/2455
37	YE	0.24	0/1817	0.51	0/2455
37	YF	0.19	0/1817	0.49	2/2455 (0.1%)
37	YG	0.21	0/1817	0.53	0/2455
37	YH	0.22	0/1817	0.56	2/2455 (0.1%)
38	Z1	0.27	0/288	0.73	0/387
39	a	0.32	0/2512	0.69	2/3331 (0.1%)
39	a6	0.20	0/575	0.56	1/767 (0.1%)
39	b	0.34	0/2105	0.71	4/2785 (0.1%)
39	c	0.27	0/3549	0.63	0/4707
39	d	0.29	0/1162	0.55	0/1538
40	a1	0.18	0/1313	0.47	0/1779
40	a2	0.29	0/1313	0.57	0/1779
40	a3	0.23	0/1313	0.53	0/1779
40	a4	0.29	0/1313	0.65	2/1779 (0.1%)
41	b1	0.38	0/1095	0.72	0/1465

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	b2	0.37	2/3141 (0.1%)	0.58	3/4226 (0.1%)
41	b3	0.21	0/3152	0.45	0/4240
41	b4	0.31	0/3152	0.55	1/4240 (0.0%)
41	b5	0.31	0/2749	0.62	3/3697 (0.1%)
42	e	0.17	0/4786	0.44	1/6472 (0.0%)
42	f	0.20	0/4786	0.49	4/6472 (0.1%)
42	g	0.22	0/4786	0.51	1/6472 (0.0%)
43	h	0.25	0/2057	0.52	1/2757 (0.0%)
43	i	0.28	0/2042	0.54	1/2737 (0.0%)
43	j	0.24	0/2036	0.53	1/2729 (0.0%)
43	k	0.29	1/2042 (0.0%)	0.57	1/2737 (0.0%)
44	h1	0.29	0/809	0.67	0/1091
44	h2	0.32	0/831	0.60	0/1119
44	h3	0.35	0/831	0.66	0/1119
44	h4	0.24	0/820	0.64	0/1105
45	i1	0.19	0/937	0.46	0/1281
45	l	0.24	0/937	0.48	0/1281
45	m	0.19	0/937	0.43	0/1281
45	n	0.22	0/937	0.53	0/1281
46	i2	0.18	0/1526	0.46	0/2039
46	i3	0.23	0/1526	0.52	0/2039
46	i4	0.21	0/1526	0.49	0/2039
47	o	0.32	0/1707	0.72	6/2264 (0.3%)
47	p	0.31	0/3334	0.67	5/4428 (0.1%)
48	q	0.22	0/614	0.54	0/827
48	r	0.33	0/640	0.69	1/862 (0.1%)
48	s	0.22	0/640	0.50	0/862
49	y	0.27	0/942	0.64	1/1279 (0.1%)
All	All	0.23	23/1674605 (0.0%)	0.49	425/2267788 (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
2	2	0	2
3	3	0	1
4	5	0	1
4	j1	0	1
8	AM	0	1
8	CM	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	EE	0	1
8	FA	0	1
8	IE	0	1
8	JE	0	1
8	JM	0	1
8	NG	0	1
8	VE	0	1
8	VM	0	1
8	WI	0	1
9	AJ	0	1
9	AL	0	1
9	BD	0	1
9	HN	0	1
9	IB	0	1
9	JF	0	1
9	LF	0	1
9	LH	0	1
9	NL	0	1
9	NN	0	1
9	OF	0	1
9	PF	0	1
11	B5	0	1
12	S0	0	1
12	S3	0	1
12	S5	0	1
12	S6	0	1
12	S9	0	1
14	D3	0	1
14	T2	0	1
17	O8	0	1
22	M1	0	1
24	O3	0	1
25	O5	0	1
28	Q1	0	1
28	Q2	0	1
28	Q3	0	1
28	Q4	0	1
28	Q5	0	1
30	U3	0	1
30	U8	0	1
31	Z	0	1
35	XF	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
36	Y5	0	1
40	a4	0	1
46	i3	0	1
All	All	0	52

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	LE	175	PRO	CG-CD	-8.11	1.23	1.50
18	I1	87	PRO	CG-CD	-7.92	1.23	1.50
30	V0	403	PRO	CG-CD	-7.00	1.26	1.50
9	IL	32	PRO	CG-CD	-6.84	1.27	1.50
41	b2	270	PRO	CA-C	-6.50	1.48	1.51

The worst 5 of 425 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	V0	403	PRO	CA-N-CD	-13.52	93.07	112.00
28	Q1	158	ALA	O-C-N	-13.37	107.98	123.22
18	I1	87	PRO	CA-N-CD	-13.02	93.77	112.00
9	IP	171	PRO	CA-N-CD	-12.92	93.91	112.00
9	TD	80	PRO	CA-N-CD	-12.88	93.97	112.00

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	277	ARG	Sidechain
2	2	503	ARG	Sidechain
3	3	339	GLN	Mainchain
4	5	62	ARG	Sidechain
9	AJ	262	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	670	0	664	37	0
1	7	1174	0	1127	52	0
2	1	3738	0	3656	105	0
2	2	2160	0	2156	101	0
3	3	4023	0	4087	150	0
3	4	1230	0	1250	36	0
4	5	2975	0	2950	82	0
4	6	2975	0	2950	86	0
4	j1	2975	0	2950	110	0
5	8	1470	0	1442	43	0
6	A	806	0	806	28	0
6	N1	806	0	806	37	0
7	A0	444	0	449	18	0
7	A1	2935	0	2976	62	0
7	A2	3288	0	3322	63	0
7	A3	3288	0	3322	59	0
7	A4	3274	0	3304	46	0
7	A5	1400	0	1386	39	0
8	AA	3424	0	3339	83	0
8	AC	3424	0	3339	85	0
8	AE	3431	0	3348	104	0
8	AG	3440	0	3354	91	0
8	AI	3431	0	3348	76	0
8	AK	3418	0	3334	97	0
8	AM	3431	0	3348	98	0
8	AO	3431	0	3348	108	0
8	BC	3374	0	3289	82	0
8	BE	3440	0	3354	106	0
8	BG	3396	0	3309	83	0
8	BI	3440	0	3354	81	0
8	BK	3390	0	3304	87	0
8	BM	3424	0	3339	96	0
8	BO	3396	0	3309	91	0
8	CC	3424	0	3339	100	0
8	CE	3424	0	3339	88	0
8	CG	3424	0	3339	87	0
8	CI	3424	0	3339	83	0
8	CK	3424	0	3339	76	0
8	CM	3431	0	3348	115	0
8	CO	3424	0	3339	89	0
8	CQ	3410	0	3330	92	0
8	DC	3382	0	3300	125	0
8	DE	3366	0	3285	72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	DG	3366	0	3285	78	0
8	DI	3374	0	3296	81	0
8	DK	3373	0	3294	73	0
8	DM	3380	0	3294	77	0
8	DO	3372	0	3290	75	0
8	DQ	3360	0	3280	87	0
8	EA	3424	0	3339	83	0
8	EC	3418	0	3334	97	0
8	EE	3424	0	3339	81	0
8	EG	3424	0	3339	81	0
8	EI	3424	0	3339	86	0
8	EK	3424	0	3339	77	0
8	EM	3424	0	3339	95	0
8	EO	3410	0	3330	98	0
8	FA	3366	0	3285	120	0
8	FC	3366	0	3285	97	0
8	FE	3366	0	3285	97	0
8	FG	3351	0	3274	85	0
8	FI	3366	0	3285	105	0
8	FK	3373	0	3294	97	0
8	FM	3366	0	3285	94	0
8	FO	3355	0	3273	102	0
8	GA	3368	0	3284	99	0
8	GC	3373	0	3294	109	0
8	GE	3373	0	3294	118	0
8	GG	3431	0	3348	145	0
8	GI	3387	0	3303	106	0
8	GK	3387	0	3303	110	0
8	GM	3395	0	3307	134	0
8	GO	3395	0	3307	89	0
8	HA	3371	0	3295	98	0
8	HC	3389	0	3304	134	0
8	HE	3431	0	3348	107	0
8	HG	3431	0	3348	117	0
8	HI	3431	0	3348	91	0
8	HK	3366	0	3285	125	0
8	HM	3389	0	3304	122	0
8	HO	3381	0	3298	123	0
8	IA	3380	0	3294	126	0
8	IC	3431	0	3348	144	0
8	IE	3440	0	3354	142	0
8	IG	3387	0	3303	149	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	II	3399	0	3310	122	0
8	IK	3411	0	3327	158	0
8	IM	3391	0	3306	111	0
8	IO	3431	0	3348	147	0
8	JC	3388	0	3300	114	0
8	JE	3424	0	3339	146	0
8	JG	3360	0	3279	93	0
8	JI	3390	0	3304	131	0
8	JK	3381	0	3298	97	0
8	JM	3366	0	3285	98	0
8	JO	3379	0	3299	128	0
8	JQ	3403	0	3323	112	0
8	KA	3380	0	3294	98	0
8	KC	3389	0	3307	94	0
8	KE	3397	0	3311	113	0
8	KG	3380	0	3294	100	0
8	KI	3374	0	3289	103	0
8	KK	3372	0	3290	97	0
8	KM	3380	0	3294	118	0
8	KO	3389	0	3307	99	0
8	LA	3396	0	3309	102	0
8	LC	3374	0	3289	93	0
8	LE	3388	0	3305	84	0
8	LG	3440	0	3354	91	0
8	LI	3440	0	3354	75	0
8	LK	3440	0	3354	98	0
8	LM	3404	0	3313	97	0
8	LO	3366	0	3285	120	0
8	MA	3374	0	3289	73	0
8	MC	3374	0	3289	68	0
8	ME	3424	0	3339	76	0
8	MG	3380	0	3294	96	0
8	MI	3378	0	3292	79	0
8	MK	3390	0	3304	93	0
8	MM	3380	0	3294	98	0
8	MO	3352	0	3276	116	0
8	NA	3353	0	3271	97	0
8	NC	3352	0	3276	99	0
8	NE	3394	0	3307	108	0
8	NG	3382	0	3300	134	0
8	NI	3373	0	3294	104	0
8	NK	3373	0	3294	148	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	NM	3382	0	3300	170	0
8	NO	3382	0	3300	115	0
8	OA	3374	0	3289	95	0
8	OC	3366	0	3285	107	0
8	OE	3372	0	3290	96	0
8	OG	3366	0	3285	108	0
8	OI	3360	0	3280	100	0
8	OK	3374	0	3289	123	0
8	OM	3352	0	3276	109	0
8	OO	3330	0	3251	114	0
8	PC	3352	0	3276	103	0
8	PE	3330	0	3254	90	0
8	PG	3366	0	3285	94	0
8	PI	3366	0	3285	110	0
8	PK	3367	0	3282	109	0
8	PM	3380	0	3294	112	0
8	PO	3366	0	3285	100	0
8	QC	3352	0	3276	103	0
8	QE	3366	0	3285	104	0
8	QG	3352	0	3276	100	0
8	QI	3345	0	3269	119	0
8	QK	3345	0	3267	86	0
8	QM	3338	0	3260	117	0
8	QO	3345	0	3266	100	0
8	RC	3352	0	3276	89	0
8	RE	3353	0	3273	96	0
8	RG	3352	0	3276	105	0
8	RI	3360	0	3280	93	0
8	RK	3368	0	3283	101	0
8	RM	3361	0	3277	112	0
8	RO	3353	0	3273	101	0
8	SA	3359	0	3276	80	0
8	SC	3352	0	3276	105	0
8	SE	3352	0	3276	114	0
8	SG	3345	0	3267	103	0
8	SI	3360	0	3280	105	0
8	SK	3345	0	3267	98	0
8	SM	3333	0	3260	97	0
8	TA	3342	0	3259	92	0
8	TC	3337	0	3263	126	0
8	TE	3357	0	3274	95	0
8	TG	3341	0	3264	90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	TI	3349	0	3268	100	0
8	TK	3352	0	3276	87	0
8	TM	3341	0	3264	104	0
8	UA	3327	0	3248	97	0
8	UC	3351	0	3272	99	0
8	UE	3351	0	3272	112	0
8	UG	3353	0	3271	70	0
8	UI	3352	0	3276	81	0
8	UK	3353	0	3271	91	0
8	UM	3359	0	3276	103	0
8	UO	3347	0	3269	99	0
8	VA	3345	0	3267	83	0
8	VC	3410	0	3330	81	0
8	VE	3358	0	3281	116	0
8	VG	3410	0	3330	121	0
8	VI	3360	0	3280	122	0
8	VK	3418	0	3334	105	0
8	VM	3359	0	3278	102	0
8	VO	3403	0	3321	93	0
8	WA	3403	0	3321	103	0
8	WC	3424	0	3339	93	0
8	WE	3382	0	3295	104	0
8	WG	3418	0	3334	92	0
8	WI	3424	0	3339	85	0
8	WK	3418	0	3334	97	0
8	WM	3374	0	3289	86	0
8	WO	3358	0	3281	91	0
9	AB	3391	0	3269	103	0
9	AD	3413	0	3284	109	0
9	AF	3373	0	3257	103	0
9	AH	3404	0	3276	76	0
9	AJ	3404	0	3278	91	0
9	AL	3404	0	3276	102	0
9	AN	3404	0	3278	111	0
9	AP	3391	0	3269	92	0
9	BB	3361	0	3245	92	0
9	BD	3373	0	3257	67	0
9	BF	3368	0	3251	93	0
9	BH	3373	0	3257	81	0
9	BJ	3382	0	3263	82	0
9	BL	3373	0	3257	90	0
9	BN	3373	0	3257	89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	BP	3373	0	3257	90	0
9	CB	3356	0	3240	108	0
9	CD	3382	0	3263	101	0
9	CF	3382	0	3263	68	0
9	CH	3382	0	3263	67	0
9	CJ	3361	0	3245	58	0
9	CL	3368	0	3252	98	0
9	CN	3382	0	3263	104	0
9	CP	3373	0	3257	79	0
9	DB	3368	0	3252	96	0
9	DD	3368	0	3252	86	0
9	DF	3373	0	3257	73	0
9	DH	3373	0	3257	66	0
9	DJ	3373	0	3257	64	0
9	DL	3382	0	3263	83	0
9	DN	3361	0	3245	70	0
9	DP	3373	0	3257	73	0
9	EB	3361	0	3245	101	0
9	ED	3361	0	3245	87	0
9	EF	3361	0	3245	89	0
9	EH	3361	0	3245	85	0
9	EJ	3356	0	3240	84	0
9	EL	3361	0	3243	89	0
9	EN	3361	0	3245	99	0
9	FB	3373	0	3257	116	0
9	FD	3373	0	3257	81	0
9	FF	3373	0	3257	77	0
9	FH	3373	0	3257	94	0
9	FJ	3368	0	3252	100	0
9	FL	3368	0	3252	89	0
9	FN	3373	0	3257	121	0
9	GB	3356	0	3240	122	0
9	GD	3373	0	3257	115	0
9	GF	3373	0	3257	110	0
9	GH	3382	0	3263	99	0
9	GJ	3373	0	3257	94	0
9	GL	3382	0	3263	119	0
9	GN	3382	0	3263	101	0
9	HB	3373	0	3257	126	0
9	HD	3356	0	3240	142	0
9	HF	3373	0	3257	99	0
9	HH	3382	0	3263	106	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	HJ	3373	0	3257	127	0
9	HL	3382	0	3263	128	0
9	HN	3373	0	3256	111	0
9	HP	3356	0	3240	90	0
9	IB	3373	0	3257	144	0
9	ID	3373	0	3257	134	0
9	IF	3373	0	3257	123	0
9	IH	3382	0	3263	147	0
9	IJ	3368	0	3252	114	0
9	IL	3382	0	3262	134	0
9	IN	3382	0	3263	126	0
9	IP	3382	0	3263	140	0
9	JB	3356	0	3240	100	0
9	JD	3356	0	3240	144	0
9	JF	3356	0	3240	126	0
9	JH	3356	0	3240	121	0
9	JJ	3356	0	3240	117	0
9	JL	3356	0	3240	123	0
9	JN	3348	0	3236	113	0
9	JP	3356	0	3240	104	0
9	KB	3373	0	3257	93	0
9	KD	3382	0	3263	116	0
9	KF	3382	0	3263	82	0
9	KH	3382	0	3263	116	0
9	KJ	3373	0	3257	93	0
9	KL	3373	0	3257	107	0
9	KN	3373	0	3257	130	0
9	KP	3361	0	3245	115	0
9	LB	3433	0	3299	106	0
9	LD	3382	0	3263	95	0
9	LF	3451	0	3311	92	0
9	LH	3382	0	3263	81	0
9	LJ	3433	0	3299	92	0
9	LL	3361	0	3245	102	0
9	LN	3391	0	3269	99	0
9	LP	3368	0	3252	77	0
9	MB	3382	0	3263	77	0
9	MD	3382	0	3263	94	0
9	MF	3356	0	3240	74	0
9	MH	3382	0	3263	95	0
9	MJ	3373	0	3257	61	0
9	ML	3373	0	3257	104	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	MN	3382	0	3261	80	0
9	MP	3382	0	3263	101	0
9	NB	3361	0	3245	111	0
9	ND	3382	0	3263	101	0
9	NF	3361	0	3245	139	0
9	NH	3356	0	3240	116	0
9	NJ	3373	0	3257	154	0
9	NL	3361	0	3245	137	0
9	NN	3373	0	3257	130	0
9	NP	3356	0	3240	91	0
9	OB	3361	0	3245	138	0
9	OD	3361	0	3245	134	0
9	OF	3368	0	3252	128	0
9	OH	3361	0	3245	129	0
9	OJ	3368	0	3252	138	0
9	OL	3356	0	3240	140	0
9	ON	3356	0	3240	112	0
9	OP	3348	0	3236	114	0
9	PB	3361	0	3245	80	0
9	PD	3361	0	3245	127	0
9	PF	3361	0	3245	105	0
9	PH	3361	0	3245	94	0
9	PJ	3356	0	3240	109	0
9	PL	3361	0	3245	99	0
9	PN	3361	0	3245	93	0
9	PP	3356	0	3240	70	0
9	QB	3348	0	3236	112	0
9	QD	3356	0	3240	103	0
9	QF	3356	0	3240	103	0
9	QH	3356	0	3240	126	0
9	QJ	3356	0	3240	109	0
9	QL	3356	0	3240	94	0
9	QN	3356	0	3240	111	0
9	QP	3348	0	3236	95	0
9	RD	3361	0	3245	99	0
9	RF	3361	0	3245	91	0
9	RH	3361	0	3245	99	0
9	RJ	3361	0	3245	105	0
9	RL	3361	0	3243	91	0
9	RN	3356	0	3240	84	0
9	RP	3361	0	3245	64	0
9	SB	3348	0	3236	97	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	SD	3361	0	3245	103	0
9	SF	3348	0	3236	117	0
9	SH	3356	0	3240	113	0
9	SJ	3356	0	3240	109	0
9	SL	3348	0	3236	99	0
9	SN	3348	0	3236	97	0
9	TB	3348	0	3236	99	0
9	TD	3348	0	3236	92	0
9	TF	3348	0	3236	94	0
9	TH	3356	0	3240	105	0
9	TJ	3361	0	3245	110	0
9	TL	3356	0	3240	105	0
9	TN	3348	0	3236	95	0
9	UB	3348	0	3236	112	0
9	UD	3348	0	3236	95	0
9	UF	3348	0	3236	94	0
9	UH	3356	0	3240	98	0
9	UJ	3356	0	3240	97	0
9	UL	3348	0	3236	101	0
9	UN	3348	0	3236	97	0
9	VB	3348	0	3236	95	0
9	VD	3348	0	3236	85	0
9	VF	3348	0	3236	106	0
9	VH	3356	0	3240	130	0
9	VJ	3356	0	3240	105	0
9	VL	3361	0	3245	99	0
9	VN	3348	0	3236	108	0
9	WB	3356	0	3240	96	0
9	WD	3356	0	3240	86	0
9	WF	3373	0	3257	93	0
9	WH	3361	0	3245	90	0
9	WJ	3361	0	3245	84	0
9	WL	3356	0	3240	92	0
9	WN	3356	0	3240	92	0
9	WP	3356	0	3240	85	0
10	B	2769	0	2797	72	0
10	C	2408	0	2452	83	0
11	B0	334	0	319	22	0
11	B1	2984	0	2999	77	0
11	B2	3401	0	3418	79	0
11	B3	3401	0	3418	89	0
11	B4	3412	0	3431	84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B5	1675	0	1700	70	0
11	R0	1612	0	1644	61	0
11	R1	3412	0	3431	112	0
11	R2	3412	0	3431	83	0
11	R3	3412	0	3431	99	0
11	R4	3025	0	3041	133	0
11	R5	366	0	359	11	0
12	C0	1453	0	1391	38	0
12	C1	3354	0	3326	93	0
12	C2	3354	0	3326	58	0
12	C3	3332	0	3309	63	0
12	C4	2944	0	2939	70	0
12	C5	420	0	433	24	0
12	C6	354	0	339	15	0
12	S0	2675	0	2601	77	0
12	S1	3613	0	3573	94	0
12	S2	3613	0	3573	104	0
12	S3	3613	0	3573	117	0
12	S4	2459	0	2464	90	0
12	S5	2568	0	2499	70	0
12	S6	3453	0	3416	102	0
12	S7	3453	0	3416	92	0
12	S8	3435	0	3400	119	0
12	S9	2232	0	2247	111	0
13	D	622	0	603	10	0
13	K3	1460	0	1417	38	0
14	D0	889	0	824	28	0
14	D1	3370	0	3310	76	0
14	D2	3480	0	3416	81	0
14	D3	3480	0	3416	87	0
14	D4	3480	0	3416	84	0
14	D5	715	0	731	34	0
14	T0	957	0	898	51	0
14	T1	3594	0	3541	128	0
14	T2	3594	0	3541	118	0
14	T3	3606	0	3550	87	0
14	T4	3260	0	3205	104	0
14	T5	975	0	991	63	0
15	E	2372	0	2363	54	0
15	F	2363	0	2355	57	0
15	N2	2363	0	2355	59	0
16	G	724	0	695	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	H	1316	0	1274	39	0
17	I	1429	0	1382	47	0
17	J	1307	0	1261	25	0
17	K	1420	0	1369	29	0
17	L	1316	0	1274	43	0
17	M	1413	0	1362	38	0
17	N	1316	0	1274	38	0
17	O7	1413	0	1362	56	0
17	O8	837	0	822	42	0
17	O9	837	0	822	36	0
17	P8	837	0	822	32	0
17	P9	837	0	822	42	0
17	Z2	412	0	396	7	0
17	Z3	412	0	396	9	0
17	Z4	412	0	396	13	0
17	Z5	405	0	388	14	0
18	I1	796	0	744	37	0
19	J1	934	0	955	41	0
19	J2	2010	0	2037	72	0
19	J3	2010	0	2037	85	0
19	J4	1992	0	2023	110	0
19	J5	1001	0	1008	53	0
20	K1	1009	0	983	37	0
20	K2	1009	0	983	26	0
21	L1	1034	0	1013	40	0
22	M1	826	0	826	28	0
22	M2	826	0	826	20	0
22	M3	1280	0	1265	41	0
22	M4	826	0	826	33	0
23	O	627	0	622	21	0
23	P	2875	0	2819	77	0
23	Q	858	0	833	22	0
24	O1	1332	0	1310	22	0
24	O2	1344	0	1319	29	0
24	O3	1344	0	1319	19	0
24	O4	1344	0	1319	30	0
25	O5	4047	0	3978	99	0
25	O6	383	0	370	21	0
25	T	2365	0	2316	78	0
25	U	4138	0	4066	133	0
25	V	4299	0	4232	135	0
26	P1	637	0	620	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P2	825	0	805	53	0
27	P3	1103	0	1068	89	0
27	P4	1272	0	1218	42	0
27	P5	1272	0	1218	50	0
27	P6	1263	0	1212	69	0
27	P7	447	0	424	18	0
28	Q1	1634	0	1575	55	0
28	Q2	1634	0	1575	63	0
28	Q3	1634	0	1575	45	0
28	Q4	1634	0	1575	57	0
28	Q5	152	0	145	15	0
29	R	1648	0	1612	40	0
29	S	2728	0	2675	61	0
30	U0	2897	0	2904	71	0
30	U1	3396	0	3406	97	0
30	U2	3396	0	3406	76	0
30	U3	3396	0	3406	76	0
30	U4	1664	0	1622	43	0
30	U5	2607	0	2570	72	0
30	U6	3360	0	3375	90	0
30	U7	3360	0	3375	109	0
30	U8	3360	0	3375	115	0
30	U9	1486	0	1552	50	0
30	V0	1695	0	1747	51	0
30	V1	3185	0	3186	101	0
30	V2	3185	0	3186	96	0
30	V3	3185	0	3186	105	0
30	V4	2325	0	2271	76	0
30	V5	2408	0	2410	66	0
30	V6	2980	0	2973	71	0
30	V7	2736	0	2753	118	0
30	V8	2477	0	2481	57	0
30	V9	800	0	847	28	0
30	W0	2447	0	2477	118	0
30	W2	2458	0	2495	71	0
30	W4	2662	0	2677	46	0
30	W5	2662	0	2677	57	0
30	W6	2662	0	2677	30	0
30	W7	2662	0	2677	64	0
31	W	6116	0	5999	162	0
31	X	6116	0	5999	119	0
31	Y	6124	0	6005	145	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Z	6116	0	5999	132	0
32	X0	200	0	179	4	0
32	X1	192	0	169	3	0
32	X2	192	0	169	3	0
32	X3	200	0	179	7	0
33	X4	2619	0	2523	86	0
33	X5	1041	0	1024	47	0
34	X6	2097	0	2128	74	0
34	X7	2097	0	2129	61	0
34	X8	2097	0	2129	80	0
35	XA	1540	0	1570	37	0
35	XB	1540	0	1570	58	0
35	XC	1540	0	1570	47	0
35	XD	1540	0	1570	42	0
35	XE	1540	0	1570	40	0
35	XF	1540	0	1570	49	0
35	XG	1540	0	1570	45	0
35	XH	1540	0	1570	51	0
36	Y0	483	0	492	38	0
36	Y1	1828	0	1862	129	0
36	Y2	1711	0	1742	80	0
36	Y3	483	0	492	29	0
36	Y4	1412	0	1431	104	0
36	Y5	644	0	651	50	0
37	YA	1775	0	1793	43	0
37	YB	1775	0	1793	51	0
37	YC	1775	0	1793	33	0
37	YD	1775	0	1793	30	0
37	YE	1775	0	1793	34	0
37	YF	1775	0	1793	31	0
37	YG	1775	0	1793	40	0
37	YH	1775	0	1793	49	0
38	Z1	279	0	266	14	0
39	a	2499	0	2559	134	0
39	a6	572	0	613	22	0
39	b	2092	0	2130	94	0
39	c	3528	0	3595	144	0
39	d	1155	0	1184	48	0
40	a1	1277	0	1271	36	0
40	a2	1277	0	1271	49	0
40	a3	1277	0	1271	45	0
40	a4	1277	0	1271	55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	b1	1081	0	1130	45	0
41	b2	3091	0	3189	94	0
41	b3	3102	0	3202	81	0
41	b4	3102	0	3202	117	0
41	b5	2705	0	2771	72	0
42	e	4689	0	4669	141	0
42	f	4689	0	4669	162	0
42	g	4689	0	4669	153	0
43	h	2014	0	2098	40	0
43	i	1999	0	2087	70	0
43	j	1993	0	2082	54	0
43	k	1999	0	2087	83	0
44	h1	787	0	790	37	0
44	h2	809	0	816	34	0
44	h3	809	0	816	43	0
44	h4	798	0	803	36	0
45	i1	909	0	908	32	0
45	l	909	0	908	31	0
45	m	909	0	908	30	0
45	n	909	0	908	33	0
46	i2	1500	0	1519	51	0
46	i3	1500	0	1519	54	0
46	i4	1500	0	1519	48	0
47	o	1688	0	1717	59	0
47	p	3300	0	3358	106	0
48	q	599	0	579	20	0
48	r	625	0	610	23	0
48	s	625	0	610	28	0
49	y	911	0	857	45	0
50	AA	32	0	12	0	0
50	AC	32	0	12	1	0
50	AE	32	0	12	1	0
50	AG	32	0	12	0	0
50	AI	32	0	12	0	0
50	AK	32	0	12	0	0
50	AM	32	0	12	0	0
50	AO	32	0	12	0	0
50	BC	32	0	12	1	0
50	BE	32	0	12	0	0
50	BG	32	0	12	0	0
50	BI	32	0	12	0	0
50	BK	32	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BM	32	0	12	0	0
50	BO	32	0	12	0	0
50	CC	32	0	12	0	0
50	CE	32	0	12	0	0
50	CG	32	0	12	1	0
50	CI	32	0	12	3	0
50	CK	32	0	12	2	0
50	CM	32	0	12	1	0
50	CO	32	0	12	1	0
50	CQ	32	0	12	0	0
50	DC	32	0	12	0	0
50	DE	32	0	12	1	0
50	DG	32	0	12	0	0
50	DI	32	0	12	0	0
50	DK	32	0	12	2	0
50	DM	32	0	12	1	0
50	DO	32	0	12	1	0
50	DQ	32	0	12	2	0
50	EA	32	0	12	1	0
50	EC	32	0	12	0	0
50	EE	32	0	12	1	0
50	EG	32	0	12	1	0
50	EI	32	0	12	1	0
50	EK	32	0	12	1	0
50	EM	32	0	12	0	0
50	EO	32	0	12	0	0
50	FA	32	0	12	0	0
50	FC	32	0	12	1	0
50	FE	32	0	12	1	0
50	FG	32	0	12	0	0
50	FI	32	0	12	1	0
50	FK	32	0	12	1	0
50	FM	32	0	12	1	0
50	FO	32	0	12	1	0
50	GA	32	0	12	0	0
50	GC	32	0	12	0	0
50	GE	32	0	12	0	0
50	GG	32	0	12	1	0
50	GI	32	0	12	1	0
50	GK	32	0	12	0	0
50	GM	32	0	12	2	0
50	GO	32	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	HA	32	0	12	1	0
50	HC	32	0	12	1	0
50	HE	32	0	12	2	0
50	HG	32	0	12	1	0
50	HI	32	0	12	1	0
50	HK	32	0	12	0	0
50	HM	32	0	12	0	0
50	HO	32	0	12	1	0
50	IA	32	0	12	0	0
50	IC	32	0	12	0	0
50	IE	32	0	12	1	0
50	IG	32	0	12	1	0
50	II	32	0	12	3	0
50	IK	32	0	12	0	0
50	IM	32	0	12	0	0
50	IO	32	0	12	1	0
50	JC	32	0	12	0	0
50	JE	32	0	12	0	0
50	JG	32	0	12	0	0
50	JI	32	0	12	3	0
50	JK	32	0	12	1	0
50	JM	32	0	12	0	0
50	JO	32	0	12	2	0
50	JQ	32	0	12	1	0
50	KA	32	0	12	1	0
50	KC	32	0	12	4	0
50	KE	32	0	12	0	0
50	KG	32	0	12	3	0
50	KI	32	0	12	0	0
50	KK	32	0	12	1	0
50	KM	32	0	12	1	0
50	KO	32	0	12	0	0
50	LA	32	0	12	0	0
50	LC	32	0	12	0	0
50	LE	32	0	12	1	0
50	LG	32	0	12	0	0
50	LI	32	0	12	2	0
50	LK	32	0	12	1	0
50	LM	32	0	12	1	0
50	LO	32	0	12	1	0
50	MA	32	0	12	0	0
50	MC	32	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	ME	32	0	12	0	0
50	MG	32	0	12	0	0
50	MI	32	0	12	1	0
50	MK	32	0	12	1	0
50	MM	32	0	12	1	0
50	MO	32	0	12	1	0
50	NA	32	0	12	0	0
50	NC	32	0	12	1	0
50	NE	32	0	12	2	0
50	NG	32	0	12	1	0
50	NI	32	0	12	1	0
50	NK	32	0	12	0	0
50	NM	32	0	12	3	0
50	NO	32	0	12	1	0
50	OA	32	0	12	0	0
50	OC	32	0	12	1	0
50	OE	32	0	12	0	0
50	OG	32	0	12	0	0
50	OI	32	0	12	1	0
50	OK	32	0	12	0	0
50	OM	32	0	12	1	0
50	OO	32	0	12	1	0
50	PC	32	0	12	0	0
50	PE	32	0	12	0	0
50	PG	32	0	12	3	0
50	PI	32	0	12	1	0
50	PK	32	0	12	0	0
50	PM	32	0	12	0	0
50	PO	32	0	12	0	0
50	QC	32	0	12	2	0
50	QE	32	0	12	1	0
50	QG	32	0	12	2	0
50	QI	32	0	12	3	0
50	QK	32	0	12	2	0
50	QM	32	0	12	2	0
50	QO	32	0	12	6	0
50	RC	32	0	12	0	0
50	RE	32	0	12	2	0
50	RG	32	0	12	1	0
50	RI	32	0	12	3	0
50	RK	32	0	12	2	0
50	RM	32	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	RO	32	0	12	0	0
50	SA	32	0	12	0	0
50	SC	32	0	12	0	0
50	SE	32	0	12	2	0
50	SG	32	0	12	1	0
50	SI	32	0	12	0	0
50	SK	32	0	12	1	0
50	SM	32	0	12	2	0
50	TA	32	0	12	0	0
50	TC	32	0	12	2	0
50	TE	32	0	12	1	0
50	TG	32	0	12	1	0
50	TI	32	0	12	1	0
50	TK	32	0	12	2	0
50	TM	32	0	12	1	0
50	UA	32	0	12	0	0
50	UC	32	0	12	2	0
50	UE	32	0	12	1	0
50	UG	32	0	12	1	0
50	UI	32	0	12	0	0
50	UK	32	0	12	2	0
50	UM	32	0	12	1	0
50	UO	32	0	12	1	0
50	VA	32	0	12	0	0
50	VC	32	0	12	0	0
50	VE	32	0	12	0	0
50	VG	32	0	12	1	0
50	VI	32	0	12	0	0
50	VK	32	0	12	1	0
50	VM	32	0	12	0	0
50	VO	32	0	12	1	0
50	WA	32	0	12	1	0
50	WC	32	0	12	1	0
50	WE	32	0	12	0	0
50	WG	32	0	12	1	0
50	WI	32	0	12	2	0
50	WK	32	0	12	0	0
50	WM	32	0	12	1	0
50	WO	32	0	12	2	0
51	AA	1	0	0	0	0
51	AC	1	0	0	0	0
51	AE	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	AG	1	0	0	0	0
51	AI	1	0	0	0	0
51	AK	1	0	0	0	0
51	AM	1	0	0	0	0
51	AO	1	0	0	0	0
51	BC	1	0	0	0	0
51	BE	1	0	0	0	0
51	BG	1	0	0	0	0
51	BI	1	0	0	0	0
51	BK	1	0	0	0	0
51	BM	1	0	0	0	0
51	BO	1	0	0	0	0
51	CC	1	0	0	0	0
51	CE	1	0	0	0	0
51	CG	1	0	0	0	0
51	CI	1	0	0	0	0
51	CK	1	0	0	0	0
51	CM	1	0	0	0	0
51	CO	1	0	0	0	0
51	CQ	1	0	0	0	0
51	DC	1	0	0	0	0
51	DE	1	0	0	0	0
51	DG	1	0	0	0	0
51	DI	1	0	0	0	0
51	DK	1	0	0	0	0
51	DM	1	0	0	0	0
51	DO	1	0	0	0	0
51	DQ	1	0	0	0	0
51	EA	1	0	0	0	0
51	EC	1	0	0	0	0
51	EE	1	0	0	0	0
51	EG	1	0	0	0	0
51	EI	1	0	0	0	0
51	EK	1	0	0	0	0
51	EM	1	0	0	0	0
51	EO	1	0	0	0	0
51	FA	1	0	0	0	0
51	FC	1	0	0	0	0
51	FE	1	0	0	0	0
51	FG	1	0	0	0	0
51	FI	1	0	0	0	0
51	FK	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	FM	1	0	0	0	0
51	FO	1	0	0	0	0
51	GA	1	0	0	0	0
51	GC	1	0	0	0	0
51	GE	1	0	0	0	0
51	GG	1	0	0	0	0
51	GI	1	0	0	0	0
51	GK	1	0	0	0	0
51	GM	1	0	0	0	0
51	GO	1	0	0	0	0
51	HA	1	0	0	0	0
51	HC	1	0	0	0	0
51	HE	1	0	0	0	0
51	HG	1	0	0	0	0
51	HI	1	0	0	0	0
51	HK	1	0	0	0	0
51	HM	1	0	0	0	0
51	HO	1	0	0	0	0
51	IA	1	0	0	0	0
51	IC	1	0	0	0	0
51	IE	1	0	0	0	0
51	IG	1	0	0	0	0
51	II	1	0	0	0	0
51	IK	1	0	0	0	0
51	IM	1	0	0	0	0
51	IO	1	0	0	0	0
51	JC	1	0	0	0	0
51	JE	1	0	0	0	0
51	JG	1	0	0	0	0
51	JI	1	0	0	0	0
51	JK	1	0	0	0	0
51	JM	1	0	0	0	0
51	JO	1	0	0	0	0
51	JQ	1	0	0	0	0
51	KA	1	0	0	0	0
51	KC	1	0	0	0	0
51	KE	1	0	0	0	0
51	KG	1	0	0	0	0
51	KI	1	0	0	0	0
51	KK	1	0	0	0	0
51	KM	1	0	0	0	0
51	KO	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	LA	1	0	0	0	0
51	LC	1	0	0	0	0
51	LE	1	0	0	0	0
51	LG	1	0	0	0	0
51	LI	1	0	0	0	0
51	LK	1	0	0	0	0
51	LM	1	0	0	0	0
51	LO	1	0	0	0	0
51	MA	1	0	0	0	0
51	MC	1	0	0	0	0
51	ME	1	0	0	0	0
51	MG	1	0	0	0	0
51	MI	1	0	0	0	0
51	MK	1	0	0	0	0
51	MM	1	0	0	0	0
51	MO	1	0	0	0	0
51	NA	1	0	0	0	0
51	NC	1	0	0	0	0
51	NE	1	0	0	0	0
51	NG	1	0	0	0	0
51	NI	1	0	0	0	0
51	NK	1	0	0	0	0
51	NM	1	0	0	0	0
51	NO	1	0	0	0	0
51	OA	1	0	0	0	0
51	OC	1	0	0	0	0
51	OE	1	0	0	0	0
51	OG	1	0	0	0	0
51	OI	1	0	0	0	0
51	OK	1	0	0	0	0
51	OM	1	0	0	0	0
51	OO	1	0	0	0	0
51	PC	1	0	0	0	0
51	PE	1	0	0	0	0
51	PG	1	0	0	0	0
51	PI	1	0	0	0	0
51	PK	1	0	0	0	0
51	PM	1	0	0	0	0
51	PO	1	0	0	0	0
51	QC	1	0	0	0	0
51	QE	1	0	0	0	0
51	QG	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	QI	1	0	0	0	0
51	QK	1	0	0	0	0
51	QM	1	0	0	0	0
51	QO	1	0	0	0	0
51	RC	1	0	0	0	0
51	RE	1	0	0	0	0
51	RG	1	0	0	0	0
51	RI	1	0	0	0	0
51	RK	1	0	0	0	0
51	RM	1	0	0	0	0
51	RO	1	0	0	0	0
51	SA	1	0	0	0	0
51	SC	1	0	0	0	0
51	SE	1	0	0	0	0
51	SG	1	0	0	0	0
51	SI	1	0	0	0	0
51	SK	1	0	0	0	0
51	SM	1	0	0	0	0
51	TA	1	0	0	0	0
51	TC	1	0	0	0	0
51	TE	1	0	0	0	0
51	TG	1	0	0	0	0
51	TI	1	0	0	0	0
51	TK	1	0	0	0	0
51	TM	1	0	0	0	0
51	UA	1	0	0	0	0
51	UC	1	0	0	0	0
51	UE	1	0	0	0	0
51	UG	1	0	0	0	0
51	UI	1	0	0	0	0
51	UK	1	0	0	0	0
51	UM	1	0	0	0	0
51	UO	1	0	0	0	0
51	VA	1	0	0	0	0
51	VC	1	0	0	0	0
51	VE	1	0	0	0	0
51	VG	1	0	0	0	0
51	VI	1	0	0	0	0
51	VK	1	0	0	0	0
51	VM	1	0	0	0	0
51	VO	1	0	0	0	0
51	WA	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	WC	1	0	0	0	0
51	WE	1	0	0	0	0
51	WG	1	0	0	0	0
51	WI	1	0	0	0	0
51	WK	1	0	0	0	0
51	WM	1	0	0	0	0
51	WO	1	0	0	0	0
52	AB	28	0	12	0	0
52	AD	28	0	12	0	0
52	AF	28	0	12	0	0
52	AH	28	0	12	1	0
52	AJ	28	0	12	0	0
52	AL	28	0	12	1	0
52	AN	28	0	12	1	0
52	AP	28	0	12	0	0
52	BB	28	0	12	0	0
52	BD	28	0	12	1	0
52	BF	28	0	12	2	0
52	BH	28	0	12	0	0
52	BJ	28	0	12	1	0
52	BL	28	0	12	0	0
52	BN	28	0	12	0	0
52	BP	28	0	12	0	0
52	CB	28	0	12	0	0
52	CD	28	0	12	0	0
52	CF	28	0	12	1	0
52	CH	28	0	12	3	0
52	CJ	28	0	12	0	0
52	CL	28	0	12	1	0
52	CN	28	0	12	0	0
52	CP	28	0	12	0	0
52	DB	28	0	12	0	0
52	DD	28	0	12	0	0
52	DF	28	0	12	0	0
52	DH	28	0	12	0	0
52	DJ	28	0	12	0	0
52	DL	28	0	12	2	0
52	DN	28	0	12	0	0
52	DP	28	0	12	0	0
52	EB	28	0	12	1	0
52	ED	28	0	12	1	0
52	EF	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	EH	28	0	12	0	0
52	EJ	28	0	12	1	0
52	EL	28	0	12	1	0
52	EN	28	0	12	0	0
52	FB	28	0	12	1	0
52	FD	28	0	12	1	0
52	FF	28	0	12	0	0
52	FH	28	0	12	0	0
52	FJ	28	0	12	6	0
52	FL	28	0	12	1	0
52	FN	28	0	12	2	0
52	GB	28	0	12	1	0
52	GD	28	0	12	2	0
52	GF	28	0	12	0	0
52	GH	28	0	12	0	0
52	GJ	28	0	12	1	0
52	GL	28	0	12	0	0
52	GN	28	0	12	0	0
52	HB	28	0	12	1	0
52	HD	28	0	12	1	0
52	HF	28	0	12	1	0
52	HH	28	0	12	3	0
52	HJ	28	0	12	0	0
52	HL	28	0	12	1	0
52	HN	28	0	12	1	0
52	HP	28	0	12	1	0
52	IB	28	0	12	0	0
52	ID	28	0	12	1	0
52	IF	28	0	12	1	0
52	IH	28	0	12	0	0
52	IJ	28	0	12	2	0
52	IL	28	0	12	3	0
52	IN	28	0	12	3	0
52	IP	28	0	12	2	0
52	JB	28	0	12	0	0
52	JD	28	0	12	1	0
52	JF	28	0	12	0	0
52	JH	28	0	12	1	0
52	JJ	28	0	12	2	0
52	JL	28	0	12	1	0
52	JN	28	0	12	1	0
52	JP	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	KB	28	0	12	2	0
52	KD	28	0	12	0	0
52	KF	28	0	12	1	0
52	KH	28	0	12	2	0
52	KJ	28	0	12	1	0
52	KL	28	0	12	1	0
52	KN	28	0	12	0	0
52	KP	28	0	12	1	0
52	LB	28	0	12	0	0
52	LD	28	0	12	0	0
52	LF	28	0	12	1	0
52	LH	28	0	12	1	0
52	LJ	28	0	12	0	0
52	LL	28	0	12	0	0
52	LN	28	0	12	0	0
52	LP	28	0	12	0	0
52	MB	28	0	12	0	0
52	MD	28	0	12	0	0
52	MF	28	0	12	0	0
52	MH	28	0	12	0	0
52	MJ	28	0	12	0	0
52	ML	28	0	12	0	0
52	MN	28	0	12	0	0
52	MP	28	0	12	0	0
52	NB	28	0	12	0	0
52	ND	28	0	12	0	0
52	NF	28	0	12	2	0
52	NH	28	0	12	3	0
52	NJ	28	0	12	1	0
52	NL	28	0	12	0	0
52	NN	28	0	12	1	0
52	NP	28	0	12	0	0
52	OB	28	0	12	4	0
52	OD	28	0	12	0	0
52	OF	28	0	12	1	0
52	OH	28	0	12	2	0
52	OJ	28	0	12	0	0
52	OL	28	0	12	0	0
52	ON	28	0	12	2	0
52	OP	28	0	12	0	0
52	PB	28	0	12	1	0
52	PD	28	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	PF	28	0	12	1	0
52	PH	28	0	12	0	0
52	PJ	28	0	12	1	0
52	PL	28	0	12	1	0
52	PN	28	0	12	2	0
52	PP	28	0	12	1	0
52	QB	28	0	12	0	0
52	QD	28	0	12	1	0
52	QF	28	0	12	0	0
52	QH	28	0	12	2	0
52	QJ	28	0	12	0	0
52	QL	28	0	12	1	0
52	QN	28	0	12	0	0
52	QP	28	0	12	1	0
52	RD	28	0	12	1	0
52	RF	28	0	12	0	0
52	RH	28	0	12	2	0
52	RJ	28	0	12	1	0
52	RL	28	0	12	1	0
52	RN	28	0	12	1	0
52	RP	28	0	12	0	0
52	SB	28	0	12	2	0
52	SD	28	0	12	0	0
52	SF	28	0	12	2	0
52	SH	28	0	12	1	0
52	SJ	28	0	12	1	0
52	SL	28	0	12	1	0
52	SN	28	0	12	0	0
52	TB	28	0	12	0	0
52	TD	28	0	12	0	0
52	TF	28	0	12	0	0
52	TH	28	0	12	0	0
52	TJ	28	0	12	0	0
52	TL	28	0	12	0	0
52	TN	28	0	12	1	0
52	UB	28	0	12	2	0
52	UD	28	0	12	0	0
52	UF	28	0	12	0	0
52	UH	28	0	12	1	0
52	UJ	28	0	12	0	0
52	UL	28	0	12	1	0
52	UN	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	VB	28	0	12	3	0
52	VD	28	0	12	1	0
52	VF	28	0	12	0	0
52	VH	28	0	12	0	0
52	VJ	28	0	12	0	0
52	VL	28	0	12	0	0
52	VN	28	0	12	2	0
52	WB	28	0	12	0	0
52	WD	28	0	12	1	0
52	WF	28	0	12	0	0
52	WH	28	0	12	0	0
52	WJ	28	0	12	1	0
52	WL	28	0	12	0	0
52	WN	28	0	12	0	0
52	WP	28	0	12	0	0
All	All	1650085	0	1606959	42893	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 42893 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)
8:UE:282:TYR:HB2	39:c:373:ARG:NH2	1.45	1.26
8:NM:54:SER:HB2	8:NM:64:ARG:CZ	1.68	1.21
9:JH:402:GLY:C	9:JH:403:MET:SD	2.36	1.08
39:c:373:ARG:O	39:c:376:GLN:HG2	1.54	1.06
8:NM:53:PHE:HB3	8:NM:61:HIS:HB2	1.10	1.05

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

5.3.2 Protein sidechains

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 532 ligands modelled in this entry, 178 are monoatomic - leaving 354 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	$\#\|Z\| > 2$
52	GDP	TJ	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
52	GDP	UF	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	6 (13%)
50	GTP	SA	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
50	GTP	PK	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
52	GDP	KP	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
52	GDP	QP	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	8 (17%)
50	GTP	FE	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
52	GDP	UJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	6 (13%)
52	GDP	ED	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	QD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	DN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	WH	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	UD	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.78	7 (15%)
52	GDP	GL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	GDP	PP	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
50	GTP	MG	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
52	GDP	AP	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	IL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
50	GTP	LC	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.61	8 (16%)
50	GTP	SG	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.54	8 (16%)
52	GDP	RD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
52	GDP	BF	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	HH	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.71	6 (13%)
50	GTP	KI	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
50	GTP	MI	501	-	33,34,34	0.88	0	50,54,54	1.55	8 (16%)
50	GTP	NK	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.56	8 (16%)
52	GDP	DB	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	KK	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.61	8 (16%)
50	GTP	EO	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
50	GTP	BK	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	JQ	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.60	8 (16%)
52	GDP	PN	502	-	29,30,30	1.15	2 (6%)	45,47,47	1.76	6 (13%)
52	GDP	AF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
50	GTP	NE	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.55	8 (16%)
50	GTP	UK	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	HB	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
52	GDP	NH	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	EC	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.63	8 (16%)
52	GDP	NN	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	DO	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
50	GTP	UI	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
52	GDP	TH	502	-	29,30,30	1.14	2 (6%)	45,47,47	1.76	7 (15%)
50	GTP	PO	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
50	GTP	VA	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.59	9 (18%)
50	GTP	AC	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
50	GTP	FK	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.55	8 (16%)
50	GTP	RK	501	-	33,34,34	0.99	3 (9%)	50,54,54	1.63	8 (16%)
52	GDP	QN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	AG	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	GDP	IH	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	6 (13%)
52	GDP	CF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	6 (13%)
50	GTP	WO	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
52	GDP	BJ	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	CO	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
52	GDP	LB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
52	GDP	TD	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
52	GDP	IB	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	JL	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	5 (11%)
50	GTP	EG	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
52	GDP	UN	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	6 (13%)
50	GTP	GE	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.54	9 (18%)
50	GTP	CC	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.59	8 (16%)
52	GDP	OF	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.79	7 (15%)
50	GTP	WG	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	BE	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.62	9 (18%)
52	GDP	LD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	KL	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	5 (11%)
50	GTP	OI	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
52	GDP	ID	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	NI	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
52	GDP	KD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	FL	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	EF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	GC	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
52	GDP	MP	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
52	GDP	SF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	FC	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
52	GDP	QJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
50	GTP	RI	501	-	33,34,34	0.99	3 (9%)	50,54,54	1.62	9 (18%)
52	GDP	OP	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
50	GTP	DG	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
50	GTP	IO	501	-	33,34,34	0.87	1 (3%)	50,54,54	1.61	8 (16%)
50	GTP	EI	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.61	9 (18%)
52	GDP	HP	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	GTP	LM	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
50	GTP	ME	501	-	33,34,34	0.89	1 (3%)	50,54,54	1.62	9 (18%)
50	GTP	DM	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.60	8 (16%)
52	GDP	DD	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
52	GDP	QH	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	6 (13%)
50	GTP	FA	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
52	GDP	KH	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	BB	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	AH	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	6 (13%)
50	GTP	FM	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
50	GTP	BG	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
52	GDP	BP	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
52	GDP	FJ	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
52	GDP	PB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	TA	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
50	GTP	QG	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.63	8 (16%)
52	GDP	MN	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	EA	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.61	9 (18%)
52	GDP	BD	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	IN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
52	GDP	VN	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.78	5 (11%)
50	GTP	FO	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	RL	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	DF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	5 (11%)
52	GDP	AJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
50	GTP	IE	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.63	10 (20%)
52	GDP	LF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
50	GTP	DE	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
52	GDP	JH	502	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	6 (13%)
52	GDP	NJ	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	NP	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
50	GTP	HO	501	-	33,34,34	0.90	2 (6%)	50,54,54	1.60	9 (18%)
50	GTP	HA	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.56	8 (16%)
50	GTP	BM	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
50	GTP	OC	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	GTP	QI	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.61	8 (16%)
50	GTP	GI	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
50	GTP	IC	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
50	GTP	QM	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.60	9 (18%)
50	GTP	MM	501	-	33,34,34	0.84	0	50,54,54	1.53	8 (16%)
52	GDP	OL	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	GF	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	EE	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
50	GTP	TG	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.55	9 (18%)
52	GDP	LH	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.72	7 (15%)
50	GTP	NC	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
52	GDP	BH	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	EB	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
52	GDP	VJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	6 (13%)
52	GDP	DP	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	WD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
50	GTP	LI	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.59	8 (16%)
50	GTP	MC	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.55	10 (20%)
50	GTP	CG	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.63	9 (18%)
52	GDP	FB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	VC	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
50	GTP	NG	501	-	33,34,34	0.89	1 (3%)	50,54,54	1.55	8 (16%)
52	GDP	GH	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	JO	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	SK	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
50	GTP	PM	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
52	GDP	DH	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	6 (13%)
50	GTP	CQ	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.60	9 (18%)
50	GTP	GM	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
52	GDP	RN	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
52	GDP	CN	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	6 (13%)
52	GDP	KF	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
50	GTP	WI	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
50	GTP	PI	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.61	9 (18%)
50	GTP	QO	501	-	33,34,34	0.93	0	50,54,54	1.56	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	GTP	DK	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.61	8 (16%)
50	GTP	UE	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
52	GDP	GB	502	-	29,30,30	1.15	2 (6%)	45,47,47	1.71	7 (15%)
52	GDP	VD	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.80	6 (13%)
50	GTP	PE	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	LN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
50	GTP	OK	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	MF	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	AM	501	-	33,34,34	0.89	1 (3%)	50,54,54	1.57	8 (16%)
52	GDP	IP	502	-	29,30,30	1.11	3 (10%)	45,47,47	1.79	8 (17%)
50	GTP	SC	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.58	8 (16%)
50	GTP	KO	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.58	8 (16%)
52	GDP	FD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
50	GTP	IK	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.65	9 (18%)
50	GTP	UG	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	RH	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	UM	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
52	GDP	FF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	RJ	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
50	GTP	JM	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	MO	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.54	8 (16%)
52	GDP	SJ	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.71	7 (15%)
52	GDP	DJ	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	6 (13%)
50	GTP	VM	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
50	GTP	AE	501	-	33,34,34	0.89	1 (3%)	50,54,54	1.62	8 (16%)
50	GTP	AO	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.59	8 (16%)
50	GTP	UC	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	JF	502	-	29,30,30	1.11	3 (10%)	45,47,47	1.85	8 (17%)
50	GTP	VG	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
50	GTP	GG	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
52	GDP	AD	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
52	GDP	TN	502	-	29,30,30	1.14	2 (6%)	45,47,47	1.75	6 (13%)
50	GTP	MA	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.55	9 (18%)
52	GDP	AN	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
52	GDP	JP	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	GTP	FI	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
52	GDP	UH	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.79	6 (13%)
50	GTP	JC	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.60	9 (18%)
52	GDP	BL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	NL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	6 (13%)
52	GDP	CJ	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	HI	501	-	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
52	GDP	HL	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	6 (13%)
52	GDP	CL	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	6 (13%)
52	GDP	AL	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	ML	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.75	7 (15%)
50	GTP	HM	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
50	GTP	TC	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
50	GTP	CE	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
50	GTP	LA	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	UO	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	ON	502	-	29,30,30	1.17	2 (6%)	45,47,47	1.75	6 (13%)
52	GDP	EL	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
52	GDP	JJ	502	-	29,30,30	1.13	4 (13%)	45,47,47	1.76	5 (11%)
50	GTP	JE	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.59	8 (16%)
52	GDP	VB	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	HG	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.55	8 (16%)
52	GDP	NB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	LE	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.63	8 (16%)
52	GDP	JD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
52	GDP	LL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
52	GDP	JN	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	5 (11%)
50	GTP	NO	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
52	GDP	GN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
52	GDP	IJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	6 (13%)
50	GTP	WM	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
50	GTP	RE	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.61	8 (16%)
52	GDP	WP	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	DI	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
52	GDP	CB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	GTP	KM	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.59	8 (16%)
52	GDP	VF	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	5 (11%)
52	GDP	HJ	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
52	GDP	CP	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	RP	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	SI	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.53	8 (16%)
50	GTP	OO	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
50	GTP	QK	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
50	GTP	GK	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.51	8 (16%)
50	GTP	WE	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.60	9 (18%)
52	GDP	QB	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
50	GTP	LG	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.61	8 (16%)
52	GDP	UB	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.79	6 (13%)
52	GDP	VH	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	KC	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
50	GTP	FG	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
50	GTP	EK	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
52	GDP	MB	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.72	6 (13%)
50	GTP	AI	501	-	33,34,34	0.88	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	UA	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	PJ	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.78	7 (15%)
50	GTP	PC	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.55	9 (18%)
52	GDP	KB	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
50	GTP	TM	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
50	GTP	SE	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.55	9 (18%)
50	GTP	PG	501	-	33,34,34	0.87	0	50,54,54	1.58	10 (20%)
52	GDP	GD	502	-	29,30,30	1.21	3 (10%)	45,47,47	1.79	5 (11%)
50	GTP	DC	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
50	GTP	TI	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
52	GDP	OH	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	WF	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
52	GDP	PD	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	6 (13%)
50	GTP	KA	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	BO	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.59	8 (16%)
50	GTP	RM	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.61	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	GTP	LK	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
50	GTP	SM	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
50	GTP	KE	501	-	33,34,34	0.94	0	50,54,54	1.59	10 (20%)
50	GTP	KG	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
52	GDP	JB	502	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
52	GDP	TL	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	WJ	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
50	GTP	II	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
50	GTP	EM	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.59	8 (16%)
50	GTP	HK	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
50	GTP	OM	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
50	GTP	LO	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)
52	GDP	LJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
50	GTP	WK	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
50	GTP	BI	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.60	8 (16%)
52	GDP	OJ	502	-	29,30,30	1.11	3 (10%)	45,47,47	1.81	8 (17%)
50	GTP	WC	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
52	GDP	HF	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.74	7 (15%)
52	GDP	NF	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	BN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
52	GDP	PF	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	6 (13%)
52	GDP	MJ	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	RG	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.61	9 (18%)
50	GTP	TK	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
50	GTP	CM	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
50	GTP	CK	501	-	33,34,34	0.92	2 (6%)	50,54,54	1.63	9 (18%)
52	GDP	EH	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
50	GTP	QC	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.62	8 (16%)
52	GDP	EN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	DL	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
52	GDP	SH	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
50	GTP	OA	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
50	GTP	RO	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
52	GDP	UL	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	WA	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	GTP	JK	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.63	8 (16%)
50	GTP	AA	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
50	GTP	HC	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	TE	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
52	GDP	OD	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.78	7 (15%)
52	GDP	QF	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	KN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	PL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	6 (13%)
50	GTP	JI	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.61	8 (16%)
52	GDP	PH	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	6 (13%)
50	GTP	IG	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.62	9 (18%)
50	GTP	DQ	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)
52	GDP	GJ	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	8 (17%)
52	GDP	SB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
50	GTP	CI	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
50	GTP	GA	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
50	GTP	HE	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
52	GDP	KJ	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
52	GDP	TF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	VI	501	-	33,34,34	1.03	3 (9%)	50,54,54	1.62	9 (18%)
52	GDP	LP	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
50	GTP	RC	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.59	9 (18%)
50	GTP	OE	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
52	GDP	MD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
52	GDP	WN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
50	GTP	MK	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
50	GTP	NM	501	-	33,34,34	0.87	0	50,54,54	1.56	8 (16%)
52	GDP	VL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	QL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	HD	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)
52	GDP	FN	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
50	GTP	IM	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
52	GDP	ND	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
52	GDP	OB	502	-	29,30,30	1.17	2 (6%)	45,47,47	1.81	6 (13%)
52	GDP	CH	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	GTP	OG	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
52	GDP	SD	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	AB	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	FH	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
52	GDP	EJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
50	GTP	AK	501	-	33,34,34	0.87	1 (3%)	50,54,54	1.56	8 (16%)
50	GTP	BC	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
52	GDP	SN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	WL	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	CD	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)
50	GTP	VO	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
52	GDP	RF	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
52	GDP	WB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
52	GDP	TB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	8 (17%)
50	GTP	GO	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
50	GTP	JG	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.59	8 (16%)
52	GDP	MH	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
50	GTP	VE	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
52	GDP	SL	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
50	GTP	QE	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
50	GTP	IA	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
50	GTP	NA	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
50	GTP	VK	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.62	8 (16%)
52	GDP	IF	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	6 (13%)
52	GDP	HN	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	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
52	GDP	TJ	502	-	-	1/16/32/32	0/3/3/3
52	GDP	UF	502	-	-	0/16/32/32	0/3/3/3
50	GTP	SA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	PK	501	-	-	8/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GDP	KP	502	-	-	2/16/32/32	0/3/3/3
52	GDP	QP	502	-	-	1/16/32/32	0/3/3/3
50	GTP	FE	501	-	-	5/22/38/38	0/3/3/3
52	GDP	UJ	502	-	-	1/16/32/32	0/3/3/3
52	GDP	ED	502	-	-	1/16/32/32	0/3/3/3
52	GDP	QD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	DN	502	-	-	1/16/32/32	0/3/3/3
52	GDP	WH	502	-	-	1/16/32/32	0/3/3/3
52	GDP	UD	502	-	-	3/16/32/32	0/3/3/3
52	GDP	GL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	PP	502	-	-	1/16/32/32	0/3/3/3
50	GTP	MG	501	-	-	6/22/38/38	0/3/3/3
52	GDP	AP	502	-	-	1/16/32/32	0/3/3/3
52	GDP	IL	502	-	-	0/16/32/32	0/3/3/3
50	GTP	LC	501	-	-	6/22/38/38	0/3/3/3
50	GTP	SG	501	-	-	8/22/38/38	0/3/3/3
52	GDP	RD	502	-	-	0/16/32/32	0/3/3/3
52	GDP	BF	502	-	-	1/16/32/32	0/3/3/3
52	GDP	HH	502	-	-	0/16/32/32	0/3/3/3
50	GTP	KI	501	-	-	7/22/38/38	0/3/3/3
50	GTP	MI	501	-	-	6/22/38/38	0/3/3/3
50	GTP	NK	501	-	-	9/22/38/38	0/3/3/3
52	GDP	DB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	KK	501	-	-	6/22/38/38	0/3/3/3
50	GTP	EO	501	-	-	8/22/38/38	0/3/3/3
50	GTP	BK	501	-	-	7/22/38/38	0/3/3/3
50	GTP	JQ	501	-	-	7/22/38/38	0/3/3/3
52	GDP	PN	502	-	-	3/16/32/32	0/3/3/3
52	GDP	AF	502	-	-	0/16/32/32	0/3/3/3
50	GTP	NE	501	-	-	7/22/38/38	0/3/3/3
50	GTP	UK	501	-	-	9/22/38/38	0/3/3/3
52	GDP	HB	502	-	-	1/16/32/32	0/3/3/3
52	GDP	NH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	EC	501	-	-	7/22/38/38	0/3/3/3
52	GDP	NN	502	-	-	4/16/32/32	0/3/3/3
50	GTP	DO	501	-	-	8/22/38/38	0/3/3/3
50	GTP	UI	501	-	-	8/22/38/38	0/3/3/3
52	GDP	TH	502	-	-	1/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GTP	PO	501	-	-	8/22/38/38	0/3/3/3
50	GTP	VA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	AC	501	-	-	6/22/38/38	0/3/3/3
50	GTP	FK	501	-	-	8/22/38/38	0/3/3/3
50	GTP	RK	501	-	-	9/22/38/38	0/3/3/3
52	GDP	QN	502	-	-	1/16/32/32	0/3/3/3
50	GTP	AG	501	-	-	6/22/38/38	0/3/3/3
52	GDP	IH	502	-	-	0/16/32/32	0/3/3/3
52	GDP	CF	502	-	-	1/16/32/32	0/3/3/3
50	GTP	WO	501	-	-	6/22/38/38	0/3/3/3
52	GDP	BJ	502	-	-	0/16/32/32	0/3/3/3
50	GTP	CO	501	-	-	8/22/38/38	0/3/3/3
52	GDP	LB	502	-	-	1/16/32/32	0/3/3/3
52	GDP	TD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	IB	502	-	-	2/16/32/32	0/3/3/3
52	GDP	JL	502	-	-	1/16/32/32	0/3/3/3
50	GTP	EG	501	-	-	7/22/38/38	0/3/3/3
52	GDP	UN	502	-	-	1/16/32/32	0/3/3/3
50	GTP	GE	501	-	-	7/22/38/38	0/3/3/3
50	GTP	CC	501	-	-	8/22/38/38	0/3/3/3
52	GDP	OF	502	-	-	2/16/32/32	0/3/3/3
50	GTP	WG	501	-	-	8/22/38/38	0/3/3/3
50	GTP	BE	501	-	-	8/22/38/38	0/3/3/3
52	GDP	LD	502	-	-	2/16/32/32	0/3/3/3
52	GDP	KL	502	-	-	1/16/32/32	0/3/3/3
50	GTP	OI	501	-	-	8/22/38/38	0/3/3/3
52	GDP	ID	502	-	-	0/16/32/32	0/3/3/3
50	GTP	NI	501	-	-	8/22/38/38	0/3/3/3
52	GDP	KD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	FL	502	-	-	0/16/32/32	0/3/3/3
52	GDP	EF	502	-	-	1/16/32/32	0/3/3/3
50	GTP	GC	501	-	-	6/22/38/38	0/3/3/3
52	GDP	MP	502	-	-	2/16/32/32	0/3/3/3
52	GDP	SF	502	-	-	1/16/32/32	0/3/3/3
50	GTP	FC	501	-	-	8/22/38/38	0/3/3/3
52	GDP	QJ	502	-	-	0/16/32/32	0/3/3/3
50	GTP	RI	501	-	-	7/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GDP	OP	502	-	-	1/16/32/32	0/3/3/3
50	GTP	DG	501	-	-	8/22/38/38	0/3/3/3
50	GTP	IO	501	-	-	8/22/38/38	0/3/3/3
50	GTP	EI	501	-	-	7/22/38/38	0/3/3/3
52	GDP	HP	502	-	-	1/16/32/32	0/3/3/3
50	GTP	LM	501	-	-	6/22/38/38	0/3/3/3
50	GTP	ME	501	-	-	5/22/38/38	0/3/3/3
50	GTP	DM	501	-	-	8/22/38/38	0/3/3/3
52	GDP	DD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	QH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	FA	501	-	-	7/22/38/38	0/3/3/3
52	GDP	KH	502	-	-	1/16/32/32	0/3/3/3
52	GDP	BB	502	-	-	0/16/32/32	0/3/3/3
52	GDP	AH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	FM	501	-	-	8/22/38/38	0/3/3/3
50	GTP	BG	501	-	-	8/22/38/38	0/3/3/3
52	GDP	BP	502	-	-	1/16/32/32	0/3/3/3
52	GDP	FJ	502	-	-	1/16/32/32	0/3/3/3
52	GDP	PB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	TA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	QG	501	-	-	8/22/38/38	0/3/3/3
52	GDP	MN	502	-	-	2/16/32/32	0/3/3/3
50	GTP	EA	501	-	-	7/22/38/38	0/3/3/3
52	GDP	BD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	IN	502	-	-	1/16/32/32	0/3/3/3
52	GDP	VN	502	-	-	1/16/32/32	0/3/3/3
50	GTP	FO	501	-	-	9/22/38/38	0/3/3/3
52	GDP	RL	502	-	-	0/16/32/32	0/3/3/3
52	GDP	DF	502	-	-	0/16/32/32	0/3/3/3
52	GDP	AJ	502	-	-	1/16/32/32	0/3/3/3
50	GTP	IE	501	-	-	8/22/38/38	0/3/3/3
52	GDP	LF	502	-	-	2/16/32/32	0/3/3/3
50	GTP	DE	501	-	-	7/22/38/38	0/3/3/3
52	GDP	JH	502	-	-	0/16/32/32	0/3/3/3
52	GDP	NJ	502	-	-	1/16/32/32	0/3/3/3
52	GDP	NP	502	-	-	1/16/32/32	0/3/3/3
50	GTP	HO	501	-	-	7/22/38/38	0/3/3/3
50	GTP	HA	501	-	-	9/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GTP	BM	501	-	-	7/22/38/38	0/3/3/3
50	GTP	OC	501	-	-	8/22/38/38	0/3/3/3
50	GTP	QI	501	-	-	8/22/38/38	0/3/3/3
50	GTP	GI	501	-	-	4/22/38/38	0/3/3/3
50	GTP	IC	501	-	-	8/22/38/38	0/3/3/3
50	GTP	QM	501	-	-	8/22/38/38	0/3/3/3
50	GTP	MM	501	-	-	9/22/38/38	0/3/3/3
52	GDP	OL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	GF	502	-	-	0/16/32/32	0/3/3/3
50	GTP	EE	501	-	-	8/22/38/38	0/3/3/3
50	GTP	TG	501	-	-	8/22/38/38	0/3/3/3
52	GDP	LH	502	-	-	3/16/32/32	0/3/3/3
50	GTP	NC	501	-	-	6/22/38/38	0/3/3/3
52	GDP	BH	502	-	-	1/16/32/32	0/3/3/3
52	GDP	EB	502	-	-	1/16/32/32	0/3/3/3
52	GDP	VJ	502	-	-	1/16/32/32	0/3/3/3
52	GDP	DP	502	-	-	4/16/32/32	0/3/3/3
52	GDP	WD	502	-	-	1/16/32/32	0/3/3/3
50	GTP	LI	501	-	-	7/22/38/38	0/3/3/3
50	GTP	MC	501	-	-	6/22/38/38	0/3/3/3
50	GTP	CG	501	-	-	6/22/38/38	0/3/3/3
52	GDP	FB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	VC	501	-	-	8/22/38/38	0/3/3/3
50	GTP	NG	501	-	-	9/22/38/38	0/3/3/3
52	GDP	GH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	JO	501	-	-	6/22/38/38	0/3/3/3
50	GTP	SK	501	-	-	8/22/38/38	0/3/3/3
50	GTP	PM	501	-	-	8/22/38/38	0/3/3/3
52	GDP	DH	502	-	-	0/16/32/32	0/3/3/3
50	GTP	CQ	501	-	-	8/22/38/38	0/3/3/3
50	GTP	GM	501	-	-	6/22/38/38	0/3/3/3
52	GDP	RN	502	-	-	0/16/32/32	0/3/3/3
52	GDP	CN	502	-	-	1/16/32/32	0/3/3/3
52	GDP	KF	502	-	-	1/16/32/32	0/3/3/3
50	GTP	WI	501	-	-	6/22/38/38	0/3/3/3
50	GTP	PI	501	-	-	8/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GTP	QO	501	-	-	7/22/38/38	0/3/3/3
50	GTP	DK	501	-	-	6/22/38/38	0/3/3/3
50	GTP	UE	501	-	-	9/22/38/38	0/3/3/3
52	GDP	GB	502	-	-	1/16/32/32	0/3/3/3
52	GDP	VD	502	-	-	1/16/32/32	0/3/3/3
50	GTP	PE	501	-	-	8/22/38/38	0/3/3/3
52	GDP	LN	502	-	-	1/16/32/32	0/3/3/3
50	GTP	OK	501	-	-	8/22/38/38	0/3/3/3
52	GDP	MF	502	-	-	1/16/32/32	0/3/3/3
50	GTP	AM	501	-	-	9/22/38/38	0/3/3/3
52	GDP	IP	502	-	-	1/16/32/32	0/3/3/3
50	GTP	SC	501	-	-	7/22/38/38	0/3/3/3
50	GTP	KO	501	-	-	5/22/38/38	0/3/3/3
52	GDP	FD	502	-	-	0/16/32/32	0/3/3/3
50	GTP	IK	501	-	-	7/22/38/38	0/3/3/3
50	GTP	UG	501	-	-	9/22/38/38	0/3/3/3
52	GDP	RH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	UM	501	-	-	8/22/38/38	0/3/3/3
52	GDP	FF	502	-	-	1/16/32/32	0/3/3/3
52	GDP	RJ	502	-	-	0/16/32/32	0/3/3/3
50	GTP	JM	501	-	-	6/22/38/38	0/3/3/3
50	GTP	MO	501	-	-	7/22/38/38	0/3/3/3
52	GDP	SJ	502	-	-	1/16/32/32	0/3/3/3
52	GDP	DJ	502	-	-	1/16/32/32	0/3/3/3
50	GTP	VM	501	-	-	7/22/38/38	0/3/3/3
50	GTP	AE	501	-	-	9/22/38/38	0/3/3/3
50	GTP	AO	501	-	-	8/22/38/38	0/3/3/3
50	GTP	UC	501	-	-	8/22/38/38	0/3/3/3
52	GDP	JF	502	-	-	0/16/32/32	0/3/3/3
50	GTP	VG	501	-	-	8/22/38/38	0/3/3/3
50	GTP	GG	501	-	-	6/22/38/38	0/3/3/3
52	GDP	AD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	TN	502	-	-	1/16/32/32	0/3/3/3
50	GTP	MA	501	-	-	7/22/38/38	0/3/3/3
52	GDP	AN	502	-	-	0/16/32/32	0/3/3/3
52	GDP	JP	502	-	-	0/16/32/32	0/3/3/3
50	GTP	FI	501	-	-	6/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GDP	UH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	JC	501	-	-	7/22/38/38	0/3/3/3
52	GDP	BL	502	-	-	2/16/32/32	0/3/3/3
52	GDP	NL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	CJ	502	-	-	1/16/32/32	0/3/3/3
50	GTP	HI	501	-	-	9/22/38/38	0/3/3/3
52	GDP	HL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	CL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	AL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	ML	502	-	-	3/16/32/32	0/3/3/3
50	GTP	HM	501	-	-	7/22/38/38	0/3/3/3
50	GTP	TC	501	-	-	8/22/38/38	0/3/3/3
50	GTP	CE	501	-	-	6/22/38/38	0/3/3/3
50	GTP	LA	501	-	-	6/22/38/38	0/3/3/3
50	GTP	UO	501	-	-	8/22/38/38	0/3/3/3
52	GDP	ON	502	-	-	3/16/32/32	0/3/3/3
52	GDP	EL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	JJ	502	-	-	2/16/32/32	0/3/3/3
50	GTP	JE	501	-	-	6/22/38/38	0/3/3/3
52	GDP	VB	502	-	-	4/16/32/32	0/3/3/3
50	GTP	HG	501	-	-	9/22/38/38	0/3/3/3
52	GDP	NB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	LE	501	-	-	5/22/38/38	0/3/3/3
52	GDP	JD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	LL	502	-	-	2/16/32/32	0/3/3/3
52	GDP	JN	502	-	-	1/16/32/32	0/3/3/3
50	GTP	NO	501	-	-	9/22/38/38	0/3/3/3
52	GDP	GN	502	-	-	1/16/32/32	0/3/3/3
52	GDP	IJ	502	-	-	0/16/32/32	0/3/3/3
50	GTP	WM	501	-	-	6/22/38/38	0/3/3/3
50	GTP	RE	501	-	-	8/22/38/38	0/3/3/3
52	GDP	WP	502	-	-	1/16/32/32	0/3/3/3
50	GTP	DI	501	-	-	8/22/38/38	0/3/3/3
52	GDP	CB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	KM	501	-	-	5/22/38/38	0/3/3/3
52	GDP	VF	502	-	-	1/16/32/32	0/3/3/3
52	GDP	HJ	502	-	-	0/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GDP	CP	502	-	-	1/16/32/32	0/3/3/3
52	GDP	RP	502	-	-	0/16/32/32	0/3/3/3
50	GTP	SI	501	-	-	9/22/38/38	0/3/3/3
50	GTP	OO	501	-	-	9/22/38/38	0/3/3/3
50	GTP	QK	501	-	-	8/22/38/38	0/3/3/3
50	GTP	GK	501	-	-	7/22/38/38	0/3/3/3
50	GTP	WE	501	-	-	7/22/38/38	0/3/3/3
52	GDP	QB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	LG	501	-	-	7/22/38/38	0/3/3/3
52	GDP	UB	502	-	-	1/16/32/32	0/3/3/3
52	GDP	VH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	KC	501	-	-	5/22/38/38	0/3/3/3
50	GTP	FG	501	-	-	6/22/38/38	0/3/3/3
50	GTP	EK	501	-	-	6/22/38/38	0/3/3/3
52	GDP	MB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	AI	501	-	-	9/22/38/38	0/3/3/3
50	GTP	UA	501	-	-	8/22/38/38	0/3/3/3
52	GDP	PJ	502	-	-	1/16/32/32	0/3/3/3
50	GTP	PC	501	-	-	8/22/38/38	0/3/3/3
52	GDP	KB	502	-	-	2/16/32/32	0/3/3/3
50	GTP	TM	501	-	-	9/22/38/38	0/3/3/3
50	GTP	SE	501	-	-	8/22/38/38	0/3/3/3
50	GTP	PG	501	-	-	8/22/38/38	0/3/3/3
52	GDP	GD	502	-	-	2/16/32/32	0/3/3/3
50	GTP	DC	501	-	-	7/22/38/38	0/3/3/3
50	GTP	TI	501	-	-	8/22/38/38	0/3/3/3
52	GDP	OH	502	-	-	2/16/32/32	0/3/3/3
52	GDP	WF	502	-	-	1/16/32/32	0/3/3/3
52	GDP	PD	502	-	-	1/16/32/32	0/3/3/3
50	GTP	KA	501	-	-	6/22/38/38	0/3/3/3
50	GTP	BO	501	-	-	8/22/38/38	0/3/3/3
50	GTP	RM	501	-	-	7/22/38/38	0/3/3/3
50	GTP	LK	501	-	-	7/22/38/38	0/3/3/3
50	GTP	SM	501	-	-	8/22/38/38	0/3/3/3
50	GTP	KE	501	-	-	7/22/38/38	0/3/3/3
50	GTP	KG	501	-	-	5/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GDP	JB	502	-	-	1/16/32/32	0/3/3/3
52	GDP	TL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	WJ	502	-	-	1/16/32/32	0/3/3/3
50	GTP	II	501	-	-	7/22/38/38	0/3/3/3
50	GTP	EM	501	-	-	7/22/38/38	0/3/3/3
50	GTP	HK	501	-	-	8/22/38/38	0/3/3/3
50	GTP	OM	501	-	-	8/22/38/38	0/3/3/3
50	GTP	LO	501	-	-	6/22/38/38	0/3/3/3
52	GDP	LJ	502	-	-	1/16/32/32	0/3/3/3
50	GTP	WK	501	-	-	7/22/38/38	0/3/3/3
50	GTP	BI	501	-	-	8/22/38/38	0/3/3/3
52	GDP	OJ	502	-	-	4/16/32/32	0/3/3/3
50	GTP	WC	501	-	-	7/22/38/38	0/3/3/3
52	GDP	HF	502	-	-	0/16/32/32	0/3/3/3
52	GDP	NF	502	-	-	1/16/32/32	0/3/3/3
52	GDP	BN	502	-	-	0/16/32/32	0/3/3/3
52	GDP	PF	502	-	-	1/16/32/32	0/3/3/3
52	GDP	MJ	502	-	-	1/16/32/32	0/3/3/3
50	GTP	RG	501	-	-	8/22/38/38	0/3/3/3
50	GTP	TK	501	-	-	8/22/38/38	0/3/3/3
50	GTP	CM	501	-	-	6/22/38/38	0/3/3/3
50	GTP	CK	501	-	-	6/22/38/38	0/3/3/3
52	GDP	EH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	QC	501	-	-	8/22/38/38	0/3/3/3
52	GDP	EN	502	-	-	1/16/32/32	0/3/3/3
52	GDP	DL	502	-	-	2/16/32/32	0/3/3/3
52	GDP	SH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	OA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	RO	501	-	-	8/22/38/38	0/3/3/3
52	GDP	UL	502	-	-	1/16/32/32	0/3/3/3
50	GTP	WA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	JK	501	-	-	4/22/38/38	0/3/3/3
50	GTP	AA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	HC	501	-	-	9/22/38/38	0/3/3/3
50	GTP	TE	501	-	-	8/22/38/38	0/3/3/3
52	GDP	OD	502	-	-	3/16/32/32	0/3/3/3
52	GDP	QF	502	-	-	1/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GDP	KN	502	-	-	1/16/32/32	0/3/3/3
52	GDP	PL	502	-	-	0/16/32/32	0/3/3/3
50	GTP	JI	501	-	-	8/22/38/38	0/3/3/3
52	GDP	PH	502	-	-	1/16/32/32	0/3/3/3
50	GTP	IG	501	-	-	9/22/38/38	0/3/3/3
50	GTP	DQ	501	-	-	8/22/38/38	0/3/3/3
52	GDP	GJ	502	-	-	3/16/32/32	0/3/3/3
52	GDP	SB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	CI	501	-	-	6/22/38/38	0/3/3/3
50	GTP	GA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	HE	501	-	-	7/22/38/38	0/3/3/3
52	GDP	KJ	502	-	-	1/16/32/32	0/3/3/3
52	GDP	TF	502	-	-	1/16/32/32	0/3/3/3
50	GTP	VI	501	-	-	8/22/38/38	0/3/3/3
52	GDP	LP	502	-	-	1/16/32/32	0/3/3/3
50	GTP	RC	501	-	-	8/22/38/38	0/3/3/3
50	GTP	OE	501	-	-	9/22/38/38	0/3/3/3
52	GDP	MD	502	-	-	4/16/32/32	0/3/3/3
52	GDP	WN	502	-	-	0/16/32/32	0/3/3/3
50	GTP	MK	501	-	-	6/22/38/38	0/3/3/3
50	GTP	NM	501	-	-	8/22/38/38	0/3/3/3
52	GDP	VL	502	-	-	1/16/32/32	0/3/3/3
52	GDP	QL	502	-	-	0/16/32/32	0/3/3/3
52	GDP	HD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	FN	502	-	-	1/16/32/32	0/3/3/3
50	GTP	IM	501	-	-	7/22/38/38	0/3/3/3
52	GDP	ND	502	-	-	1/16/32/32	0/3/3/3
52	GDP	OB	502	-	-	4/16/32/32	0/3/3/3
52	GDP	CH	502	-	-	0/16/32/32	0/3/3/3
50	GTP	OG	501	-	-	8/22/38/38	0/3/3/3
52	GDP	SD	502	-	-	1/16/32/32	0/3/3/3
52	GDP	AB	502	-	-	0/16/32/32	0/3/3/3
52	GDP	FH	502	-	-	1/16/32/32	0/3/3/3
52	GDP	EJ	502	-	-	1/16/32/32	0/3/3/3
50	GTP	AK	501	-	-	6/22/38/38	0/3/3/3
50	GTP	BC	501	-	-	8/22/38/38	0/3/3/3
52	GDP	SN	502	-	-	1/16/32/32	0/3/3/3
52	GDP	WL	502	-	-	1/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GDP	CD	502	-	-	1/16/32/32	0/3/3/3
50	GTP	VO	501	-	-	8/22/38/38	0/3/3/3
52	GDP	RF	502	-	-	1/16/32/32	0/3/3/3
52	GDP	WB	502	-	-	0/16/32/32	0/3/3/3
52	GDP	TB	502	-	-	1/16/32/32	0/3/3/3
50	GTP	GO	501	-	-	7/22/38/38	0/3/3/3
50	GTP	JG	501	-	-	6/22/38/38	0/3/3/3
52	GDP	MH	502	-	-	4/16/32/32	0/3/3/3
50	GTP	VE	501	-	-	7/22/38/38	0/3/3/3
52	GDP	SL	502	-	-	1/16/32/32	0/3/3/3
50	GTP	QE	501	-	-	7/22/38/38	0/3/3/3
50	GTP	IA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	NA	501	-	-	8/22/38/38	0/3/3/3
50	GTP	VK	501	-	-	7/22/38/38	0/3/3/3
52	GDP	IF	502	-	-	1/16/32/32	0/3/3/3
52	GDP	HN	502	-	-	0/16/32/32	0/3/3/3

The worst 5 of 712 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	OB	502	GDP	C5-C4	3.31	1.47	1.38
52	ON	502	GDP	C5-C4	3.29	1.47	1.38
52	UF	502	GDP	C5-C4	3.18	1.47	1.38
52	GD	502	GDP	C5-C4	3.17	1.47	1.38
52	NB	502	GDP	C5-C4	3.15	1.47	1.38

The worst 5 of 2671 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	GD	502	GDP	C5-C4-N3	-6.37	118.26	128.39
52	IJ	502	GDP	C5-C4-N3	-6.28	118.39	128.39
52	OB	502	GDP	C5-C4-N3	-6.25	118.44	128.39
52	QP	502	GDP	C5-C4-N3	-6.25	118.45	128.39
52	FJ	502	GDP	C5-C4-N3	-6.24	118.46	128.39

There are no chirality outliers.

5 of 1501 torsion outliers are listed below:

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

There are no ring outliers.

190 monomers are involved in 275 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	KP	502	GDP	1	0
52	QP	502	GDP	1	0
50	FE	501	GTP	1	0
52	ED	502	GDP	1	0
52	QD	502	GDP	1	0
52	PP	502	GDP	1	0
52	IL	502	GDP	3	0
50	SG	501	GTP	1	0
52	RD	502	GDP	1	0
52	BF	502	GDP	2	0
52	HH	502	GDP	3	0
50	MI	501	GTP	1	0
50	KK	501	GTP	1	0
50	JQ	501	GTP	1	0
52	PN	502	GDP	2	0
50	NE	501	GTP	2	0
50	UK	501	GTP	2	0
52	HB	502	GDP	1	0
52	NH	502	GDP	3	0
52	NN	502	GDP	1	0
50	DO	501	GTP	1	0
50	AC	501	GTP	1	0
50	FK	501	GTP	1	0
50	RK	501	GTP	2	0
52	CF	502	GDP	1	0
50	WO	501	GTP	2	0
52	BJ	502	GDP	1	0
50	CO	501	GTP	1	0
52	JL	502	GDP	1	0
50	EG	501	GTP	1	0
52	OF	502	GDP	1	0
50	WG	501	GTP	1	0
52	KL	502	GDP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	OI	501	GTP	1	0
52	ID	502	GDP	1	0
50	NI	501	GTP	1	0
52	FL	502	GDP	1	0
52	SF	502	GDP	2	0
50	FC	501	GTP	1	0
50	RI	501	GTP	3	0
50	IO	501	GTP	1	0
50	EI	501	GTP	1	0
52	HP	502	GDP	1	0
50	LM	501	GTP	1	0
50	DM	501	GTP	1	0
52	QH	502	GDP	2	0
52	KH	502	GDP	2	0
52	AH	502	GDP	1	0
50	FM	501	GTP	1	0
52	FJ	502	GDP	6	0
52	PB	502	GDP	1	0
50	QG	501	GTP	2	0
50	EA	501	GTP	1	0
52	BD	502	GDP	1	0
52	IN	502	GDP	3	0
52	VN	502	GDP	2	0
50	FO	501	GTP	1	0
52	RL	502	GDP	1	0
50	IE	501	GTP	1	0
52	LF	502	GDP	1	0
50	DE	501	GTP	1	0
52	JH	502	GDP	1	0
52	NJ	502	GDP	1	0
50	HO	501	GTP	1	0
50	HA	501	GTP	1	0
50	OC	501	GTP	1	0
50	QI	501	GTP	3	0
50	GI	501	GTP	1	0
50	QM	501	GTP	2	0
50	MM	501	GTP	1	0
50	EE	501	GTP	1	0
50	TG	501	GTP	1	0
52	LH	502	GDP	1	0
50	NC	501	GTP	1	0
52	EB	502	GDP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	WD	502	GDP	1	0
50	LI	501	GTP	2	0
50	MC	501	GTP	1	0
50	CG	501	GTP	1	0
52	FB	502	GDP	1	0
50	NG	501	GTP	1	0
50	JO	501	GTP	2	0
50	SK	501	GTP	1	0
50	GM	501	GTP	2	0
52	RN	502	GDP	1	0
52	KF	502	GDP	1	0
50	WI	501	GTP	2	0
50	PI	501	GTP	1	0
50	QO	501	GTP	6	0
50	DK	501	GTP	2	0
50	UE	501	GTP	1	0
52	GB	502	GDP	1	0
52	VD	502	GDP	1	0
52	IP	502	GDP	2	0
52	FD	502	GDP	1	0
50	UG	501	GTP	1	0
52	RH	502	GDP	2	0
50	UM	501	GTP	1	0
52	RJ	502	GDP	1	0
50	MO	501	GTP	1	0
52	SJ	502	GDP	1	0
50	AE	501	GTP	1	0
50	UC	501	GTP	2	0
50	VG	501	GTP	1	0
50	GG	501	GTP	1	0
52	TN	502	GDP	1	0
52	AN	502	GDP	1	0
50	FI	501	GTP	1	0
52	UH	502	GDP	1	0
50	HI	501	GTP	1	0
52	HL	502	GDP	1	0
52	CL	502	GDP	1	0
52	AL	502	GDP	1	0
50	TC	501	GTP	2	0
50	UO	501	GTP	1	0
52	ON	502	GDP	2	0
52	EL	502	GDP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	JJ	502	GDP	2	0
52	VB	502	GDP	3	0
50	HG	501	GTP	1	0
50	LE	501	GTP	1	0
52	JD	502	GDP	1	0
52	JN	502	GDP	1	0
50	NO	501	GTP	1	0
52	IJ	502	GDP	2	0
50	WM	501	GTP	1	0
50	RE	501	GTP	2	0
50	KM	501	GTP	1	0
50	OO	501	GTP	1	0
50	QK	501	GTP	2	0
52	UB	502	GDP	2	0
50	KC	501	GTP	4	0
50	EK	501	GTP	1	0
52	PJ	502	GDP	1	0
52	KB	502	GDP	2	0
50	TM	501	GTP	1	0
50	SE	501	GTP	2	0
50	PG	501	GTP	3	0
52	GD	502	GDP	2	0
50	TI	501	GTP	1	0
52	OH	502	GDP	2	0
52	PD	502	GDP	1	0
50	KA	501	GTP	1	0
50	LK	501	GTP	1	0
50	SM	501	GTP	2	0
50	KG	501	GTP	3	0
52	WJ	502	GDP	1	0
50	II	501	GTP	3	0
50	OM	501	GTP	1	0
50	LO	501	GTP	1	0
50	WC	501	GTP	1	0
52	HF	502	GDP	1	0
52	NF	502	GDP	2	0
52	PF	502	GDP	1	0
50	RG	501	GTP	1	0
50	TK	501	GTP	2	0
50	CM	501	GTP	1	0
50	CK	501	GTP	2	0
50	QC	501	GTP	2	0

Continued on next page...

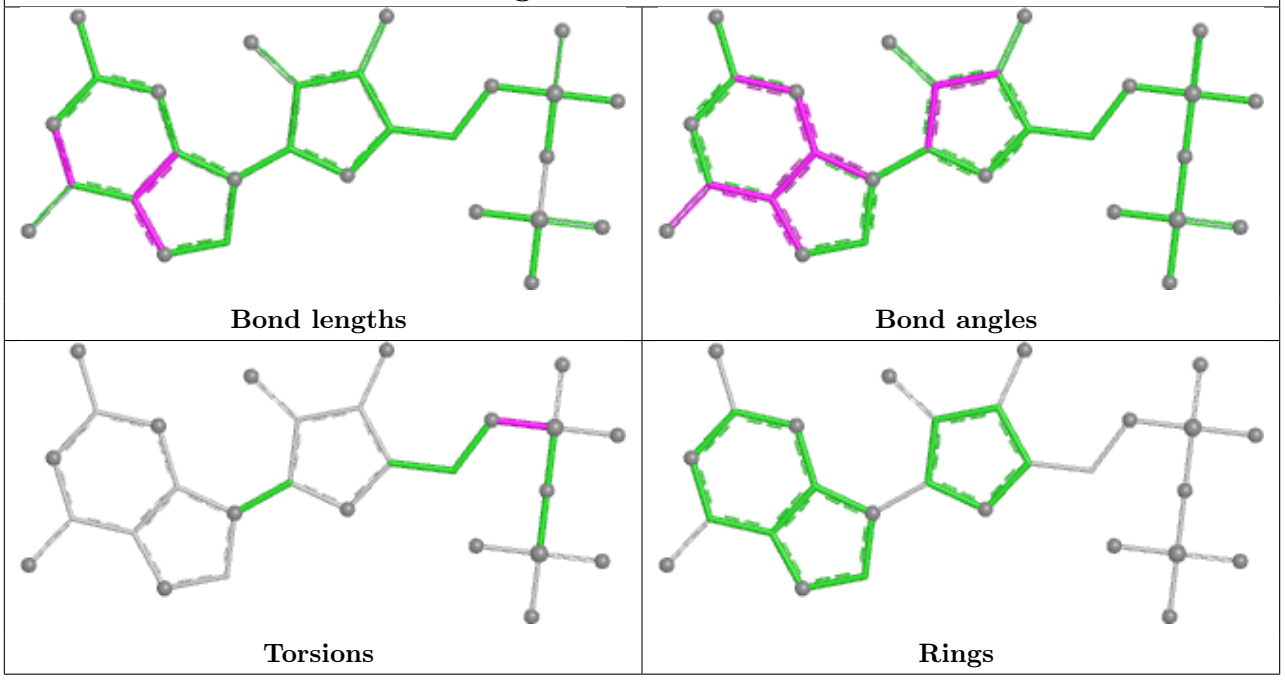
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	DL	502	GDP	2	0
52	SH	502	GDP	1	0
52	UL	502	GDP	1	0
50	WA	501	GTP	1	0
50	JK	501	GTP	1	0
50	HC	501	GTP	1	0
50	TE	501	GTP	1	0
52	PL	502	GDP	1	0
50	JI	501	GTP	3	0
50	IG	501	GTP	1	0
50	DQ	501	GTP	2	0
52	GJ	502	GDP	1	0
52	SB	502	GDP	2	0
50	CI	501	GTP	3	0
50	HE	501	GTP	2	0
52	KJ	502	GDP	1	0
50	MK	501	GTP	1	0
50	NM	501	GTP	3	0
52	QL	502	GDP	1	0
52	HD	502	GDP	1	0
52	FN	502	GDP	2	0
52	OB	502	GDP	4	0
52	CH	502	GDP	3	0
52	EJ	502	GDP	1	0
50	BC	501	GTP	1	0
50	VO	501	GTP	1	0
52	SL	502	GDP	1	0
50	QE	501	GTP	1	0
50	VK	501	GTP	1	0
52	IF	502	GDP	1	0
52	HN	502	GDP	1	0

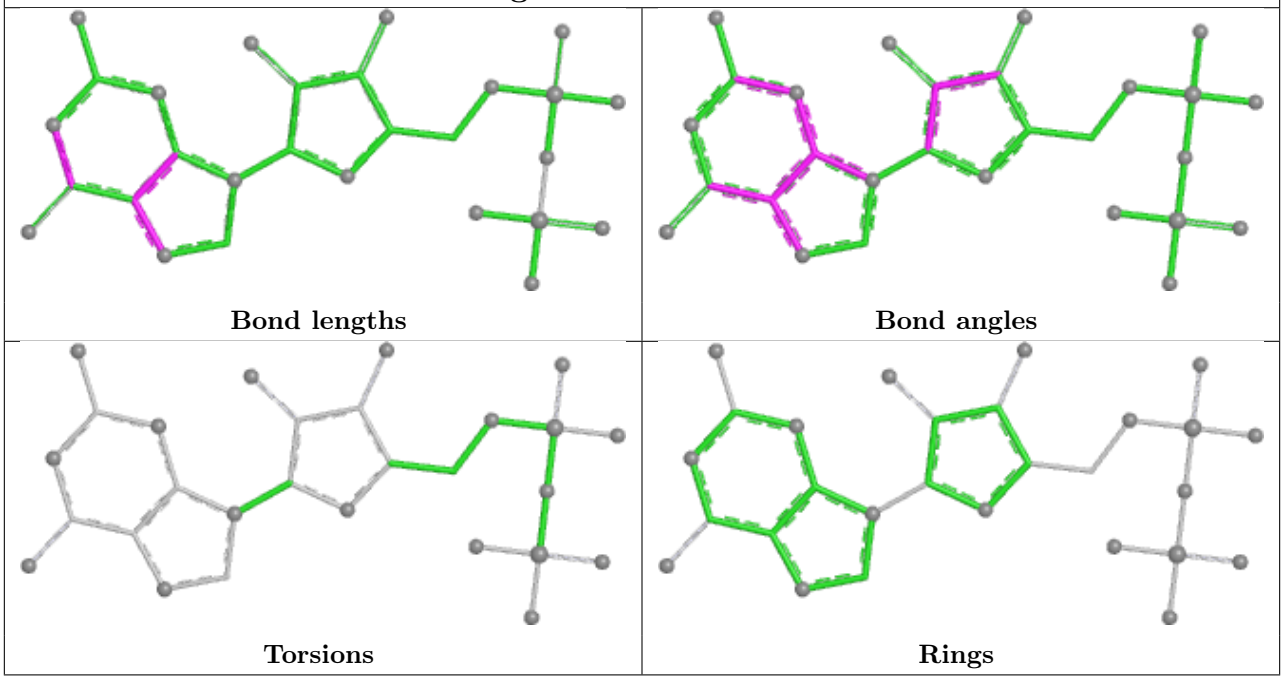
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

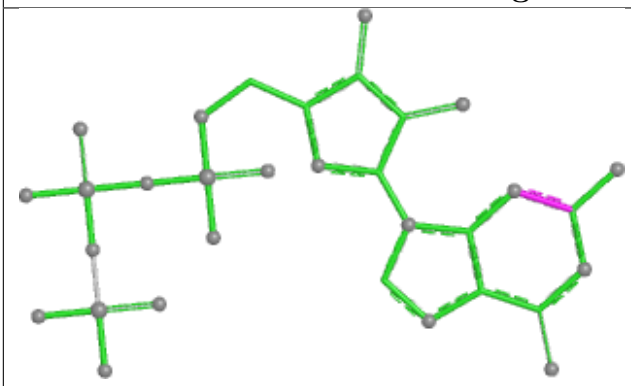
Ligand GDP TJ 502



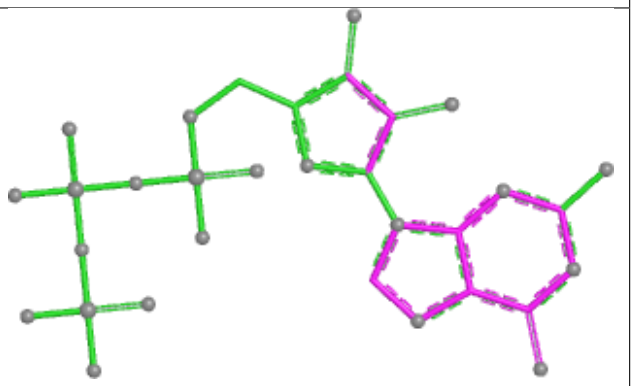
Ligand GDP UF 502



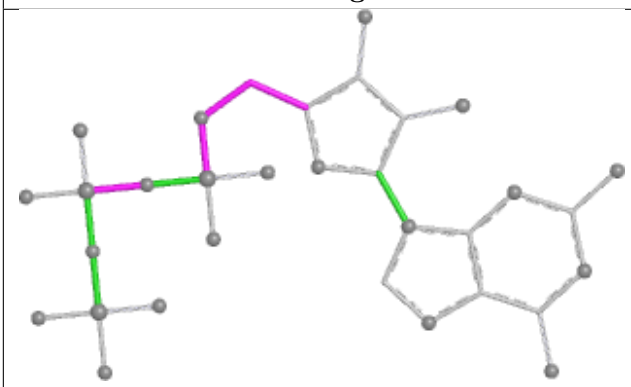
Ligand GTP SA 501



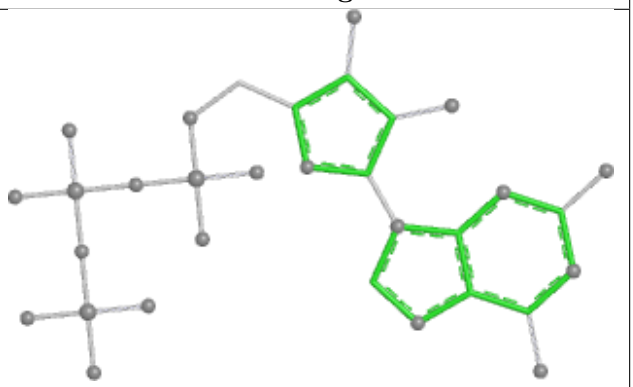
Bond lengths



Bond angles

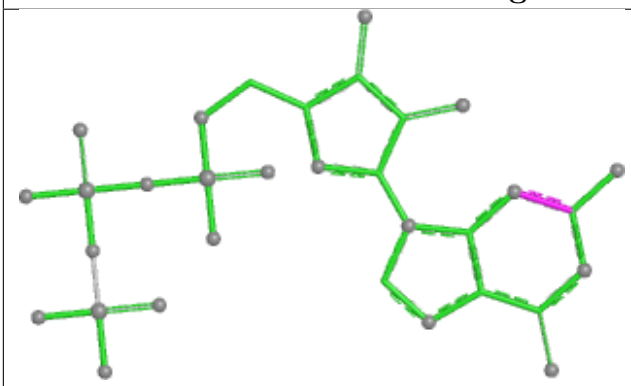


Torsions

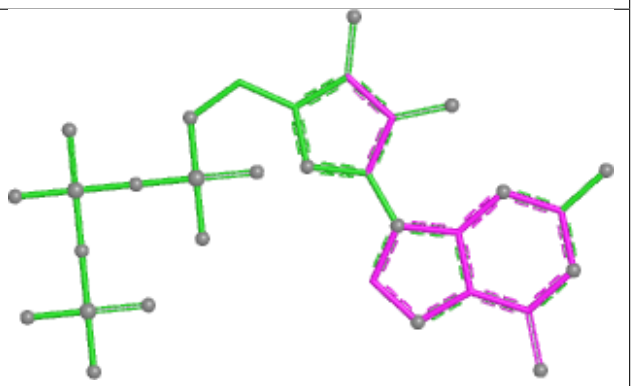


Rings

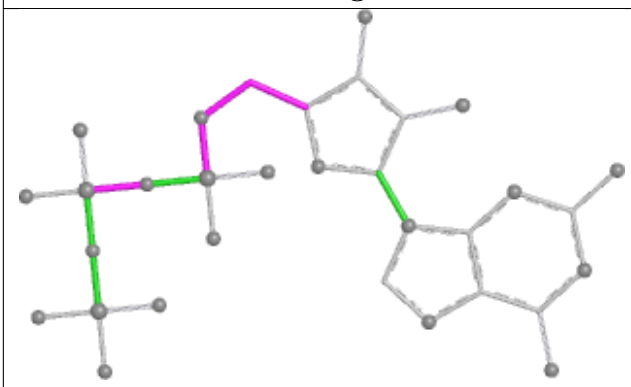
Ligand GTP PK 501



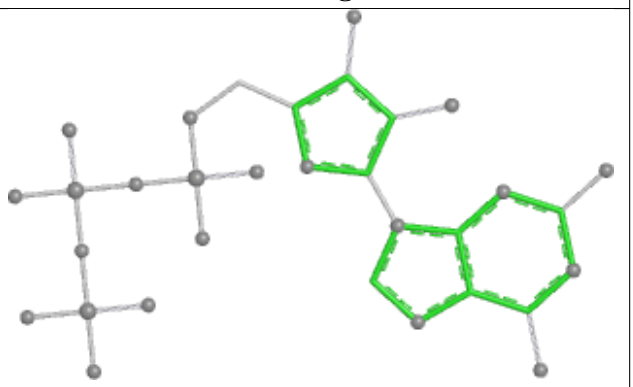
Bond lengths



Bond angles

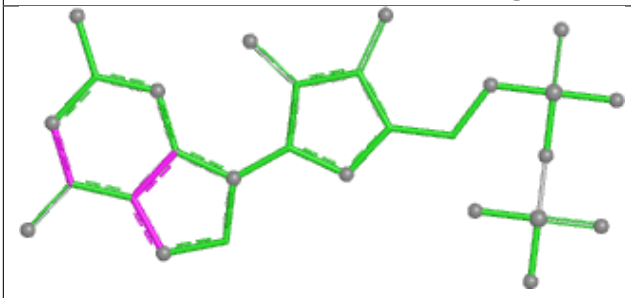


Torsions

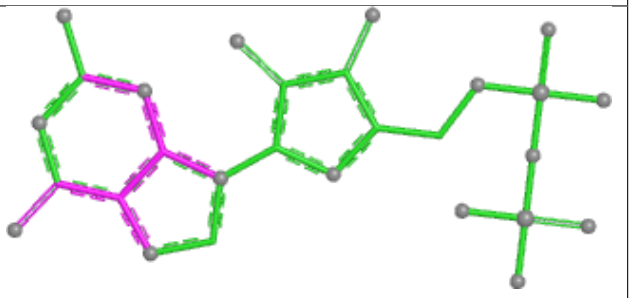


Rings

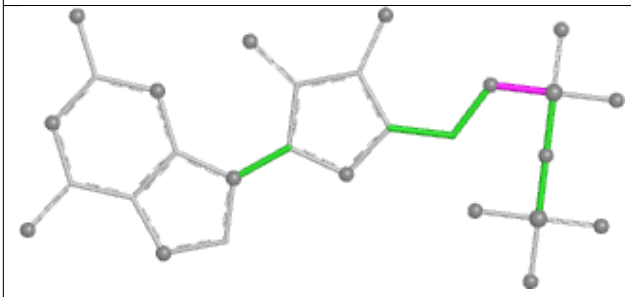
Ligand GDP KP 502



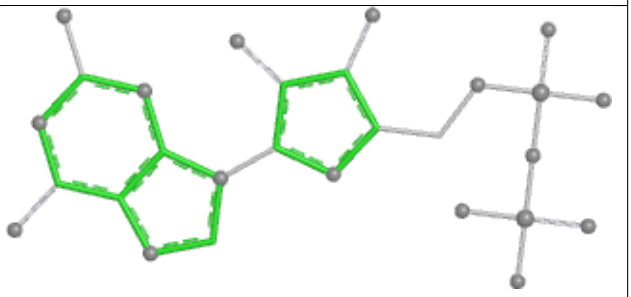
Bond lengths



Bond angles

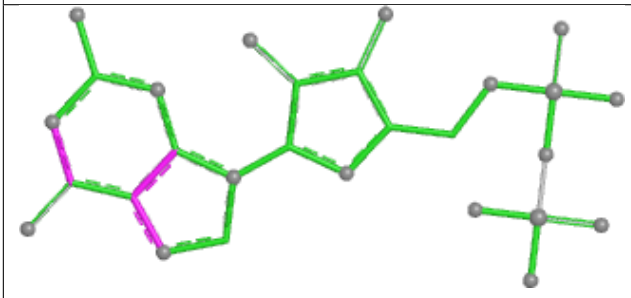


Torsions

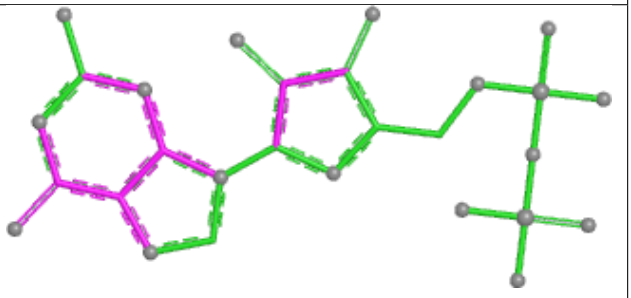


Rings

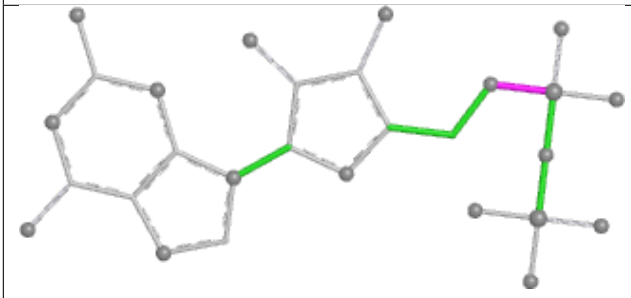
Ligand GDP QP 502



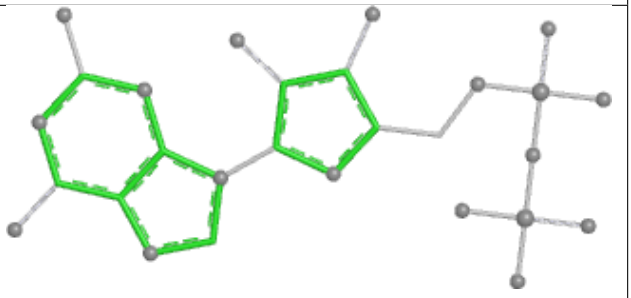
Bond lengths



Bond angles

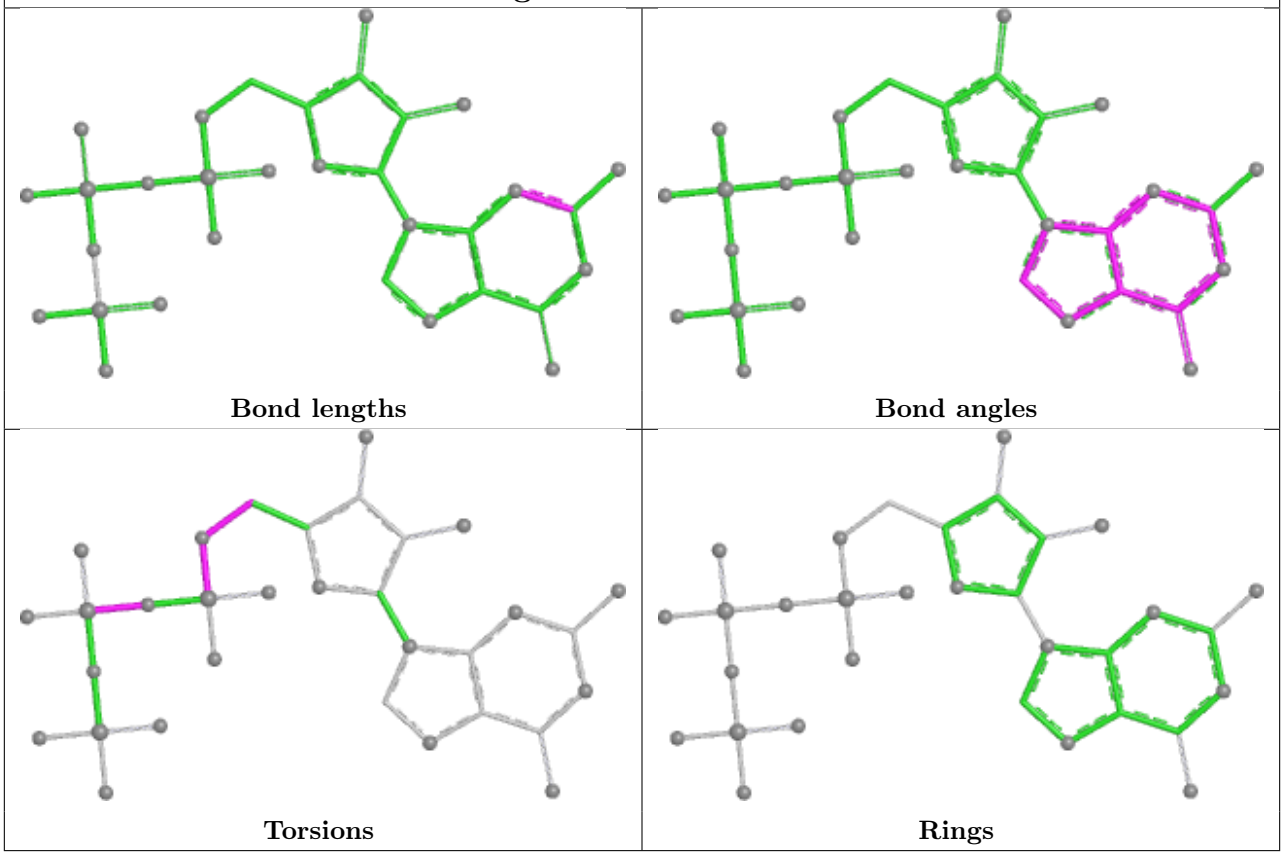


Torsions

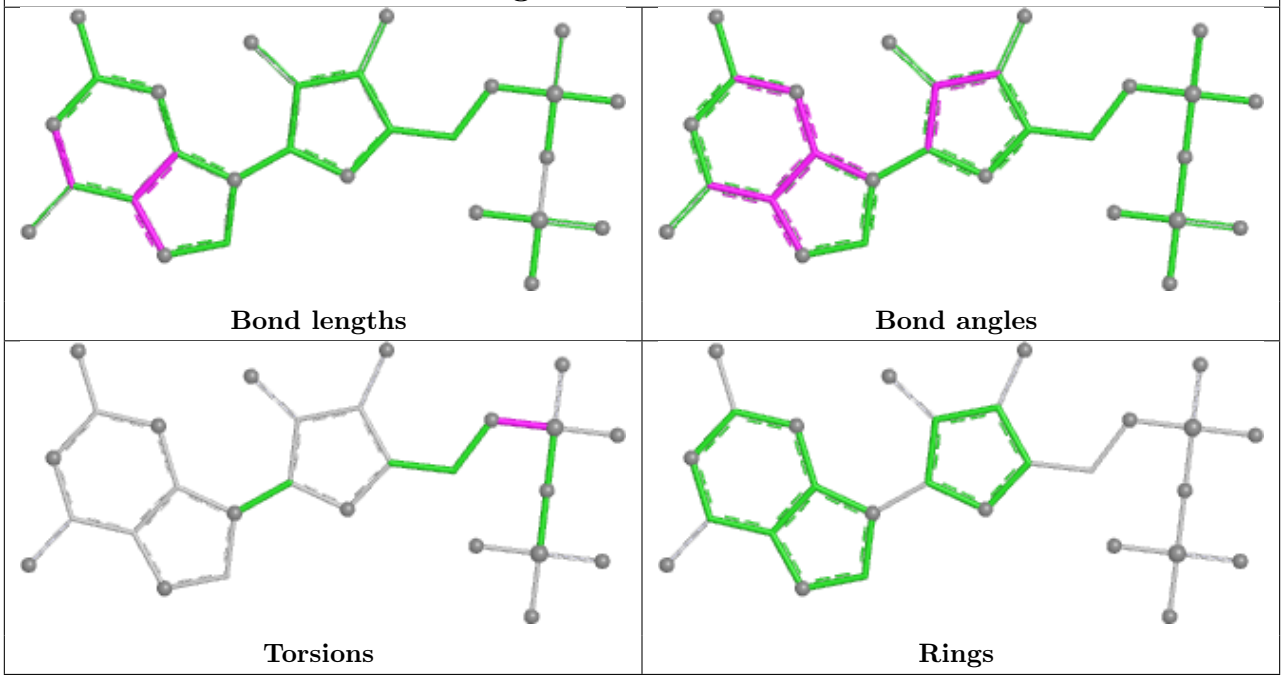


Rings

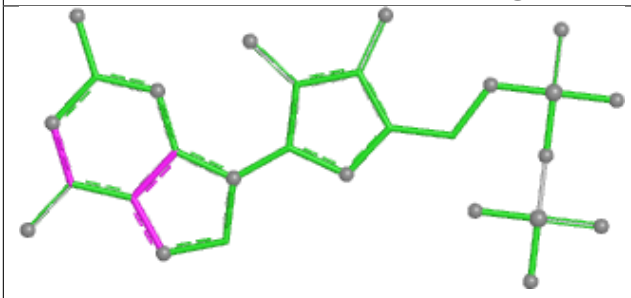
Ligand GTP FE 501



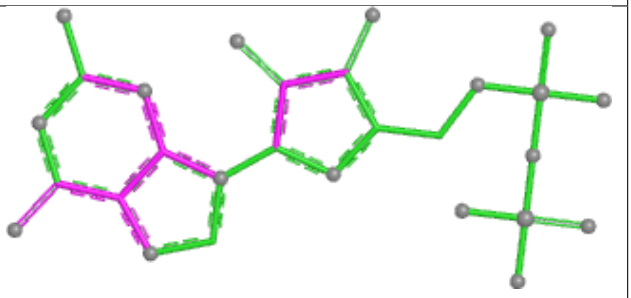
Ligand GDP UJ 502



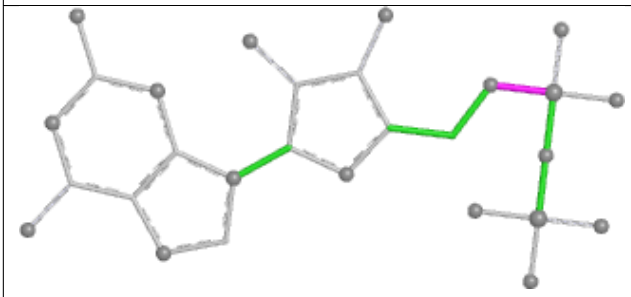
Ligand GDP ED 502



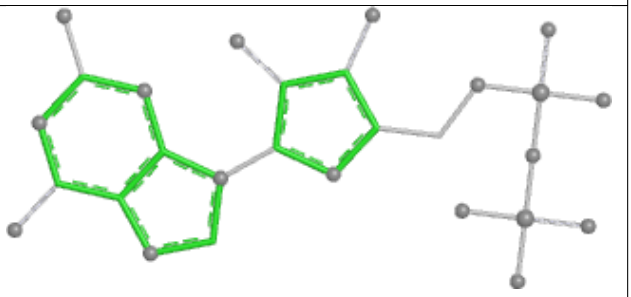
Bond lengths



Bond angles

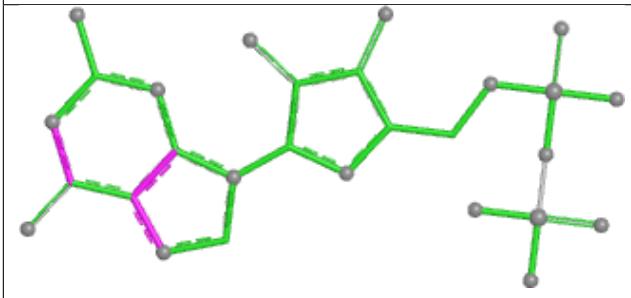


Torsions

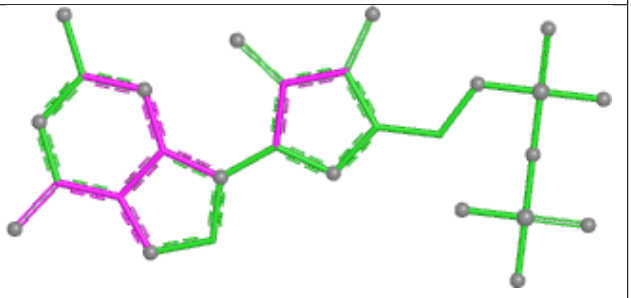


Rings

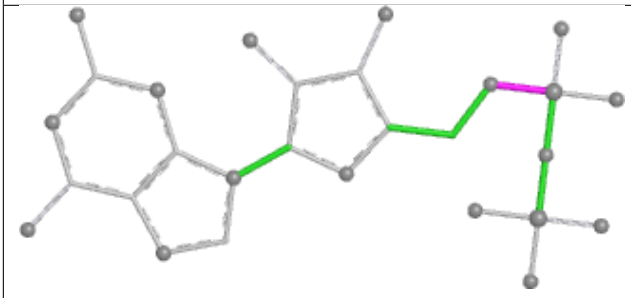
Ligand GDP QD 502



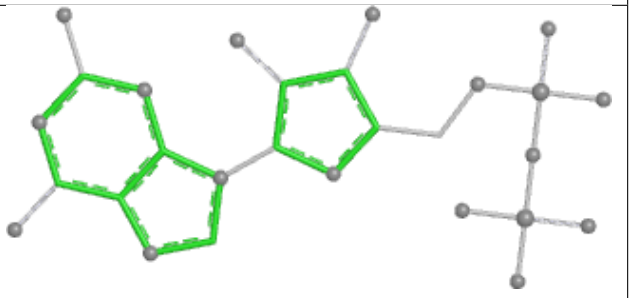
Bond lengths



Bond angles

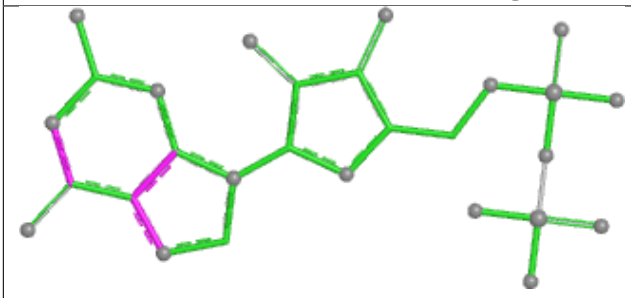


Torsions

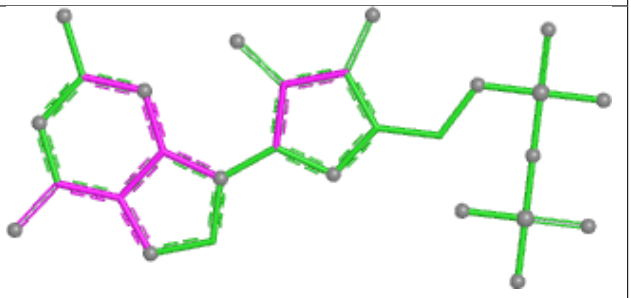


Rings

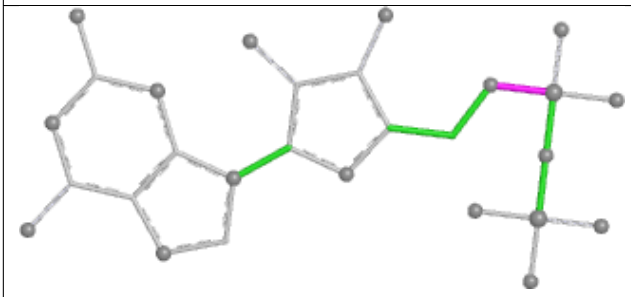
Ligand GDP DN 502



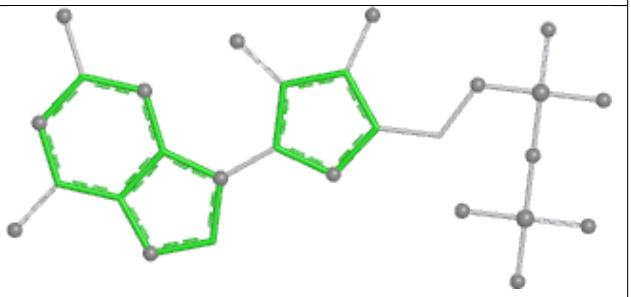
Bond lengths



Bond angles

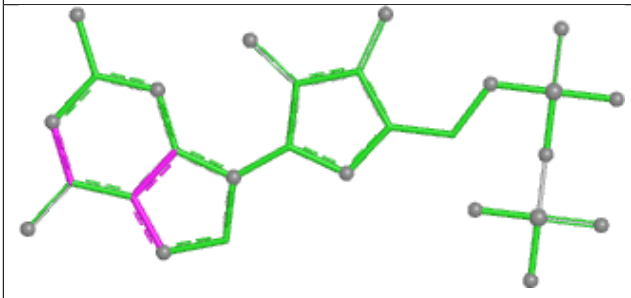


Torsions

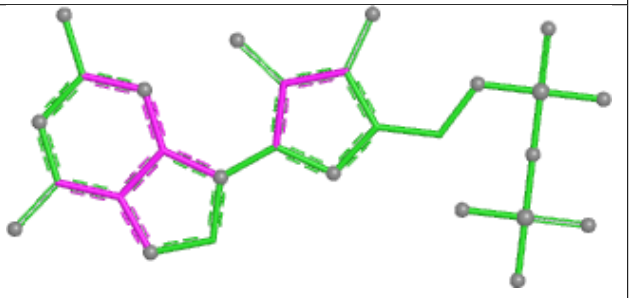


Rings

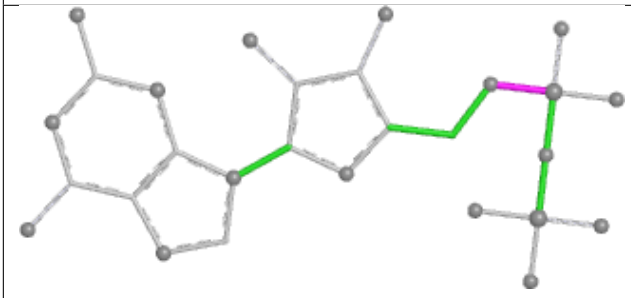
Ligand GDP WH 502



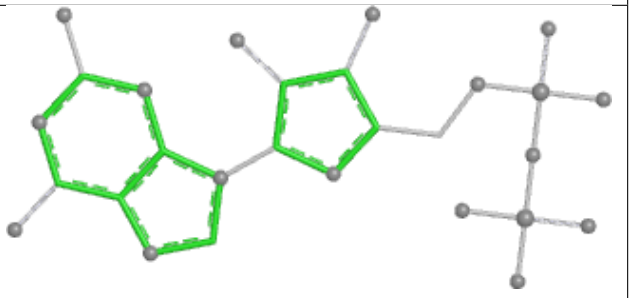
Bond lengths



Bond angles

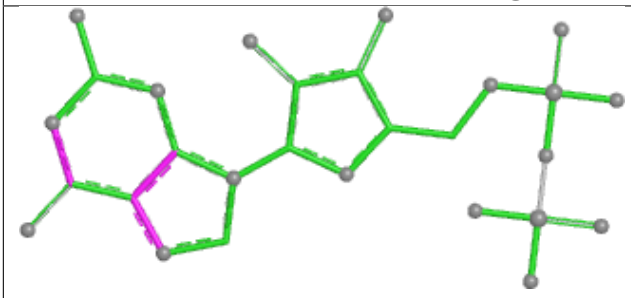


Torsions

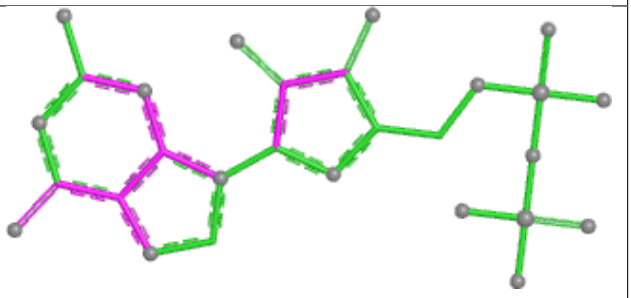


Rings

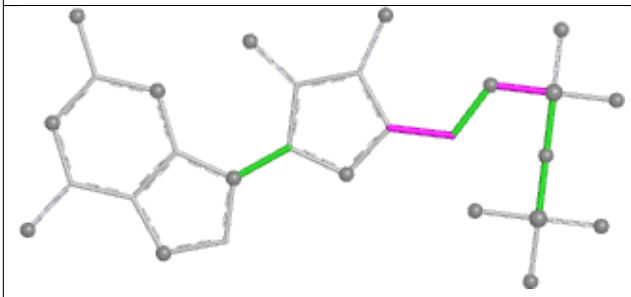
Ligand GDP UD 502



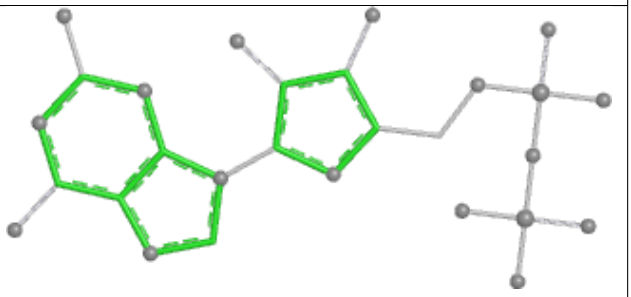
Bond lengths



Bond angles

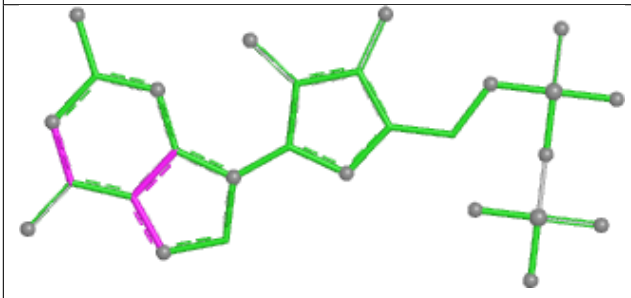


Torsions

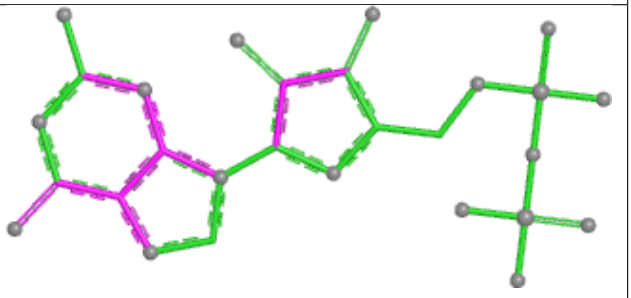


Rings

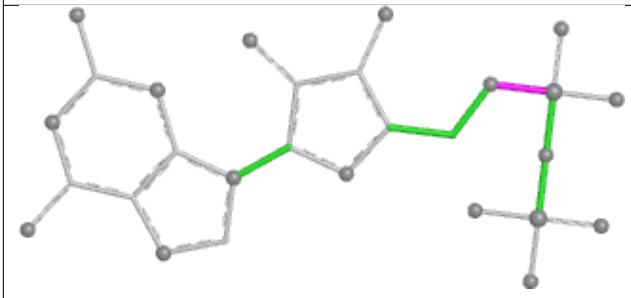
Ligand GDP GL 502



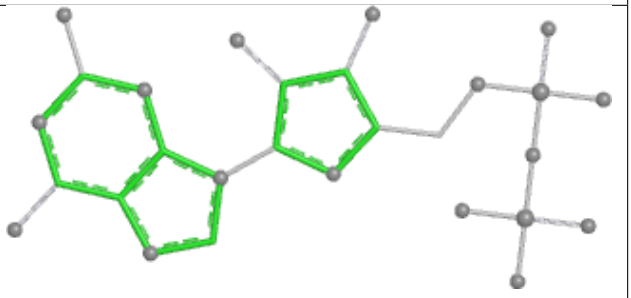
Bond lengths



Bond angles

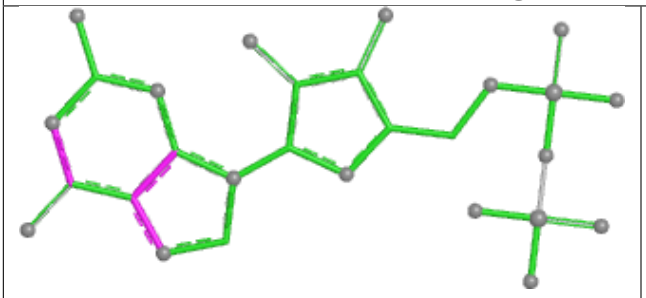


Torsions

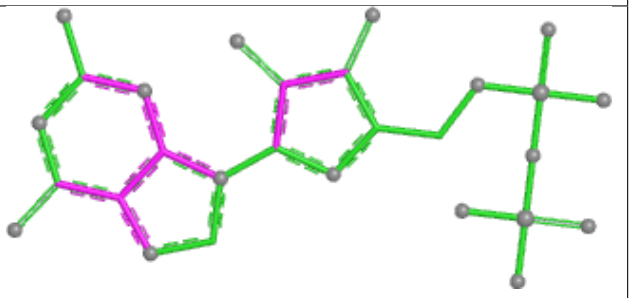


Rings

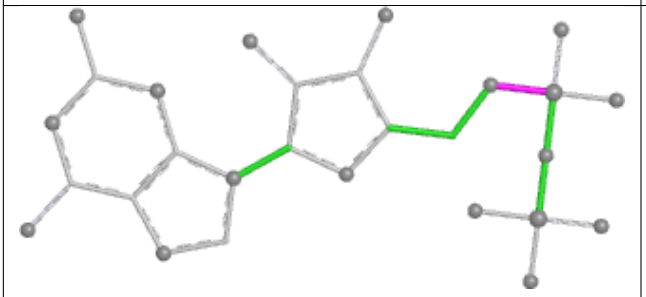
Ligand GDP PP 502



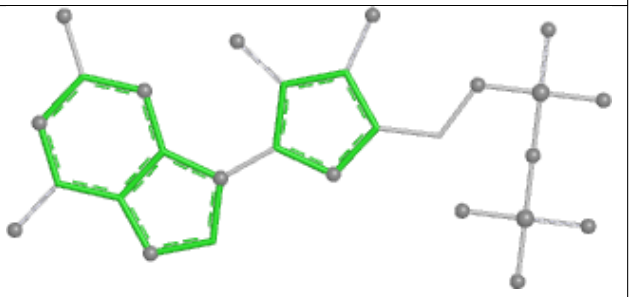
Bond lengths



Bond angles

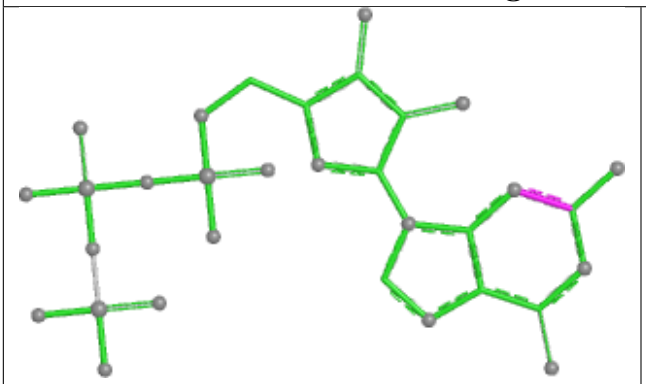


Torsions

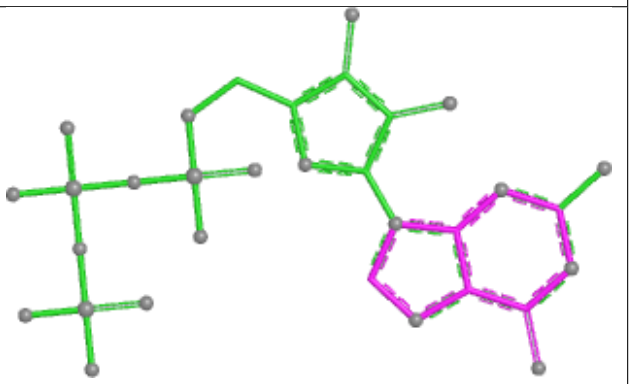


Rings

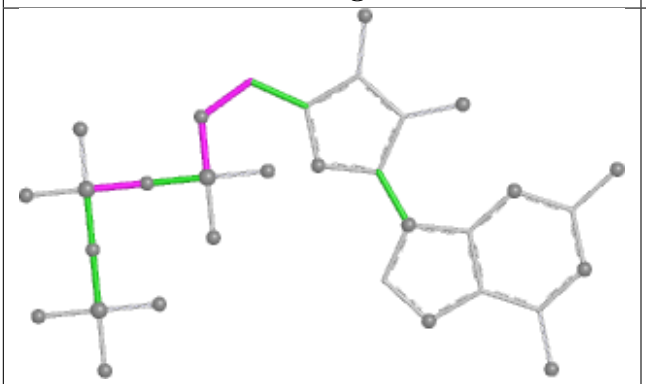
Ligand GTP MG 501



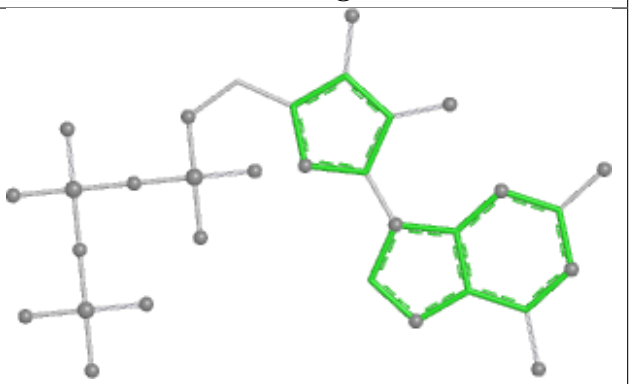
Bond lengths



Bond angles

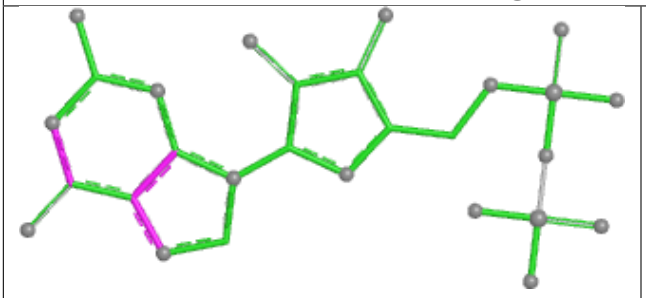


Torsions

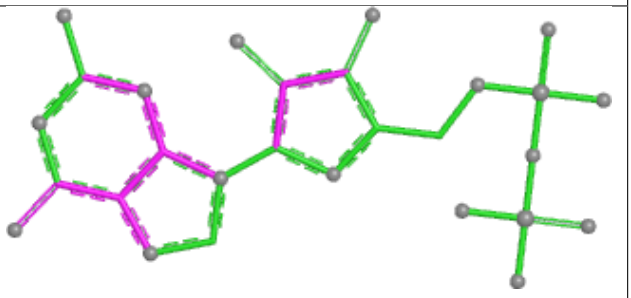


Rings

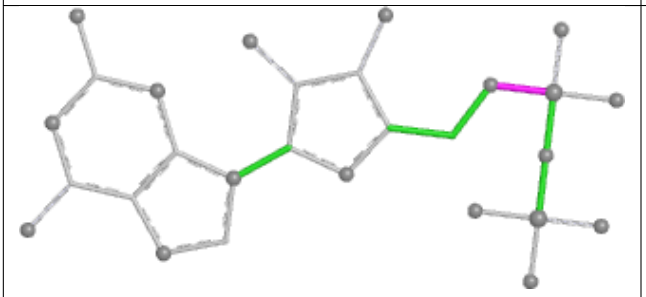
Ligand GDP AP 502



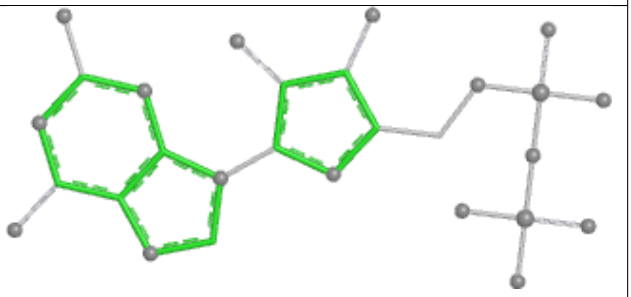
Bond lengths



Bond angles

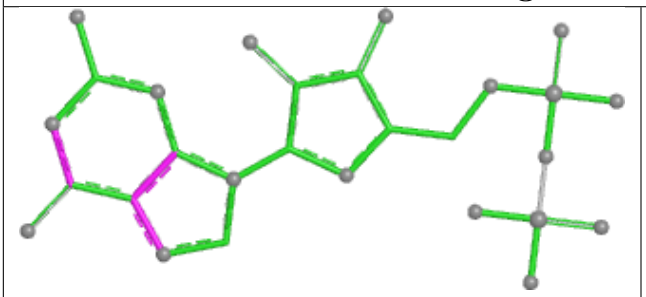


Torsions

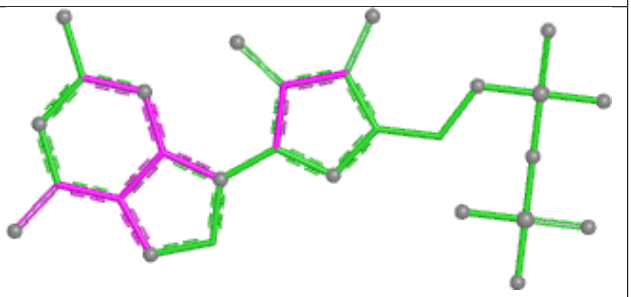


Rings

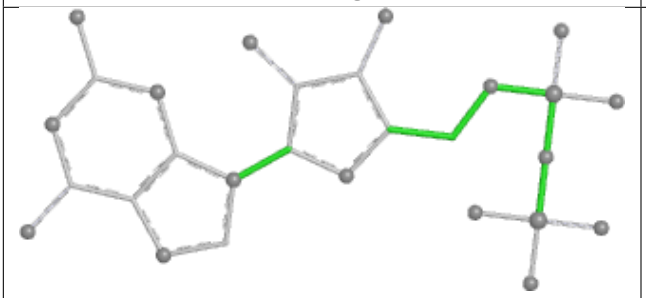
Ligand GDP IL 502



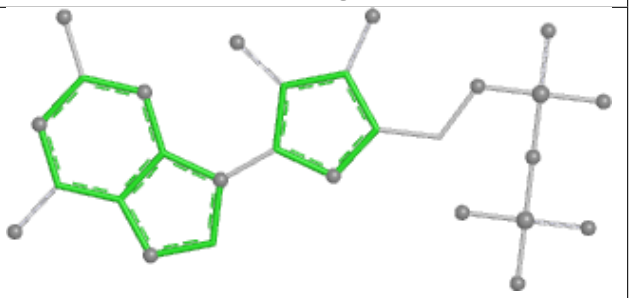
Bond lengths



Bond angles

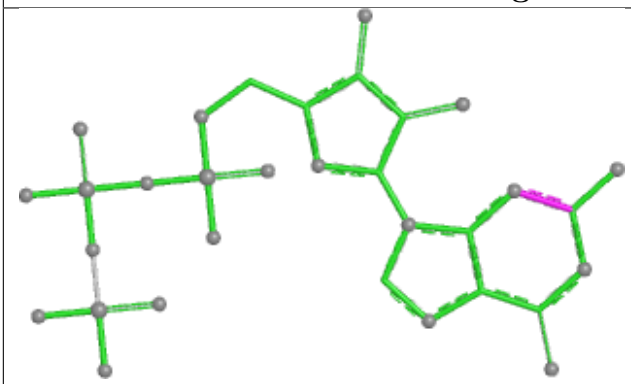


Torsions

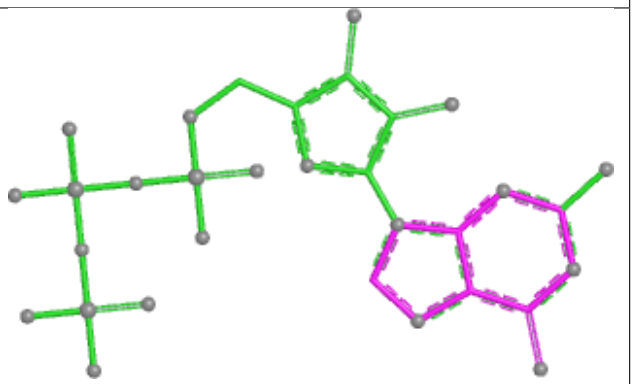


Rings

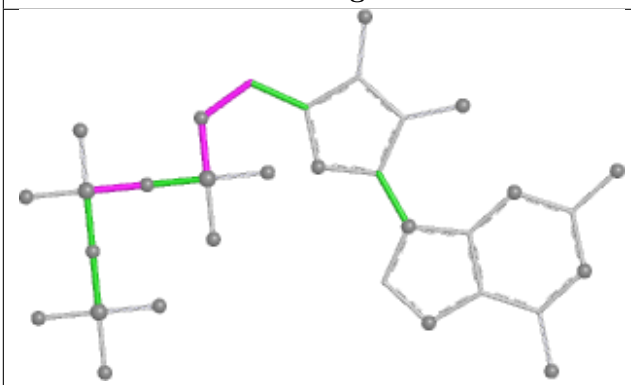
Ligand GTP LC 501



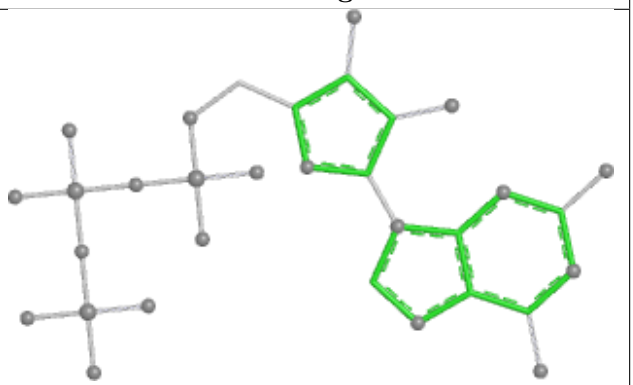
Bond lengths



Bond angles

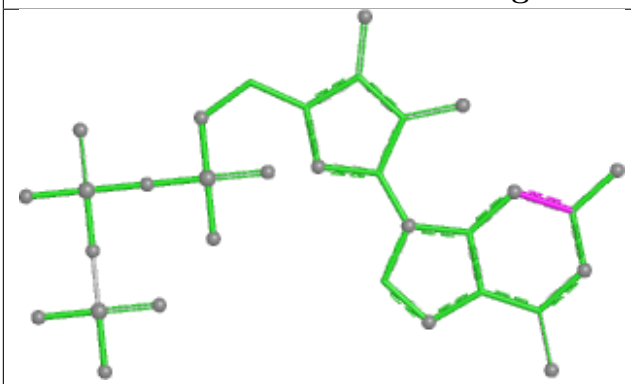


Torsions

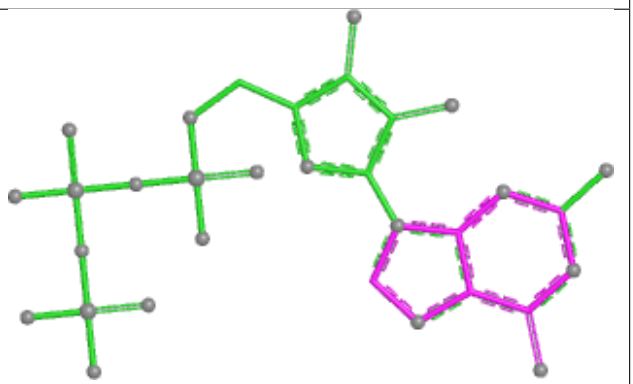


Rings

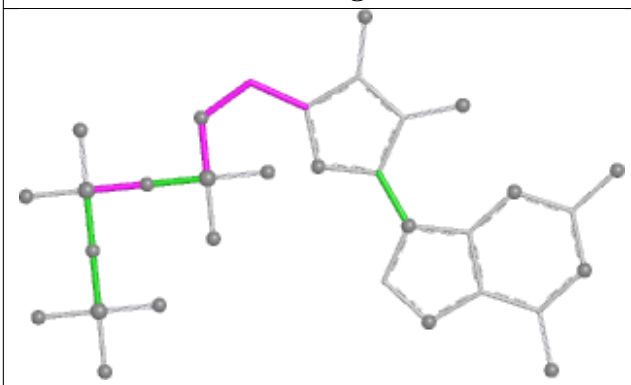
Ligand GTP SG 501



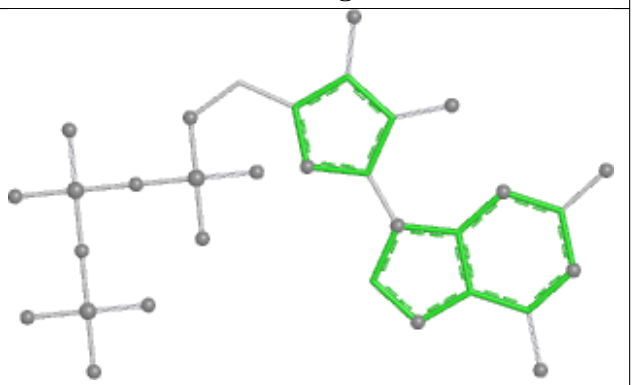
Bond lengths



Bond angles

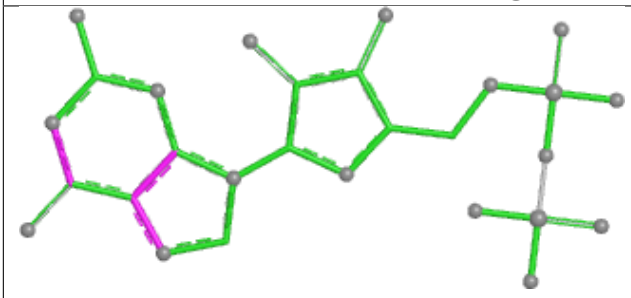


Torsions

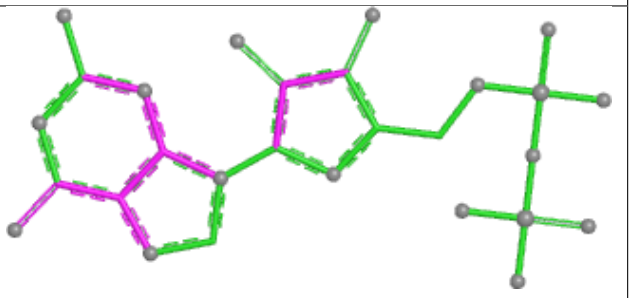


Rings

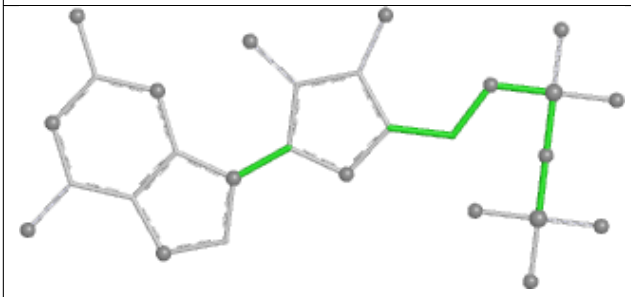
Ligand GDP RD 502



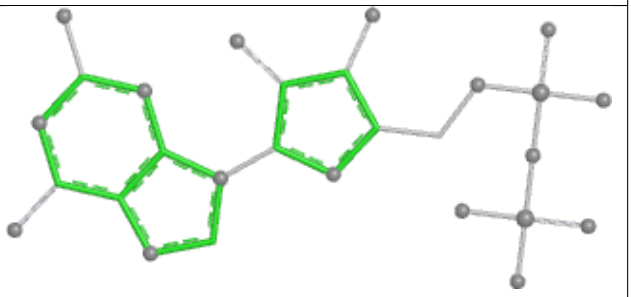
Bond lengths



Bond angles

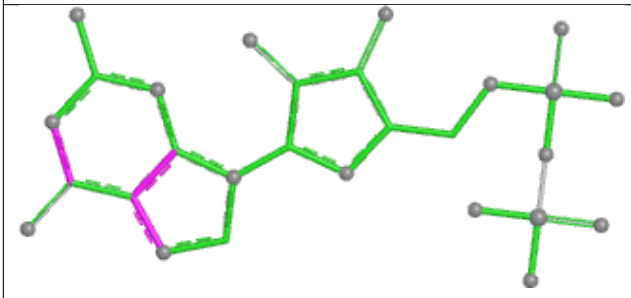


Torsions

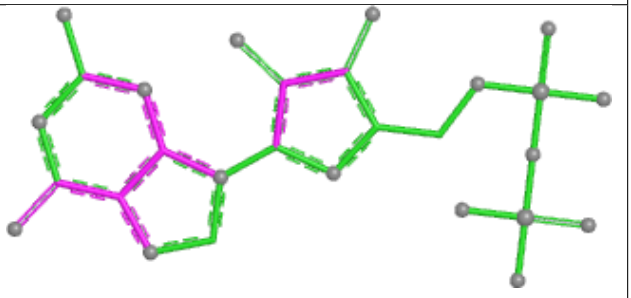


Rings

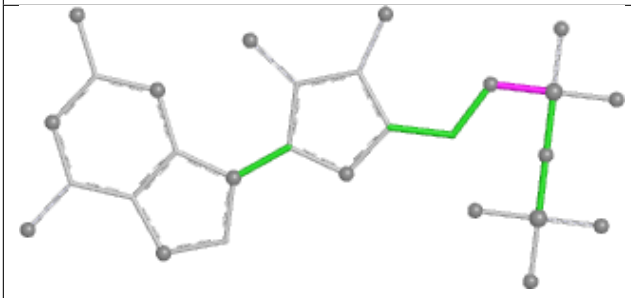
Ligand GDP BF 502



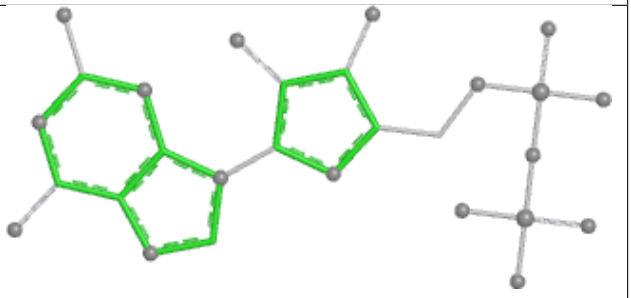
Bond lengths



Bond angles

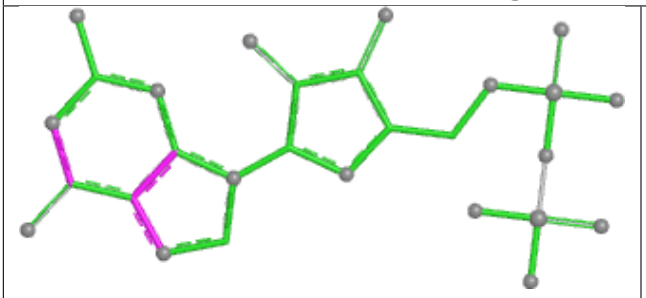


Torsions

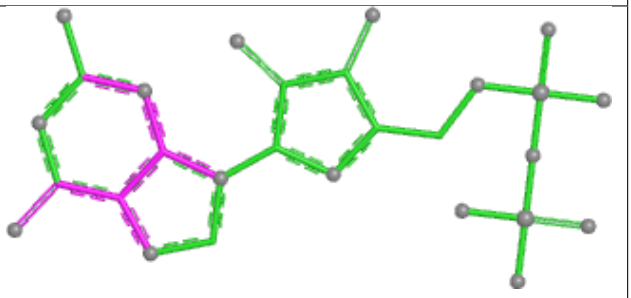


Rings

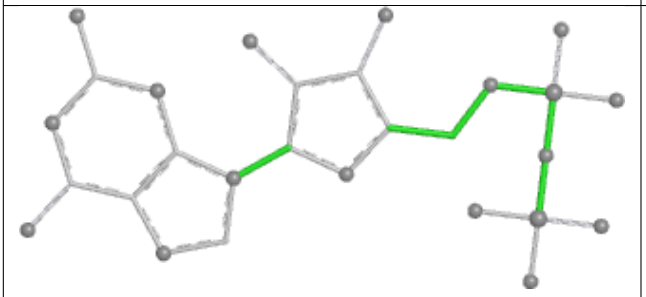
Ligand GDP HH 502



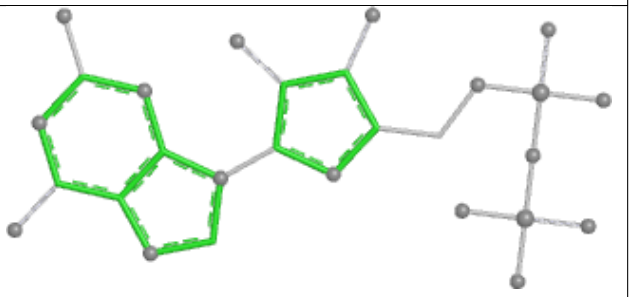
Bond lengths



Bond angles

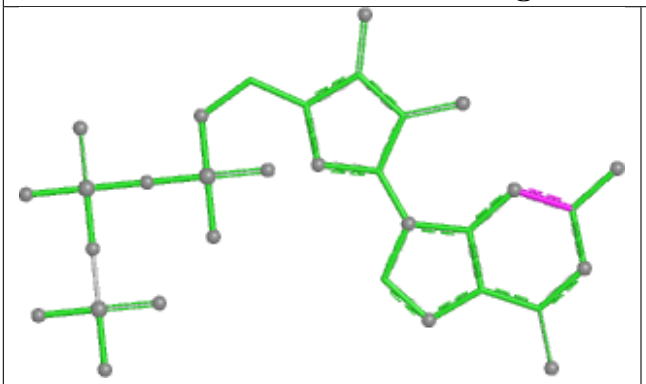


Torsions

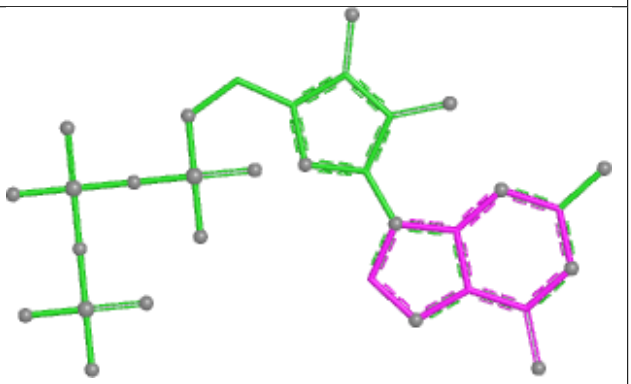


Rings

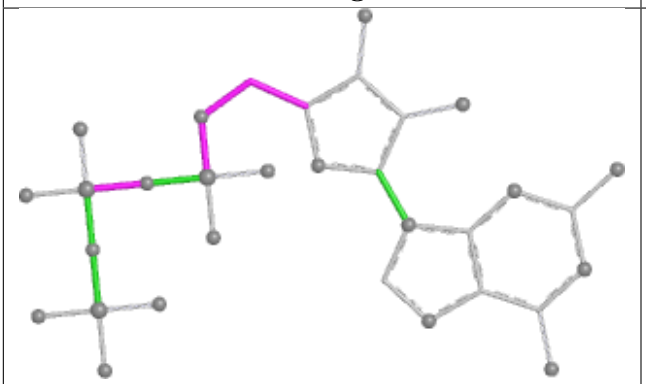
Ligand GTP KI 501



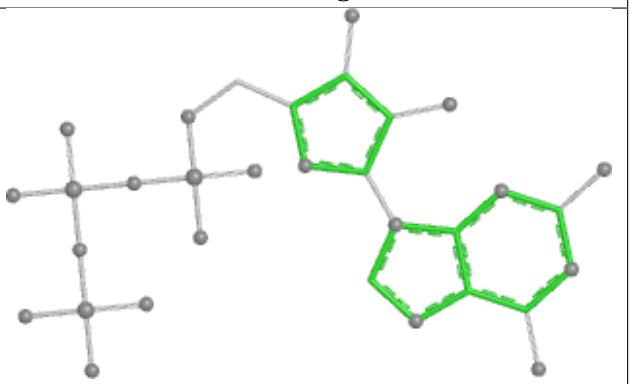
Bond lengths



Bond angles

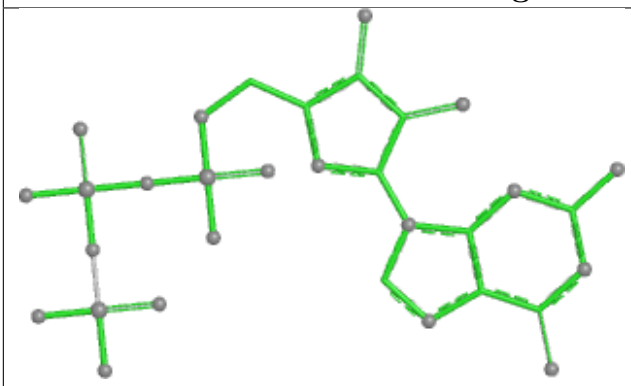


Torsions

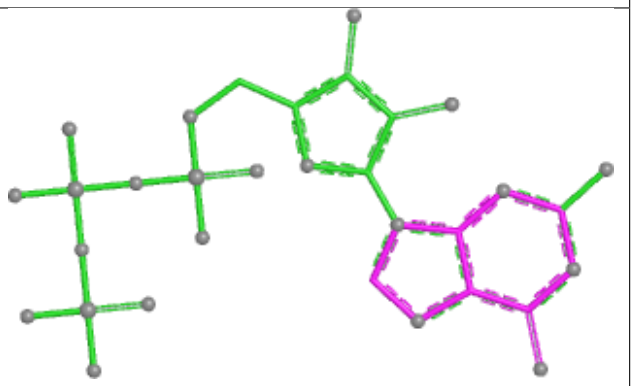


Rings

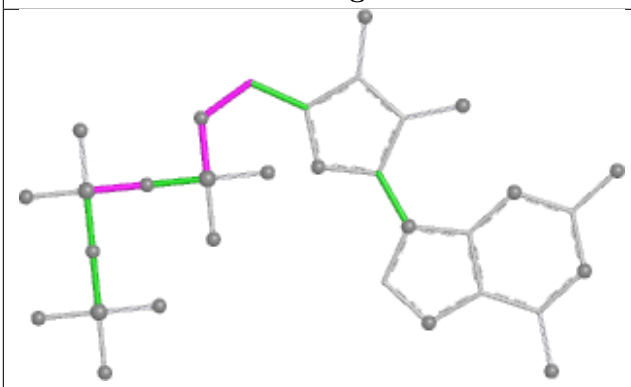
Ligand GTP MI 501



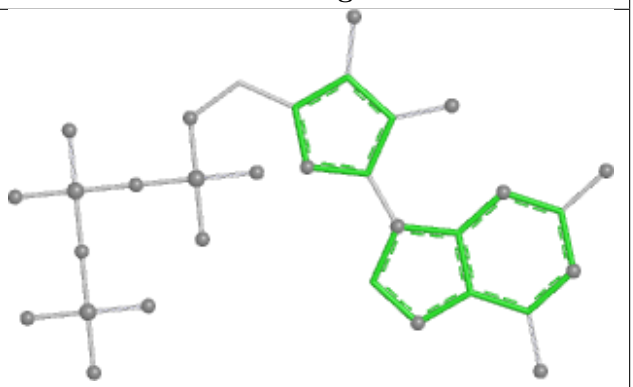
Bond lengths



Bond angles

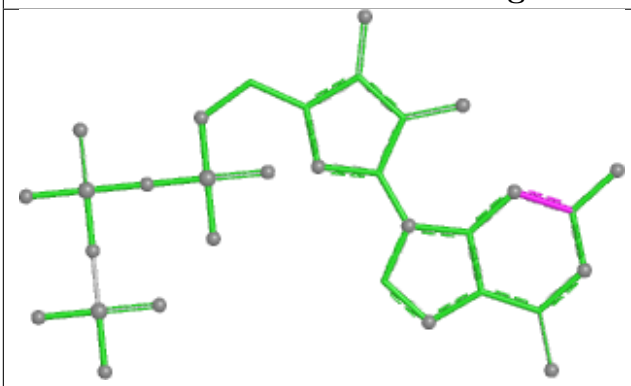


Torsions

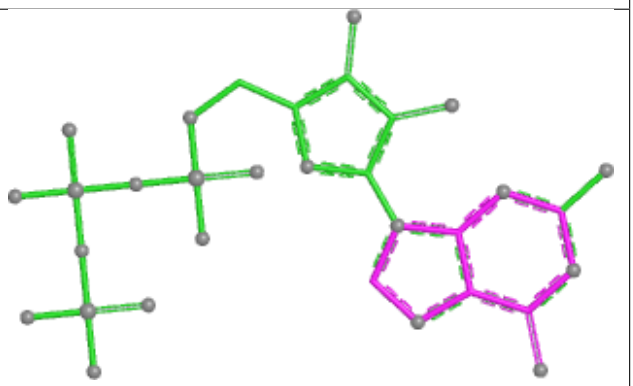


Rings

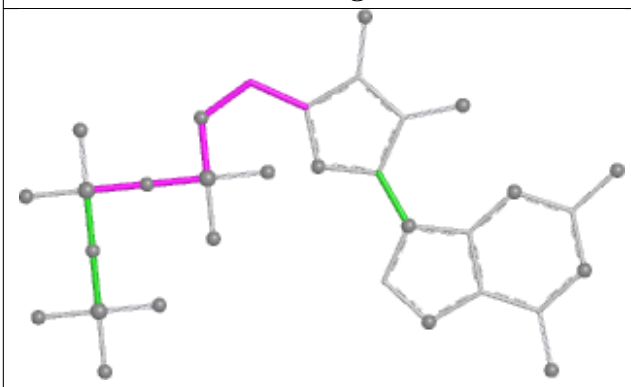
Ligand GTP NK 501



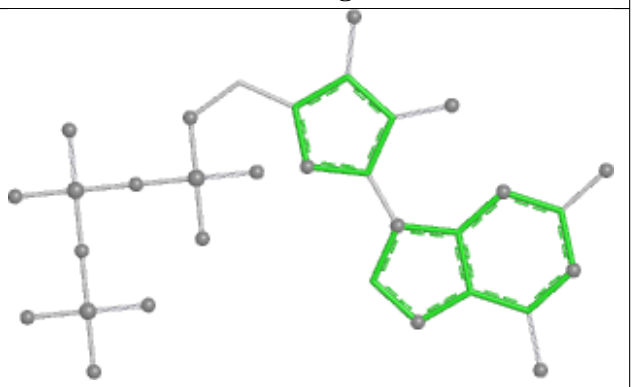
Bond lengths



Bond angles

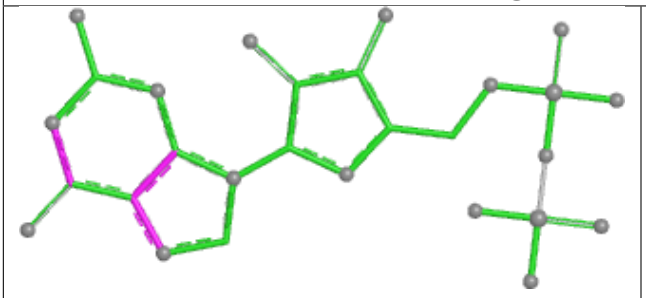


Torsions

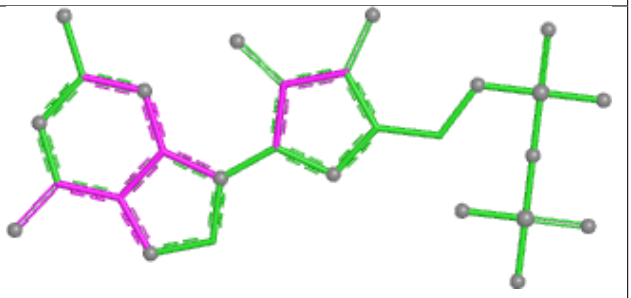


Rings

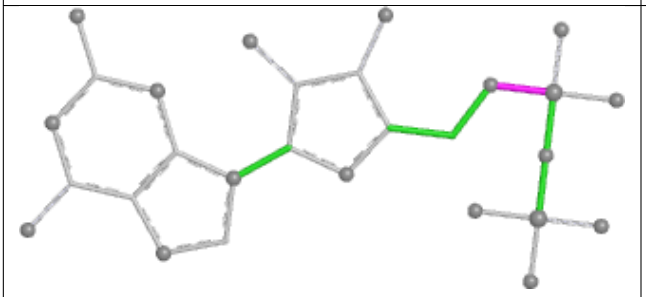
Ligand GDP DB 502



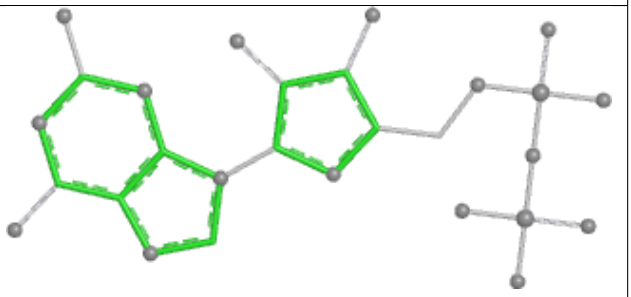
Bond lengths



Bond angles

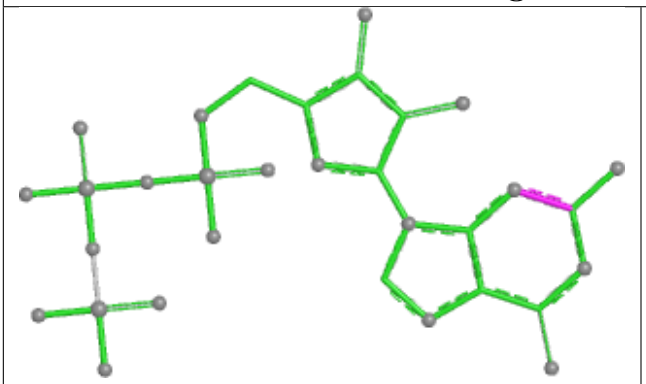


Torsions

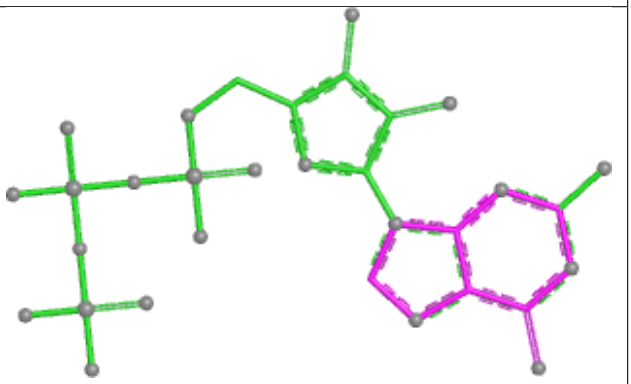


Rings

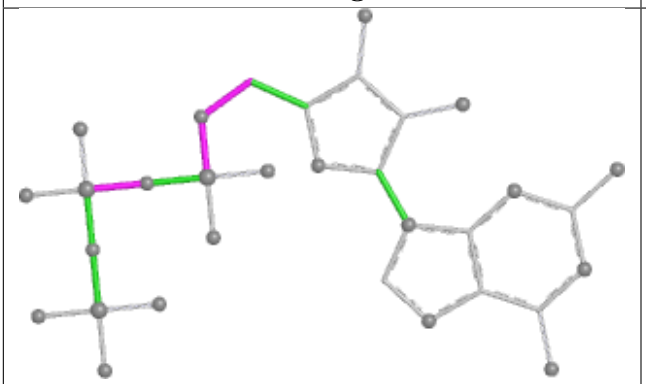
Ligand GTP KK 501



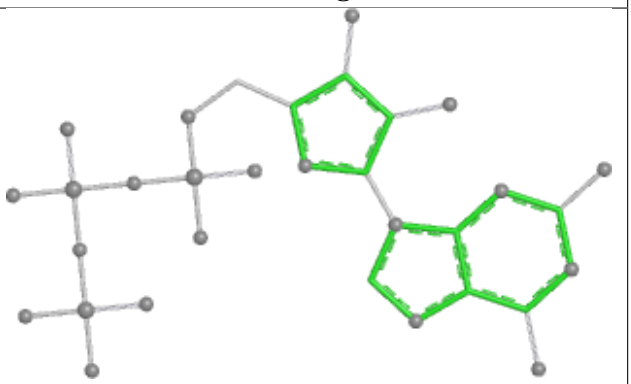
Bond lengths



Bond angles

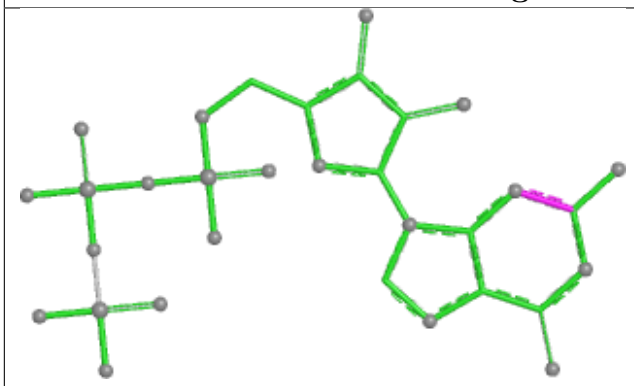


Torsions

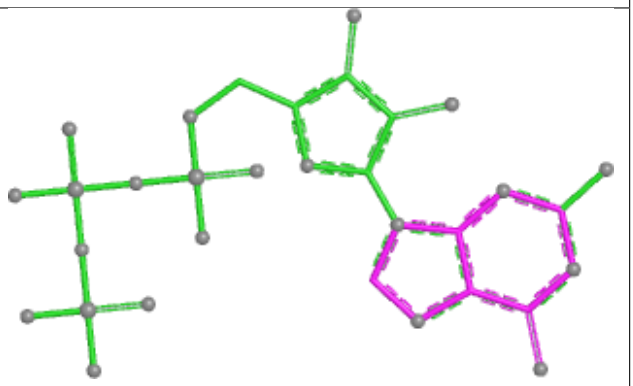


Rings

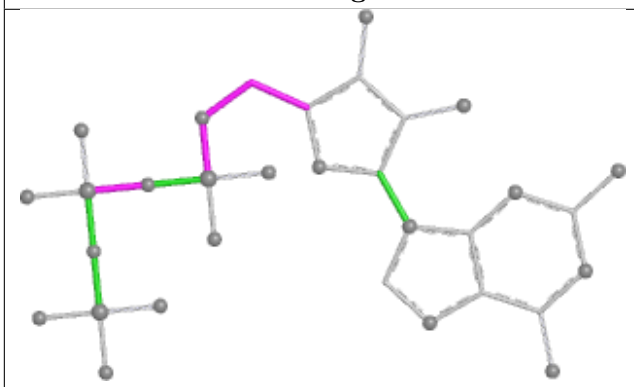
Ligand GTP EO 501



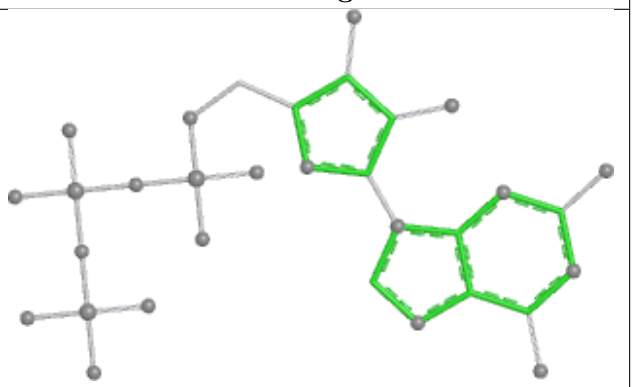
Bond lengths



Bond angles

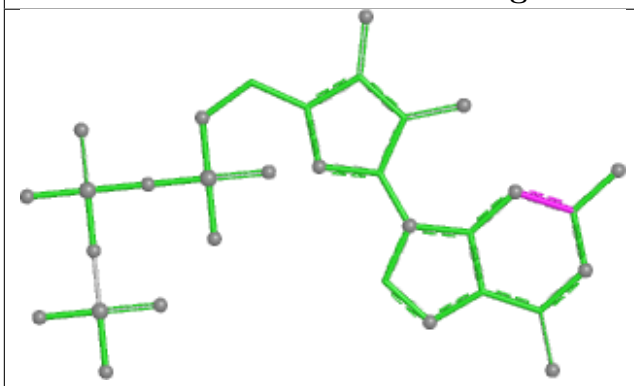


Torsions

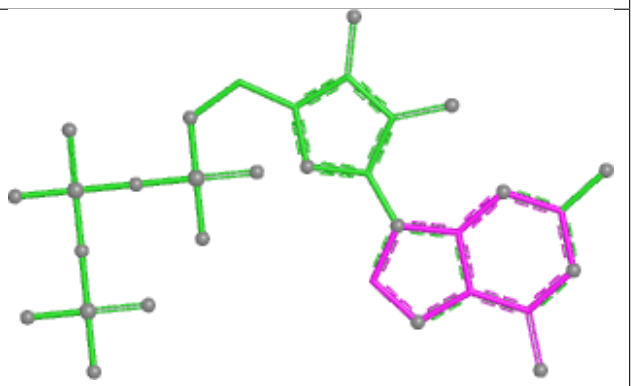


Rings

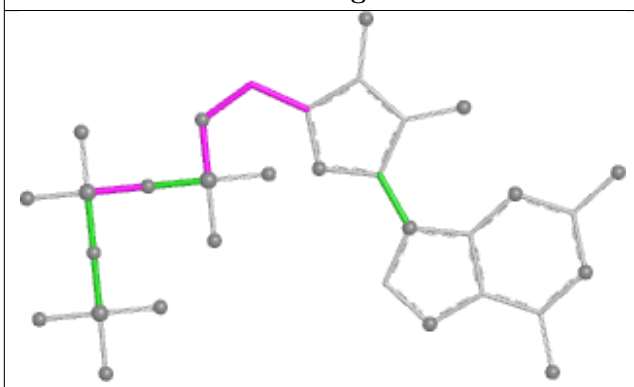
Ligand GTP BK 501



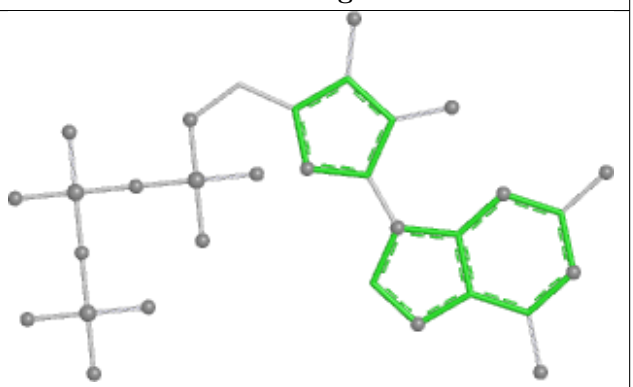
Bond lengths



Bond angles

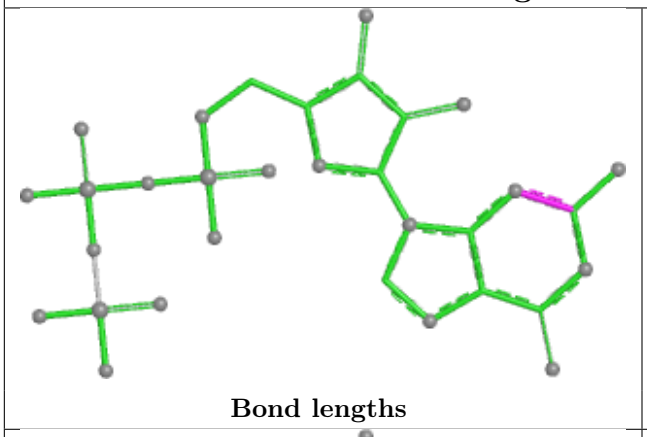


Torsions

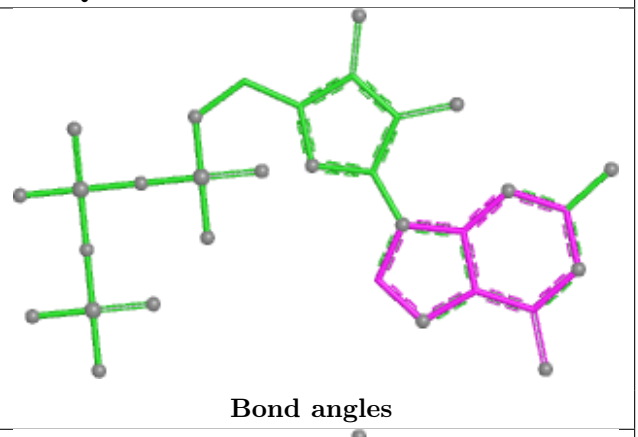


Rings

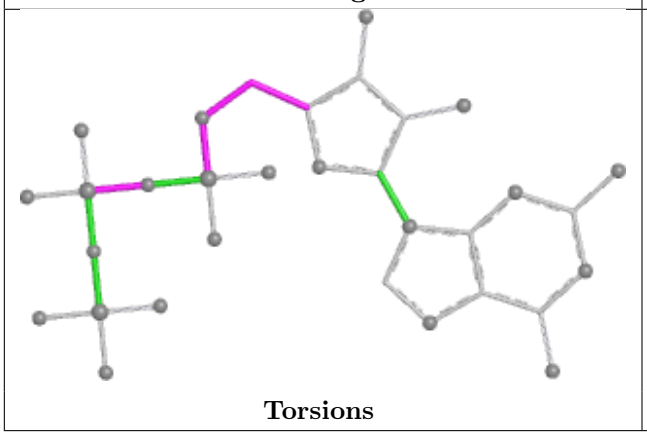
Ligand GTP JQ 501



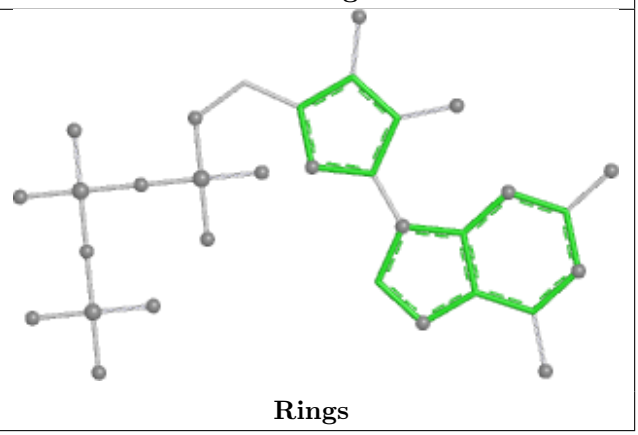
Bond lengths



Bond angles

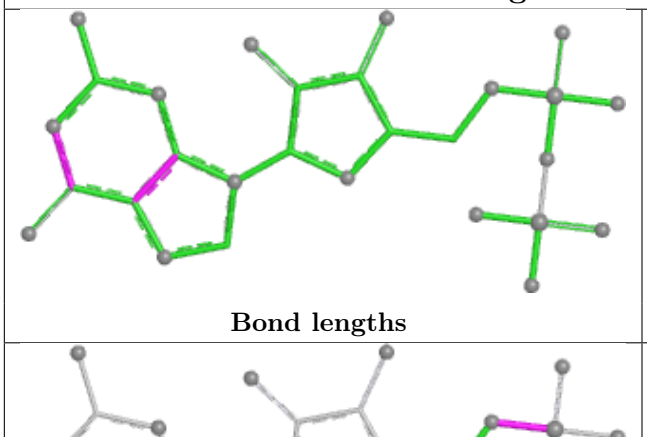


Torsions

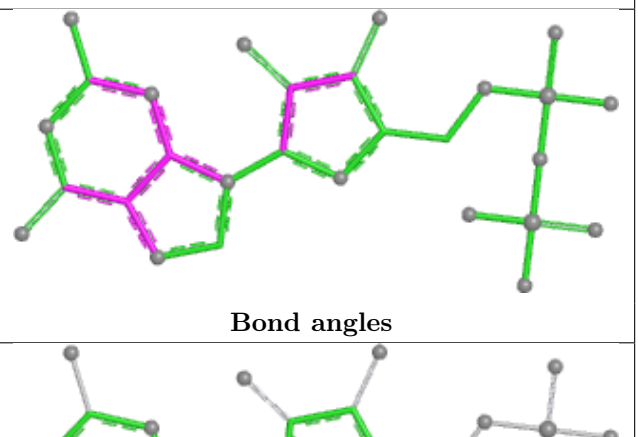


Rings

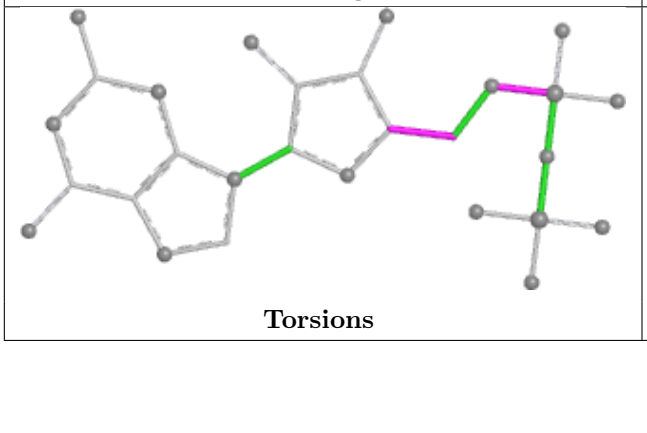
Ligand GDP PN 502



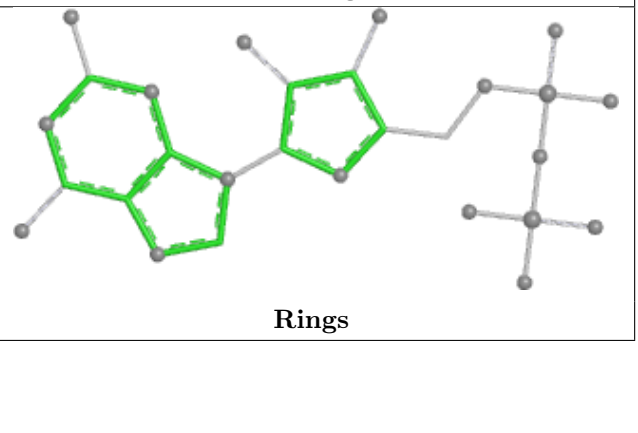
Bond lengths



Bond angles

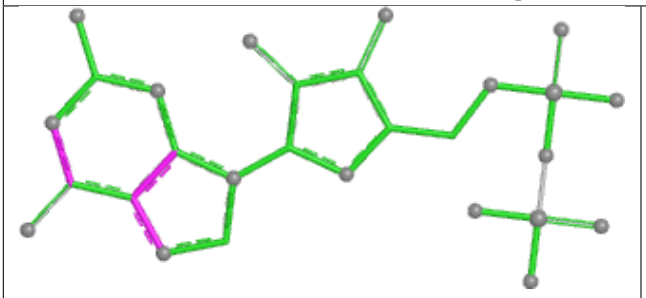


Torsions

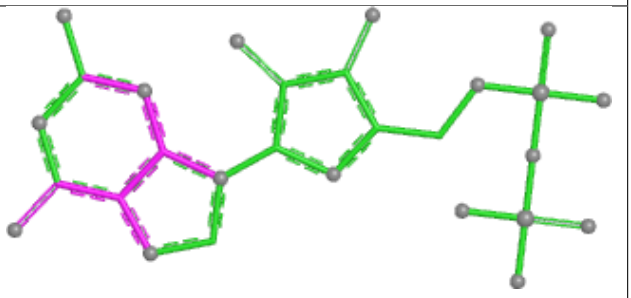


Rings

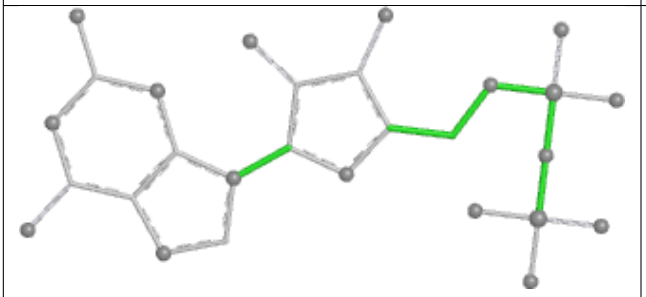
Ligand GDP AF 502



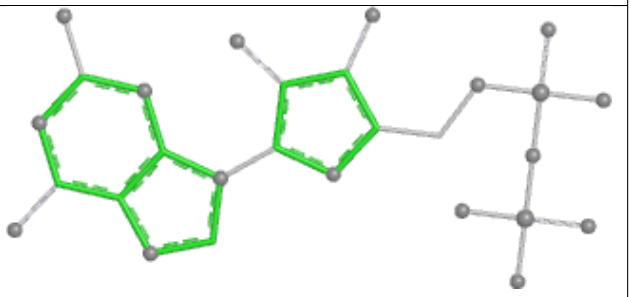
Bond lengths



Bond angles

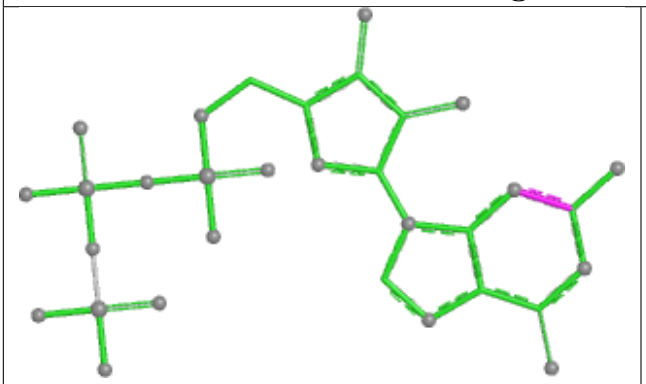


Torsions

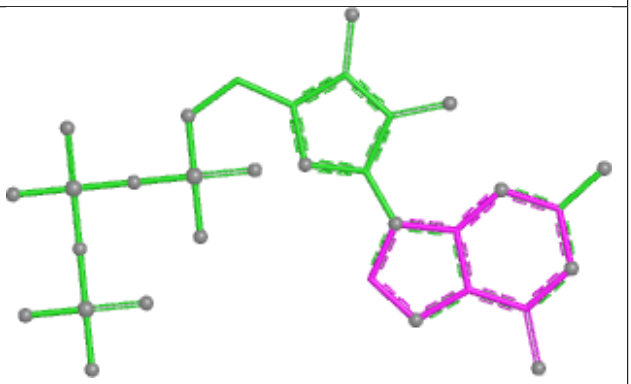


Rings

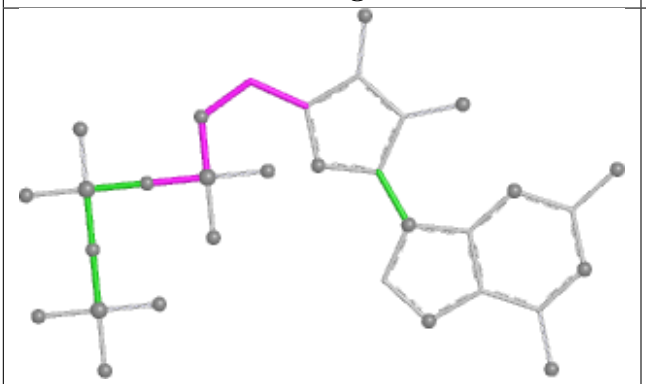
Ligand GTP NE 501



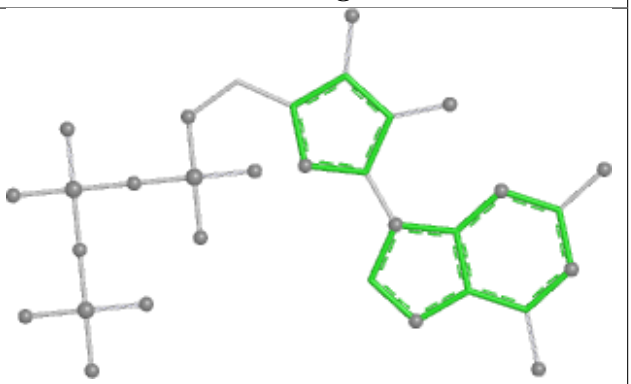
Bond lengths



Bond angles

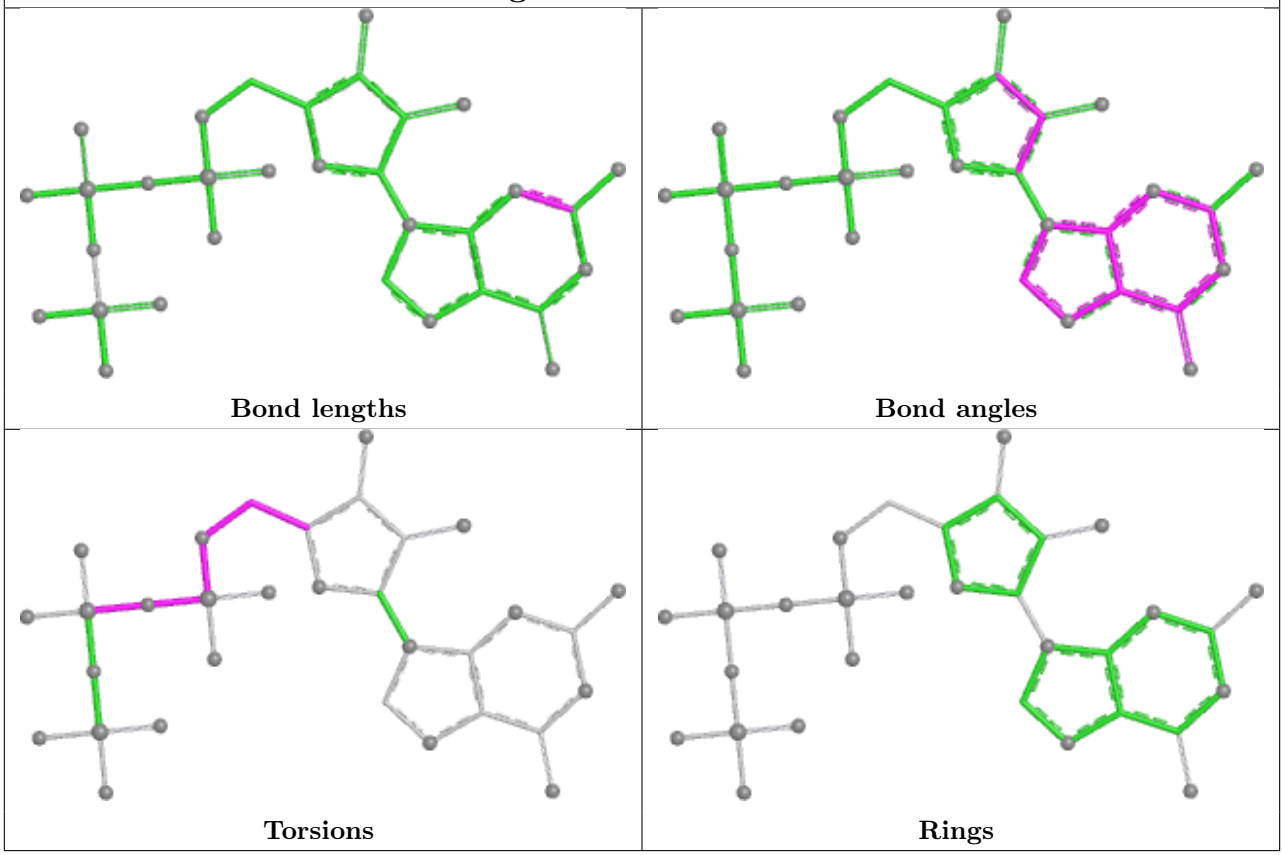


Torsions

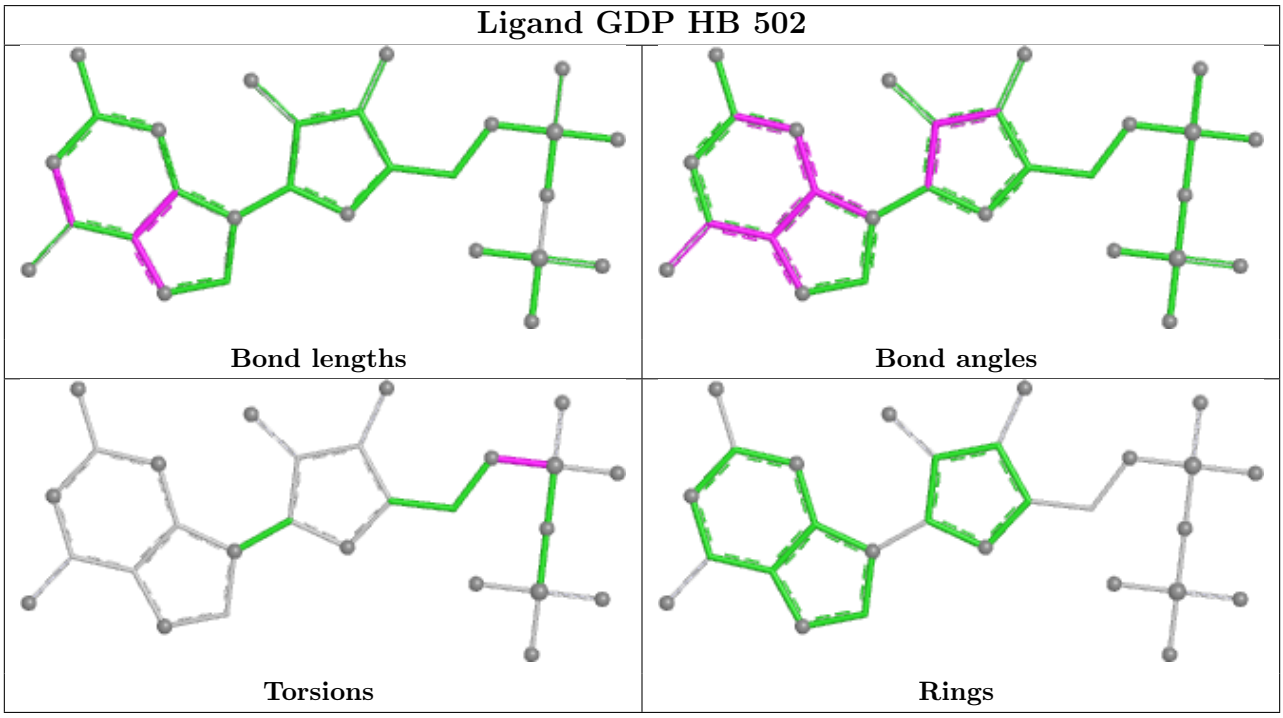


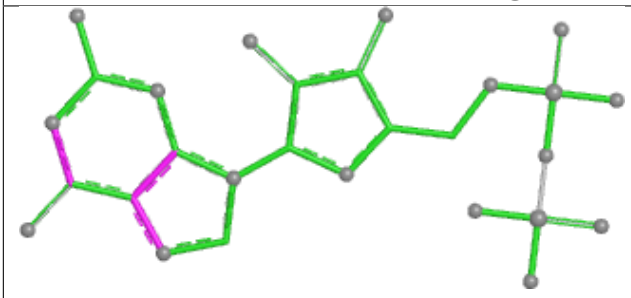
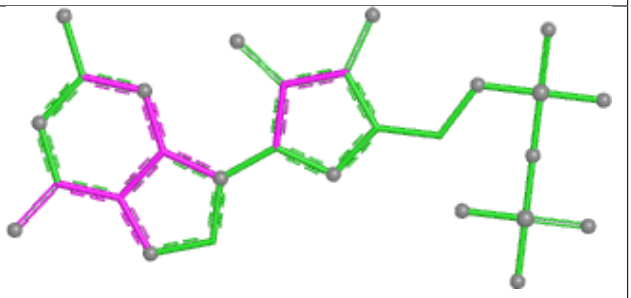
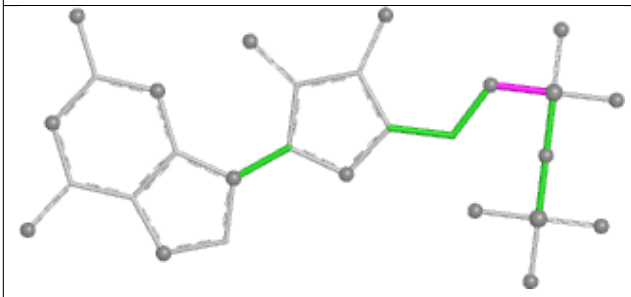
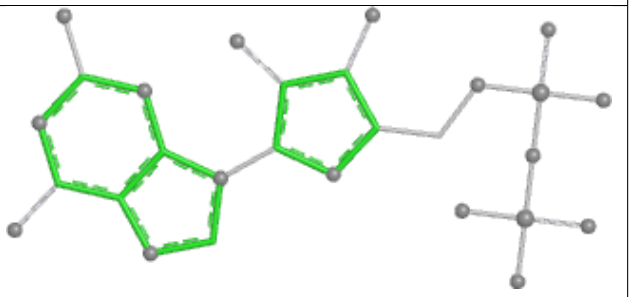
Rings

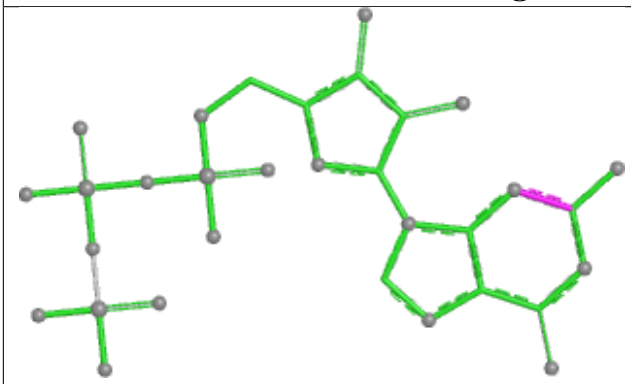
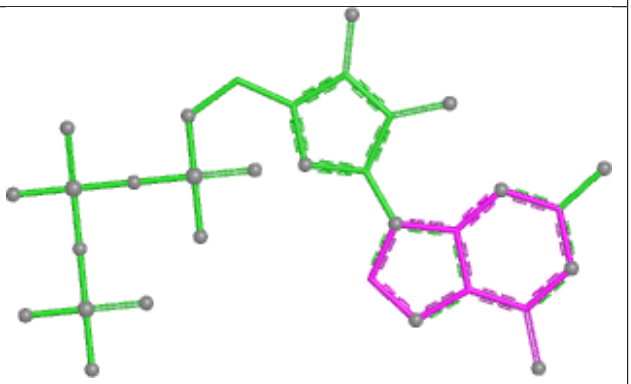
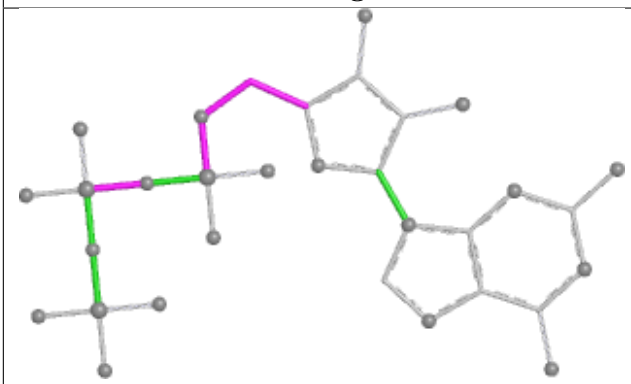
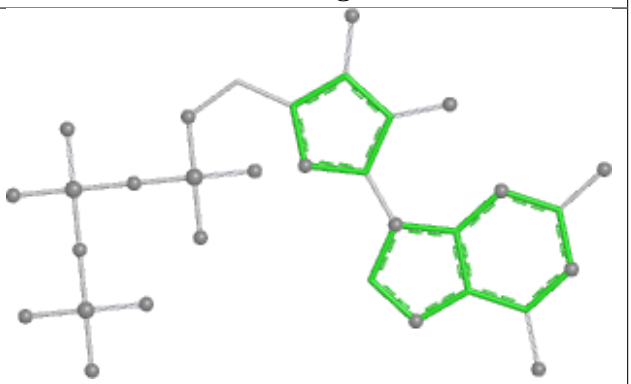
Ligand GTP UK 501



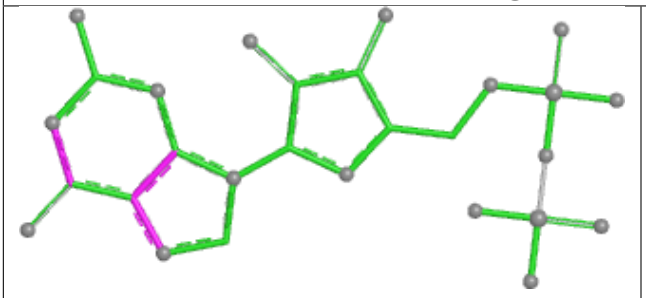
Ligand GDP HB 502



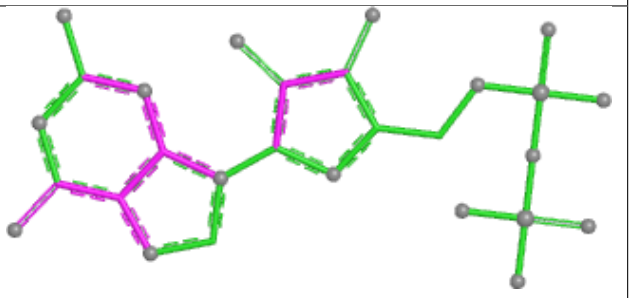
Ligand GDP NH 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP EC 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

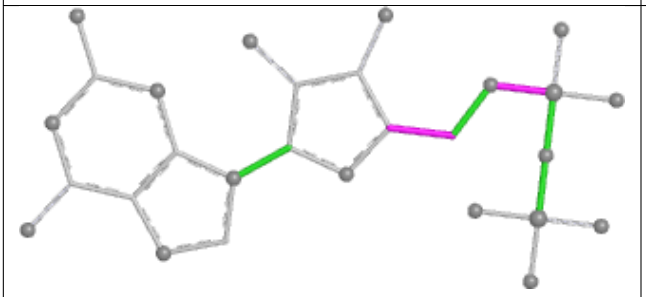
Ligand GDP NN 502



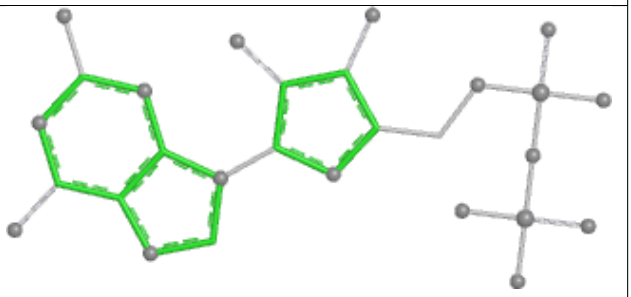
Bond lengths



Bond angles

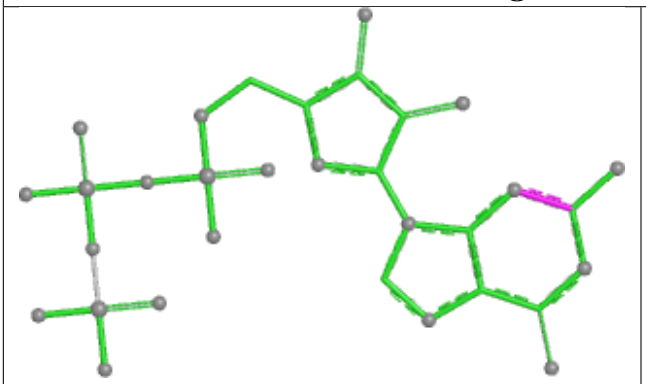


Torsions

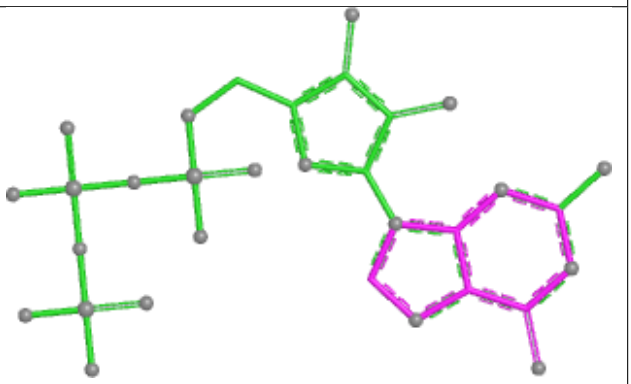


Rings

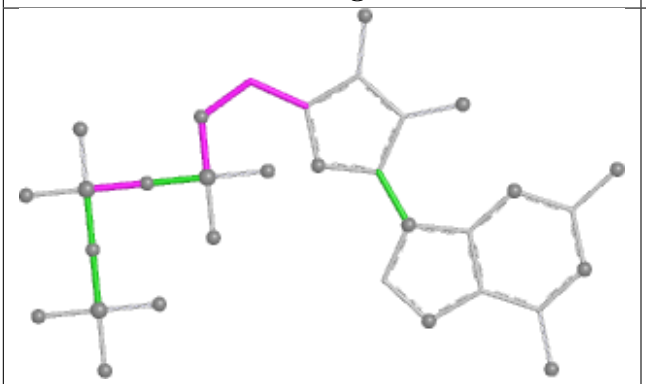
Ligand GTP DO 501



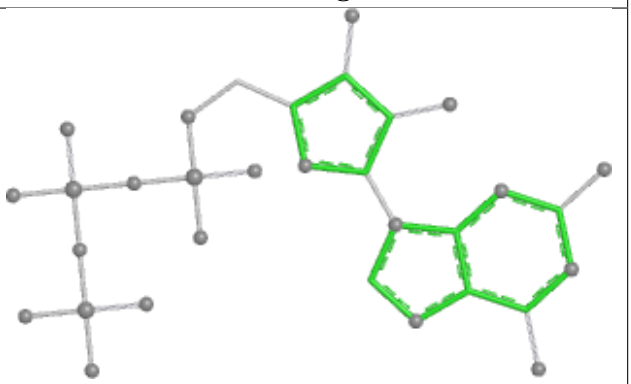
Bond lengths



Bond angles

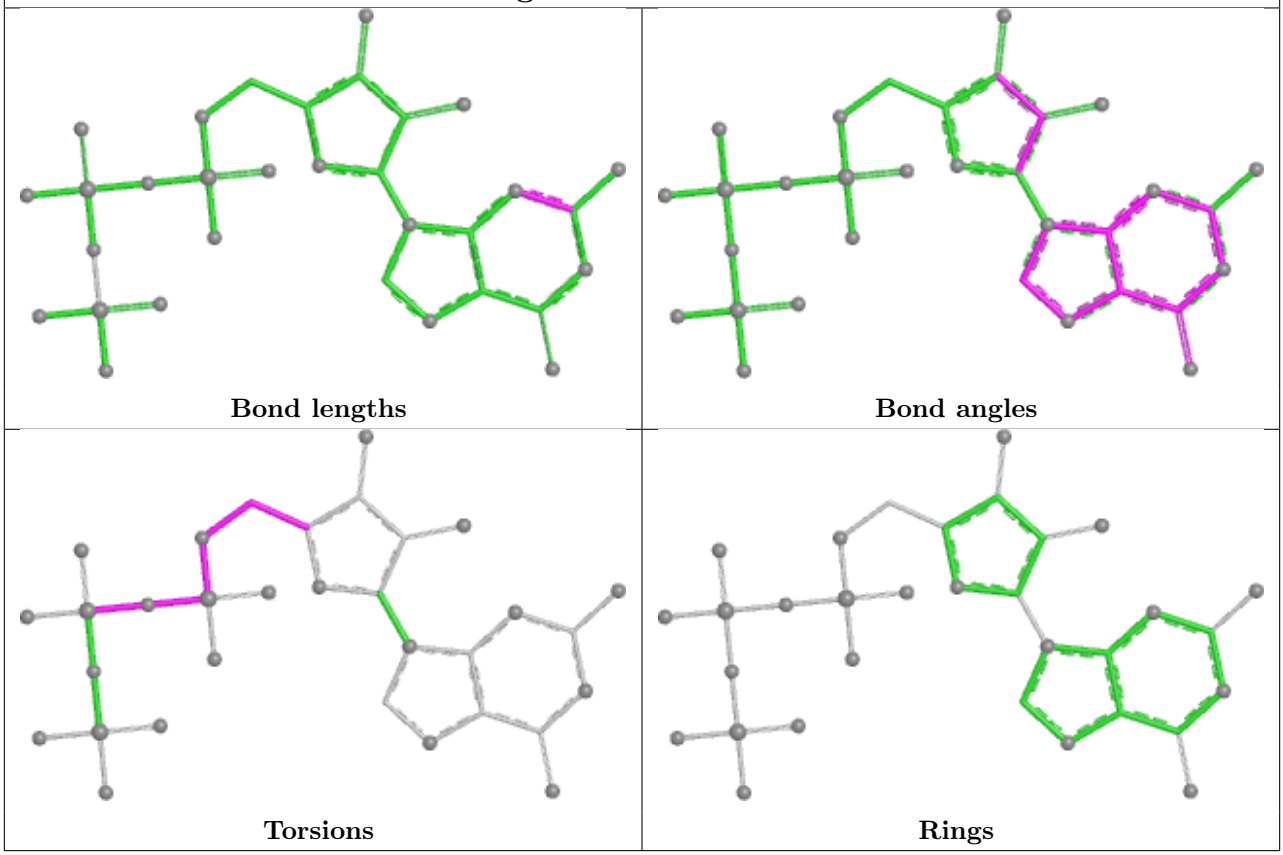


Torsions

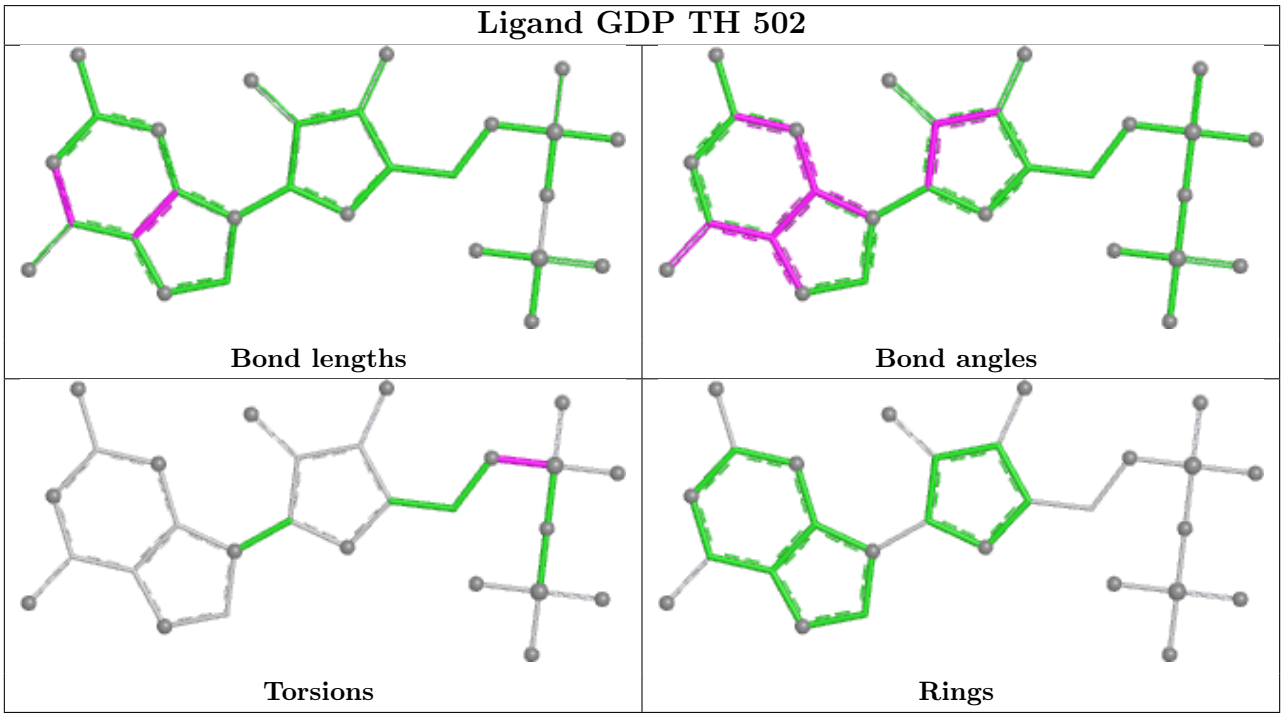


Rings

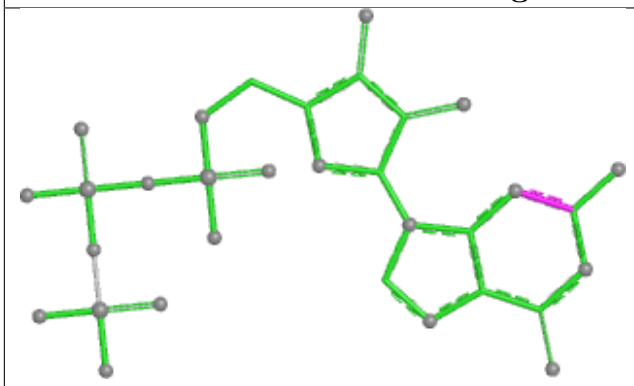
Ligand GTP UI 501



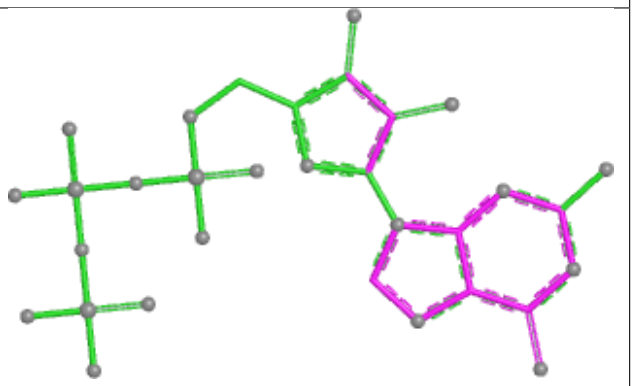
Ligand GDP TH 502



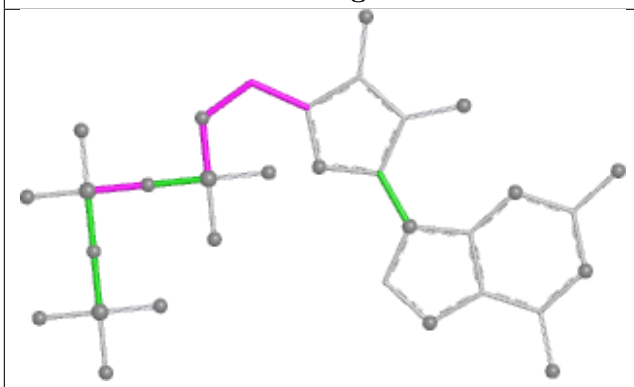
Ligand GTP PO 501



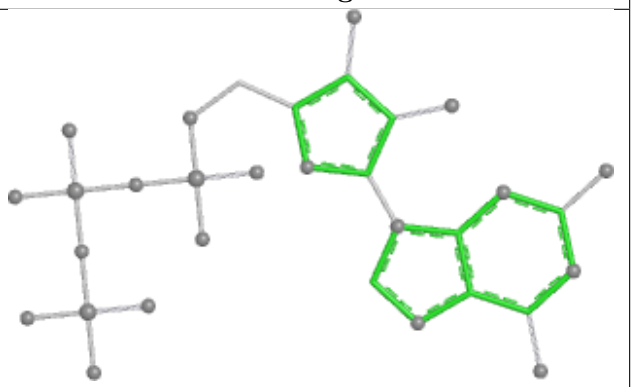
Bond lengths



Bond angles

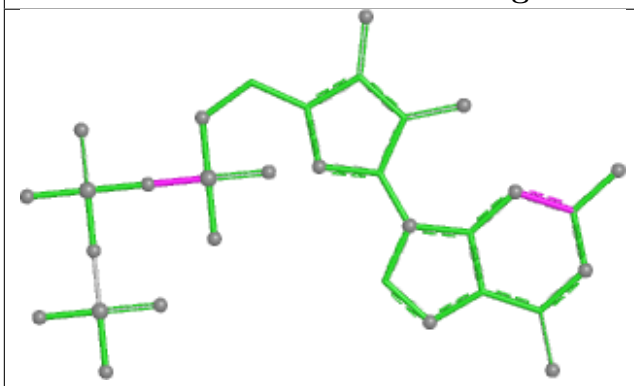


Torsions

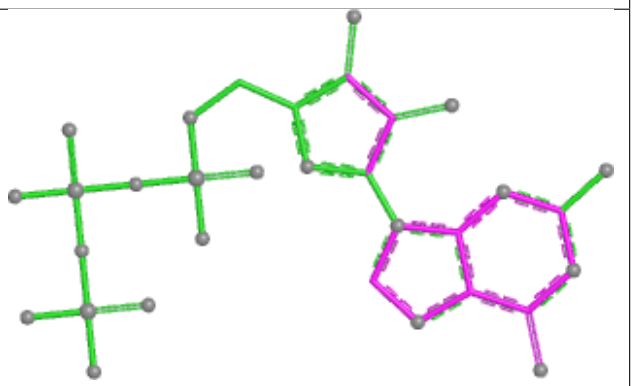


Rings

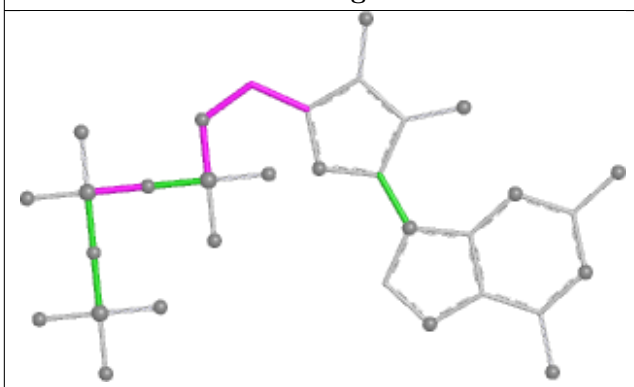
Ligand GTP VA 501



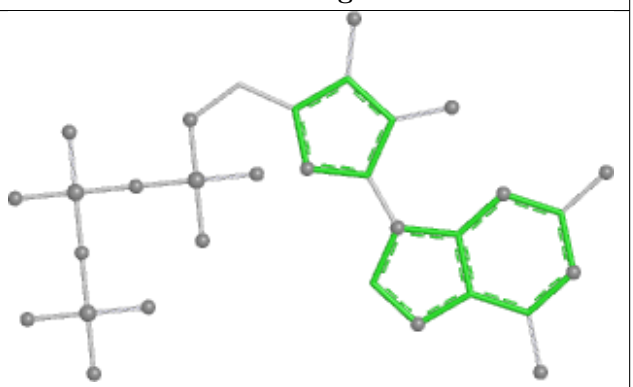
Bond lengths



Bond angles

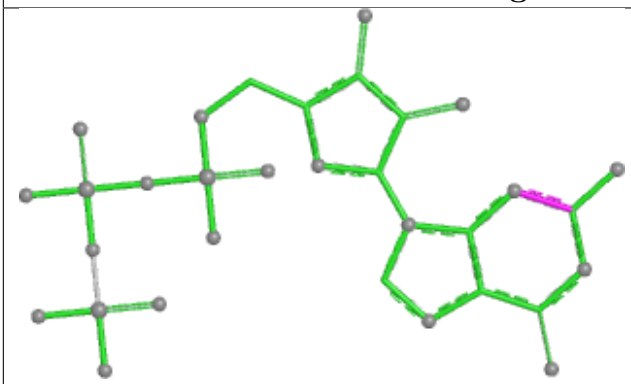


Torsions

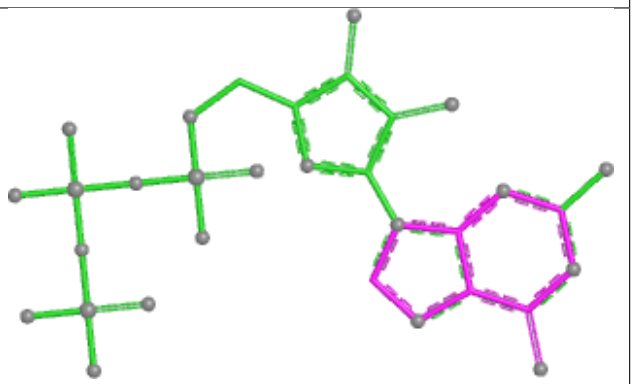


Rings

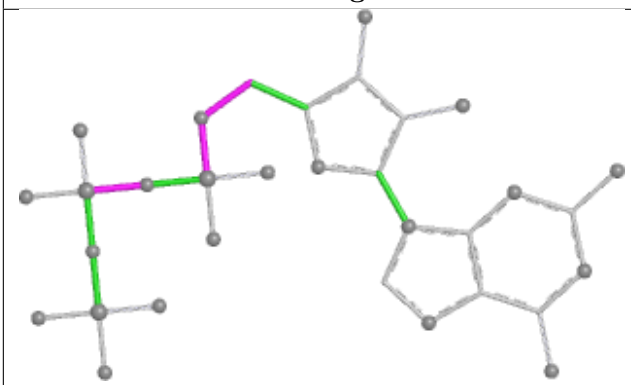
Ligand GTP AC 501



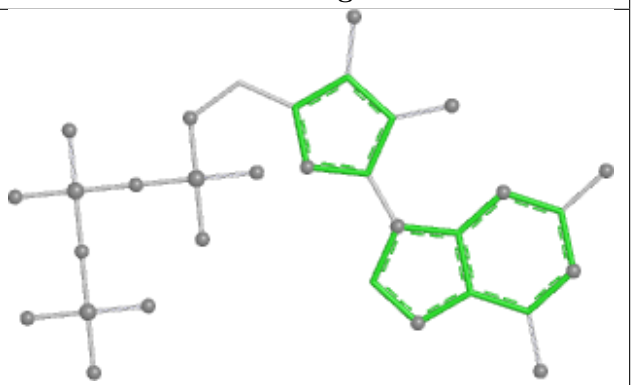
Bond lengths



Bond angles

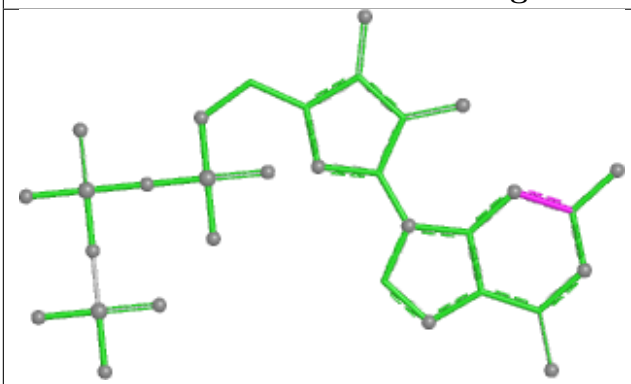


Torsions

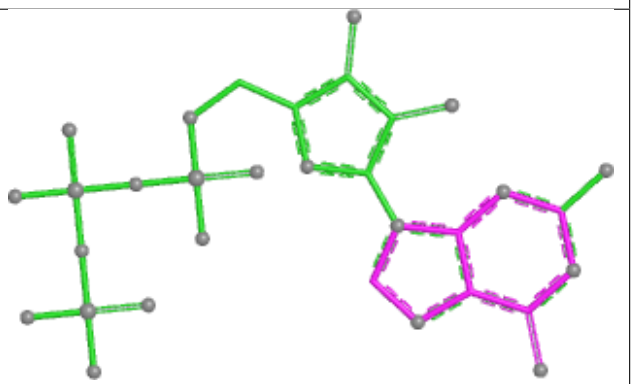


Rings

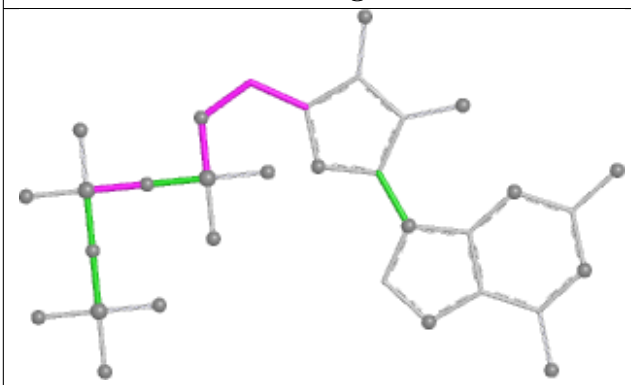
Ligand GTP FK 501



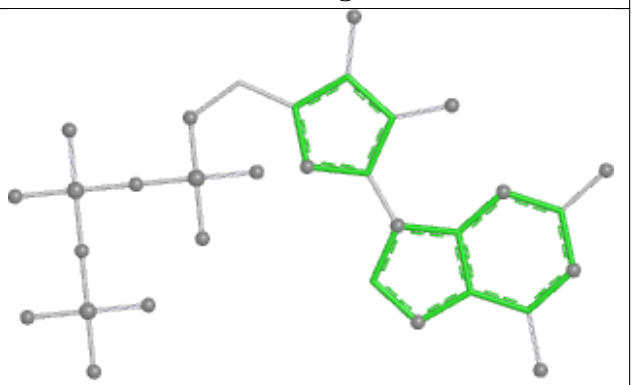
Bond lengths



Bond angles

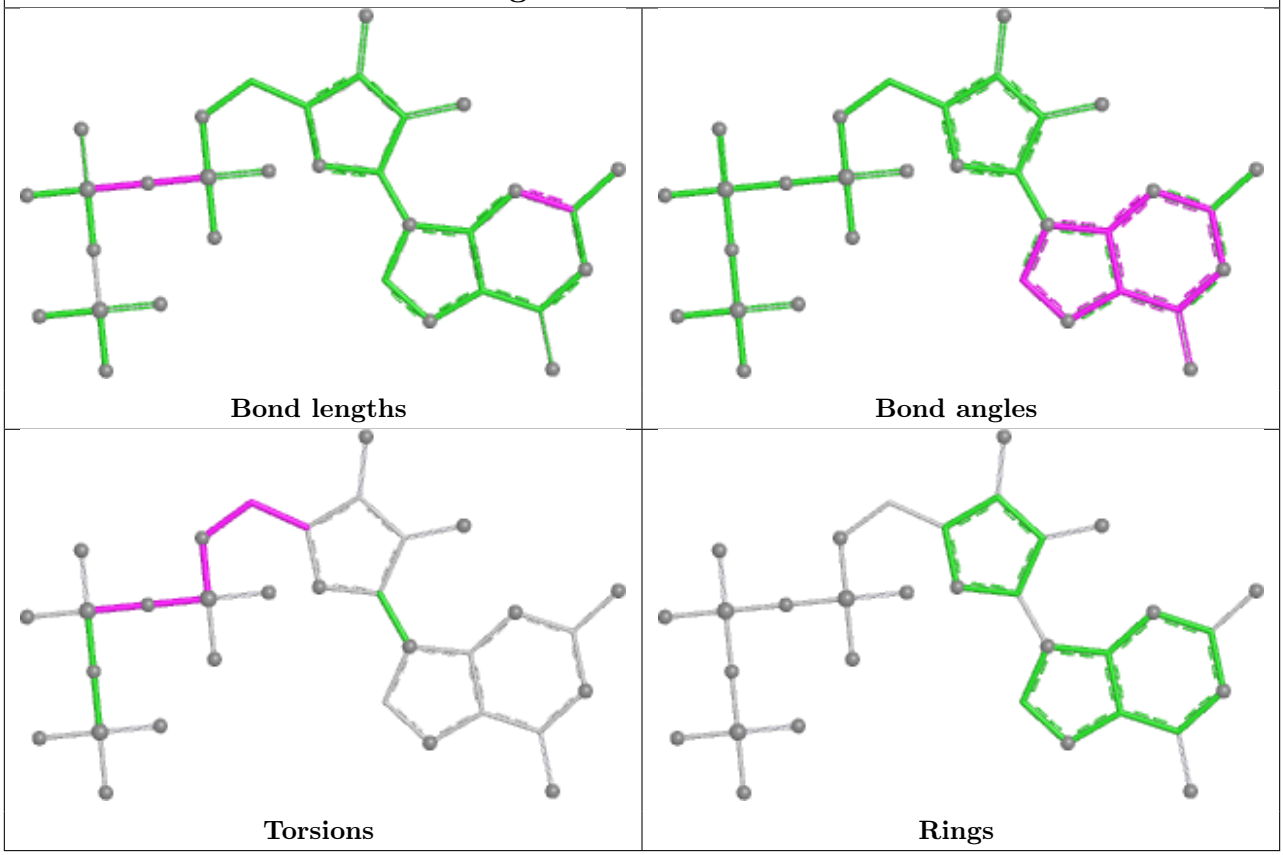


Torsions

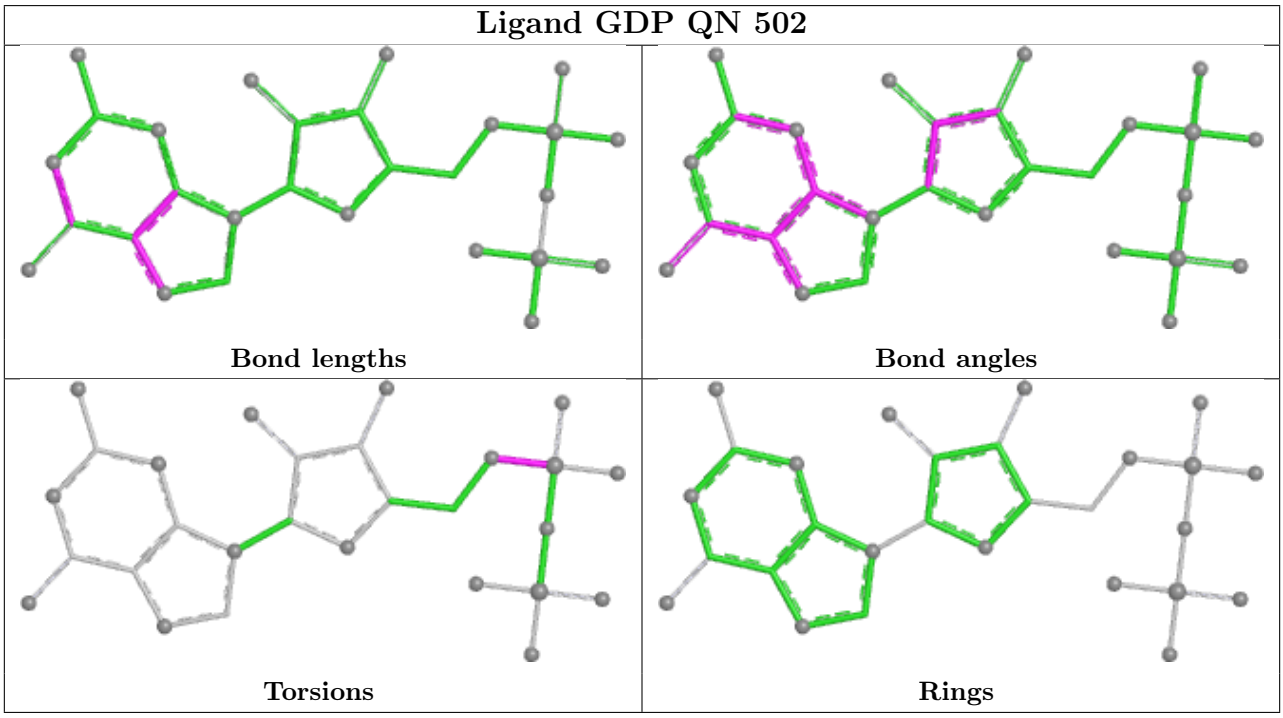


Rings

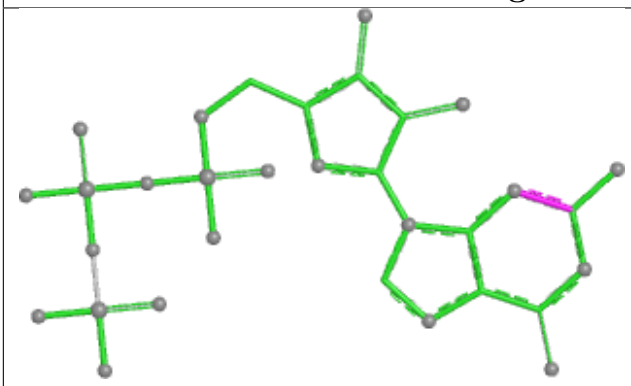
Ligand GTP RK 501



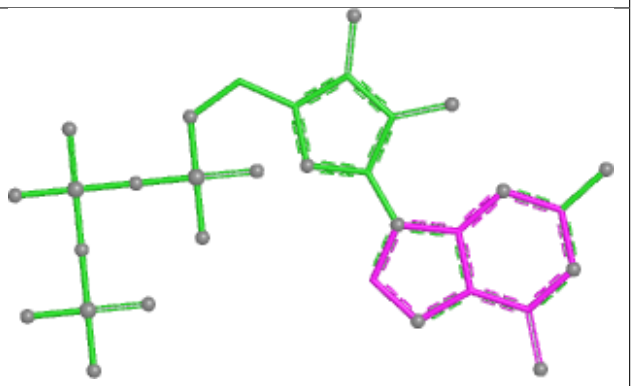
Ligand GDP QN 502



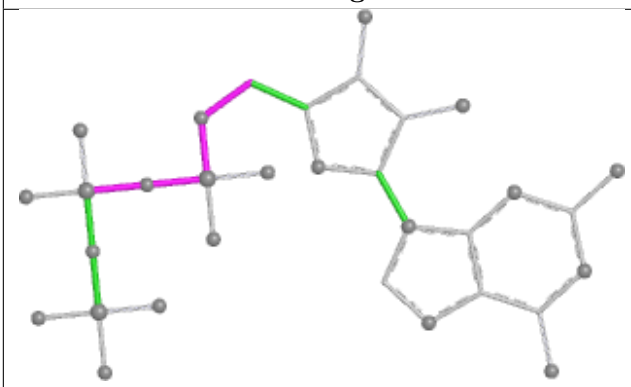
Ligand GTP AG 501



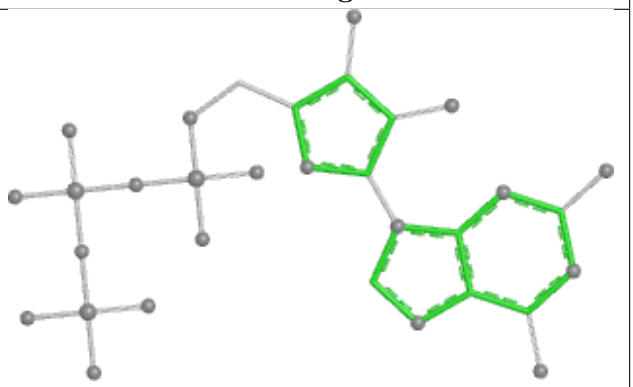
Bond lengths



Bond angles

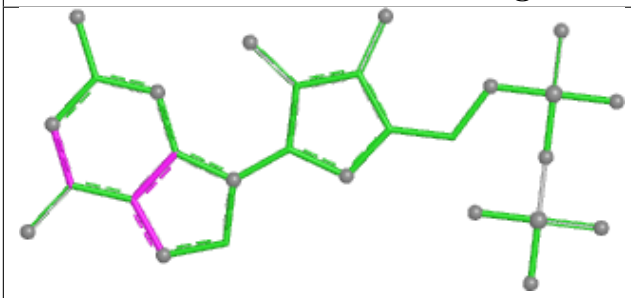


Torsions

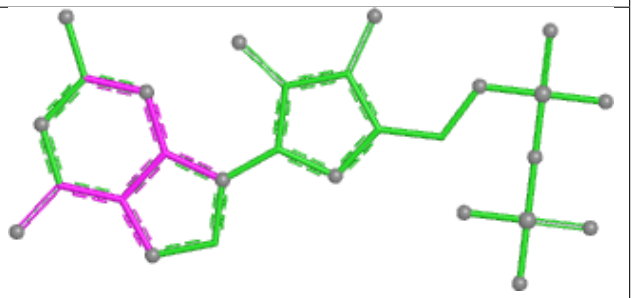


Rings

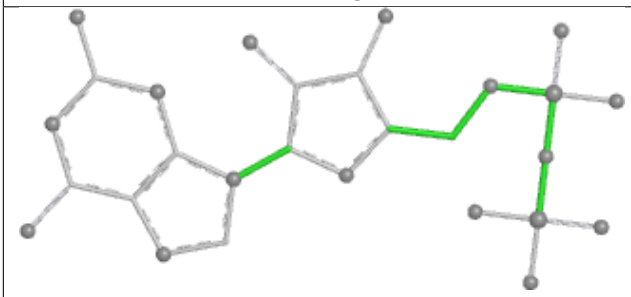
Ligand GDP IH 502



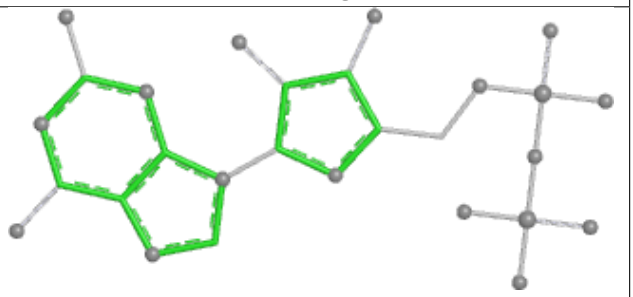
Bond lengths



Bond angles

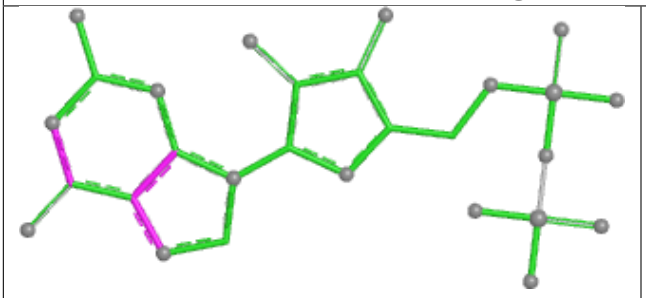


Torsions

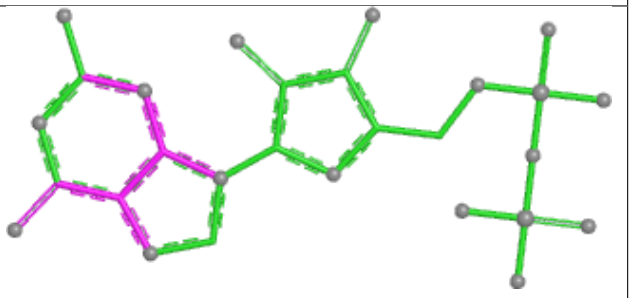


Rings

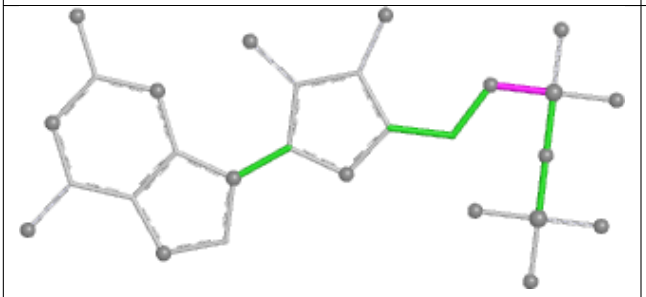
Ligand GDP CF 502



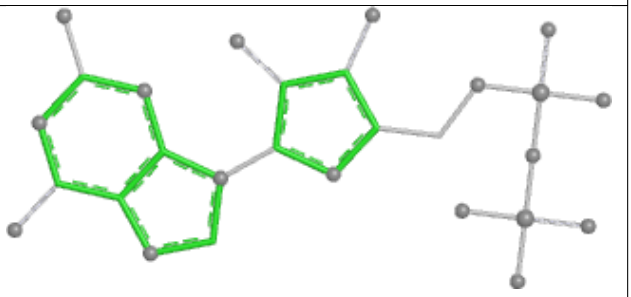
Bond lengths



Bond angles

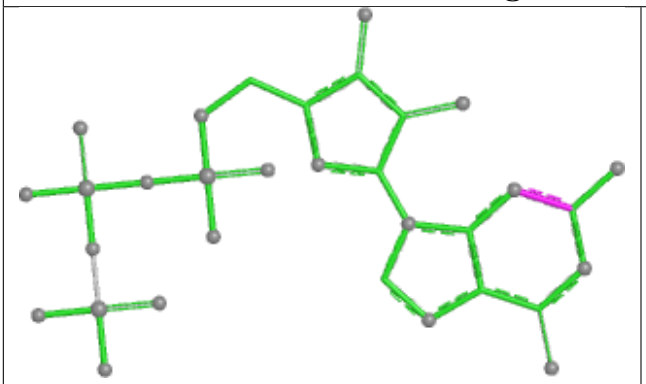


Torsions

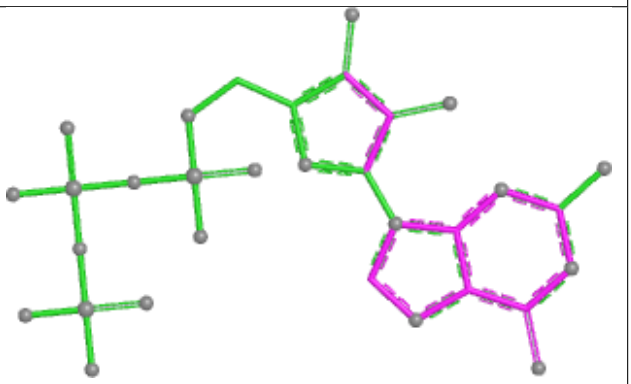


Rings

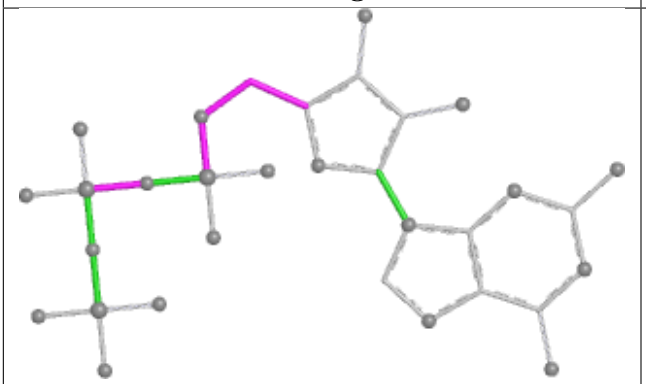
Ligand GTP WO 501



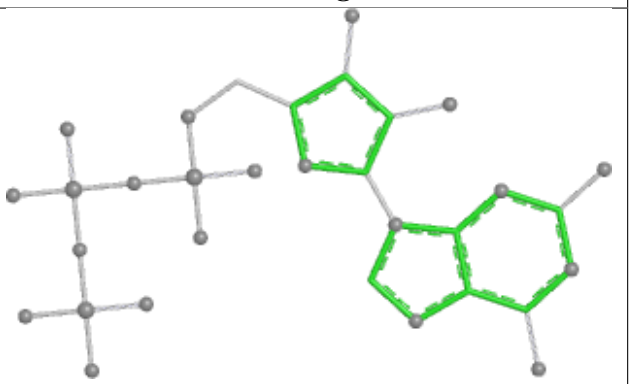
Bond lengths



Bond angles

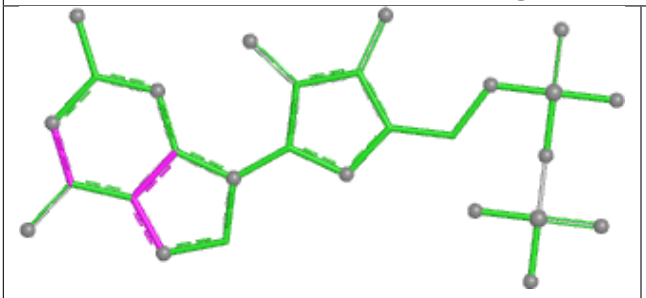


Torsions

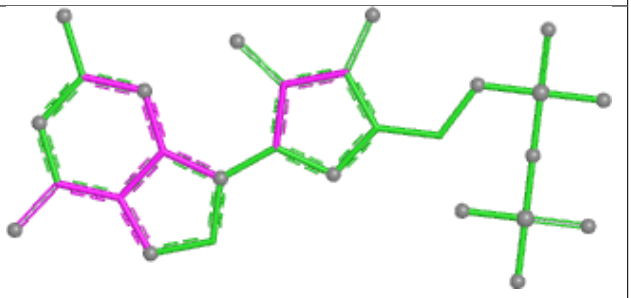


Rings

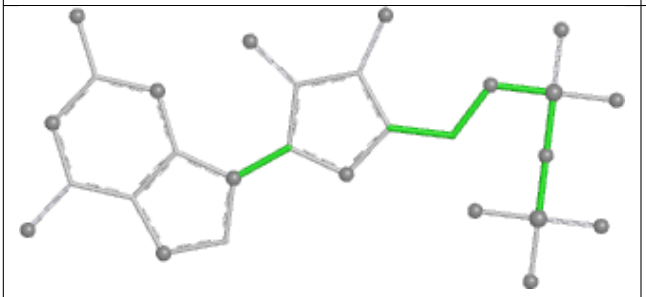
Ligand GDP BJ 502



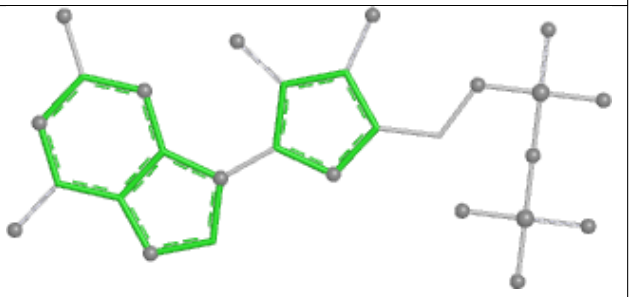
Bond lengths



Bond angles

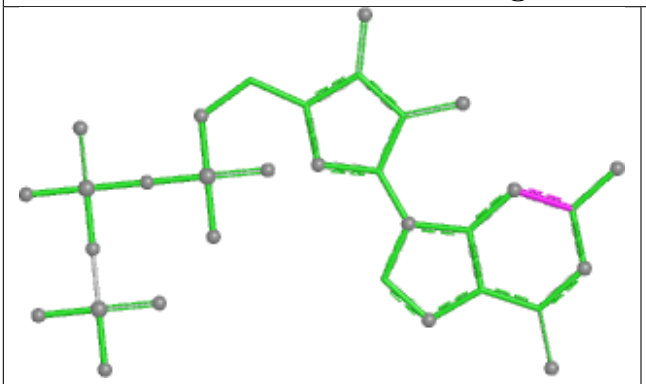


Torsions

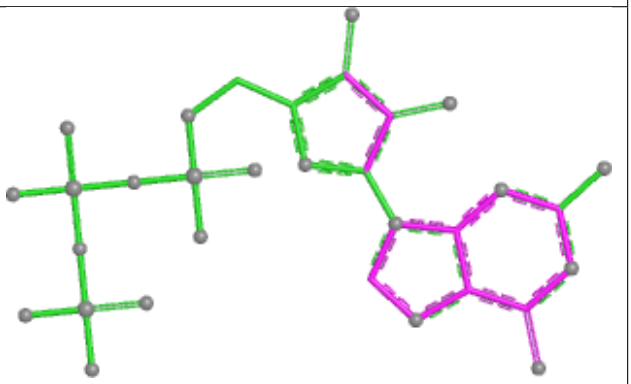


Rings

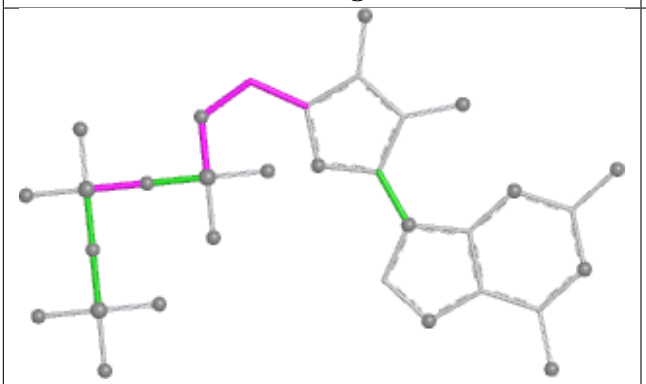
Ligand GTP CO 501



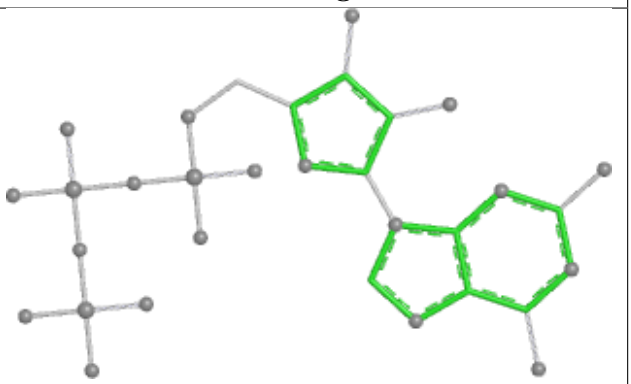
Bond lengths



Bond angles

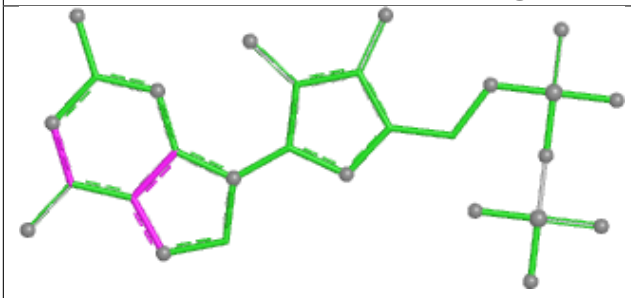


Torsions

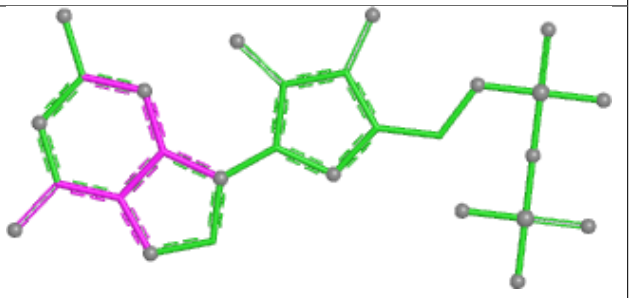


Rings

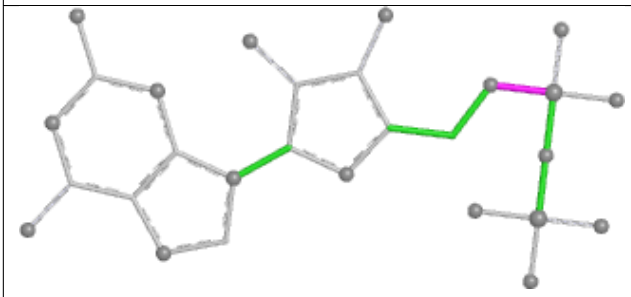
Ligand GDP LB 502



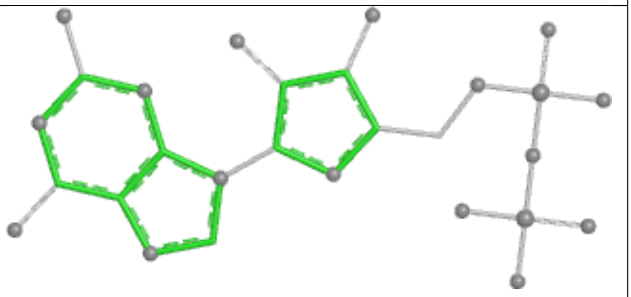
Bond lengths



Bond angles

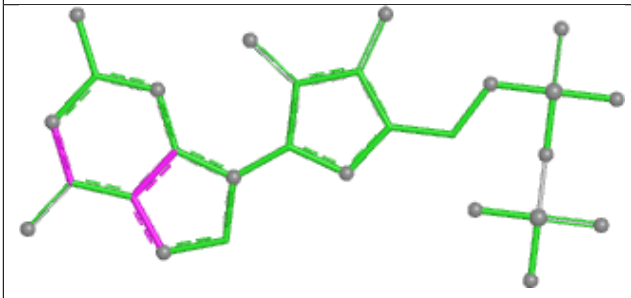


Torsions

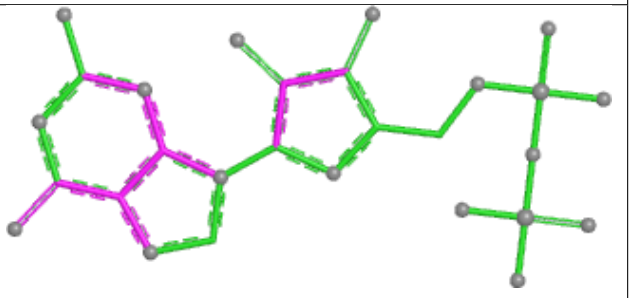


Rings

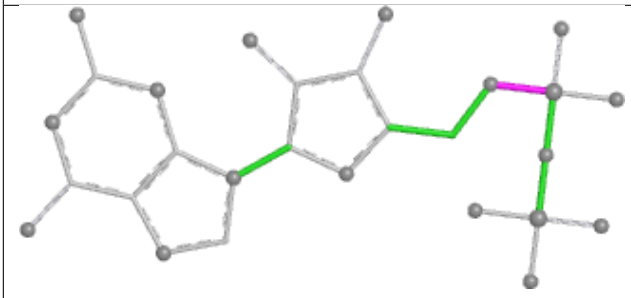
Ligand GDP TD 502



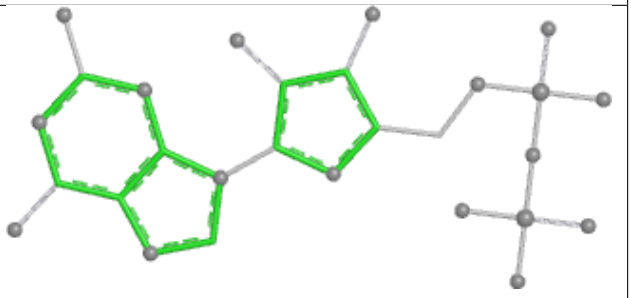
Bond lengths



Bond angles

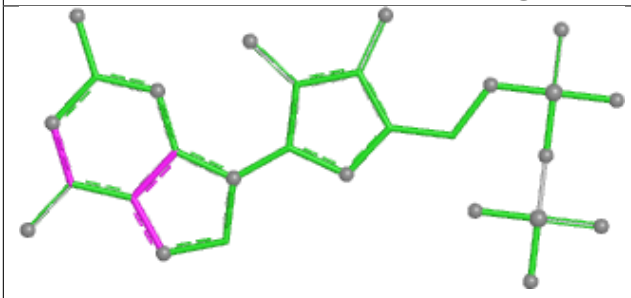


Torsions

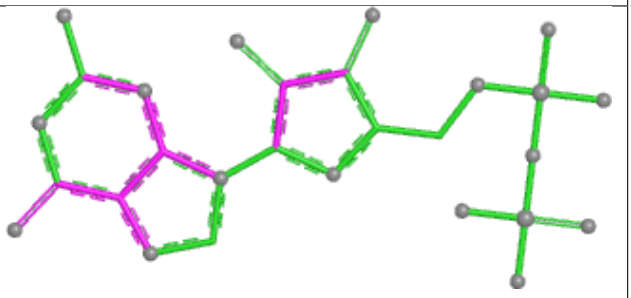


Rings

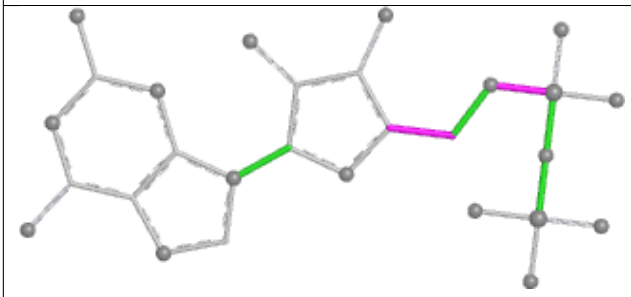
Ligand GDP IB 502



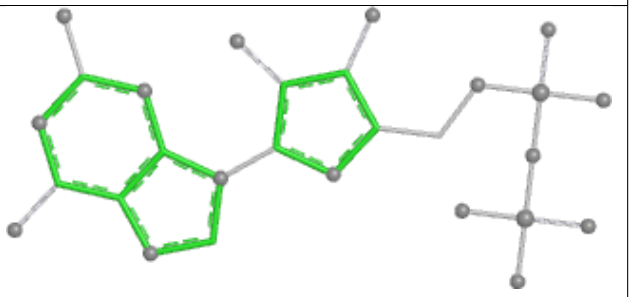
Bond lengths



Bond angles

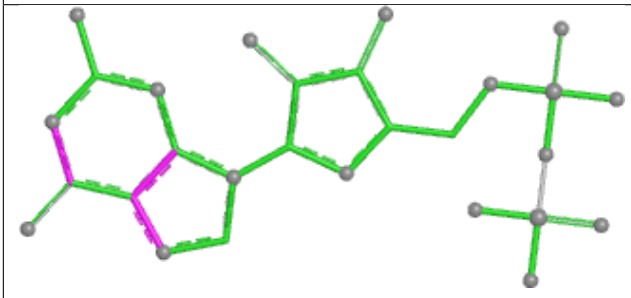


Torsions

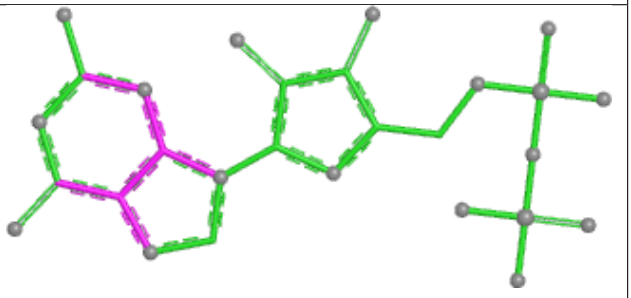


Rings

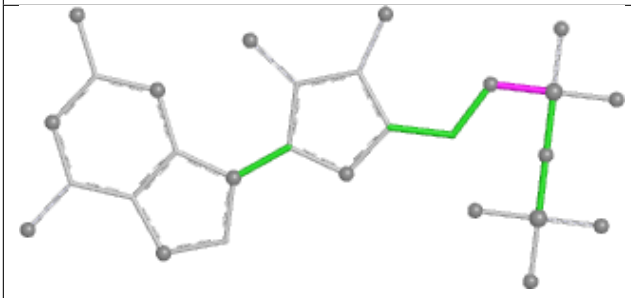
Ligand GDP JL 502



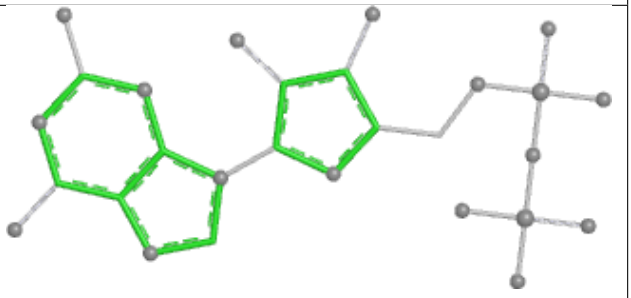
Bond lengths



Bond angles

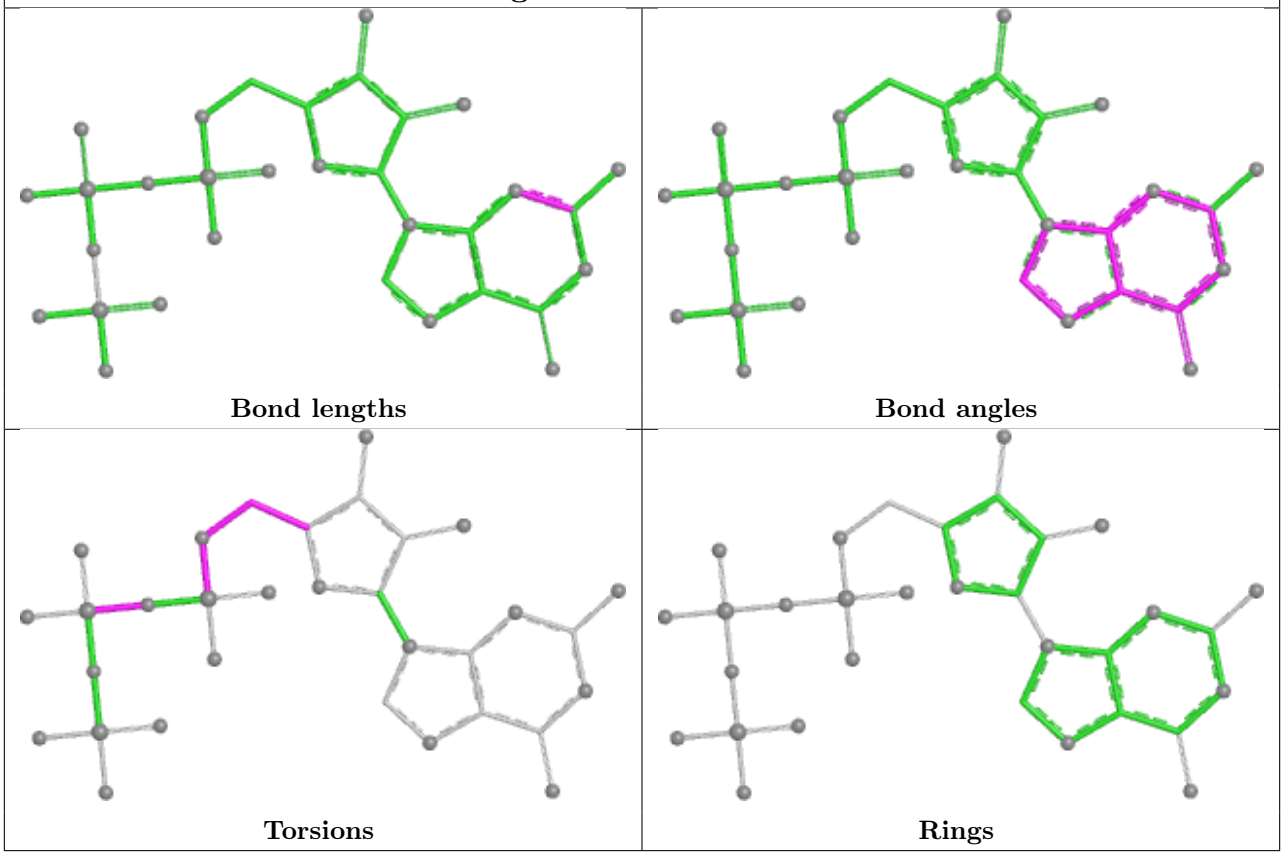


Torsions

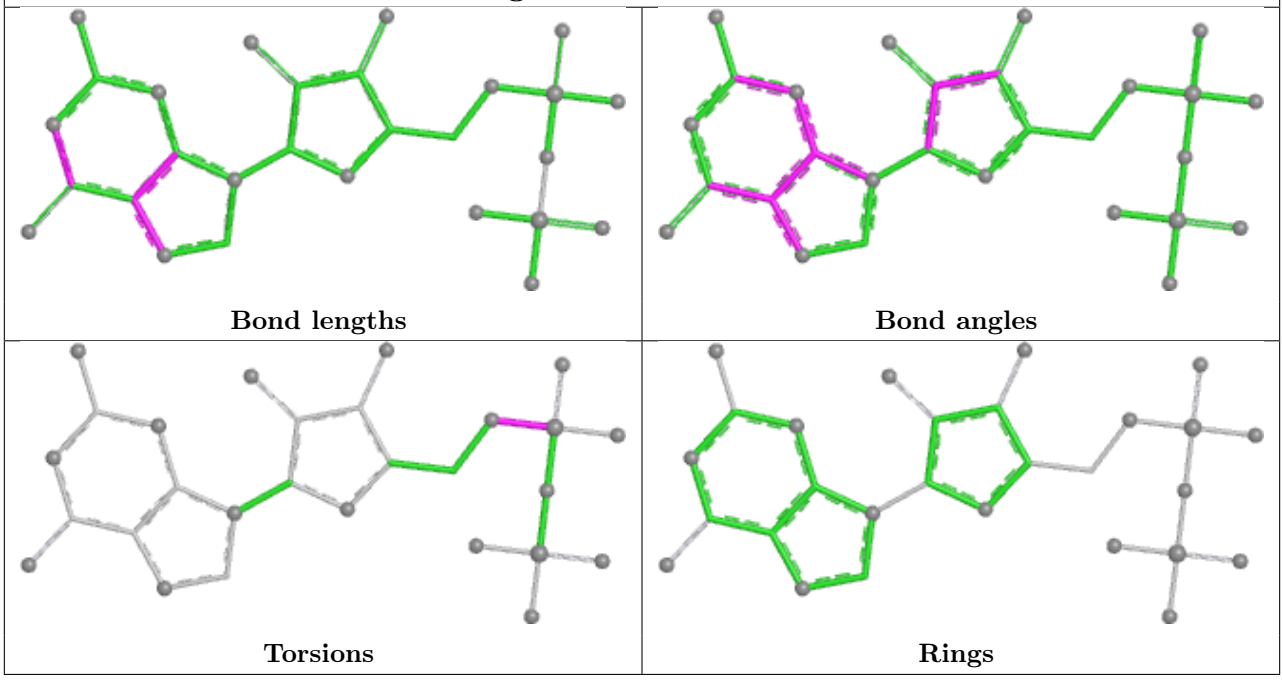


Rings

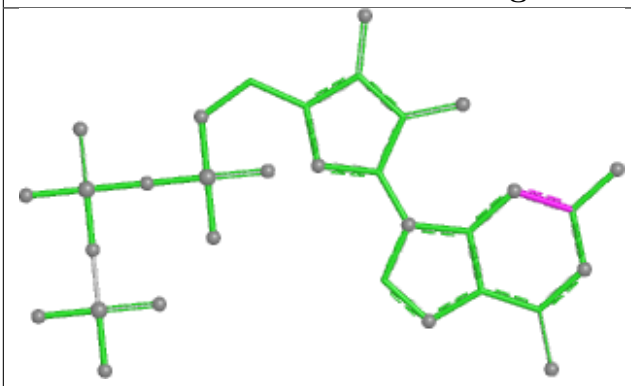
Ligand GTP EG 501



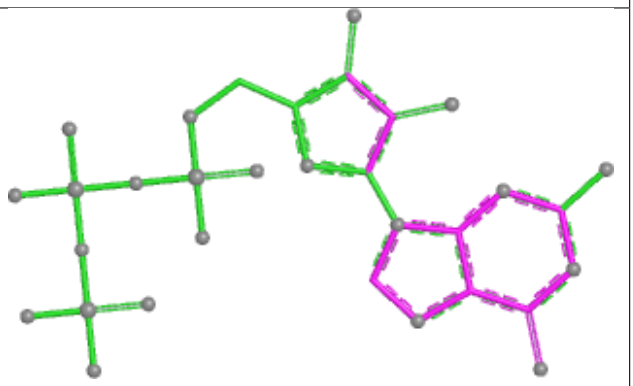
Ligand GDP UN 502



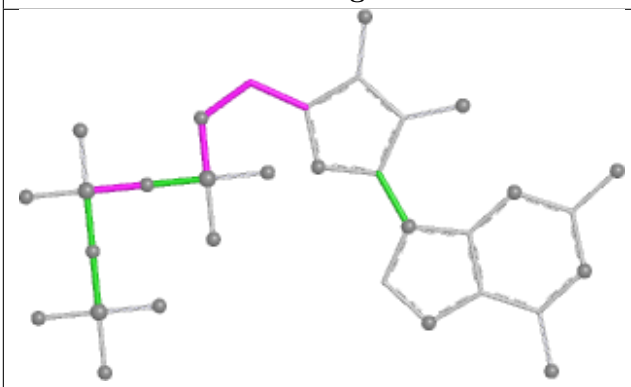
Ligand GTP GE 501



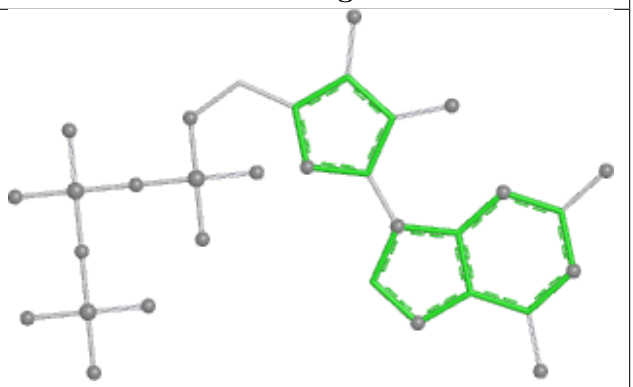
Bond lengths



Bond angles

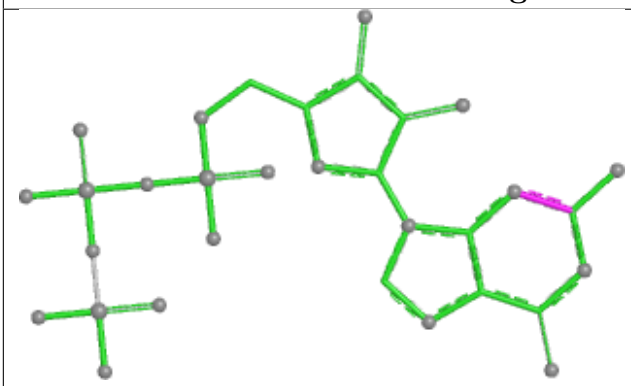


Torsions

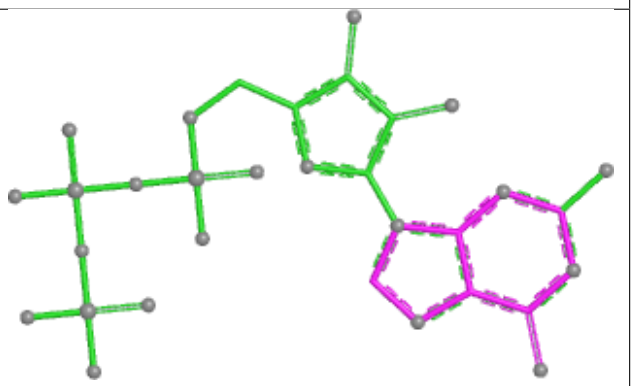


Rings

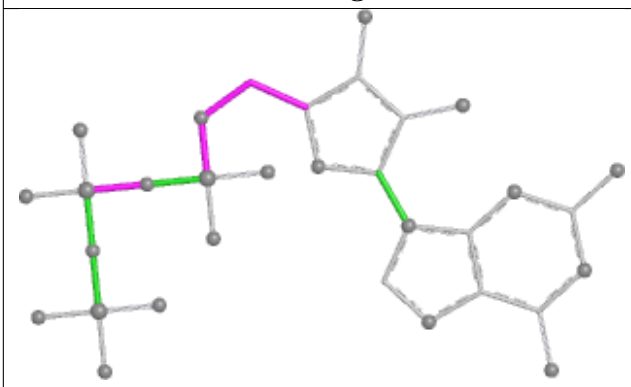
Ligand GTP CC 501



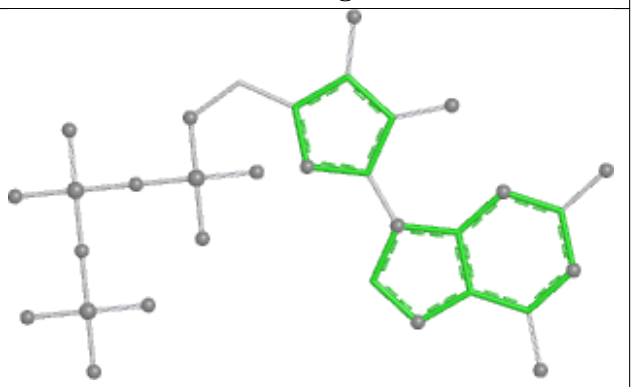
Bond lengths



Bond angles

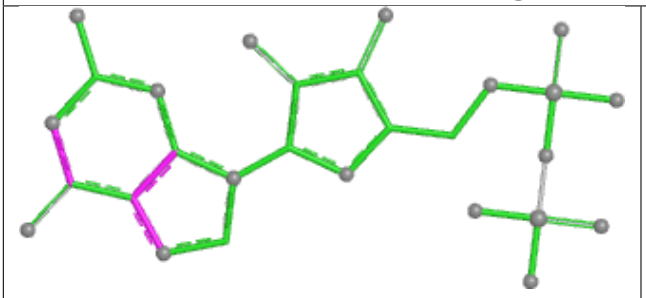


Torsions

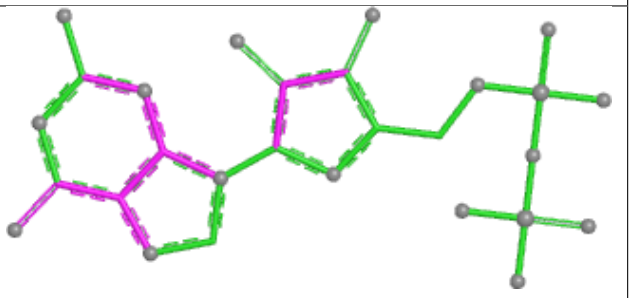


Rings

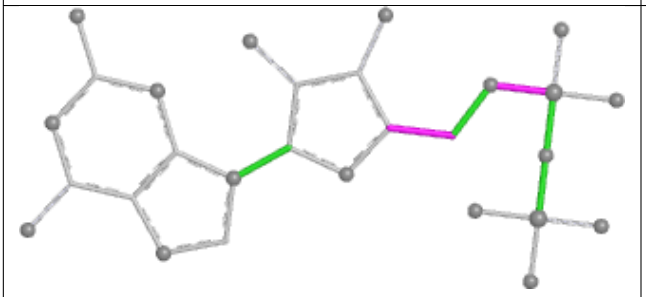
Ligand GDP OF 502



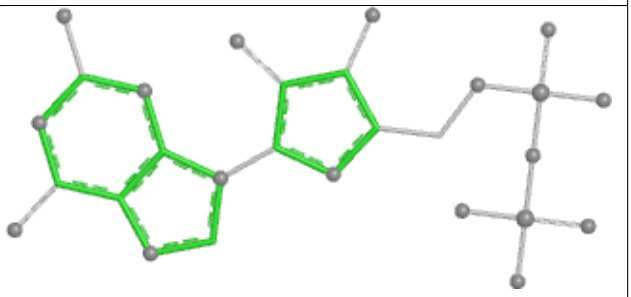
Bond lengths



Bond angles

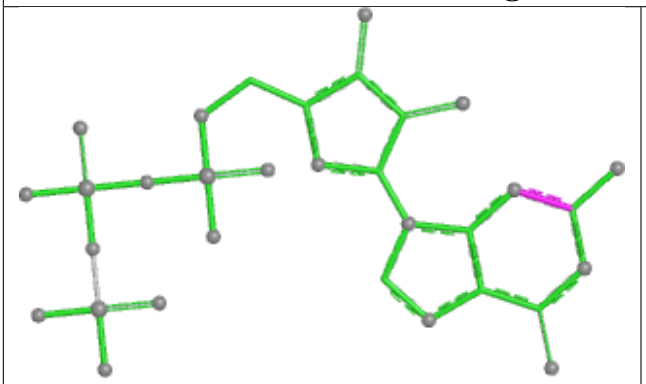


Torsions

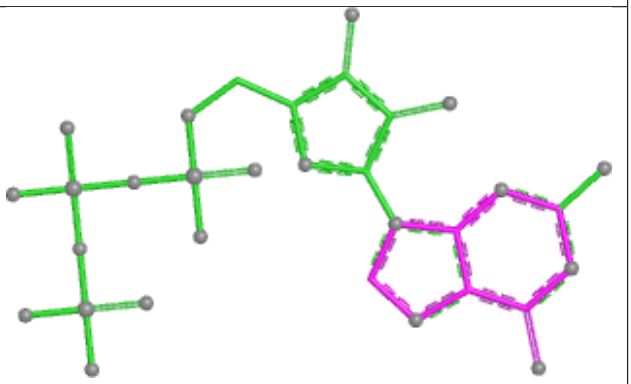


Rings

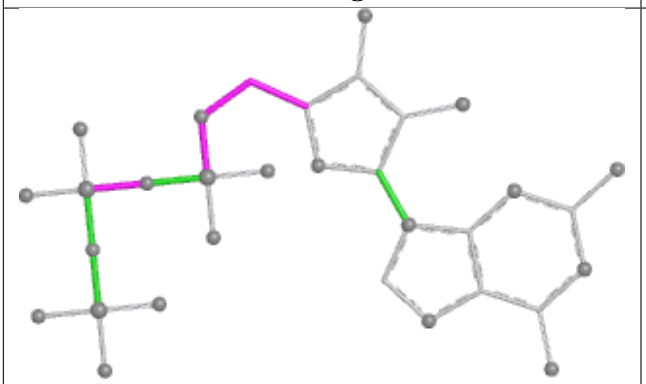
Ligand GTP WG 501



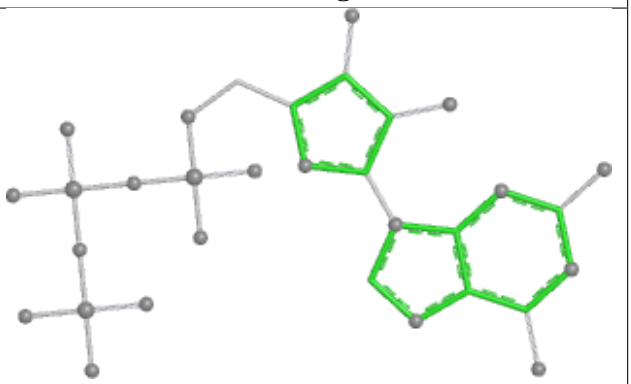
Bond lengths



Bond angles

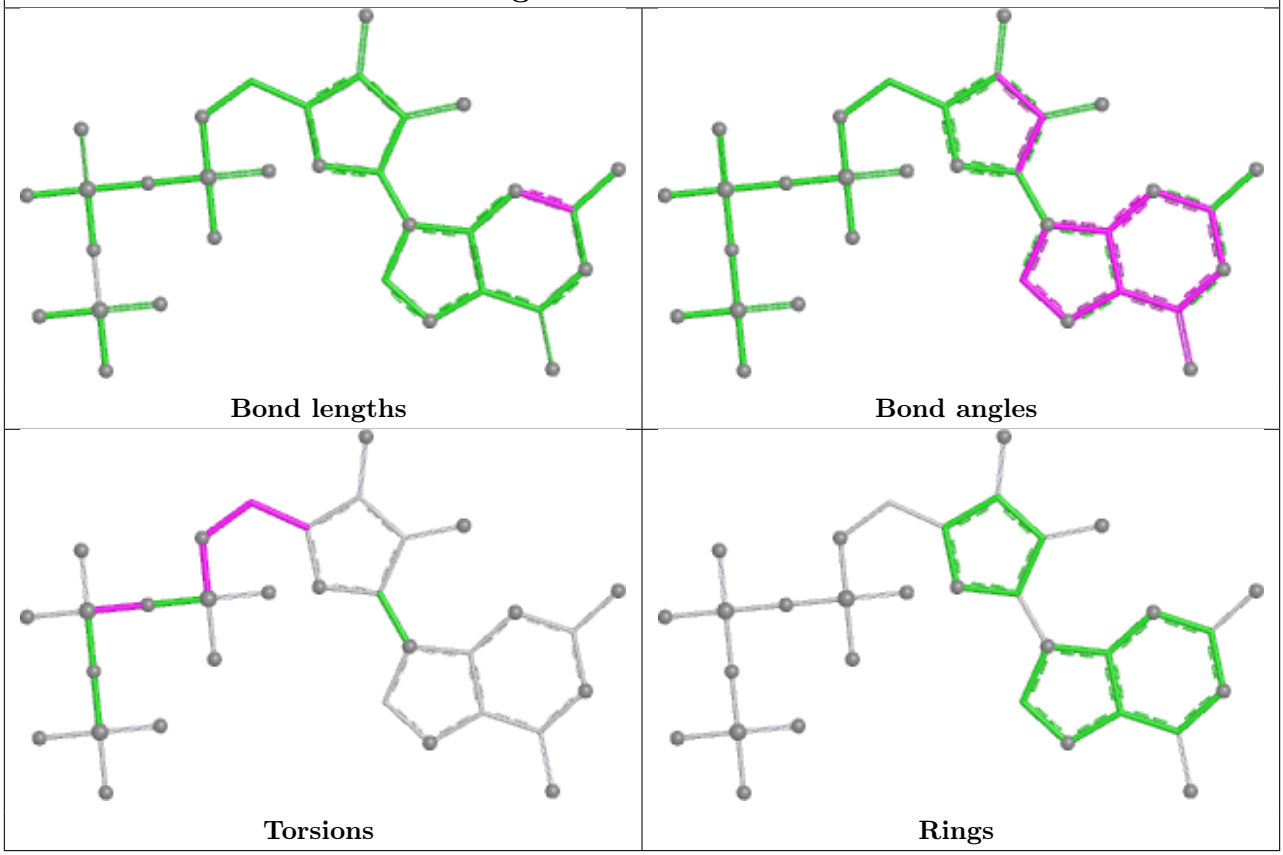


Torsions

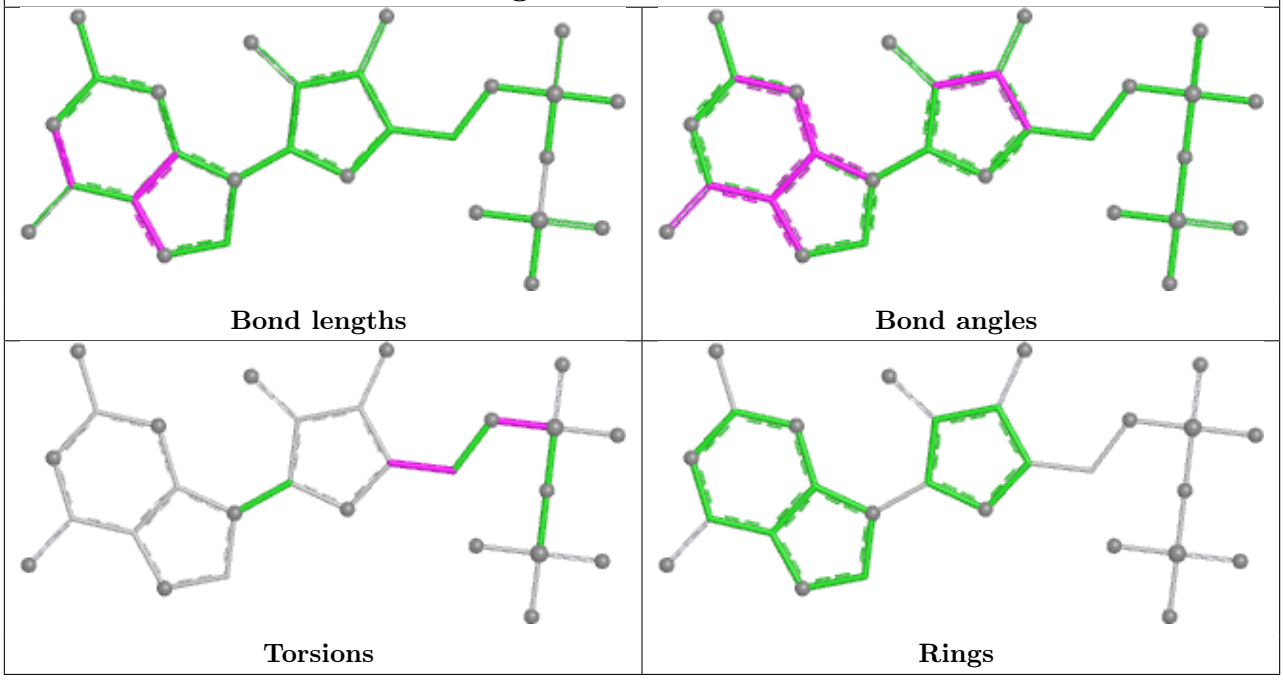


Rings

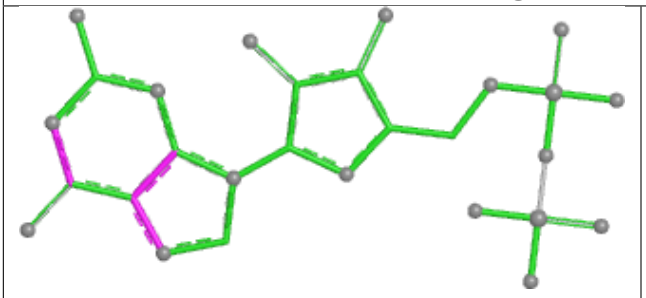
Ligand GTP BE 501



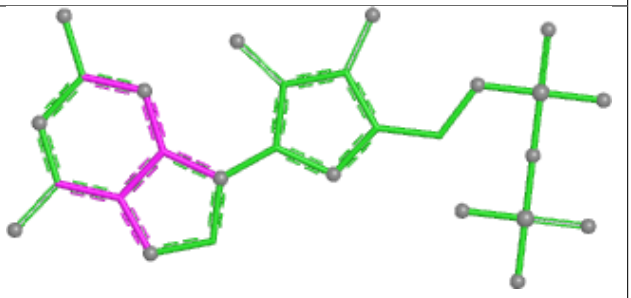
Ligand GDP LD 502



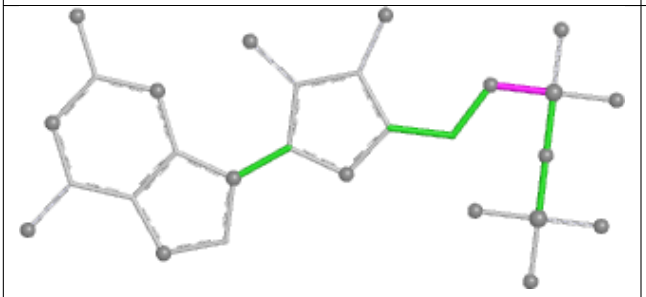
Ligand GDP KL 502



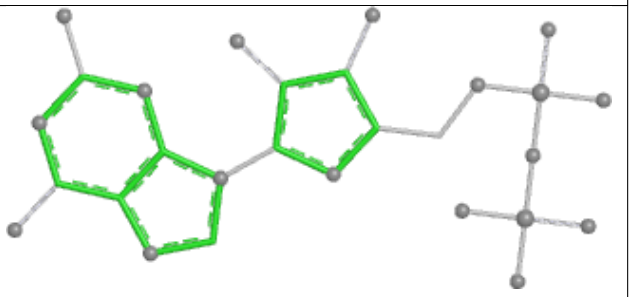
Bond lengths



Bond angles

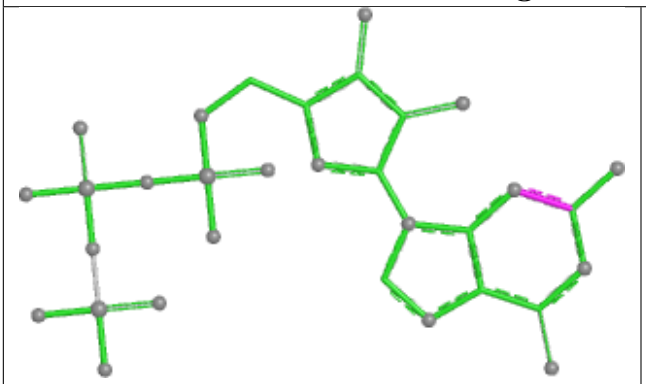


Torsions

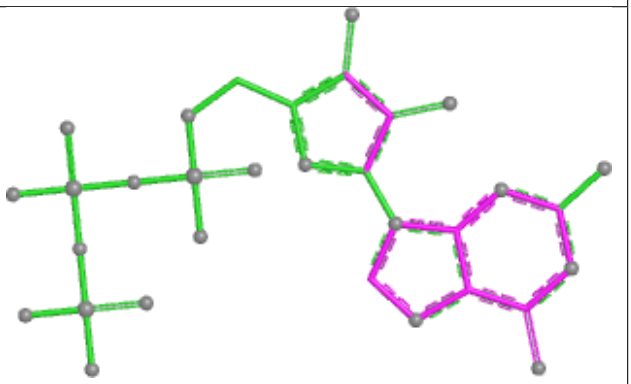


Rings

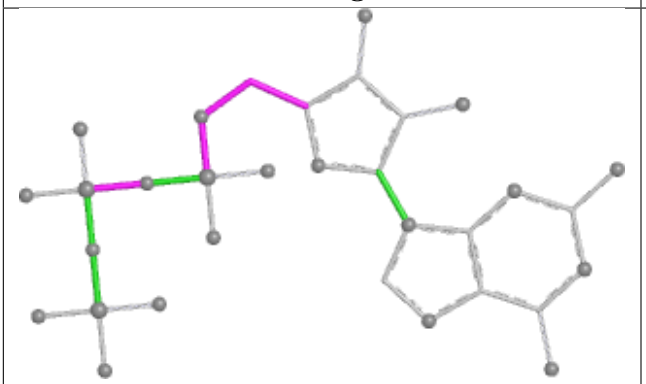
Ligand GTP OI 501



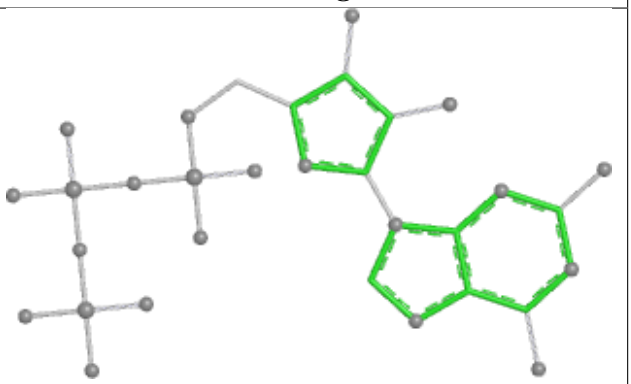
Bond lengths



Bond angles

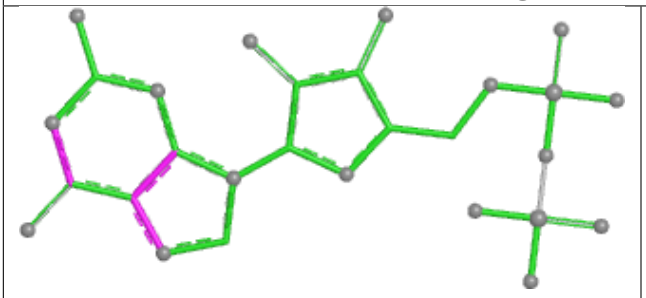


Torsions

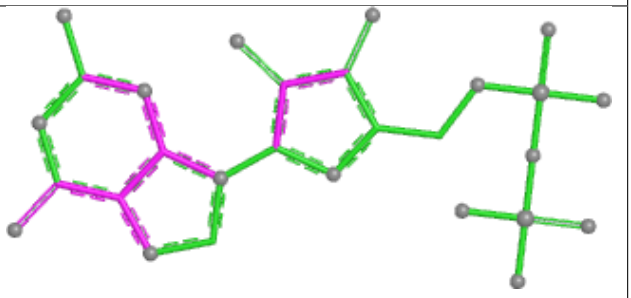


Rings

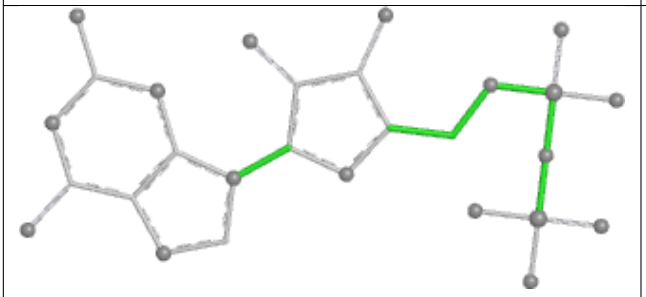
Ligand GDP ID 502



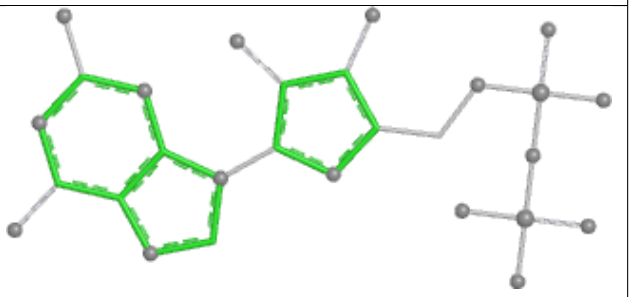
Bond lengths



Bond angles

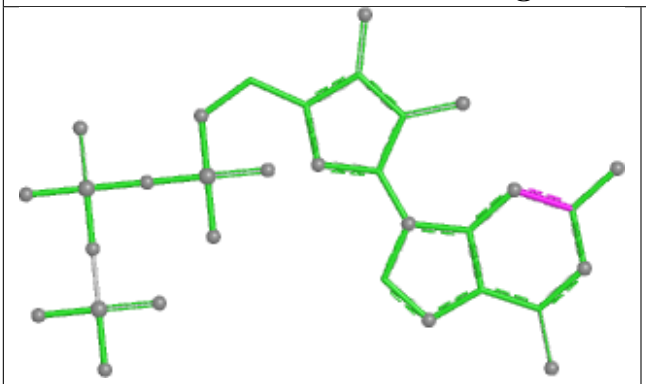


Torsions

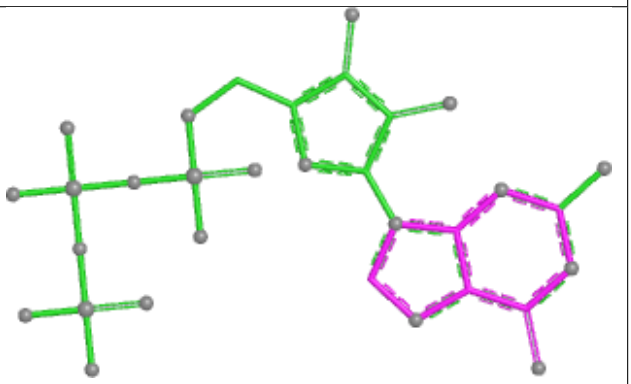


Rings

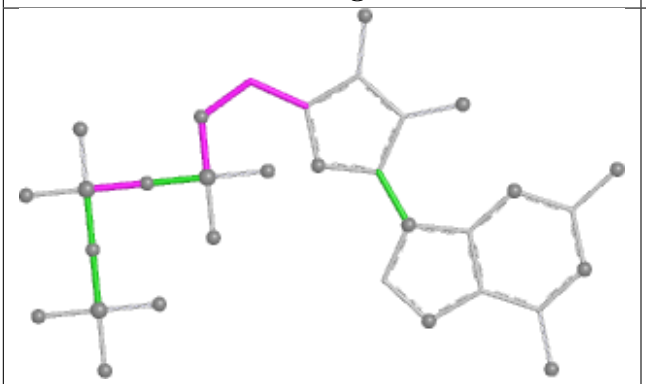
Ligand GTP NI 501



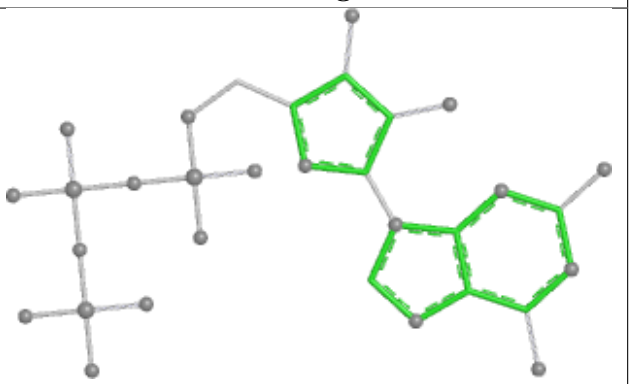
Bond lengths



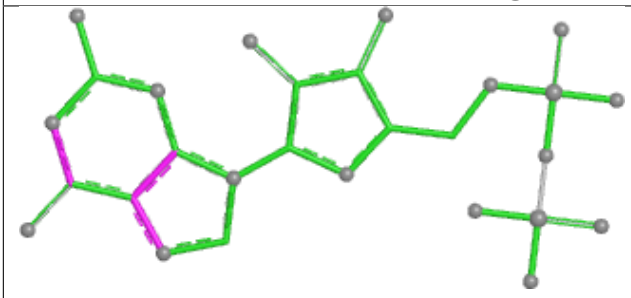
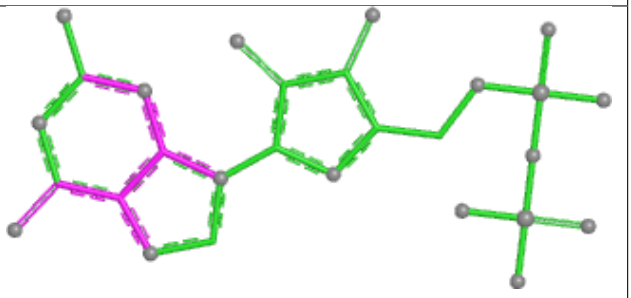
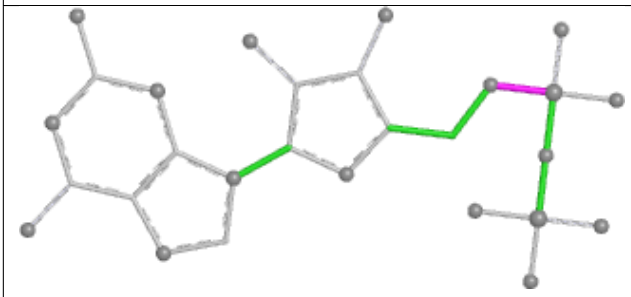
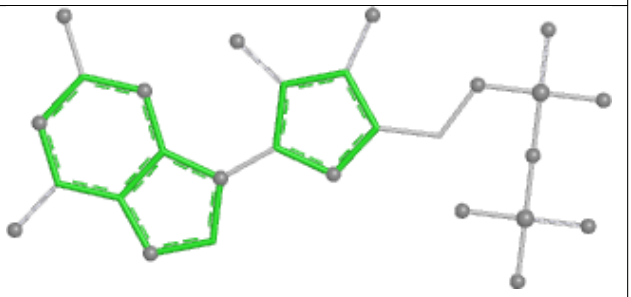
Bond angles

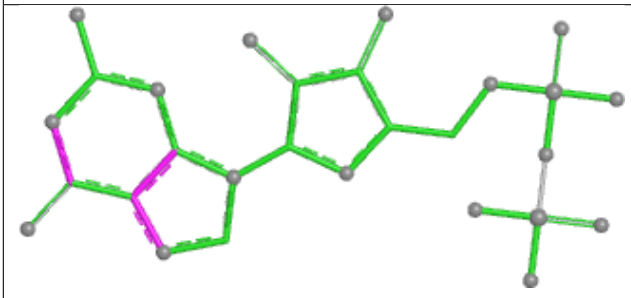
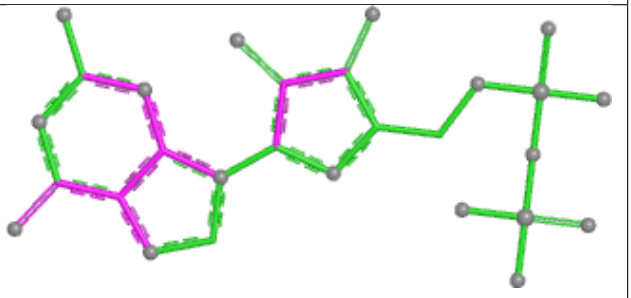
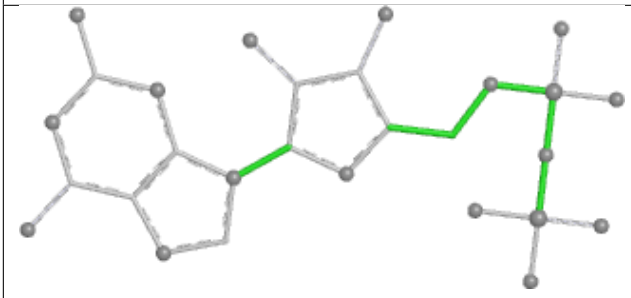
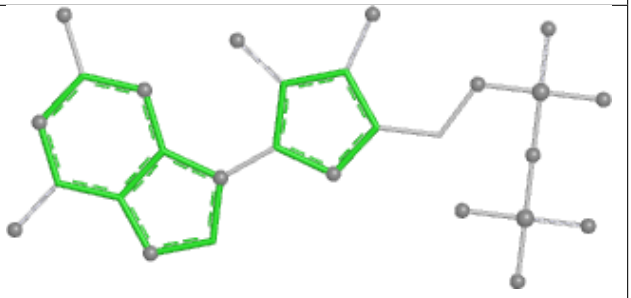


Torsions

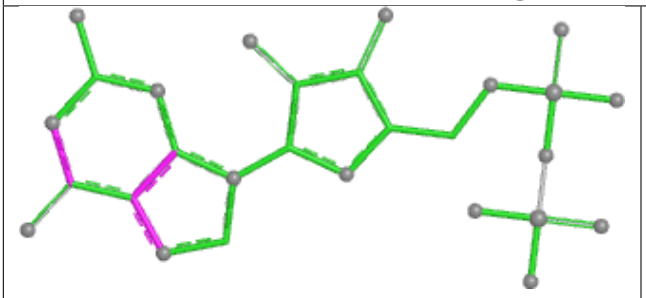


Rings

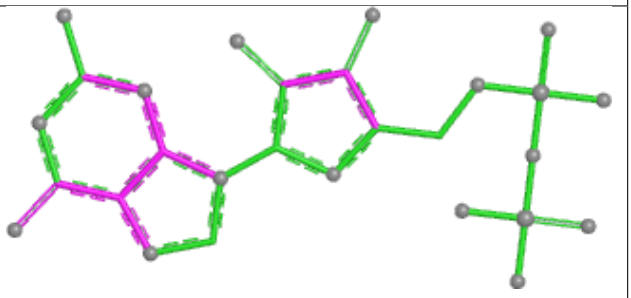
Ligand GDP KD 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP FL 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

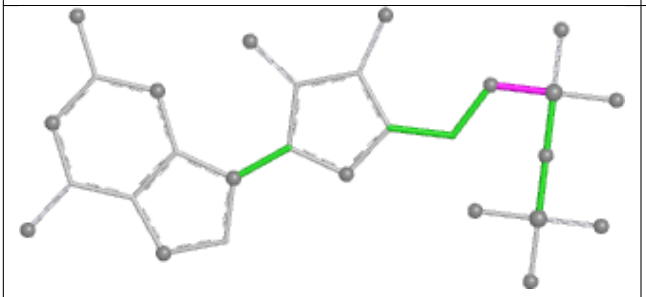
Ligand GDP EF 502



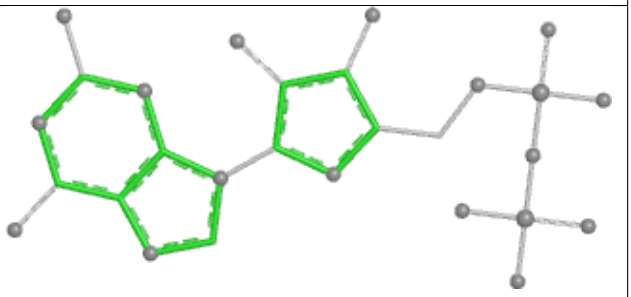
Bond lengths



Bond angles

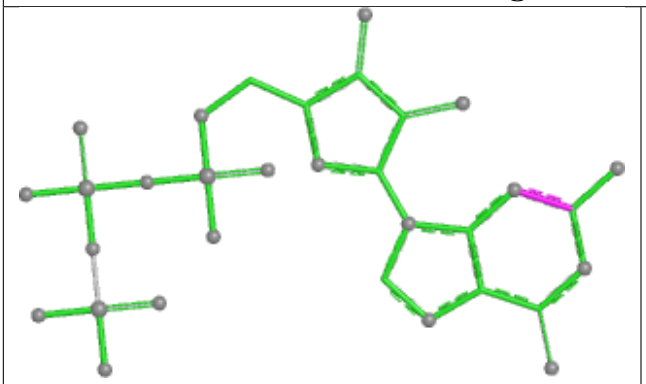


Torsions

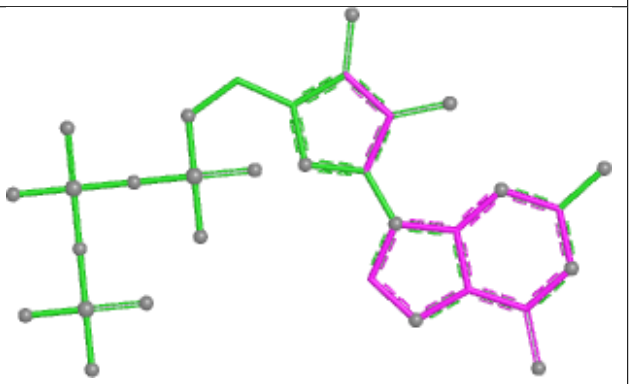


Rings

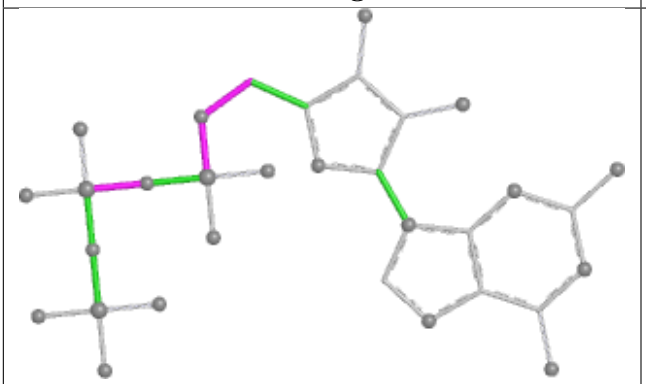
Ligand GTP GC 501



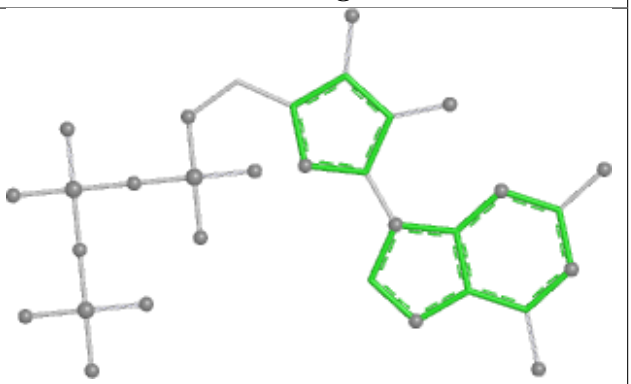
Bond lengths



Bond angles

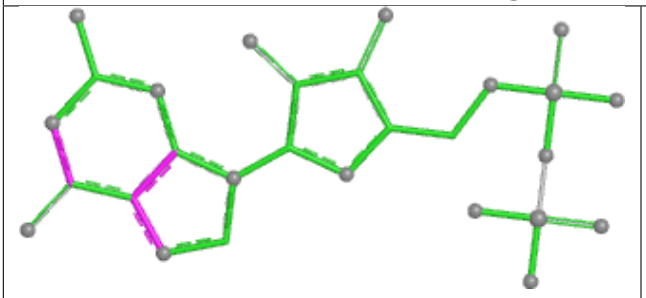


Torsions

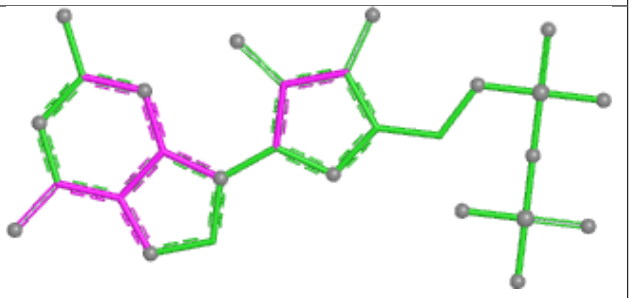


Rings

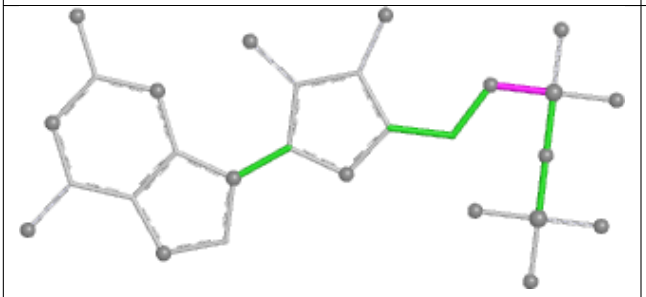
Ligand GDP MP 502



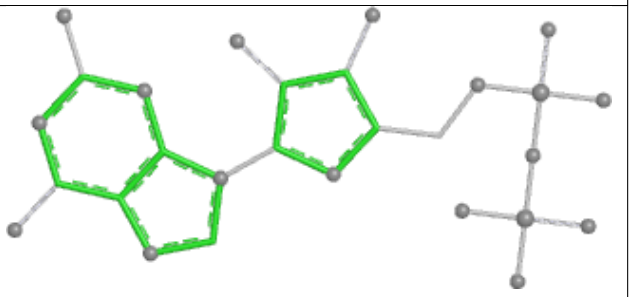
Bond lengths



Bond angles

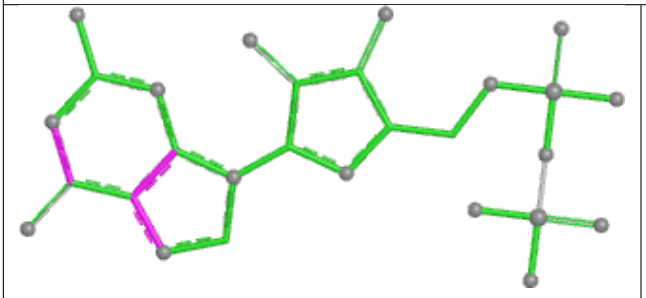


Torsions

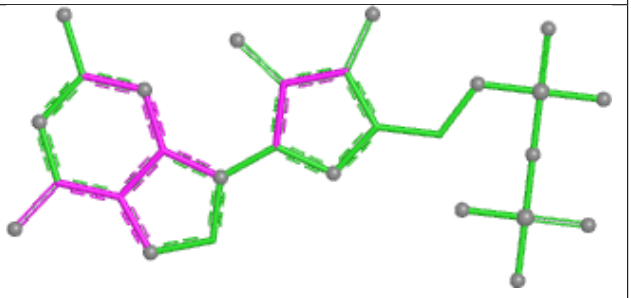


Rings

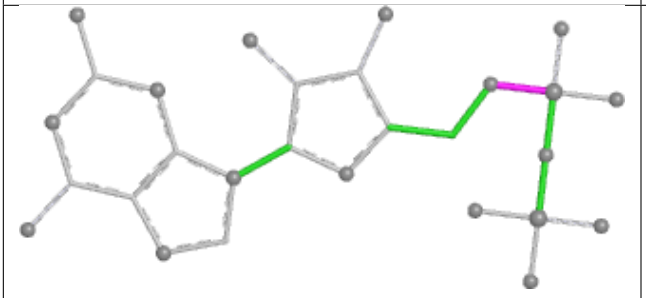
Ligand GDP SF 502



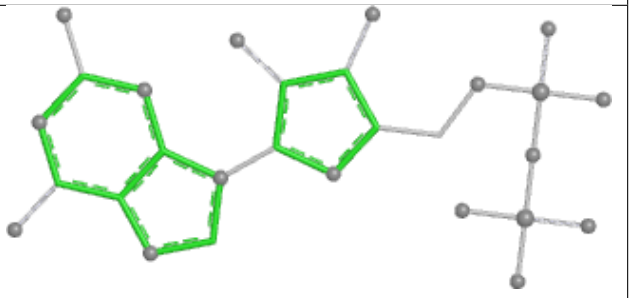
Bond lengths



Bond angles

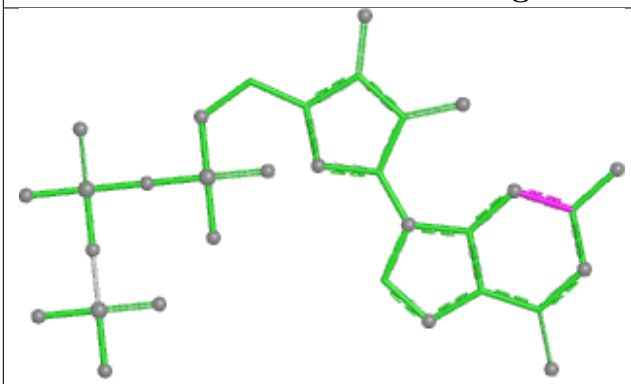


Torsions

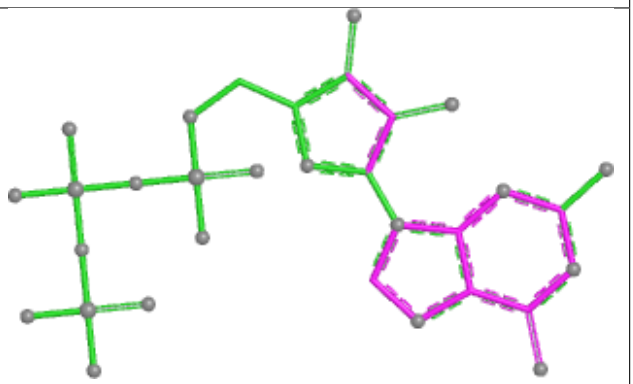


Rings

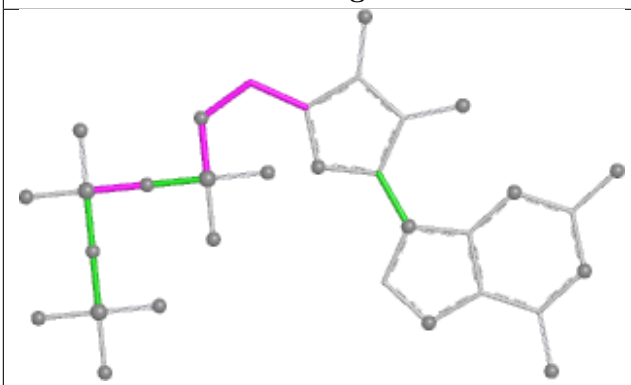
Ligand GTP FC 501



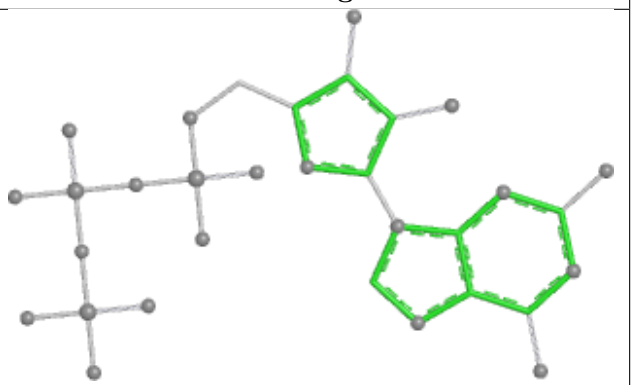
Bond lengths



Bond angles

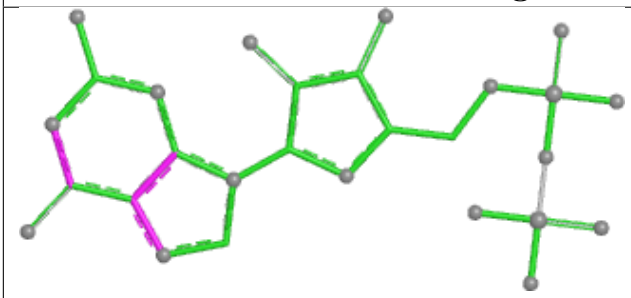


Torsions

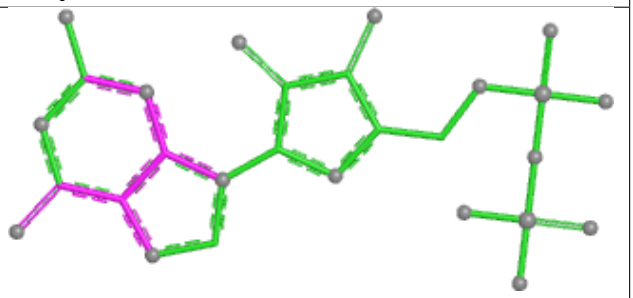


Rings

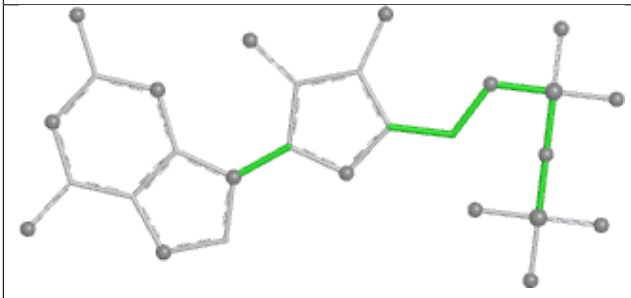
Ligand GDP QJ 502



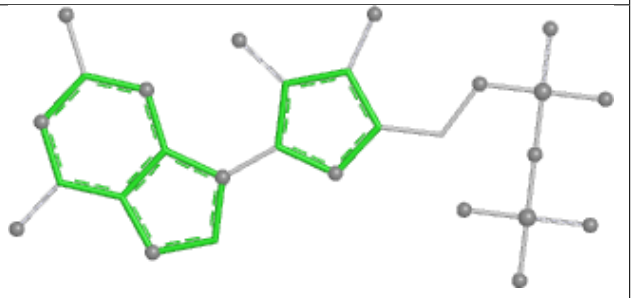
Bond lengths



Bond angles

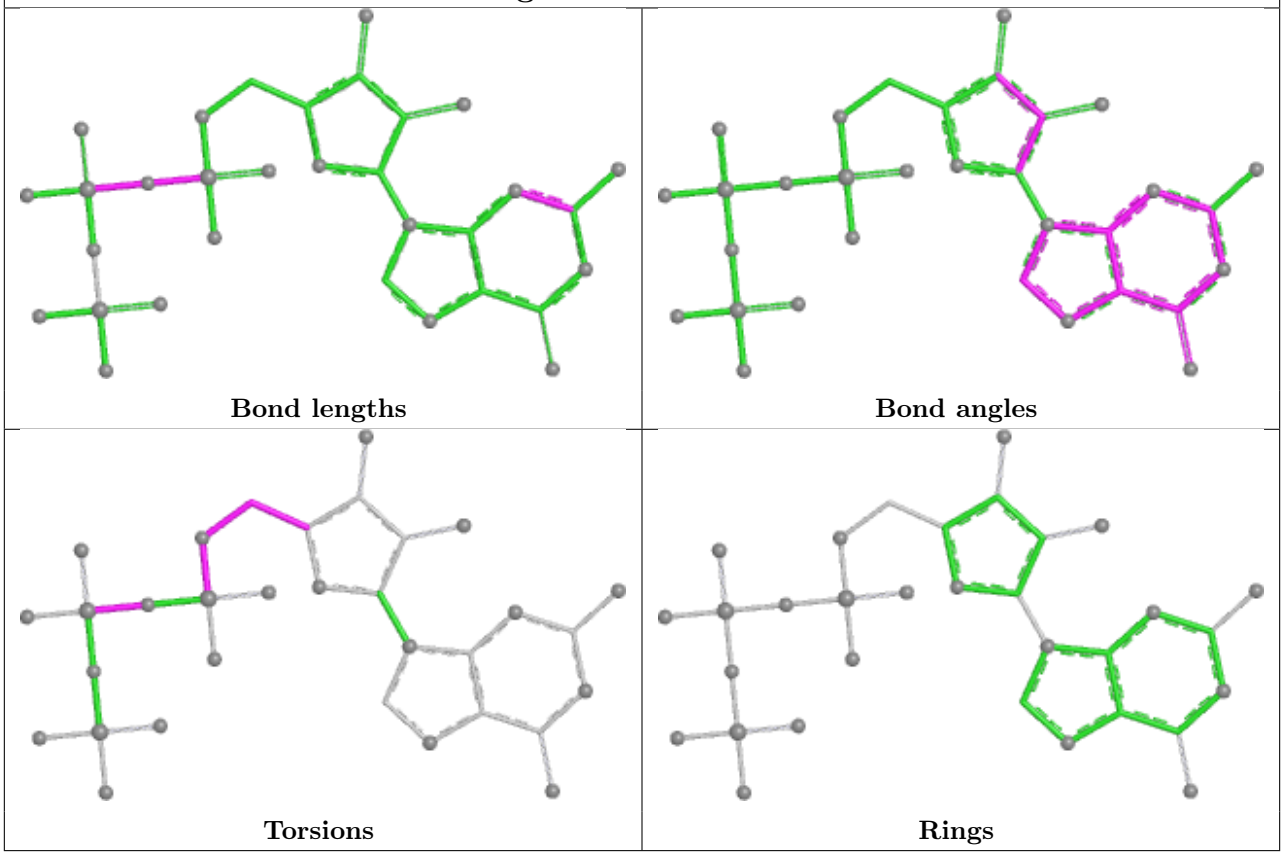


Torsions

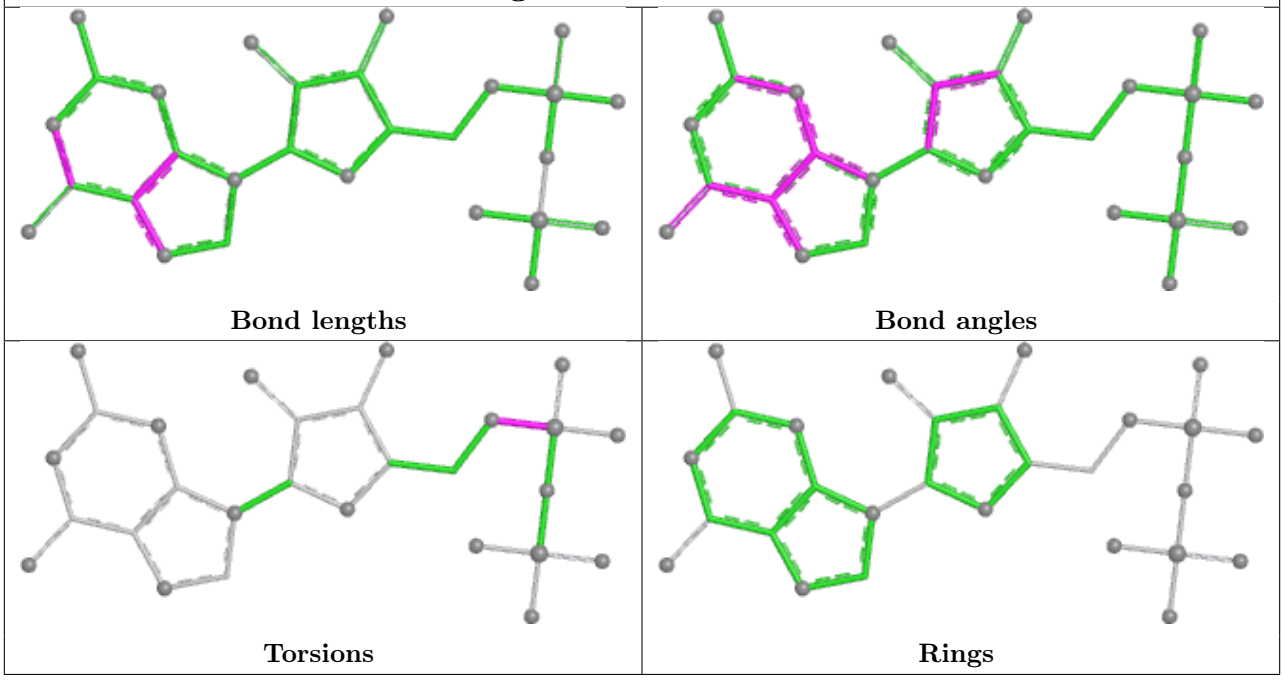


Rings

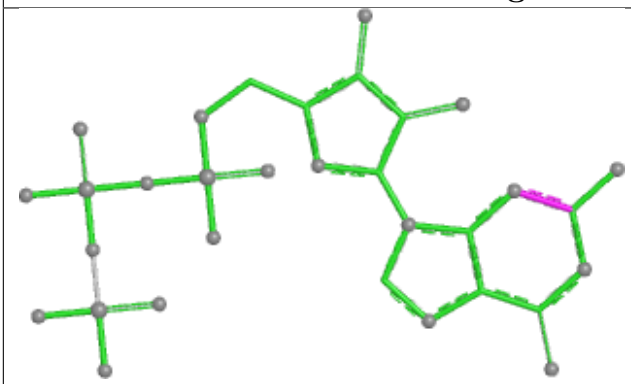
Ligand GTP RI 501



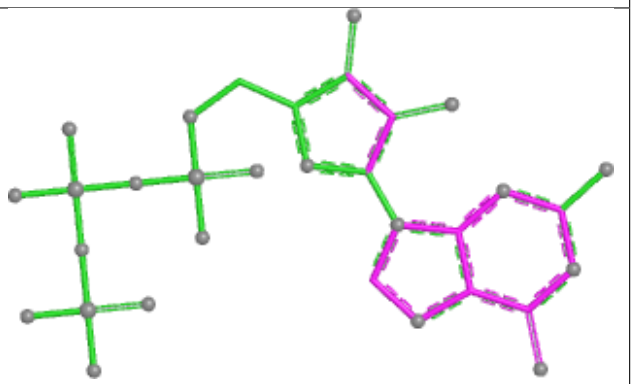
Ligand GDP OP 502



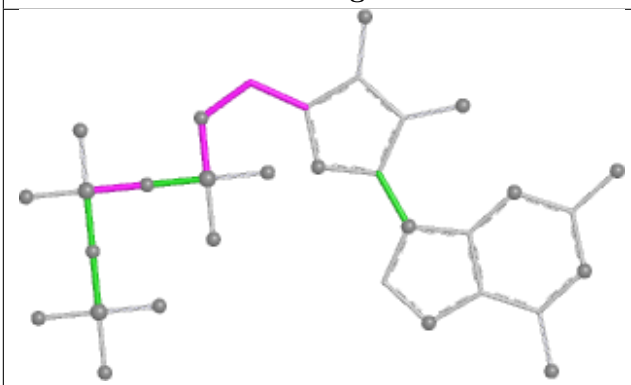
Ligand GTP DG 501



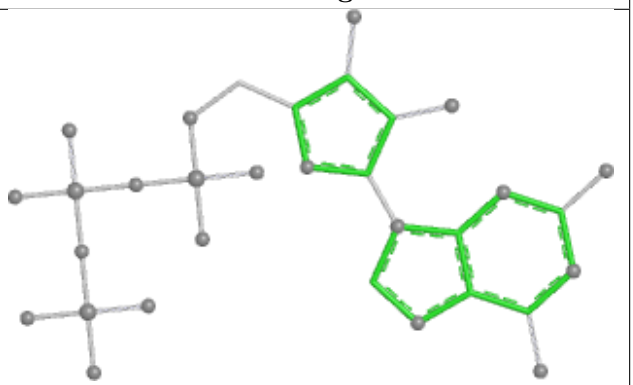
Bond lengths



Bond angles

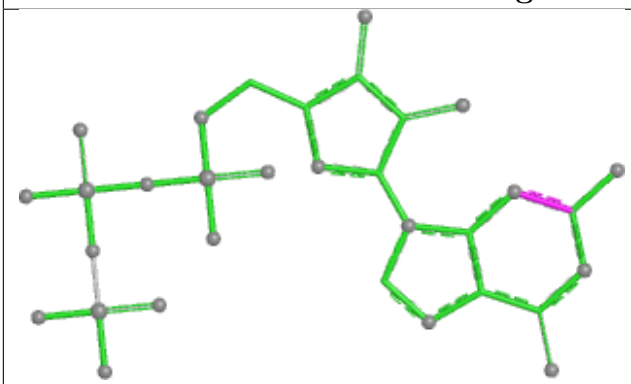


Torsions

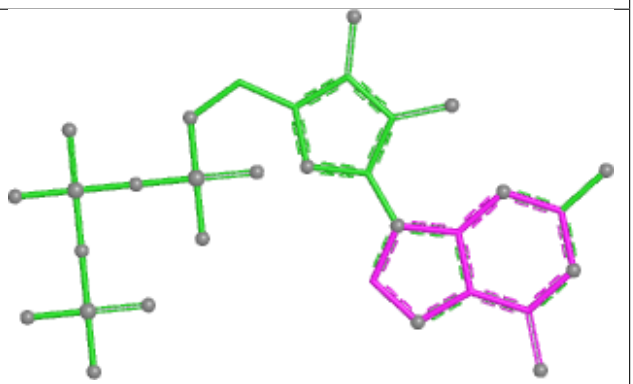


Rings

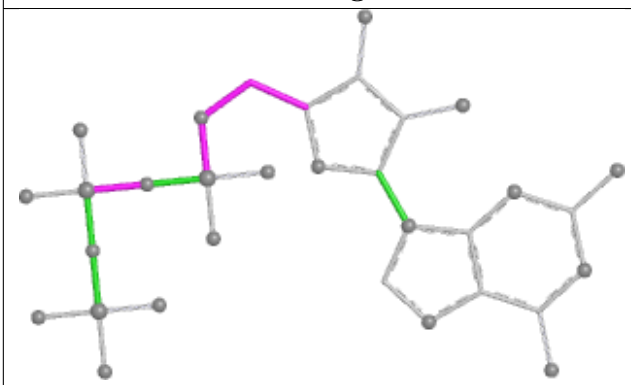
Ligand GTP IO 501



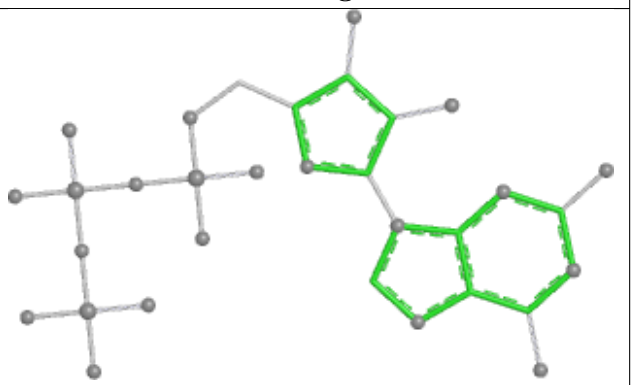
Bond lengths



Bond angles

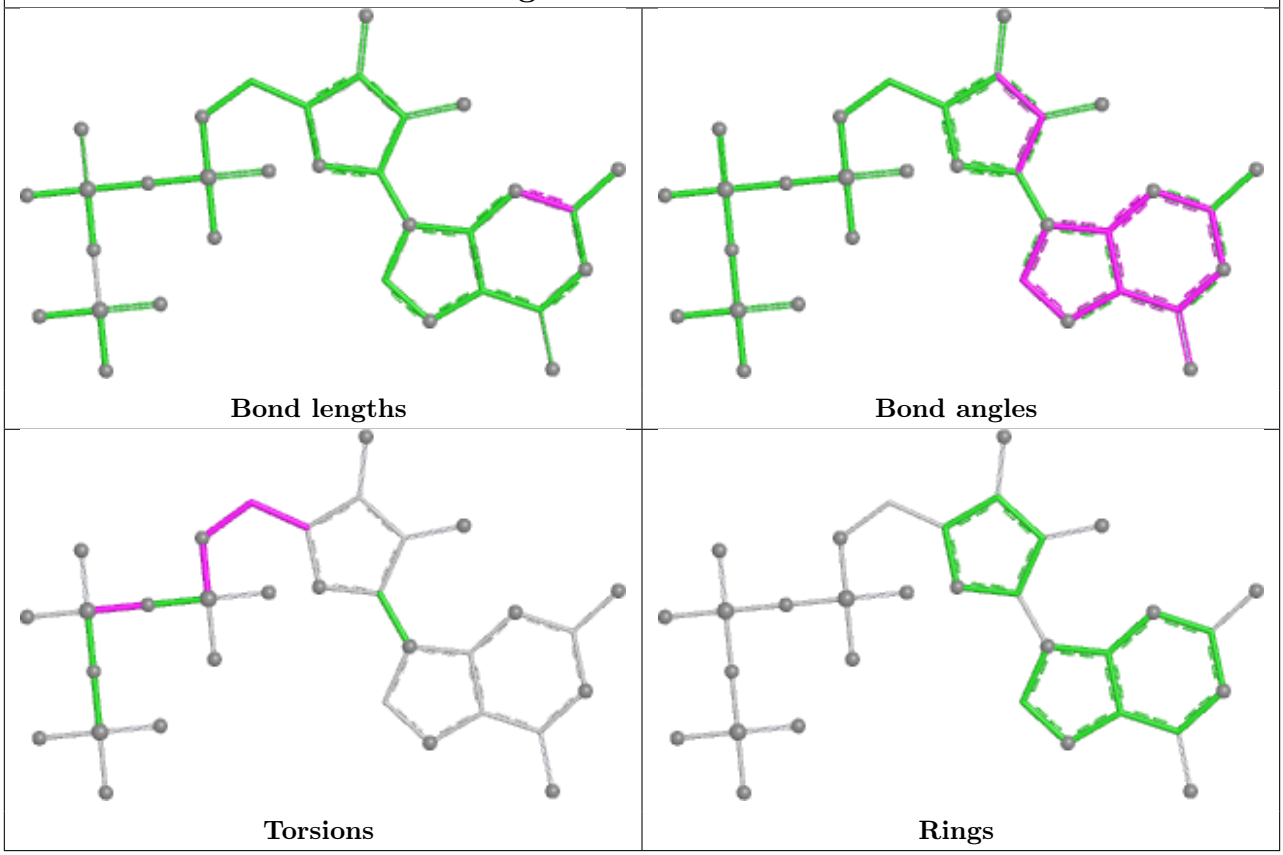


Torsions

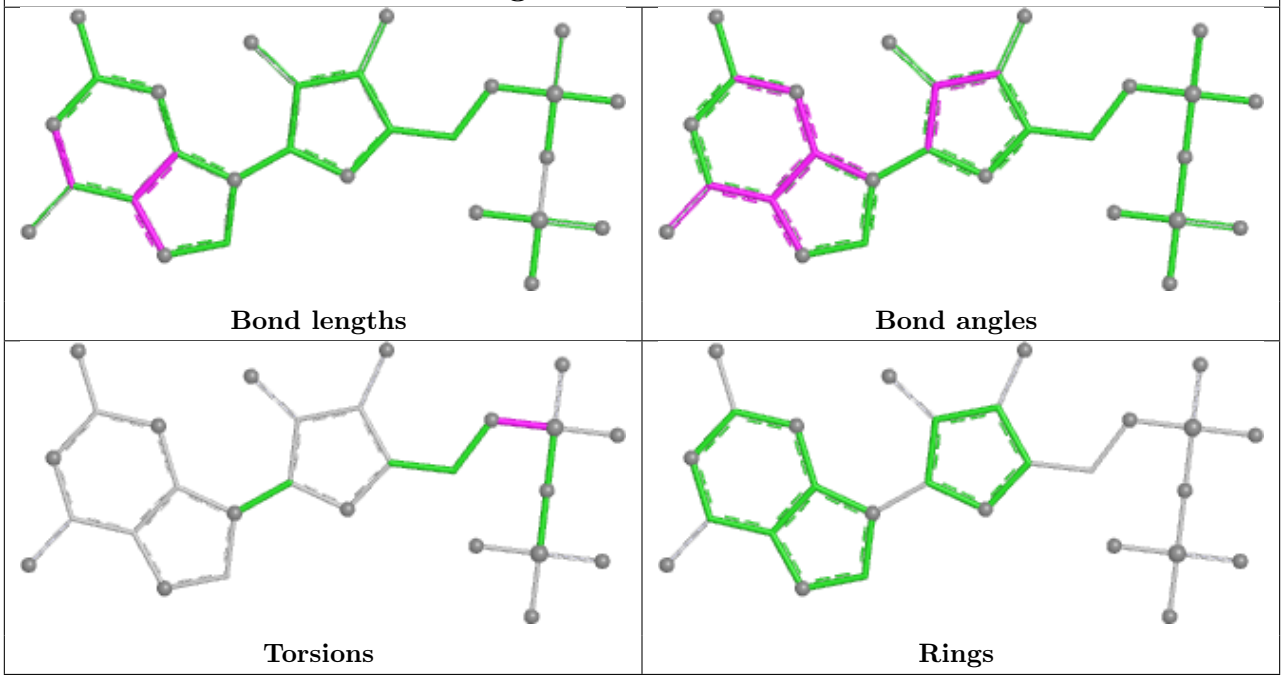


Rings

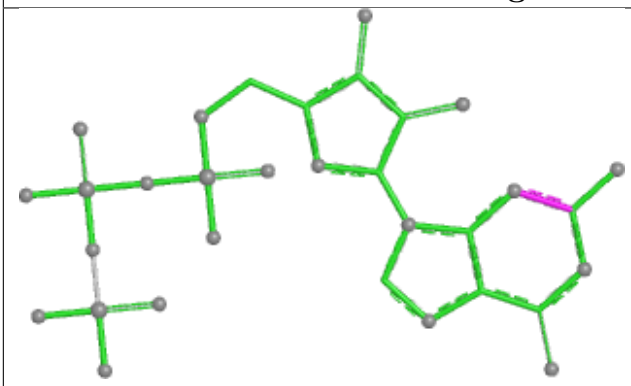
Ligand GTP EI 501



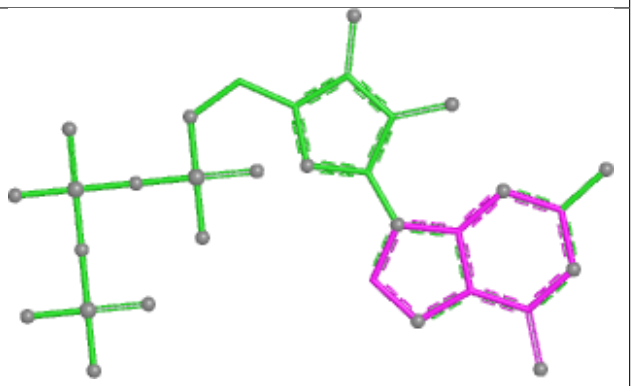
Ligand GDP HP 502



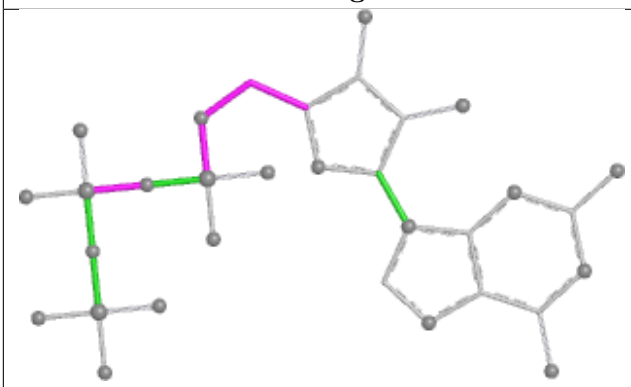
Ligand GTP LM 501



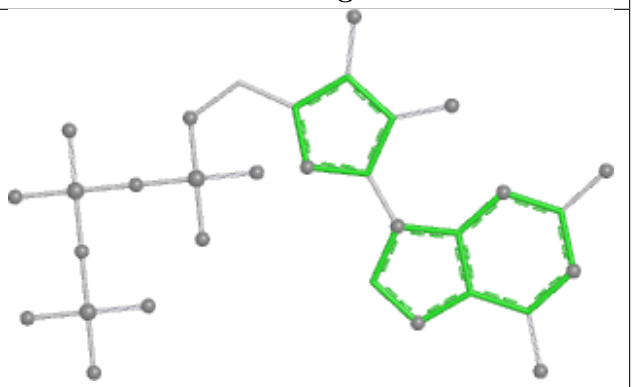
Bond lengths



Bond angles

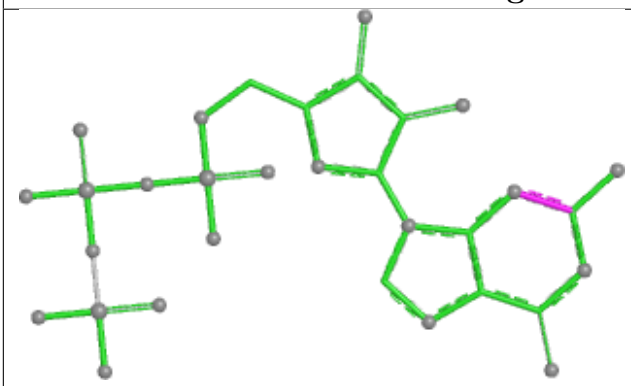


Torsions

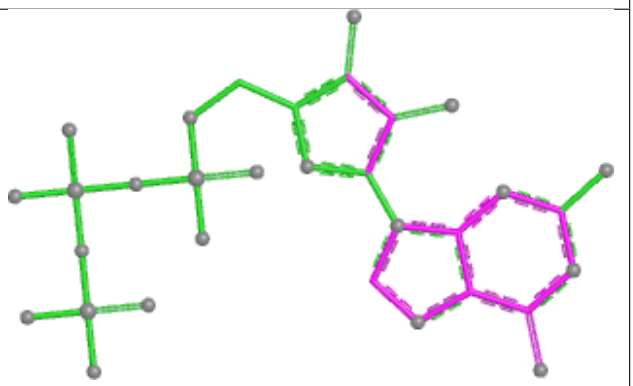


Rings

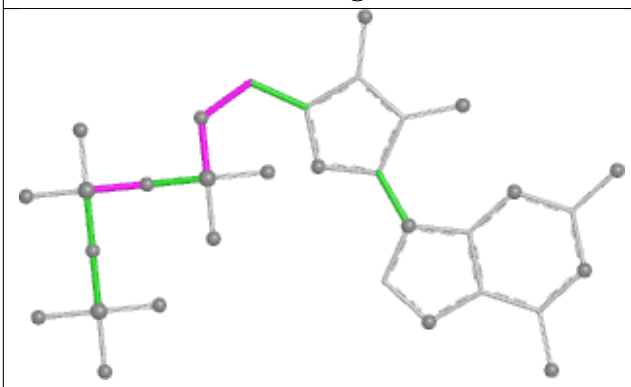
Ligand GTP ME 501



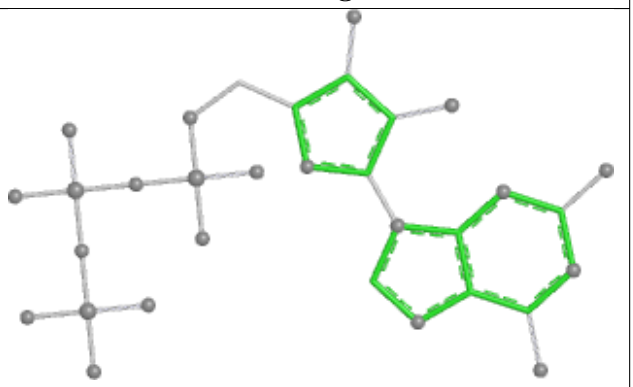
Bond lengths



Bond angles

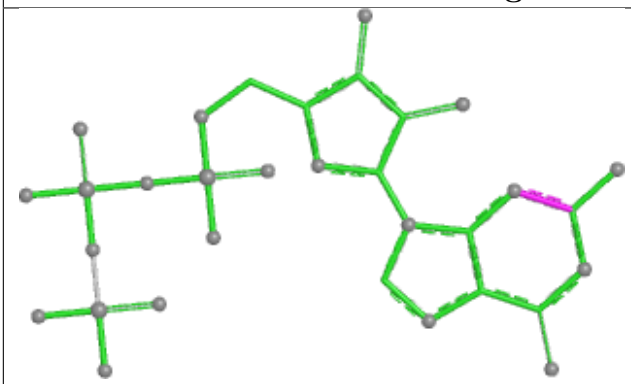


Torsions

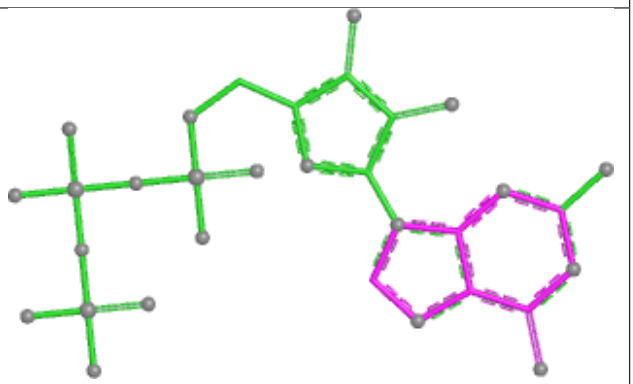


Rings

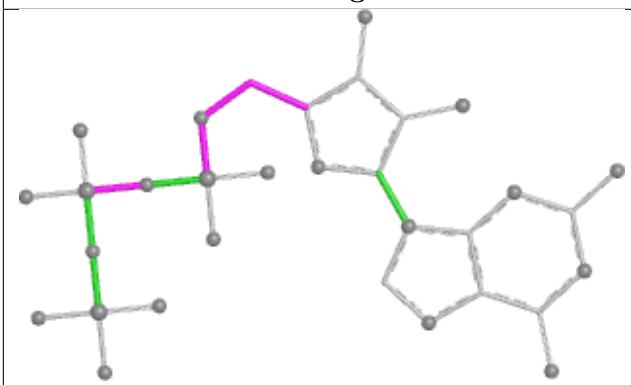
Ligand GTP DM 501



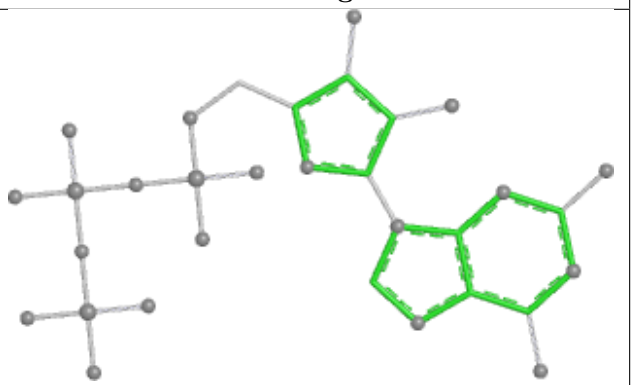
Bond lengths



Bond angles

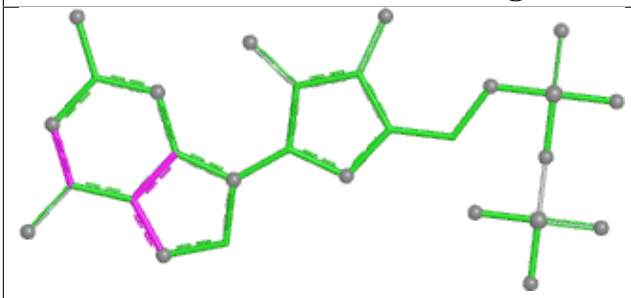


Torsions

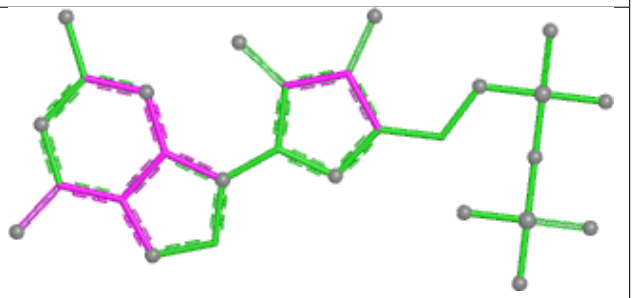


Rings

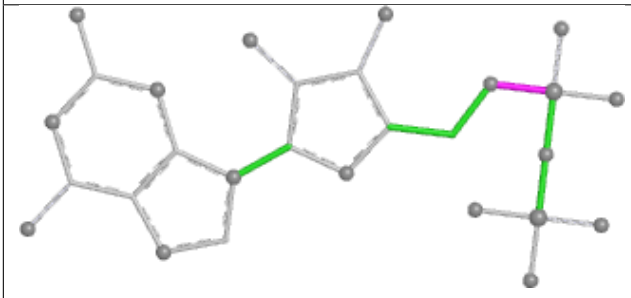
Ligand GDP DD 502



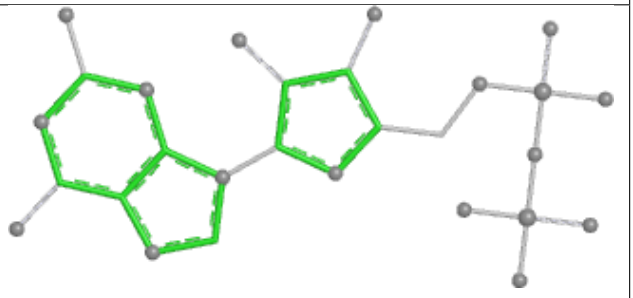
Bond lengths



Bond angles

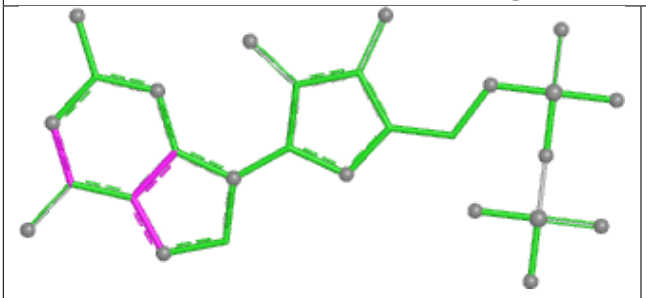


Torsions

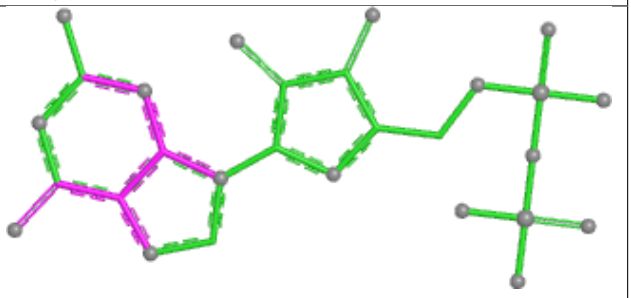


Rings

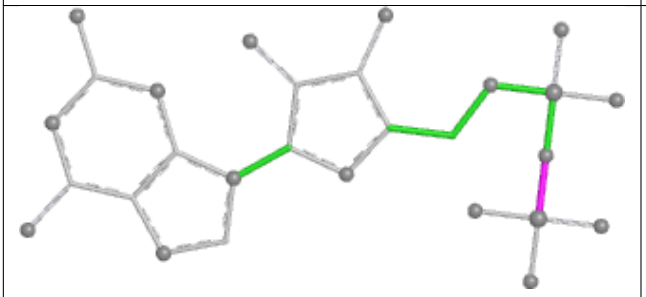
Ligand GDP QH 502



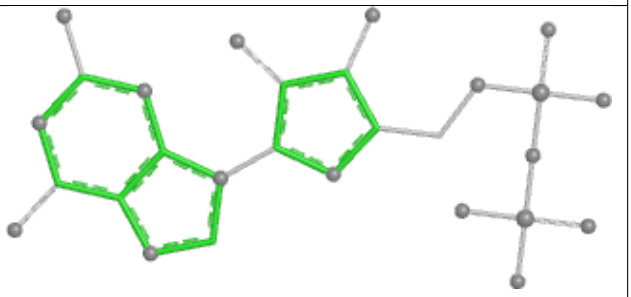
Bond lengths



Bond angles

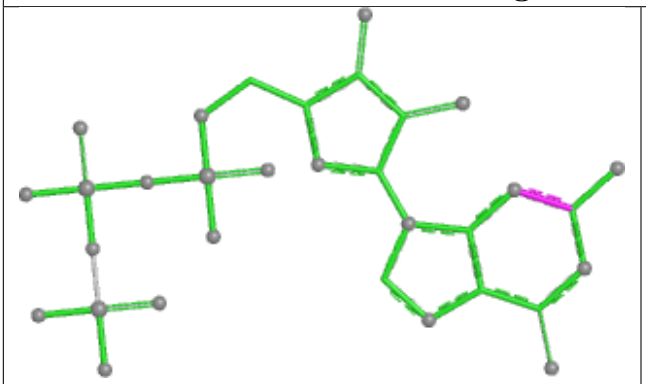


Torsions

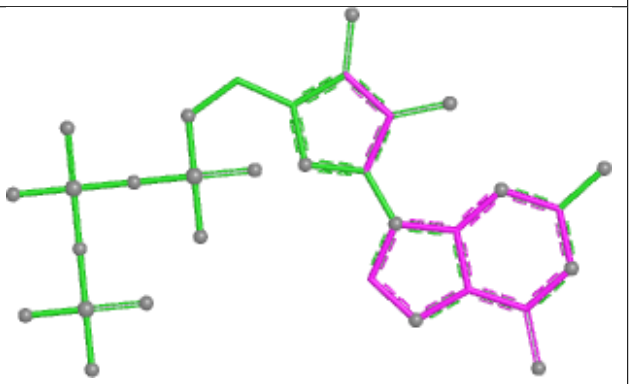


Rings

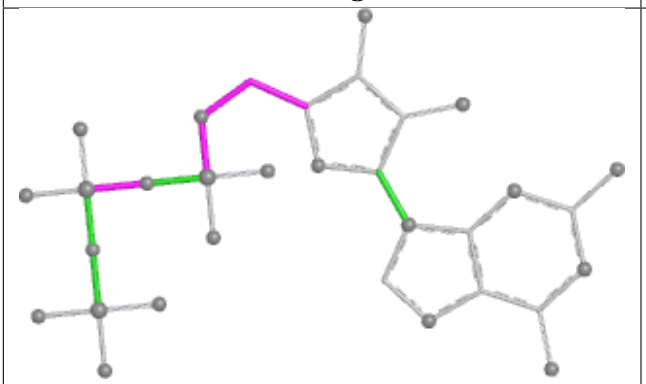
Ligand GTP FA 501



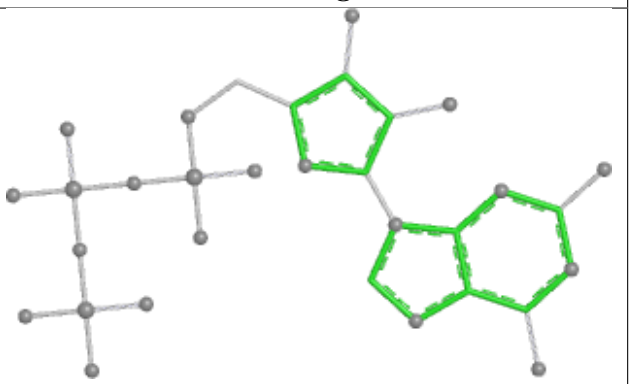
Bond lengths



Bond angles

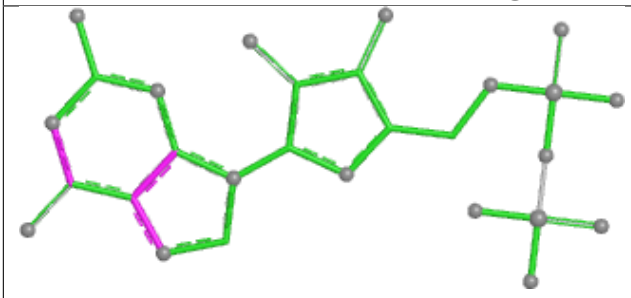


Torsions

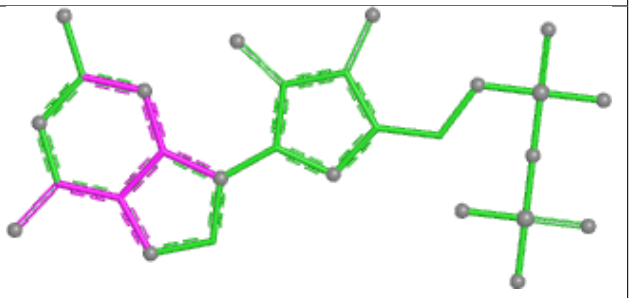


Rings

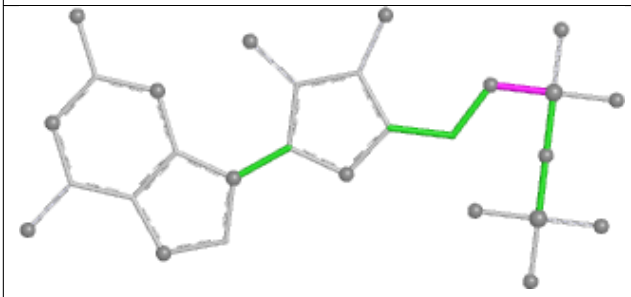
Ligand GDP KH 502



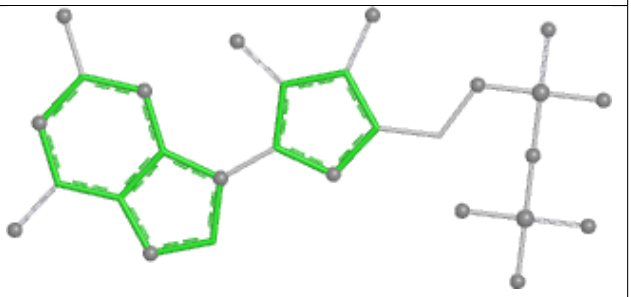
Bond lengths



Bond angles

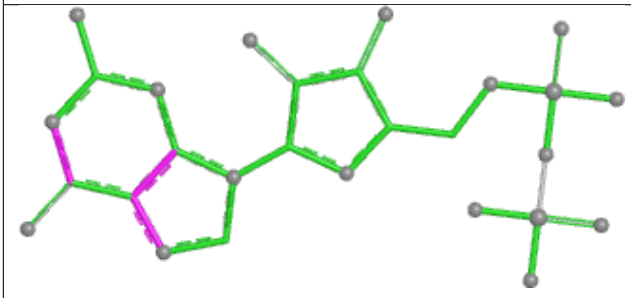


Torsions

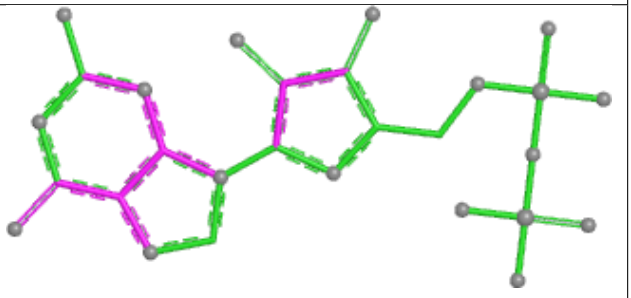


Rings

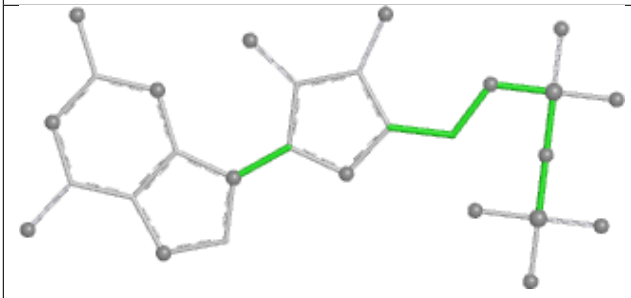
Ligand GDP BB 502



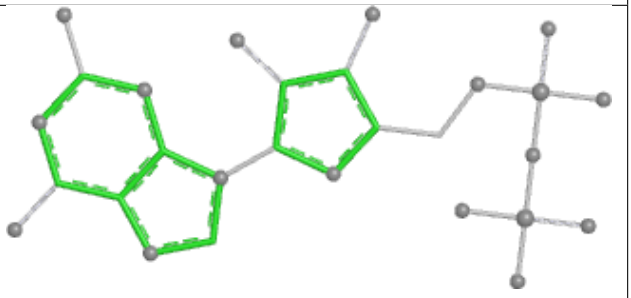
Bond lengths



Bond angles

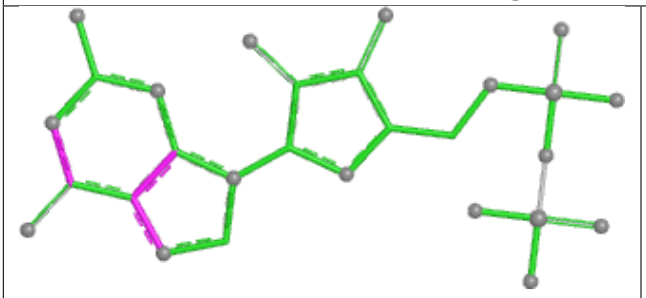


Torsions

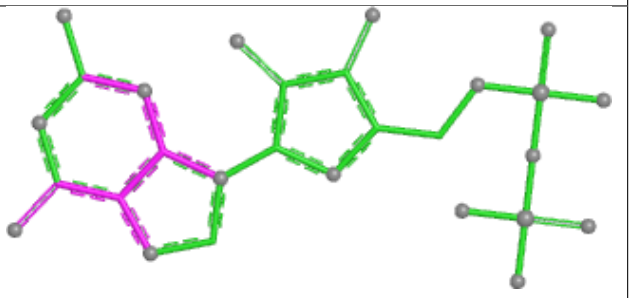


Rings

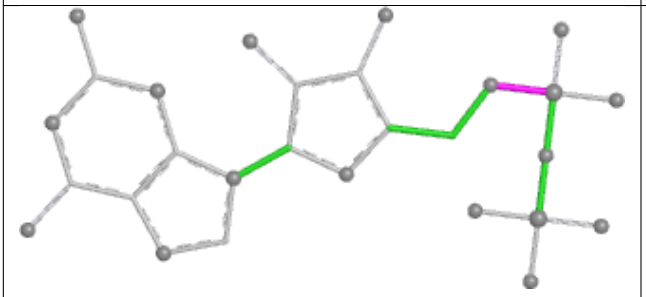
Ligand GDP AH 502



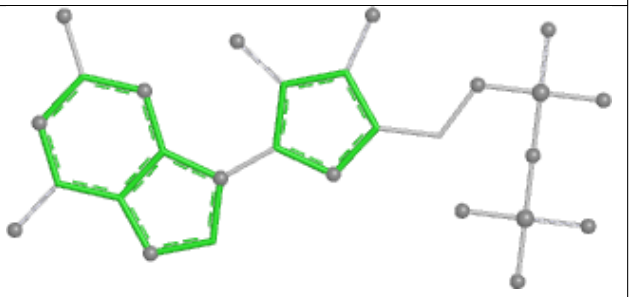
Bond lengths



Bond angles

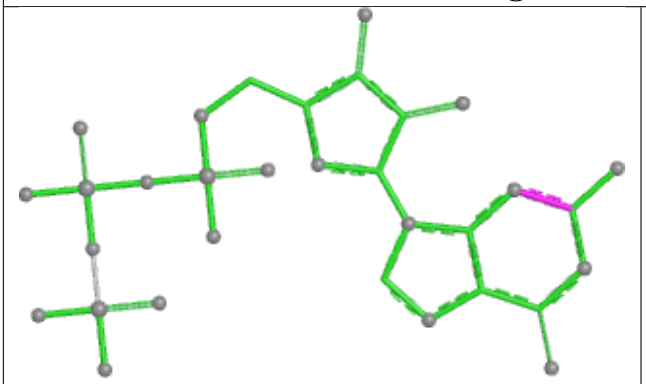


Torsions

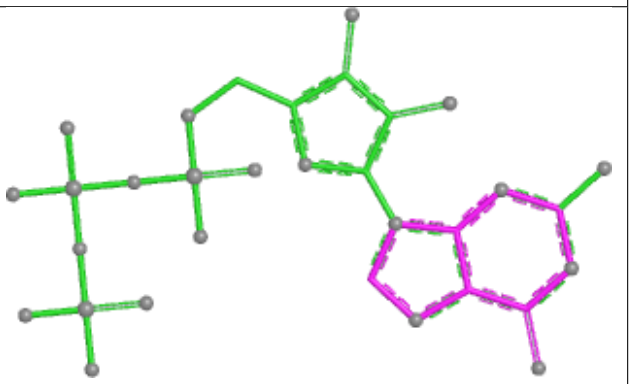


Rings

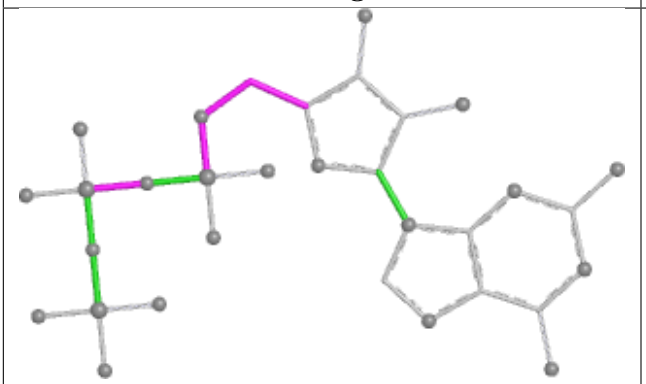
Ligand GTP FM 501



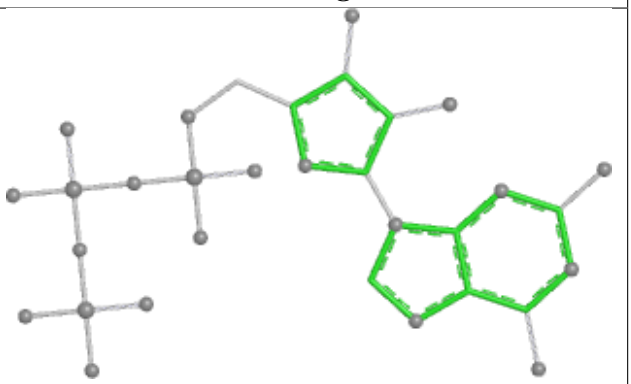
Bond lengths



Bond angles

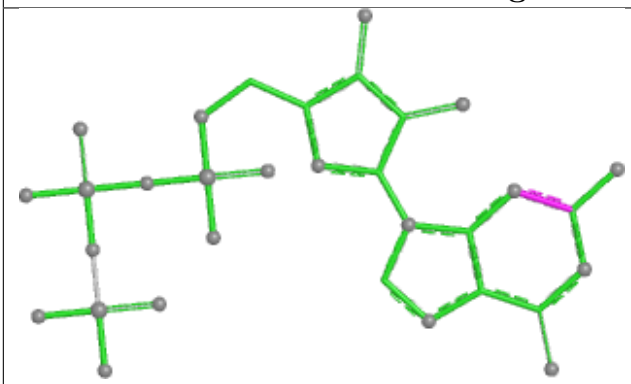


Torsions

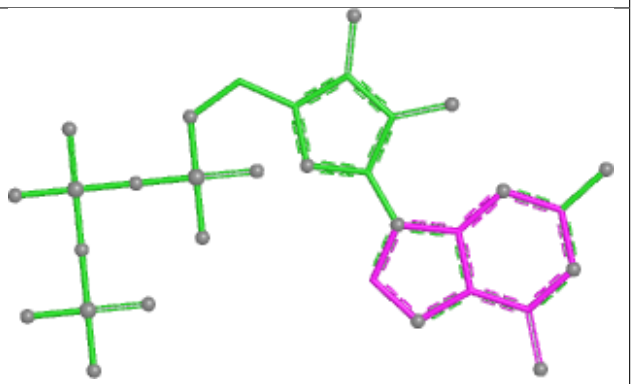


Rings

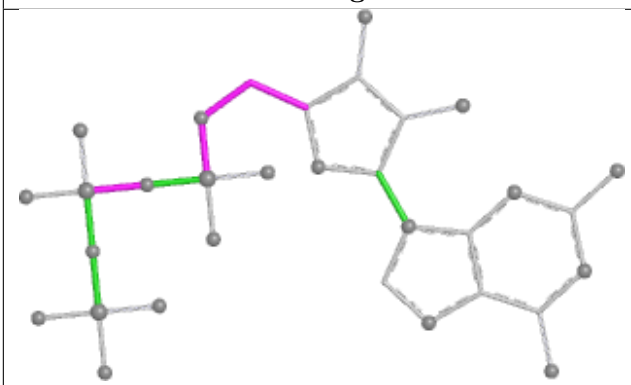
Ligand GTP BG 501



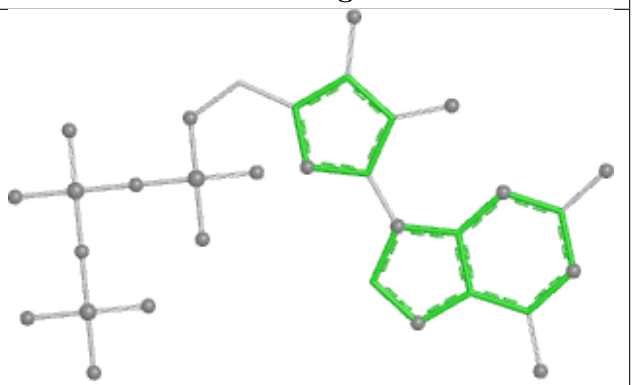
Bond lengths



Bond angles

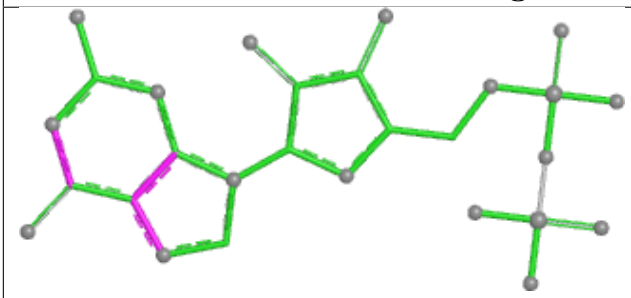


Torsions

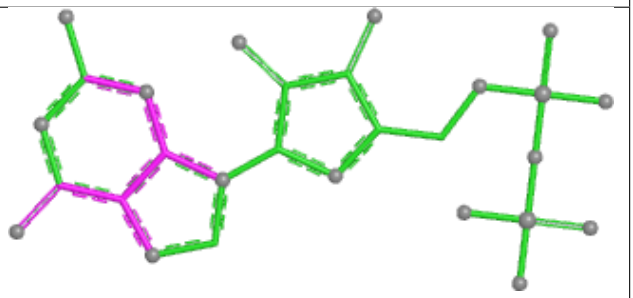


Rings

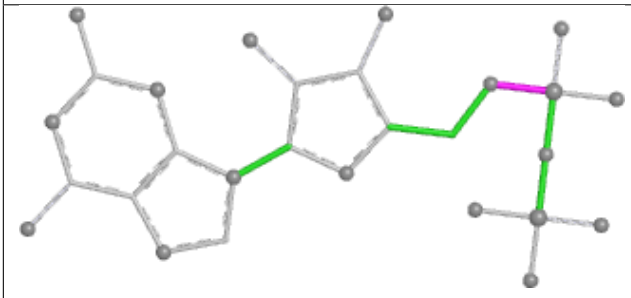
Ligand GDP BP 502



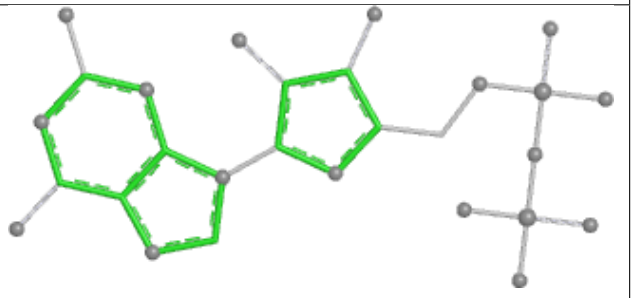
Bond lengths



Bond angles

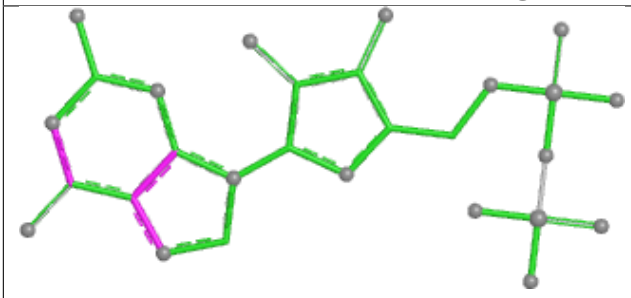


Torsions

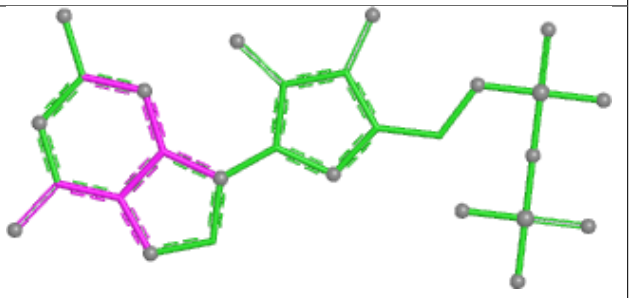


Rings

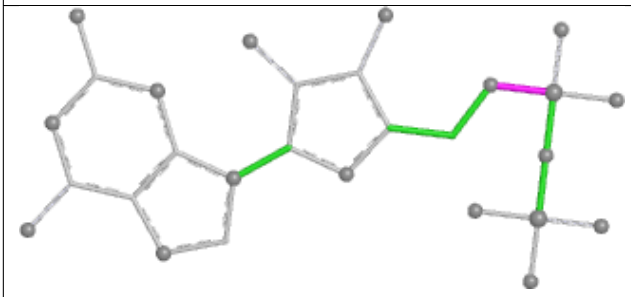
Ligand GDP FJ 502



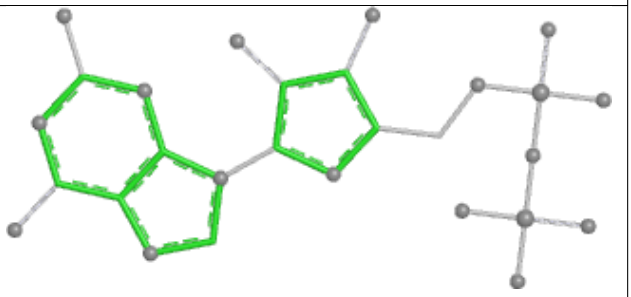
Bond lengths



Bond angles

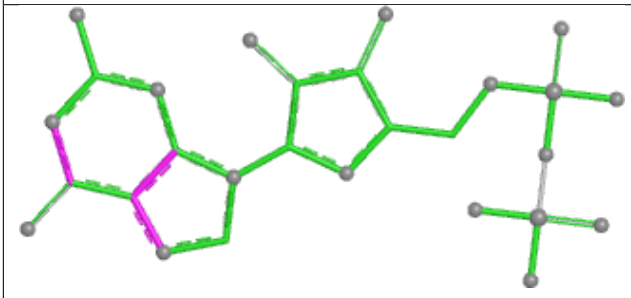


Torsions

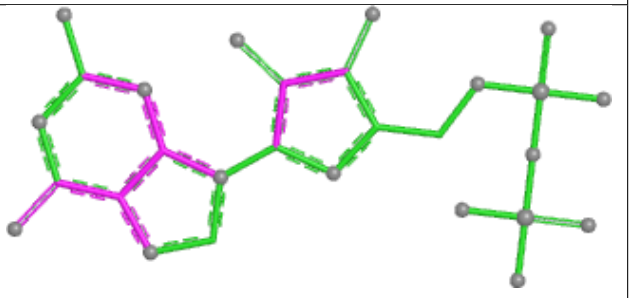


Rings

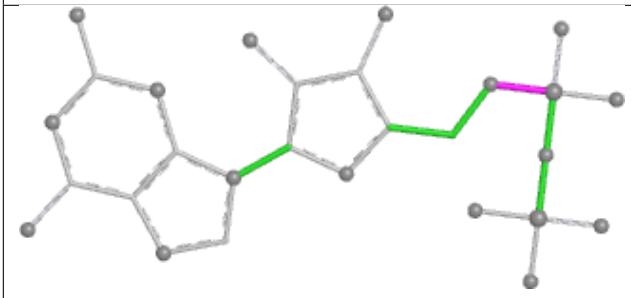
Ligand GDP PB 502



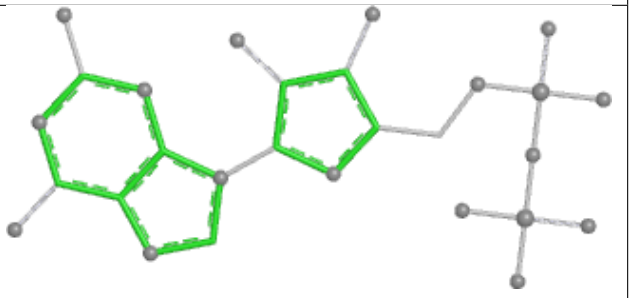
Bond lengths



Bond angles

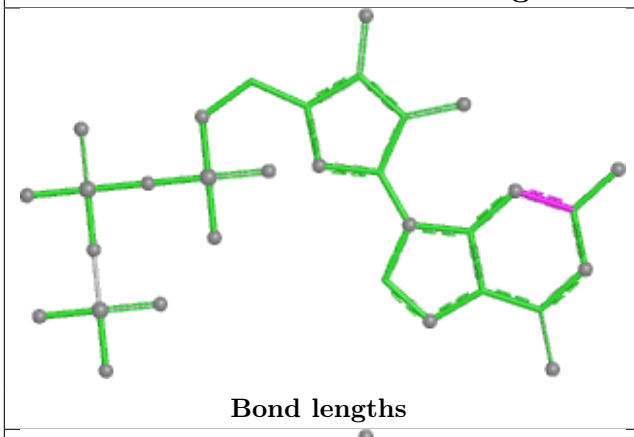


Torsions

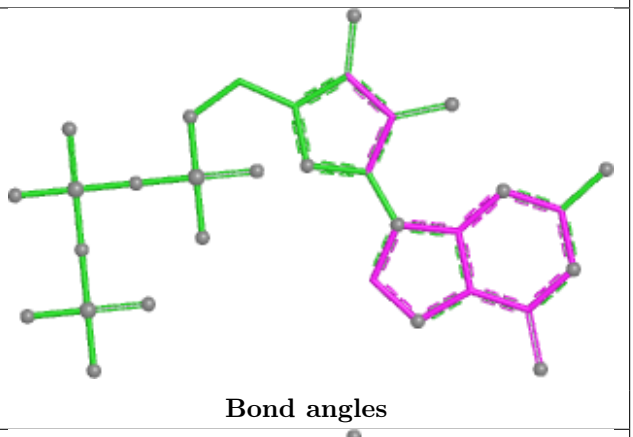


Rings

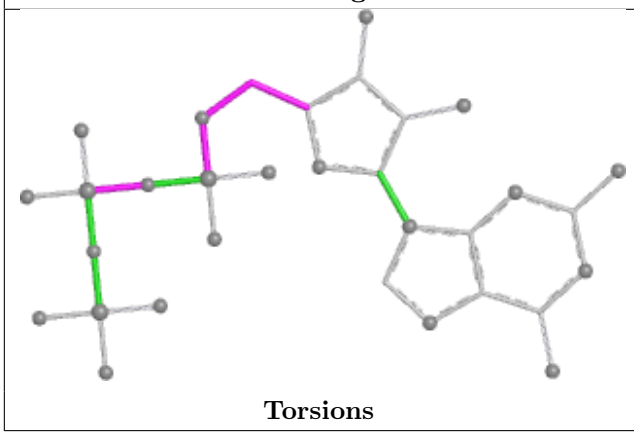
Ligand GTP TA 501



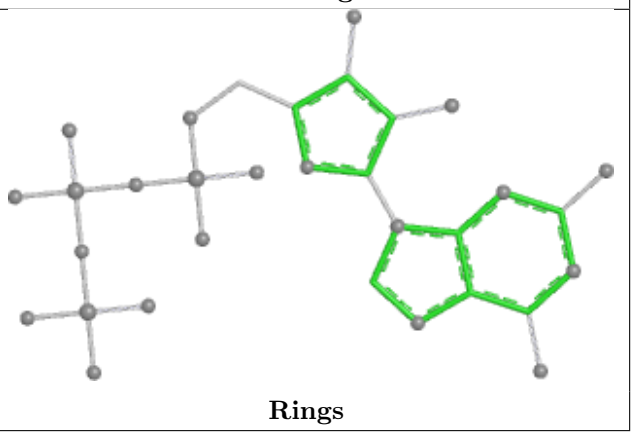
Bond lengths



Bond angles

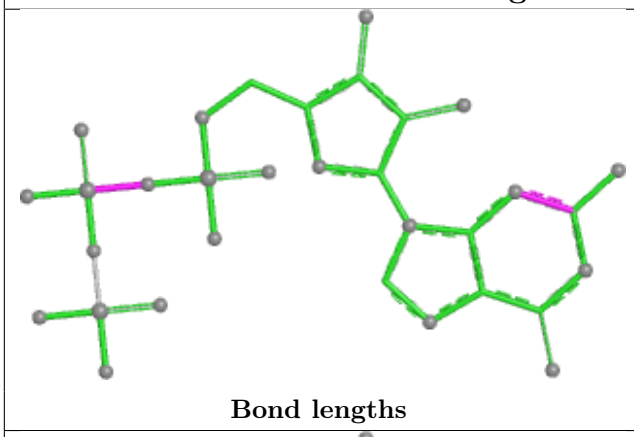


Torsions

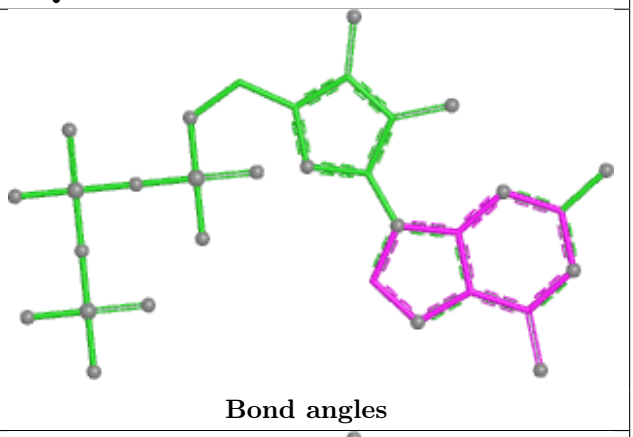


Rings

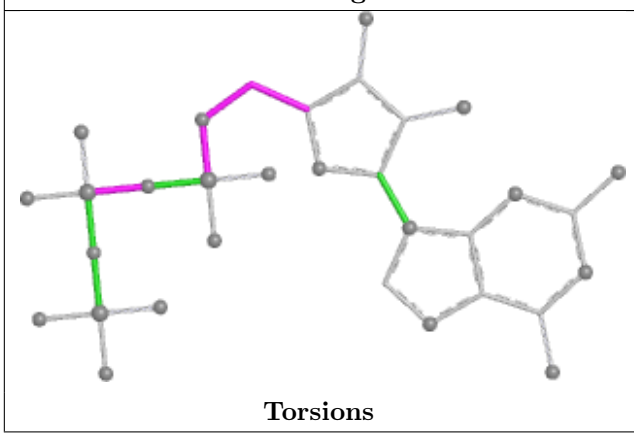
Ligand GTP QG 501



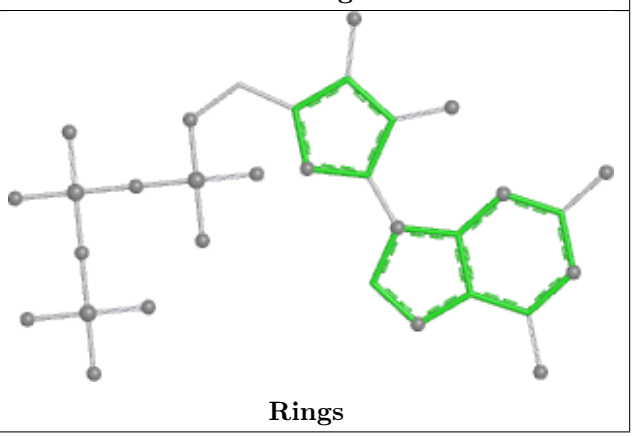
Bond lengths



Bond angles

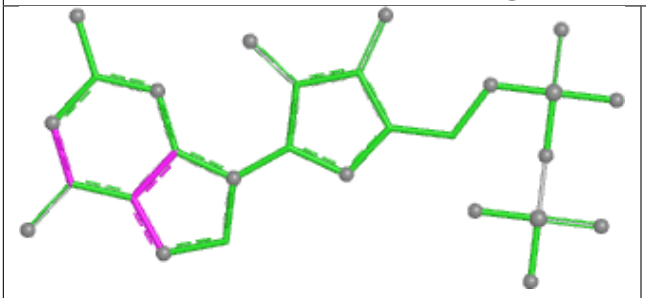


Torsions

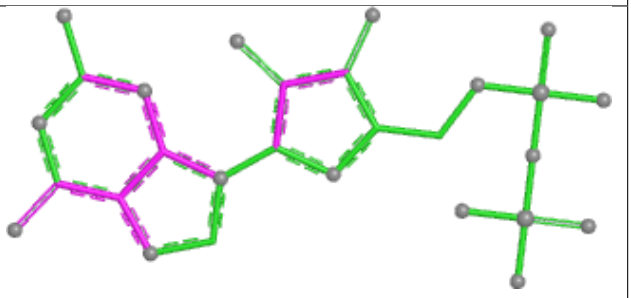


Rings

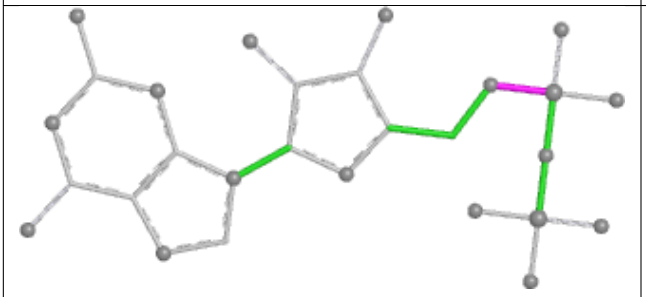
Ligand GDP MN 502



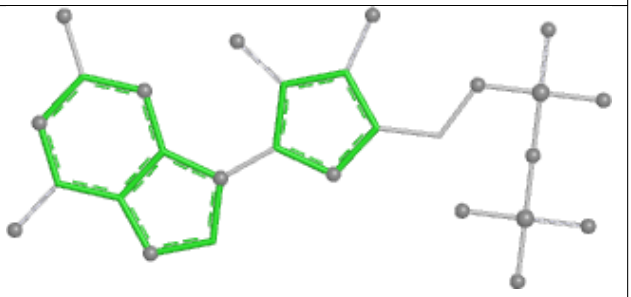
Bond lengths



Bond angles

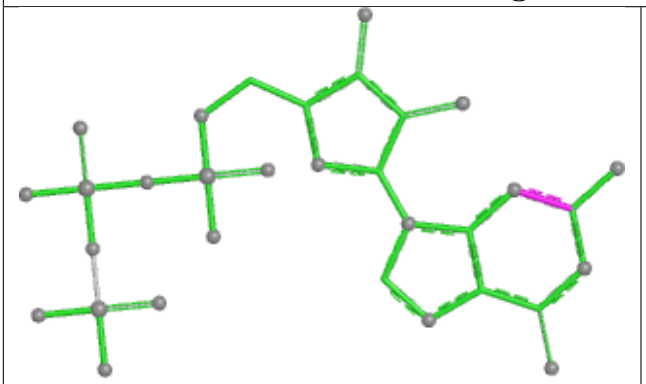


Torsions

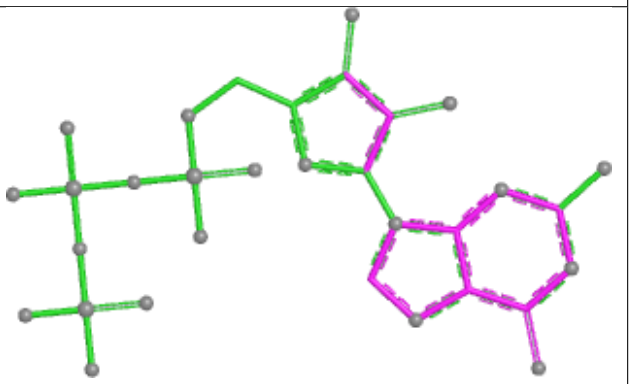


Rings

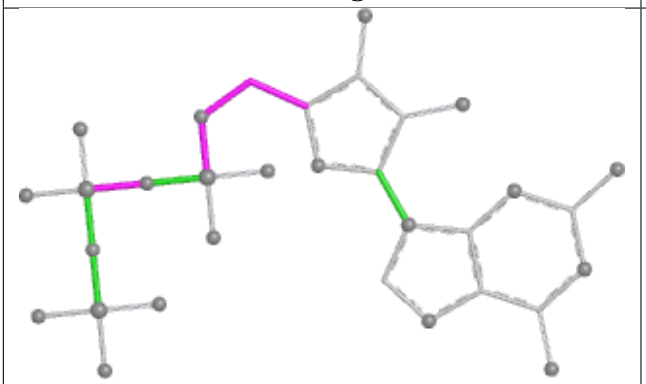
Ligand GTP EA 501



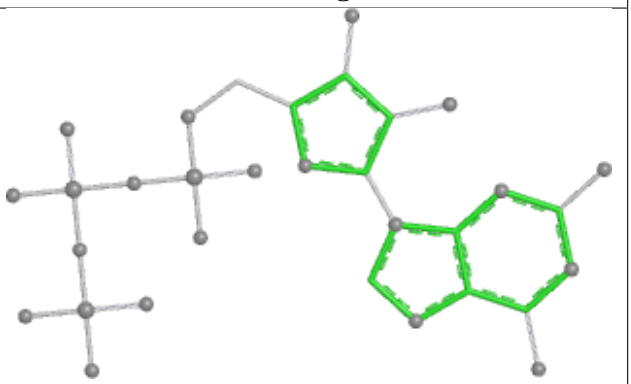
Bond lengths



Bond angles

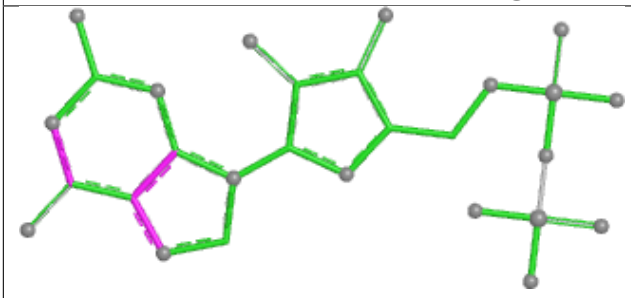


Torsions

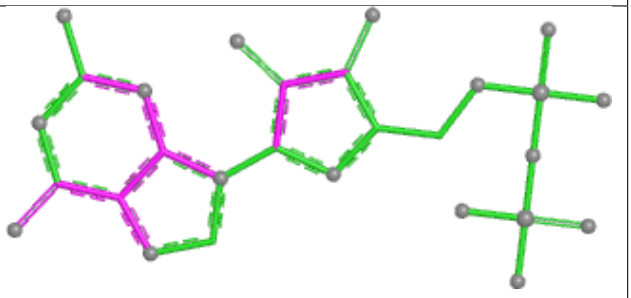


Rings

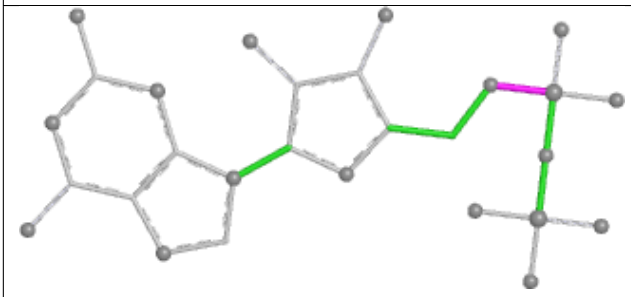
Ligand GDP BD 502



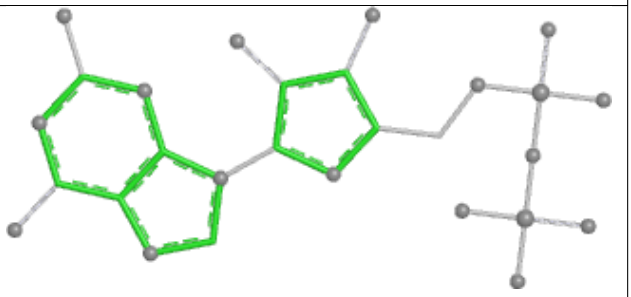
Bond lengths



Bond angles

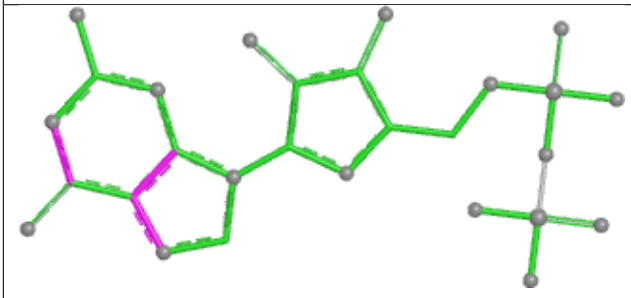


Torsions

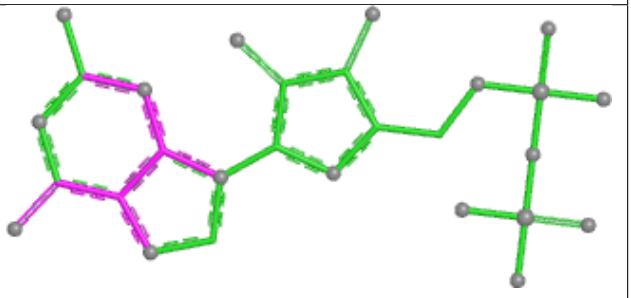


Rings

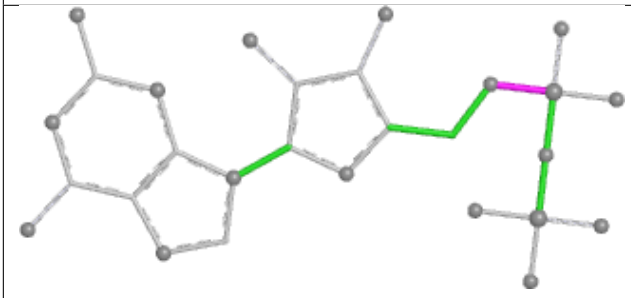
Ligand GDP IN 502



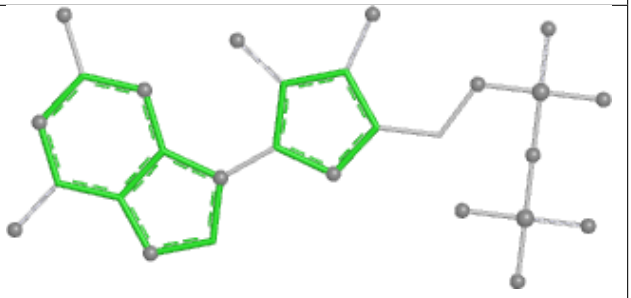
Bond lengths



Bond angles

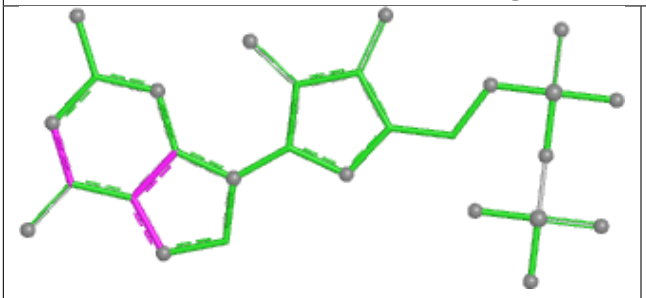


Torsions

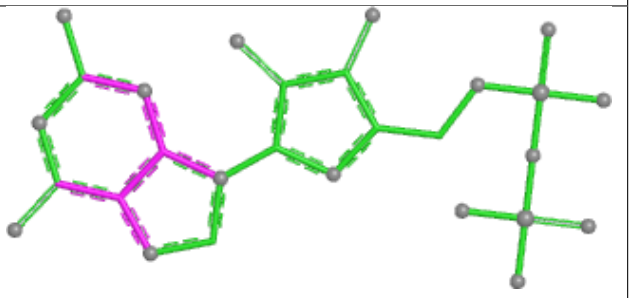


Rings

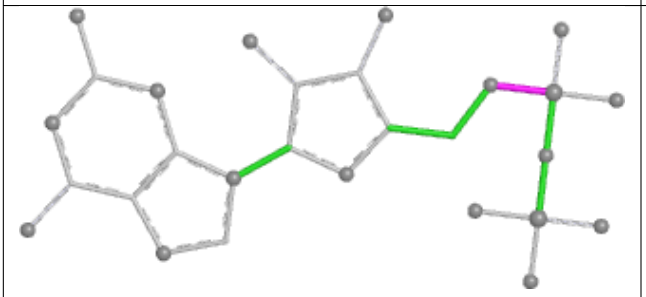
Ligand GDP VN 502



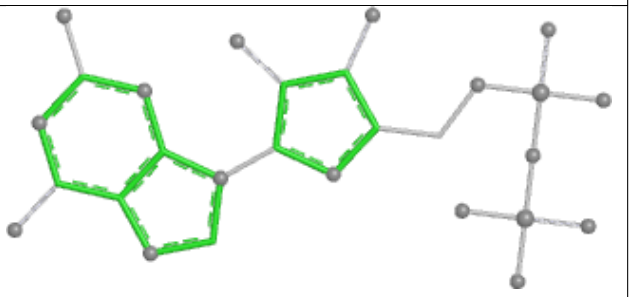
Bond lengths



Bond angles

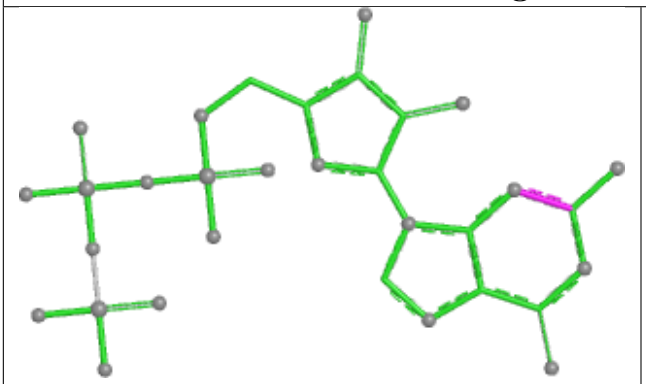


Torsions

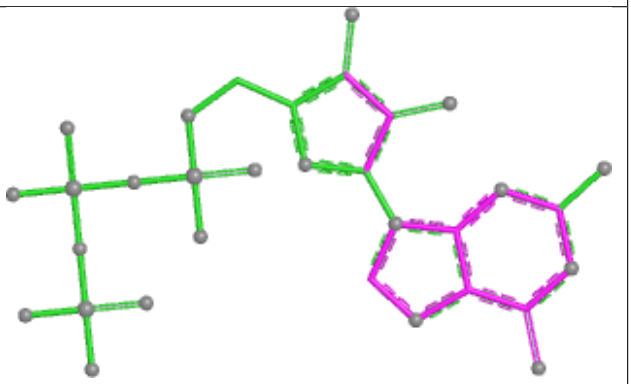


Rings

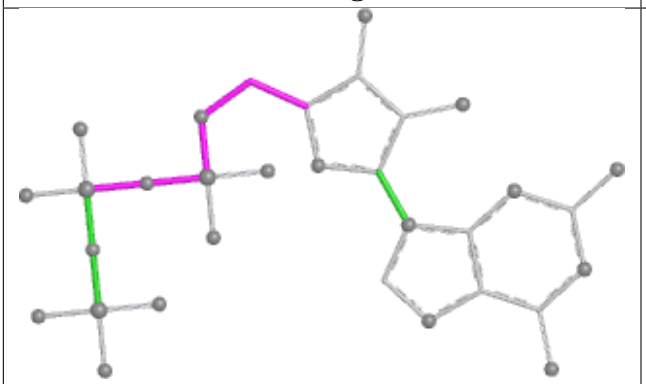
Ligand GTP FO 501



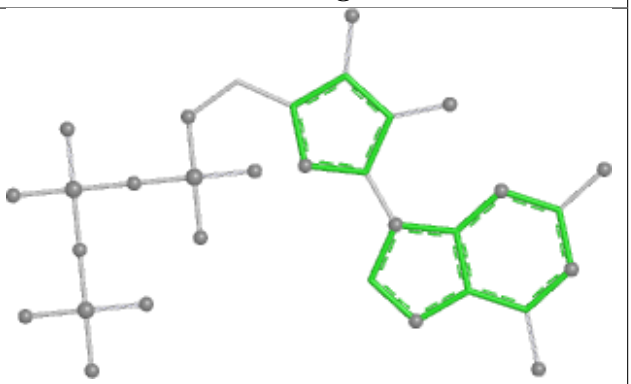
Bond lengths



Bond angles

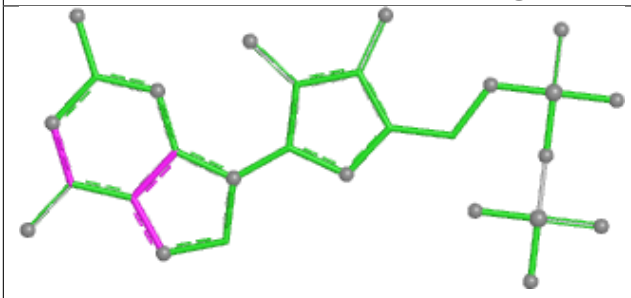


Torsions

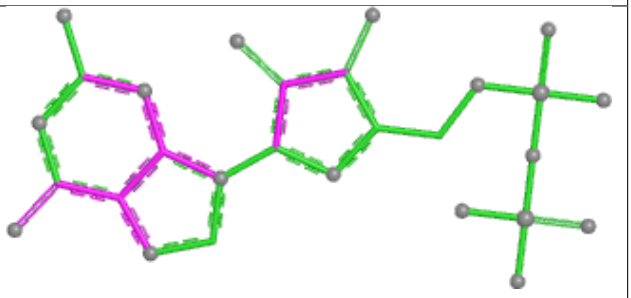


Rings

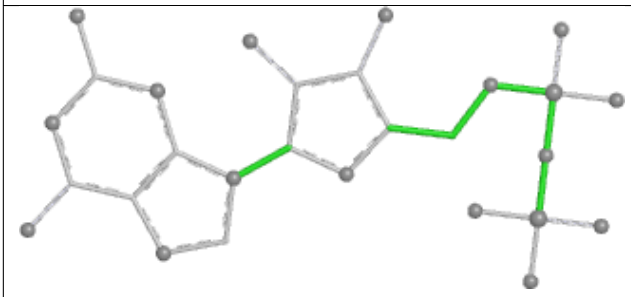
Ligand GDP RL 502



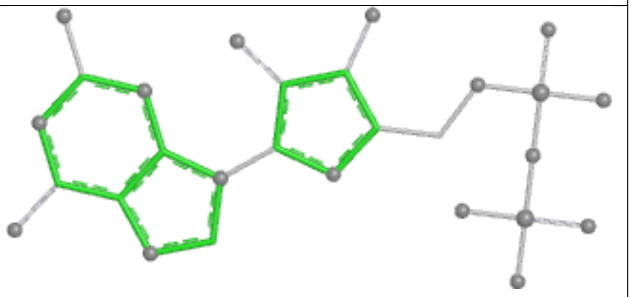
Bond lengths



Bond angles

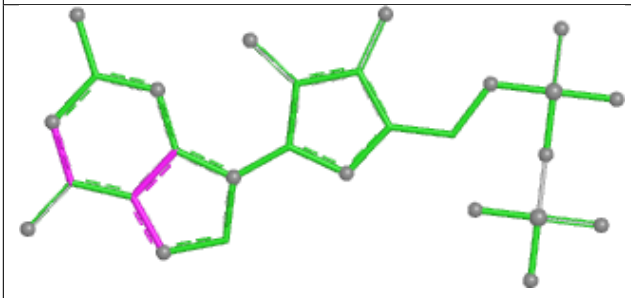


Torsions

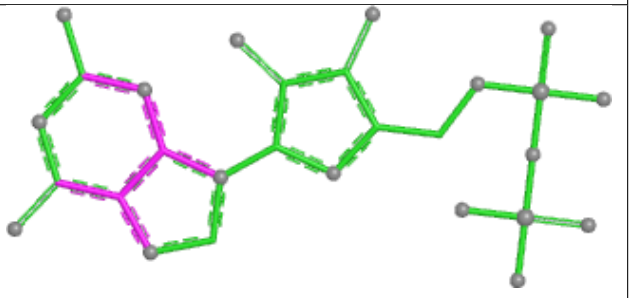


Rings

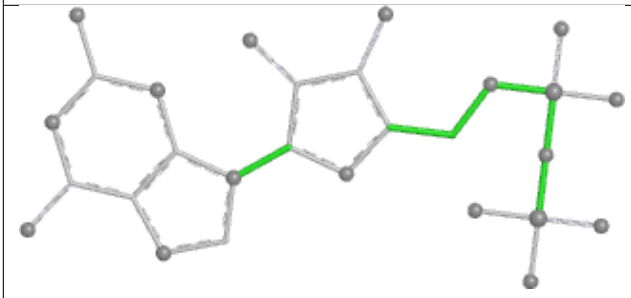
Ligand GDP DF 502



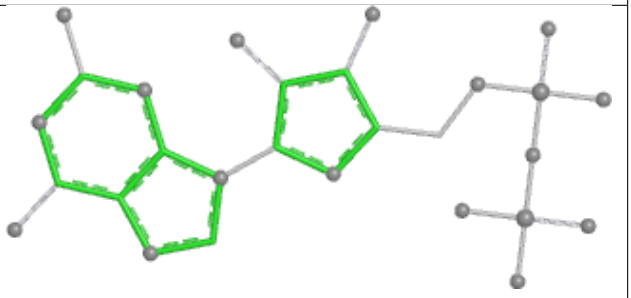
Bond lengths



Bond angles

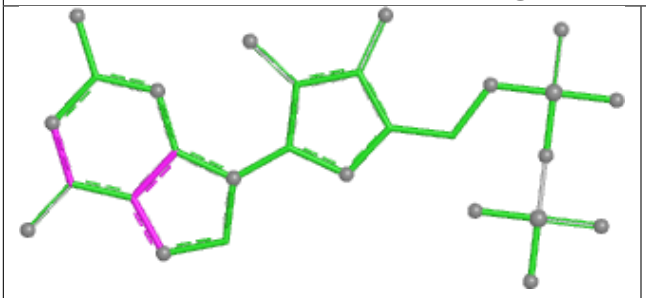


Torsions

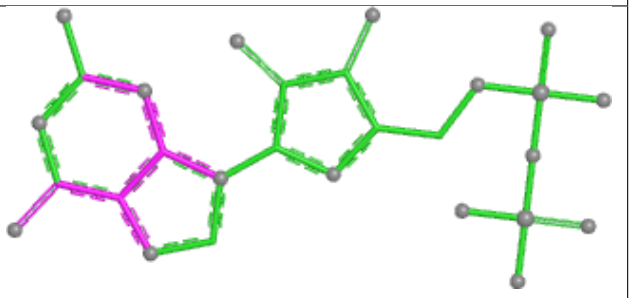


Rings

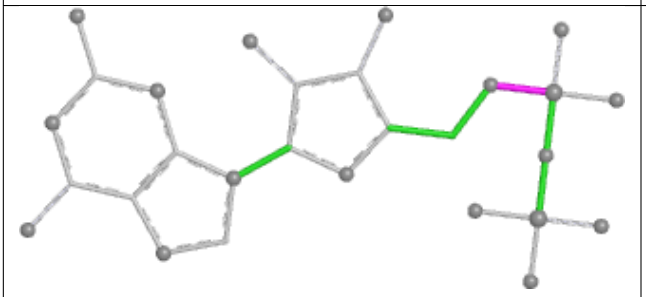
Ligand GDP AJ 502



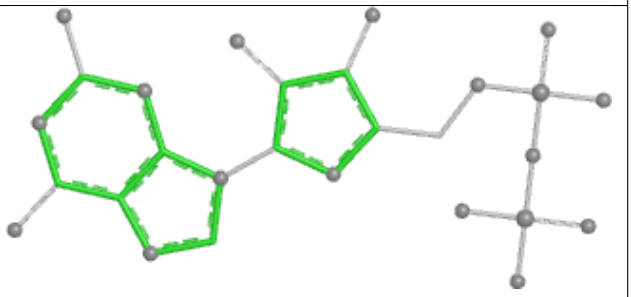
Bond lengths



Bond angles

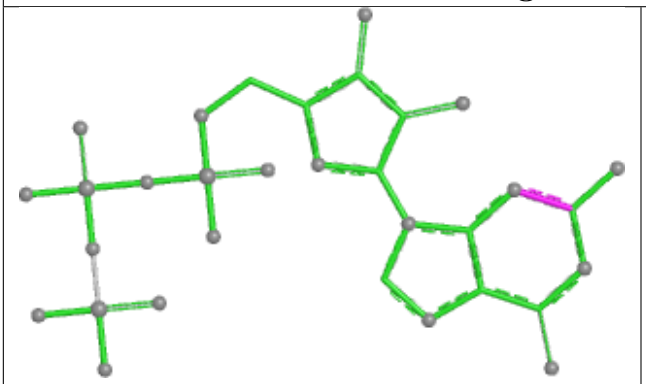


Torsions

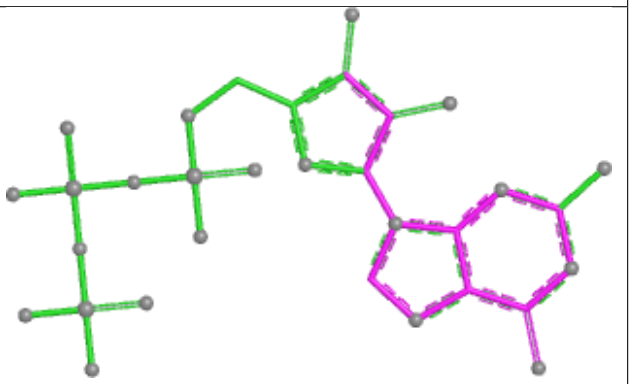


Rings

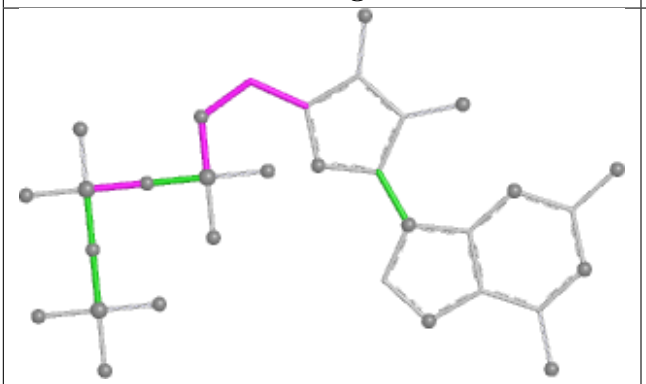
Ligand GTP IE 501



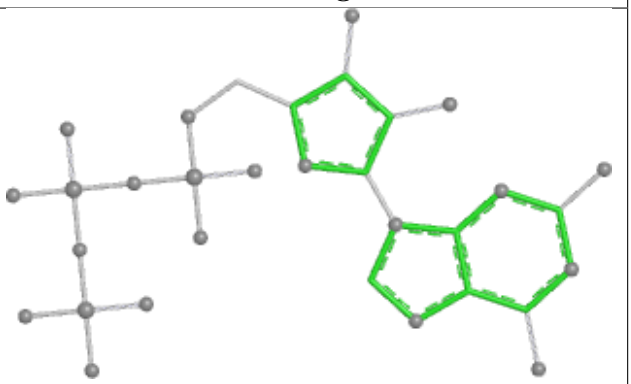
Bond lengths



Bond angles

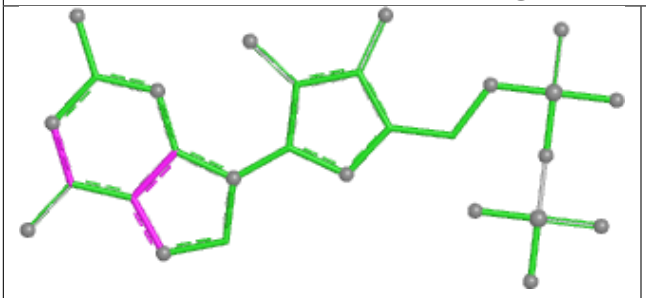


Torsions

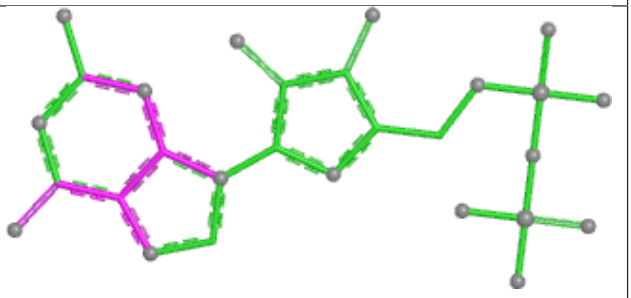


Rings

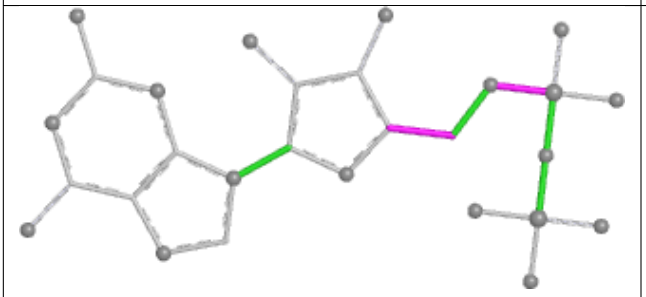
Ligand GDP LF 502



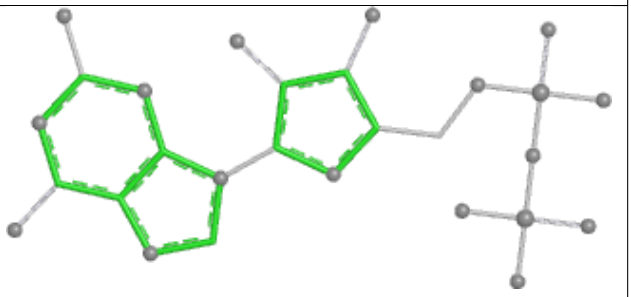
Bond lengths



Bond angles

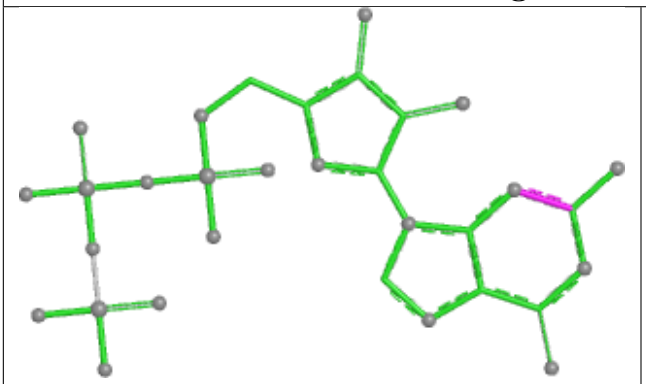


Torsions

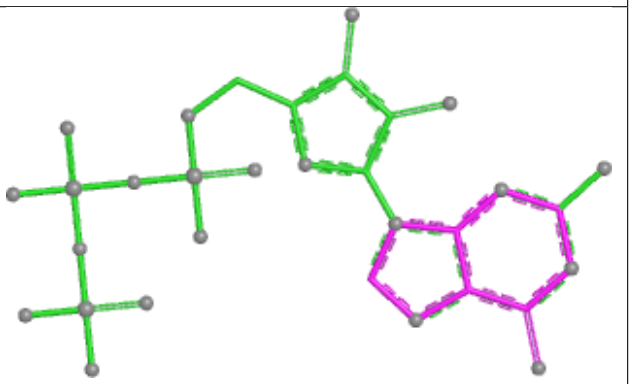


Rings

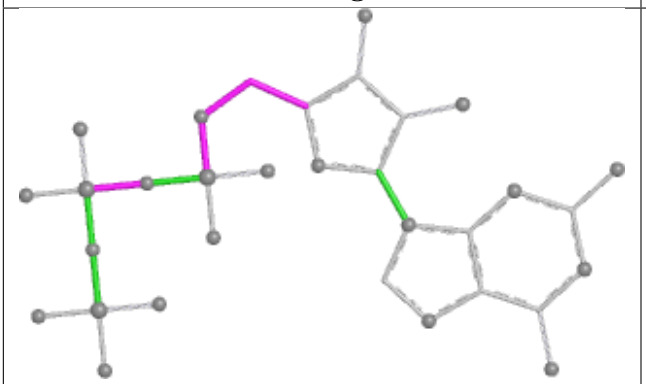
Ligand GTP DE 501



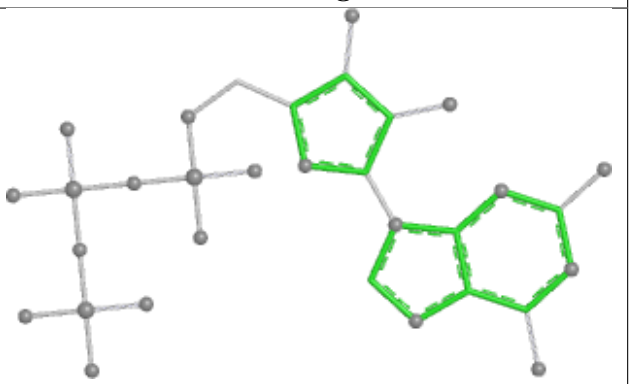
Bond lengths



Bond angles

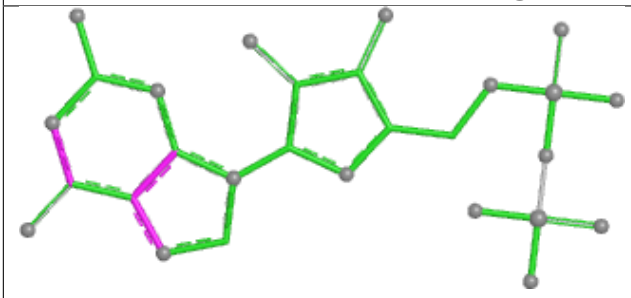


Torsions

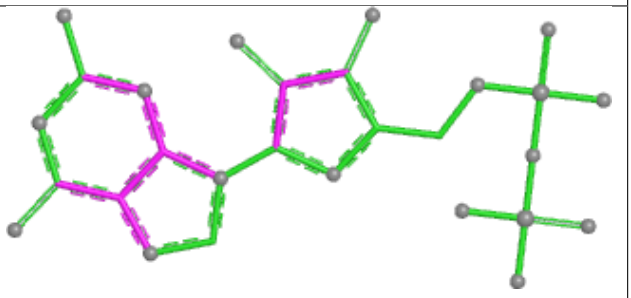


Rings

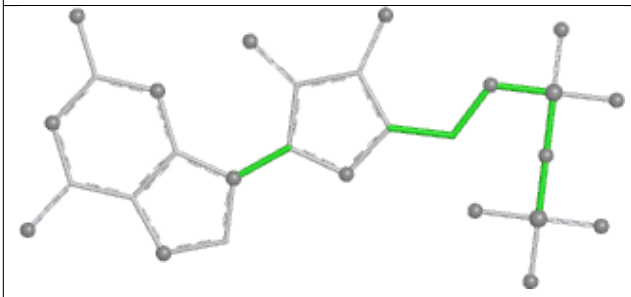
Ligand GDP JH 502



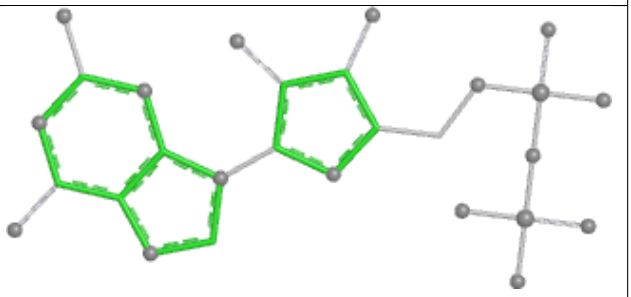
Bond lengths



Bond angles

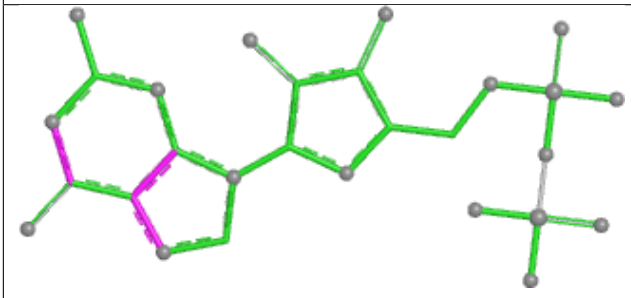


Torsions

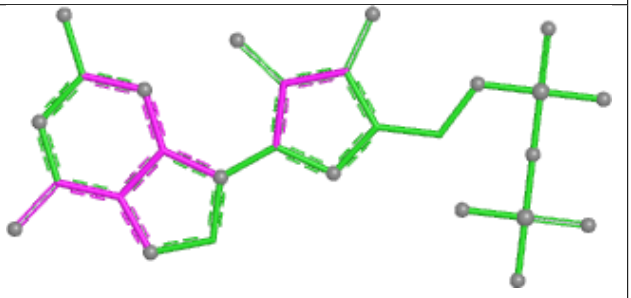


Rings

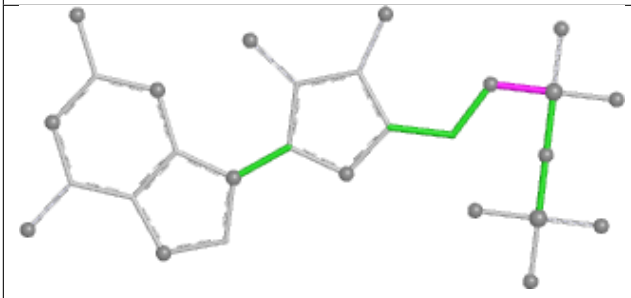
Ligand GDP NJ 502



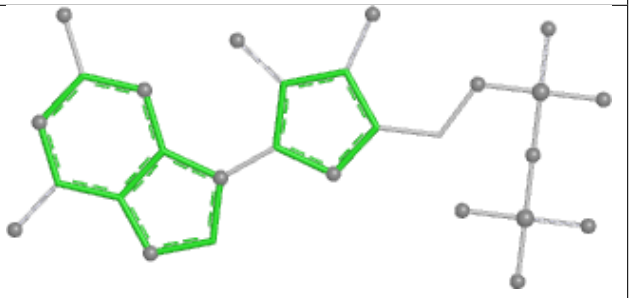
Bond lengths



Bond angles

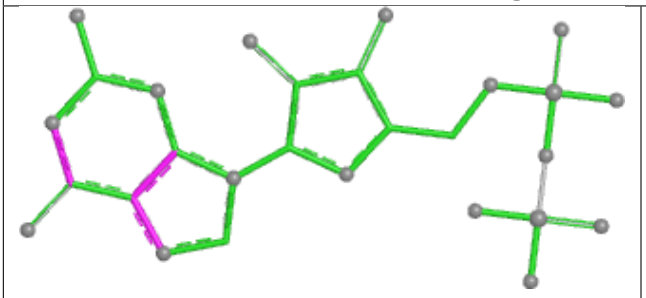


Torsions

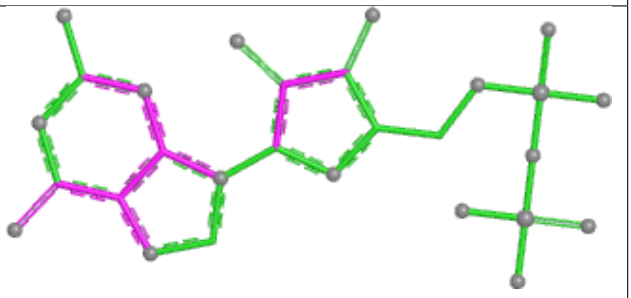


Rings

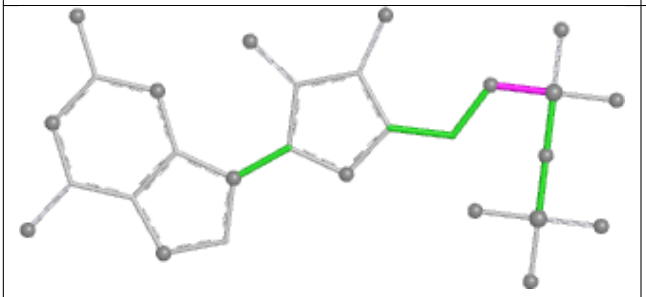
Ligand GDP NP 502



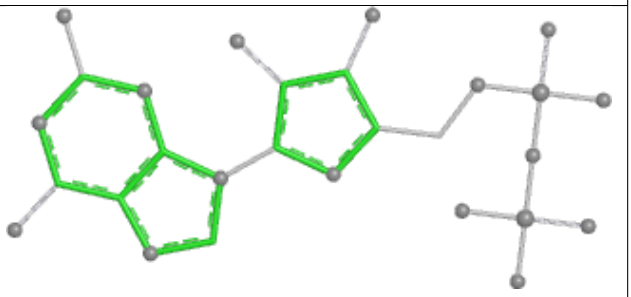
Bond lengths



Bond angles

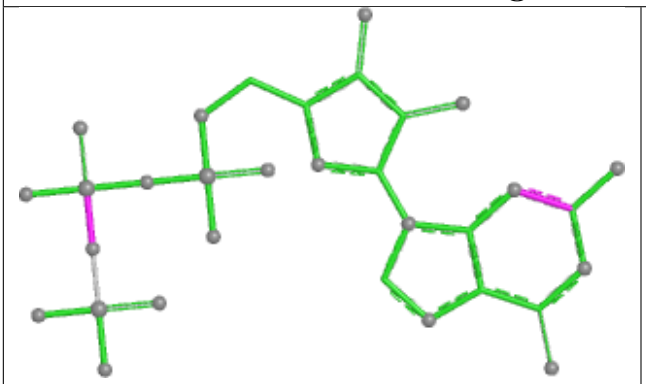


Torsions

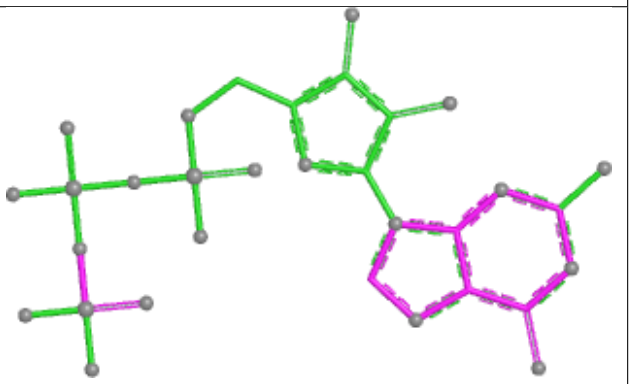


Rings

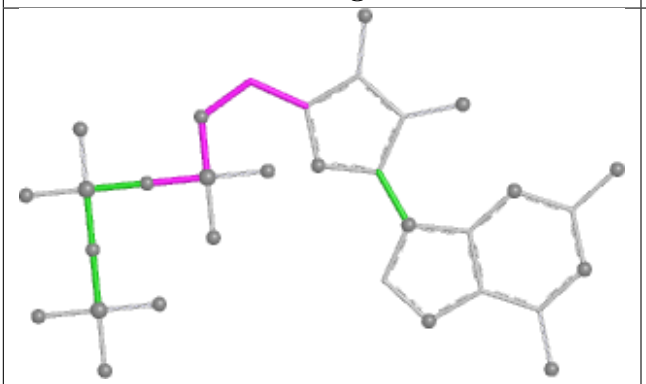
Ligand GTP HO 501



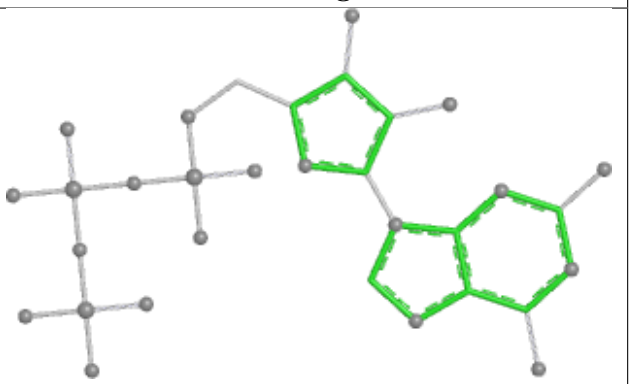
Bond lengths



Bond angles

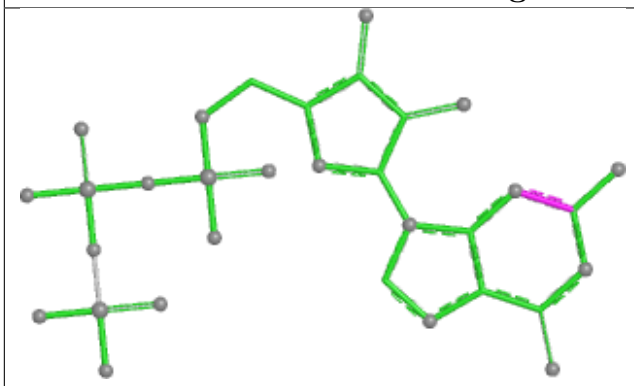


Torsions

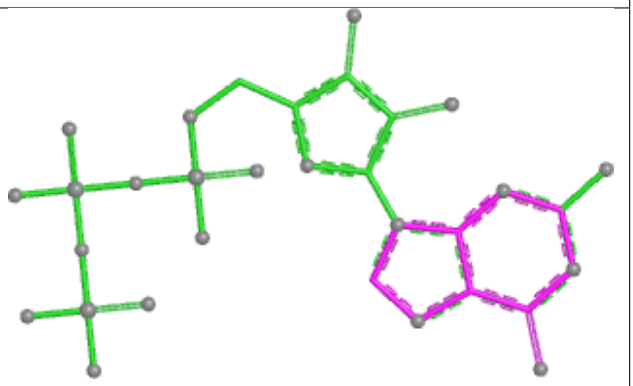


Rings

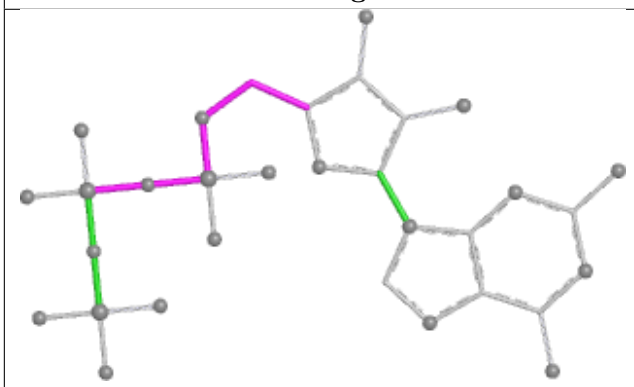
Ligand GTP HA 501



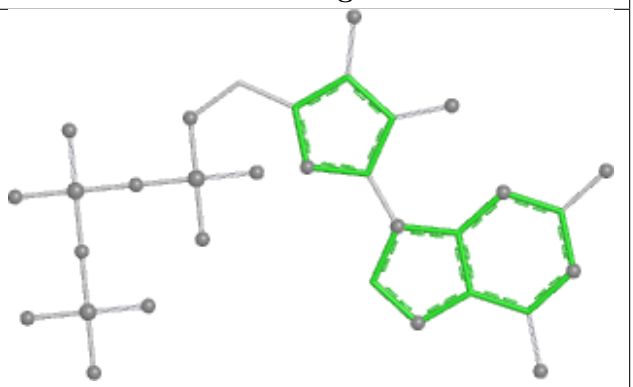
Bond lengths



Bond angles

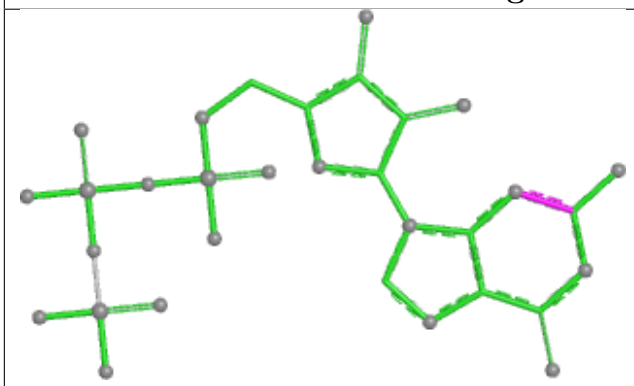


Torsions

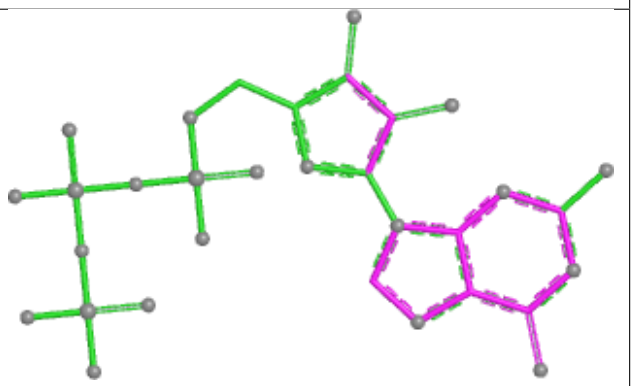


Rings

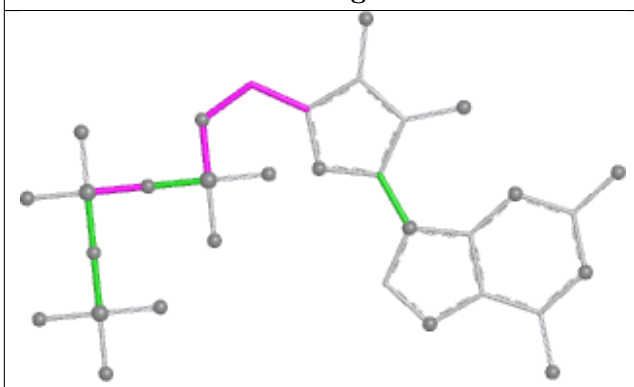
Ligand GTP BM 501



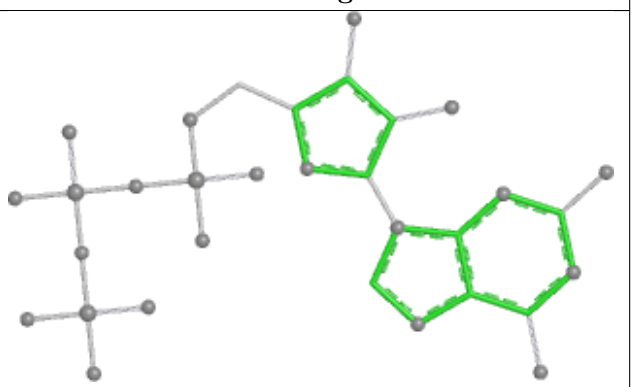
Bond lengths



Bond angles

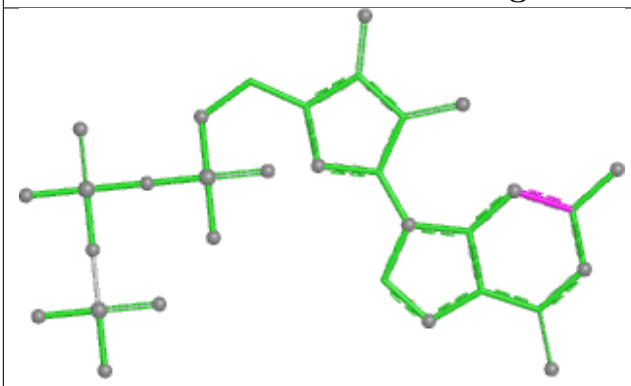


Torsions

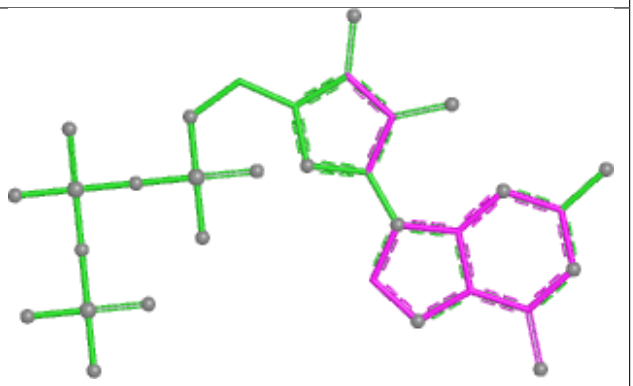


Rings

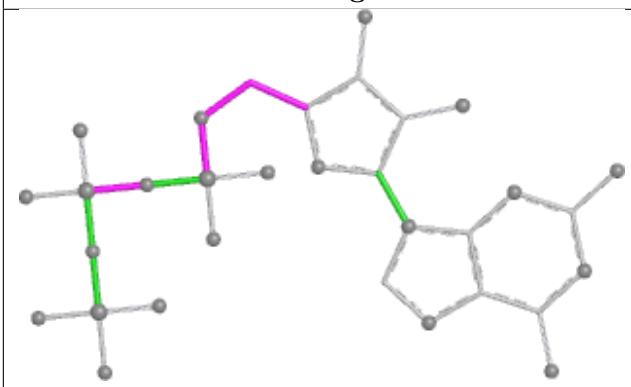
Ligand GTP OC 501



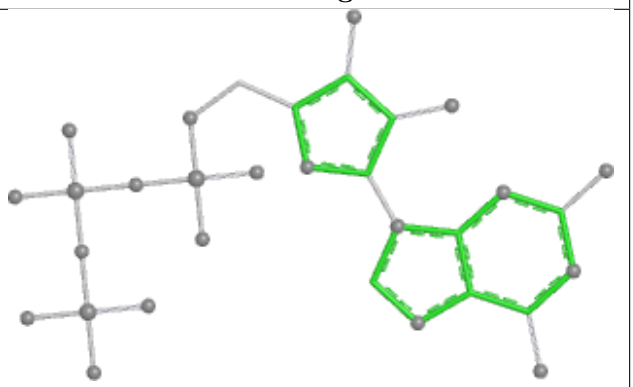
Bond lengths



Bond angles

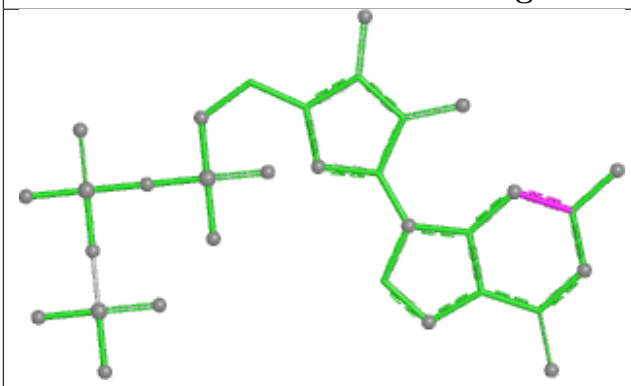


Torsions

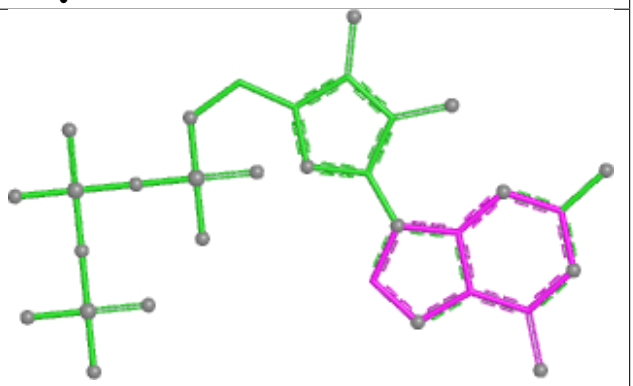


Rings

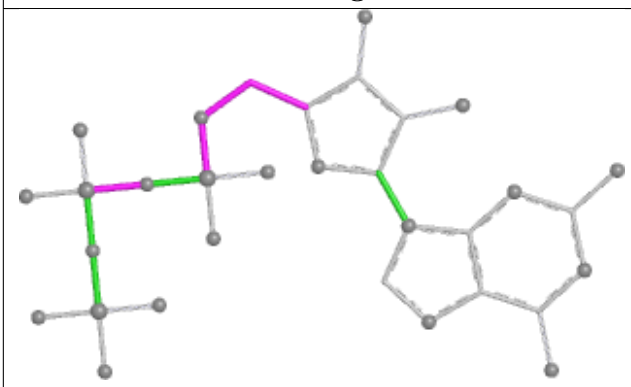
Ligand GTP QI 501



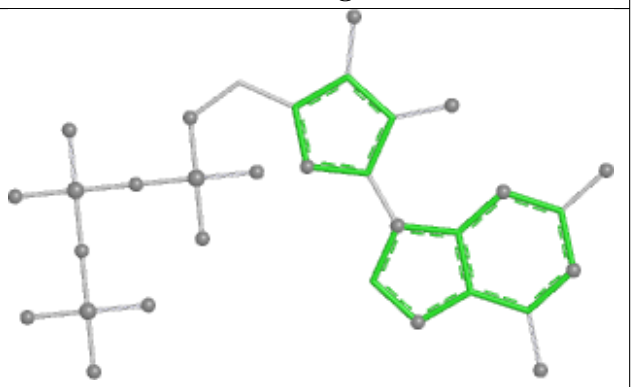
Bond lengths



Bond angles

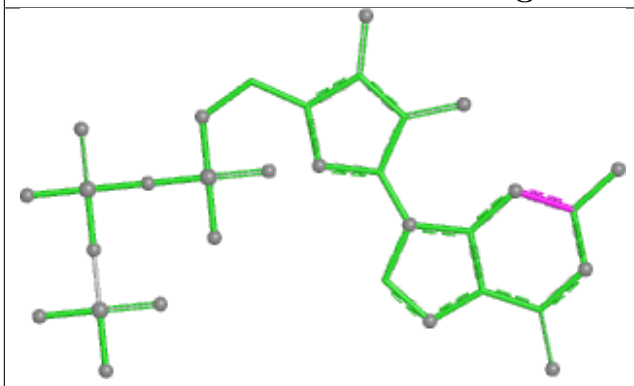


Torsions

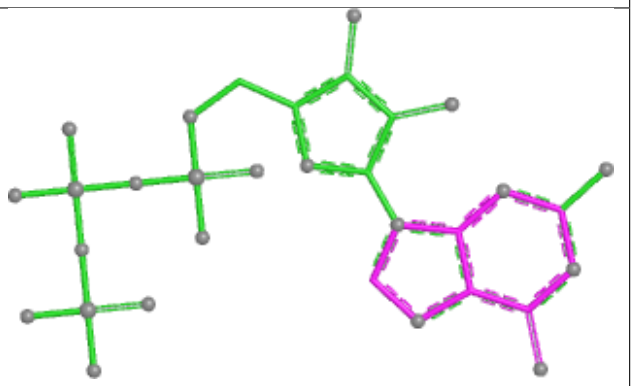


Rings

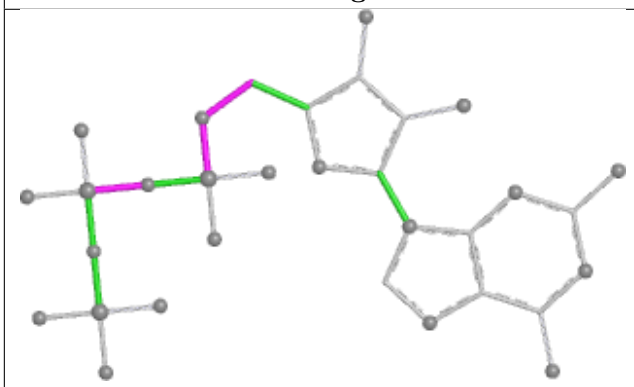
Ligand GTP GI 501



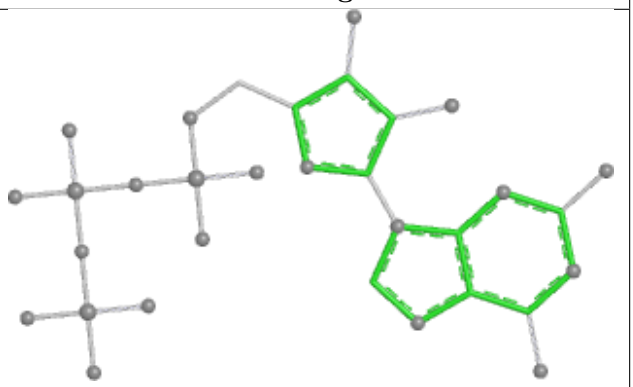
Bond lengths



Bond angles

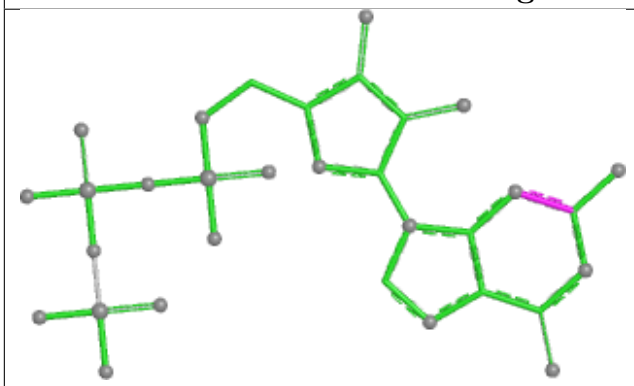


Torsions

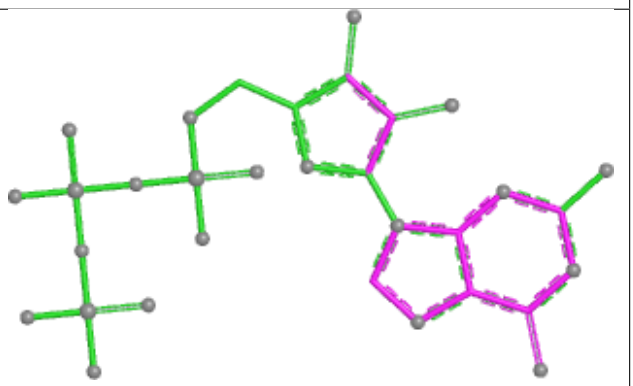


Rings

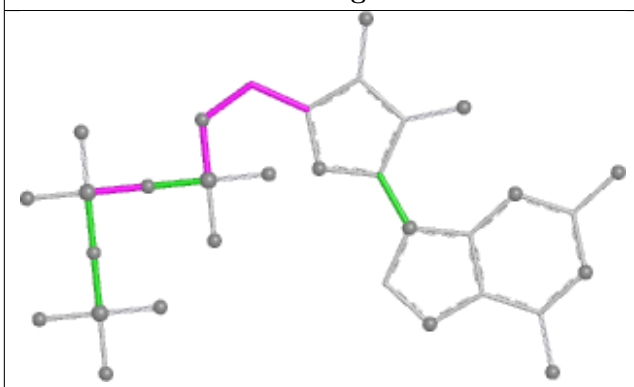
Ligand GTP IC 501



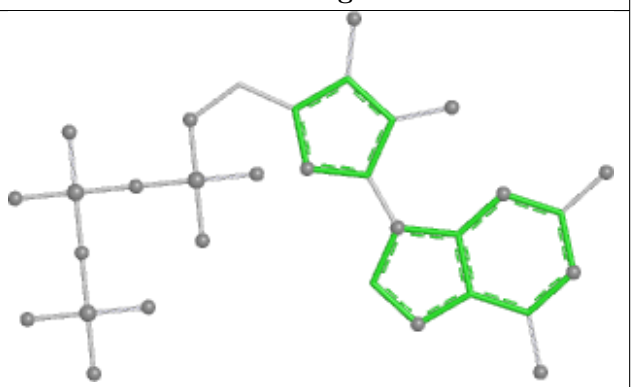
Bond lengths



Bond angles

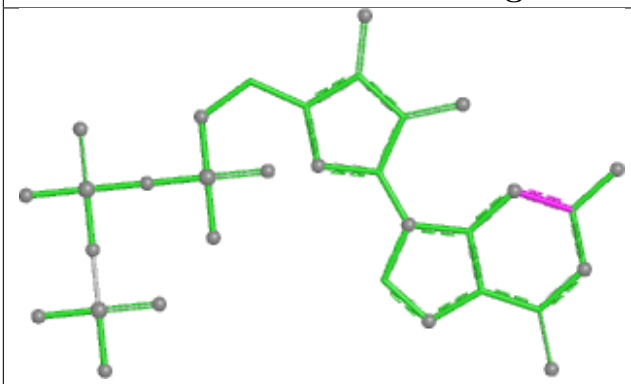


Torsions

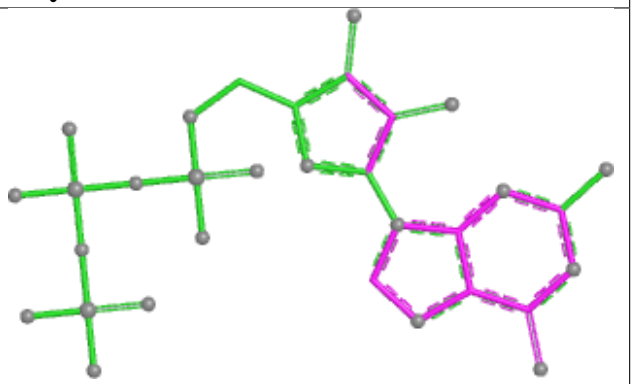


Rings

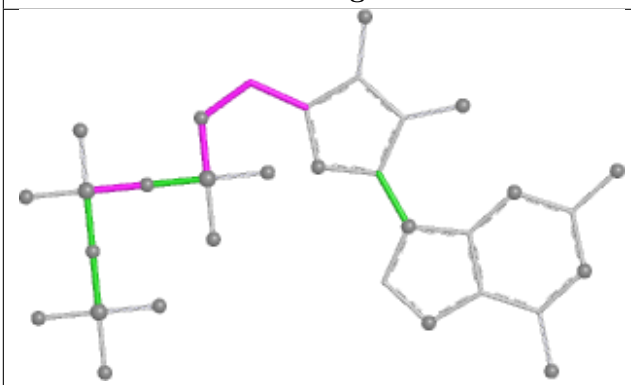
Ligand GTP QM 501



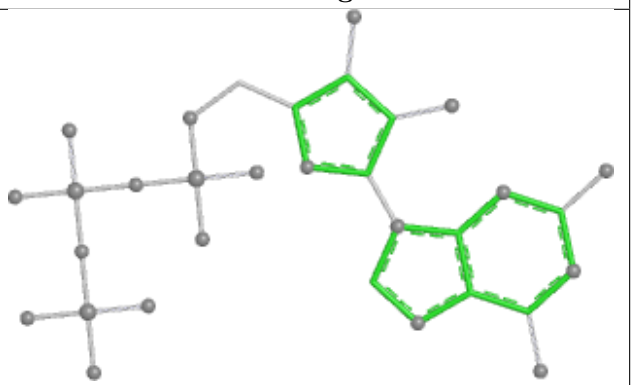
Bond lengths



Bond angles

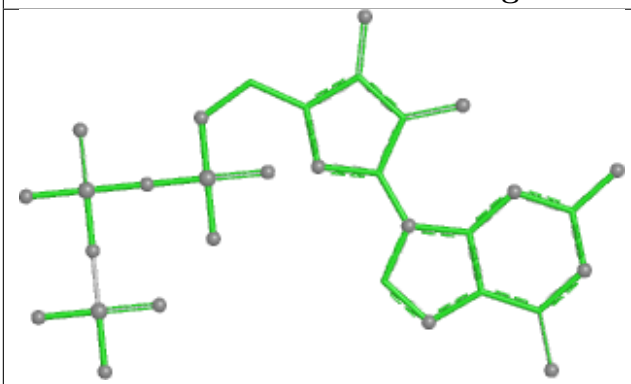


Torsions

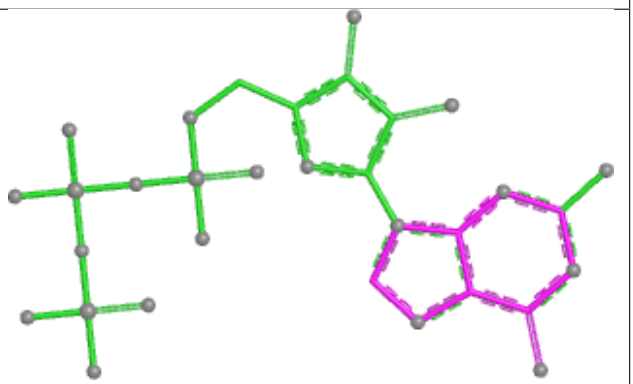


Rings

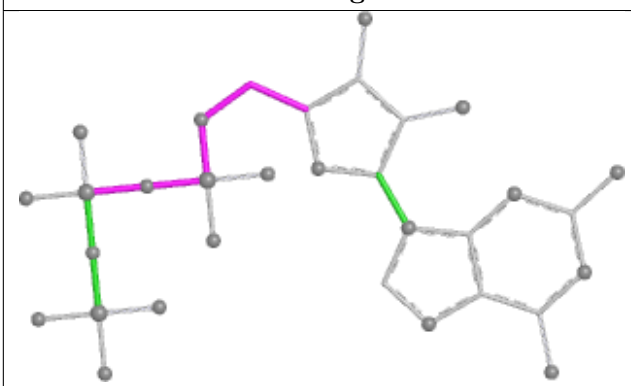
Ligand GTP MM 501



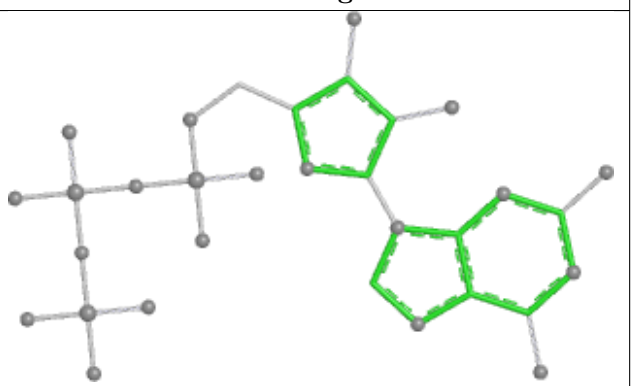
Bond lengths



Bond angles

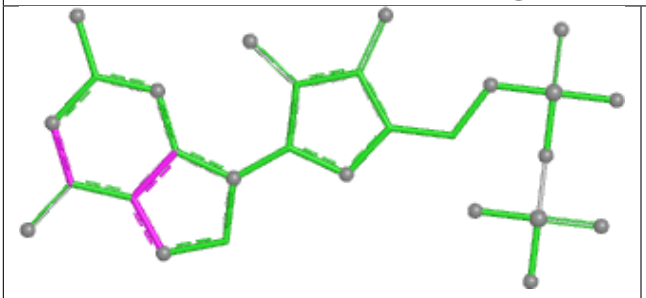


Torsions

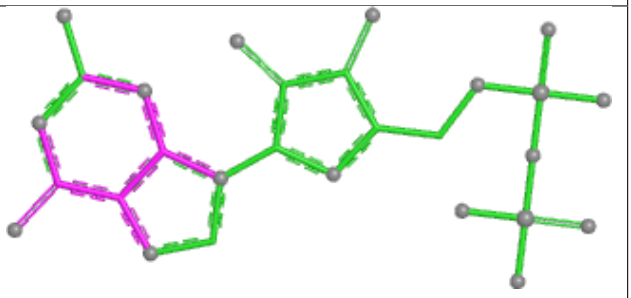


Rings

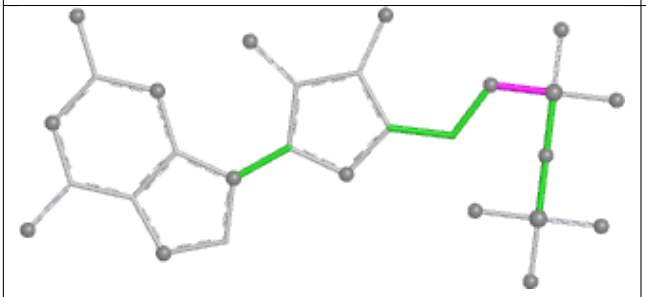
Ligand GDP OL 502



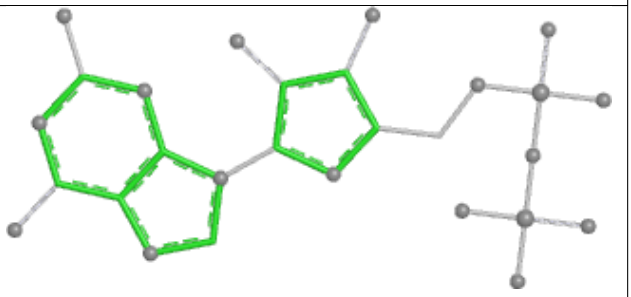
Bond lengths



Bond angles

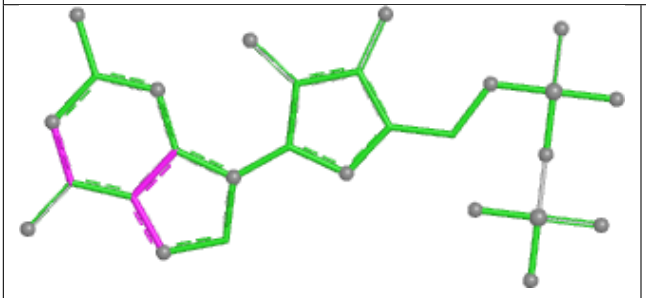


Torsions

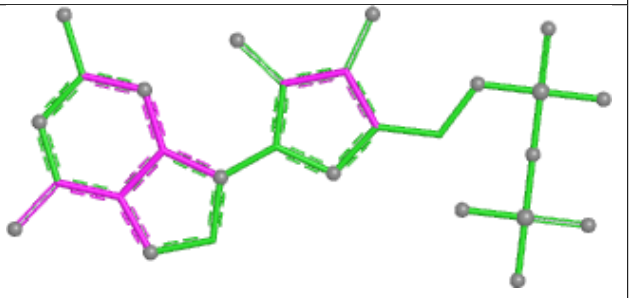


Rings

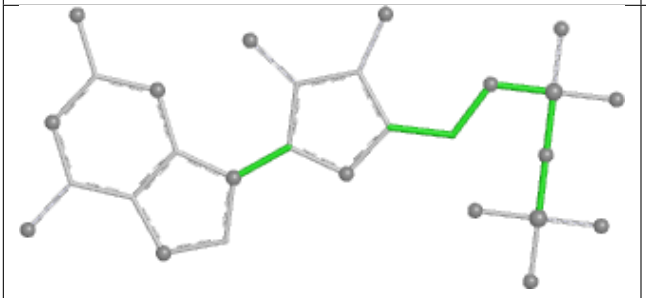
Ligand GDP GF 502



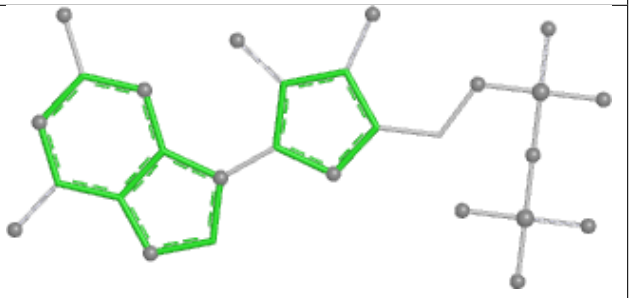
Bond lengths



Bond angles

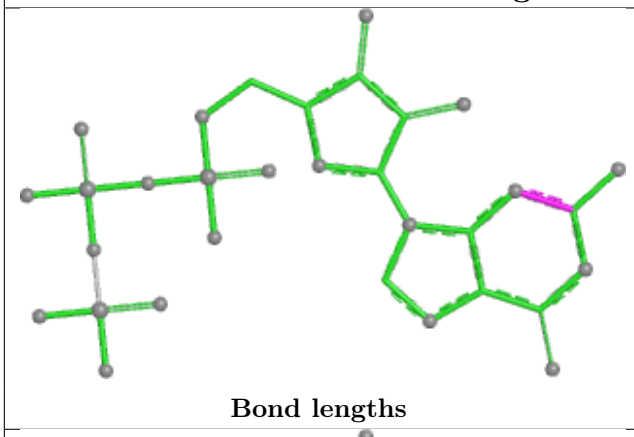


Torsions

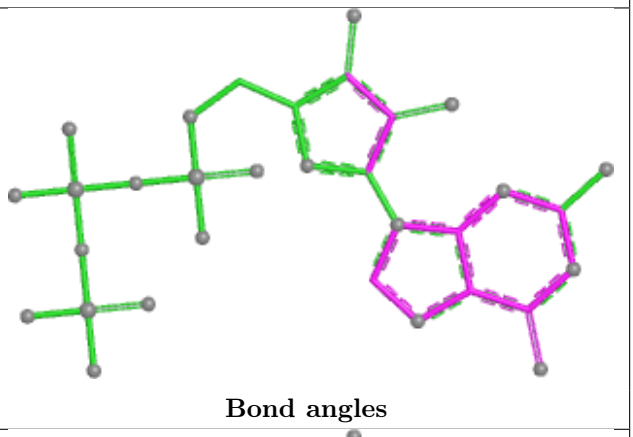


Rings

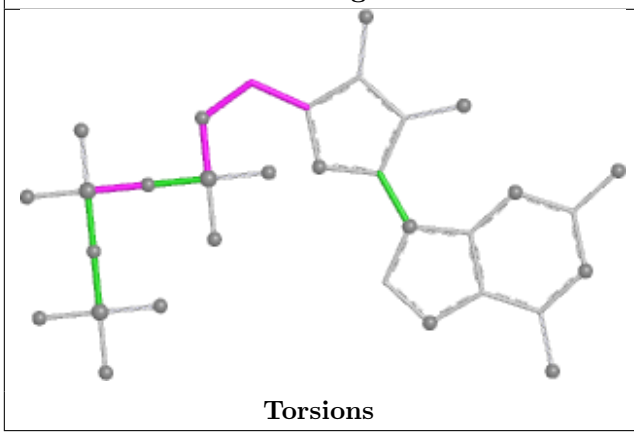
Ligand GTP EE 501



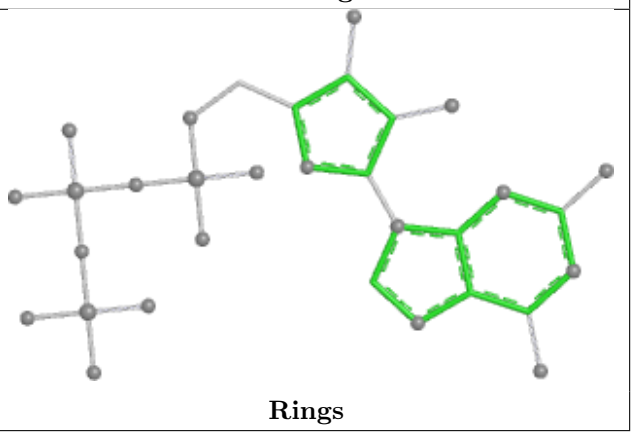
Bond lengths



Bond angles

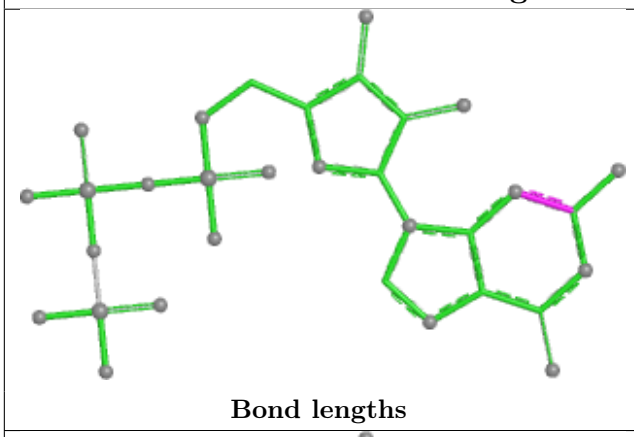


Torsions

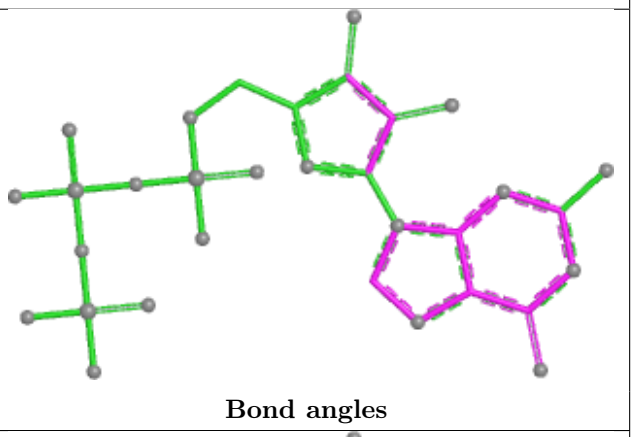


Rings

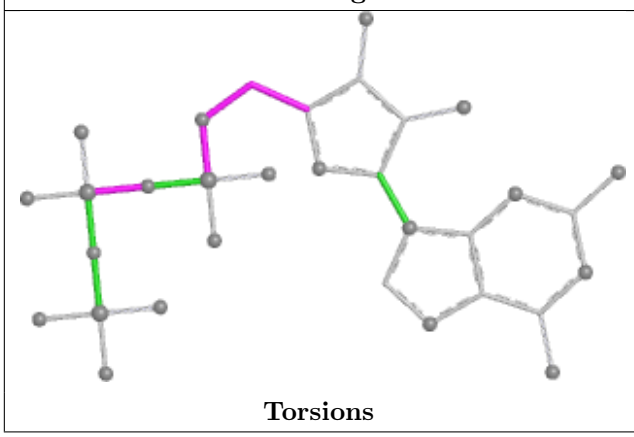
Ligand GTP TG 501



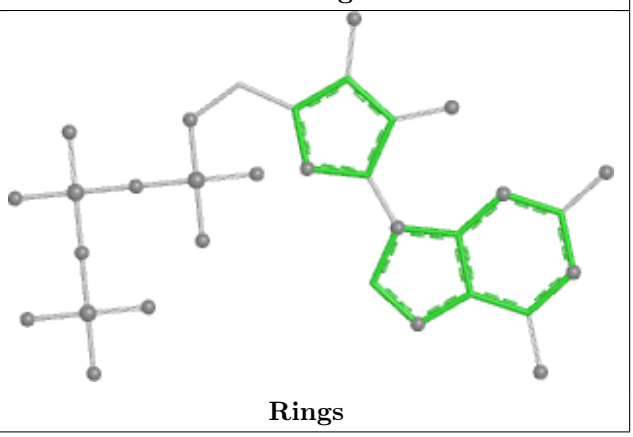
Bond lengths



Bond angles

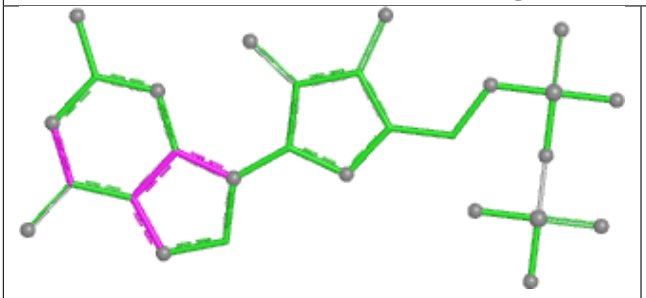


Torsions

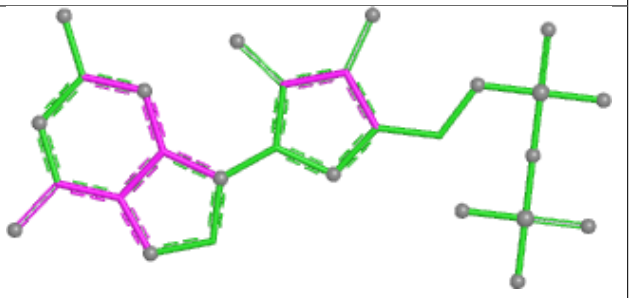


Rings

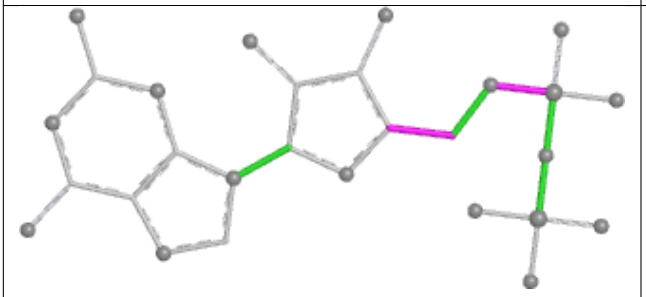
Ligand GDP LH 502



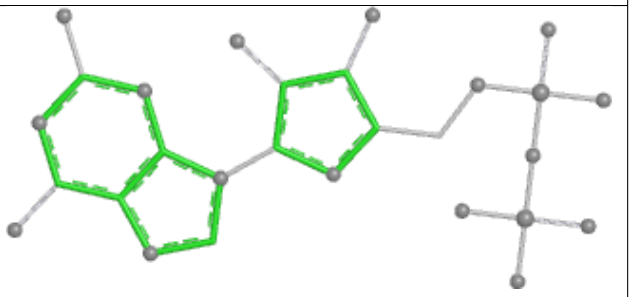
Bond lengths



Bond angles

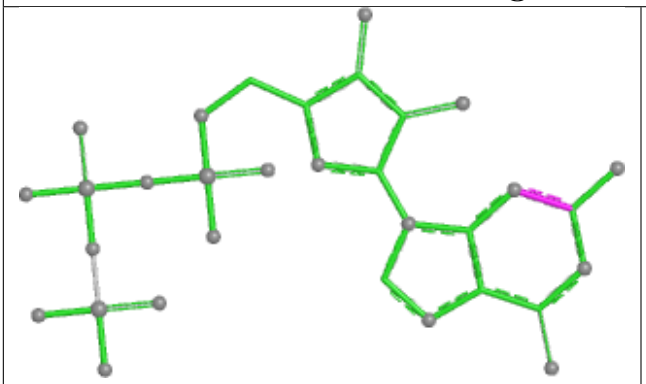


Torsions

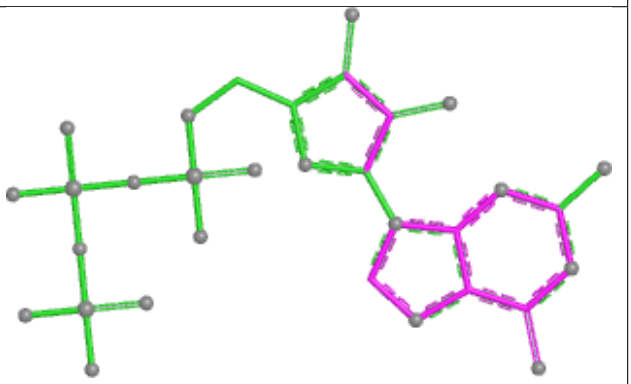


Rings

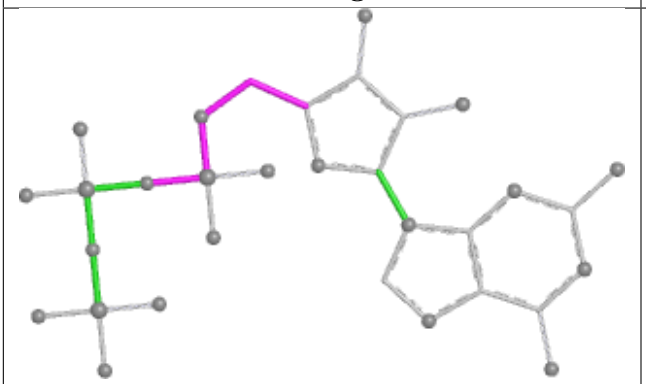
Ligand GTP NC 501



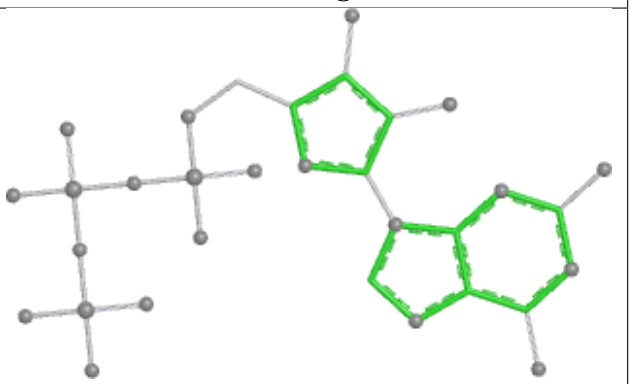
Bond lengths



Bond angles

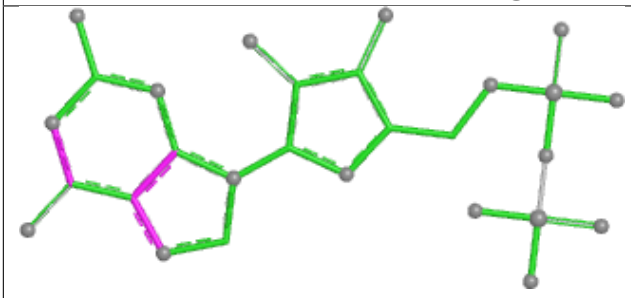


Torsions

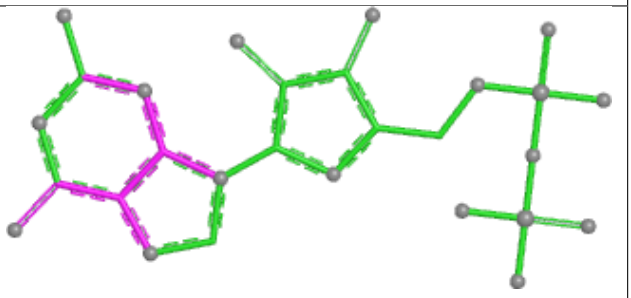


Rings

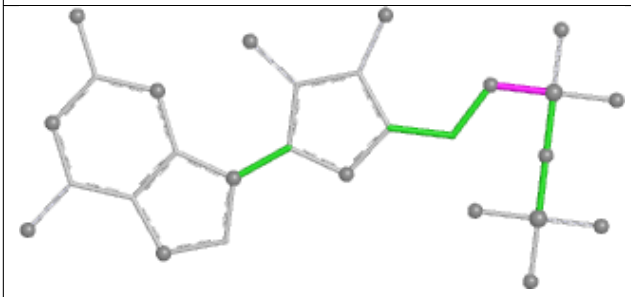
Ligand GDP BH 502



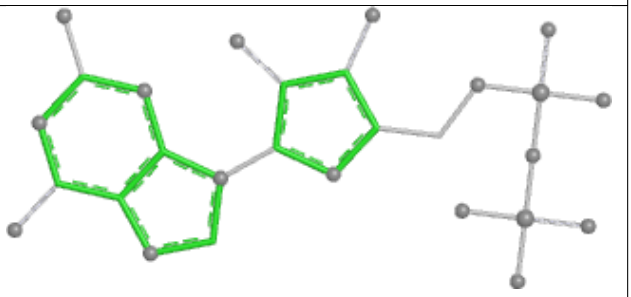
Bond lengths



Bond angles

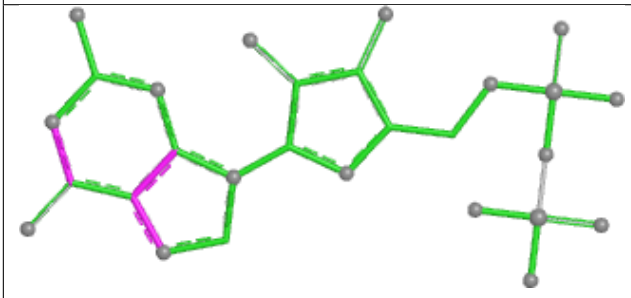


Torsions

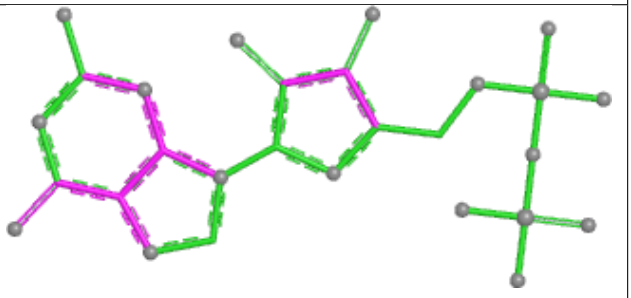


Rings

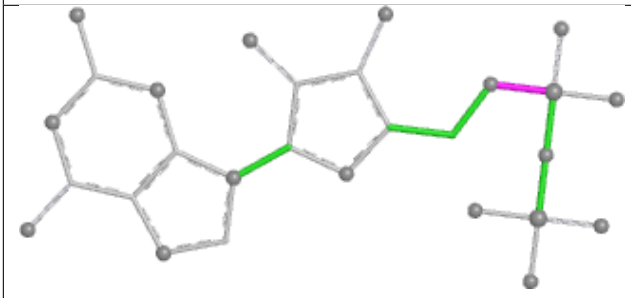
Ligand GDP EB 502



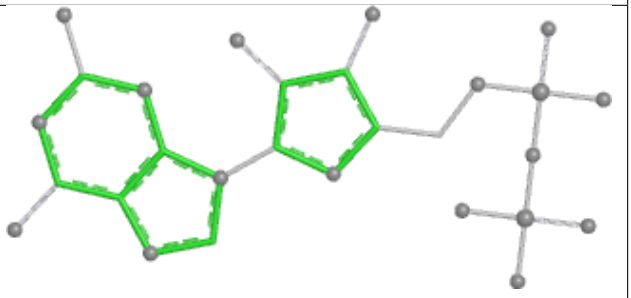
Bond lengths



Bond angles

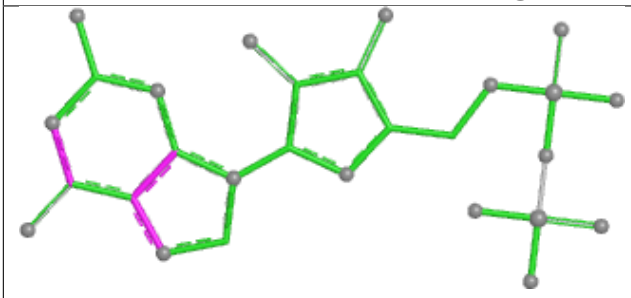


Torsions

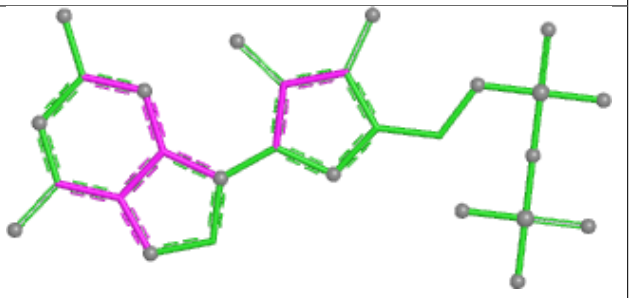


Rings

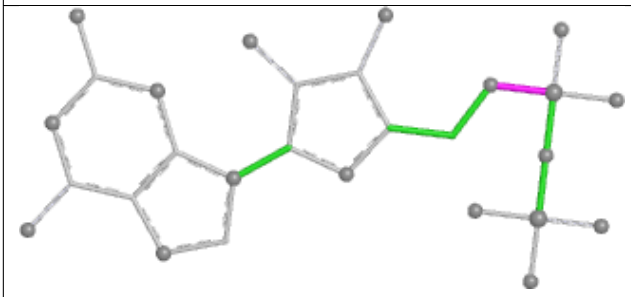
Ligand GDP VJ 502



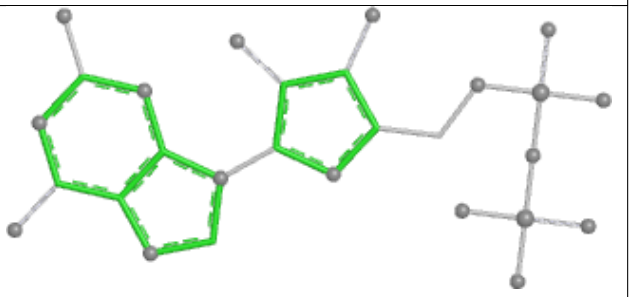
Bond lengths



Bond angles

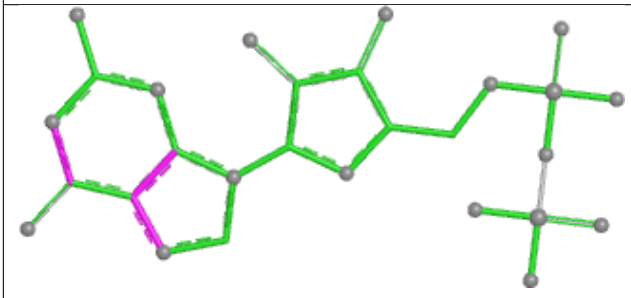


Torsions

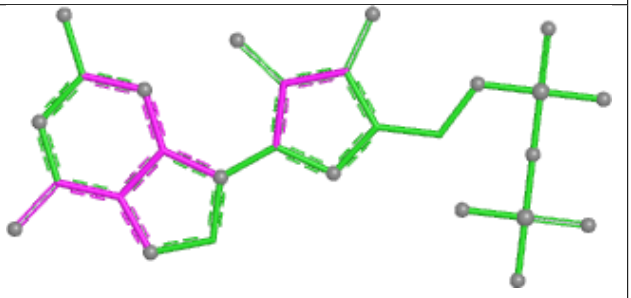


Rings

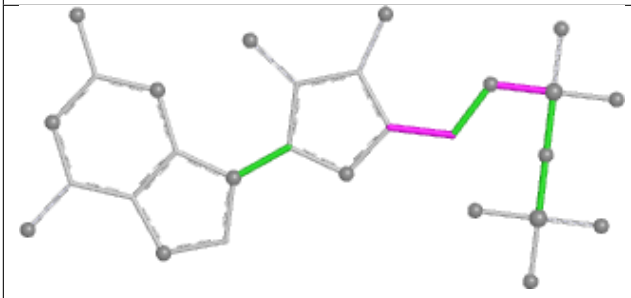
Ligand GDP DP 502



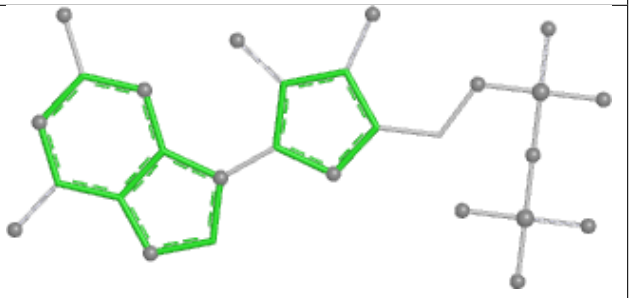
Bond lengths



Bond angles

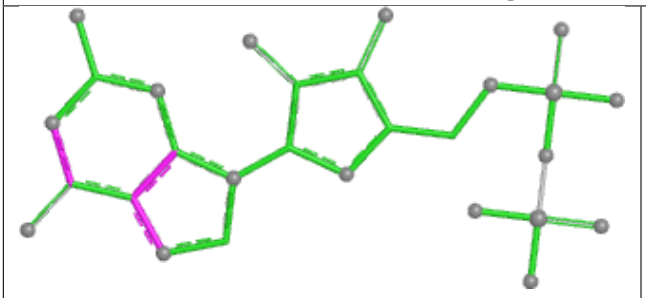


Torsions

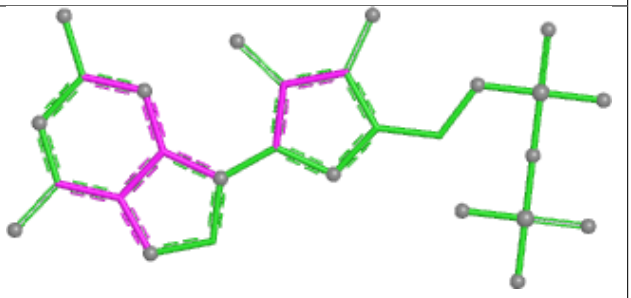


Rings

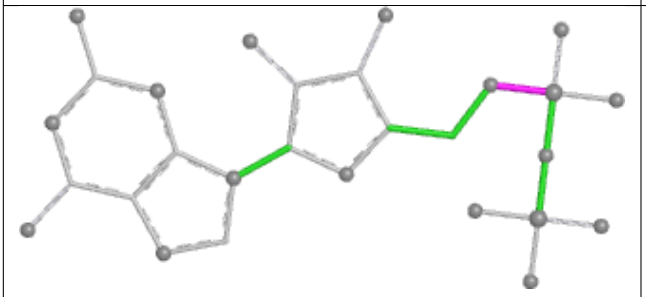
Ligand GDP WD 502



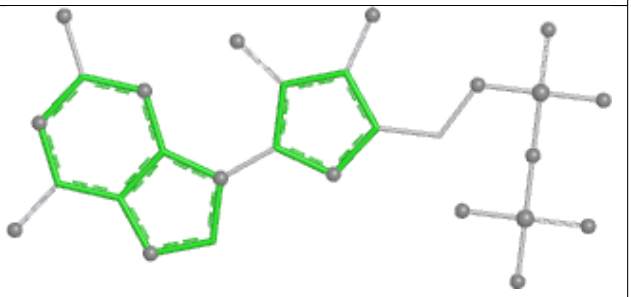
Bond lengths



Bond angles

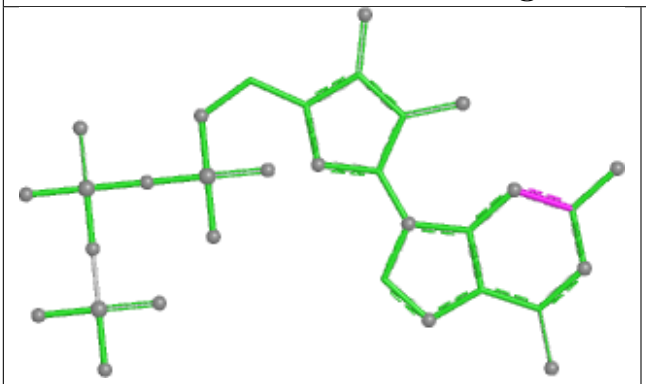


Torsions

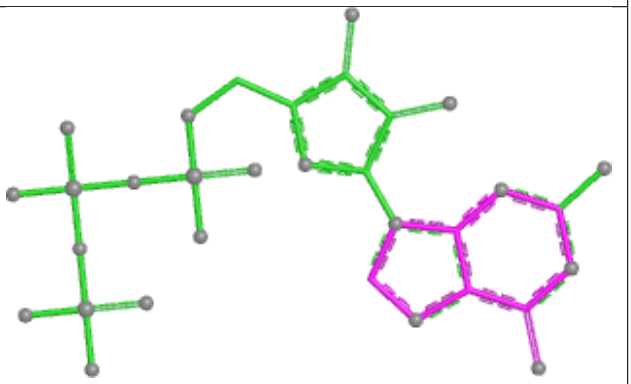


Rings

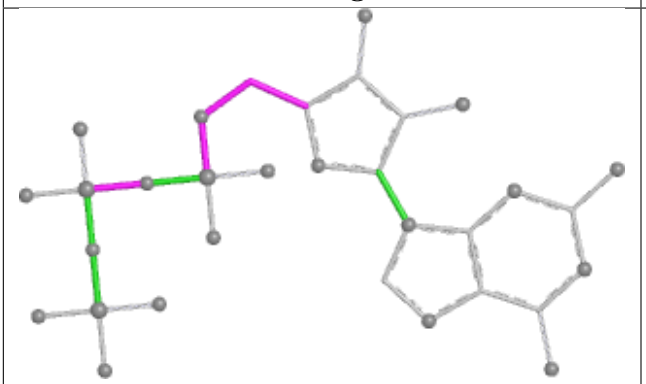
Ligand GTP LI 501



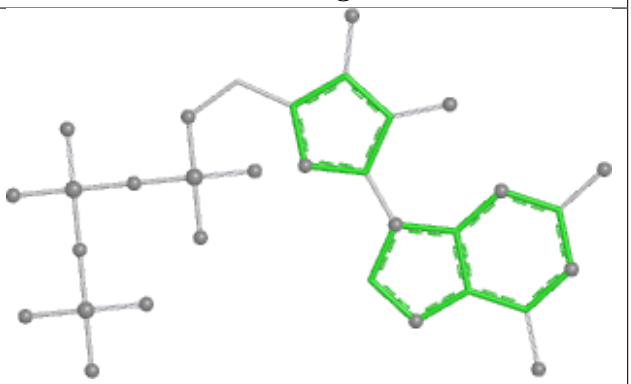
Bond lengths



Bond angles

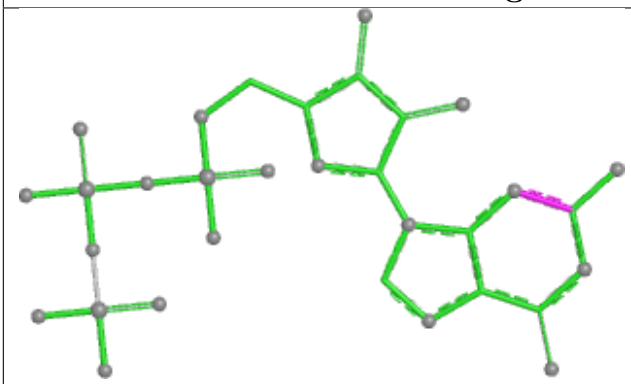


Torsions

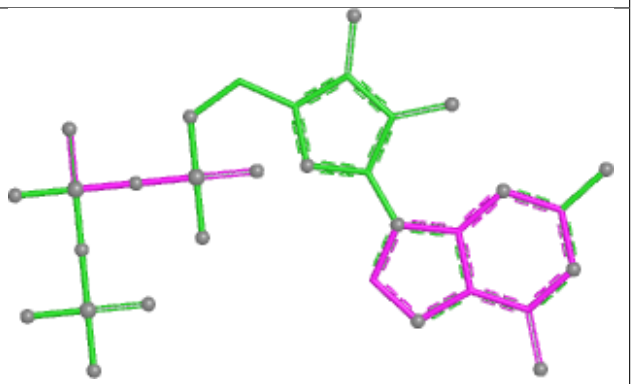


Rings

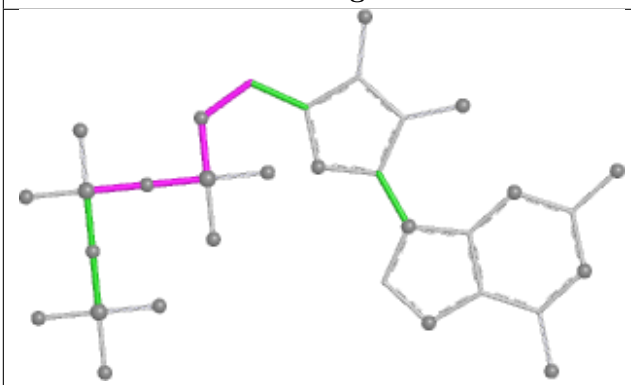
Ligand GTP MC 501



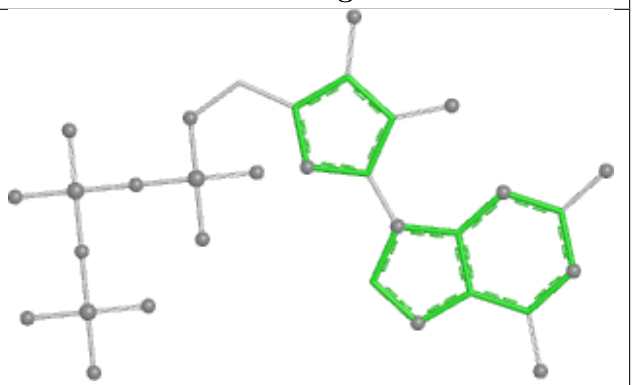
Bond lengths



Bond angles

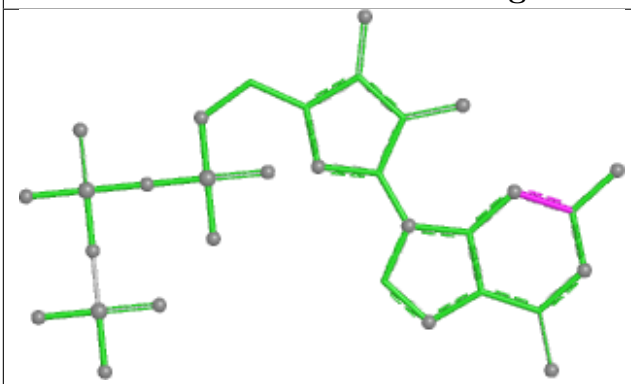


Torsions

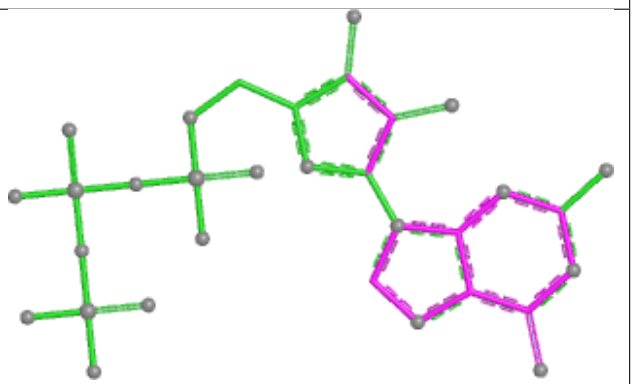


Rings

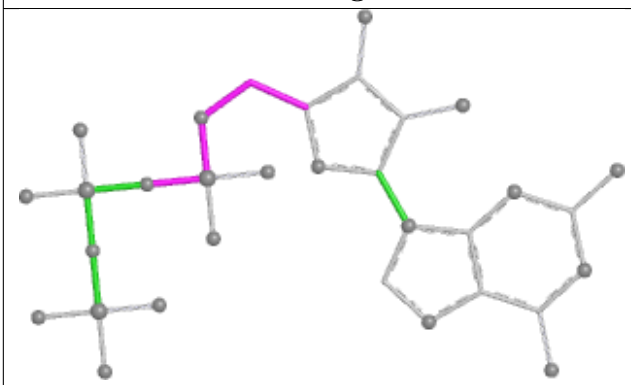
Ligand GTP CG 501



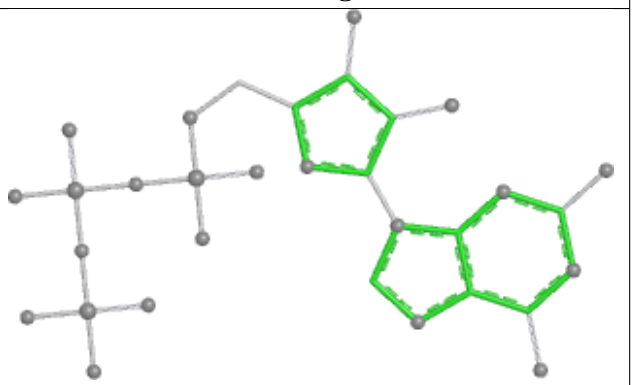
Bond lengths



Bond angles

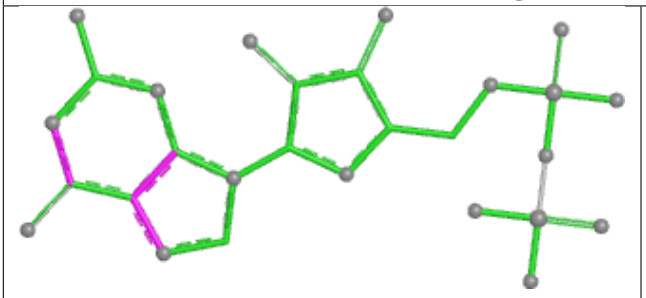


Torsions

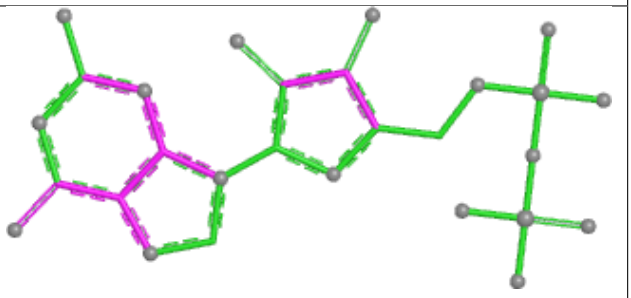


Rings

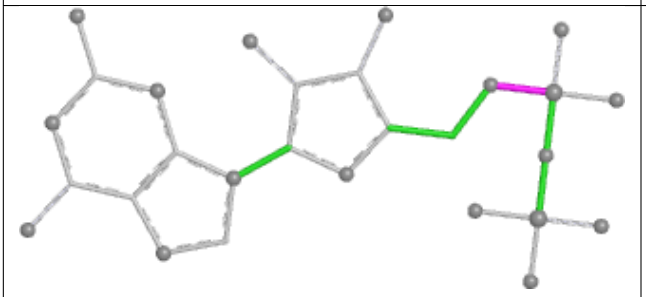
Ligand GDP FB 502



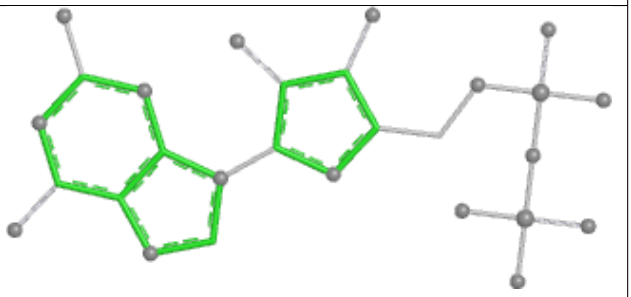
Bond lengths



Bond angles

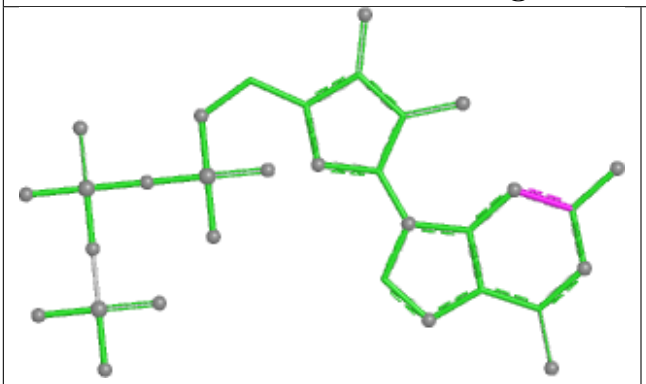


Torsions

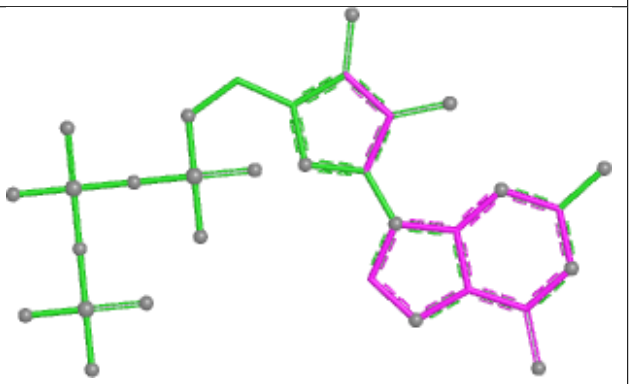


Rings

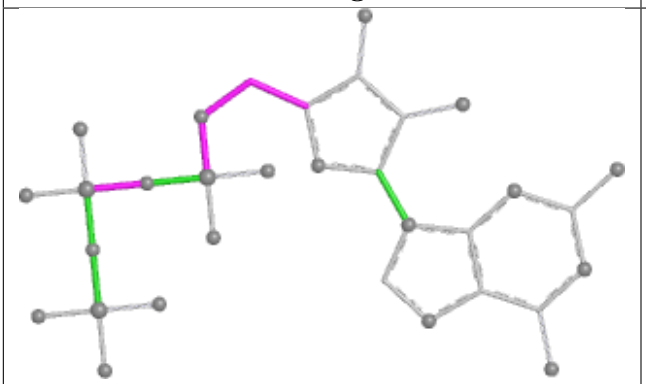
Ligand GTP VC 501



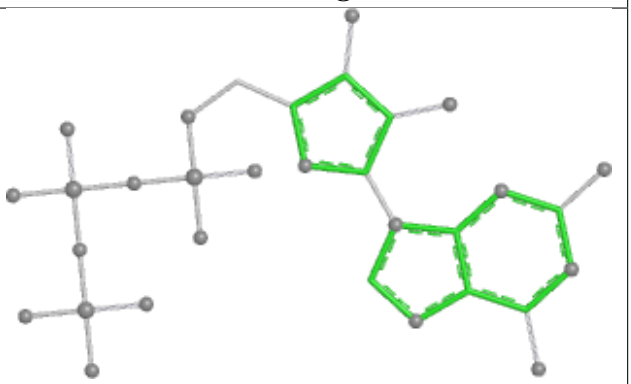
Bond lengths



Bond angles

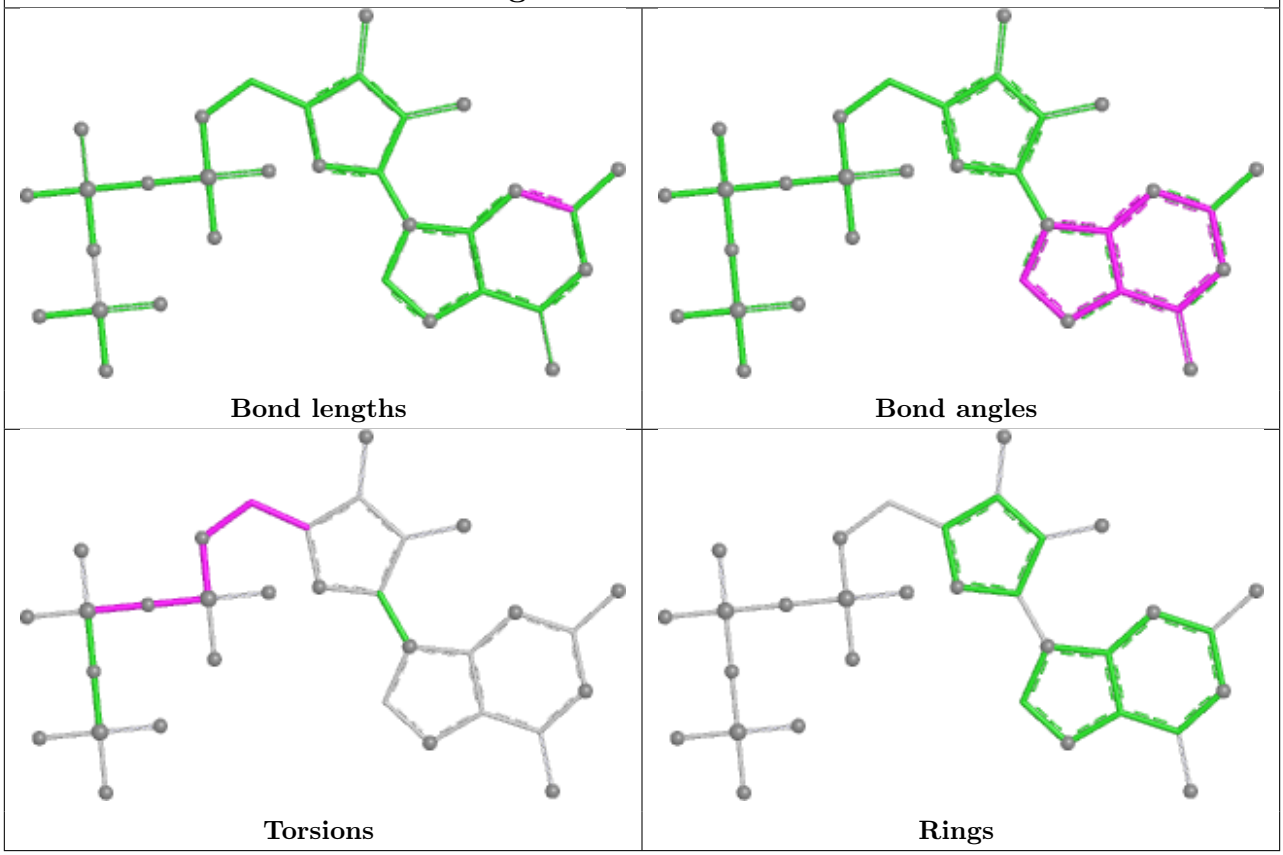


Torsions

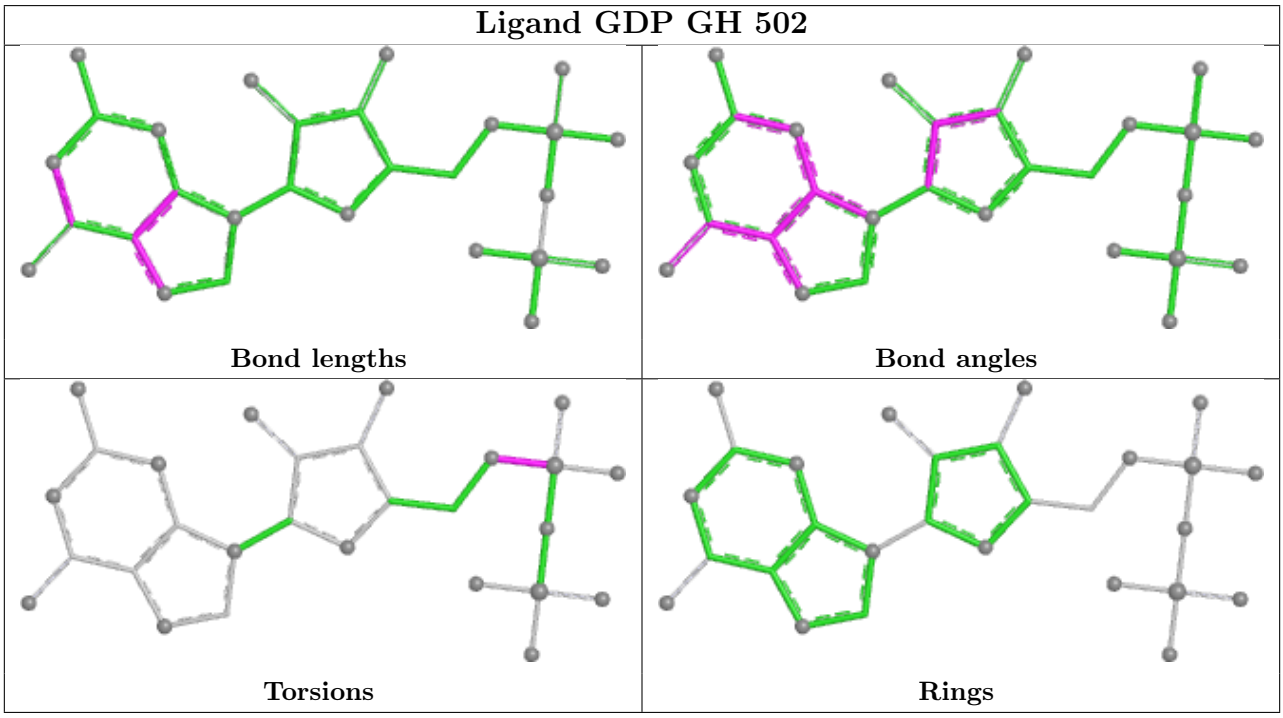


Rings

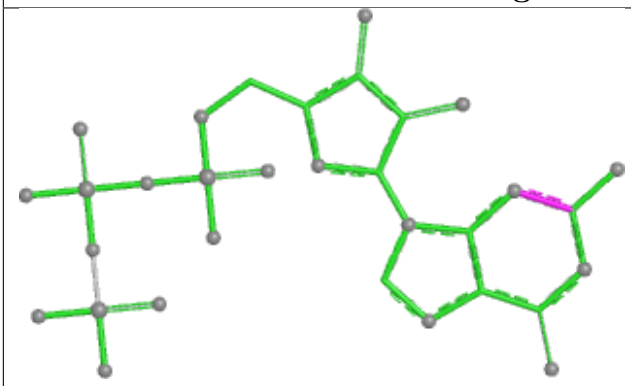
Ligand GTP NG 501



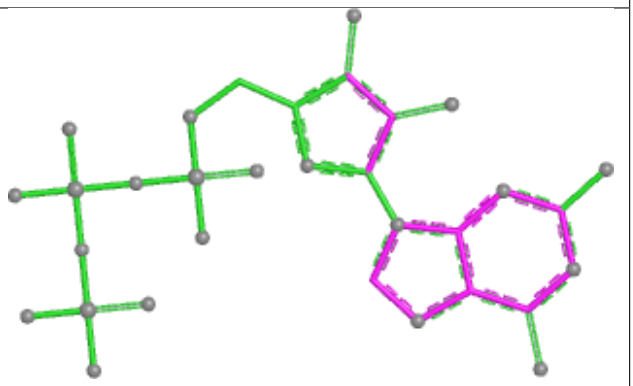
Ligand GDP GH 502



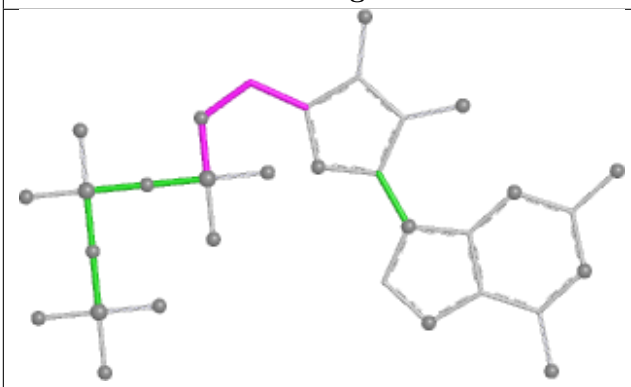
Ligand GTP JO 501



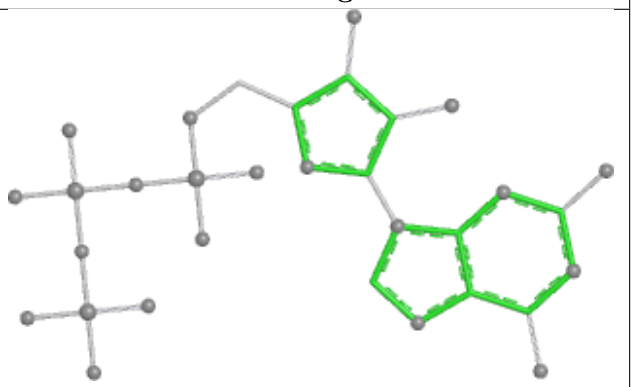
Bond lengths



Bond angles

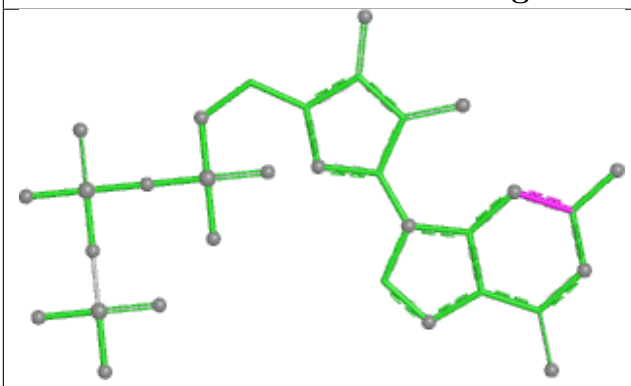


Torsions

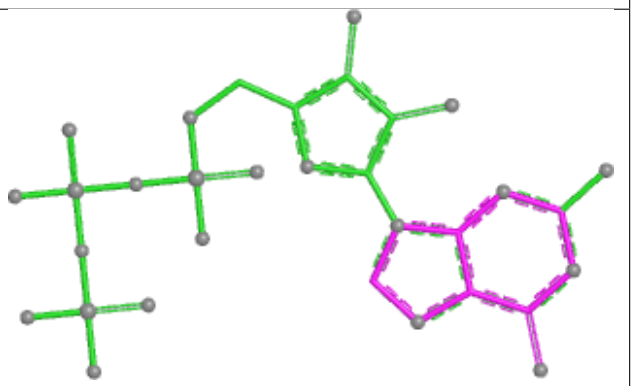


Rings

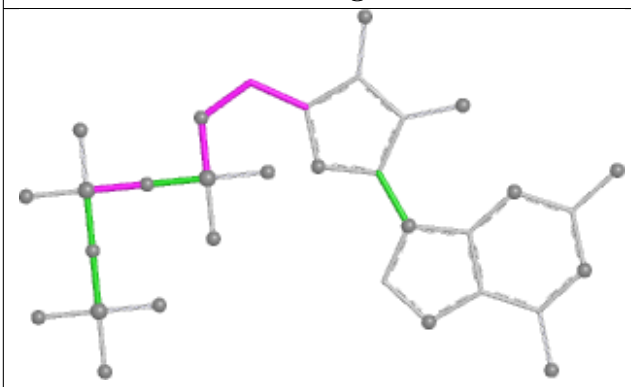
Ligand GTP SK 501



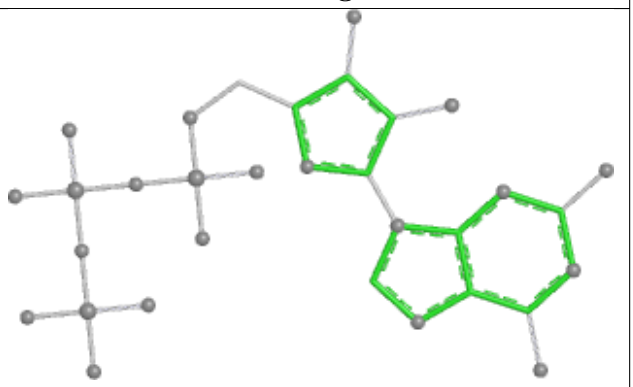
Bond lengths



Bond angles

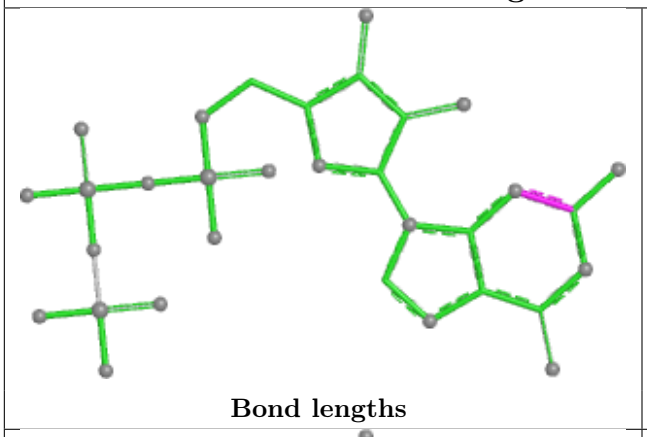


Torsions

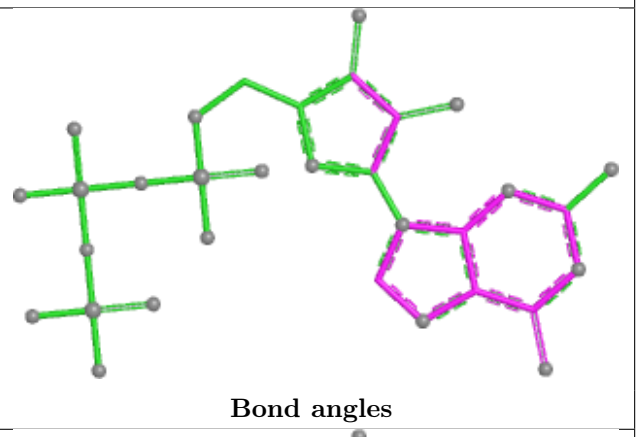


Rings

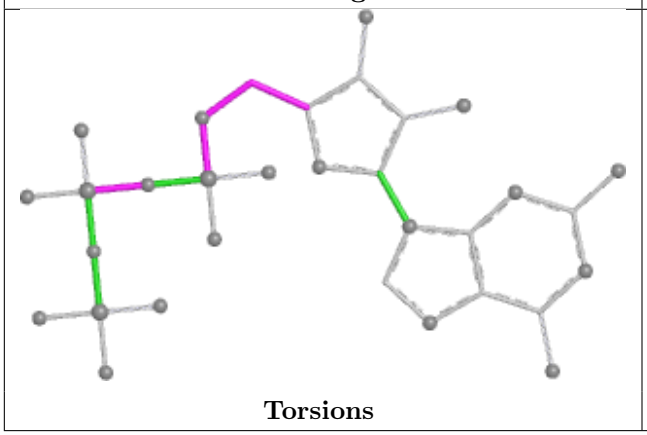
Ligand GTP PM 501



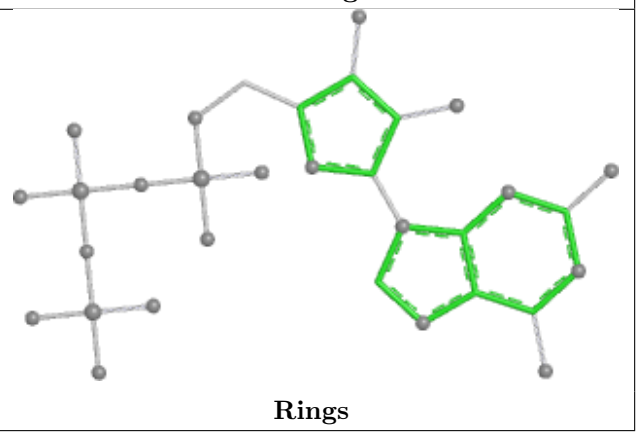
Bond lengths



Bond angles

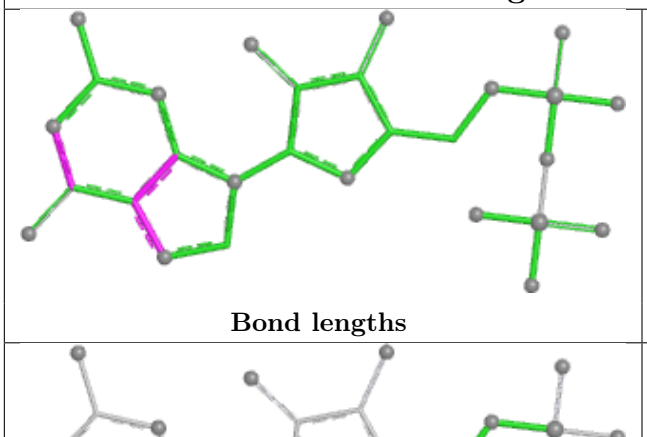


Torsions

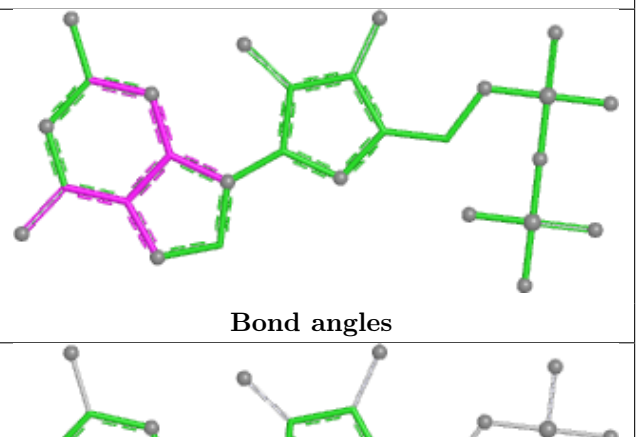


Rings

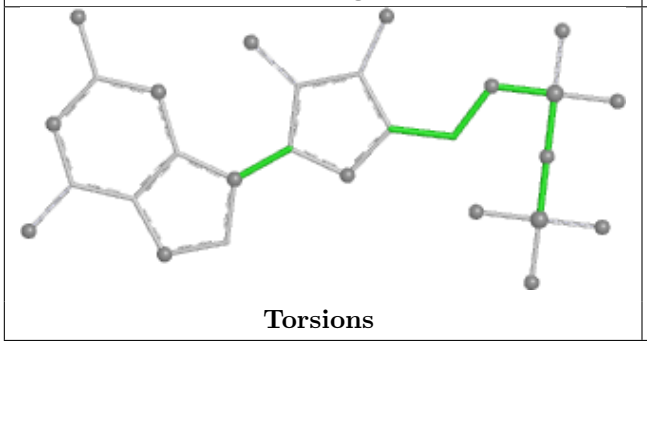
Ligand GDP DH 502



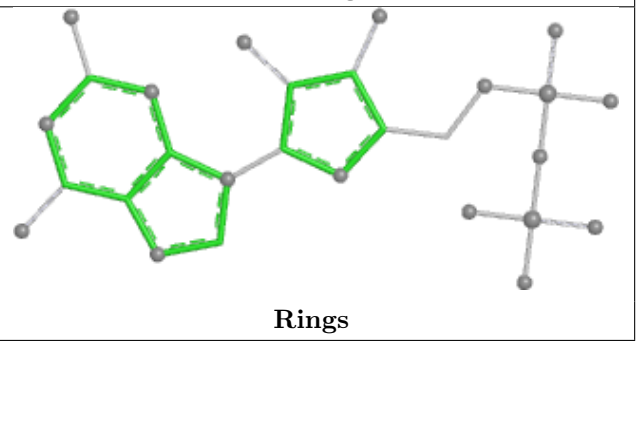
Bond lengths



Bond angles

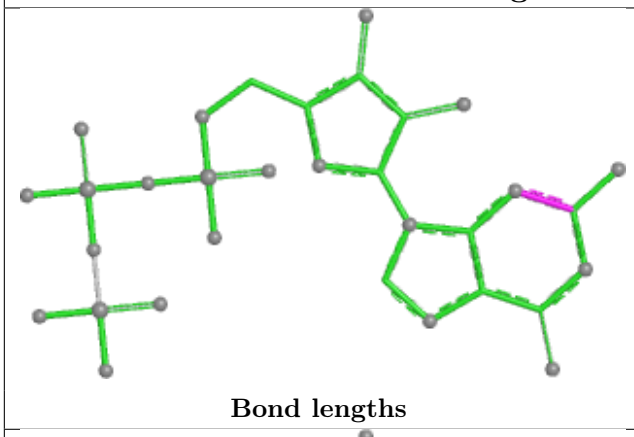


Torsions

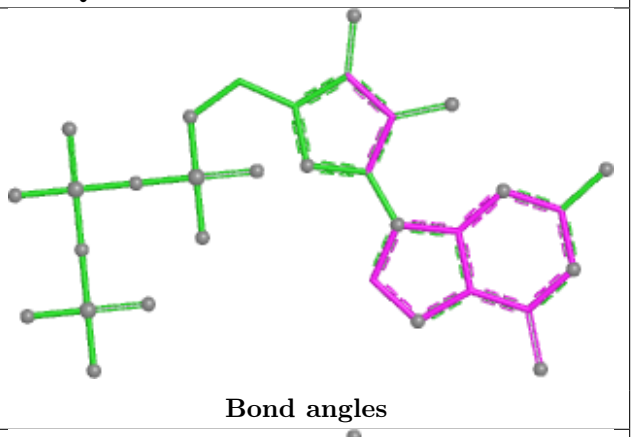


Rings

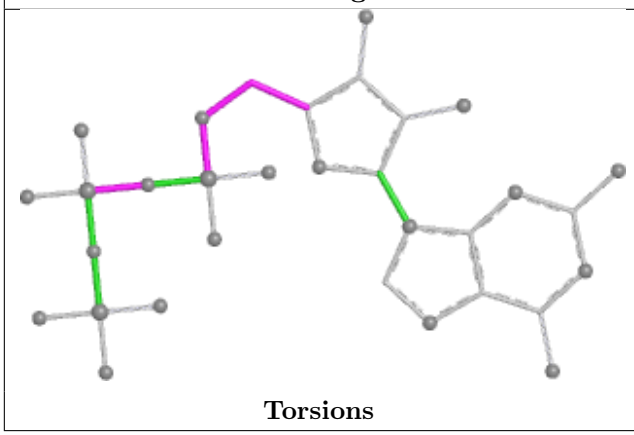
Ligand GTP CQ 501



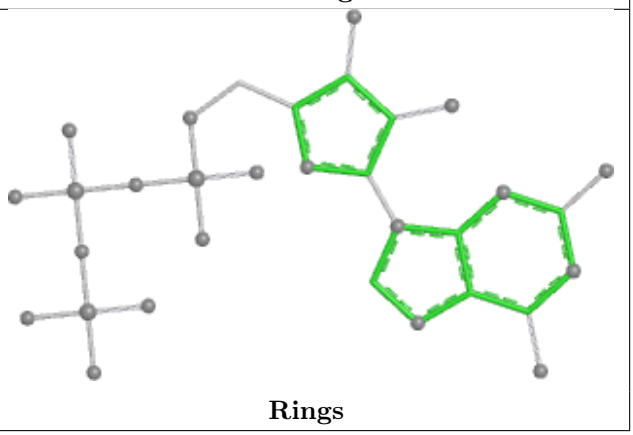
Bond lengths



Bond angles

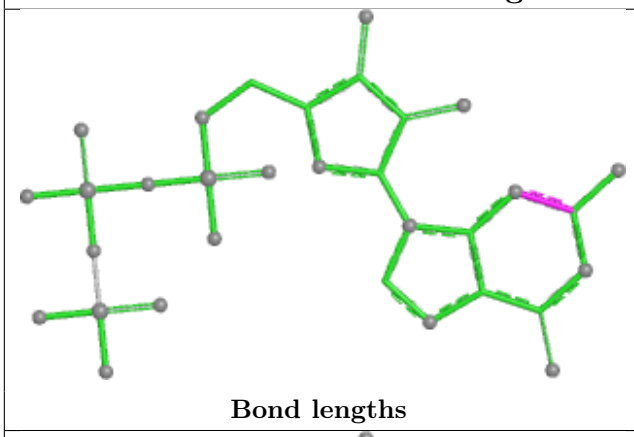


Torsions

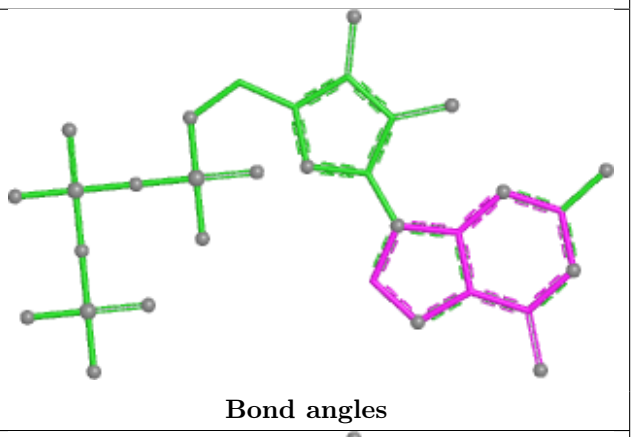


Rings

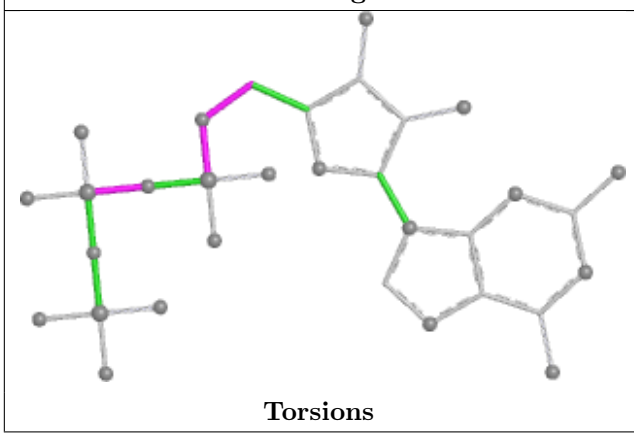
Ligand GTP GM 501



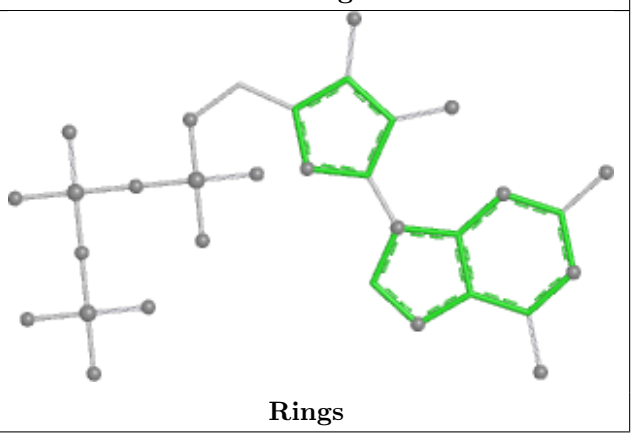
Bond lengths



Bond angles

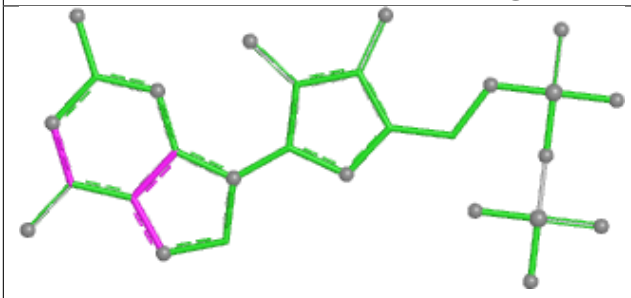


Torsions

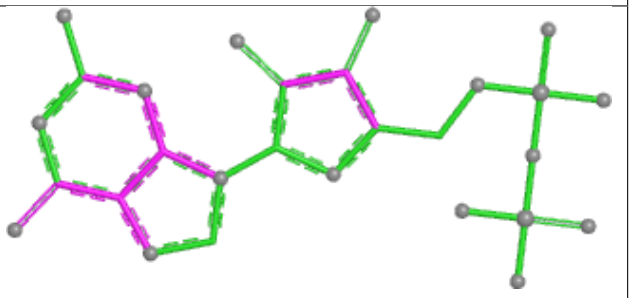


Rings

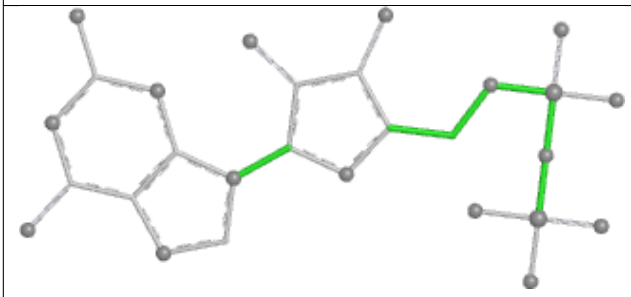
Ligand GDP RN 502



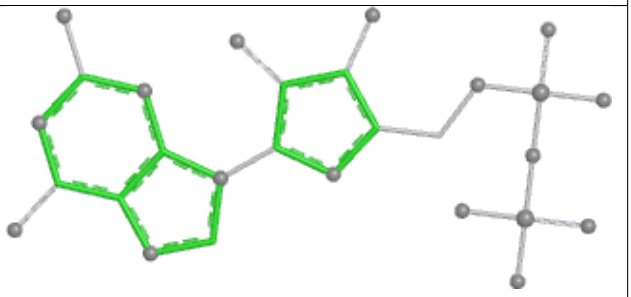
Bond lengths



Bond angles

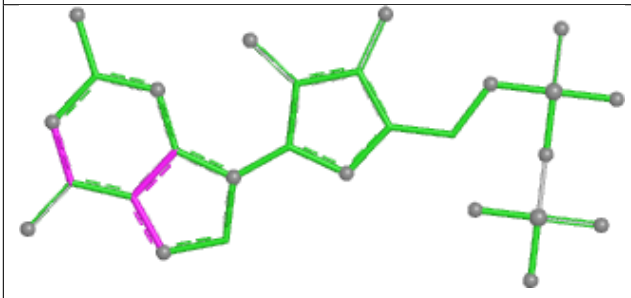


Torsions

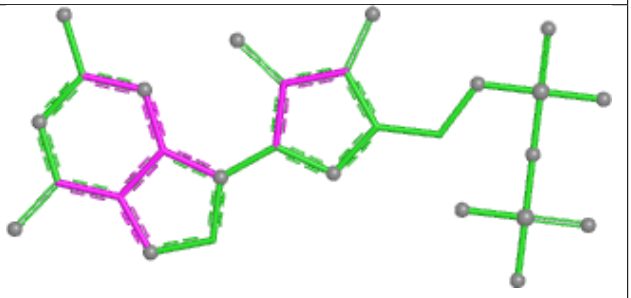


Rings

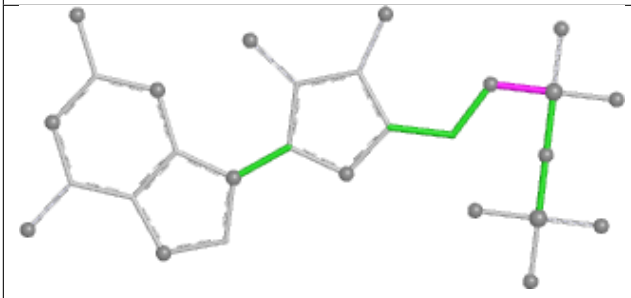
Ligand GDP CN 502



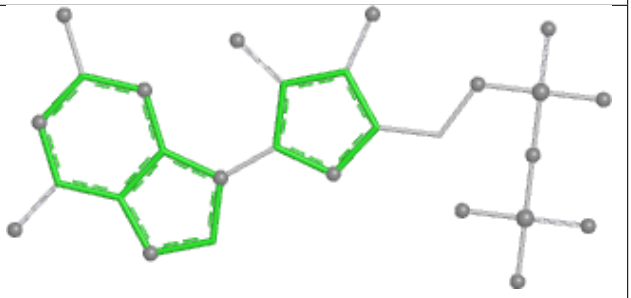
Bond lengths



Bond angles

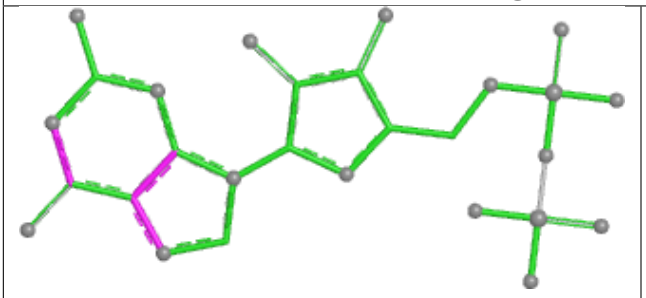


Torsions

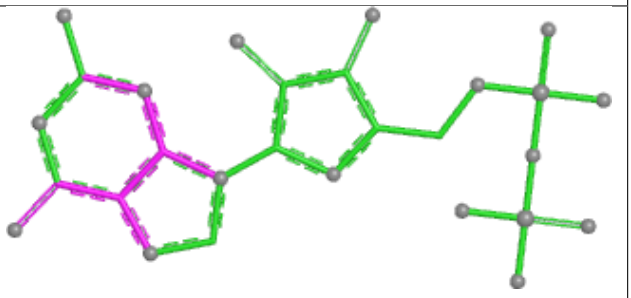


Rings

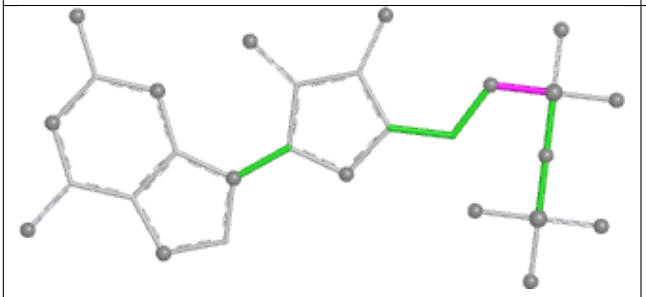
Ligand GDP KF 502



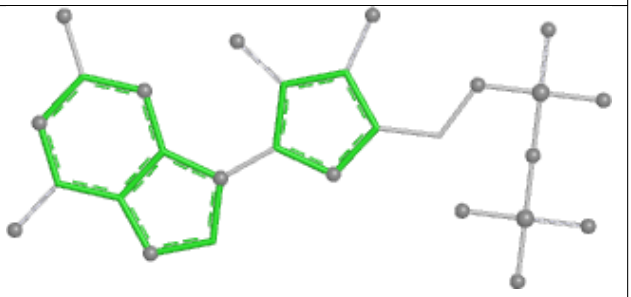
Bond lengths



Bond angles

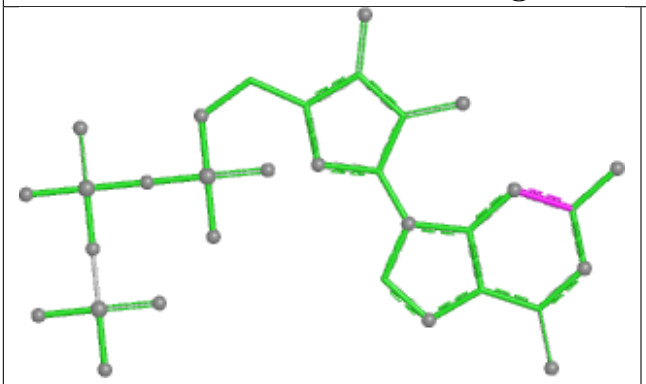


Torsions

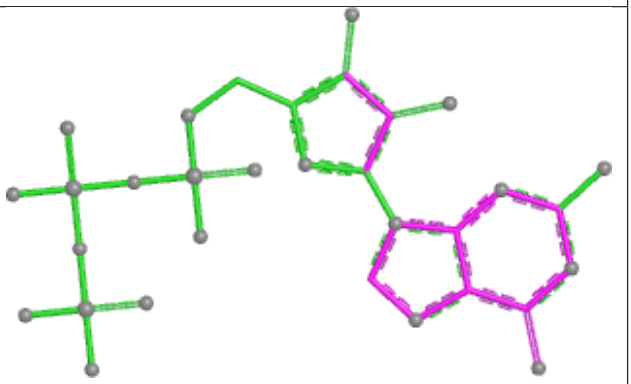


Rings

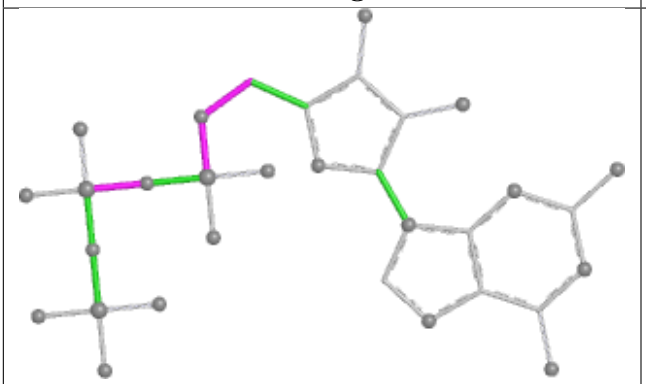
Ligand GTP WI 501



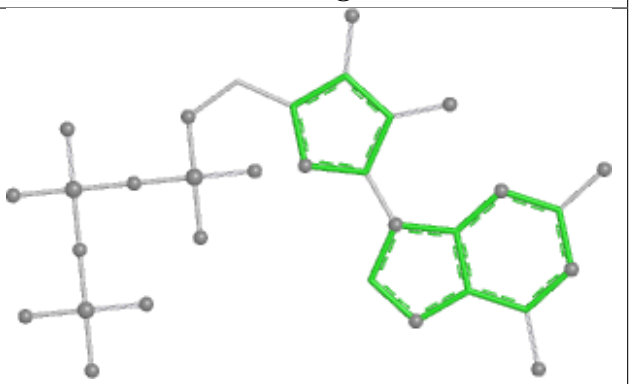
Bond lengths



Bond angles

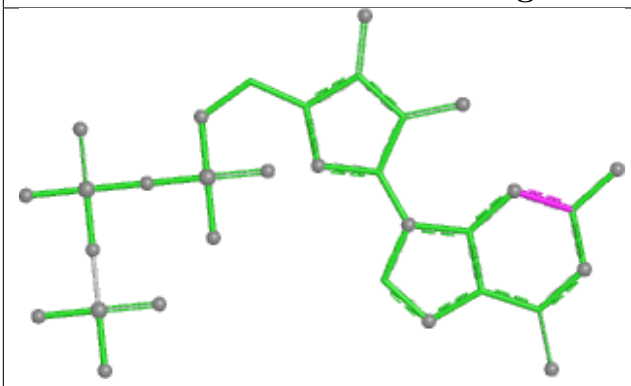


Torsions

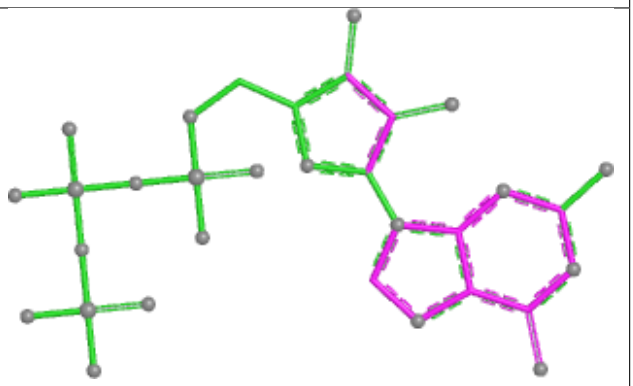


Rings

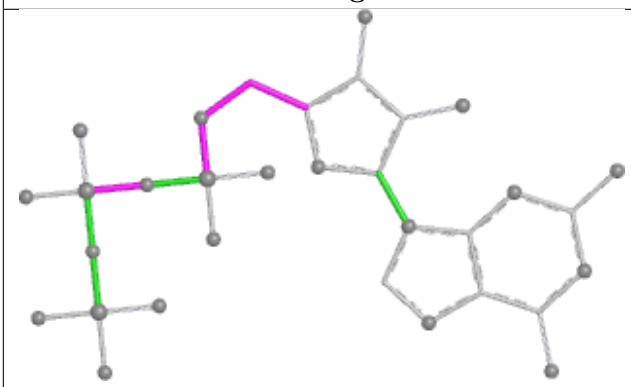
Ligand GTP PI 501



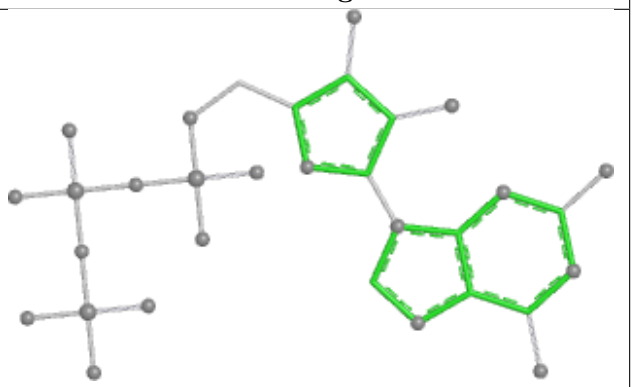
Bond lengths



Bond angles

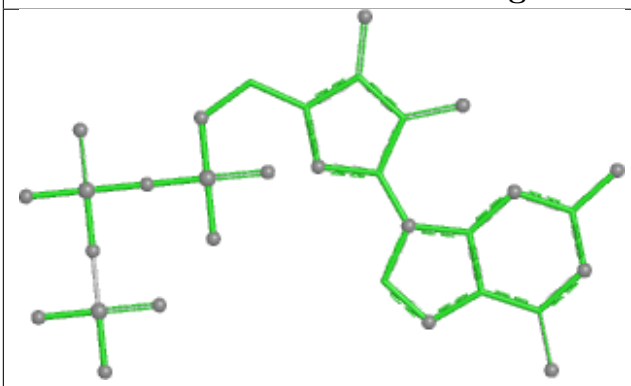


Torsions

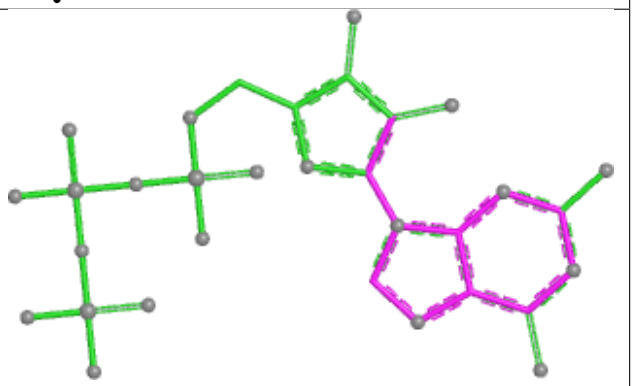


Rings

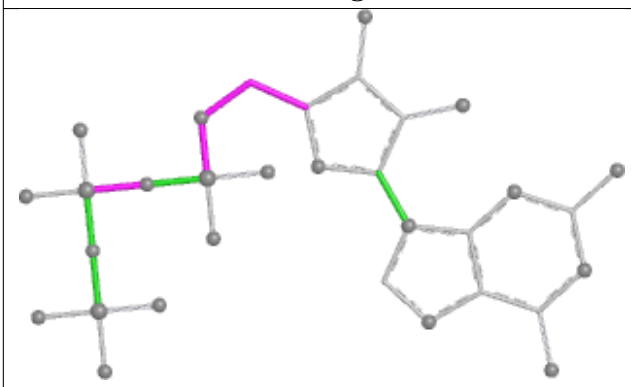
Ligand GTP QO 501



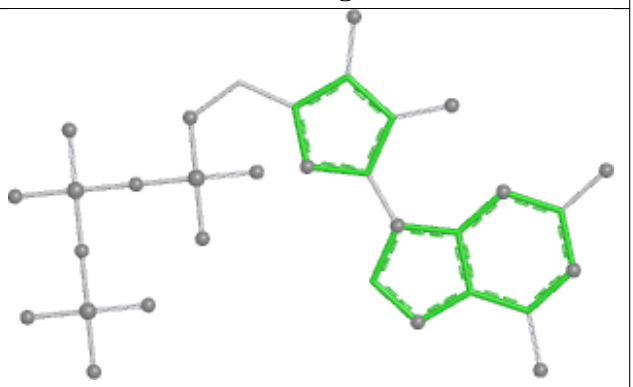
Bond lengths



Bond angles

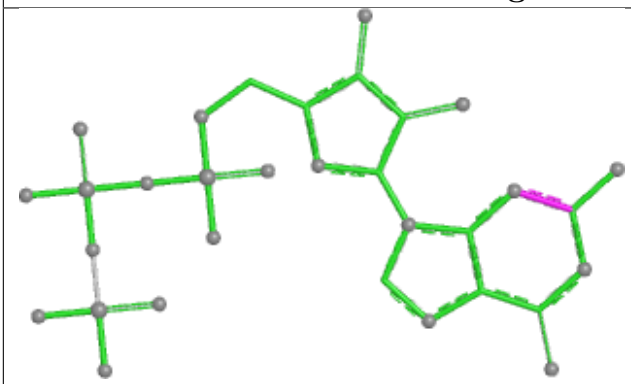


Torsions

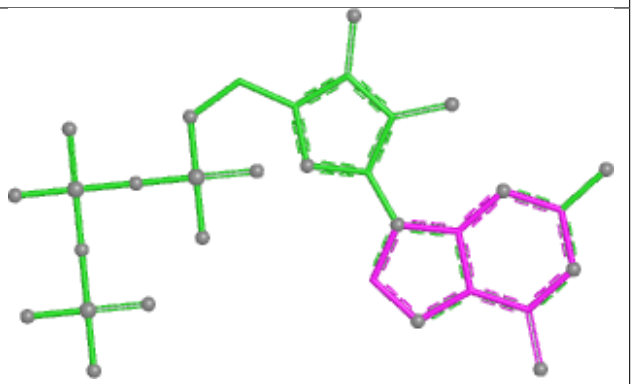


Rings

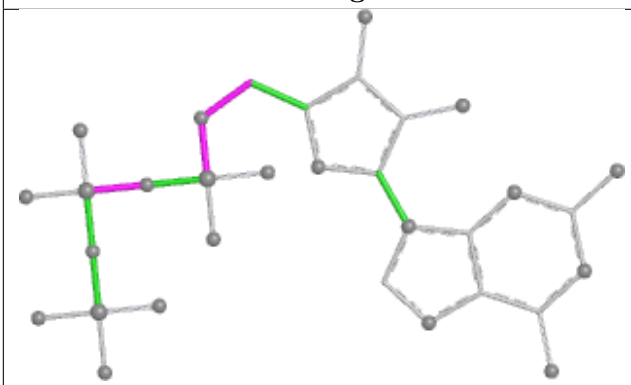
Ligand GTP DK 501



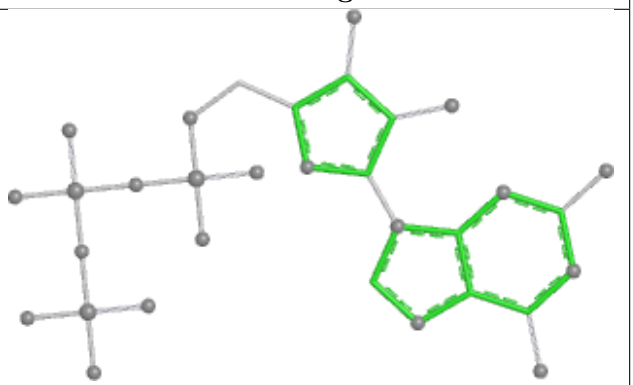
Bond lengths



Bond angles

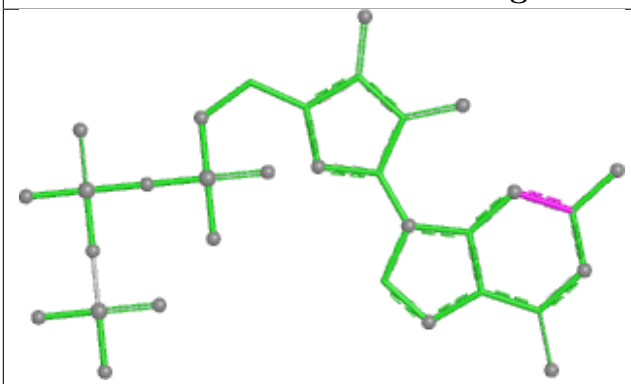


Torsions

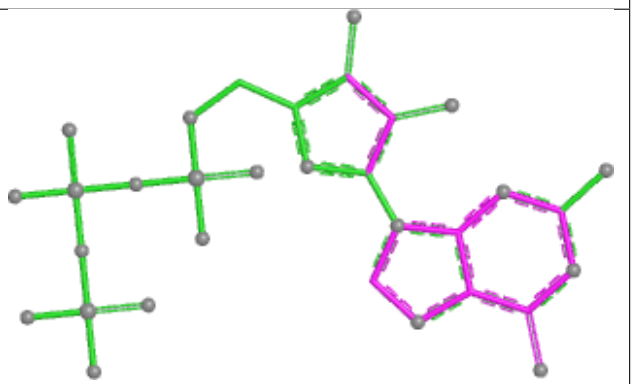


Rings

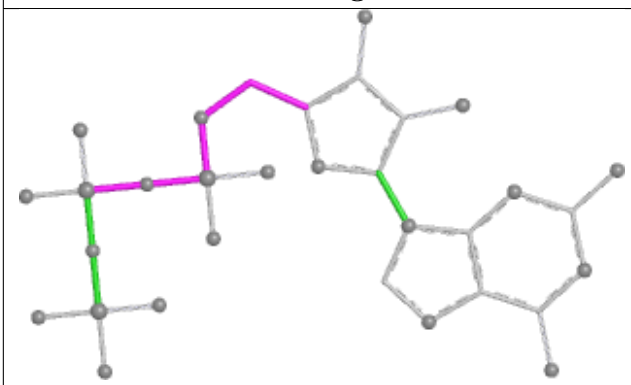
Ligand GTP UE 501



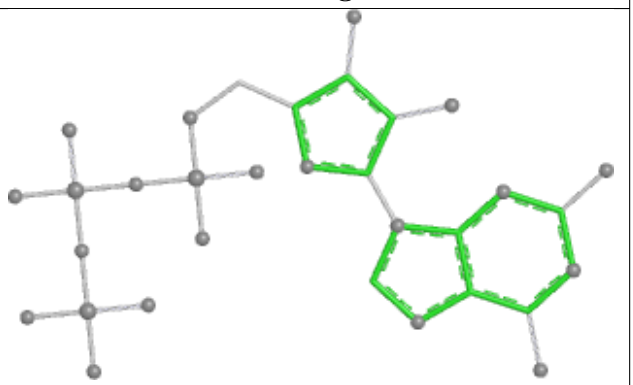
Bond lengths



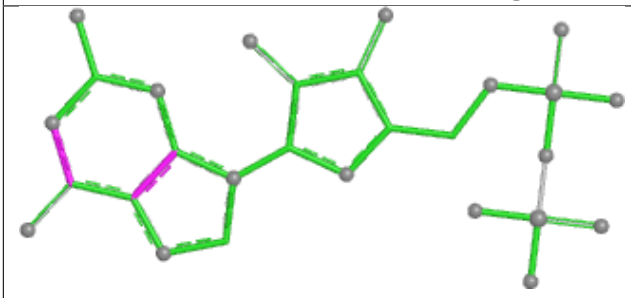
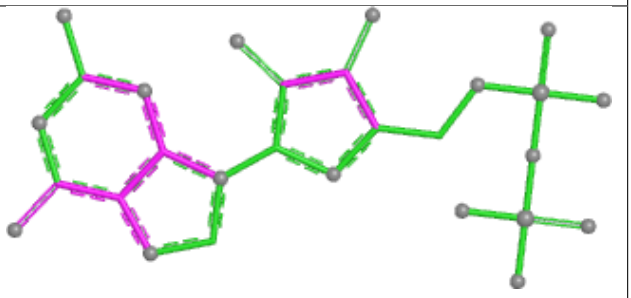
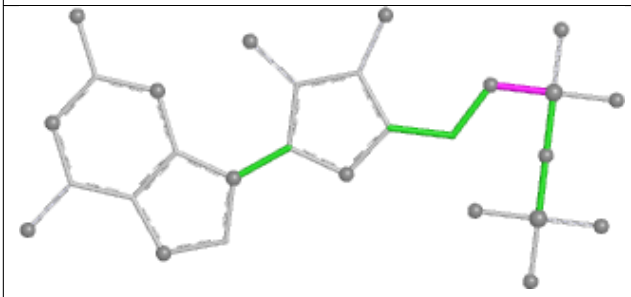
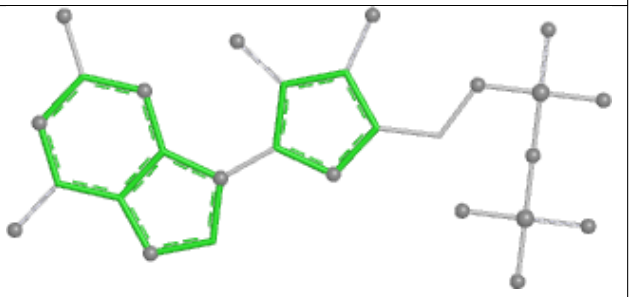
Bond angles

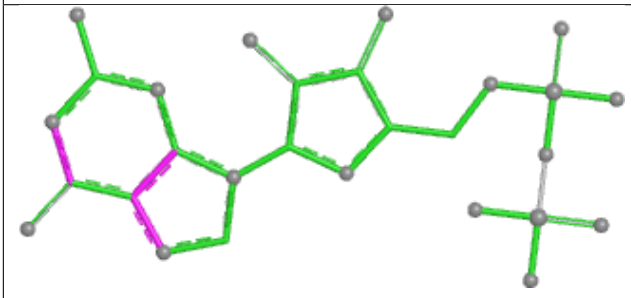
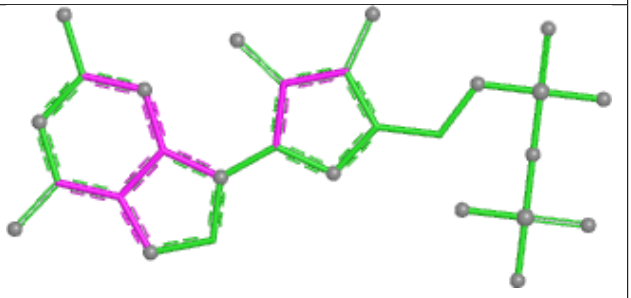
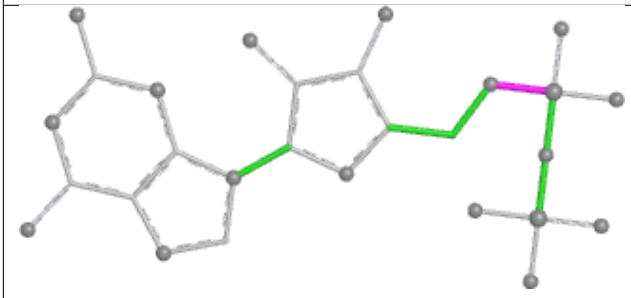
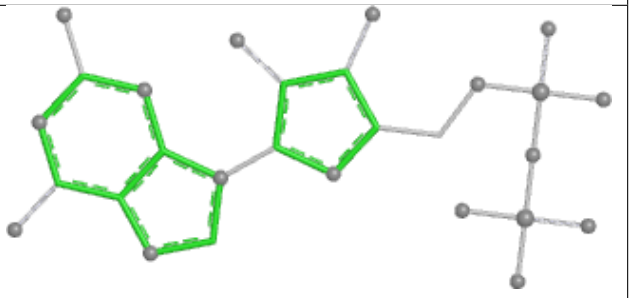


Torsions

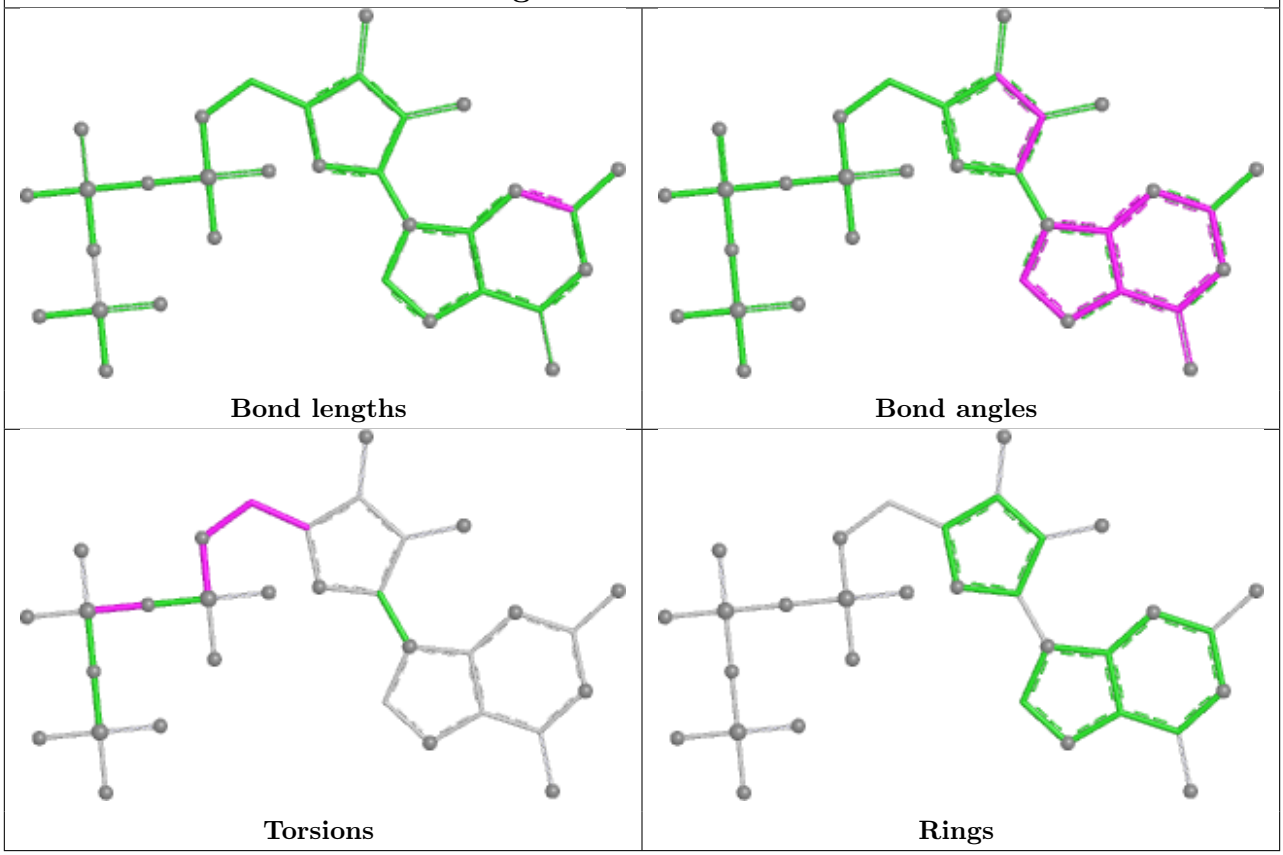


Rings

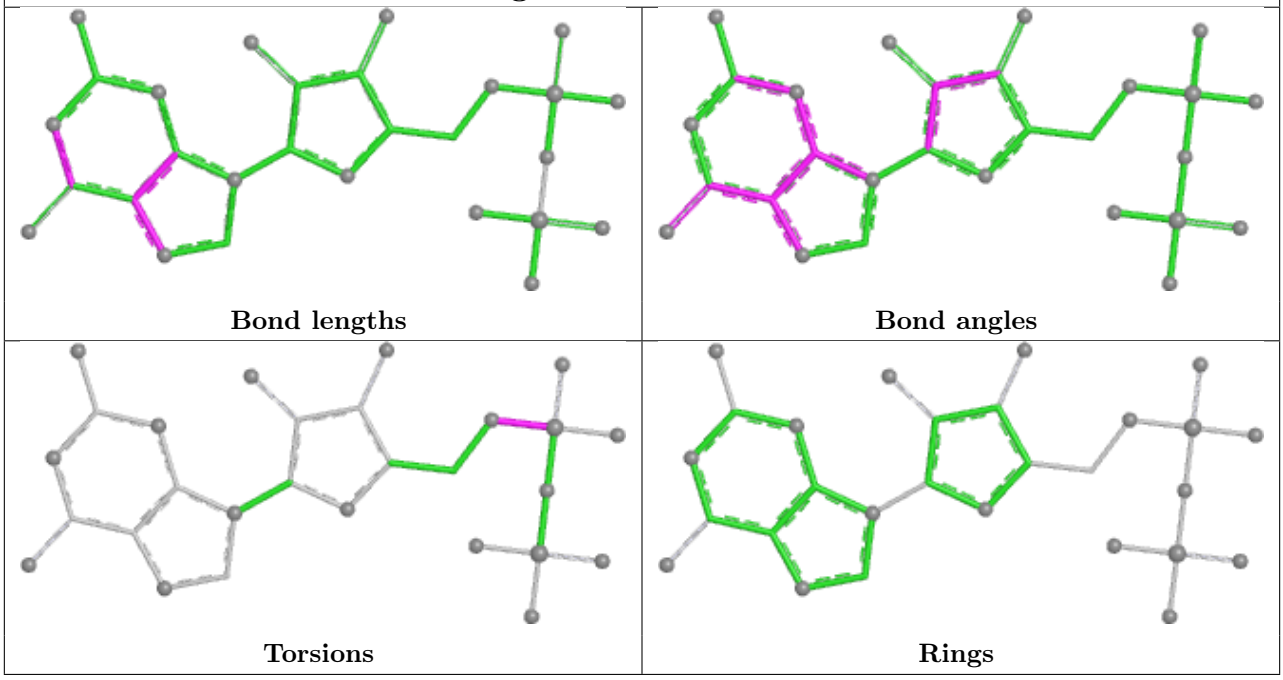
Ligand GDP GB 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP VD 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

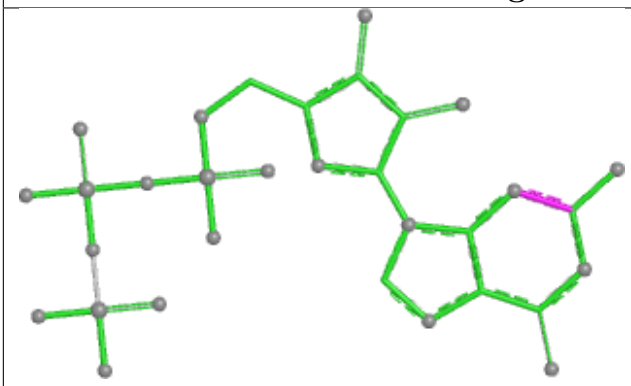
Ligand GTP PE 501



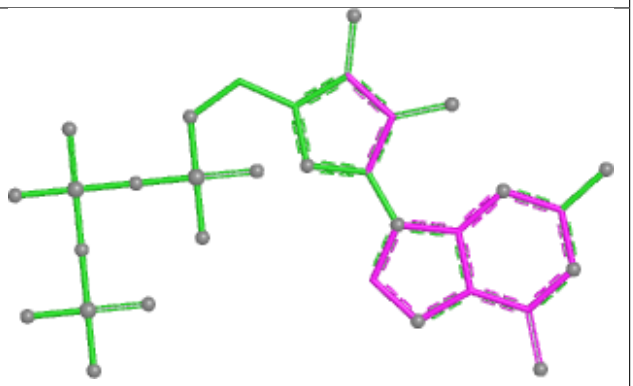
Ligand GDP LN 502



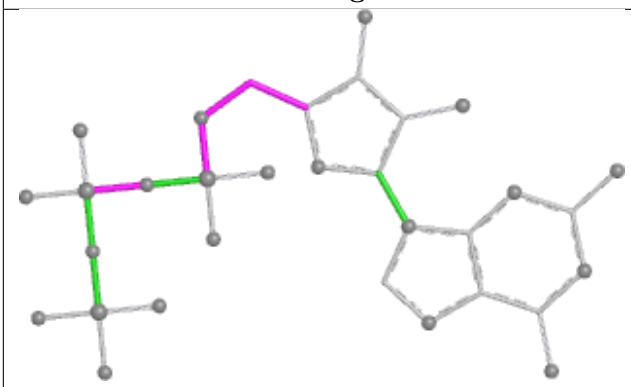
Ligand GTP OK 501



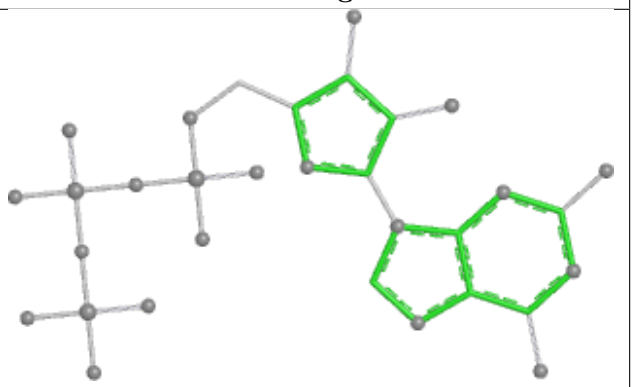
Bond lengths



Bond angles

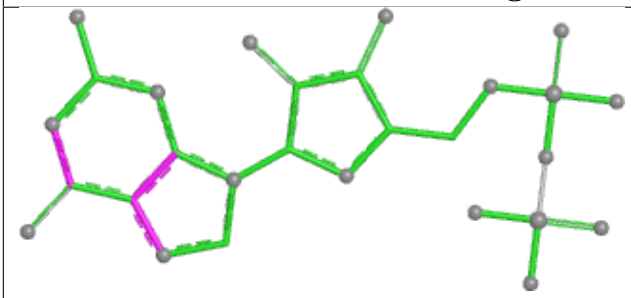


Torsions

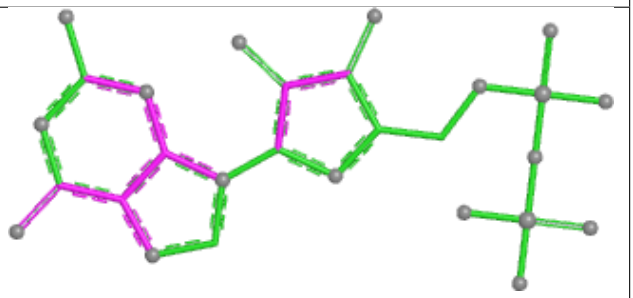


Rings

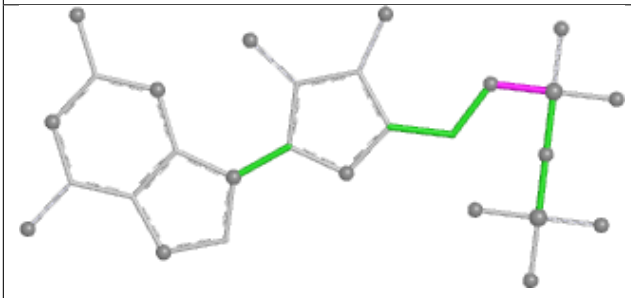
Ligand GDP MF 502



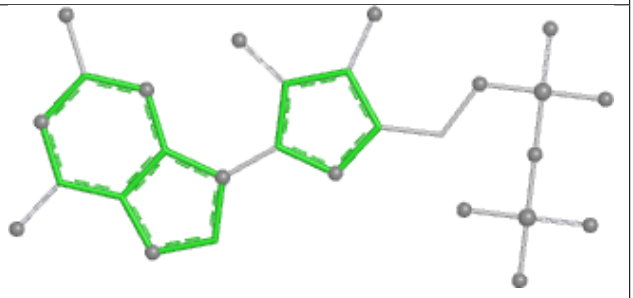
Bond lengths



Bond angles

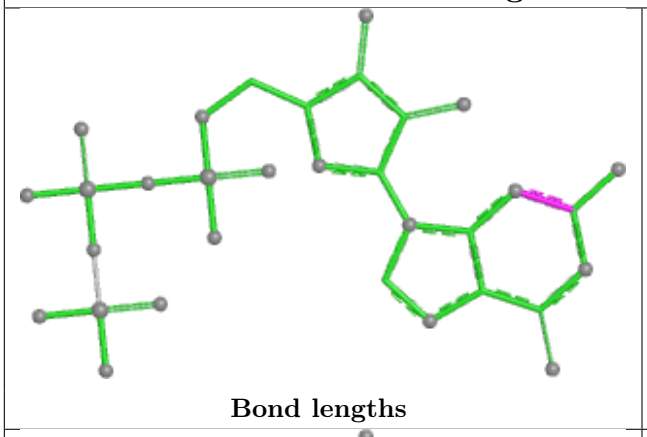


Torsions

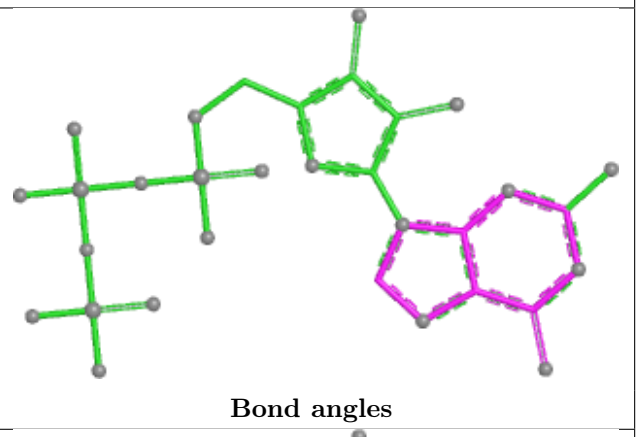


Rings

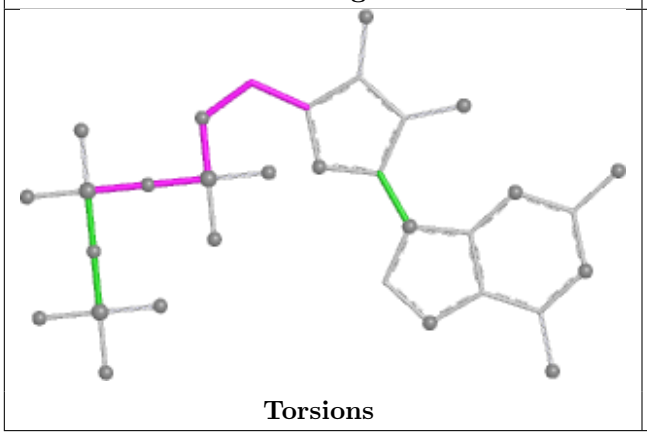
Ligand GTP AM 501



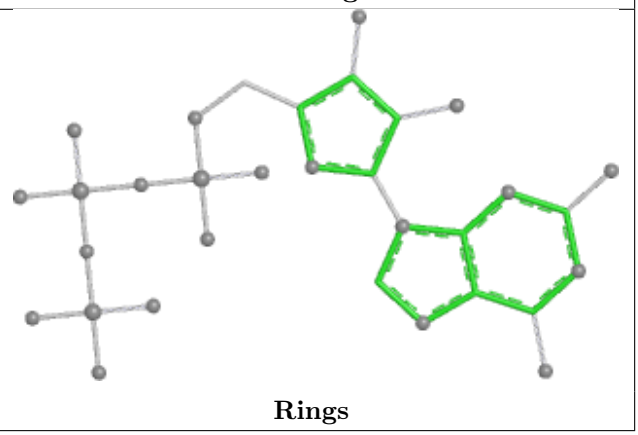
Bond lengths



Bond angles

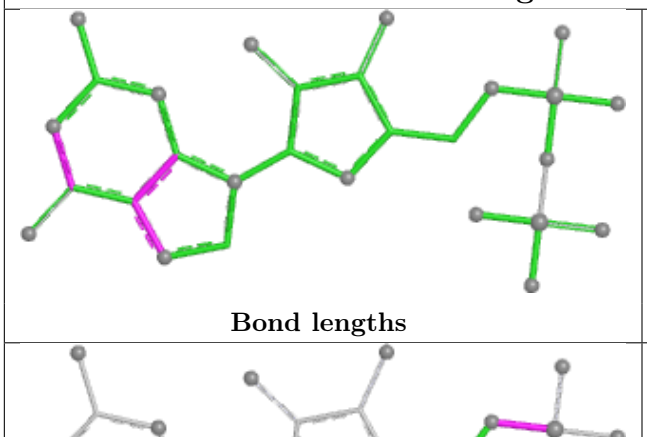


Torsions

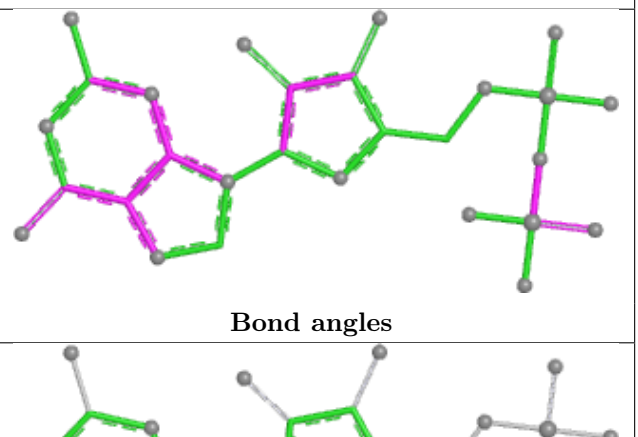


Rings

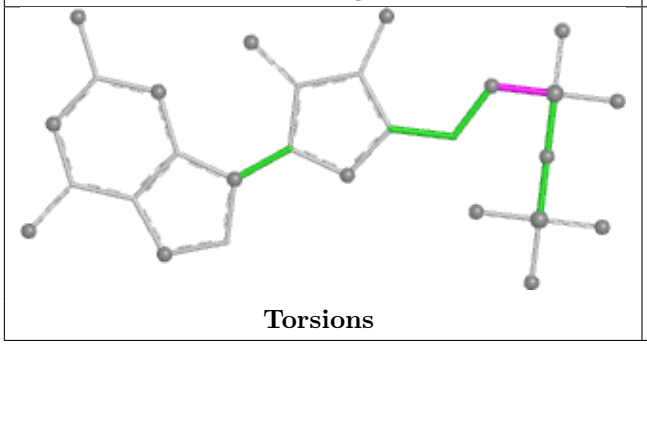
Ligand GDP IP 502



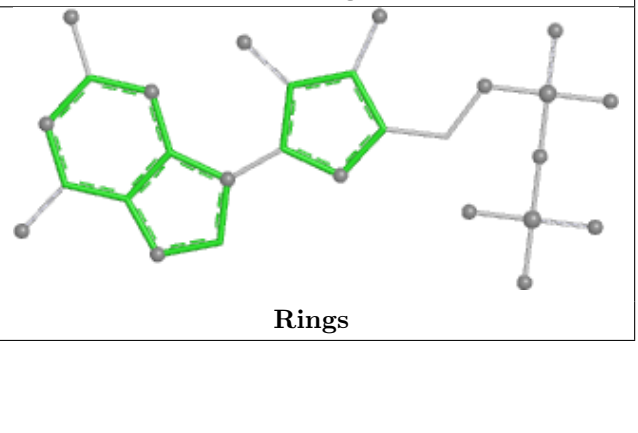
Bond lengths



Bond angles

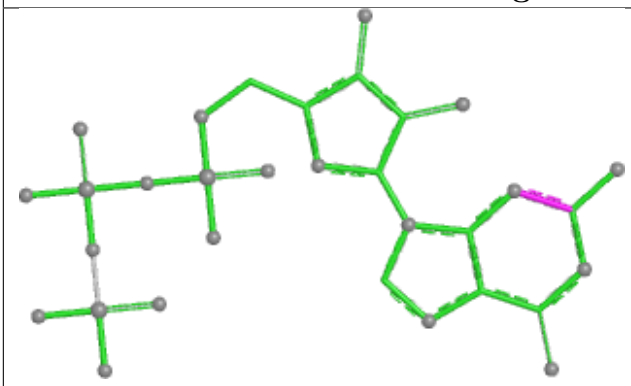


Torsions

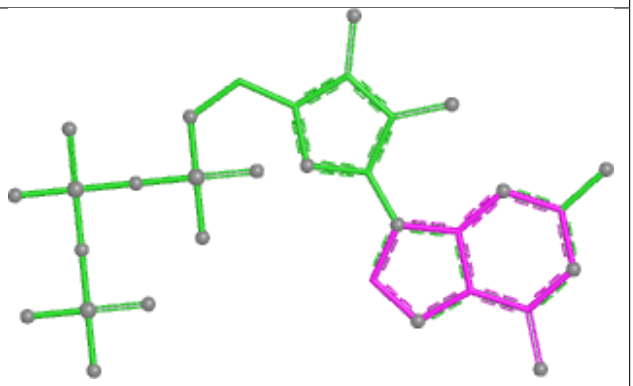


Rings

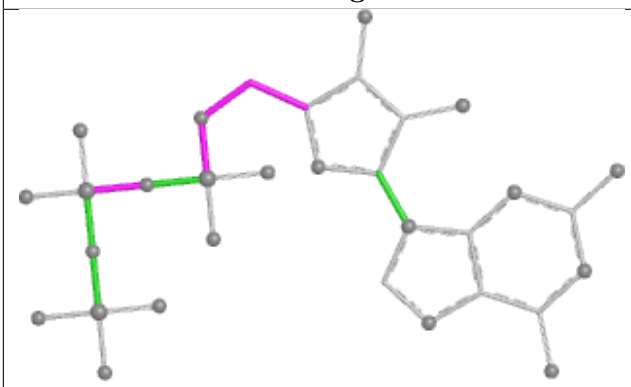
Ligand GTP SC 501



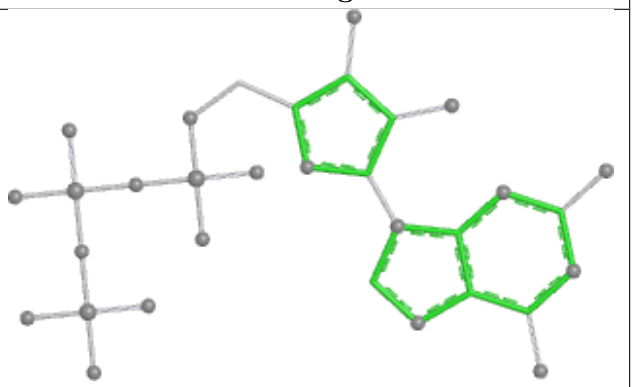
Bond lengths



Bond angles

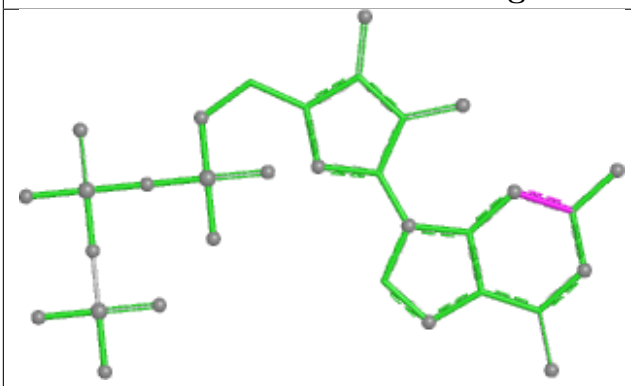


Torsions

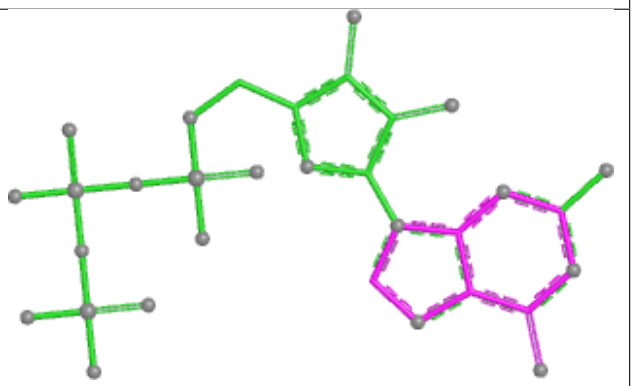


Rings

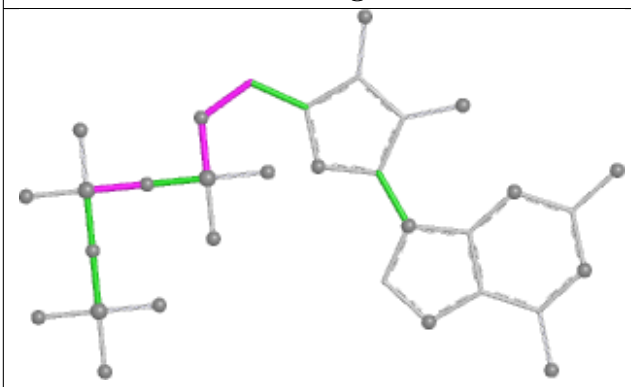
Ligand GTP KO 501



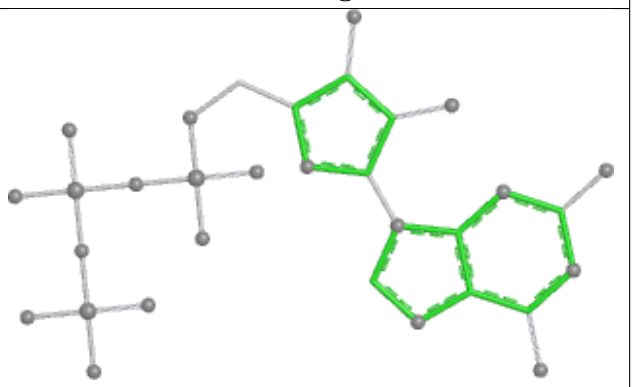
Bond lengths



Bond angles

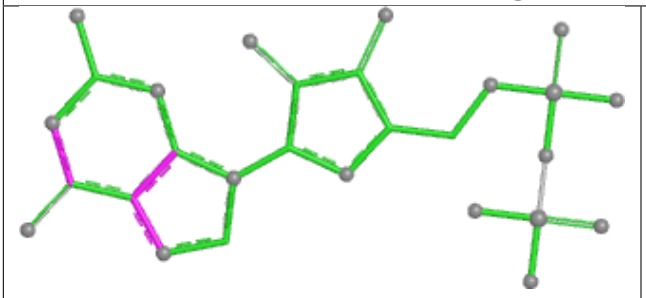


Torsions

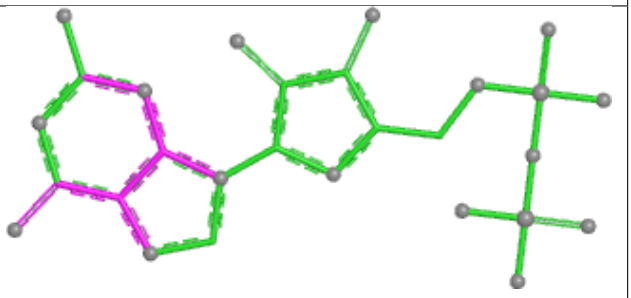


Rings

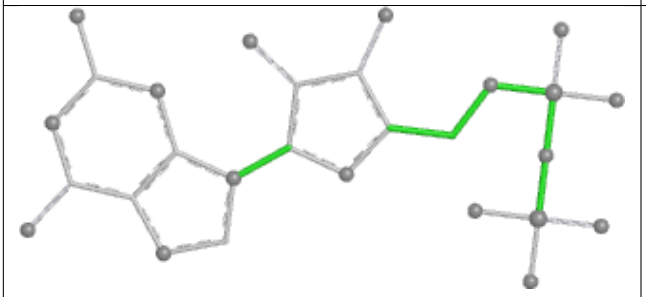
Ligand GDP FD 502



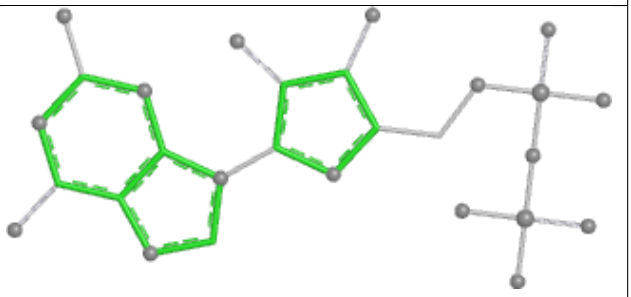
Bond lengths



Bond angles

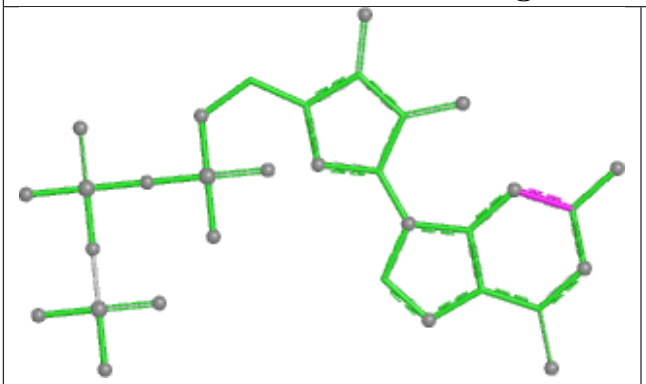


Torsions

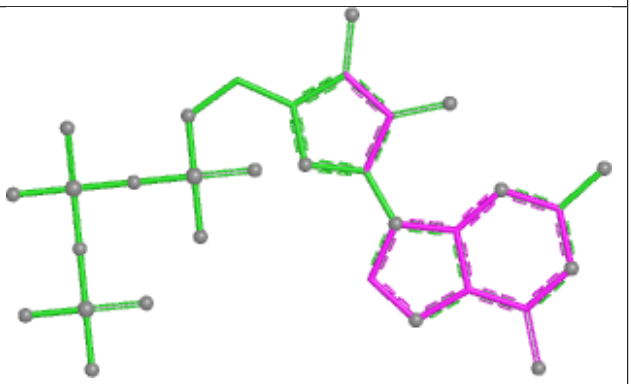


Rings

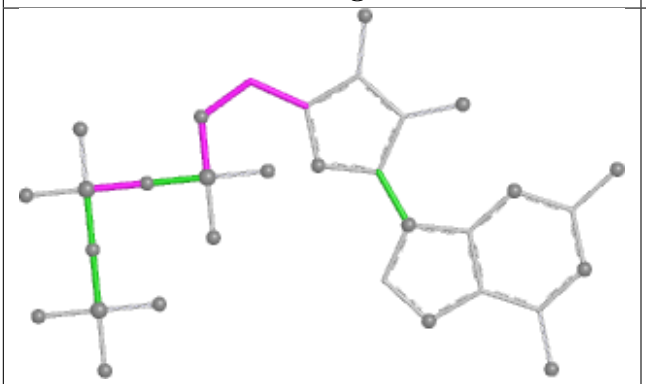
Ligand GTP IK 501



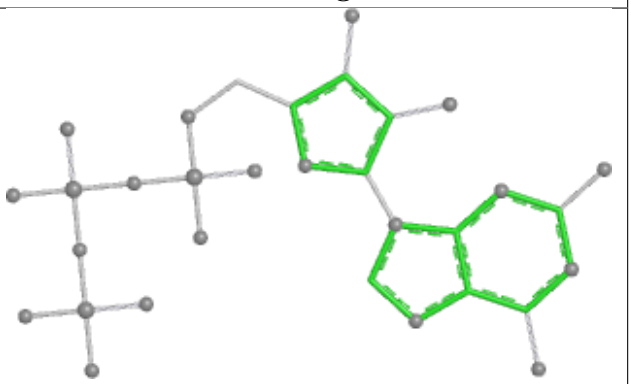
Bond lengths



Bond angles

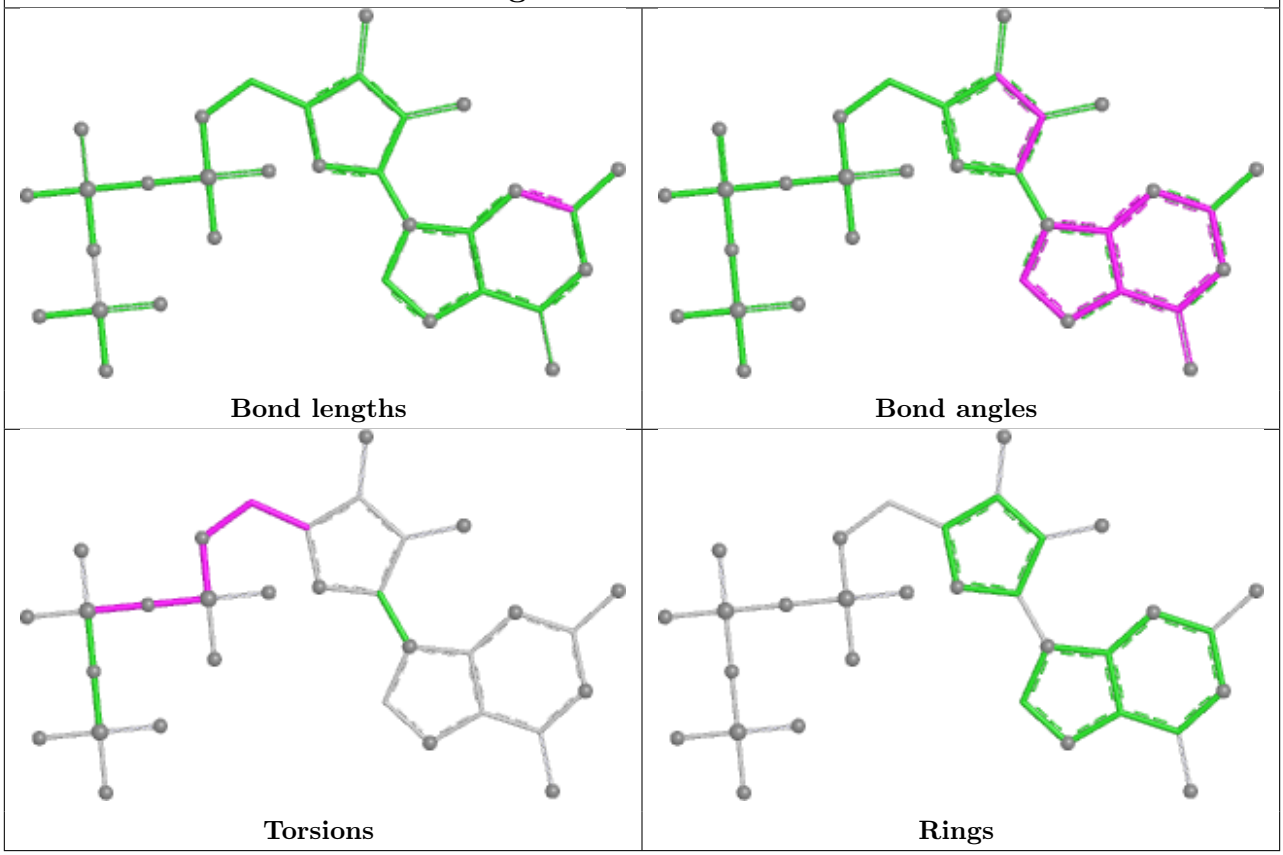


Torsions

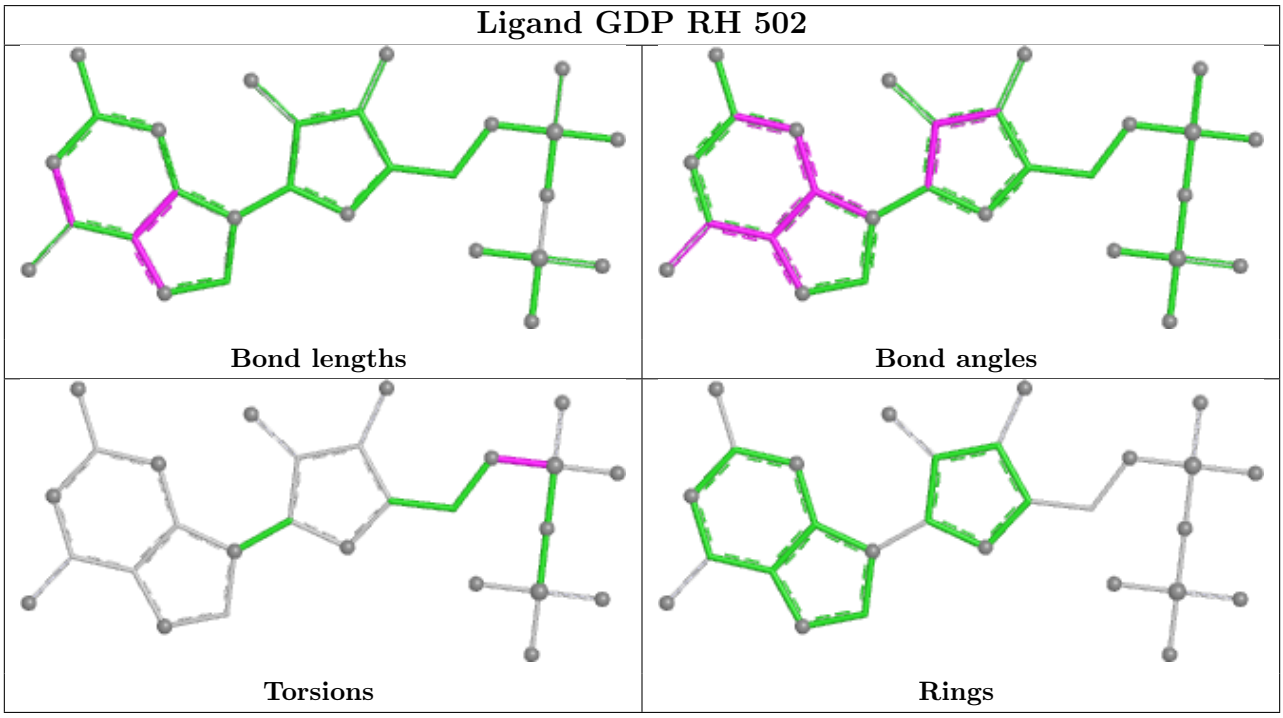


Rings

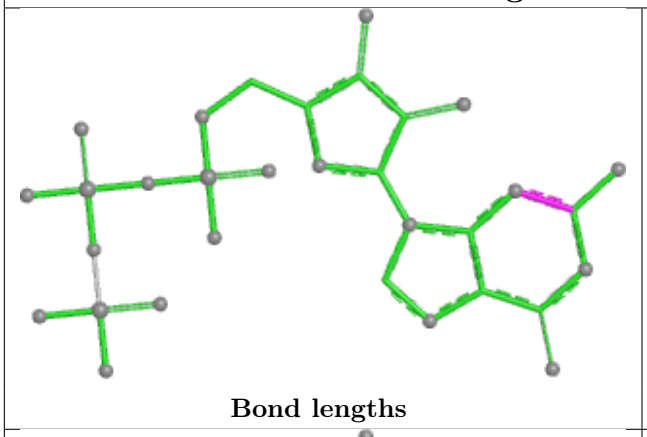
Ligand GTP UG 501



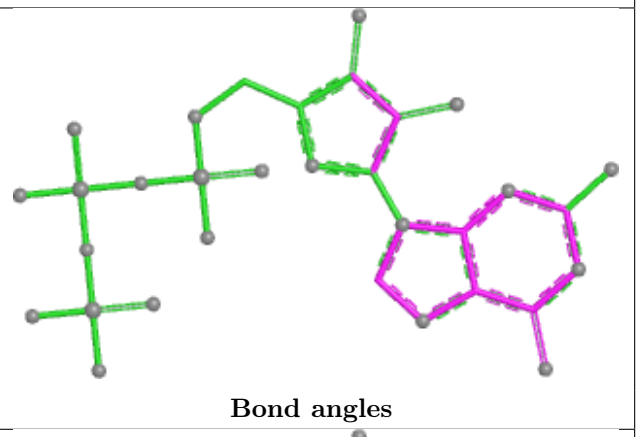
Ligand GDP RH 502



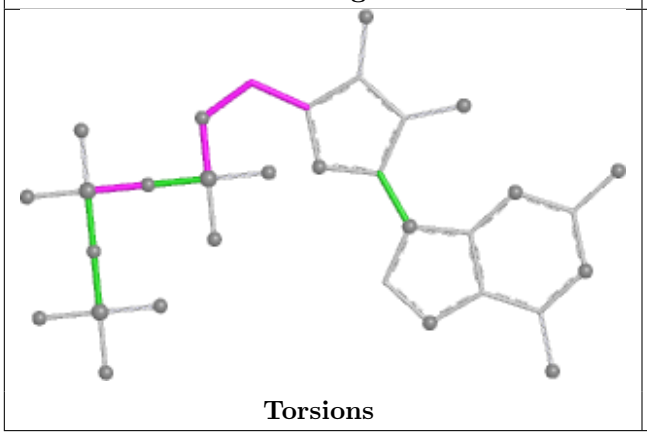
Ligand GTP UM 501



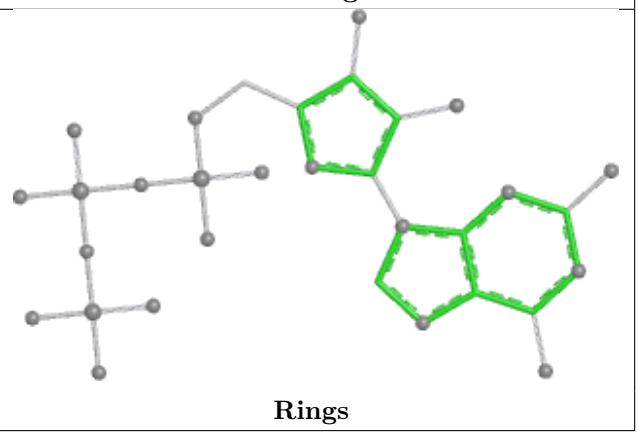
Bond lengths



Bond angles

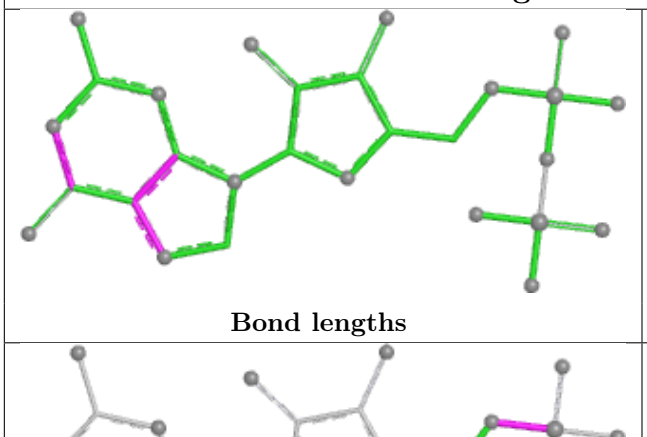


Torsions

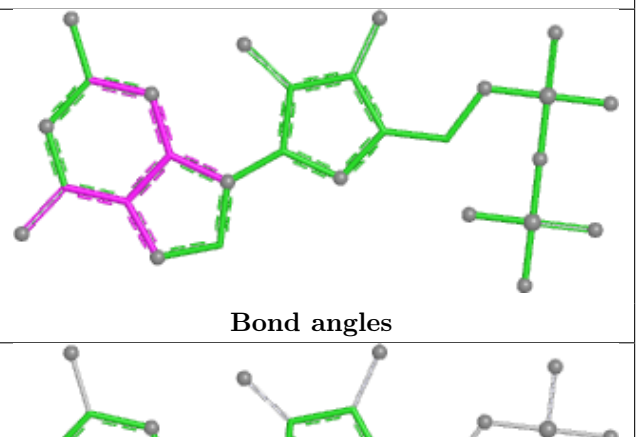


Rings

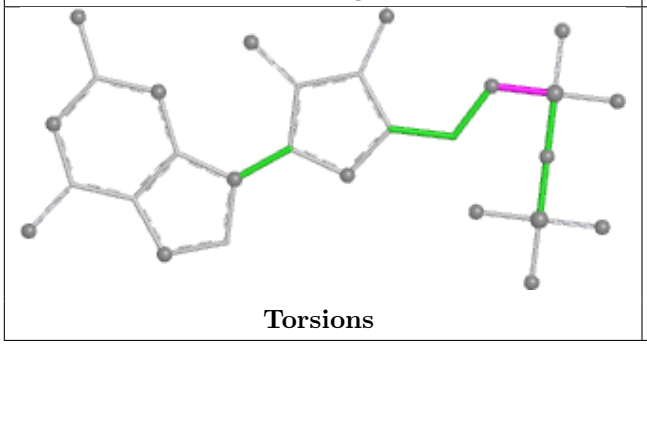
Ligand GDP FF 502



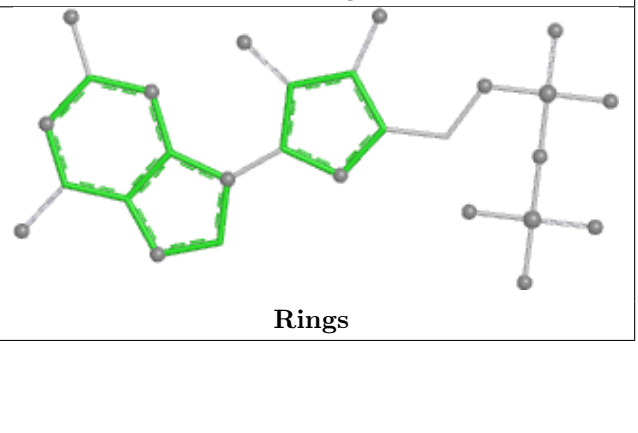
Bond lengths



Bond angles

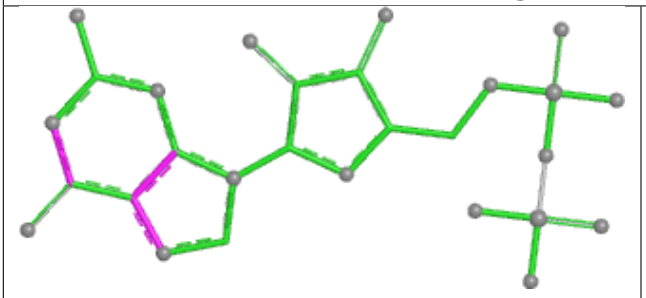


Torsions

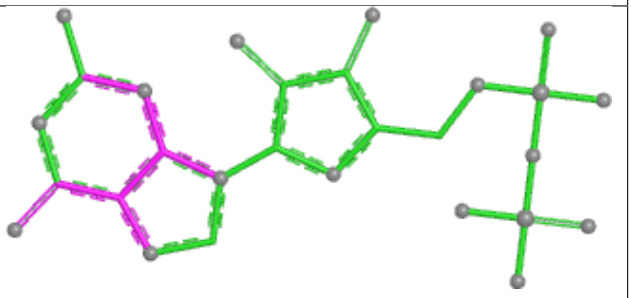


Rings

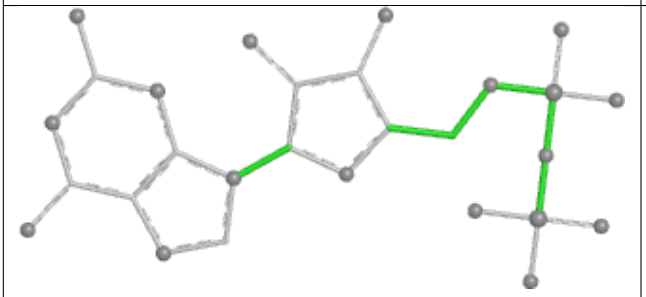
Ligand GDP RJ 502



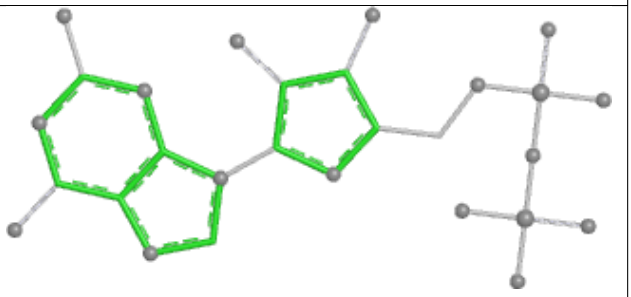
Bond lengths



Bond angles

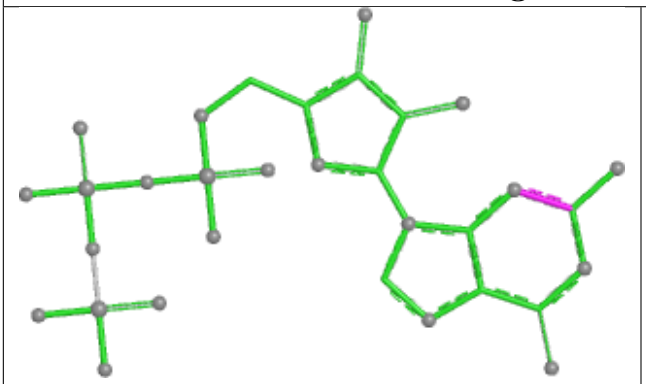


Torsions

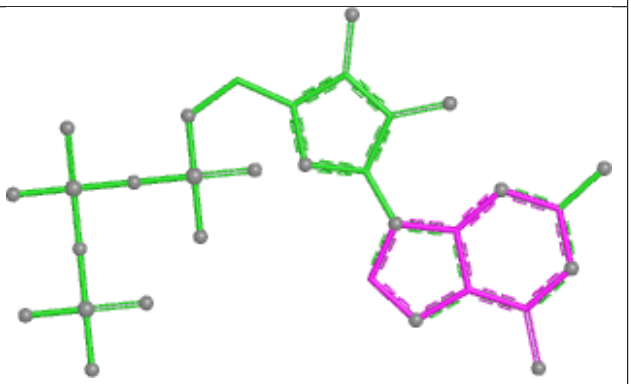


Rings

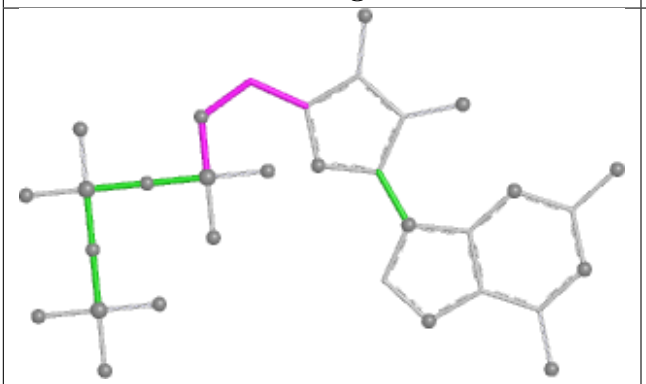
Ligand GTP JM 501



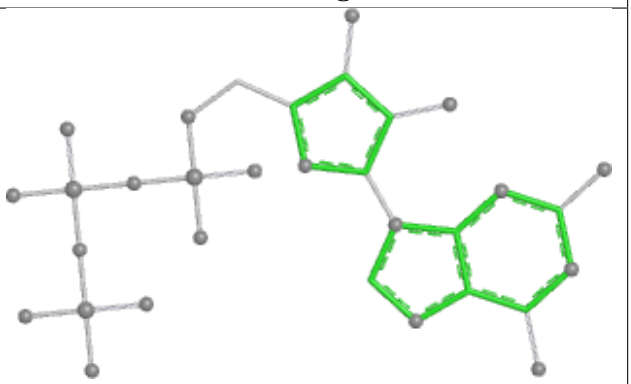
Bond lengths



Bond angles

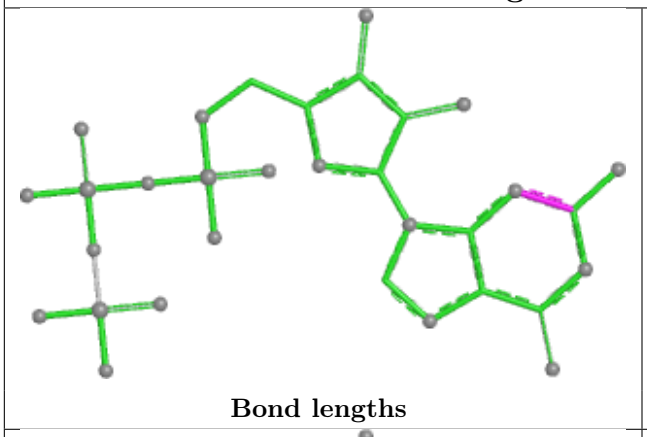


Torsions

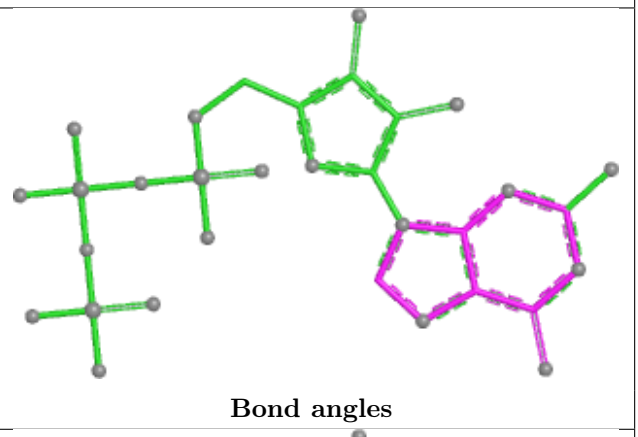


Rings

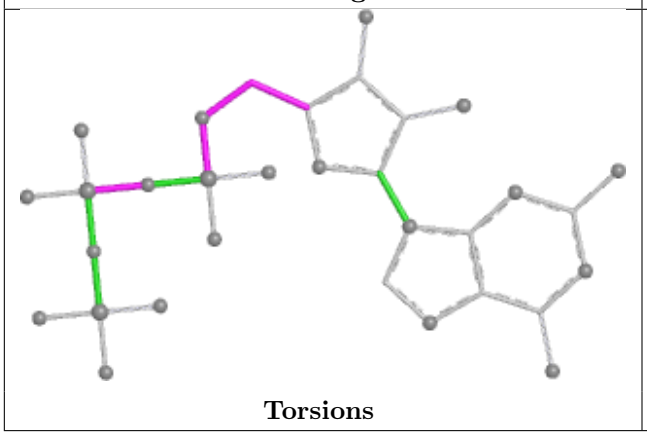
Ligand GTP MO 501



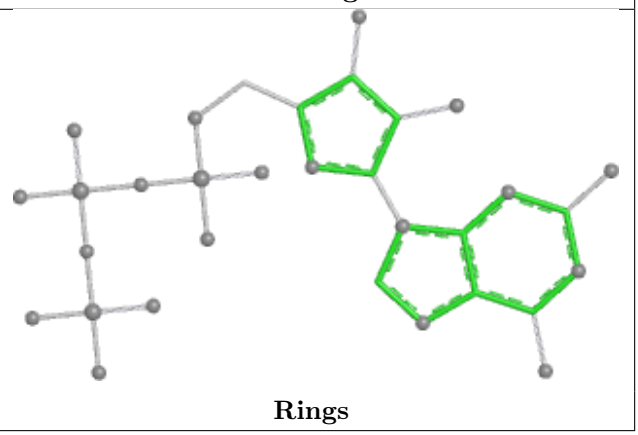
Bond lengths



Bond angles

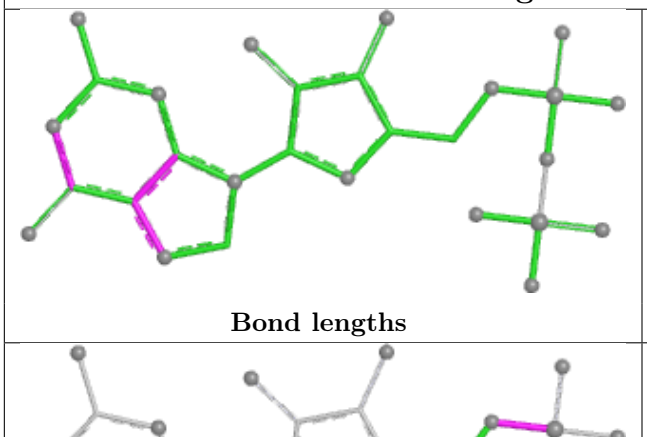


Torsions

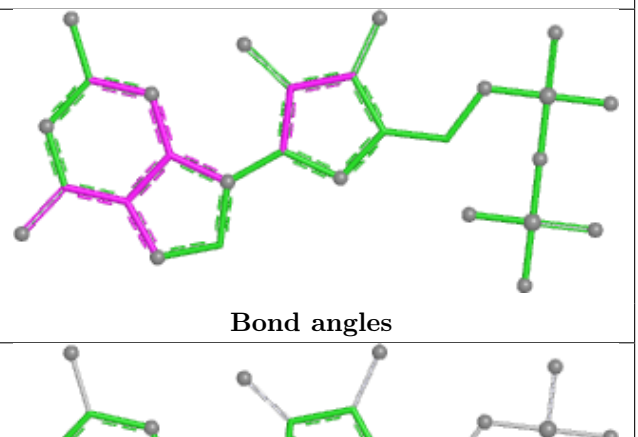


Rings

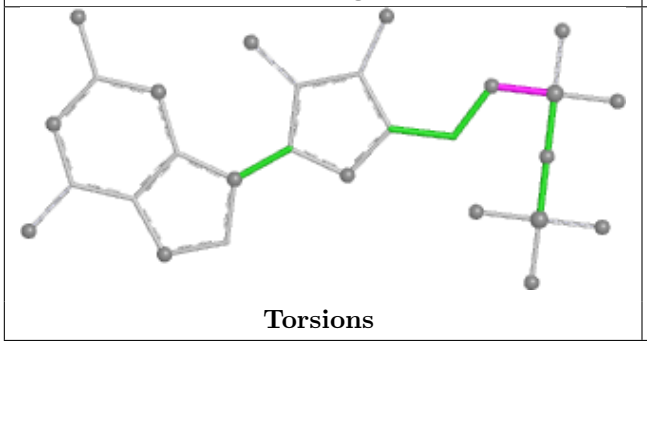
Ligand GDP SJ 502



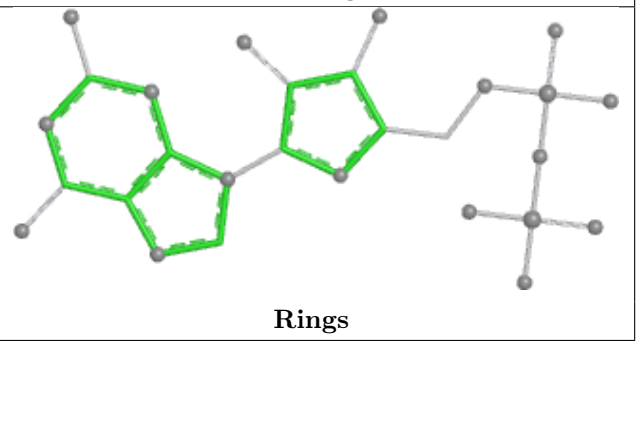
Bond lengths



Bond angles

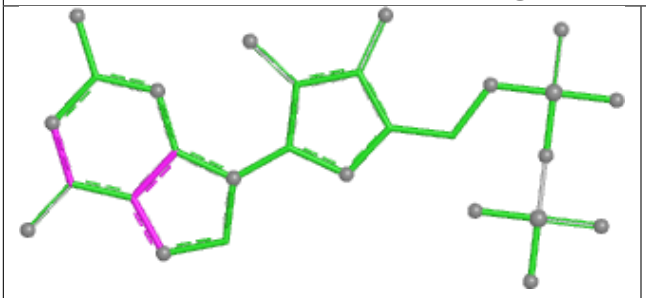


Torsions

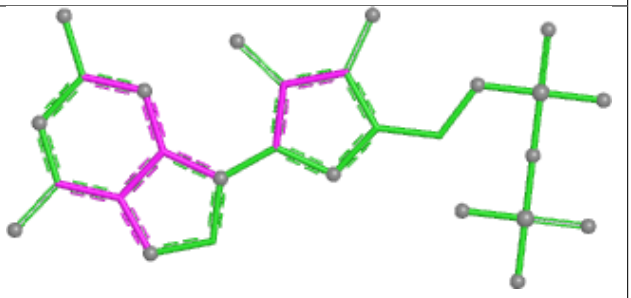


Rings

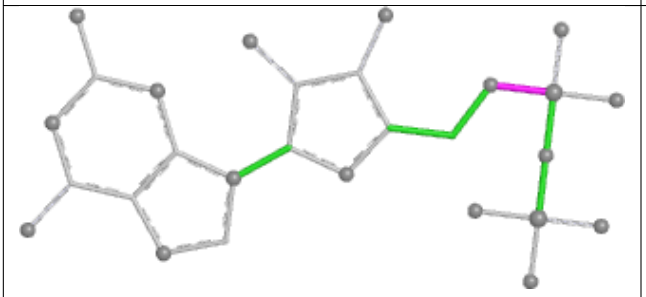
Ligand GDP DJ 502



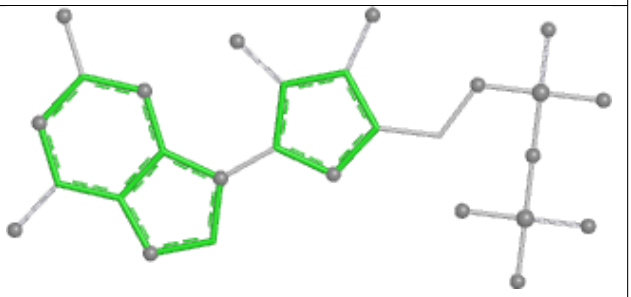
Bond lengths



Bond angles

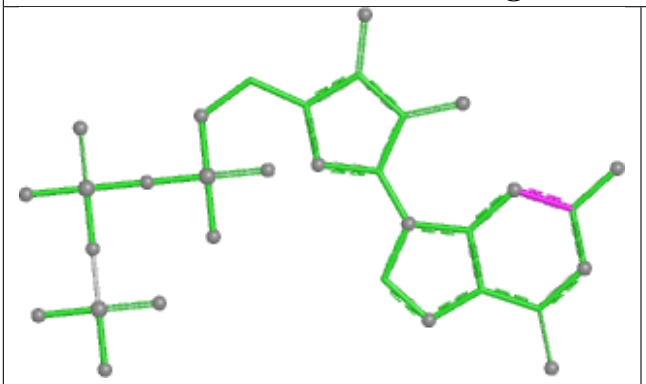


Torsions

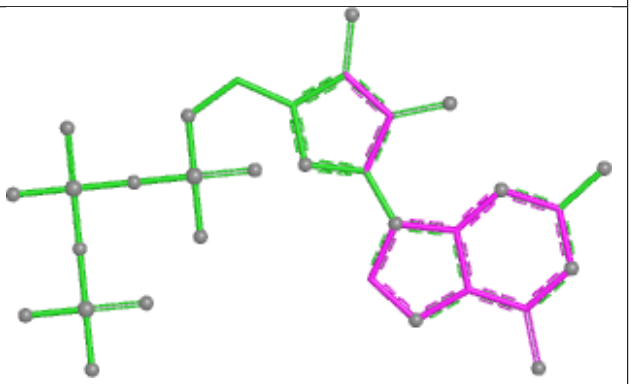


Rings

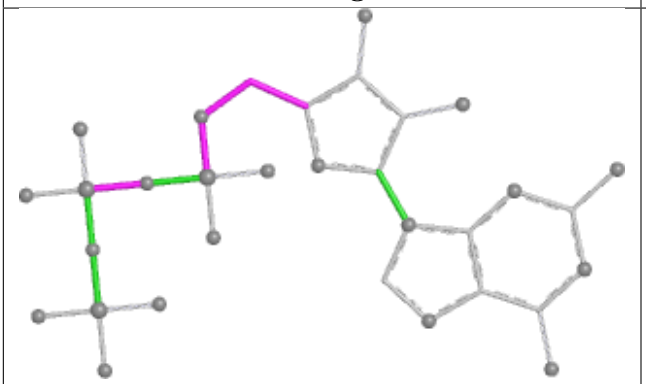
Ligand GTP VM 501



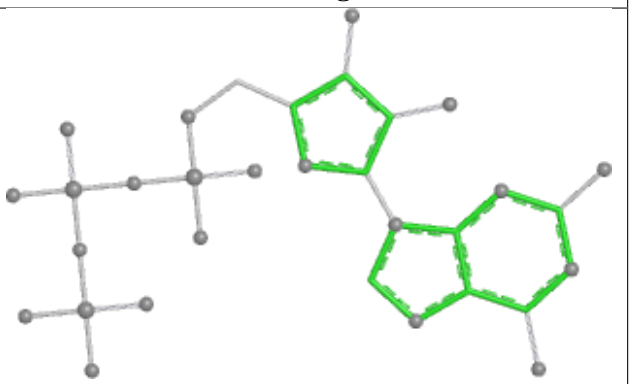
Bond lengths



Bond angles

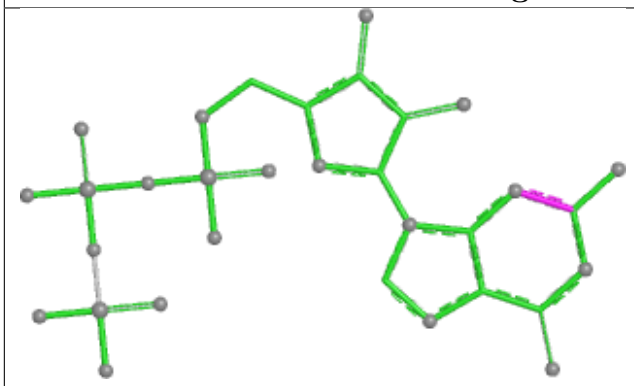


Torsions

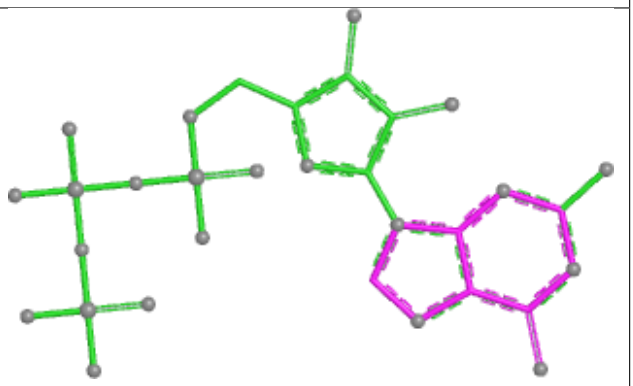


Rings

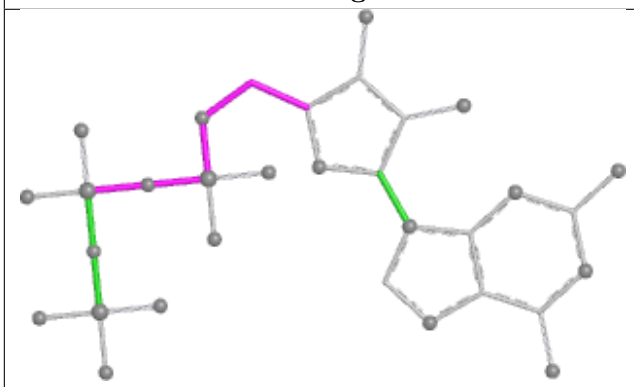
Ligand GTP AE 501



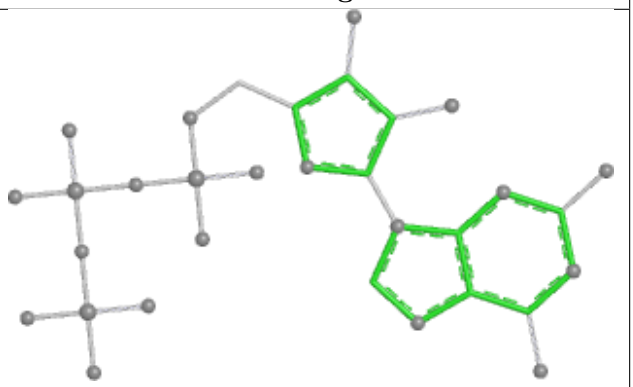
Bond lengths



Bond angles

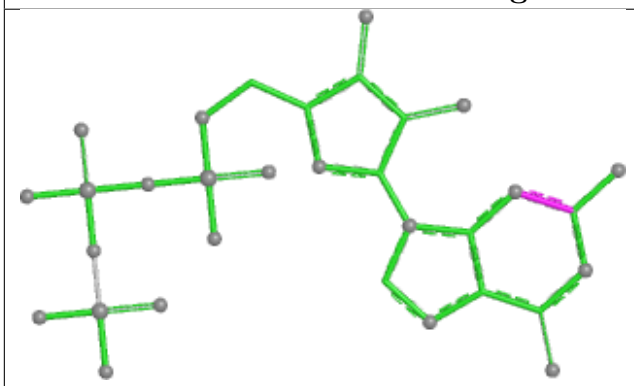


Torsions

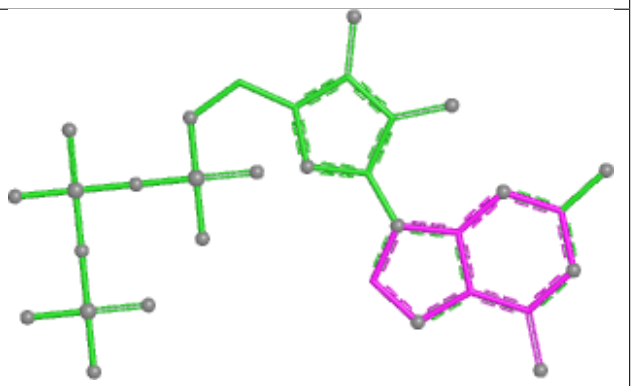


Rings

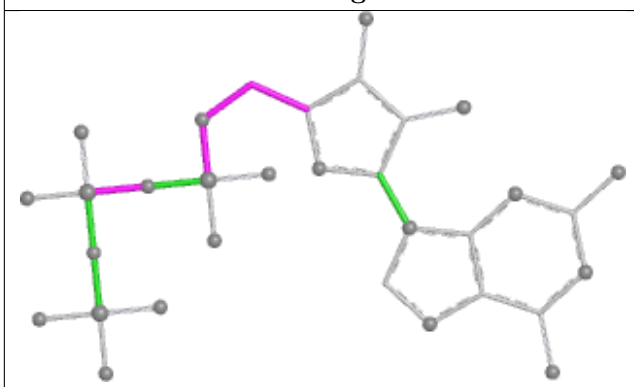
Ligand GTP AO 501



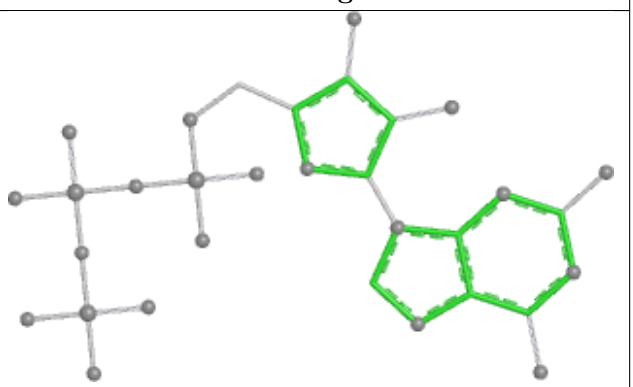
Bond lengths



Bond angles

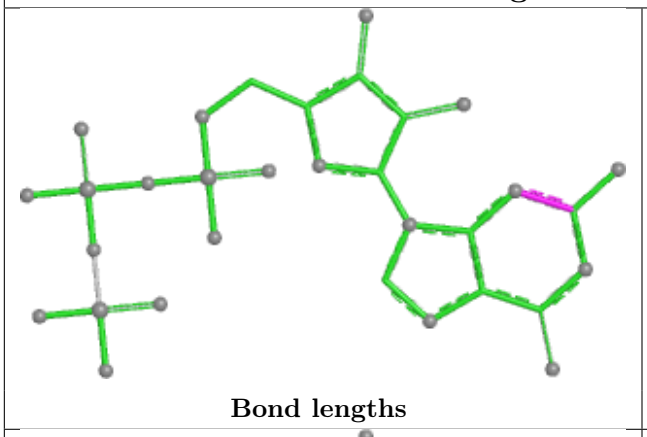


Torsions

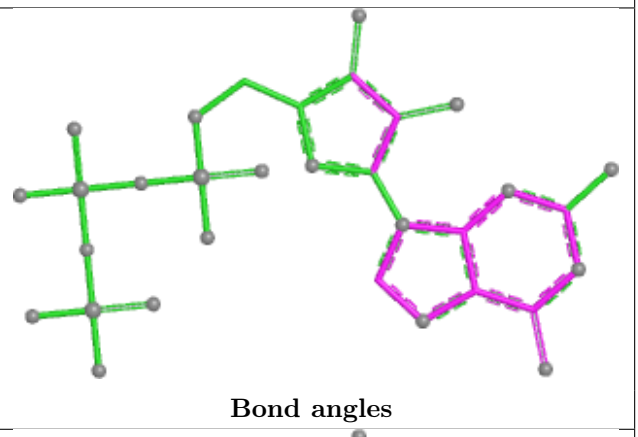


Rings

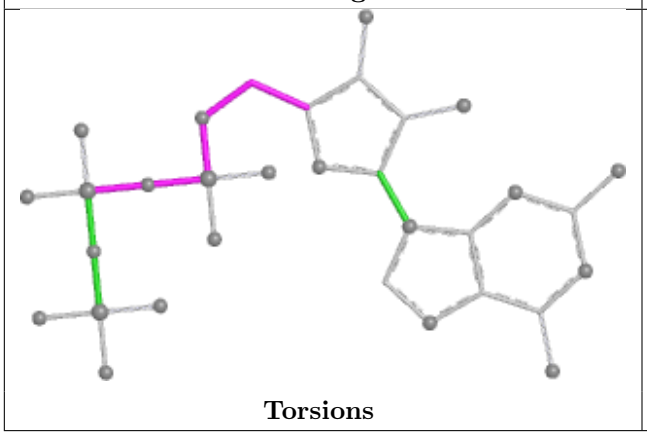
Ligand GTP UC 501



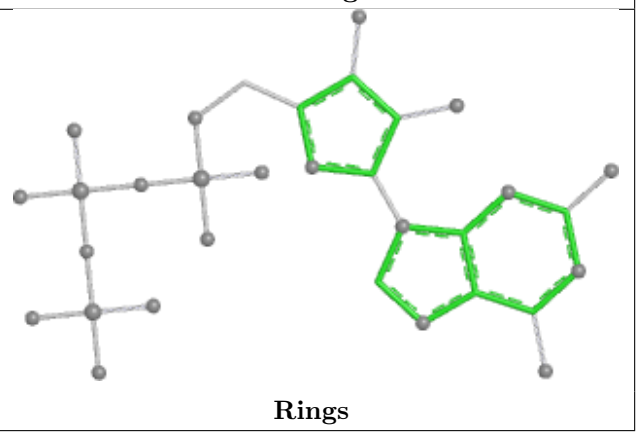
Bond lengths



Bond angles

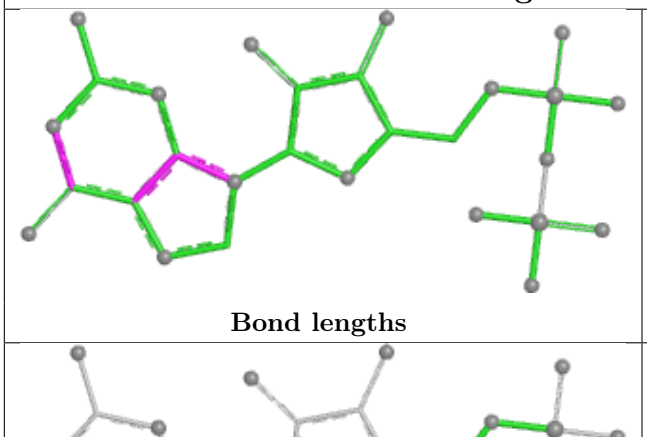


Torsions

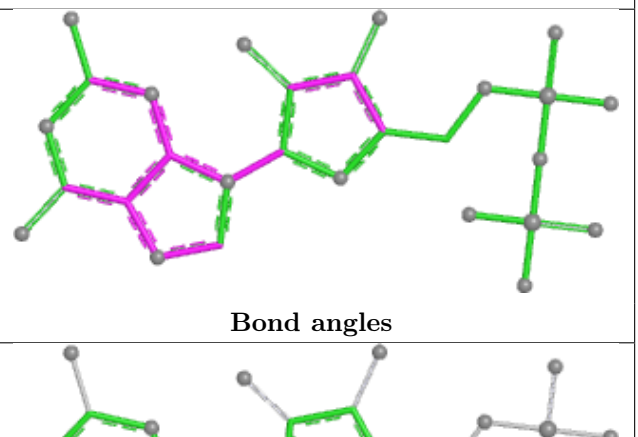


Rings

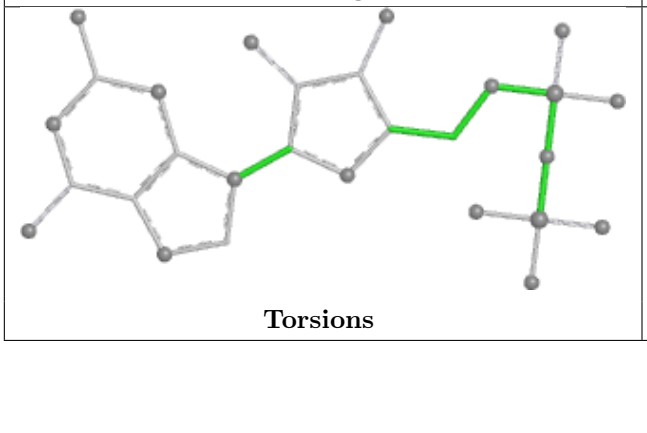
Ligand GDP JF 502



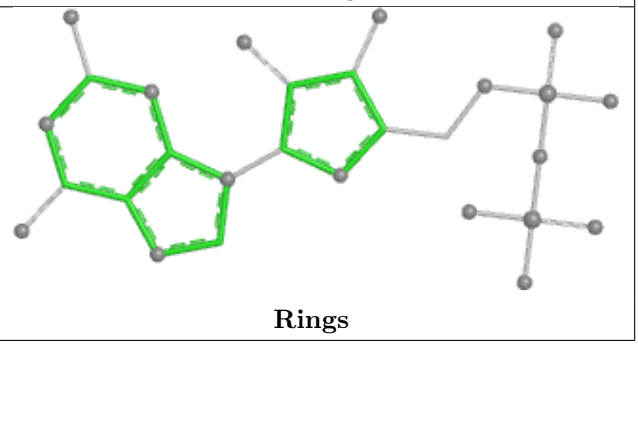
Bond lengths



Bond angles

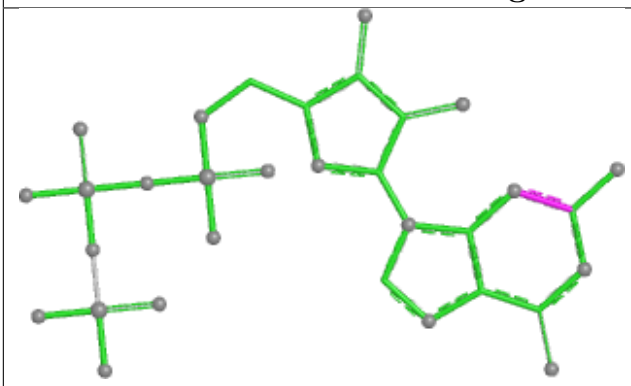


Torsions

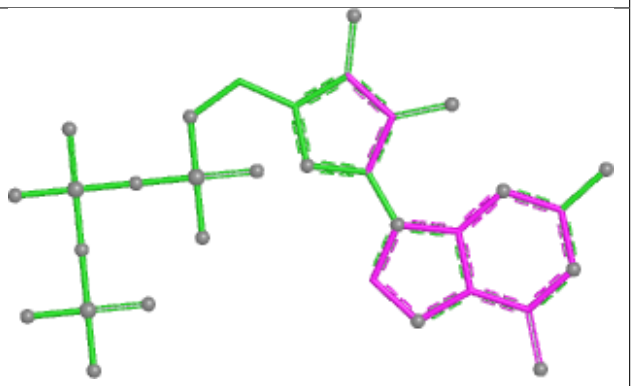


Rings

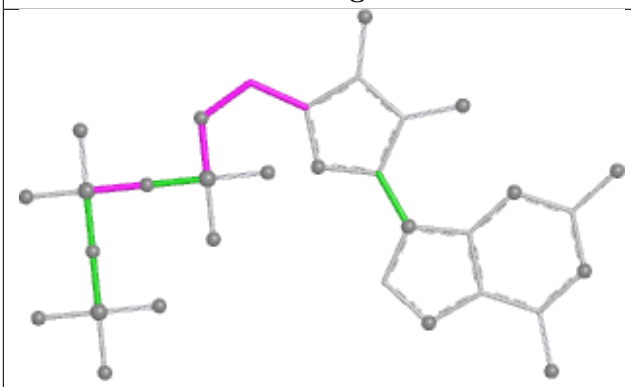
Ligand GTP VG 501



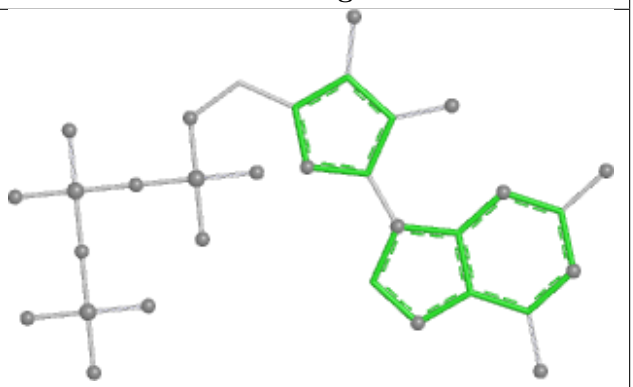
Bond lengths



Bond angles

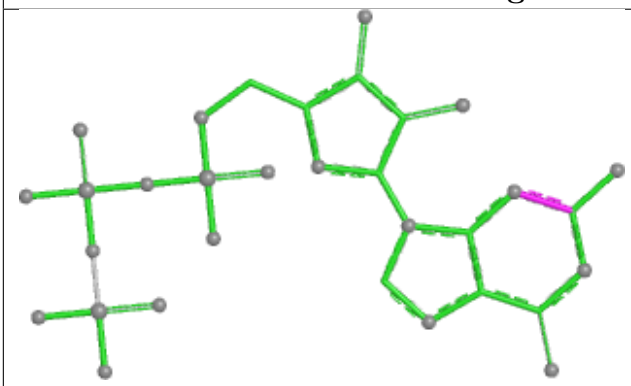


Torsions

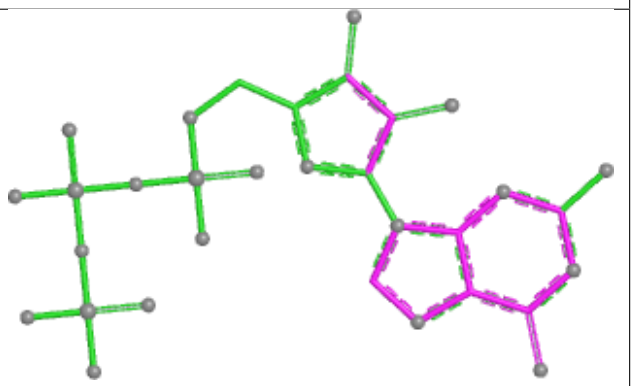


Rings

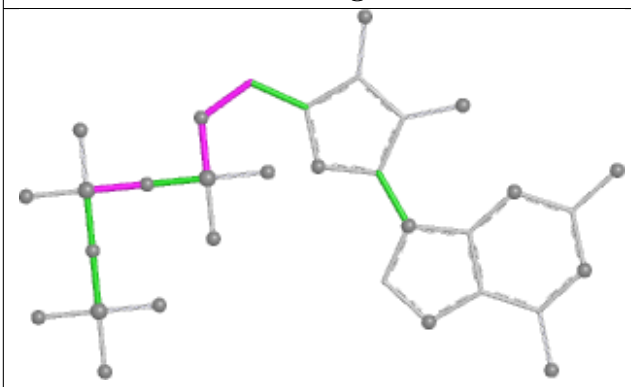
Ligand GTP GG 501



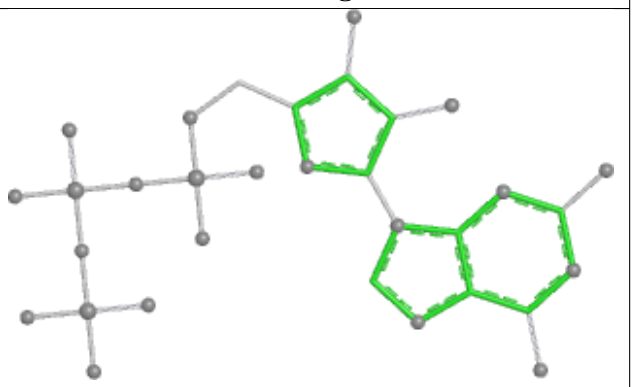
Bond lengths



Bond angles

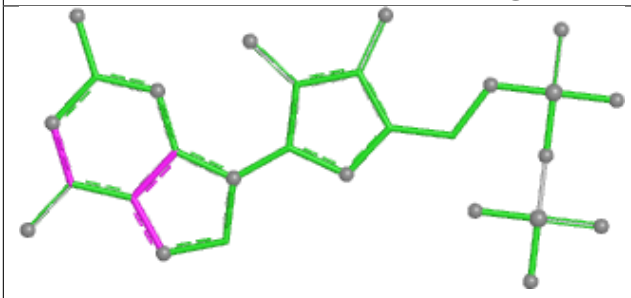


Torsions

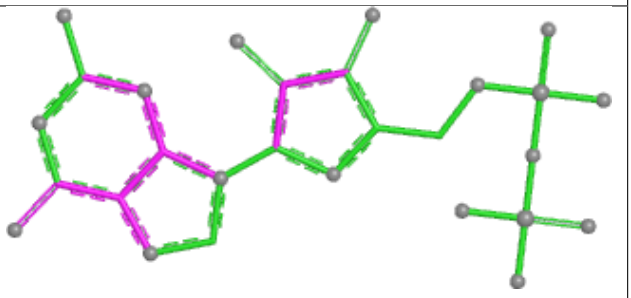


Rings

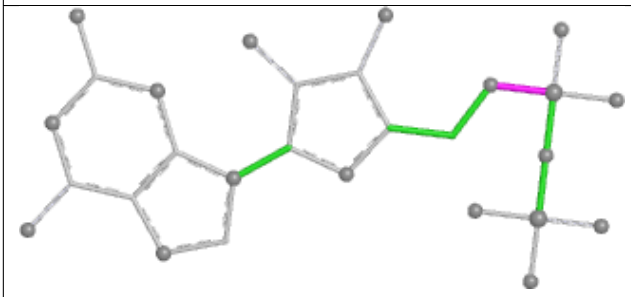
Ligand GDP AD 502



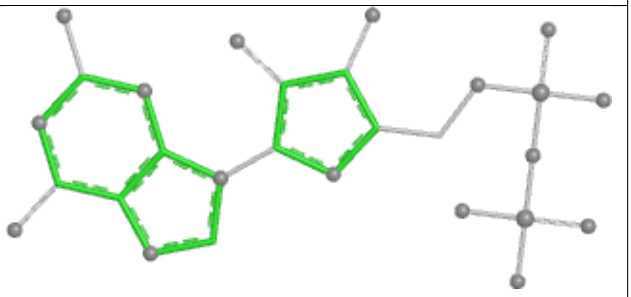
Bond lengths



Bond angles

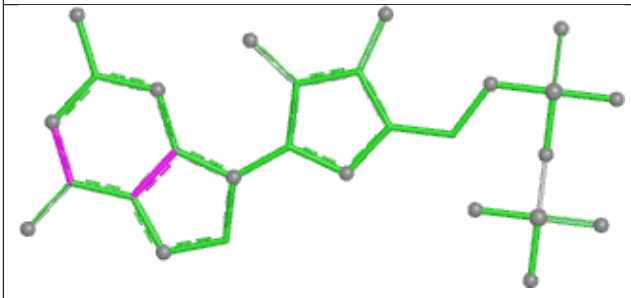


Torsions

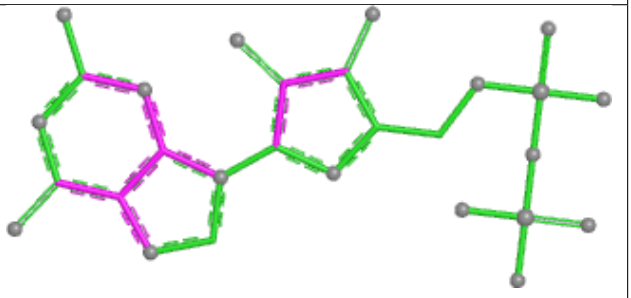


Rings

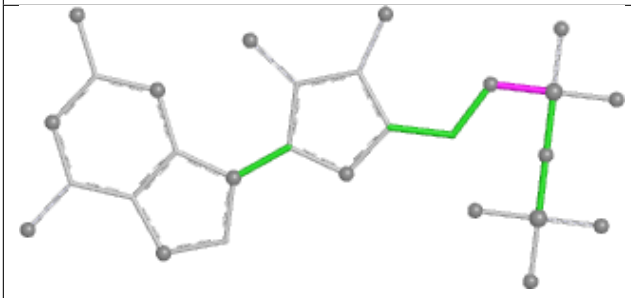
Ligand GDP TN 502



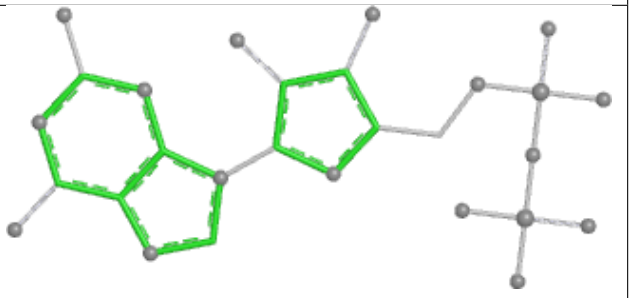
Bond lengths



Bond angles

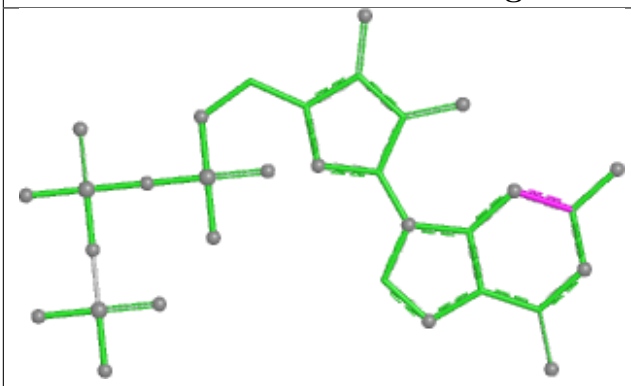


Torsions

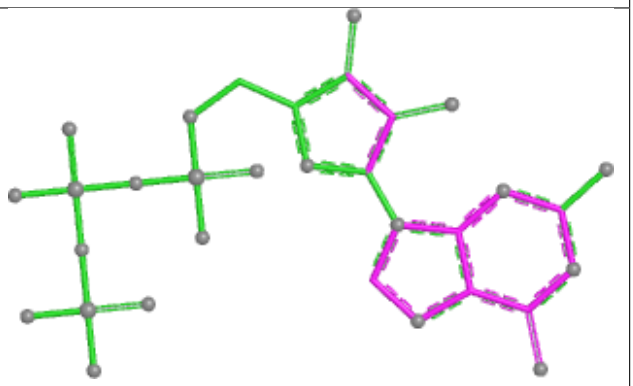


Rings

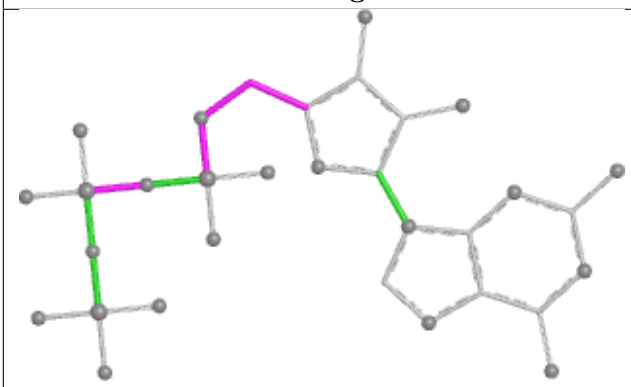
Ligand GTP MA 501



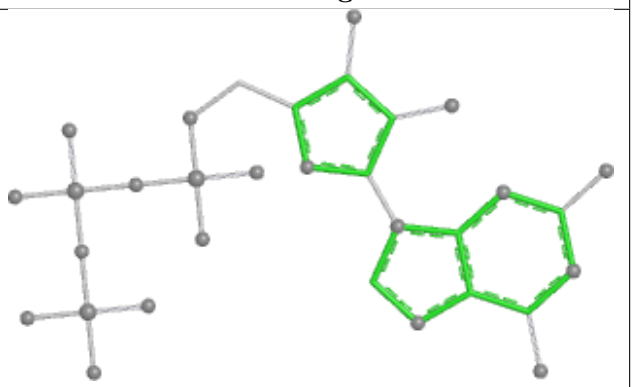
Bond lengths



Bond angles

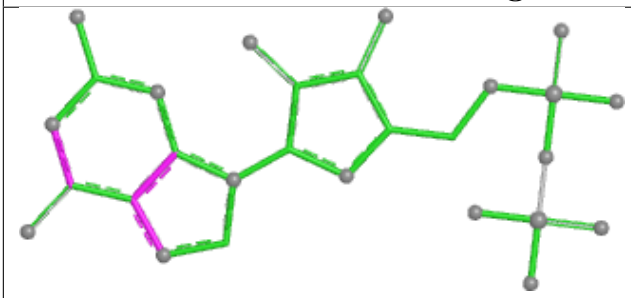


Torsions

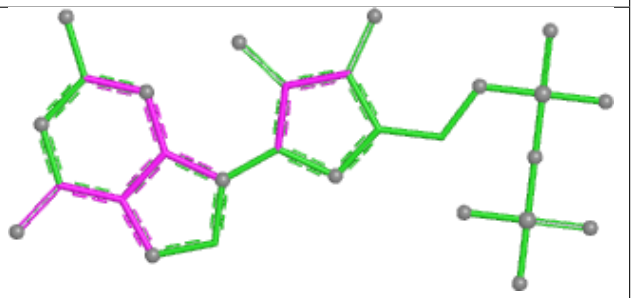


Rings

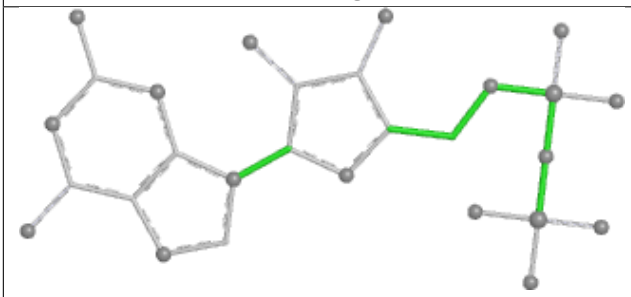
Ligand GDP AN 502



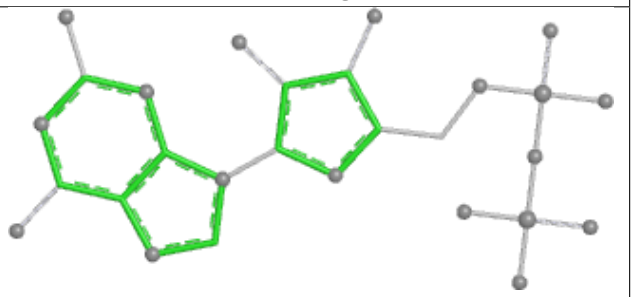
Bond lengths



Bond angles

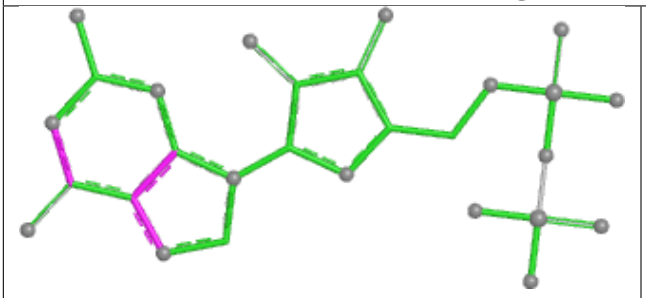


Torsions

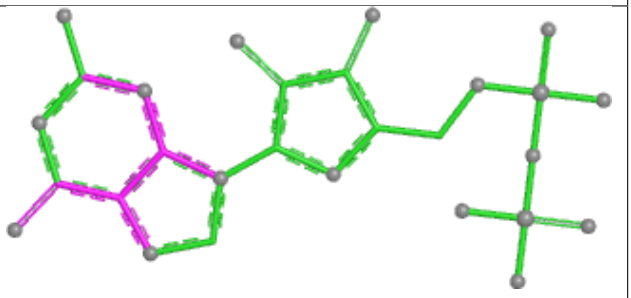


Rings

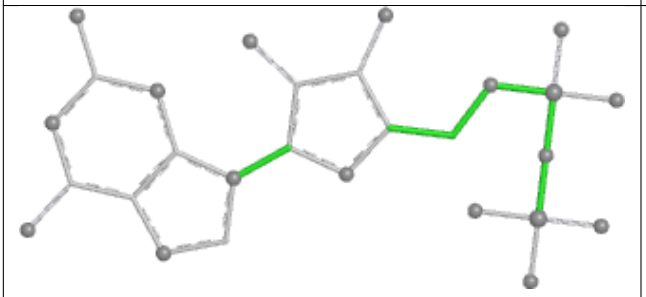
Ligand GDP JP 502



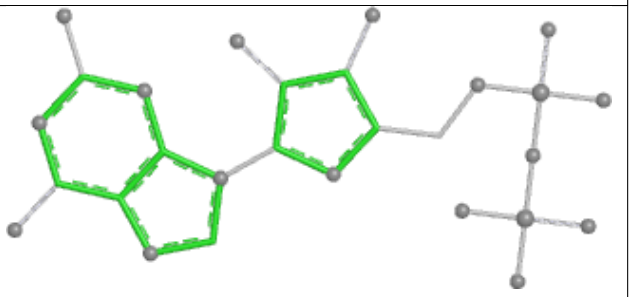
Bond lengths



Bond angles

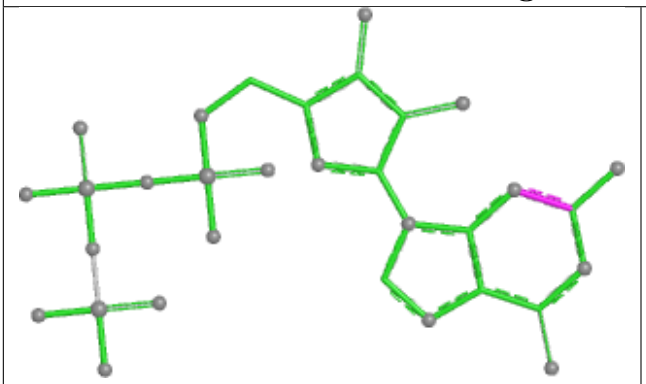


Torsions

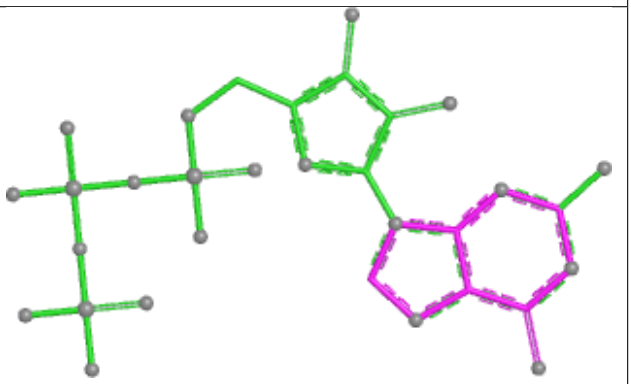


Rings

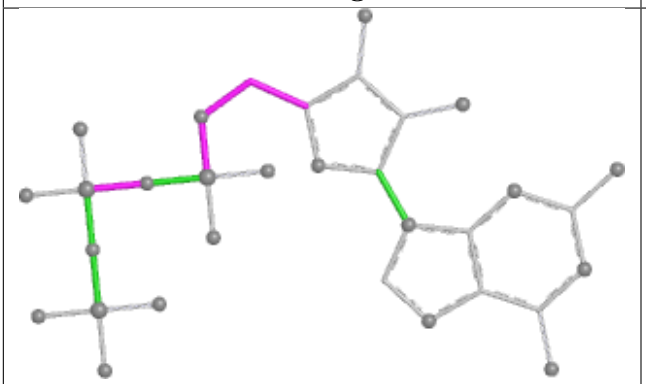
Ligand GTP FI 501



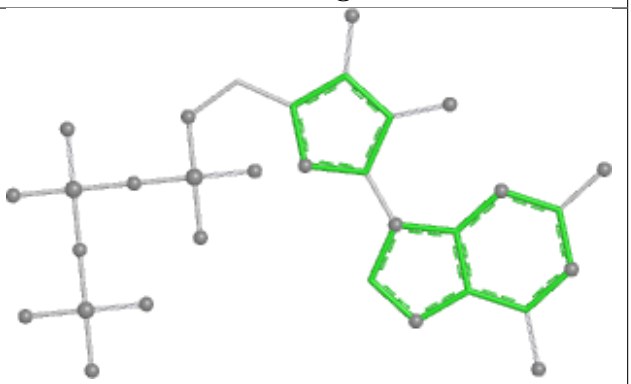
Bond lengths



Bond angles

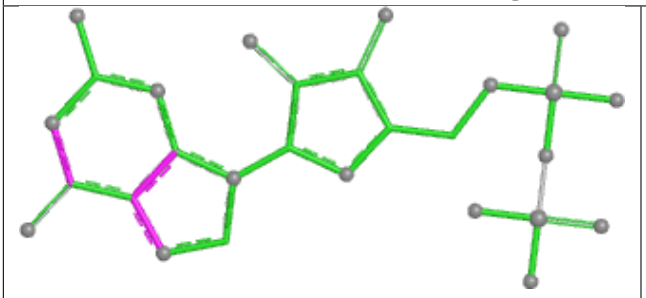


Torsions

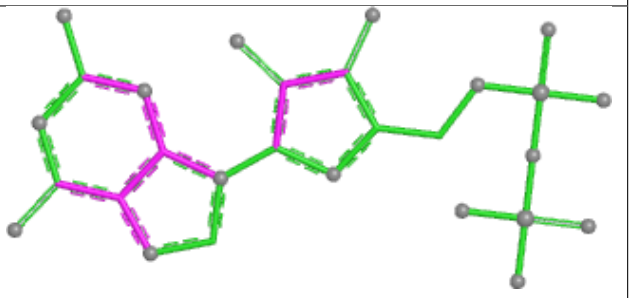


Rings

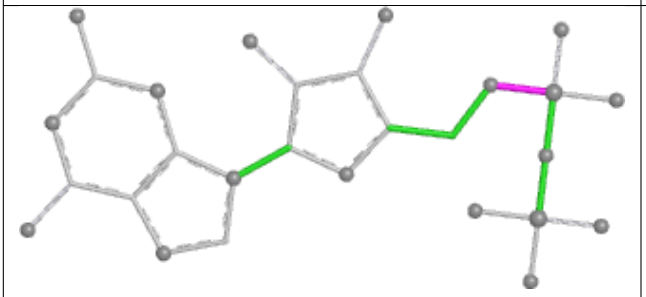
Ligand GDP UH 502



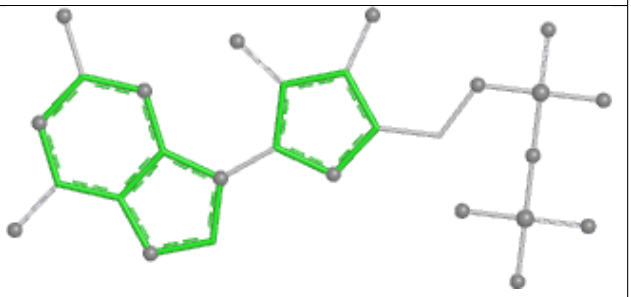
Bond lengths



Bond angles

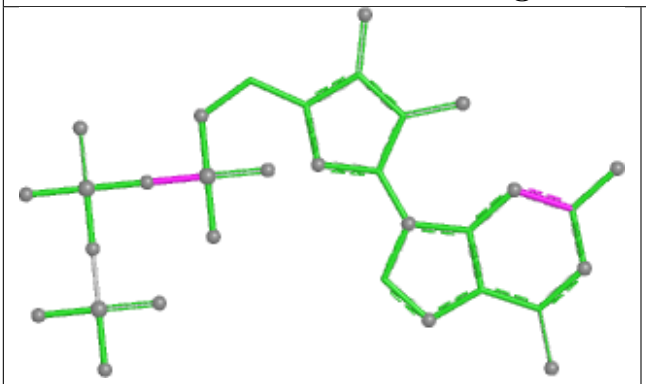


Torsions

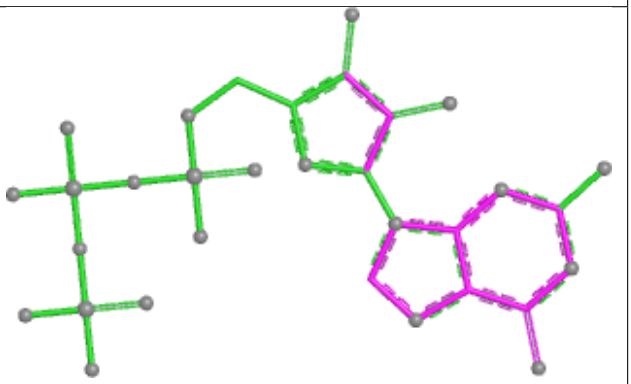


Rings

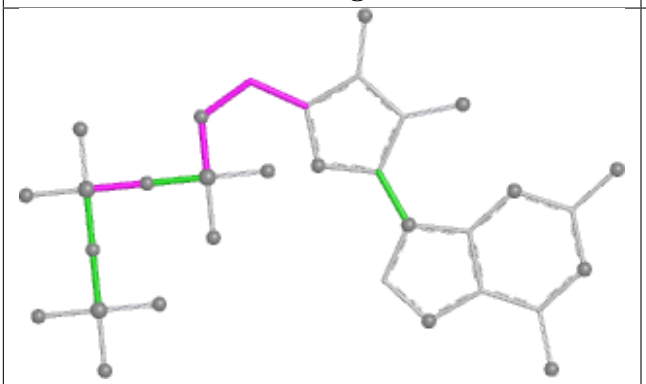
Ligand GTP JC 501



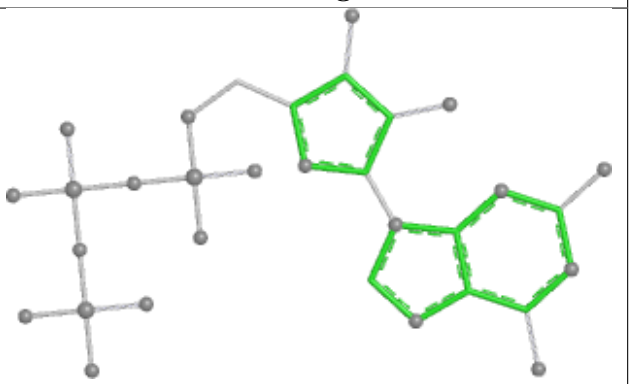
Bond lengths



Bond angles

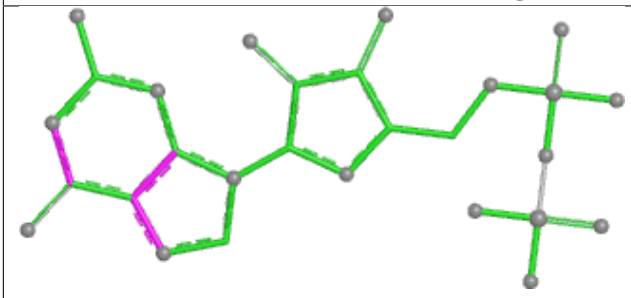


Torsions

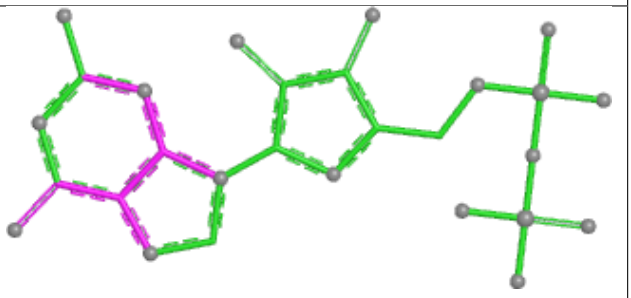


Rings

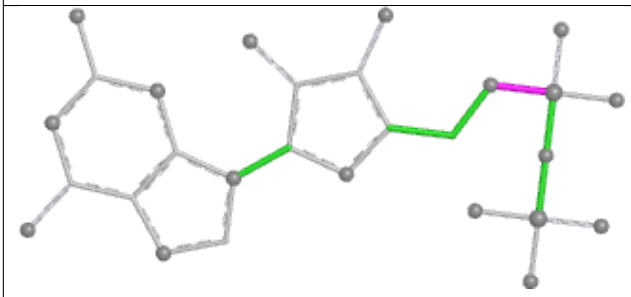
Ligand GDP BL 502



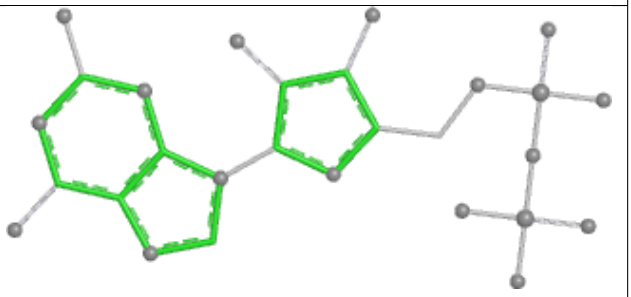
Bond lengths



Bond angles

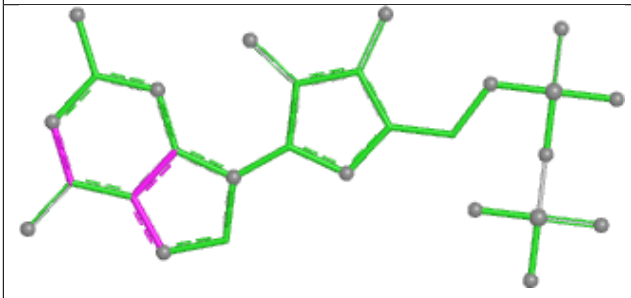


Torsions

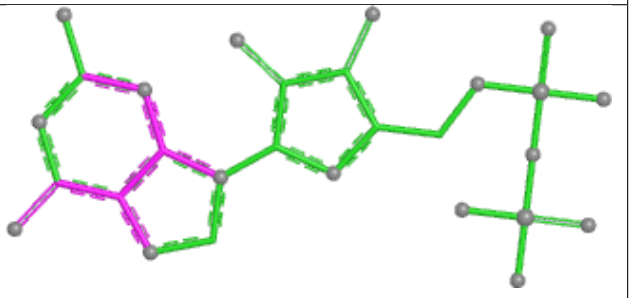


Rings

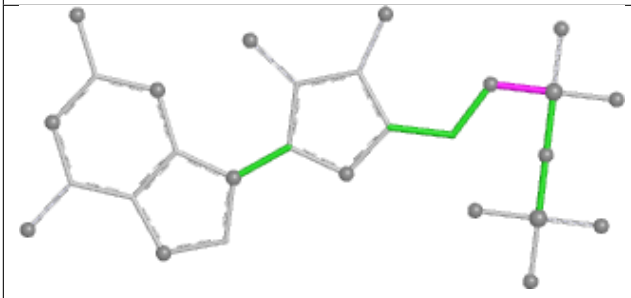
Ligand GDP NL 502



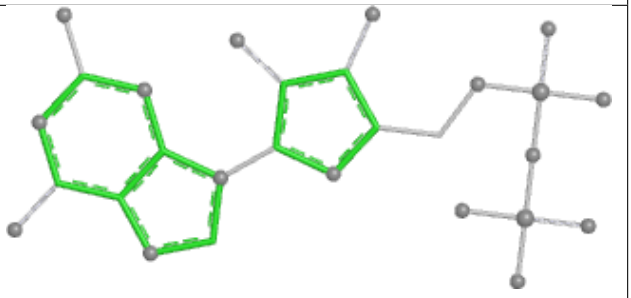
Bond lengths



Bond angles

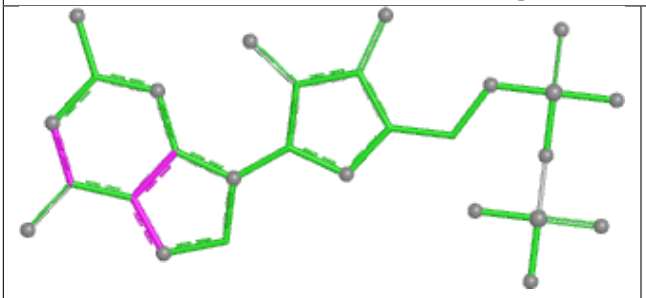


Torsions

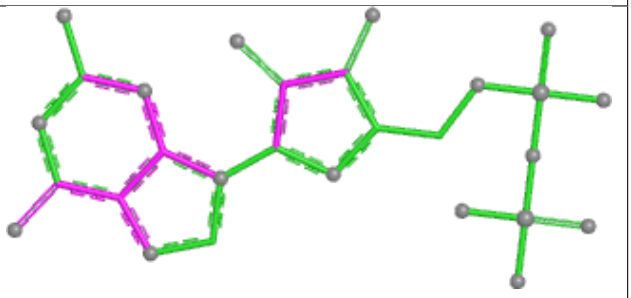


Rings

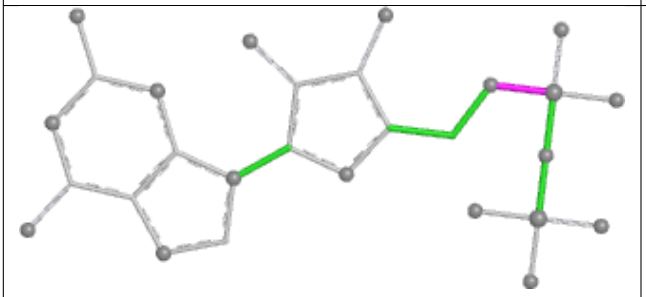
Ligand GDP CJ 502



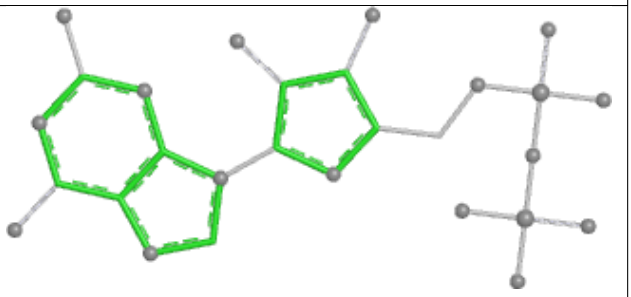
Bond lengths



Bond angles

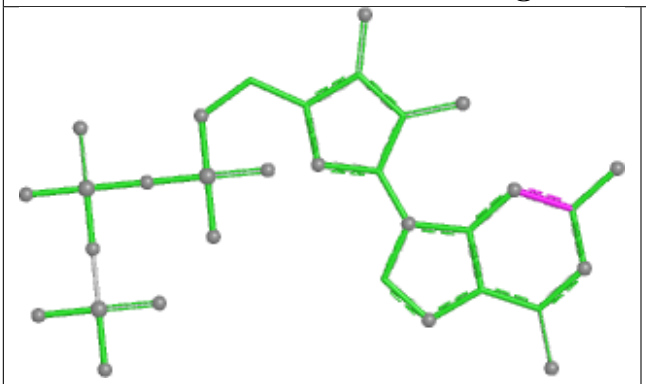


Torsions

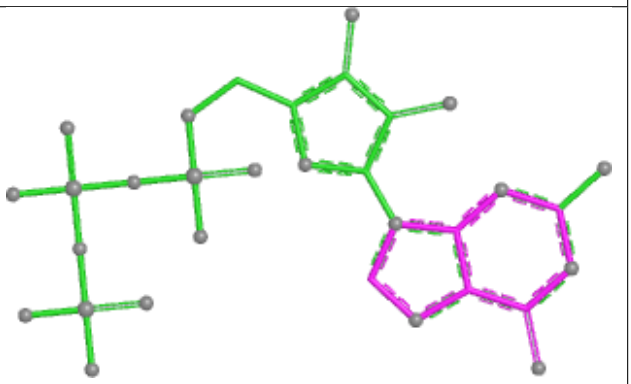


Rings

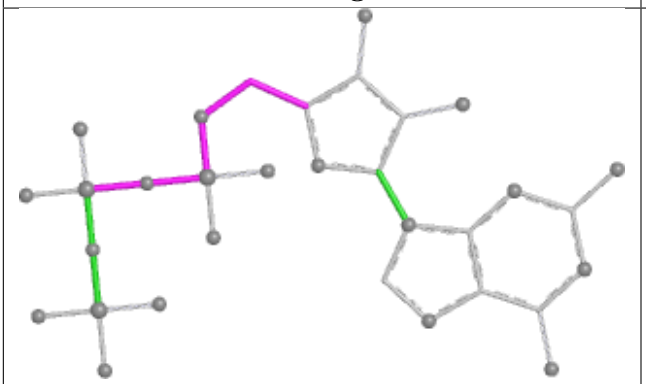
Ligand GTP HI 501



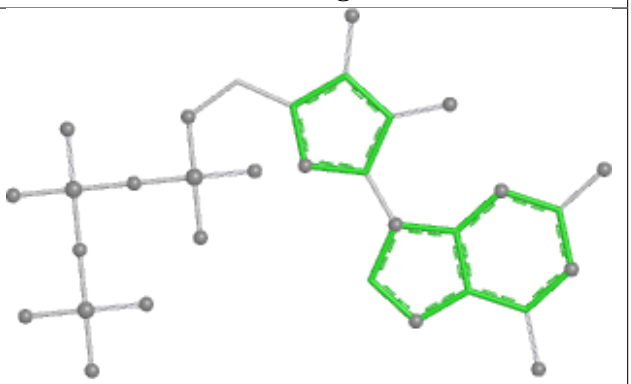
Bond lengths



Bond angles

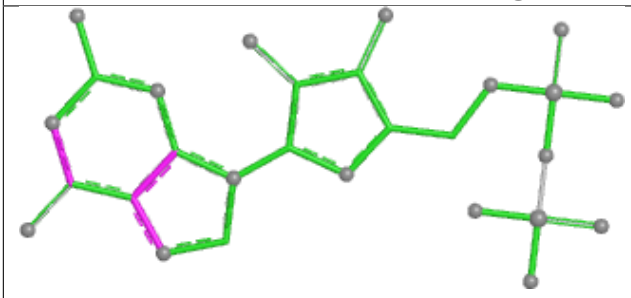


Torsions

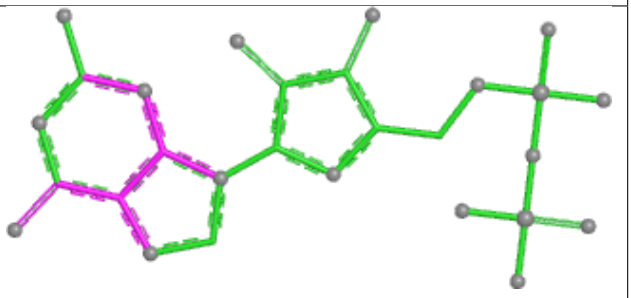


Rings

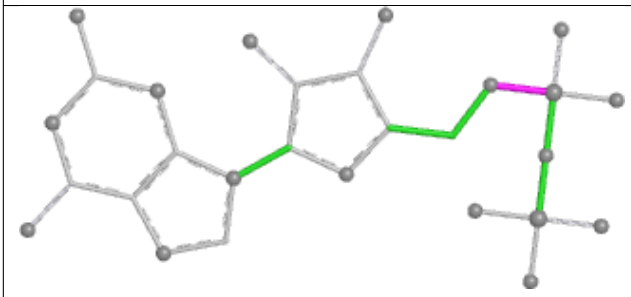
Ligand GDP HL 502



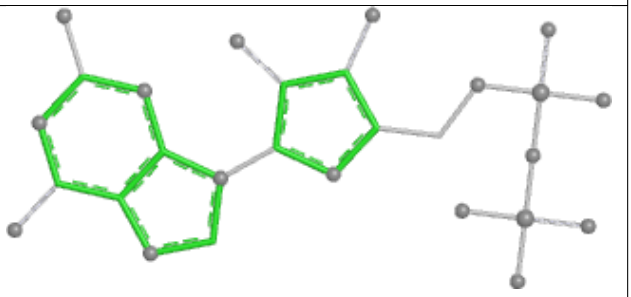
Bond lengths



Bond angles

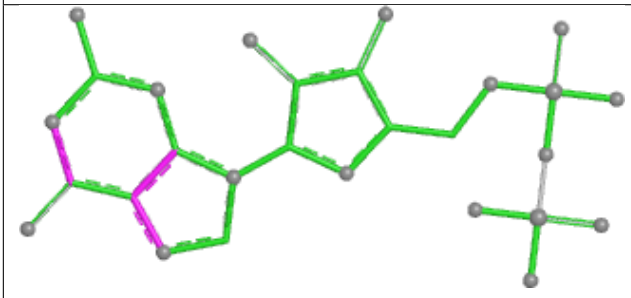


Torsions

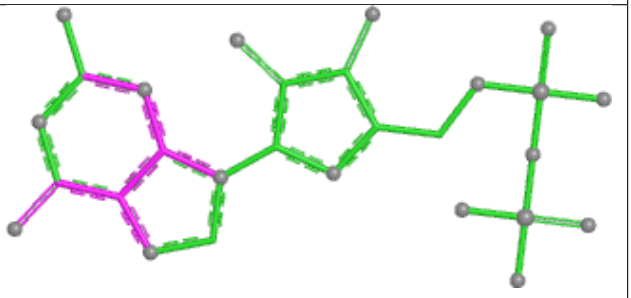


Rings

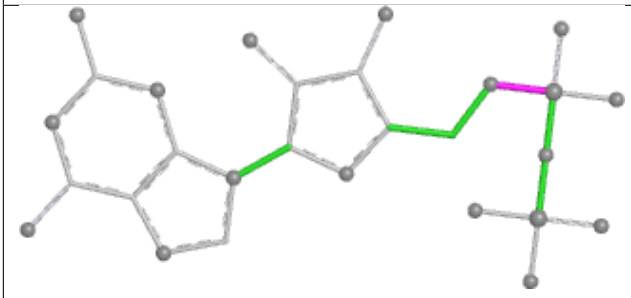
Ligand GDP CL 502



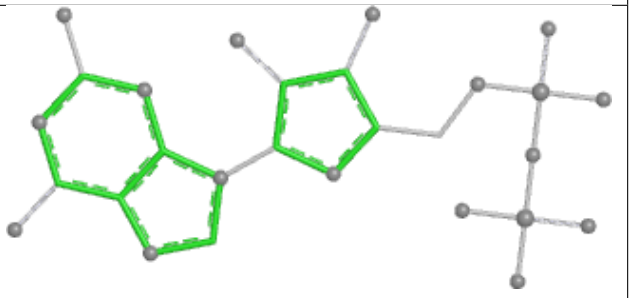
Bond lengths



Bond angles

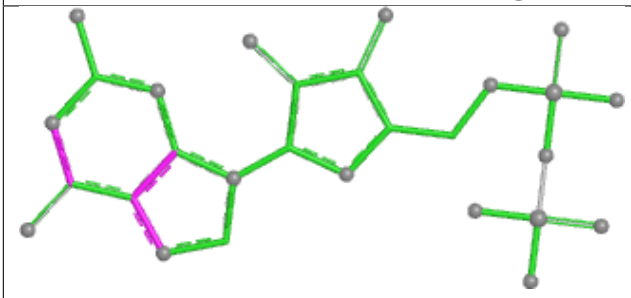


Torsions

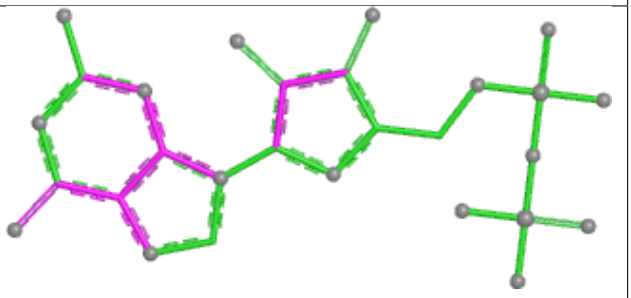


Rings

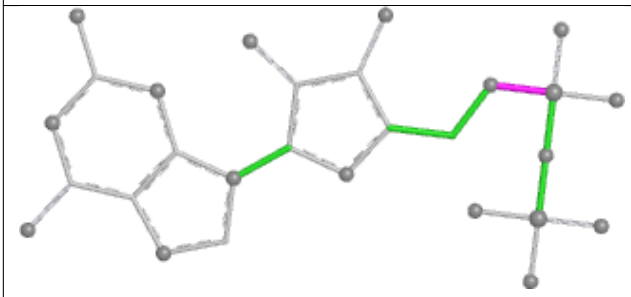
Ligand GDP AL 502



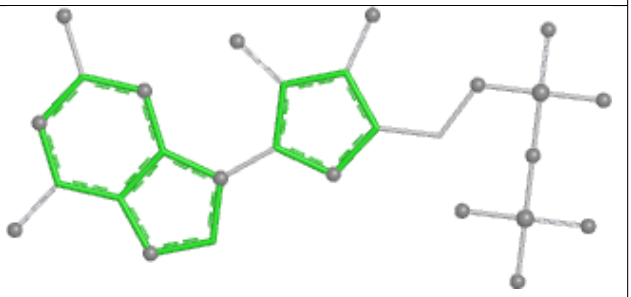
Bond lengths



Bond angles

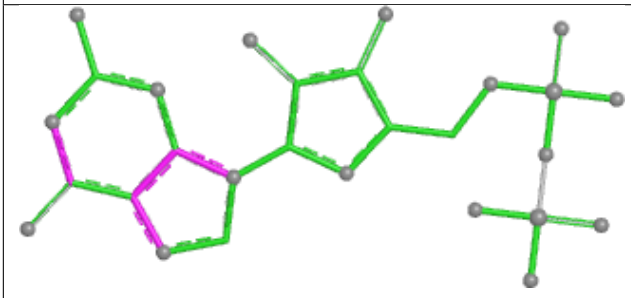


Torsions

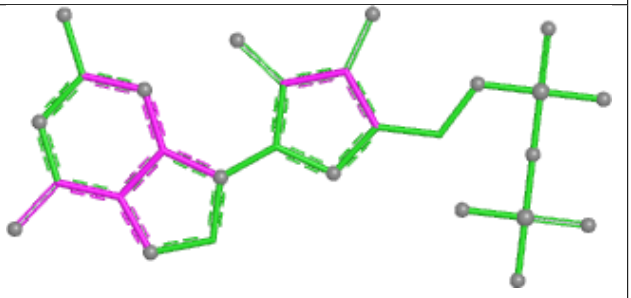


Rings

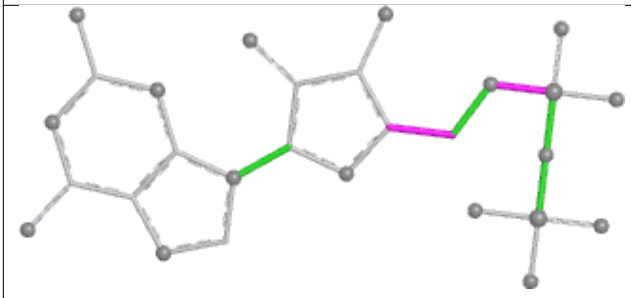
Ligand GDP ML 502



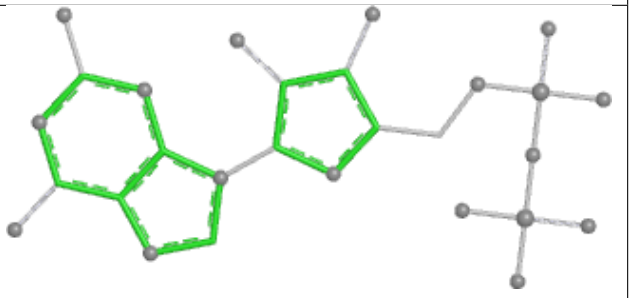
Bond lengths



Bond angles

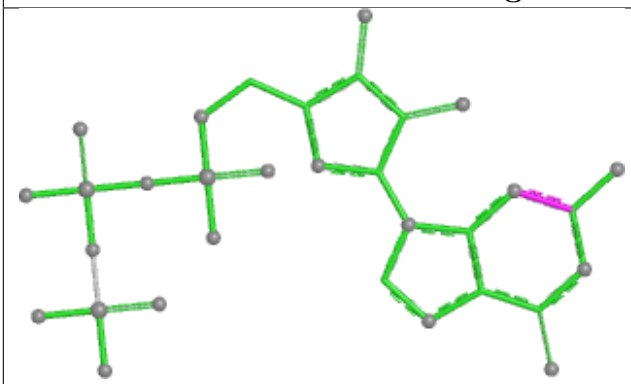


Torsions

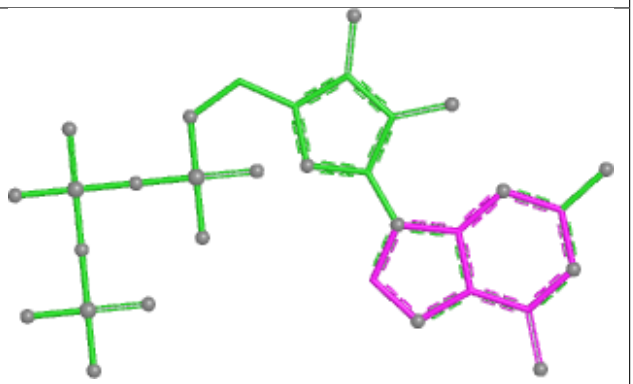


Rings

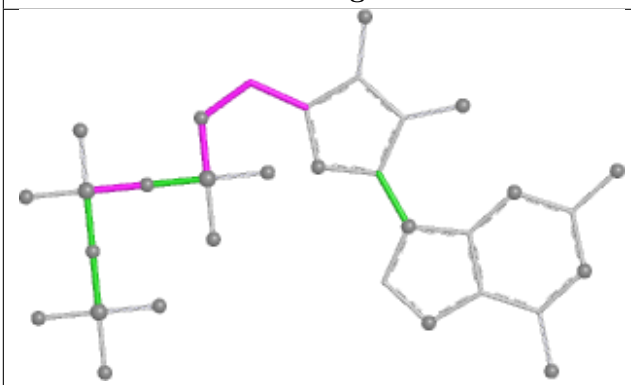
Ligand GTP HM 501



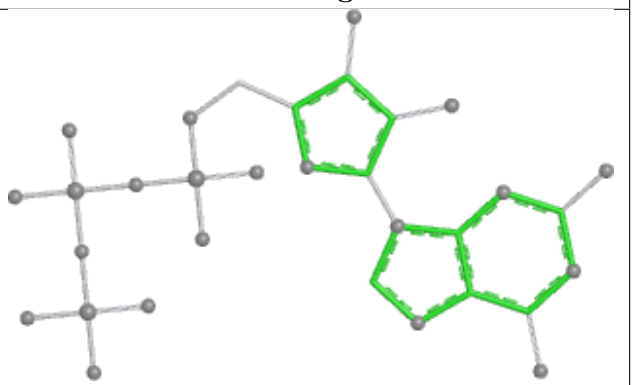
Bond lengths



Bond angles

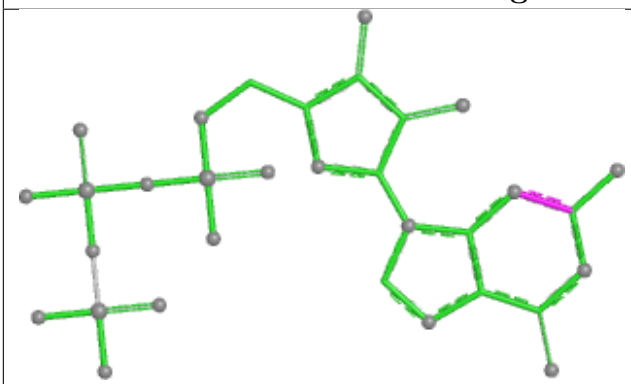


Torsions

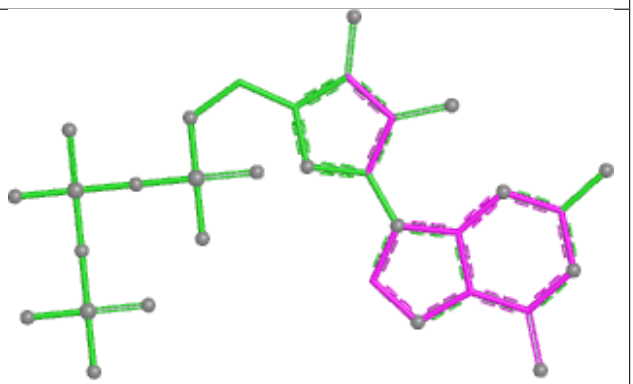


Rings

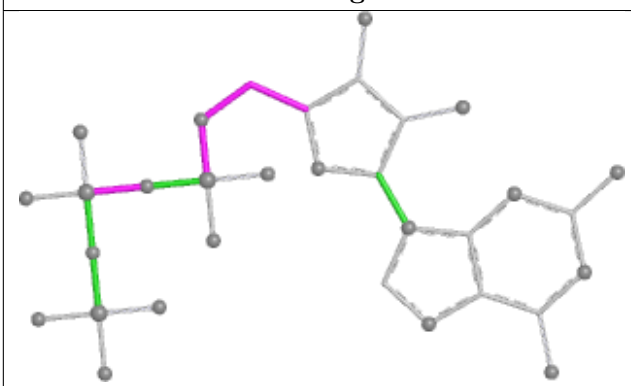
Ligand GTP TC 501



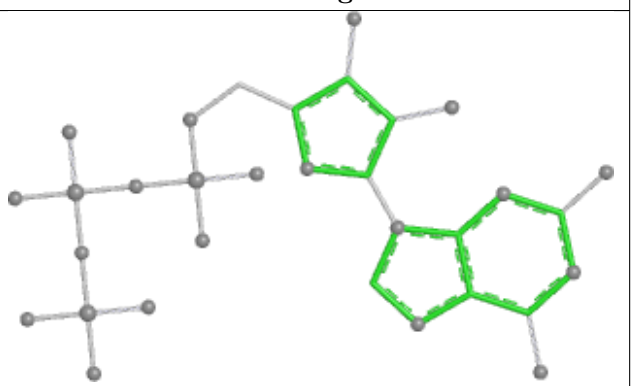
Bond lengths



Bond angles

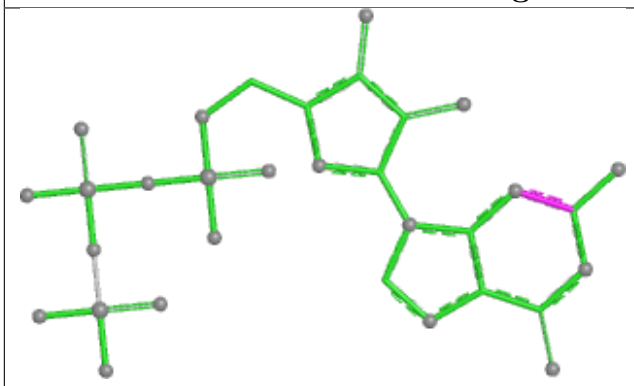


Torsions

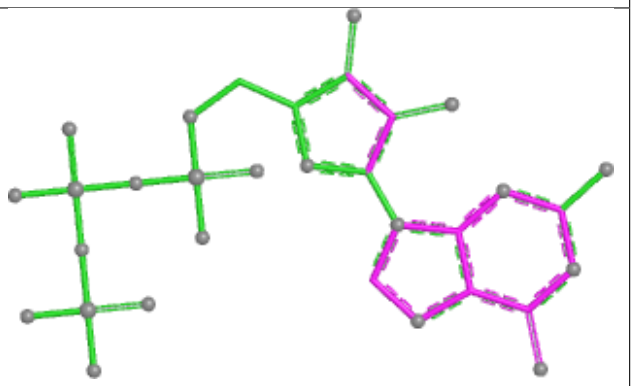


Rings

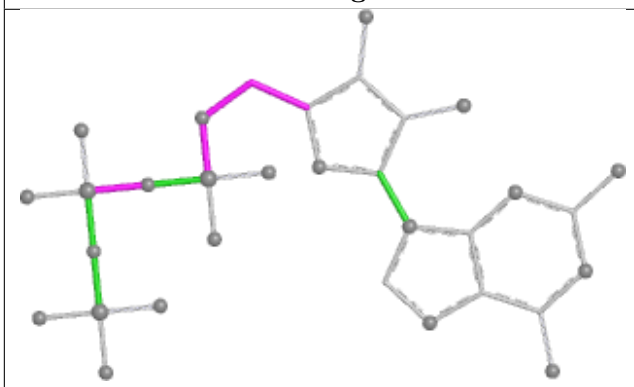
Ligand GTP CE 501



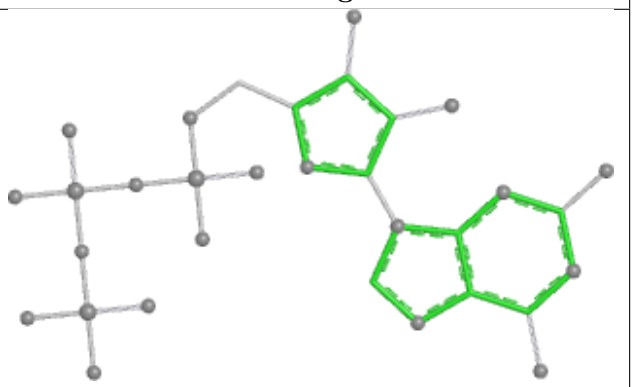
Bond lengths



Bond angles

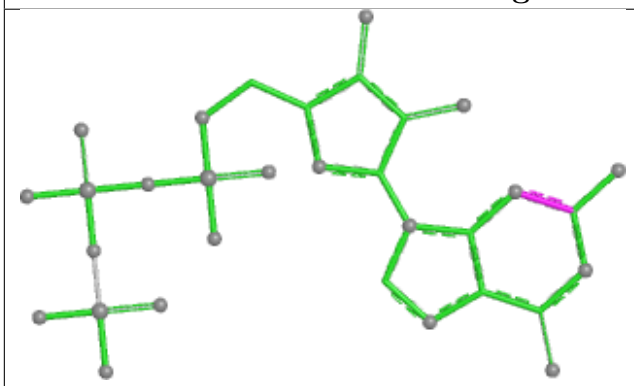


Torsions

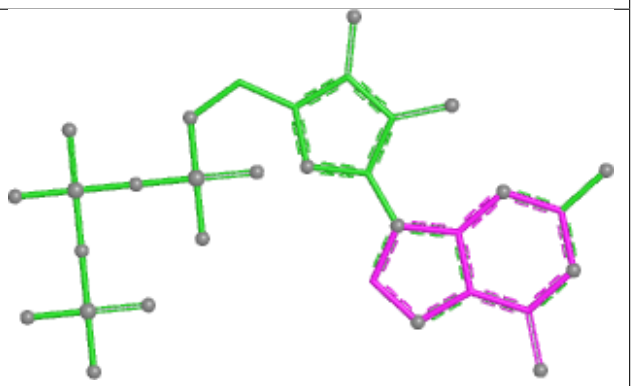


Rings

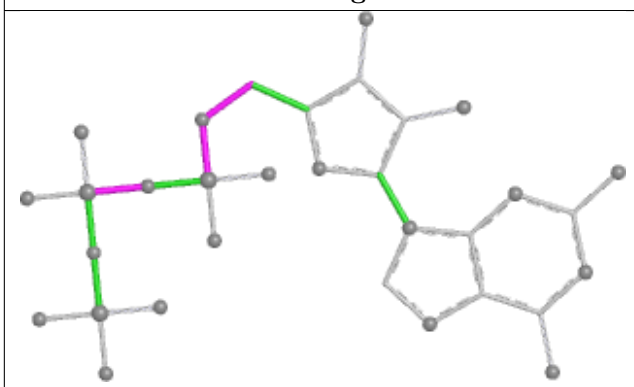
Ligand GTP LA 501



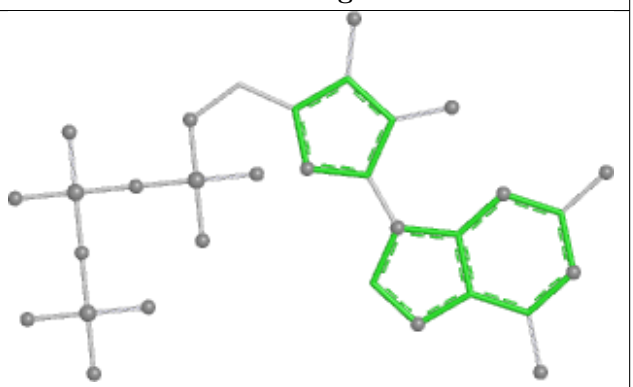
Bond lengths



Bond angles

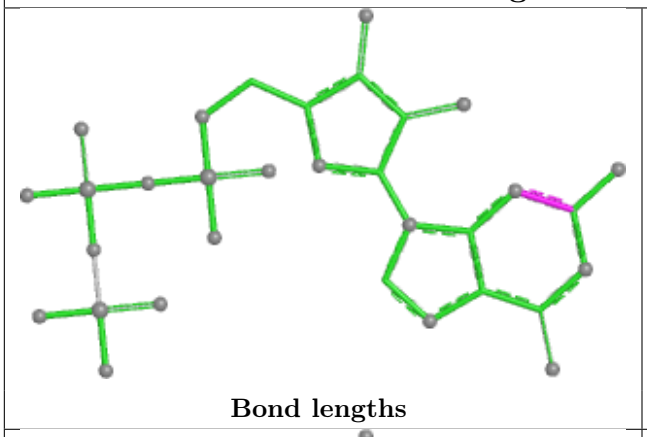


Torsions

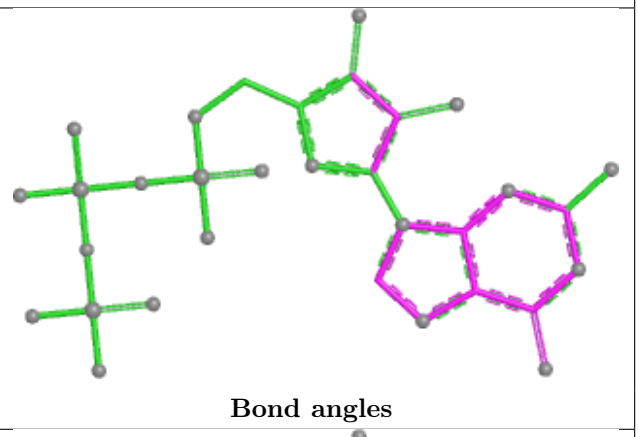


Rings

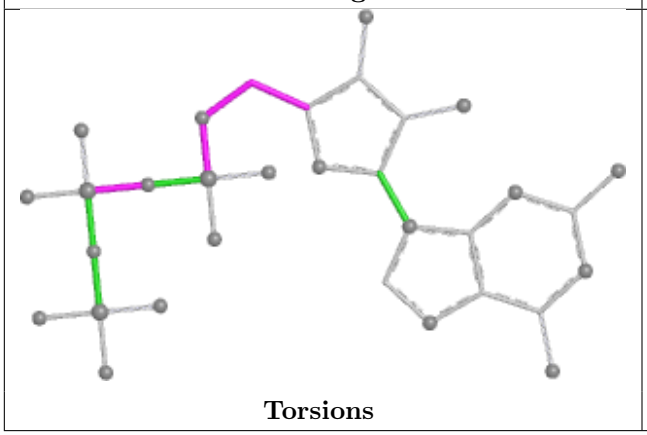
Ligand GTP UO 501



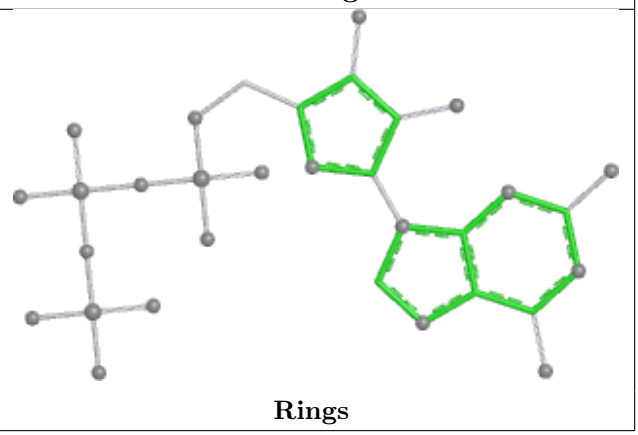
Bond lengths



Bond angles

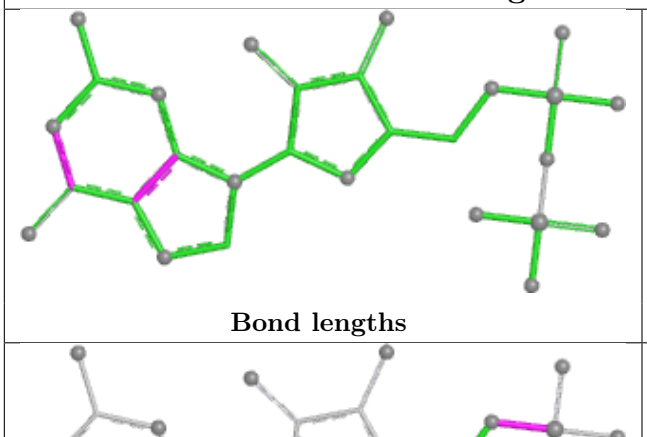


Torsions

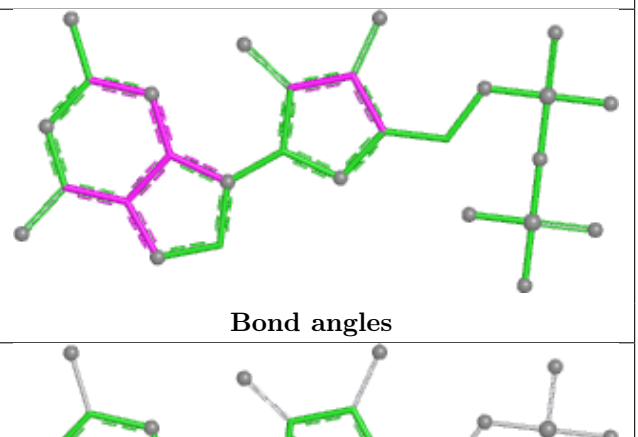


Rings

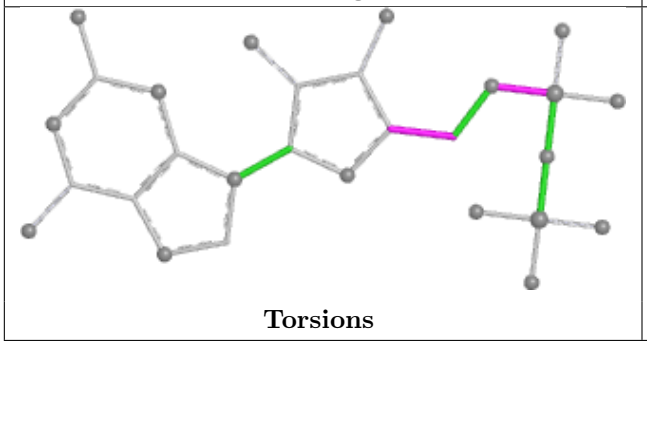
Ligand GDP ON 502



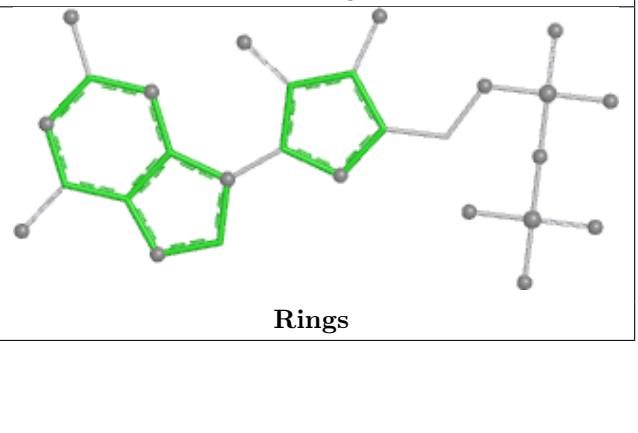
Bond lengths



Bond angles

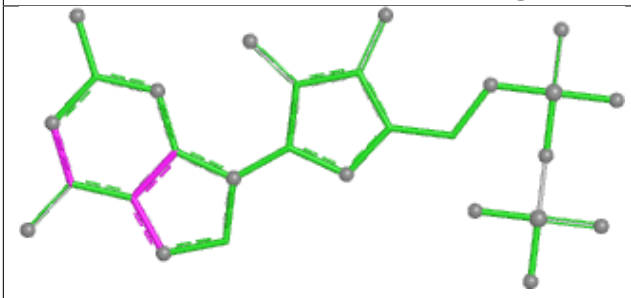


Torsions

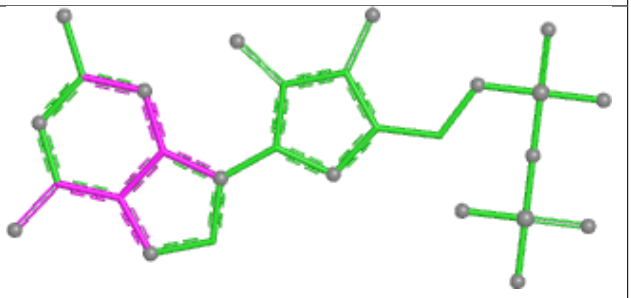


Rings

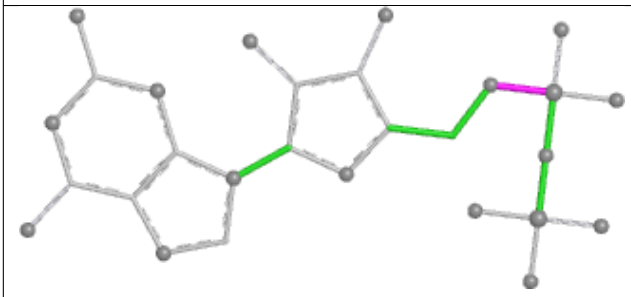
Ligand GDP EL 502



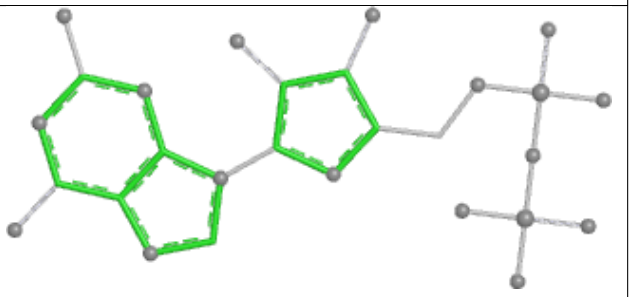
Bond lengths



Bond angles

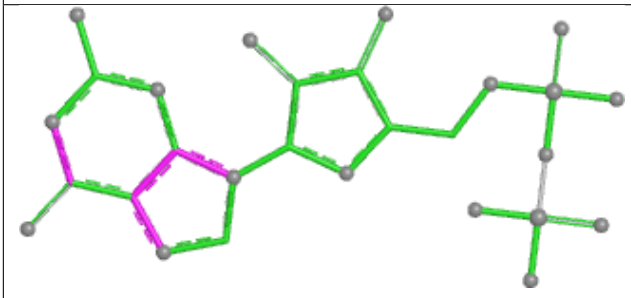


Torsions

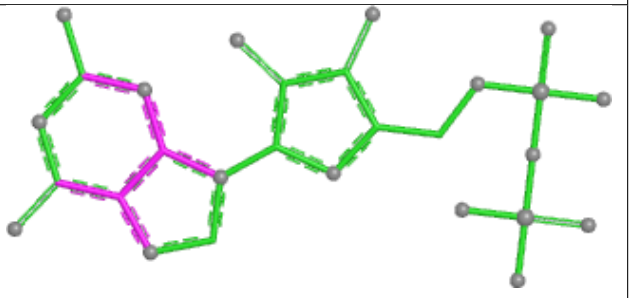


Rings

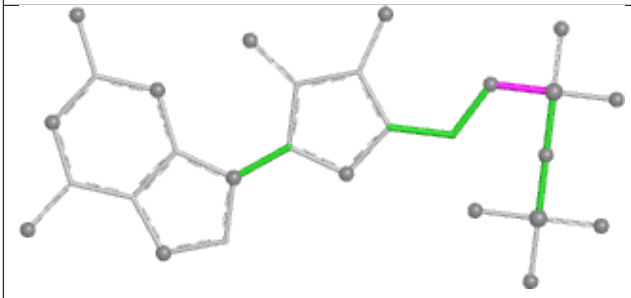
Ligand GDP JJ 502



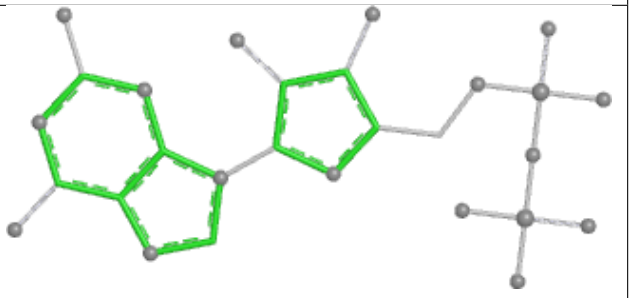
Bond lengths



Bond angles

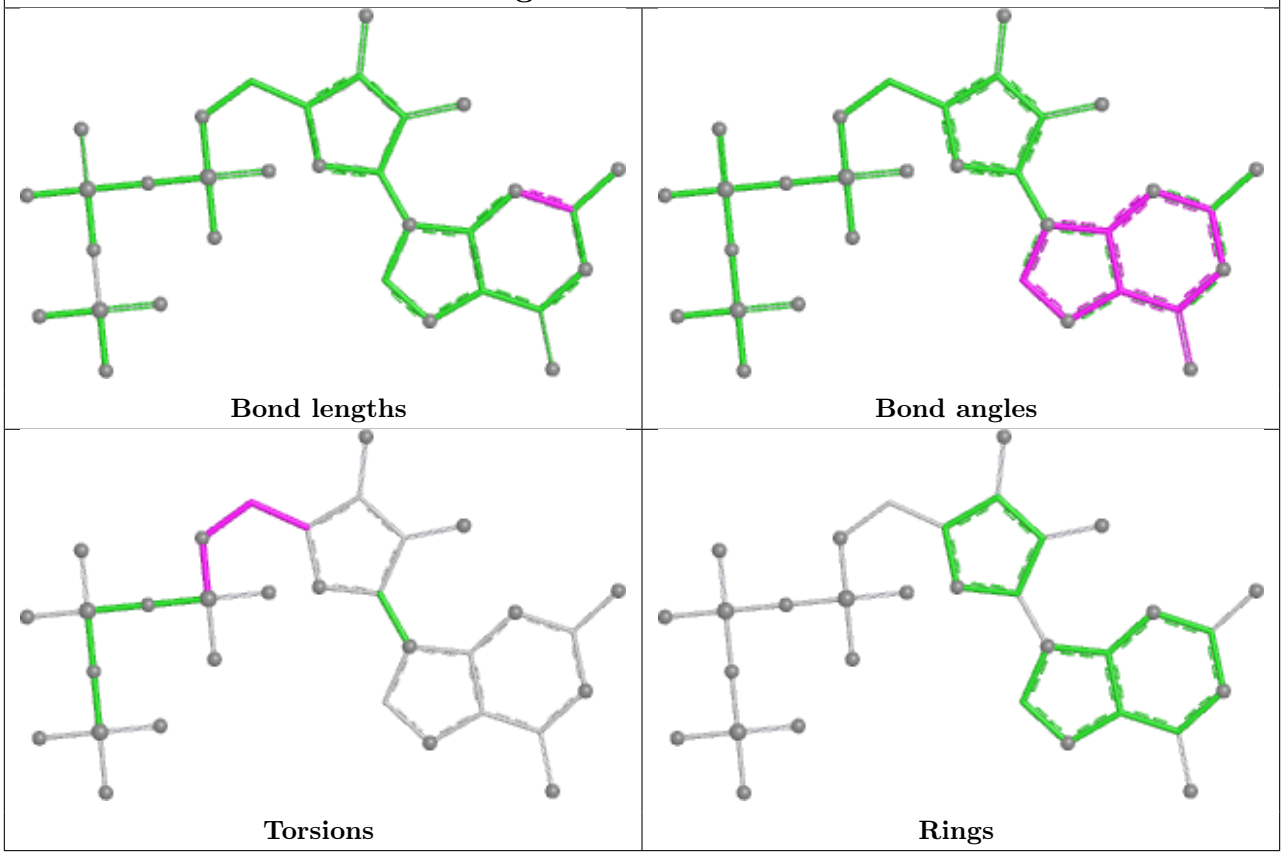


Torsions

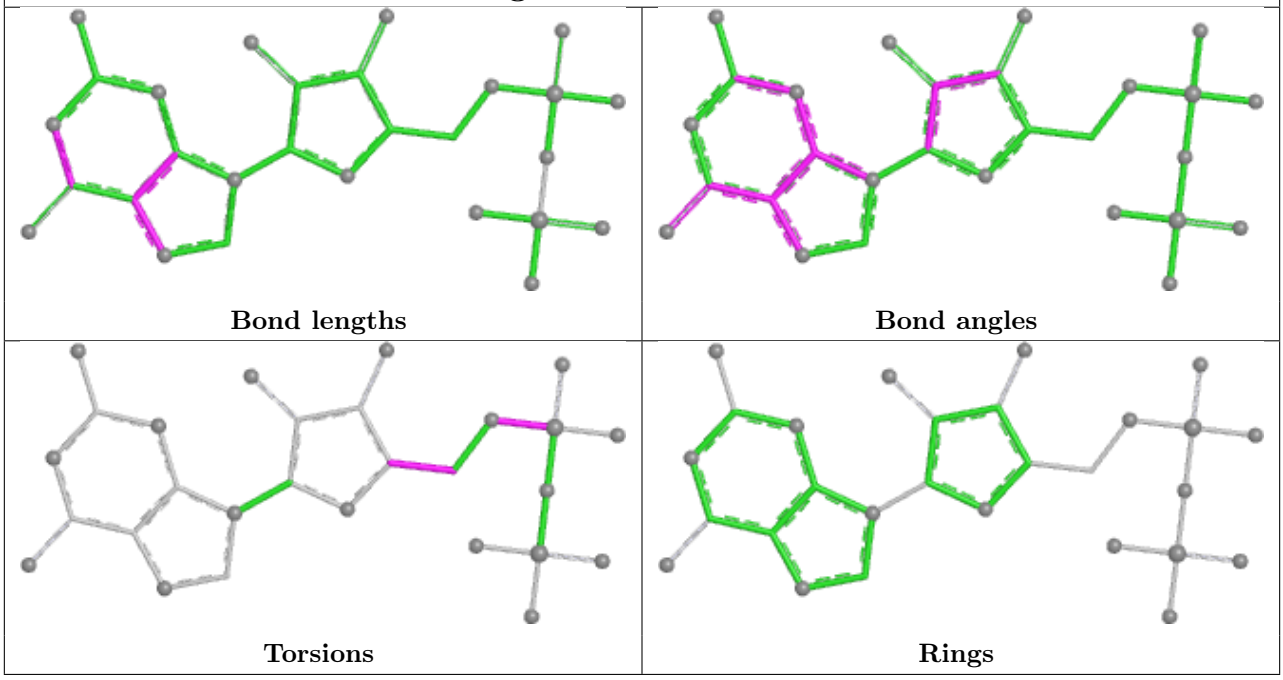


Rings

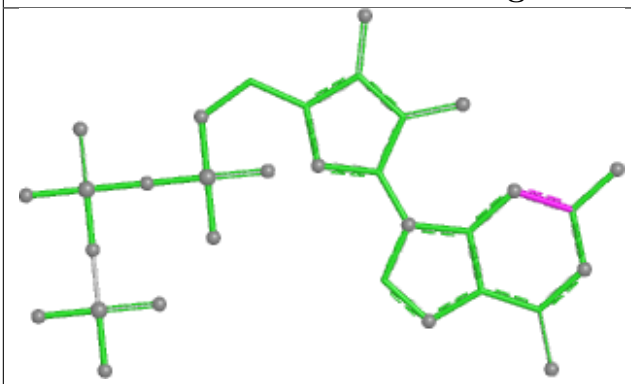
Ligand GTP JE 501



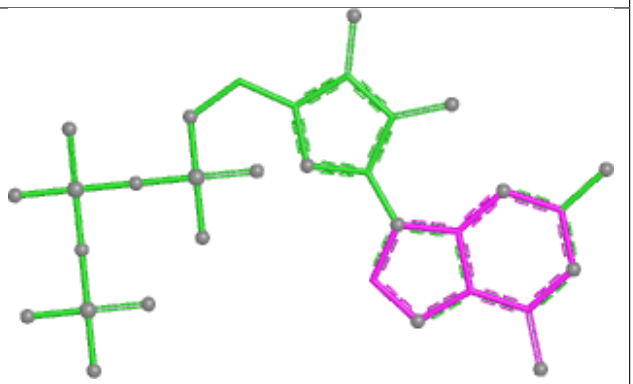
Ligand GDP VB 502



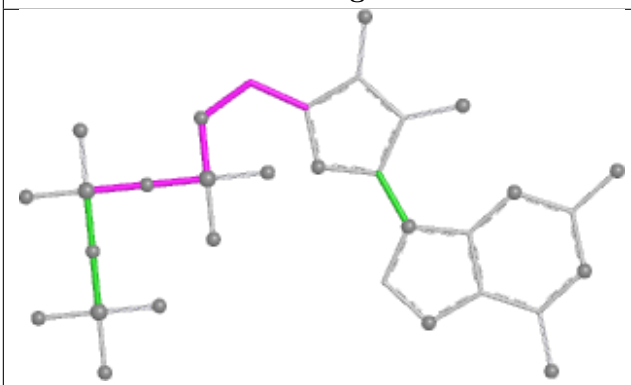
Ligand GTP HG 501



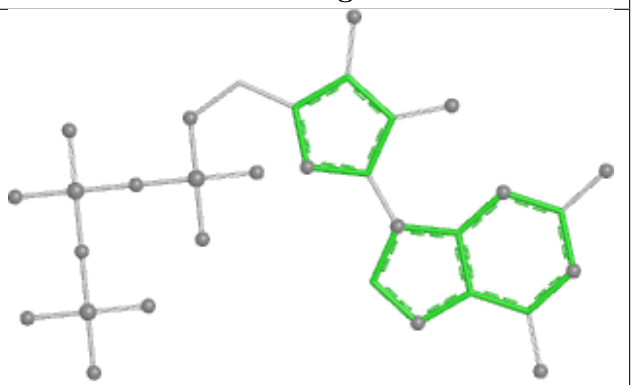
Bond lengths



Bond angles

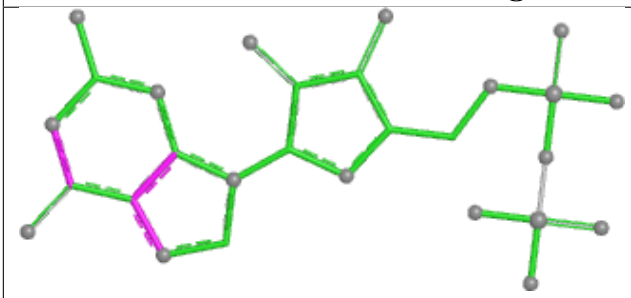


Torsions

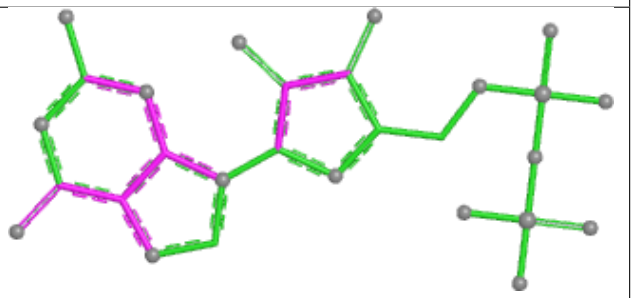


Rings

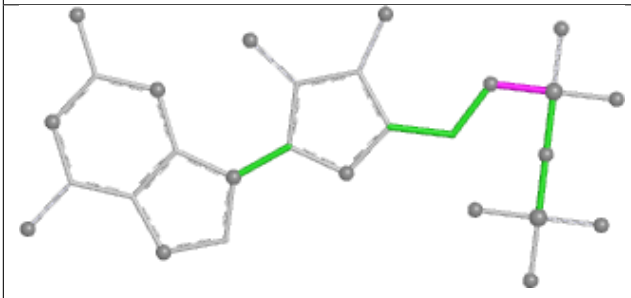
Ligand GDP NB 502



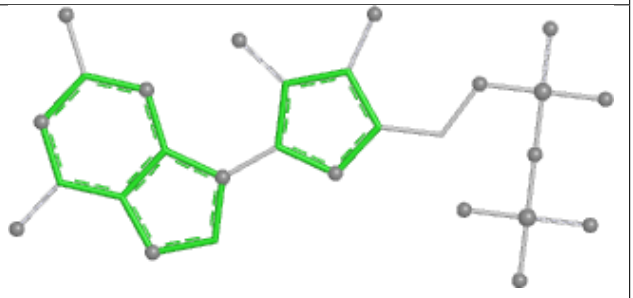
Bond lengths



Bond angles

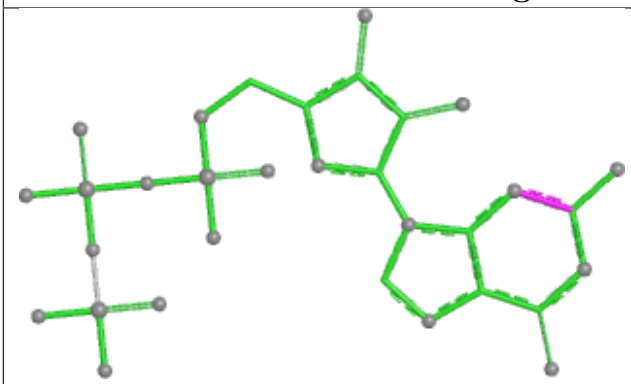


Torsions

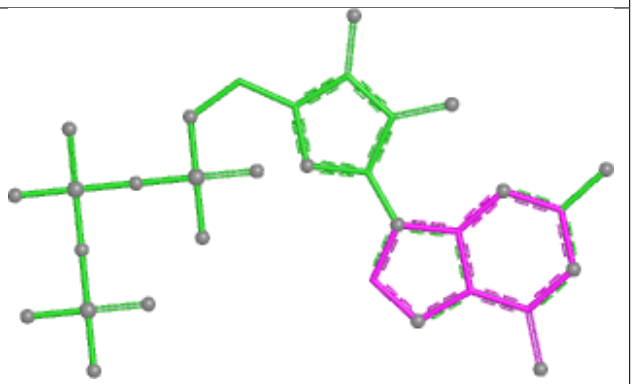


Rings

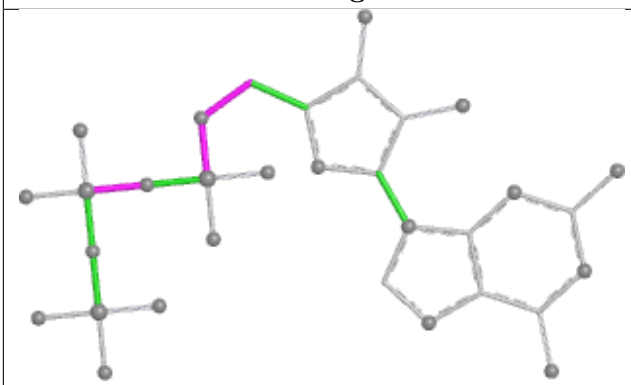
Ligand GTP LE 501



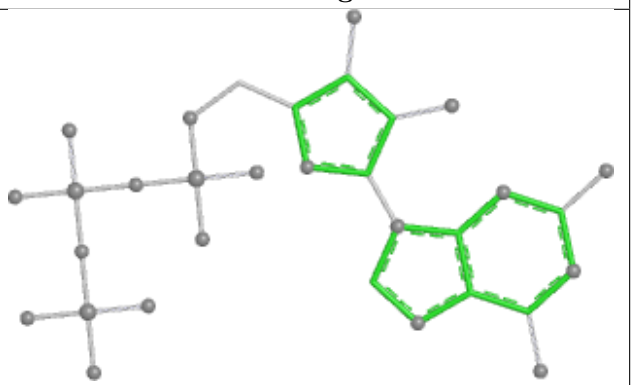
Bond lengths



Bond angles

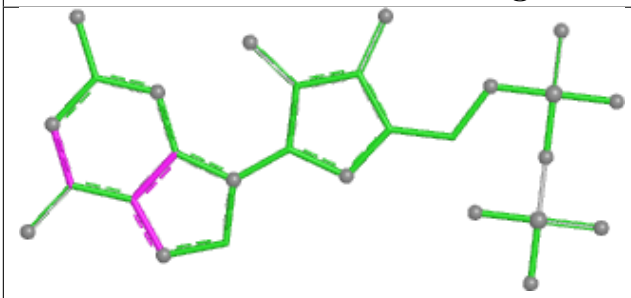


Torsions

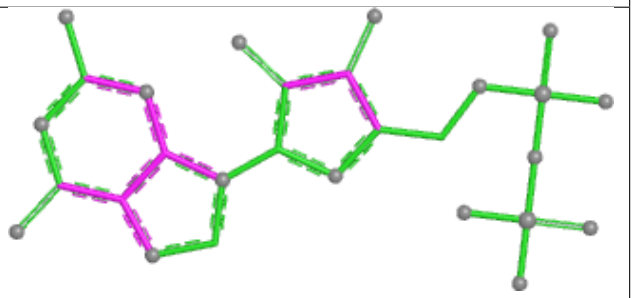


Rings

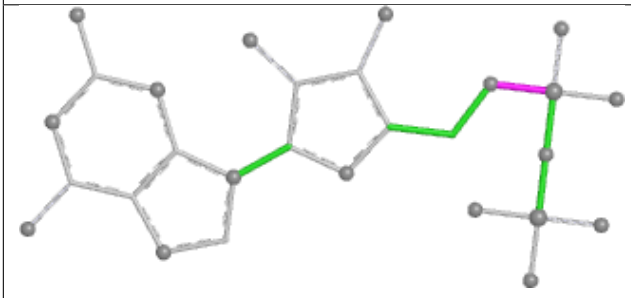
Ligand GDP JD 502



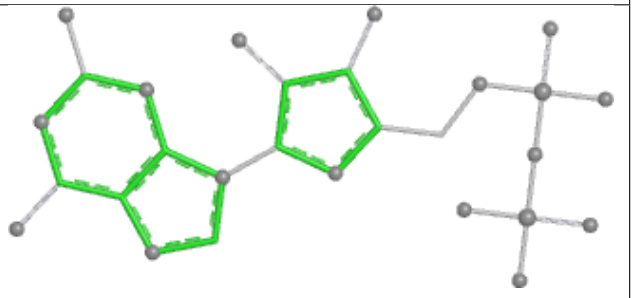
Bond lengths



Bond angles

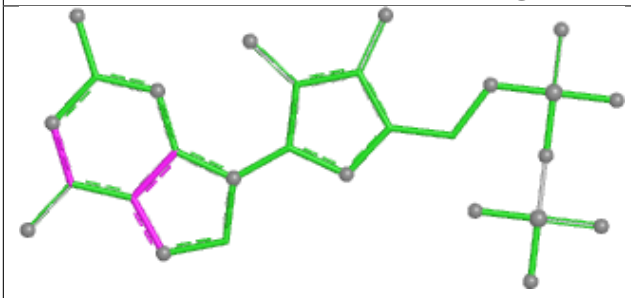


Torsions

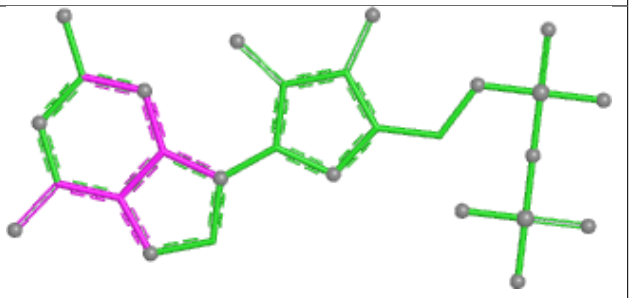


Rings

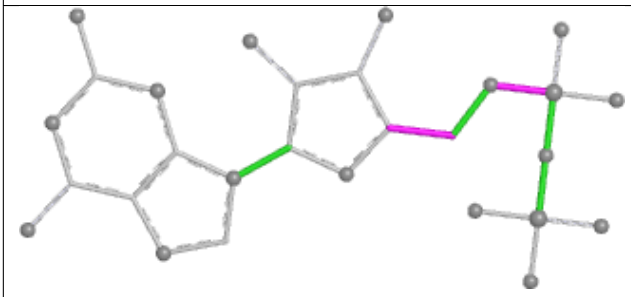
Ligand GDP LL 502



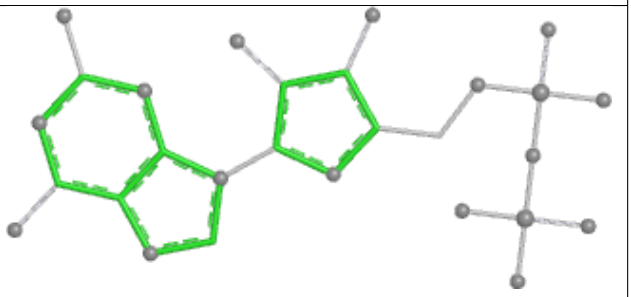
Bond lengths



Bond angles

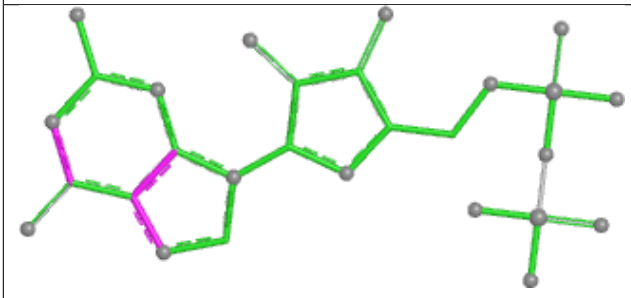


Torsions

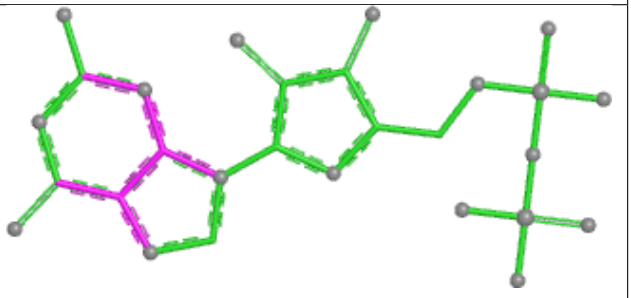


Rings

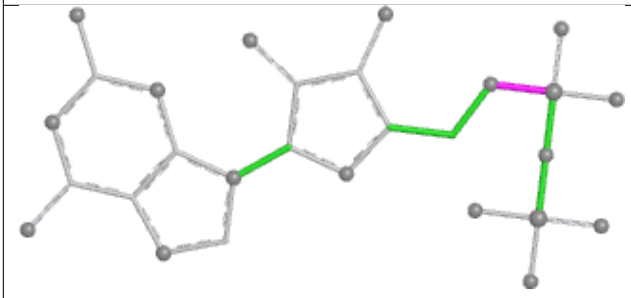
Ligand GDP JN 502



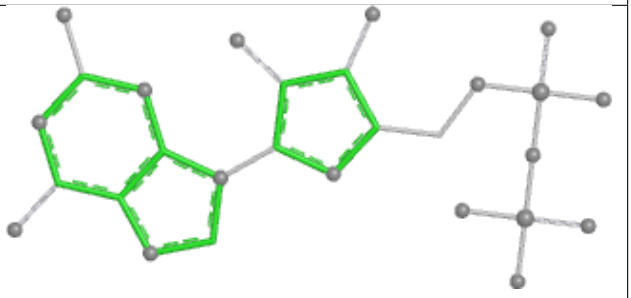
Bond lengths



Bond angles

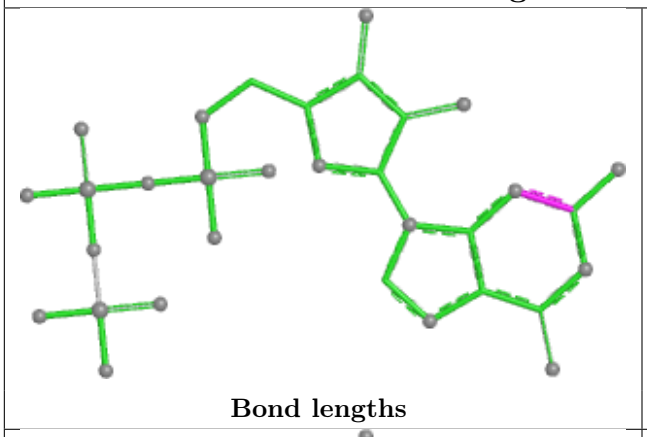


Torsions

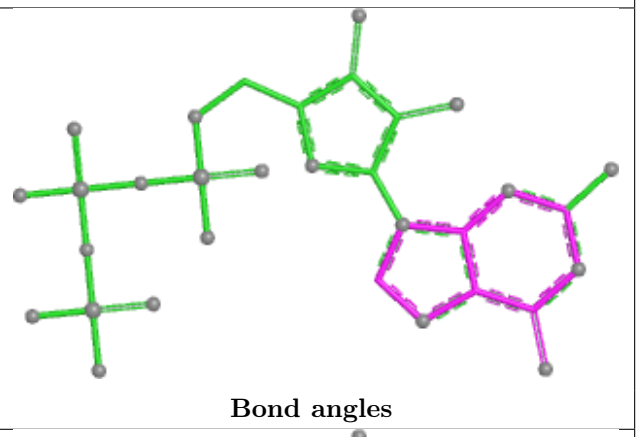


Rings

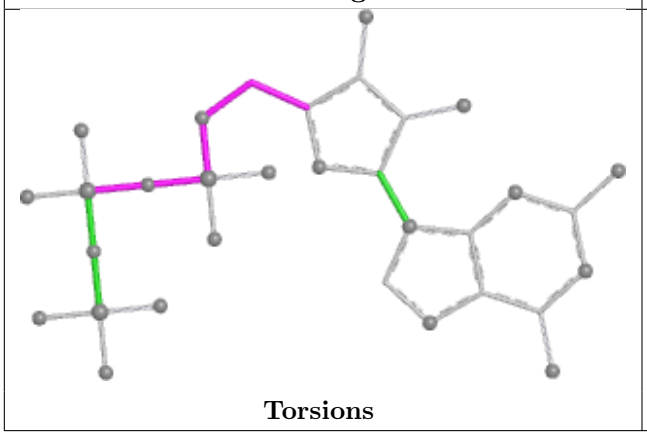
Ligand GTP NO 501



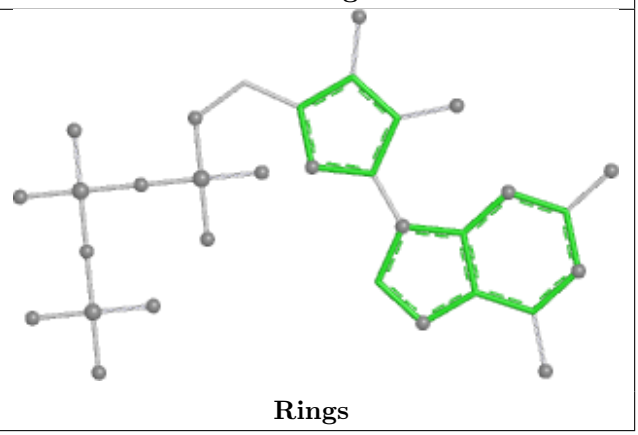
Bond lengths



Bond angles

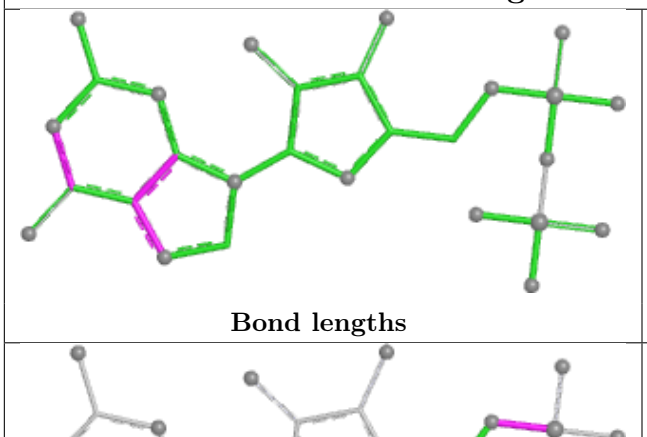


Torsions

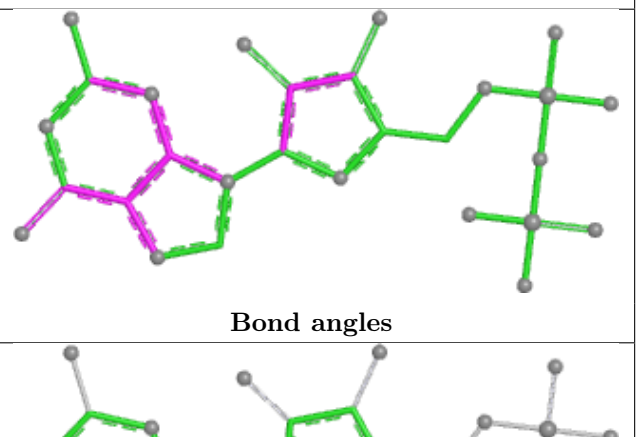


Rings

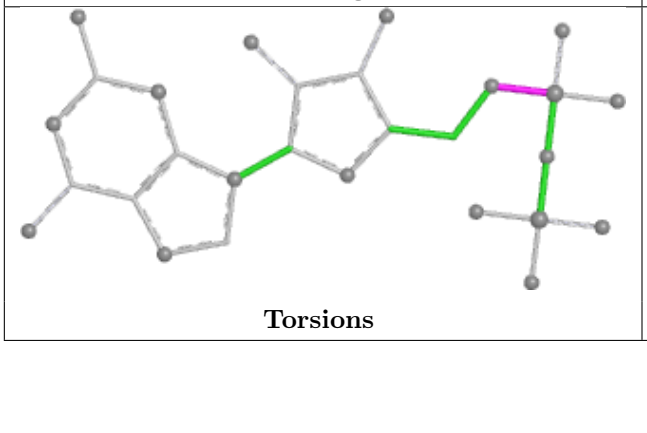
Ligand GDP GN 502



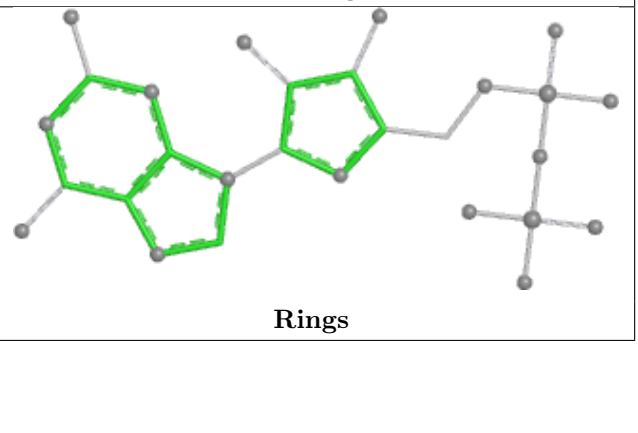
Bond lengths



Bond angles

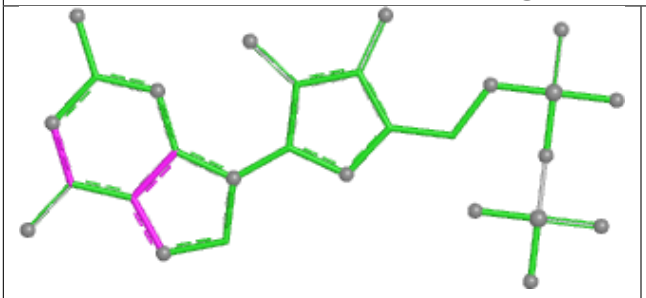


Torsions

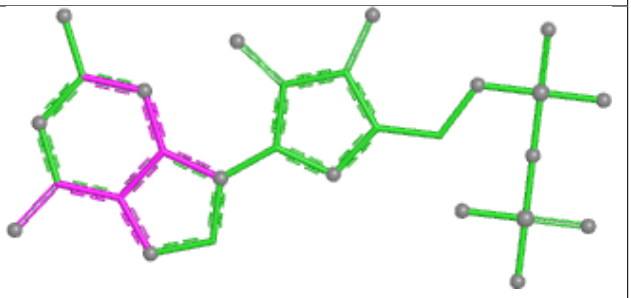


Rings

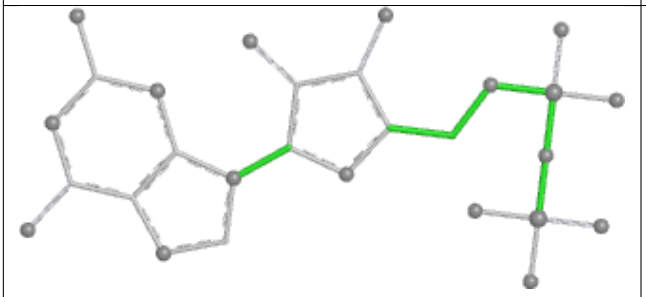
Ligand GDP IJ 502



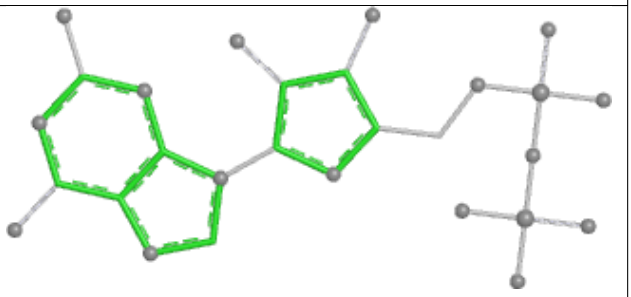
Bond lengths



Bond angles

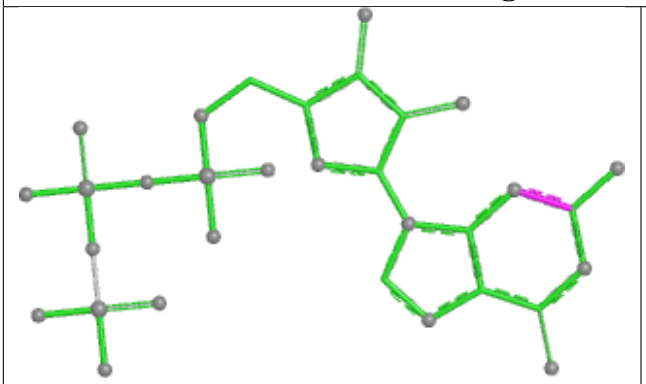


Torsions

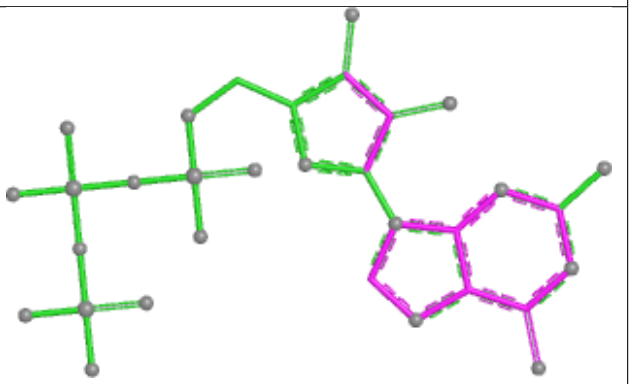


Rings

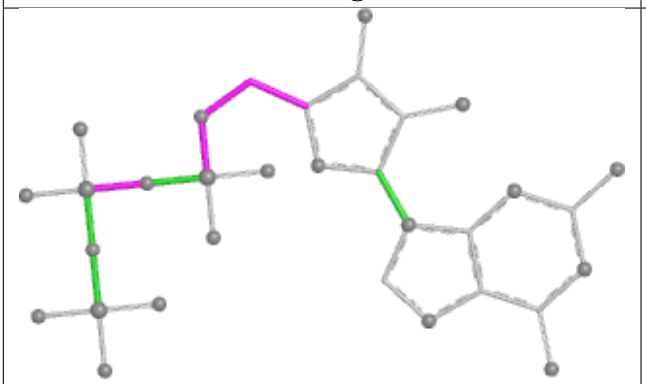
Ligand GTP WM 501



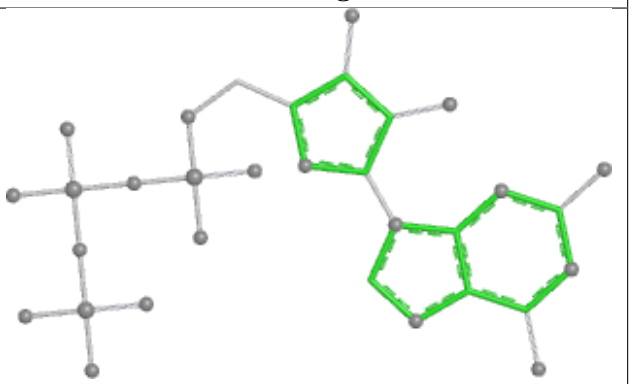
Bond lengths



Bond angles

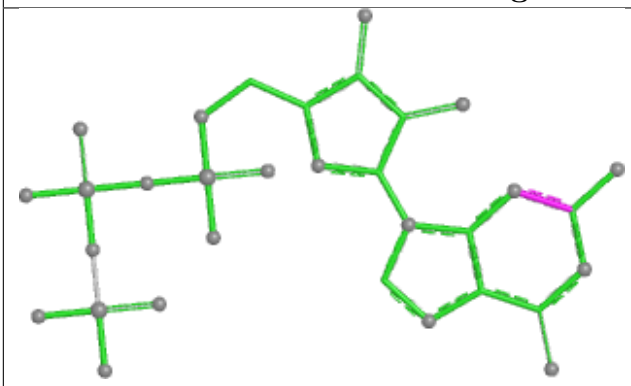


Torsions

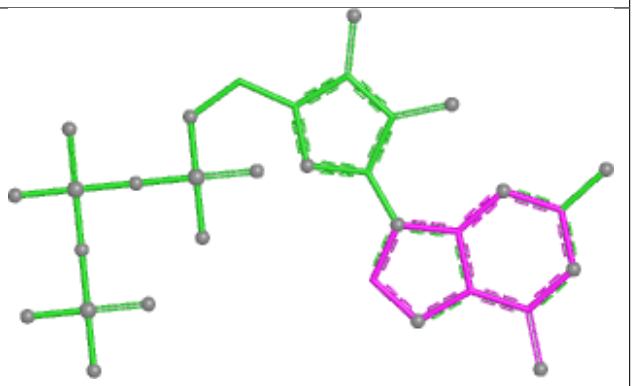


Rings

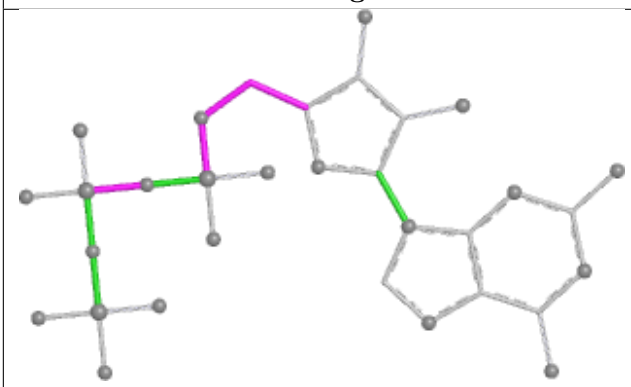
Ligand GTP RE 501



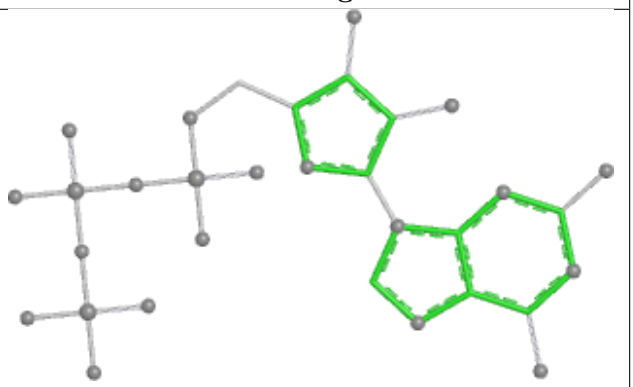
Bond lengths



Bond angles

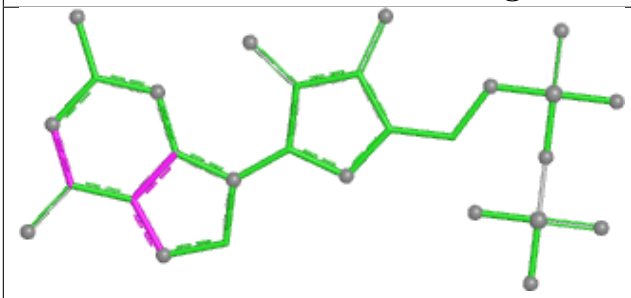


Torsions

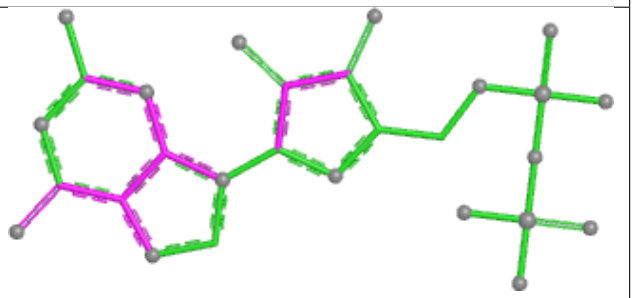


Rings

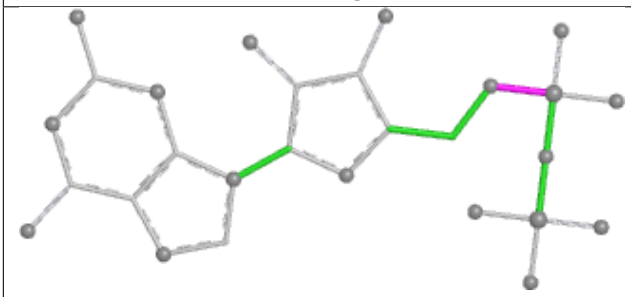
Ligand GDP WP 502



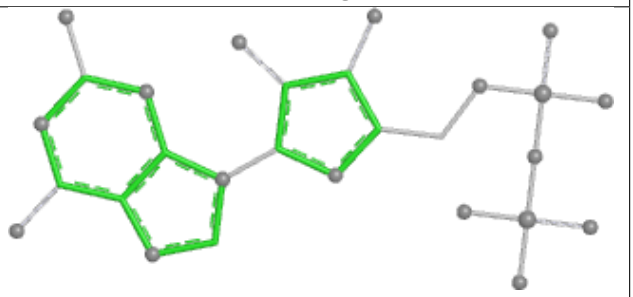
Bond lengths



Bond angles

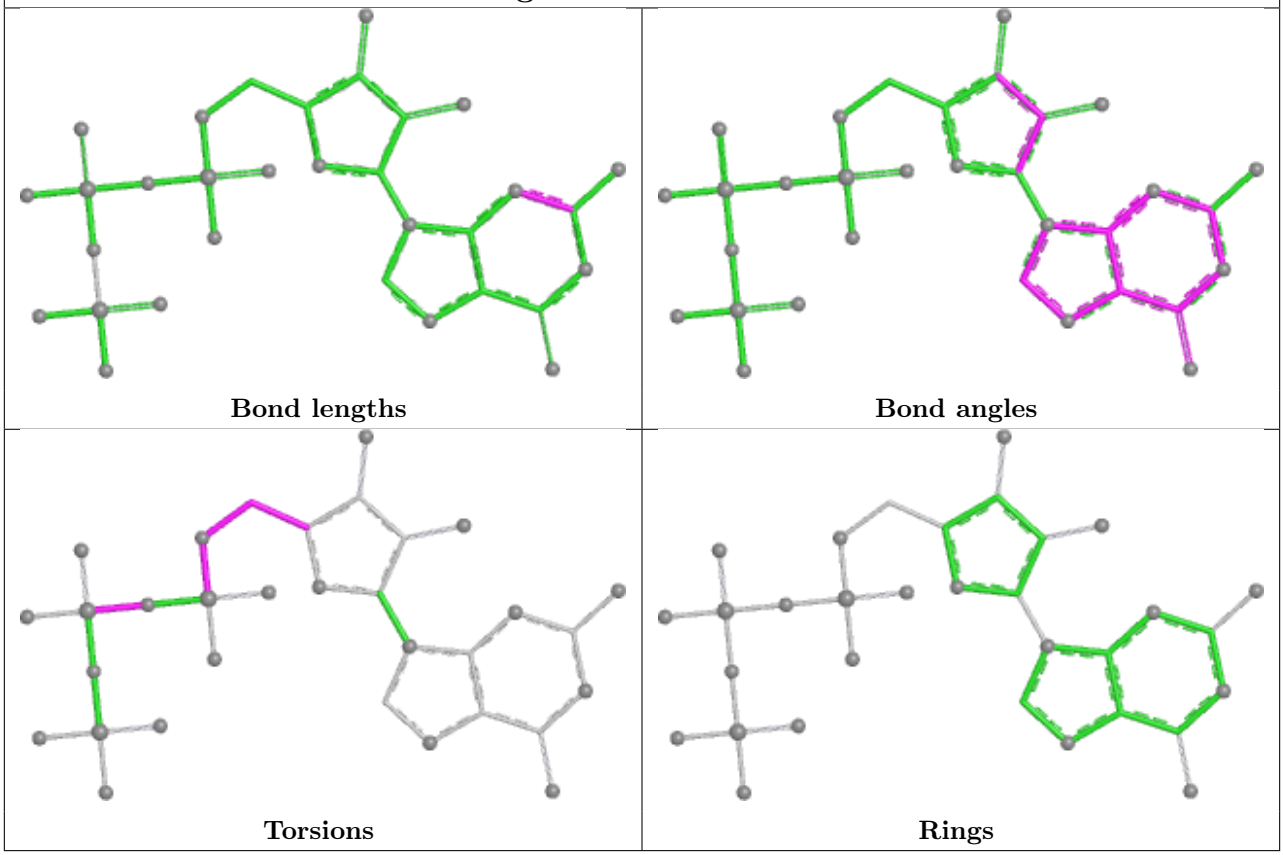


Torsions

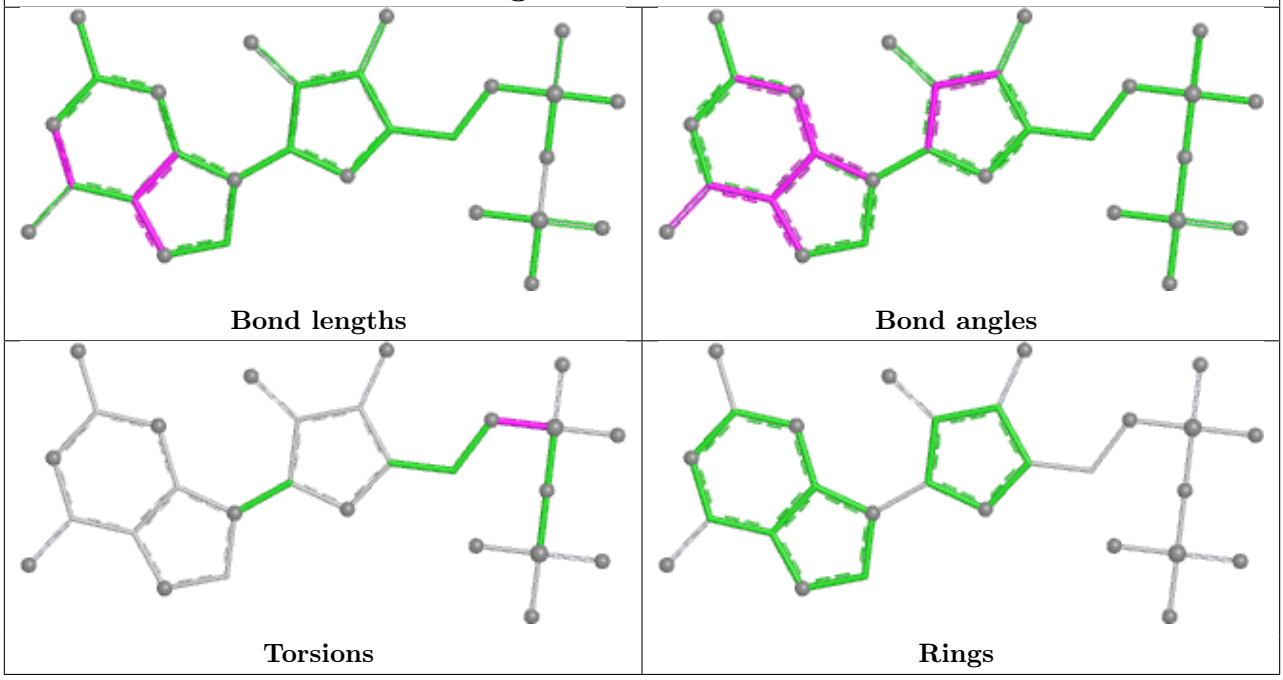


Rings

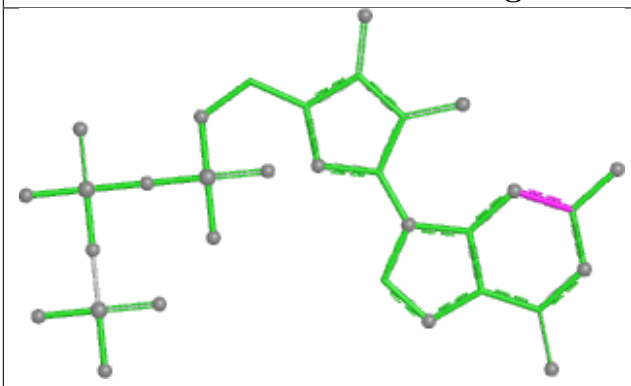
Ligand GTP DI 501



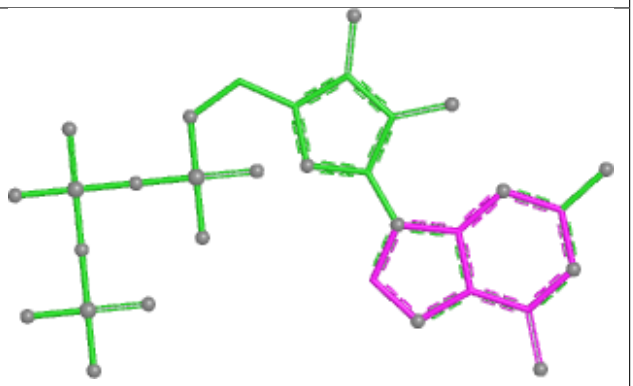
Ligand GDP CB 502



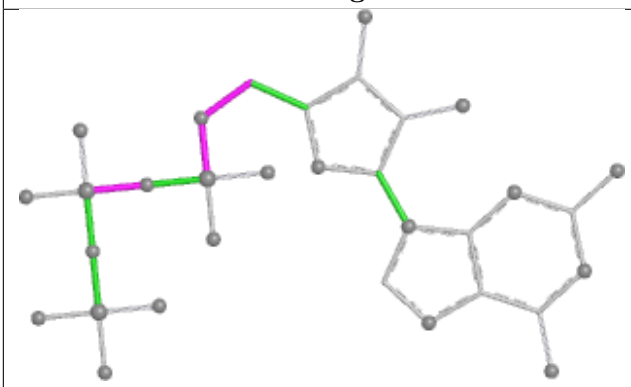
Ligand GTP KM 501



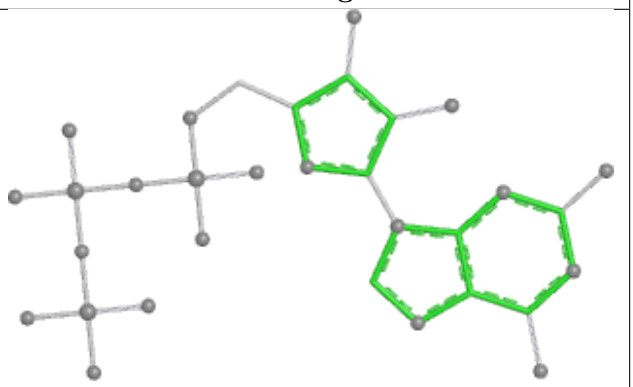
Bond lengths



Bond angles

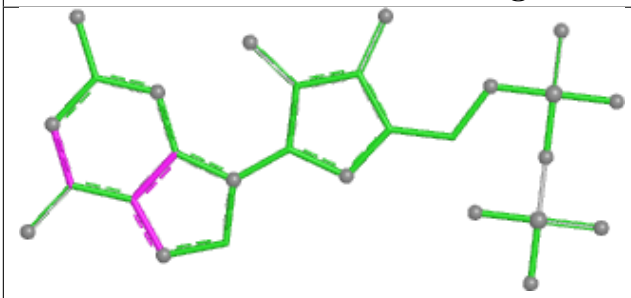


Torsions

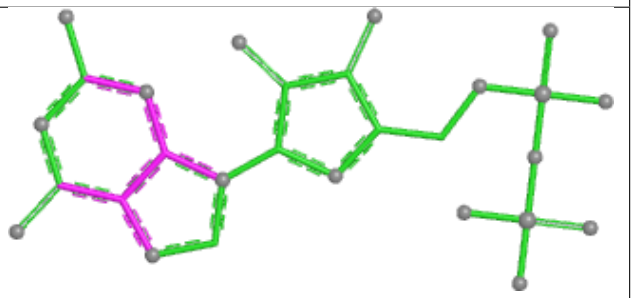


Rings

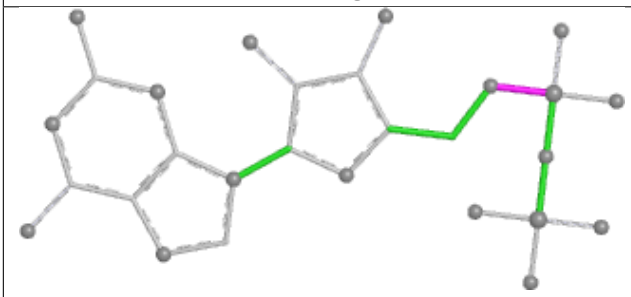
Ligand GDP VF 502



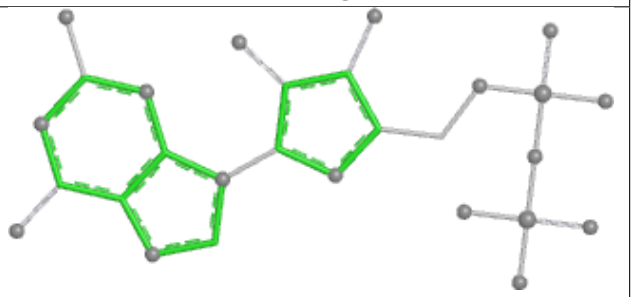
Bond lengths



Bond angles

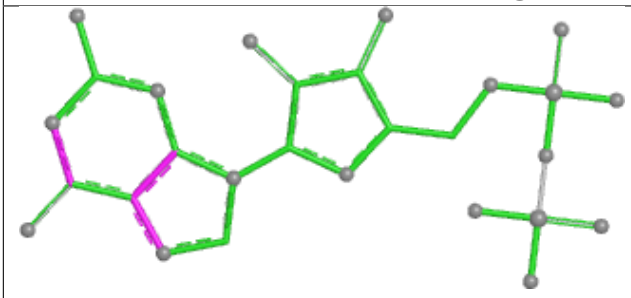


Torsions

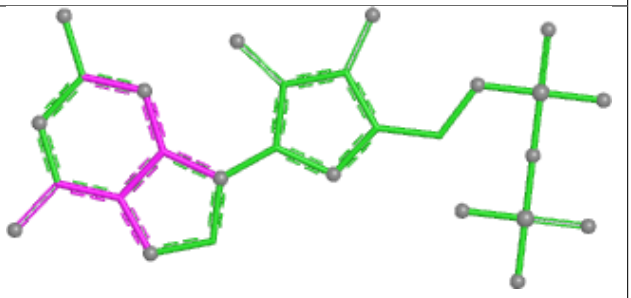


Rings

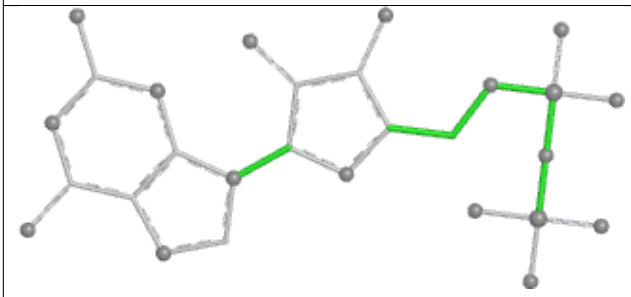
Ligand GDP HJ 502



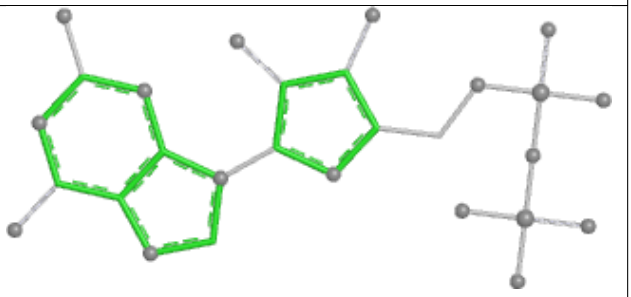
Bond lengths



Bond angles

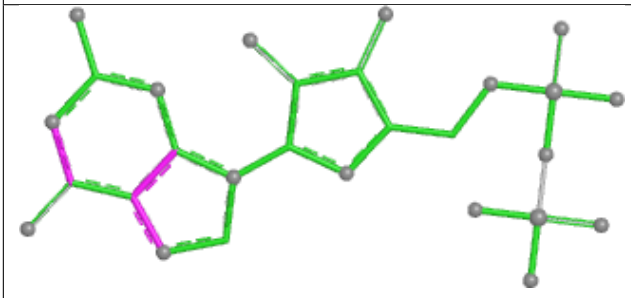


Torsions

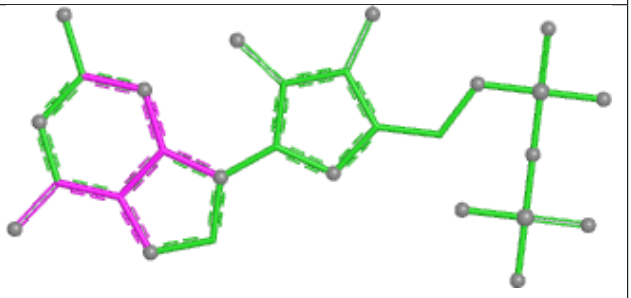


Rings

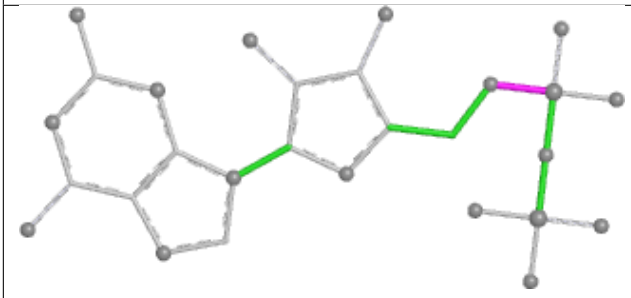
Ligand GDP CP 502



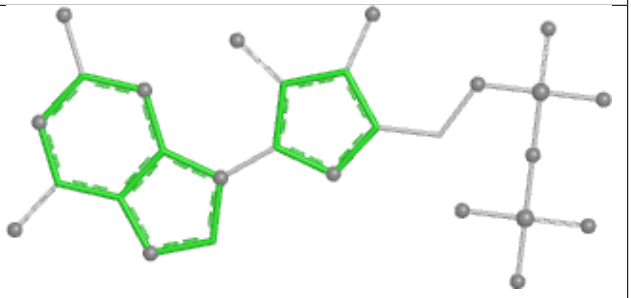
Bond lengths



Bond angles

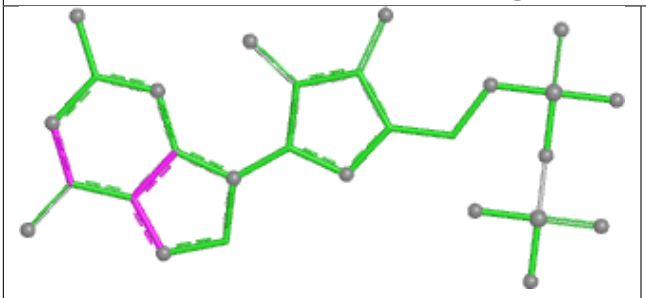


Torsions

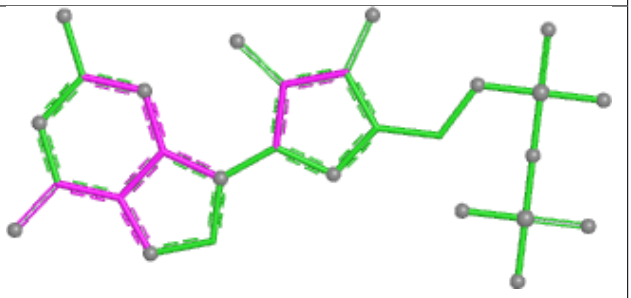


Rings

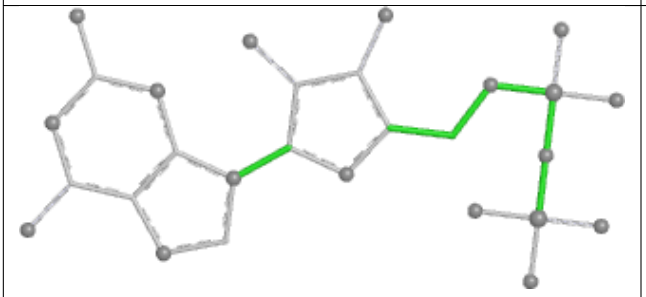
Ligand GDP RP 502



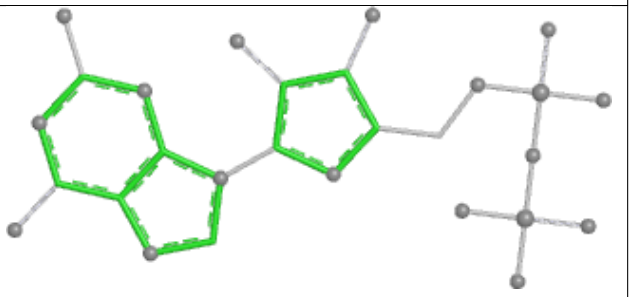
Bond lengths



Bond angles

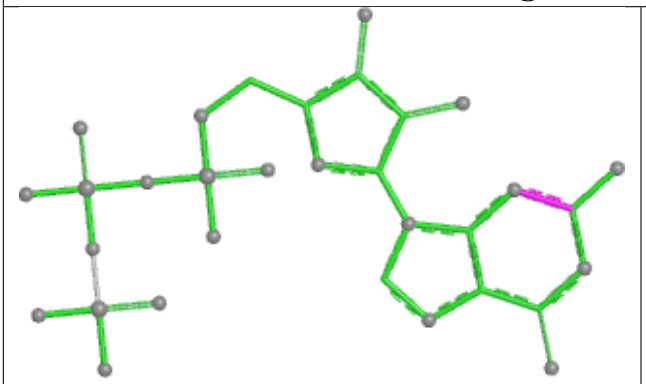


Torsions

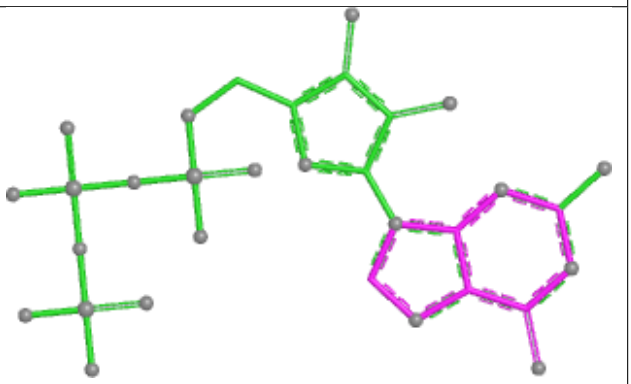


Rings

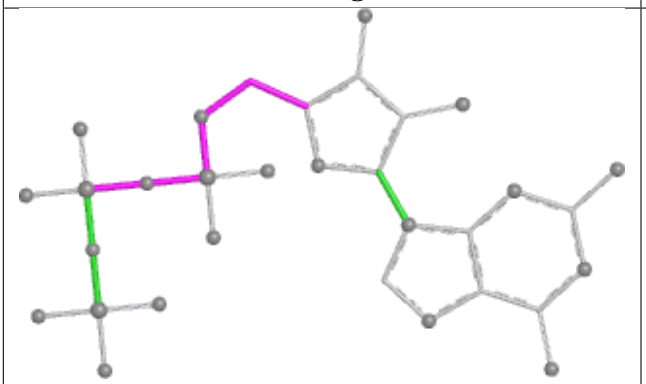
Ligand GTP SI 501



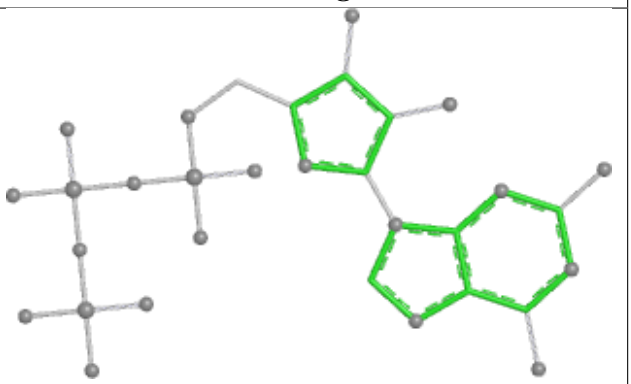
Bond lengths



Bond angles

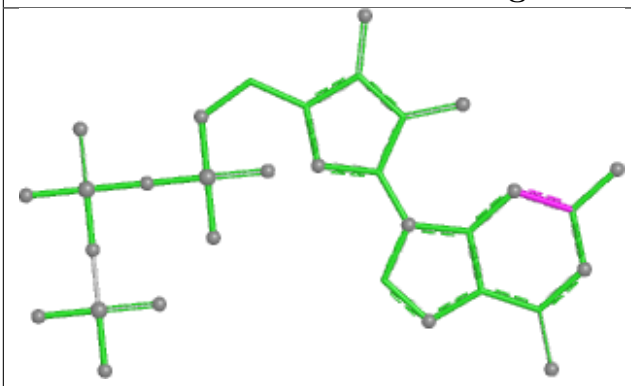


Torsions

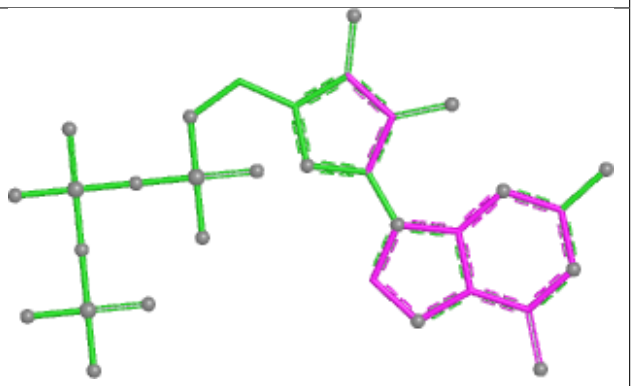


Rings

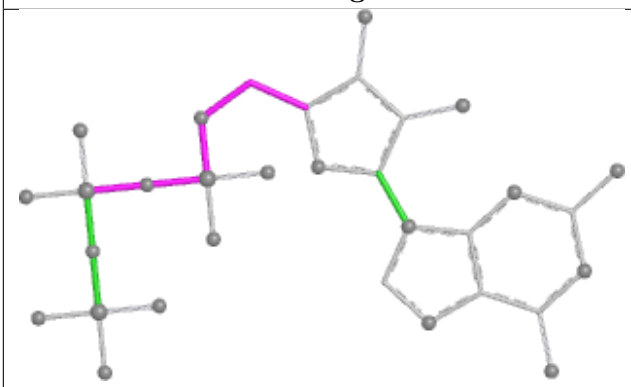
Ligand GTP OO 501



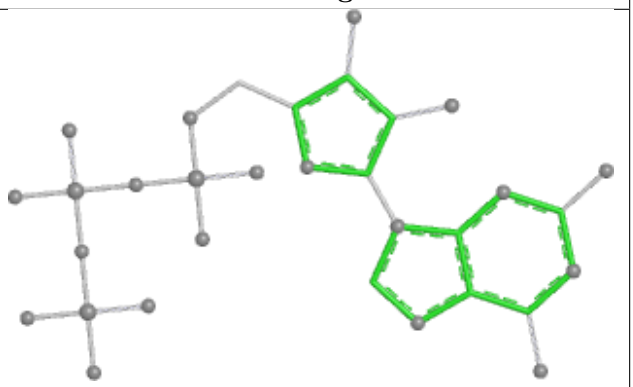
Bond lengths



Bond angles

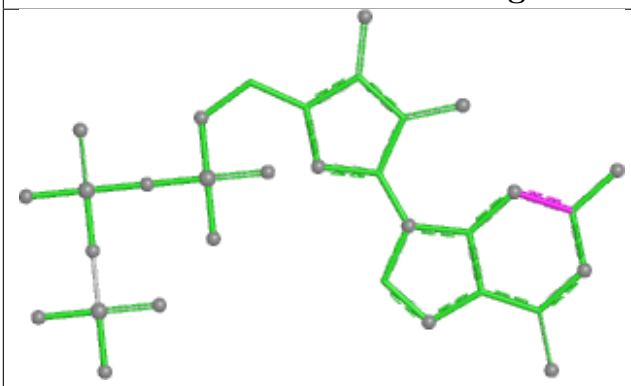


Torsions

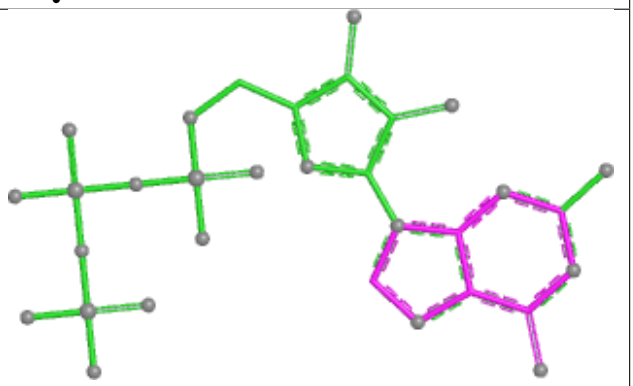


Rings

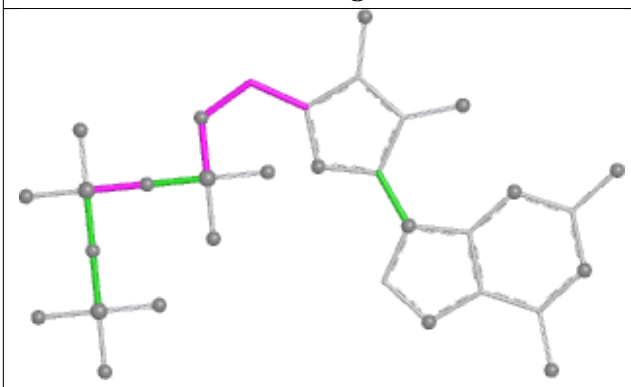
Ligand GTP QK 501



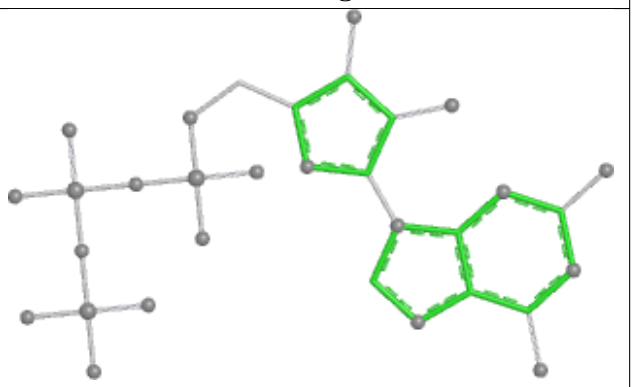
Bond lengths



Bond angles

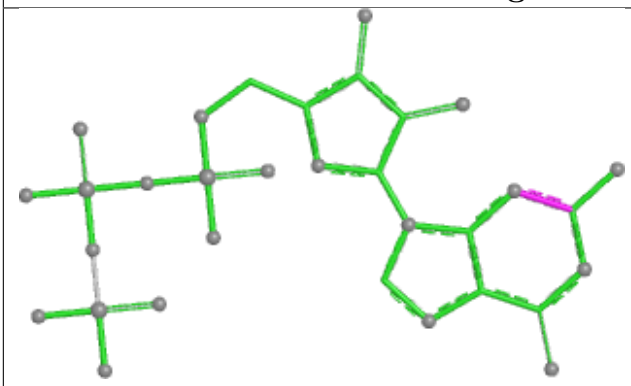


Torsions

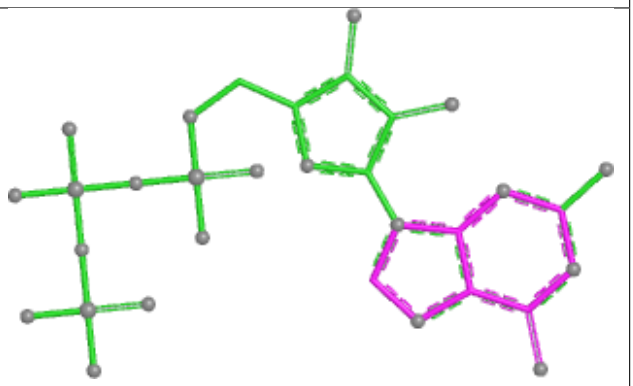


Rings

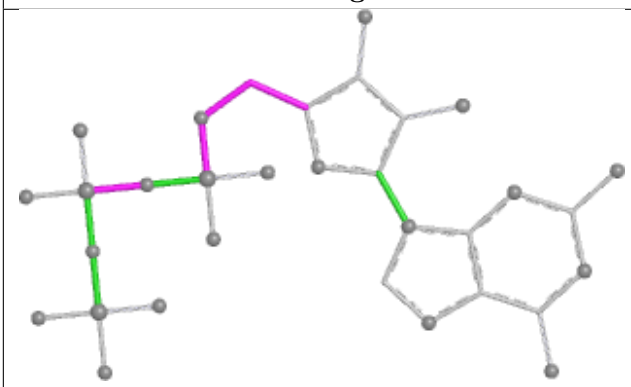
Ligand GTP GK 501



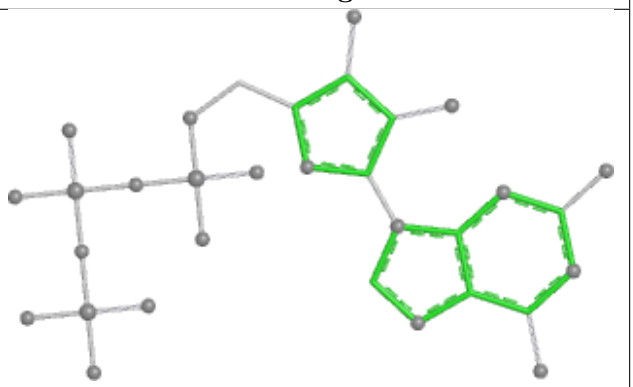
Bond lengths



Bond angles

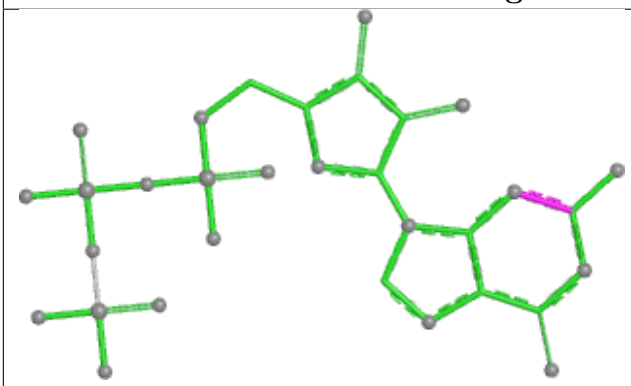


Torsions

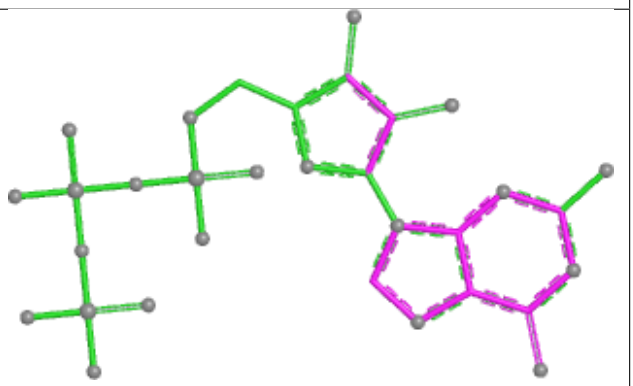


Rings

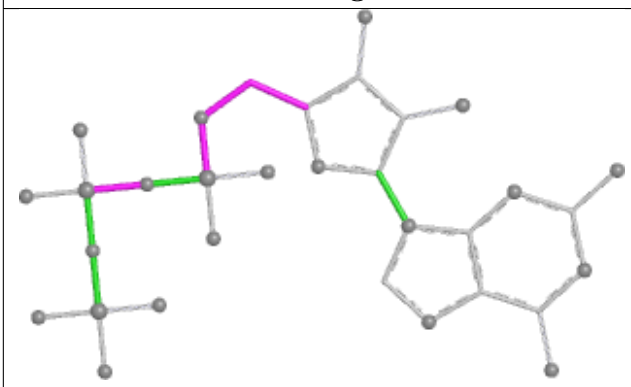
Ligand GTP WE 501



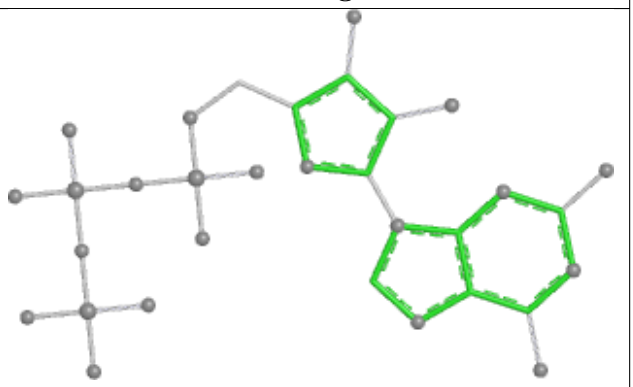
Bond lengths



Bond angles

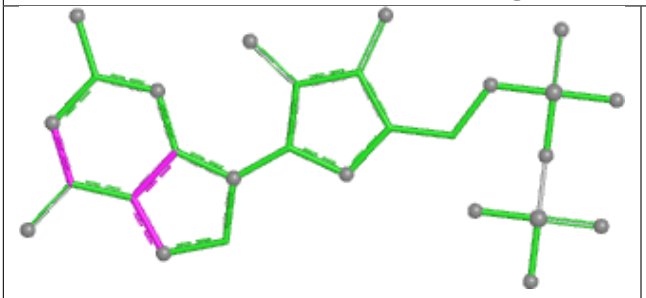


Torsions

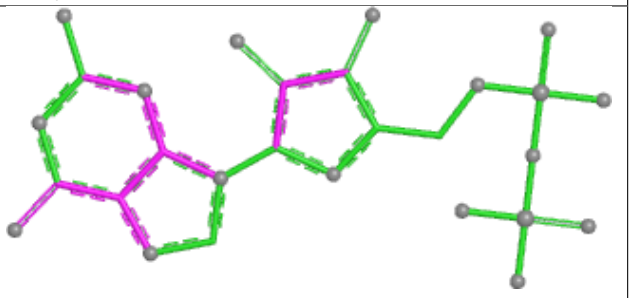


Rings

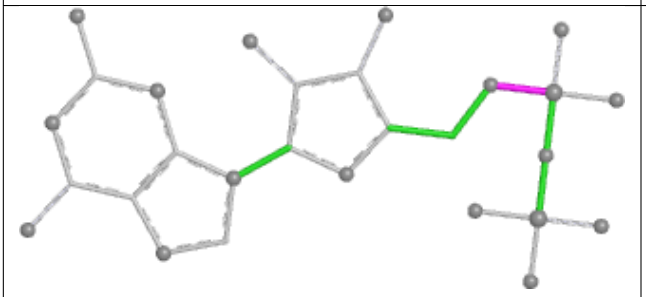
Ligand GDP QB 502



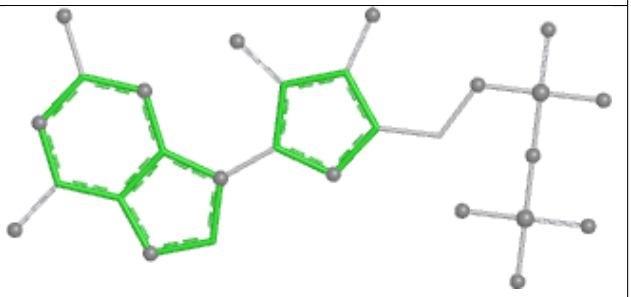
Bond lengths



Bond angles

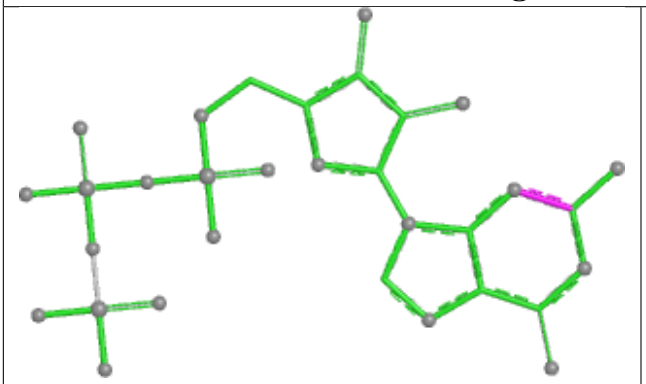


Torsions

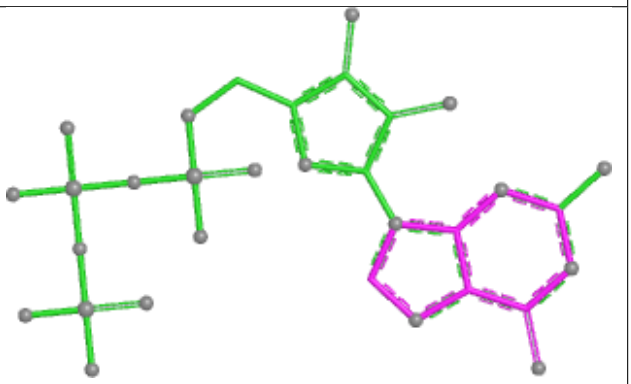


Rings

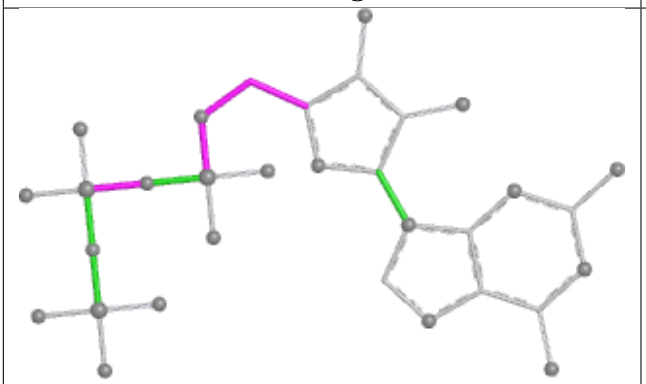
Ligand GTP LG 501



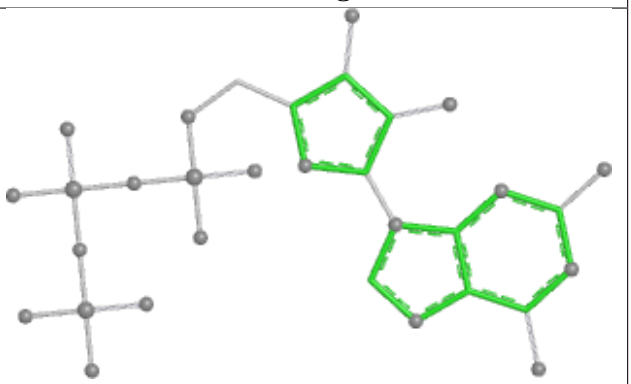
Bond lengths



Bond angles

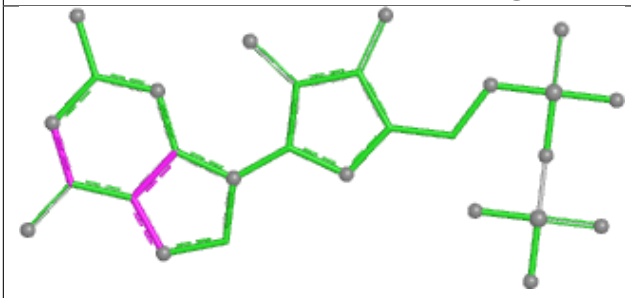


Torsions

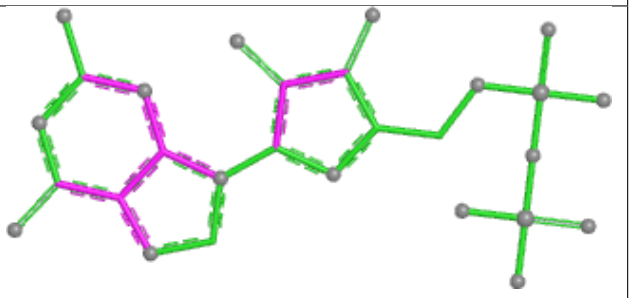


Rings

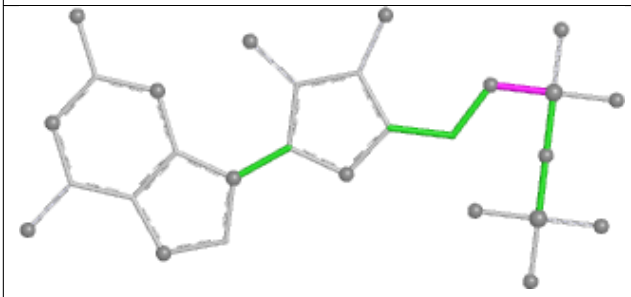
Ligand GDP UB 502



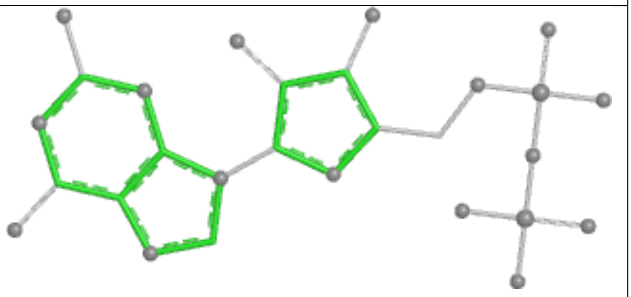
Bond lengths



Bond angles

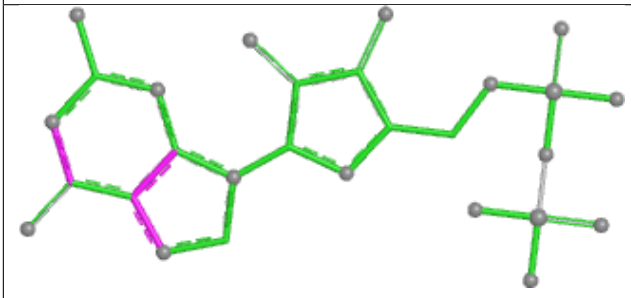


Torsions

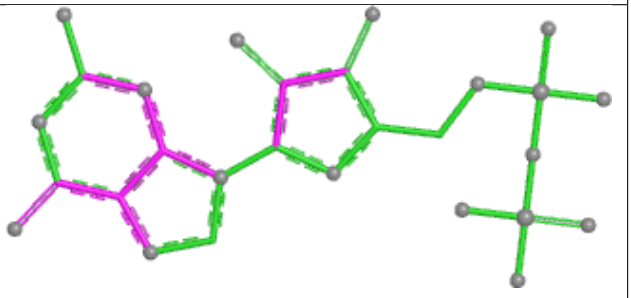


Rings

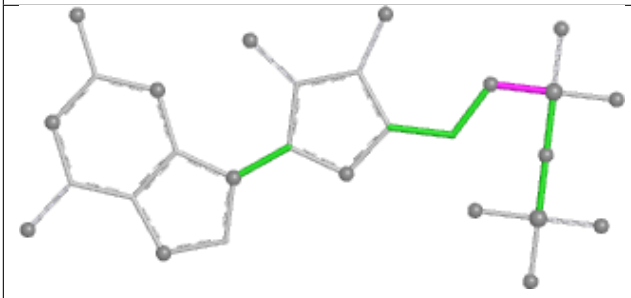
Ligand GDP VH 502



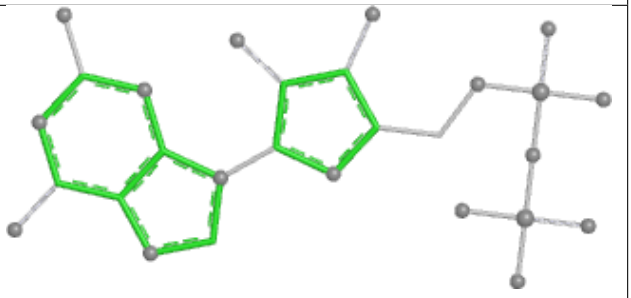
Bond lengths



Bond angles

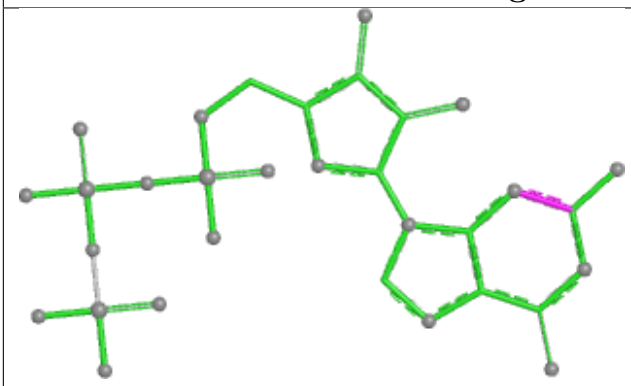


Torsions

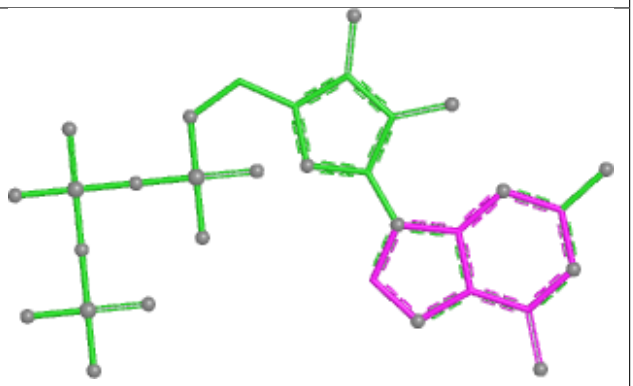


Rings

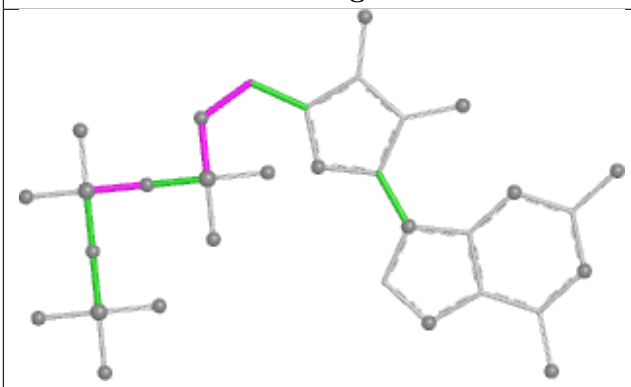
Ligand GTP KC 501



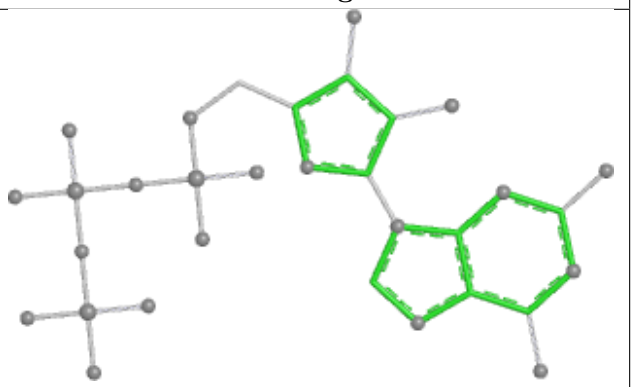
Bond lengths



Bond angles

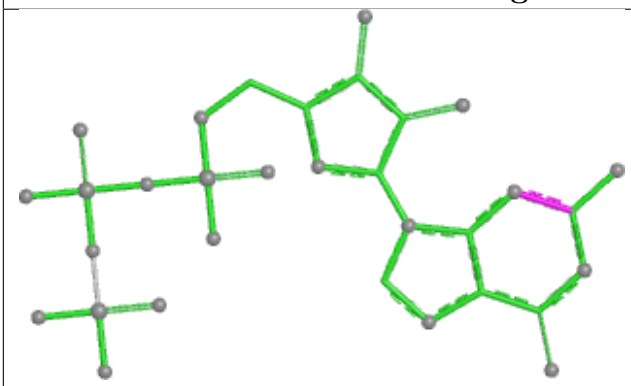


Torsions

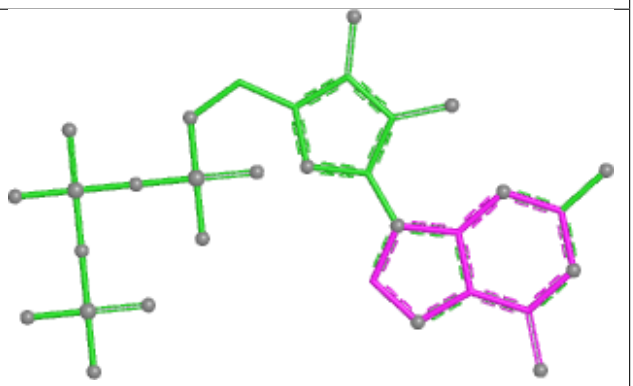


Rings

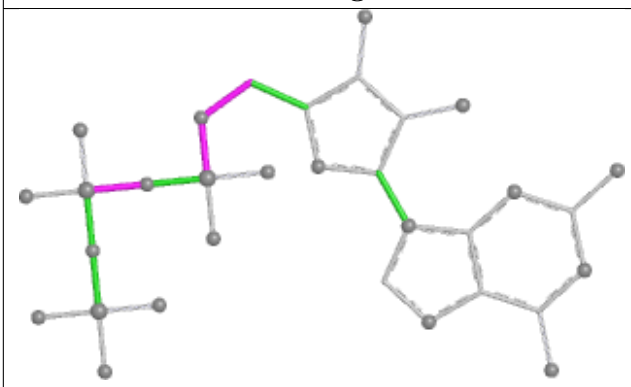
Ligand GTP FG 501



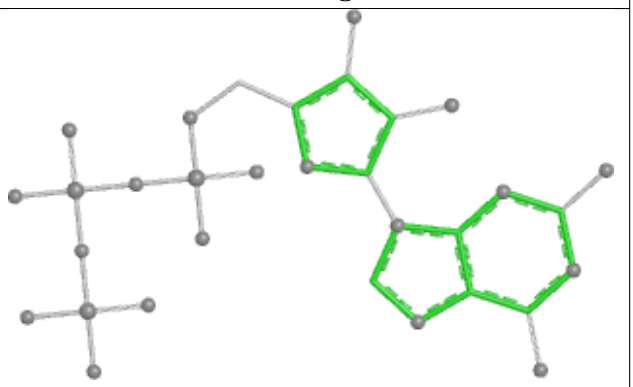
Bond lengths



Bond angles

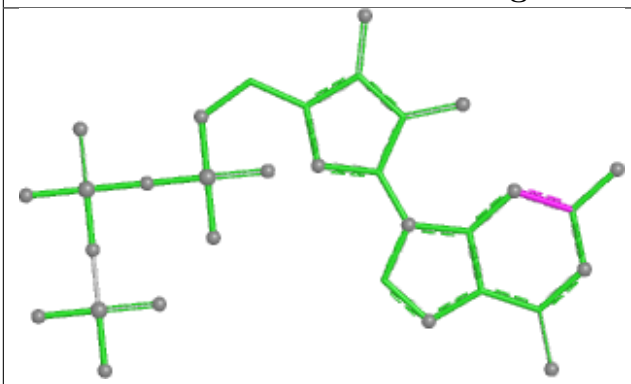


Torsions

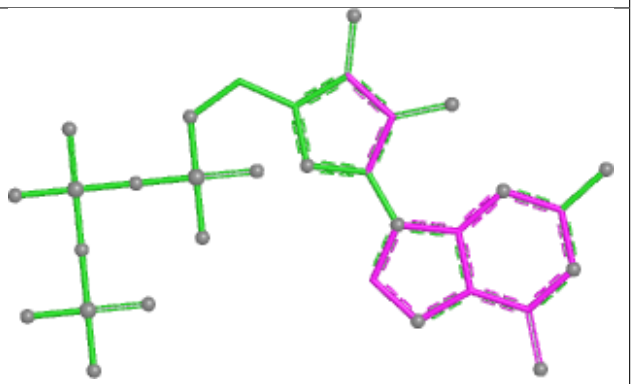


Rings

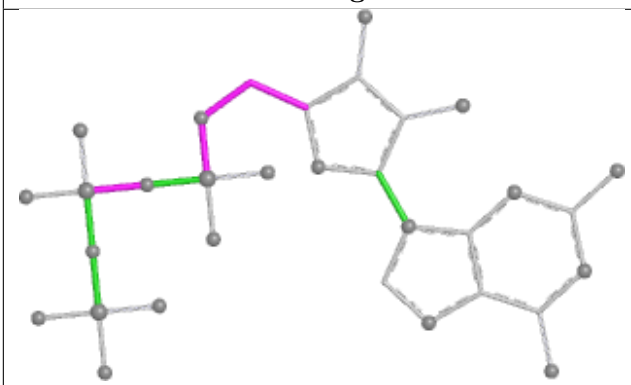
Ligand GTP EK 501



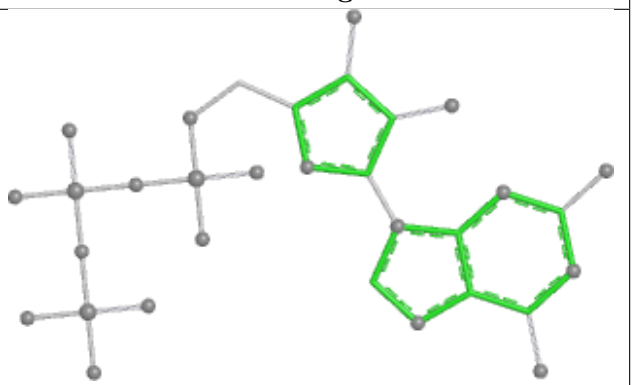
Bond lengths



Bond angles

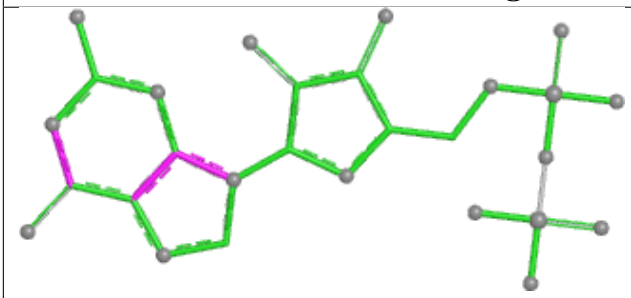


Torsions

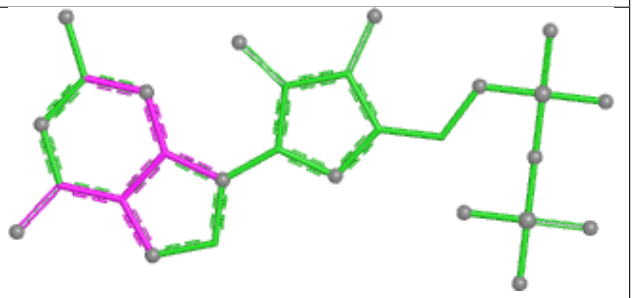


Rings

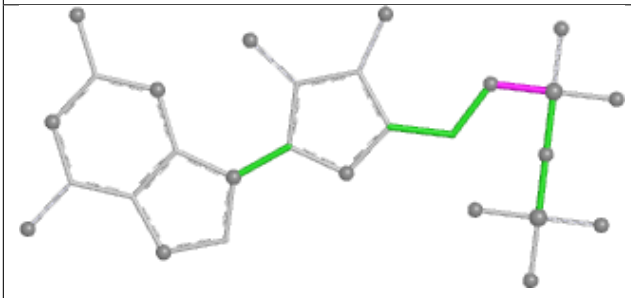
Ligand GDP MB 502



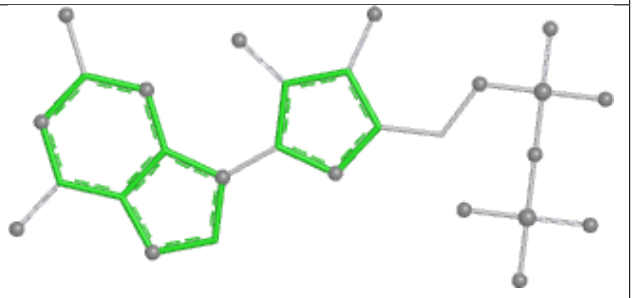
Bond lengths



Bond angles

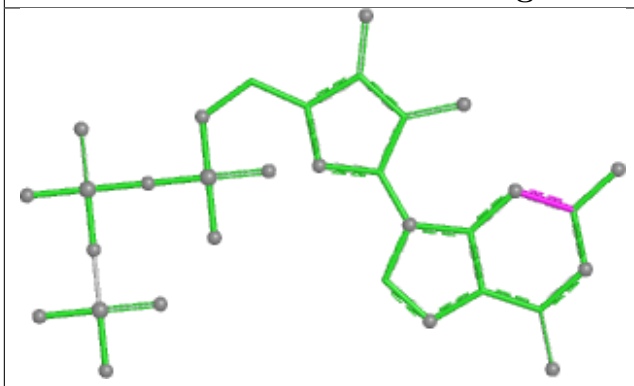


Torsions

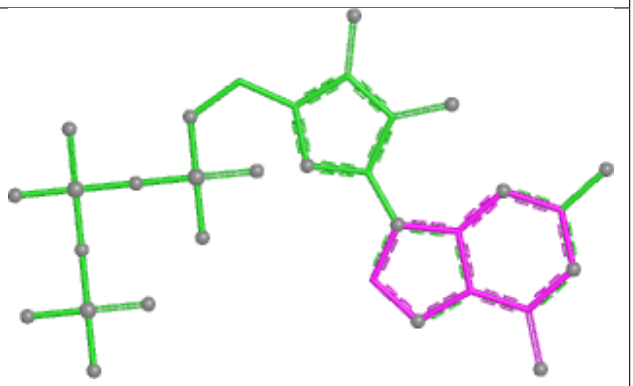


Rings

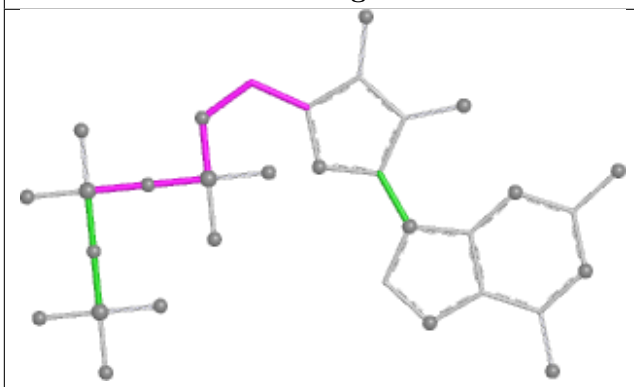
Ligand GTP AI 501



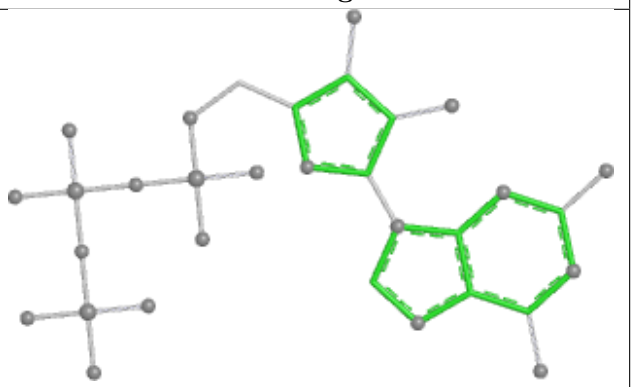
Bond lengths



Bond angles

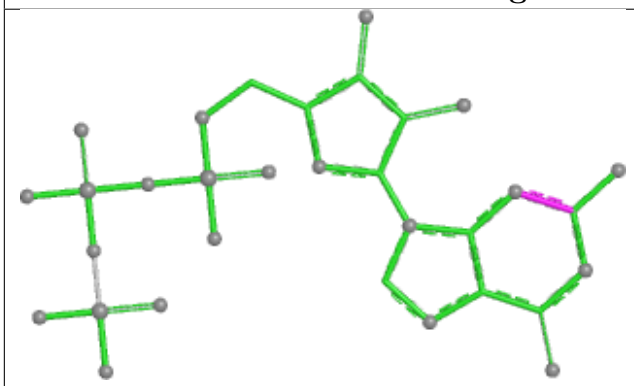


Torsions

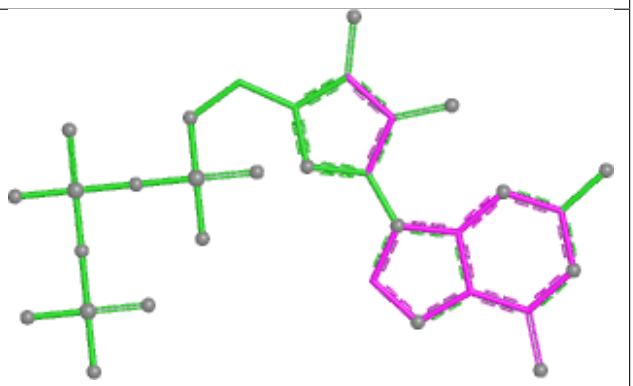


Rings

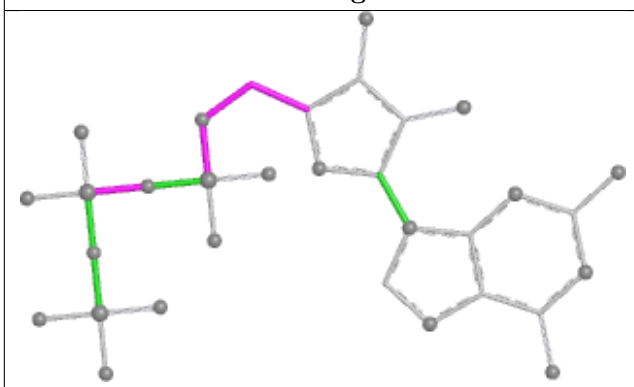
Ligand GTP UA 501



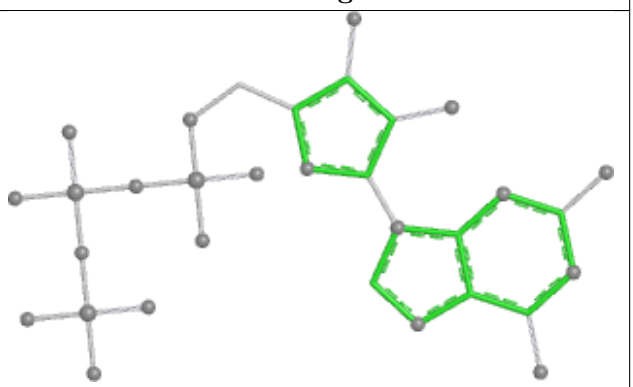
Bond lengths



Bond angles

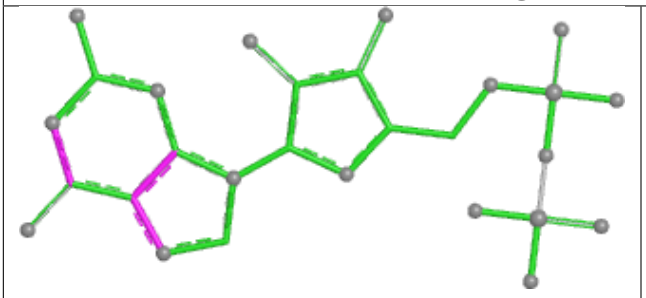


Torsions

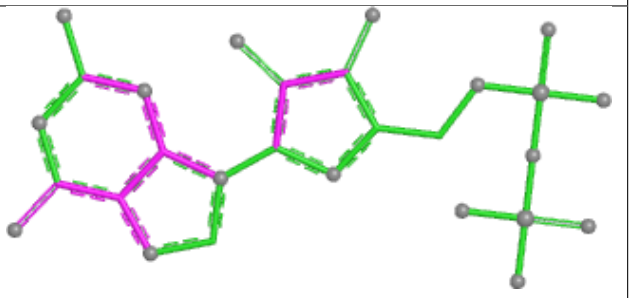


Rings

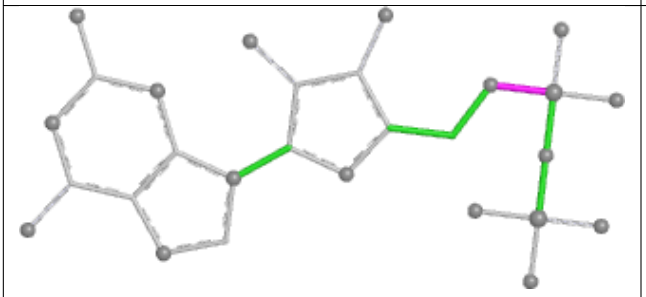
Ligand GDP PJ 502



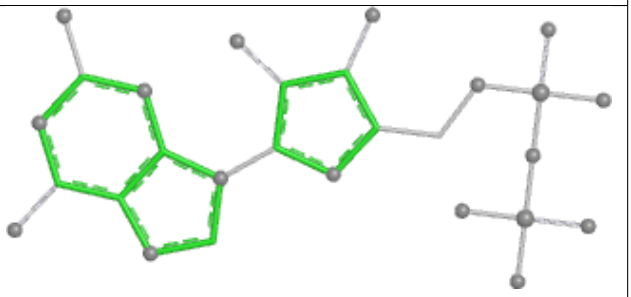
Bond lengths



Bond angles

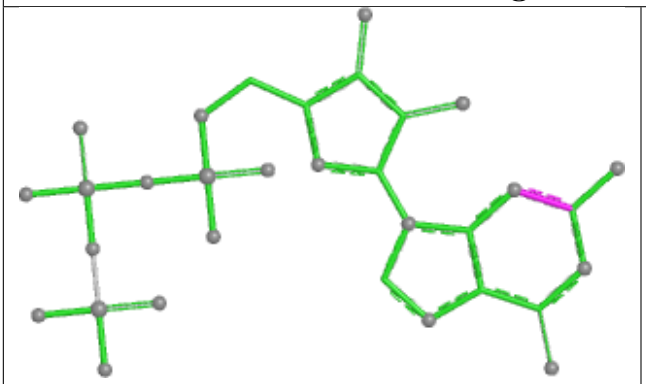


Torsions

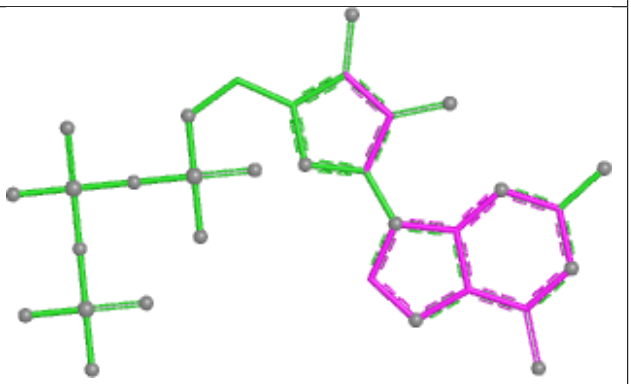


Rings

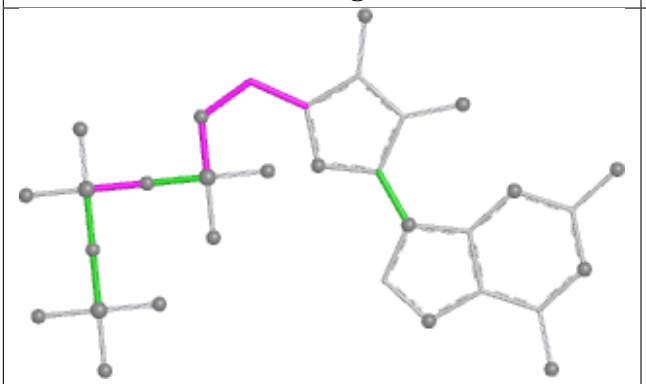
Ligand GTP PC 501



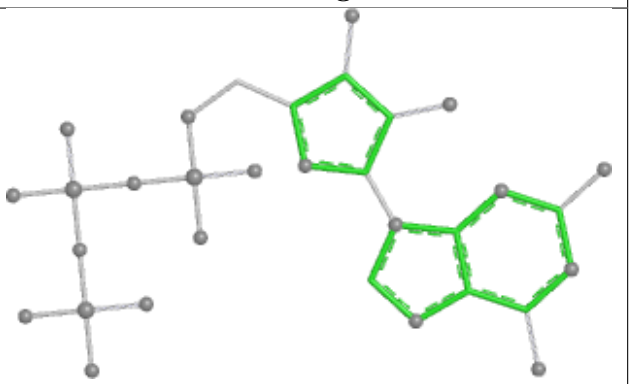
Bond lengths



Bond angles

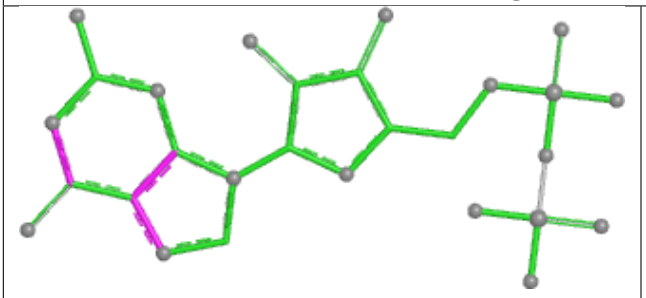


Torsions

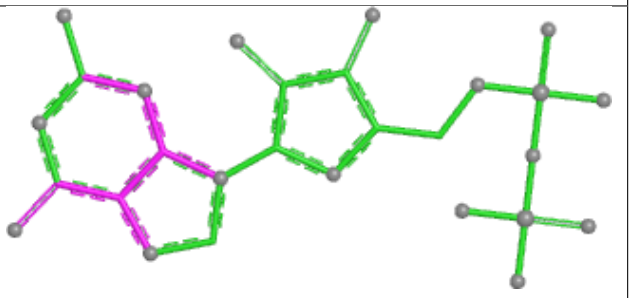


Rings

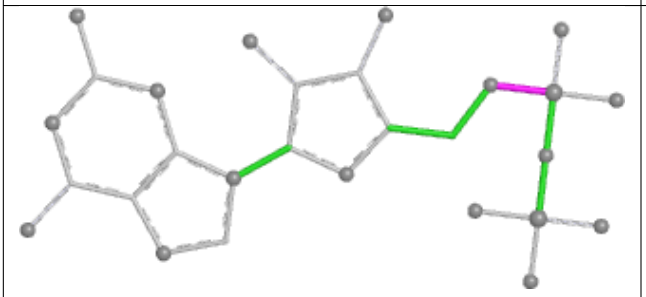
Ligand GDP KB 502



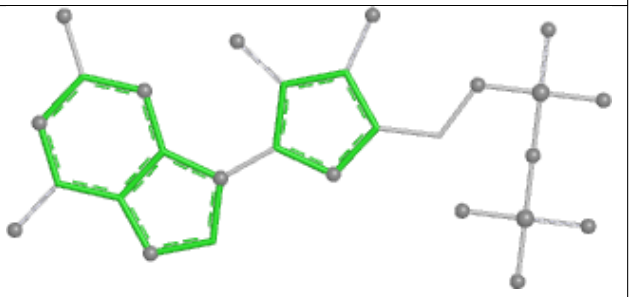
Bond lengths



Bond angles

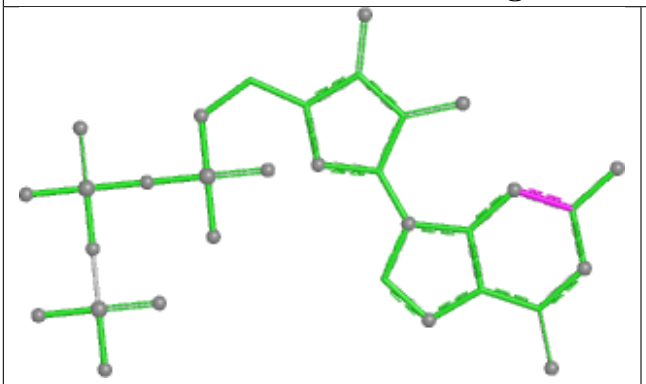


Torsions

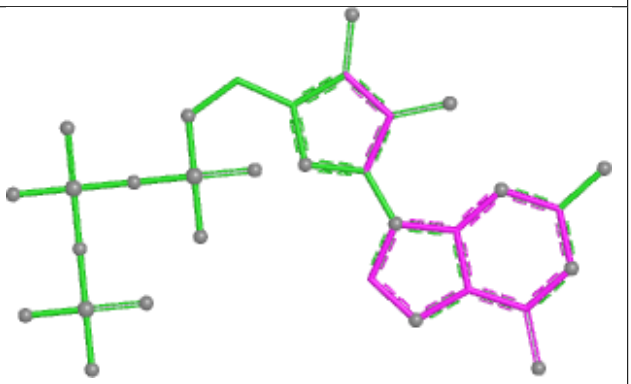


Rings

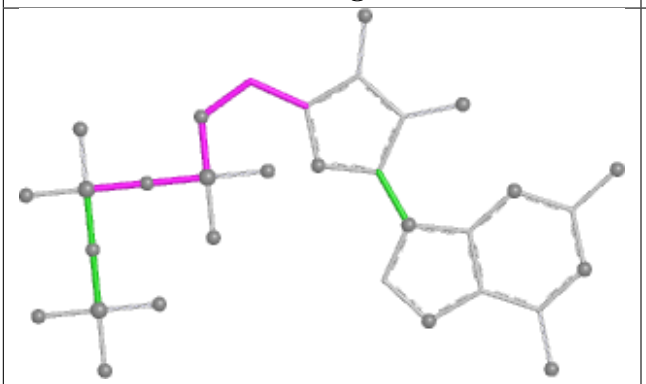
Ligand GTP TM 501



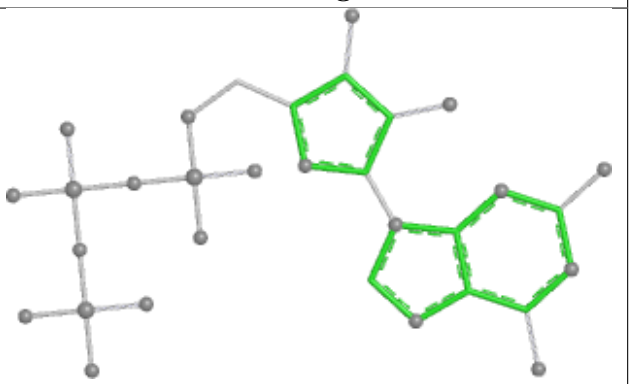
Bond lengths



Bond angles

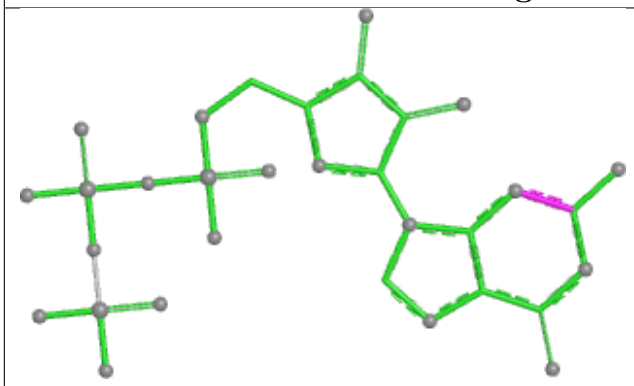


Torsions

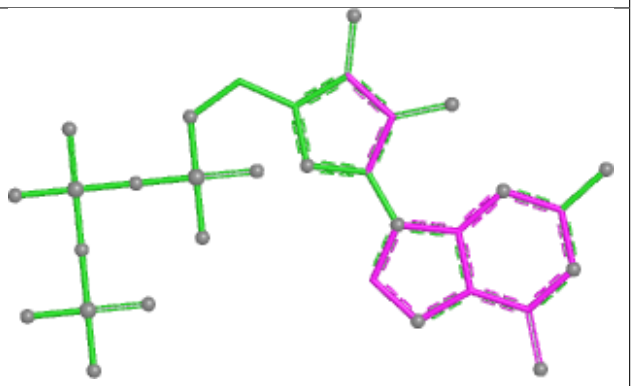


Rings

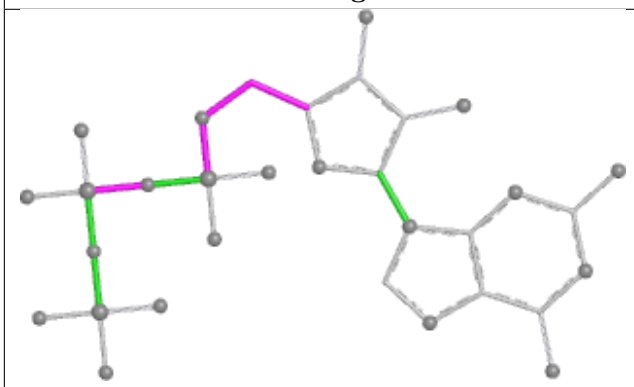
Ligand GTP SE 501



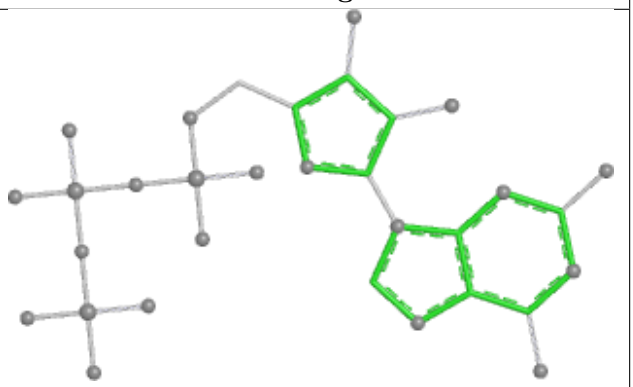
Bond lengths



Bond angles

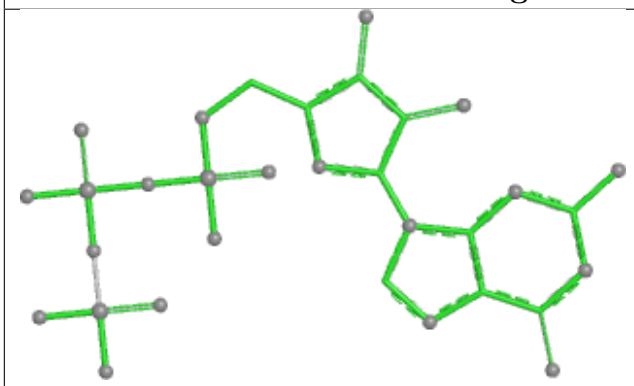


Torsions

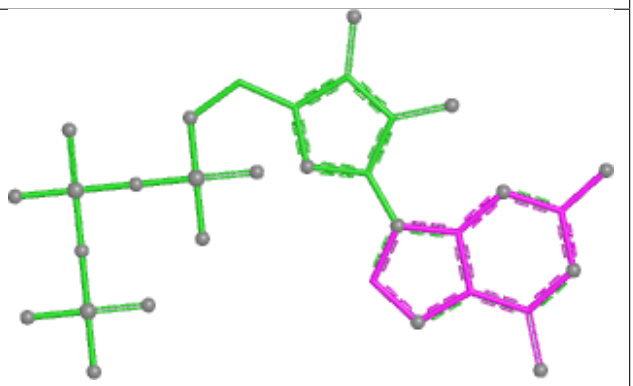


Rings

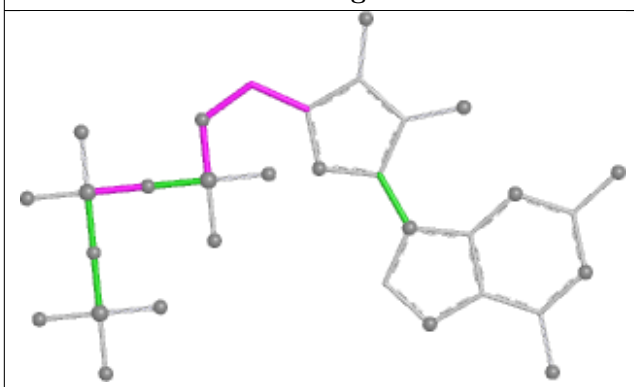
Ligand GTP PG 501



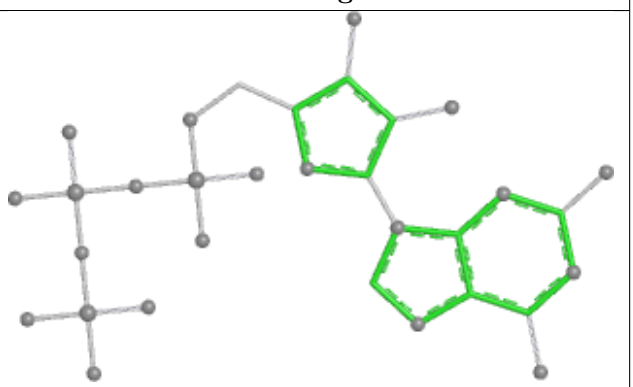
Bond lengths



Bond angles

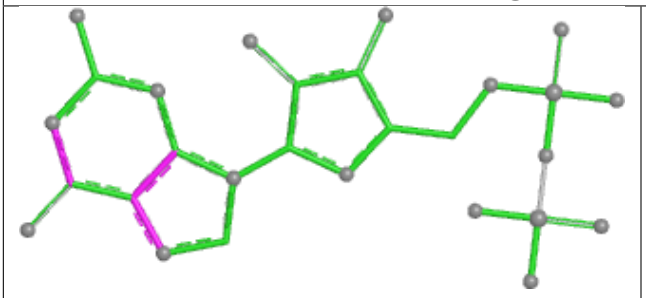


Torsions

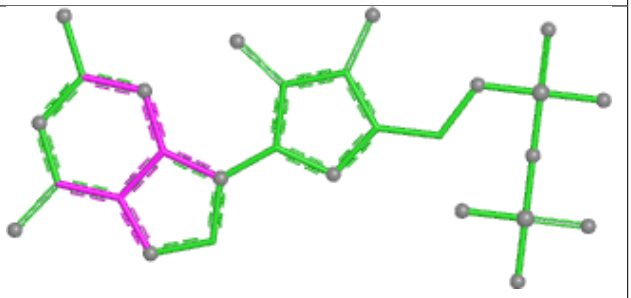


Rings

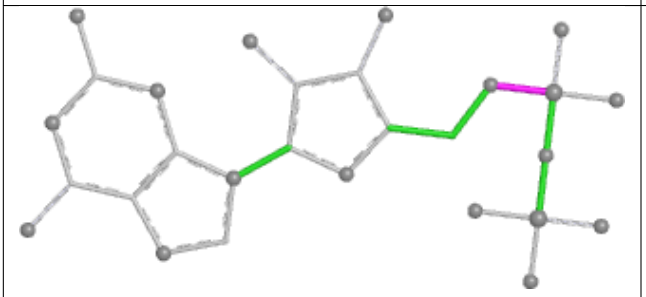
Ligand GDP GD 502



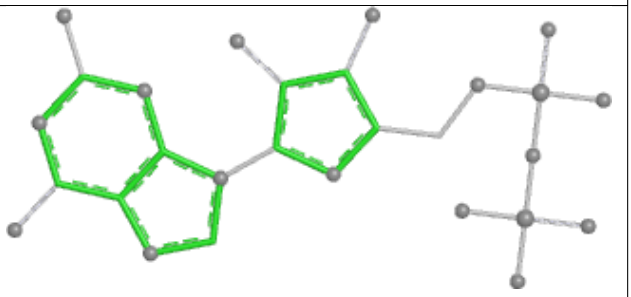
Bond lengths



Bond angles

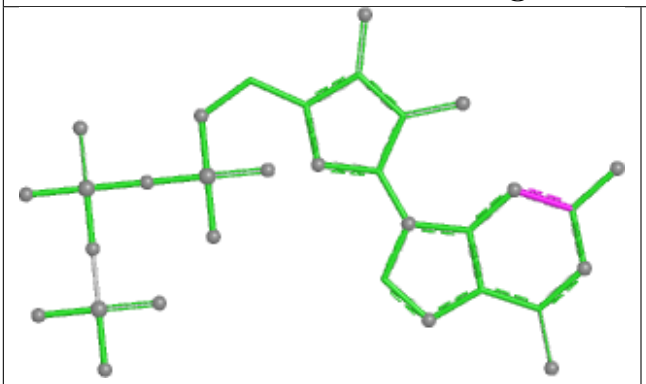


Torsions

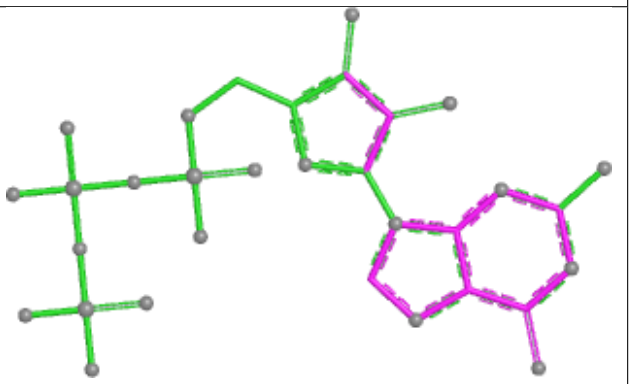


Rings

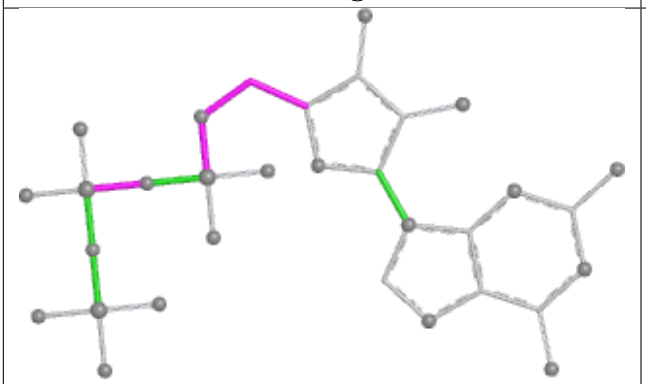
Ligand GTP DC 501



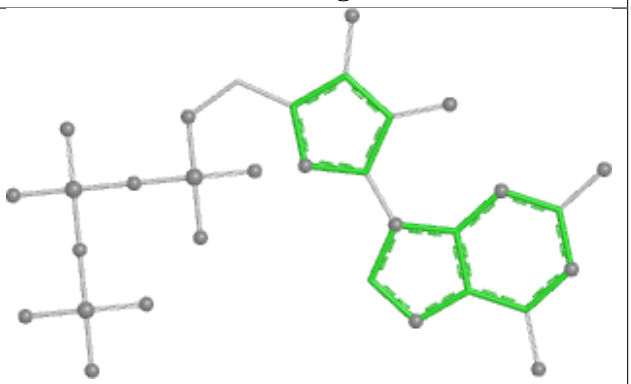
Bond lengths



Bond angles

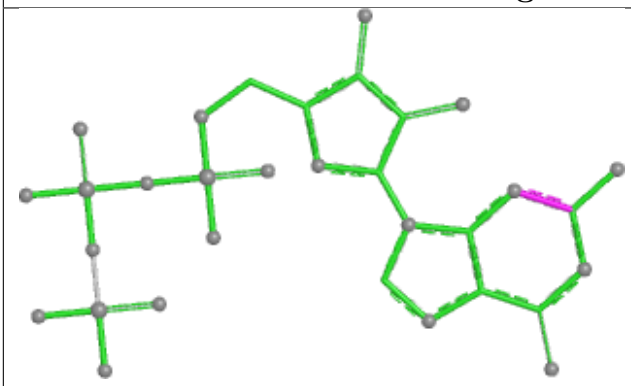


Torsions

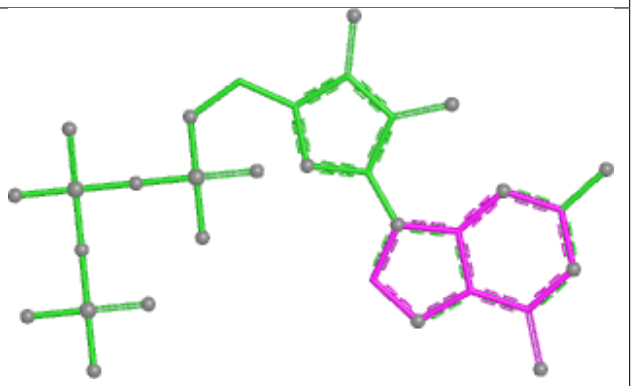


Rings

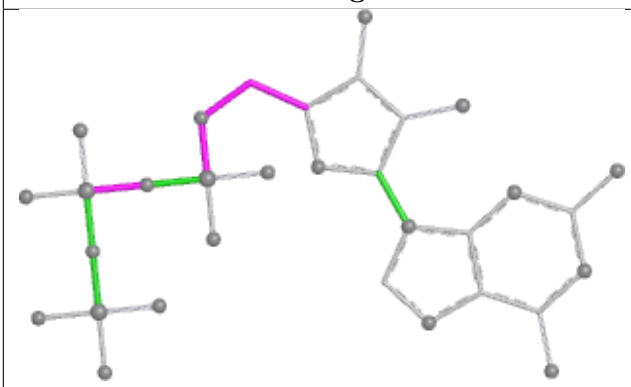
Ligand GTP TI 501



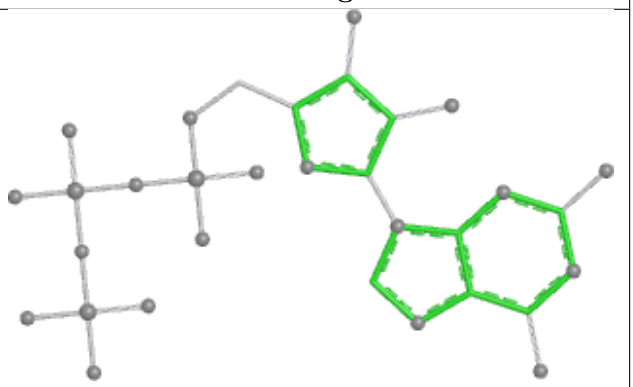
Bond lengths



Bond angles

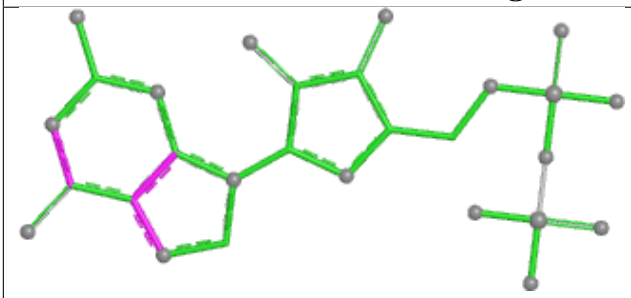


Torsions

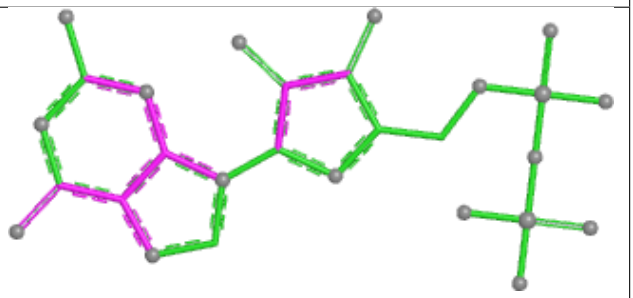


Rings

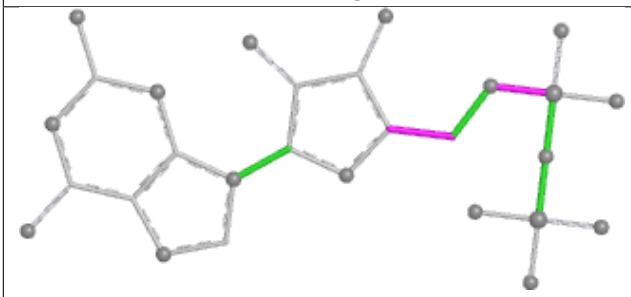
Ligand GDP OH 502



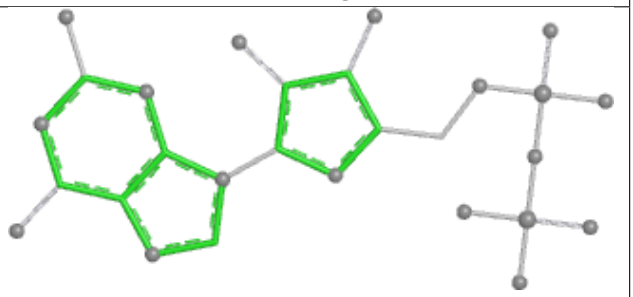
Bond lengths



Bond angles

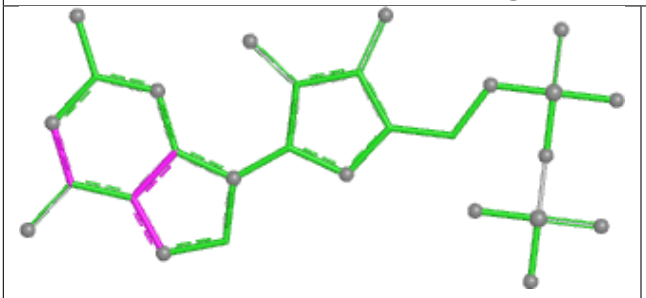


Torsions

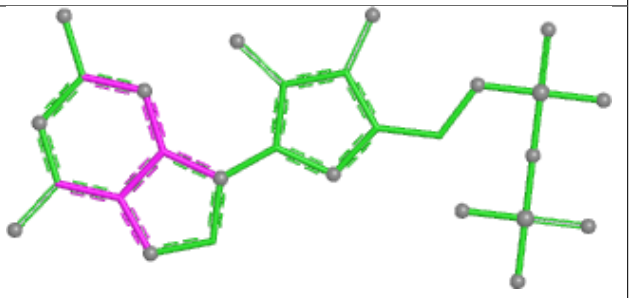


Rings

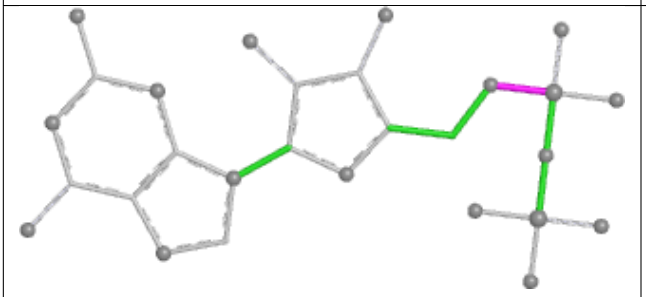
Ligand GDP WF 502



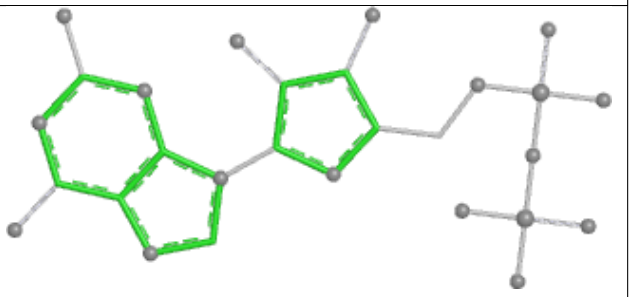
Bond lengths



Bond angles

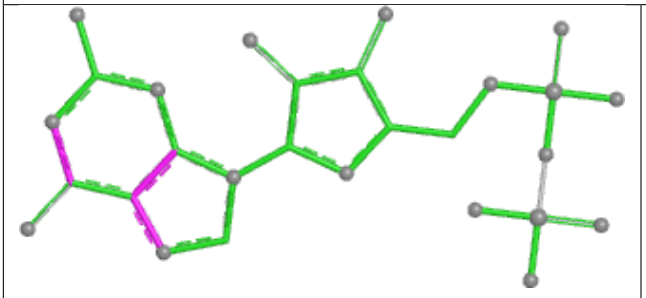


Torsions

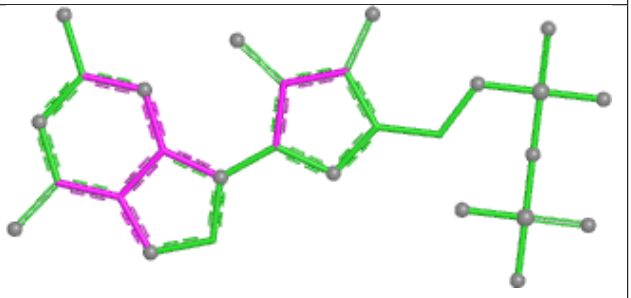


Rings

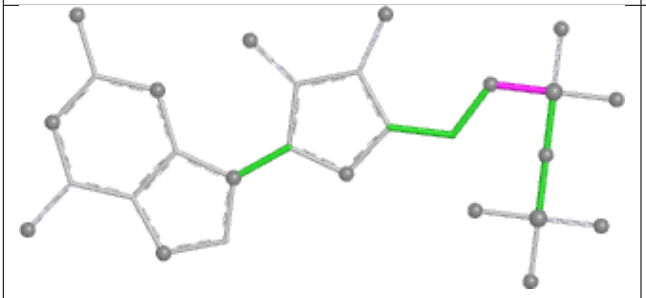
Ligand GDP PD 502



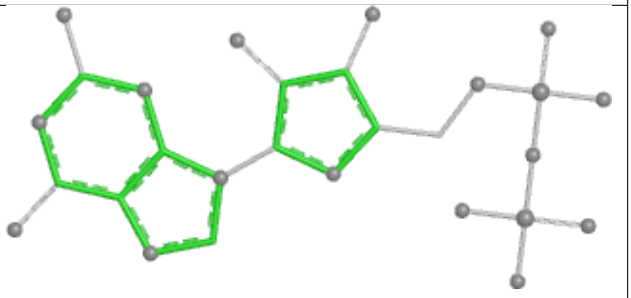
Bond lengths



Bond angles

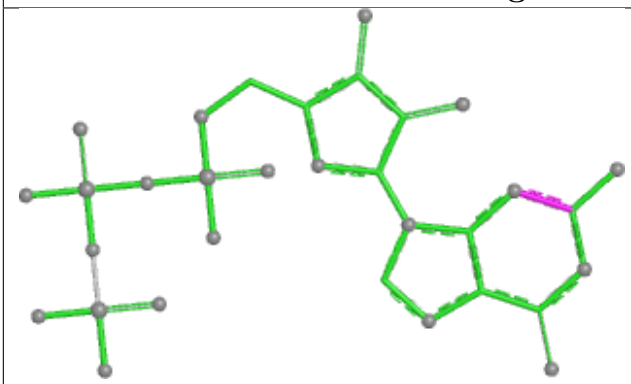


Torsions

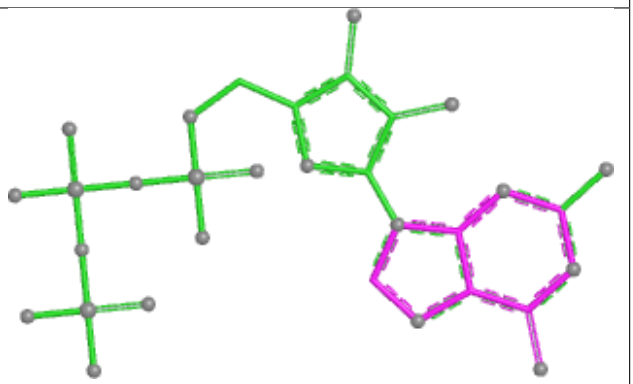


Rings

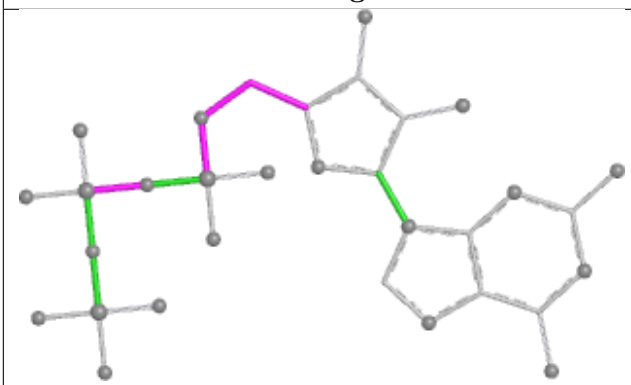
Ligand GTP KA 501



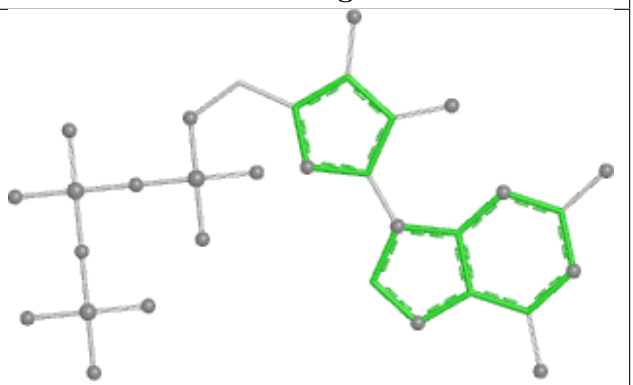
Bond lengths



Bond angles

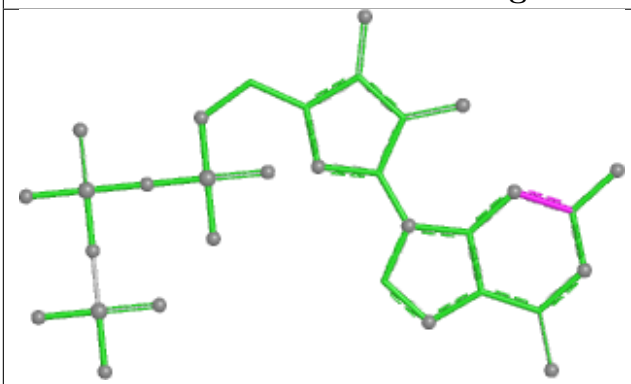


Torsions

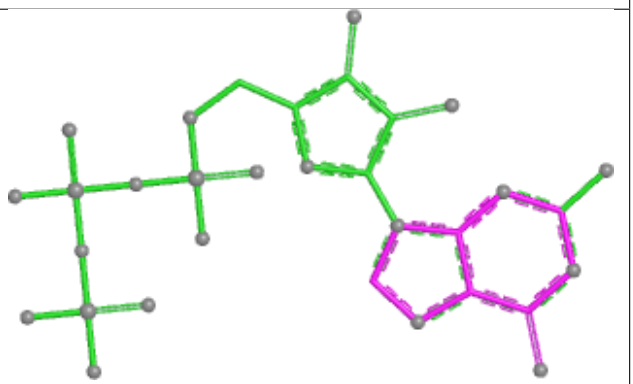


Rings

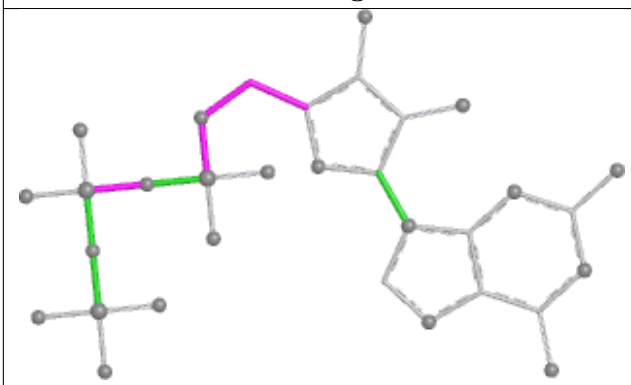
Ligand GTP BO 501



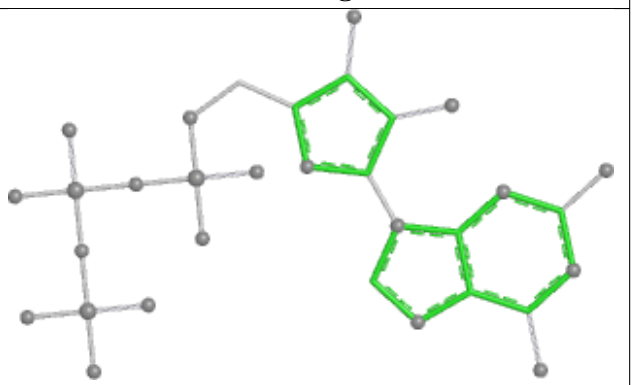
Bond lengths



Bond angles

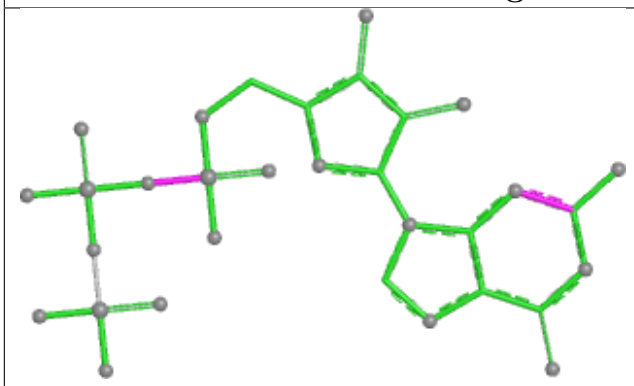


Torsions

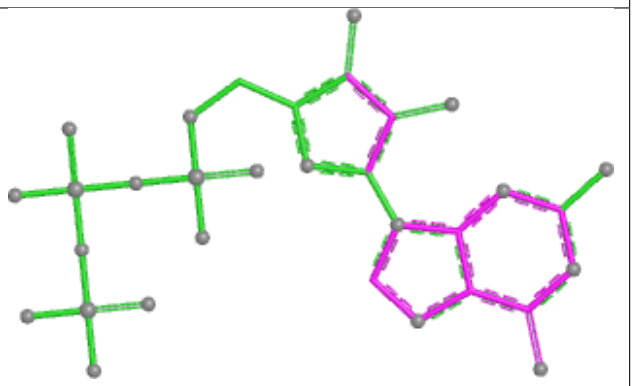


Rings

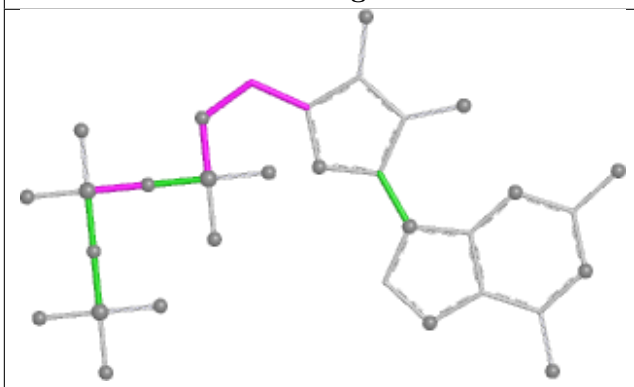
Ligand GTP RM 501



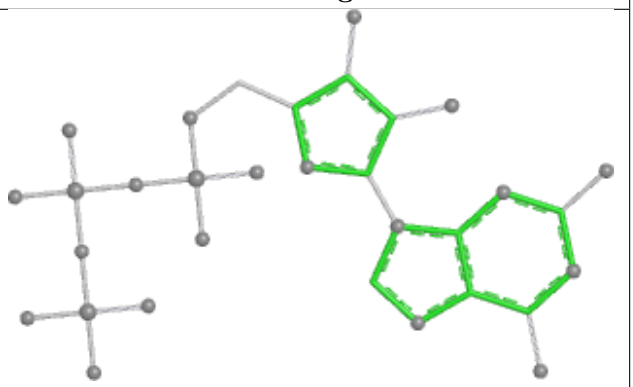
Bond lengths



Bond angles

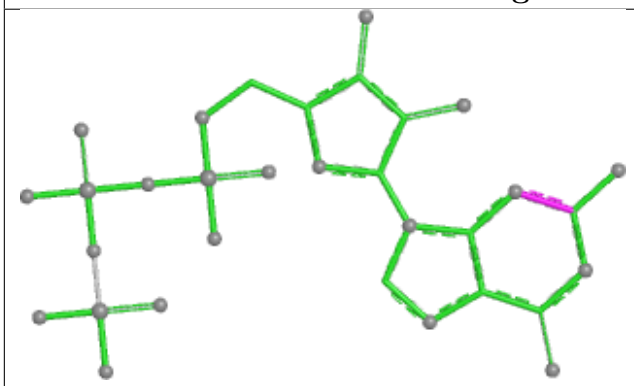


Torsions

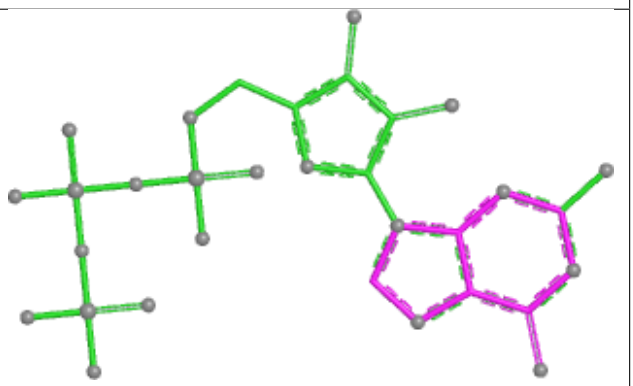


Rings

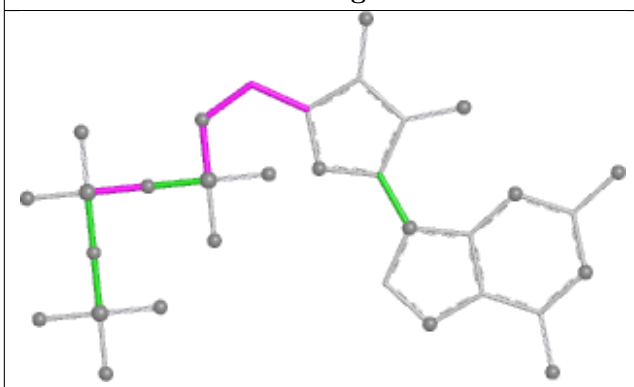
Ligand GTP LK 501



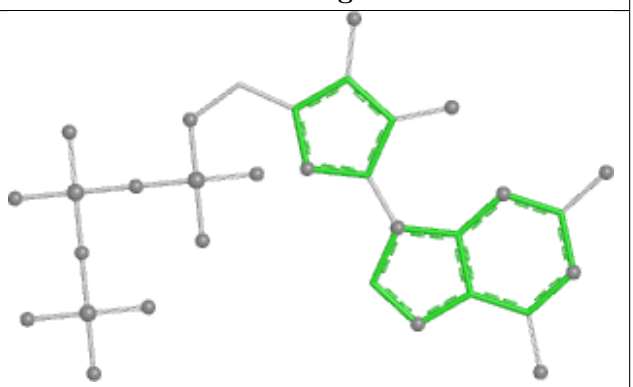
Bond lengths



Bond angles

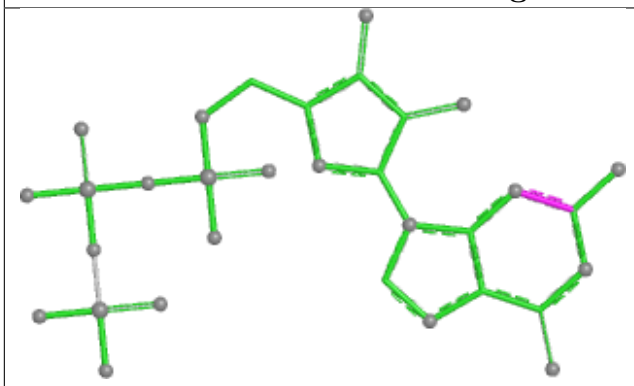


Torsions

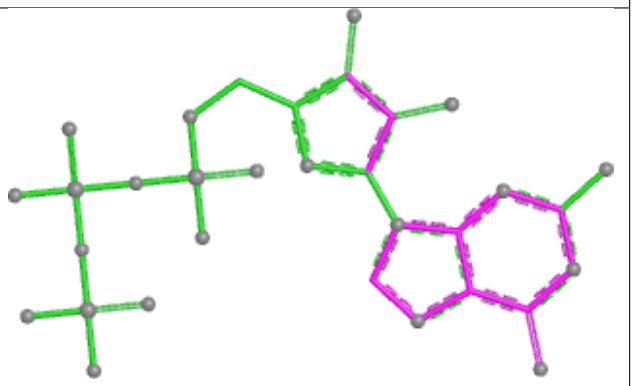


Rings

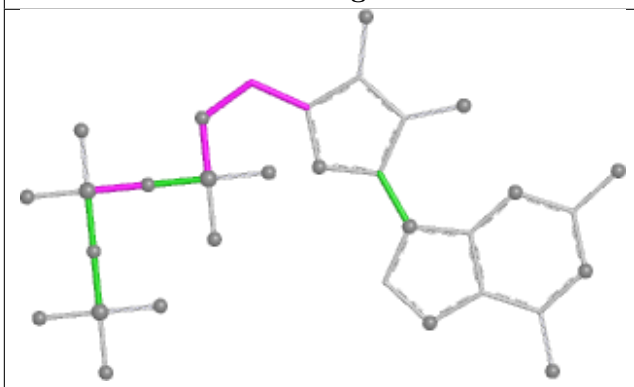
Ligand GTP SM 501



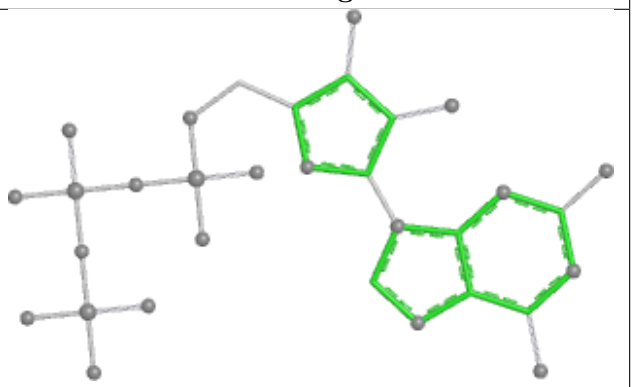
Bond lengths



Bond angles

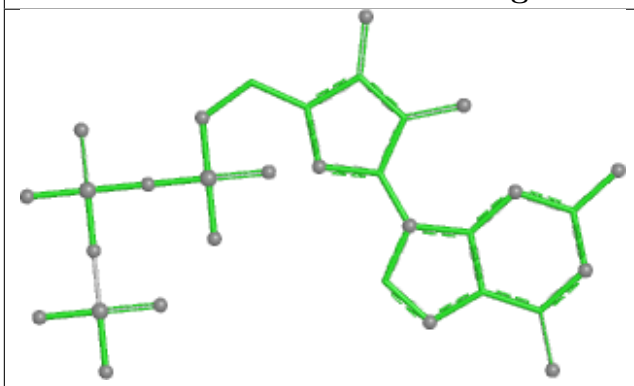


Torsions

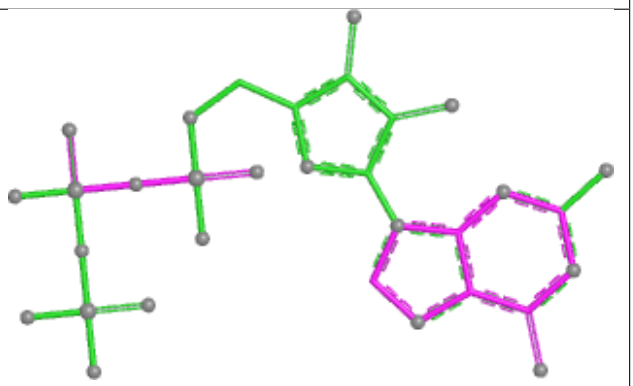


Rings

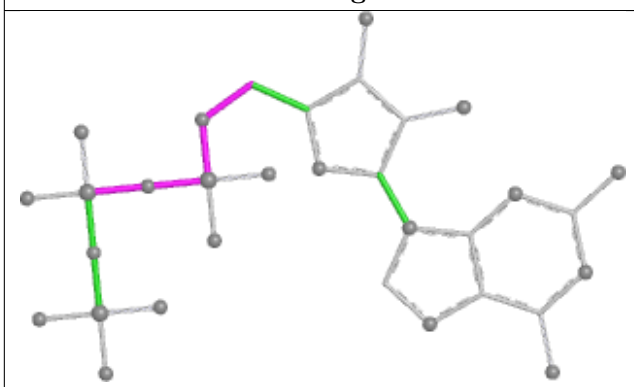
Ligand GTP KE 501



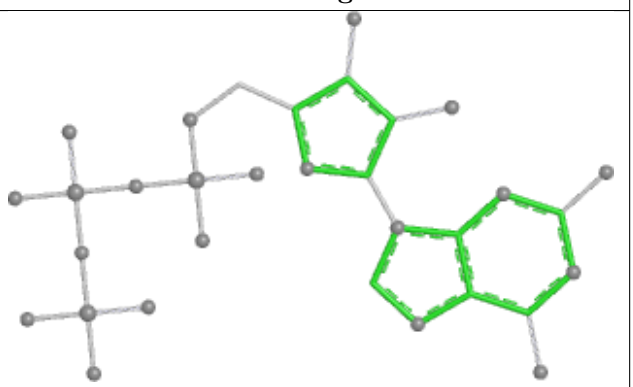
Bond lengths



Bond angles

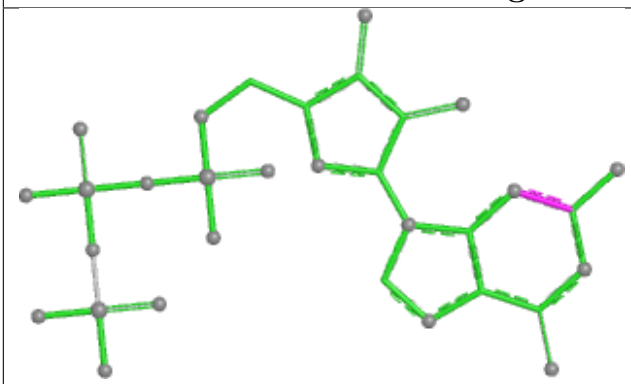


Torsions

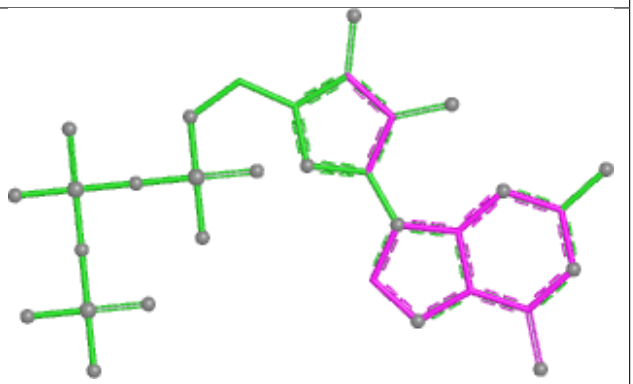


Rings

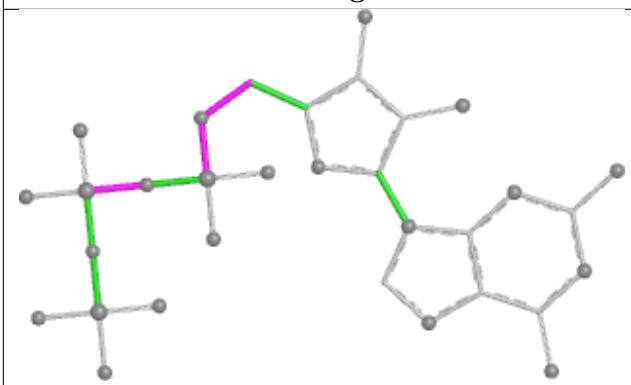
Ligand GTP KG 501



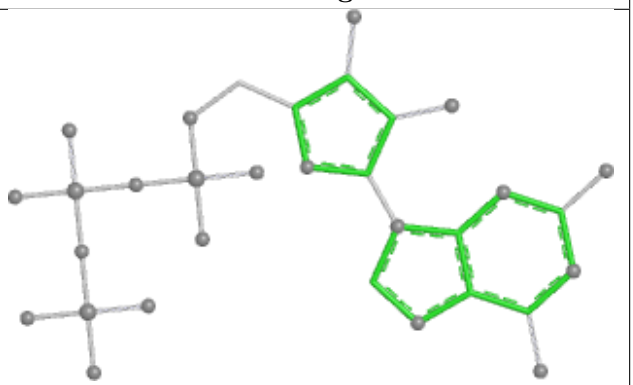
Bond lengths



Bond angles

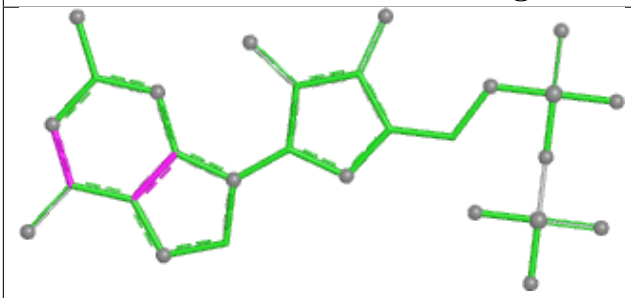


Torsions

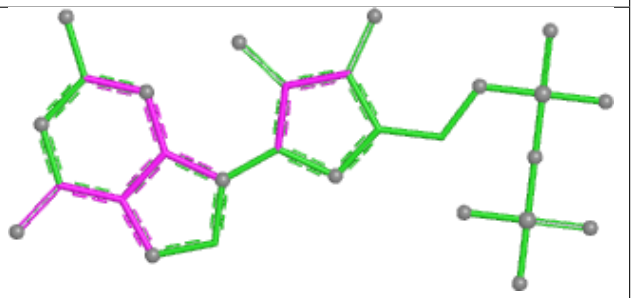


Rings

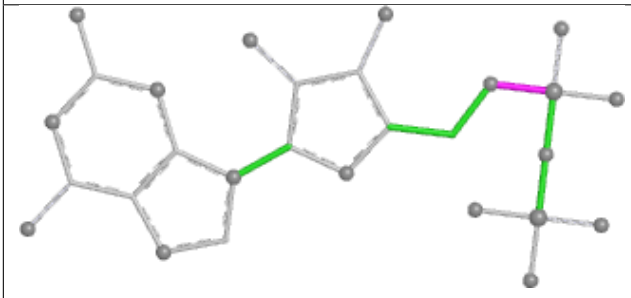
Ligand GDP JB 502



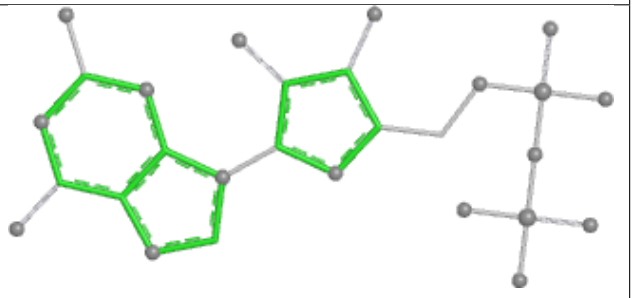
Bond lengths



Bond angles

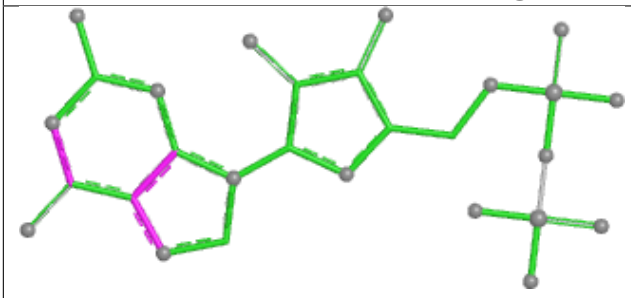


Torsions

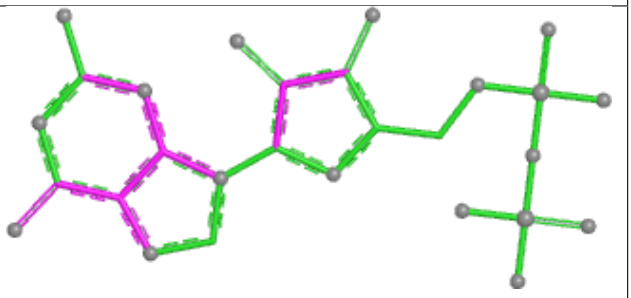


Rings

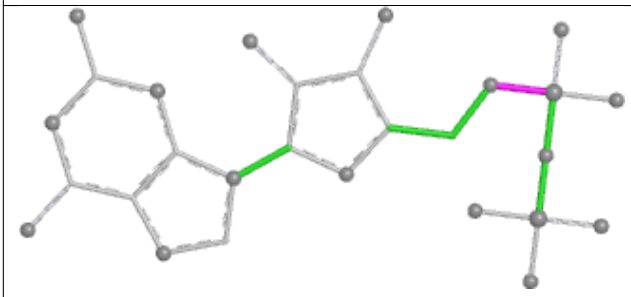
Ligand GDP TL 502



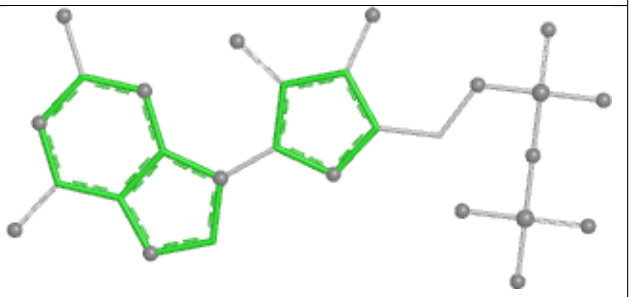
Bond lengths



Bond angles

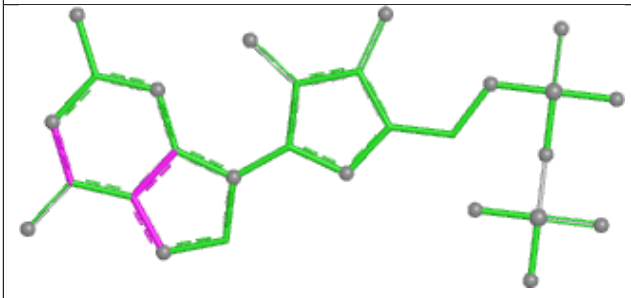


Torsions

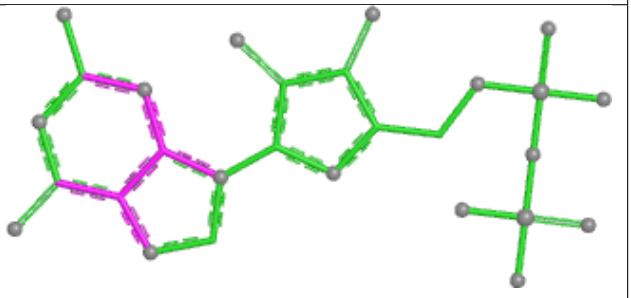


Rings

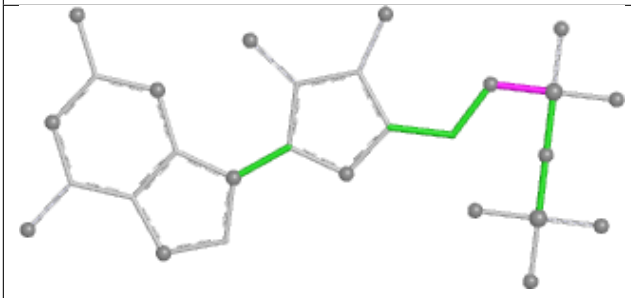
Ligand GDP WJ 502



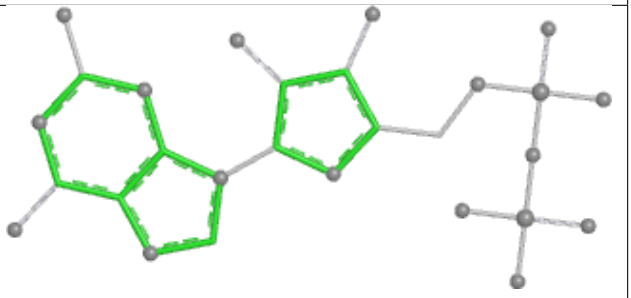
Bond lengths



Bond angles

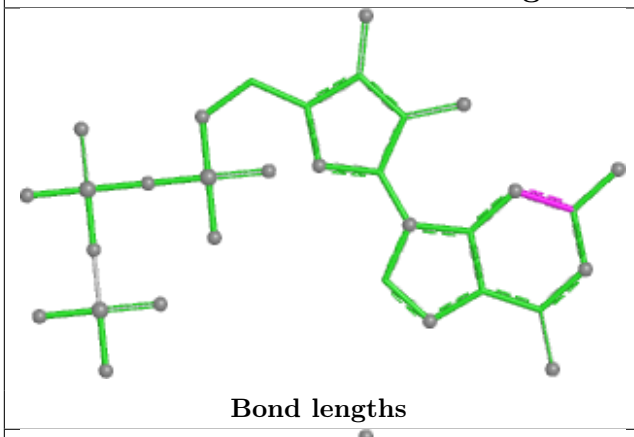


Torsions

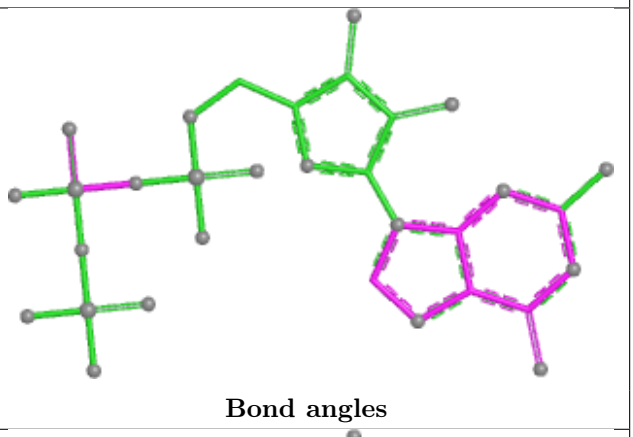


Rings

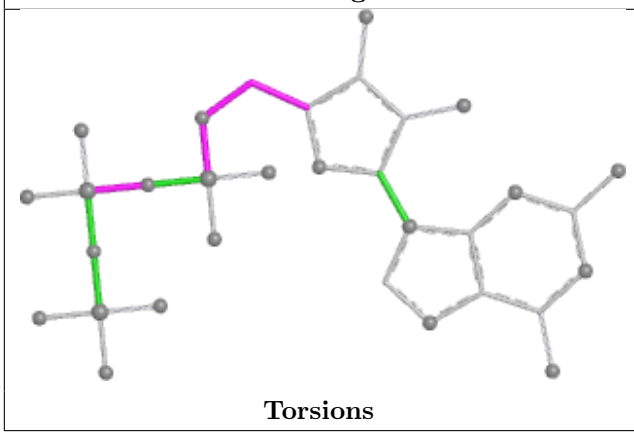
Ligand GTP II 501



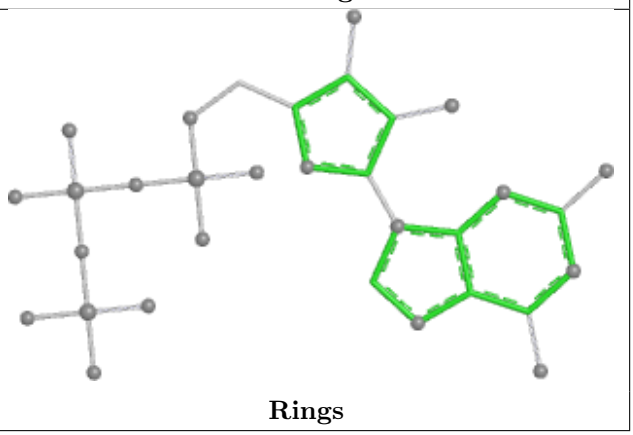
Bond lengths



Bond angles

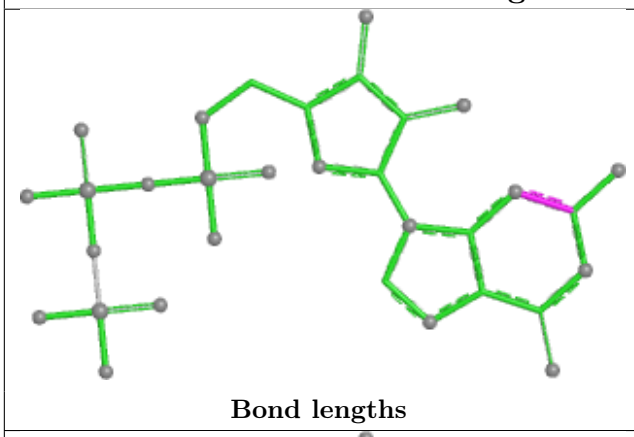


Torsions

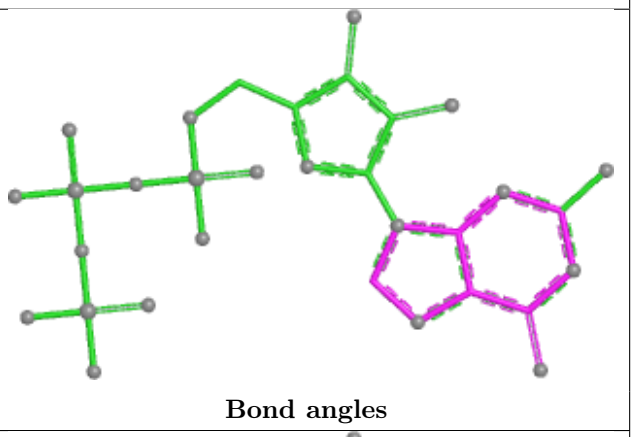


Rings

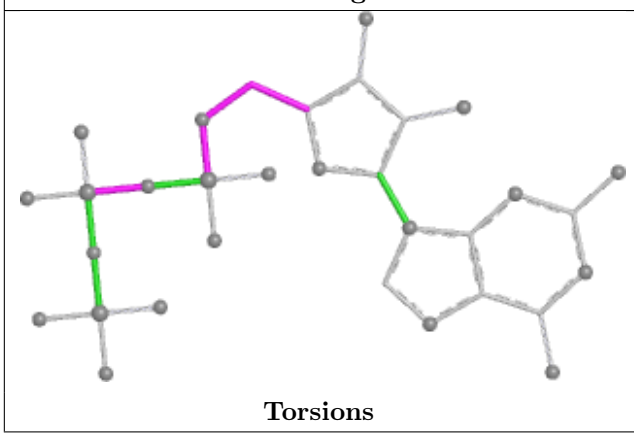
Ligand GTP EM 501



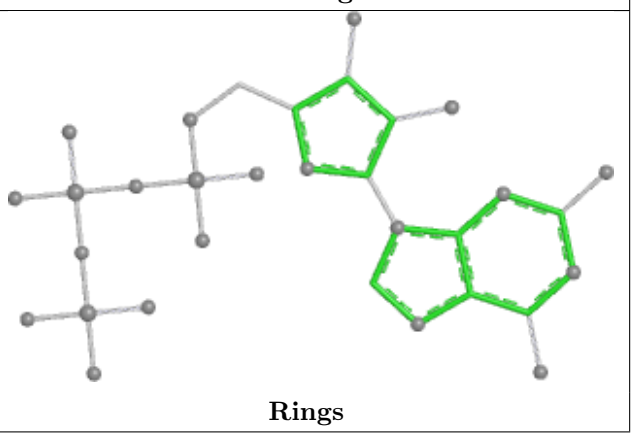
Bond lengths



Bond angles

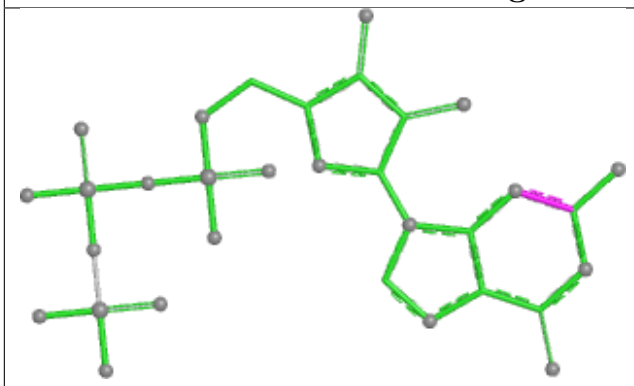


Torsions

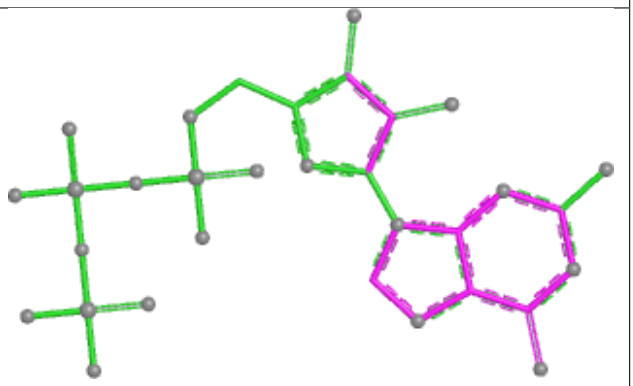


Rings

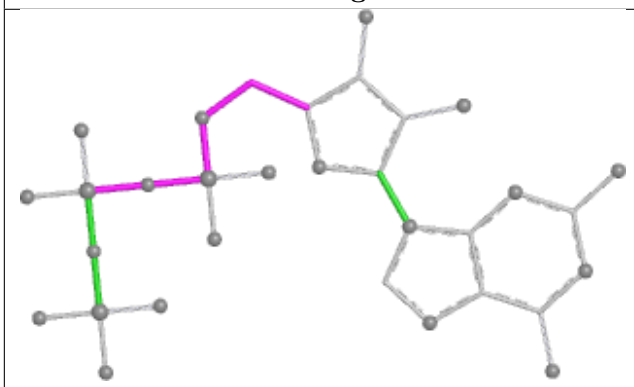
Ligand GTP HK 501



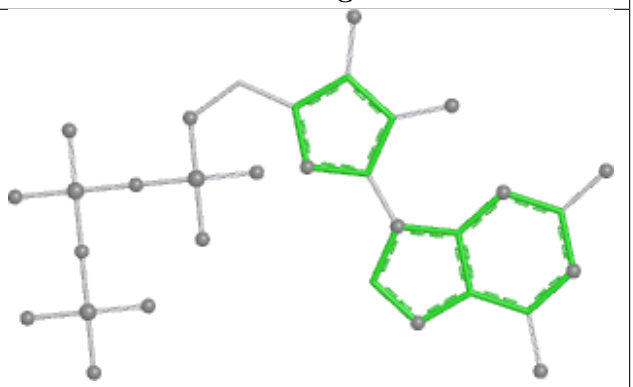
Bond lengths



Bond angles

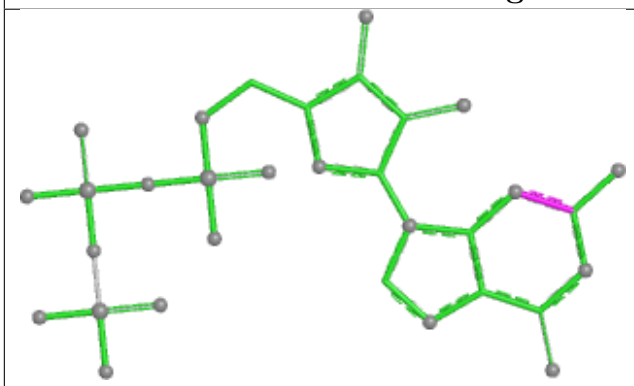


Torsions

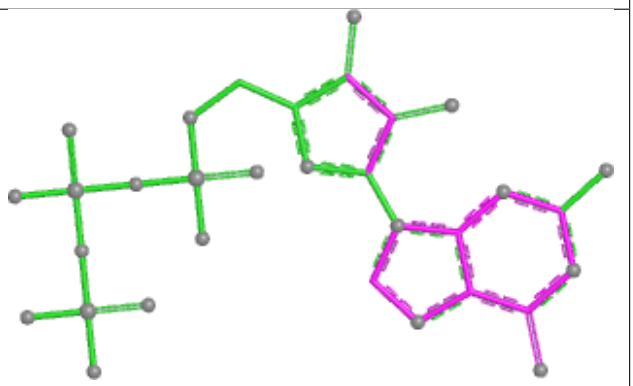


Rings

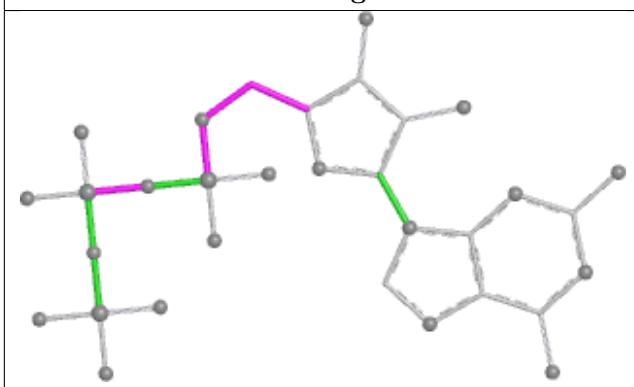
Ligand GTP OM 501



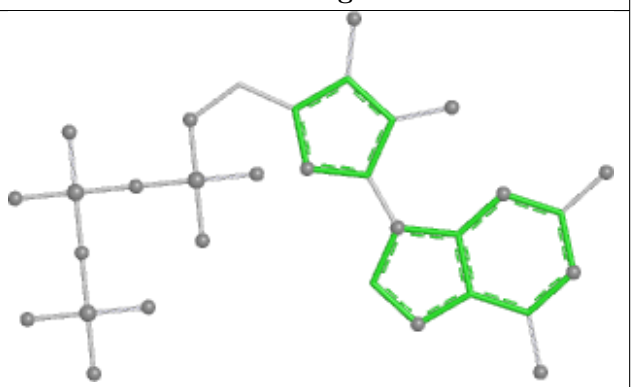
Bond lengths



Bond angles

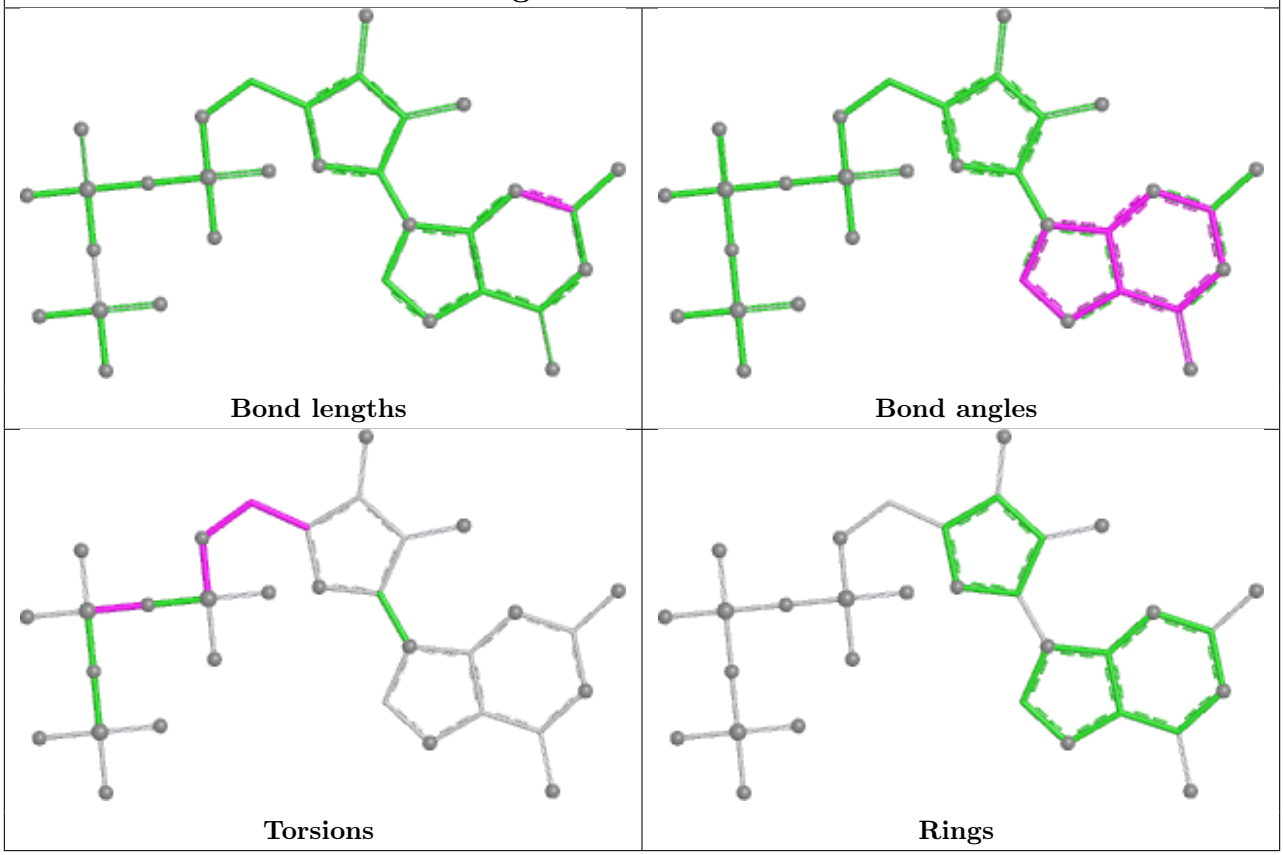


Torsions

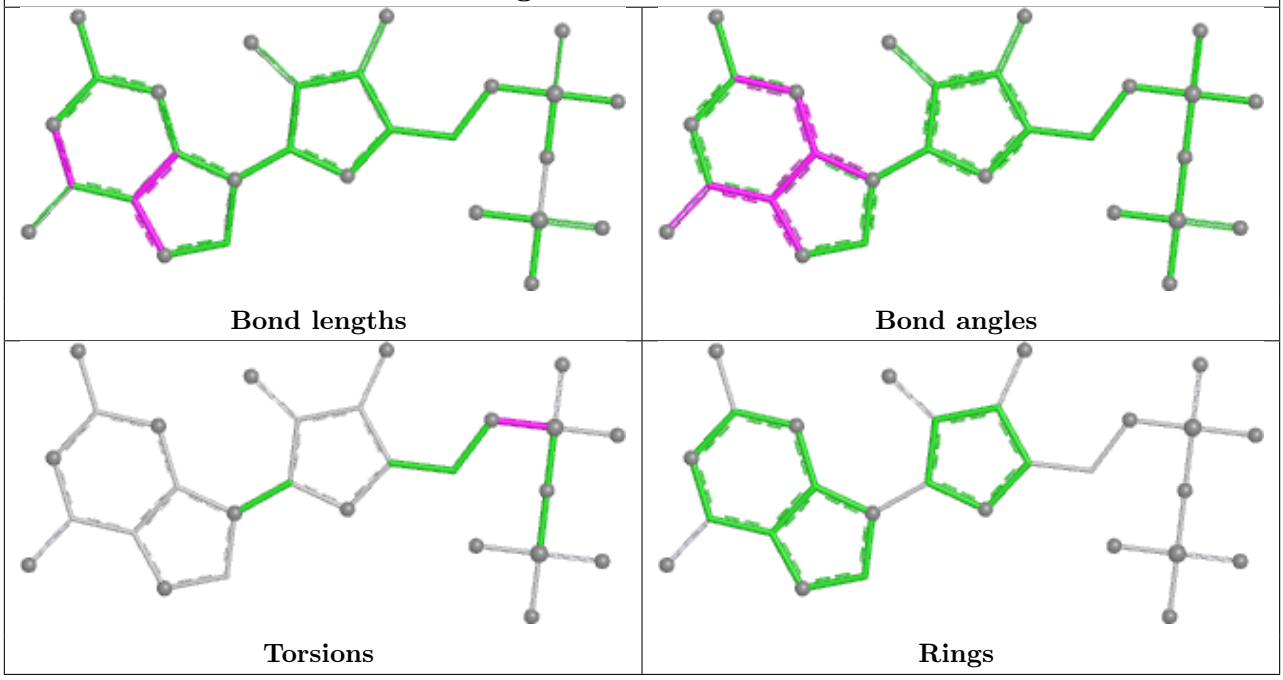


Rings

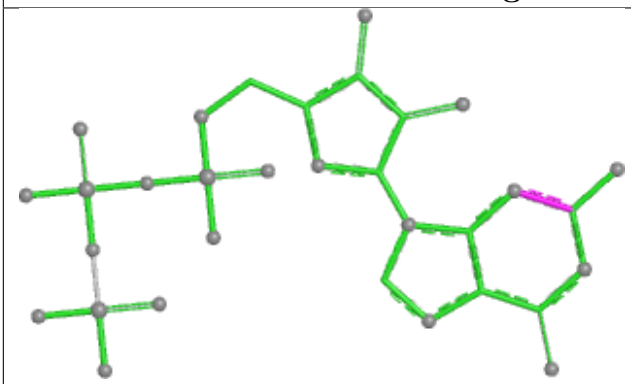
Ligand GTP LO 501



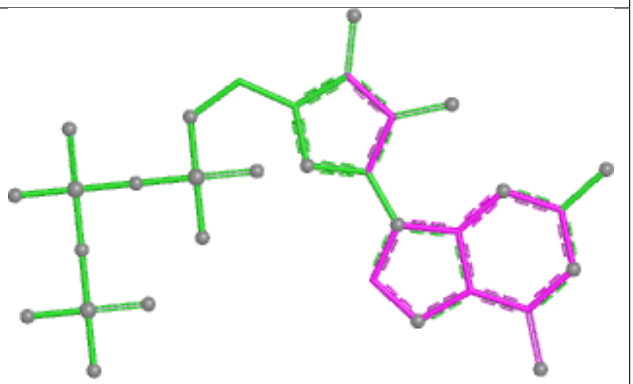
Ligand GDP LJ 502



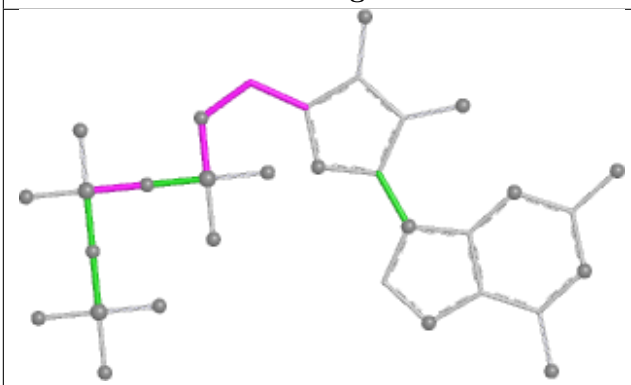
Ligand GTP WK 501



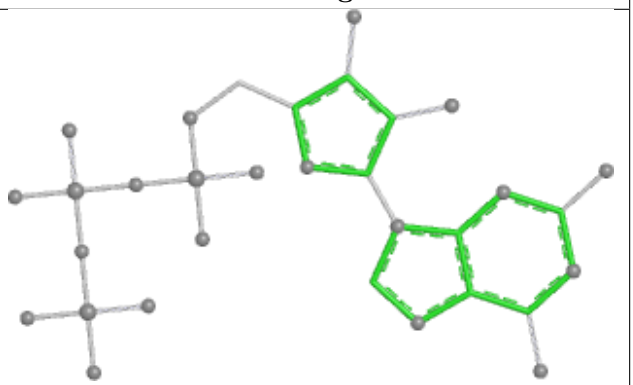
Bond lengths



Bond angles

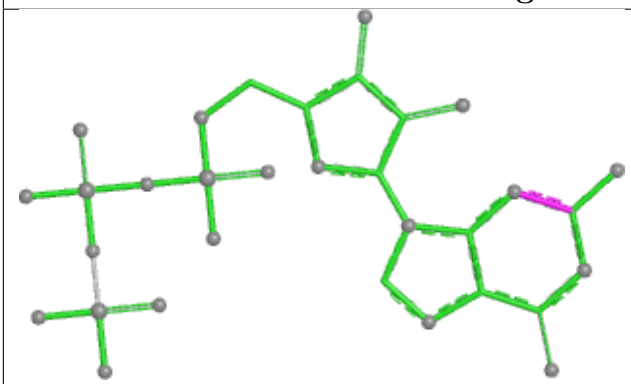


Torsions

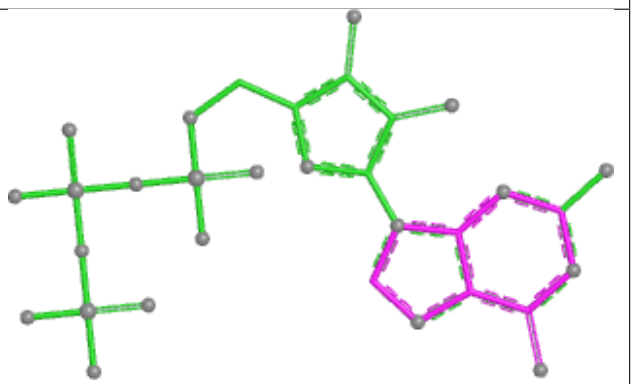


Rings

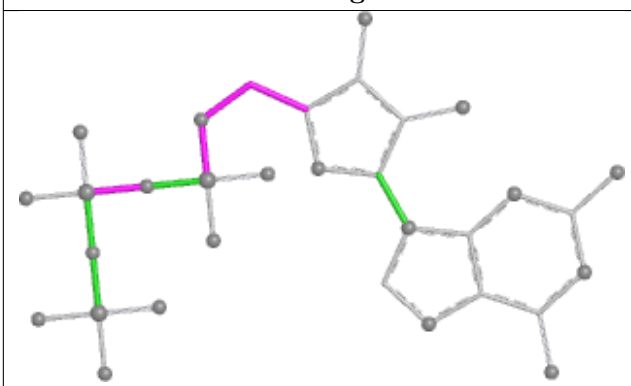
Ligand GTP BI 501



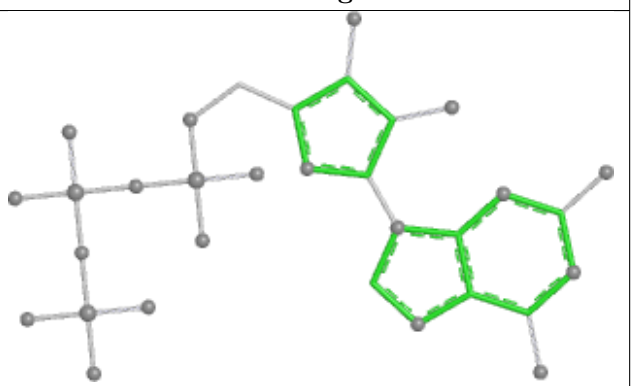
Bond lengths



Bond angles

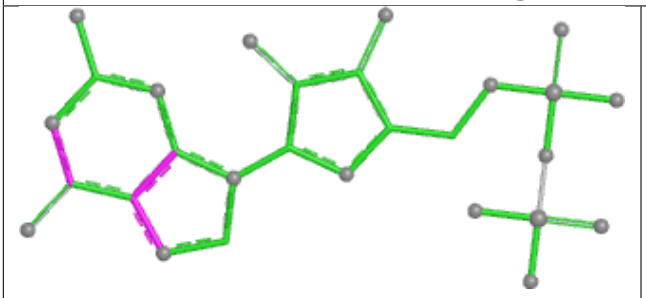


Torsions

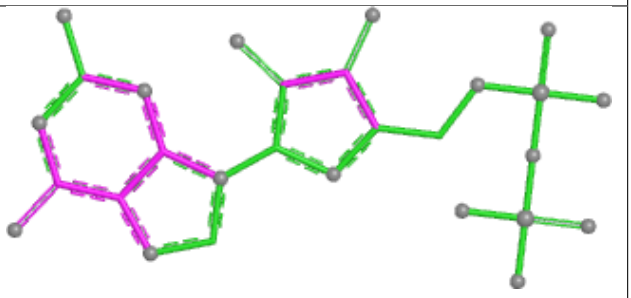


Rings

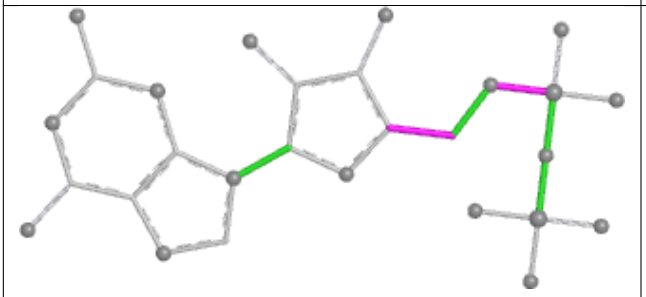
Ligand GDP OJ 502



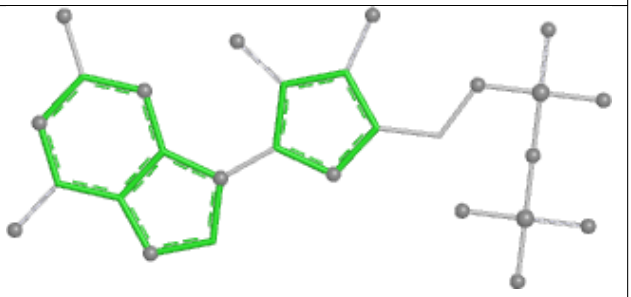
Bond lengths



Bond angles

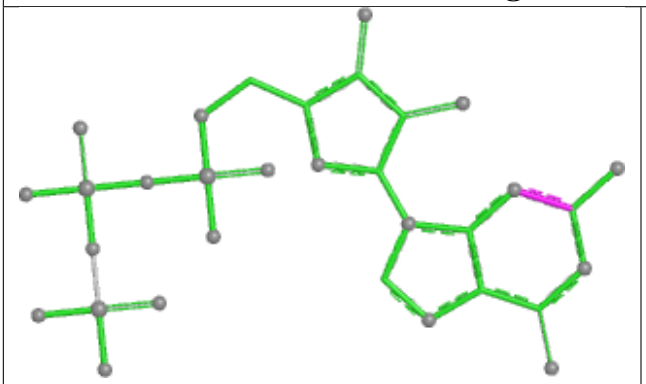


Torsions

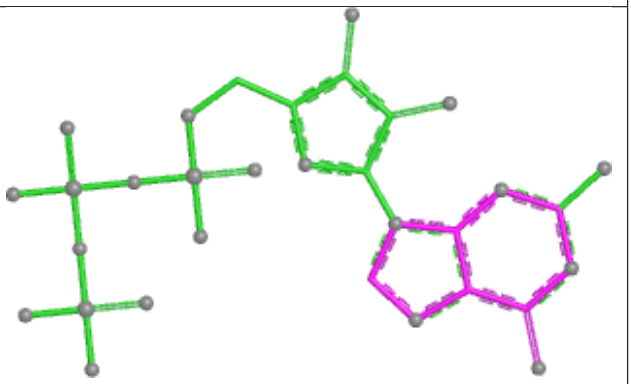


Rings

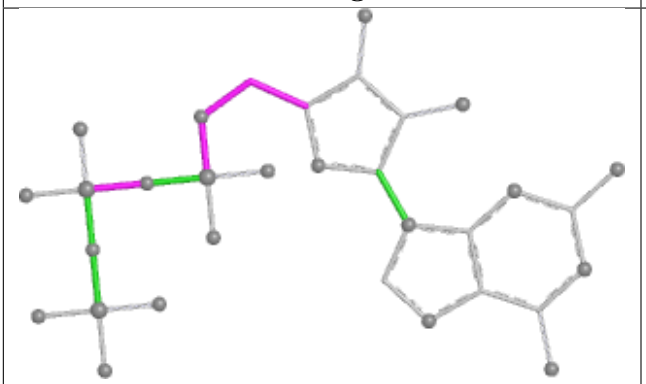
Ligand GTP WC 501



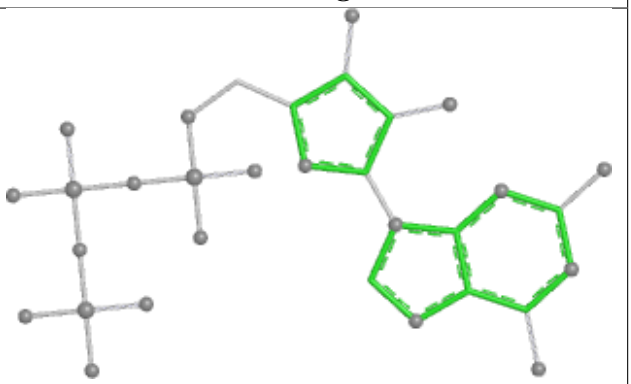
Bond lengths



Bond angles

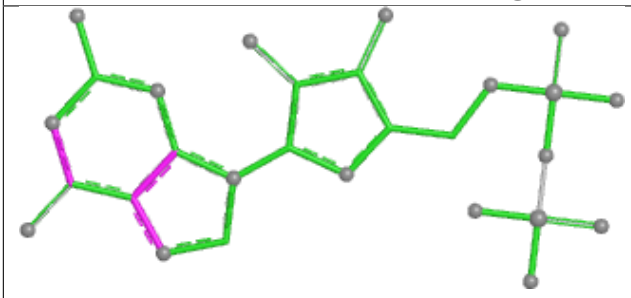


Torsions

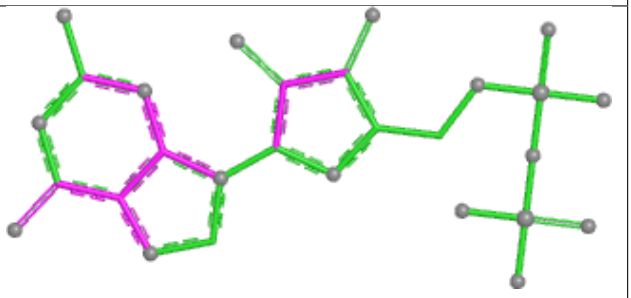


Rings

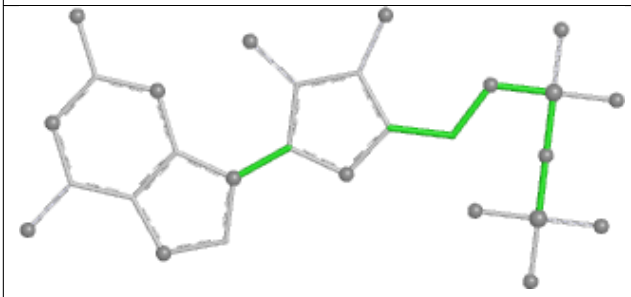
Ligand GDP HF 502



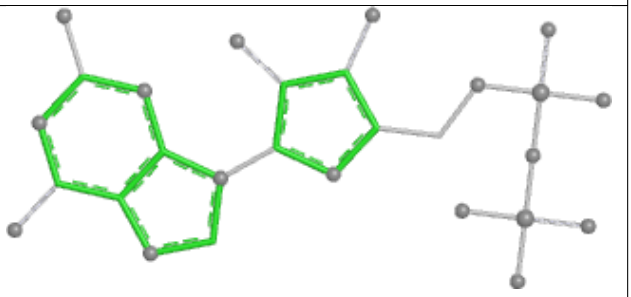
Bond lengths



Bond angles

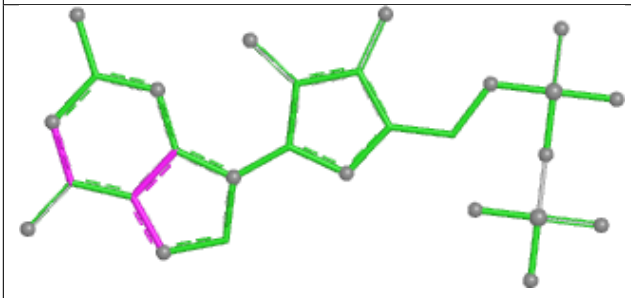


Torsions

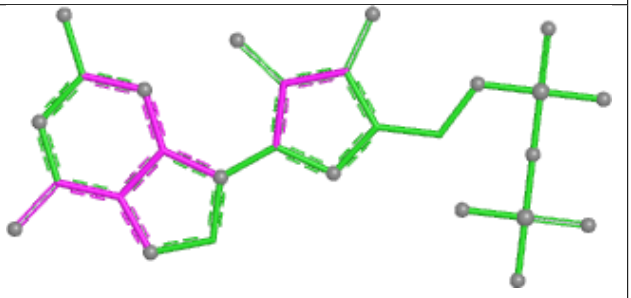


Rings

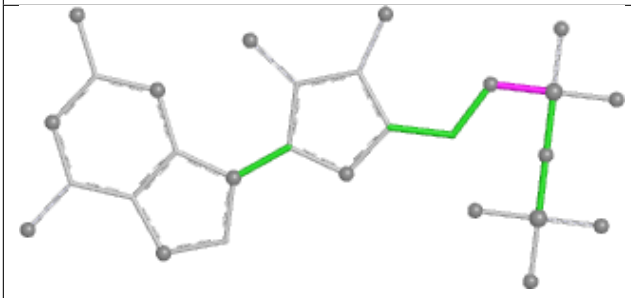
Ligand GDP NF 502



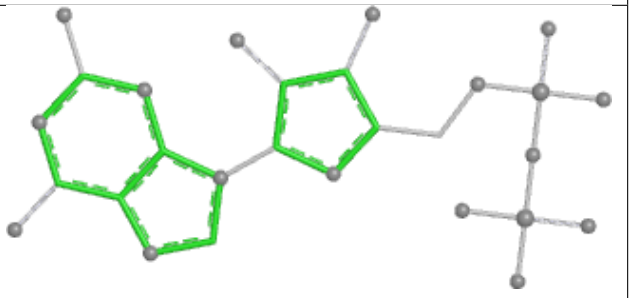
Bond lengths



Bond angles

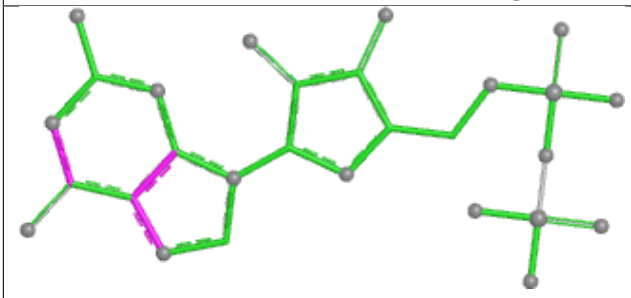


Torsions

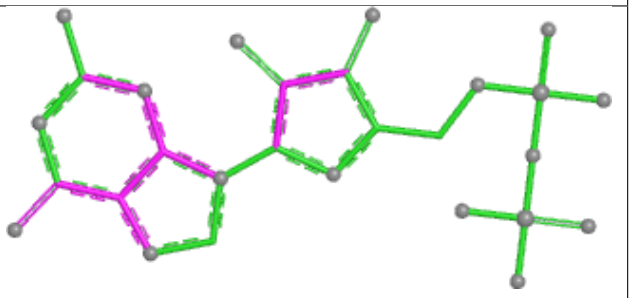


Rings

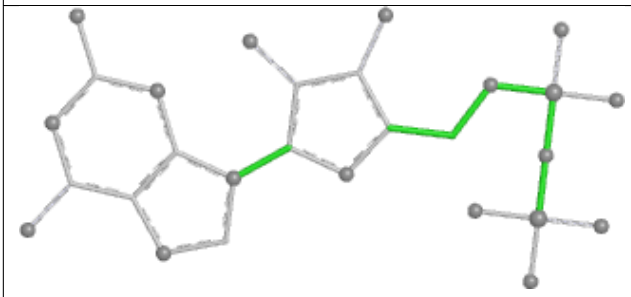
Ligand GDP BN 502



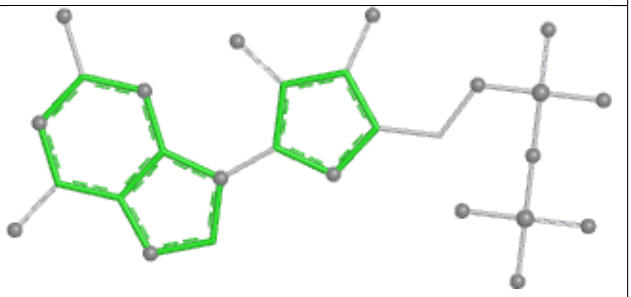
Bond lengths



Bond angles

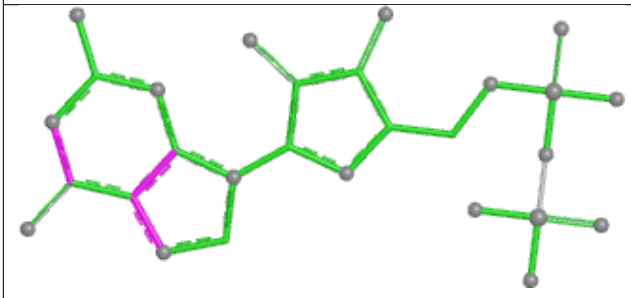


Torsions

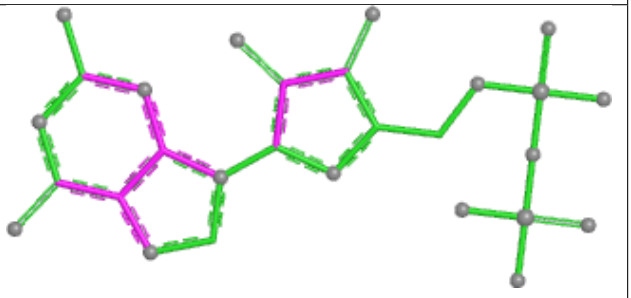


Rings

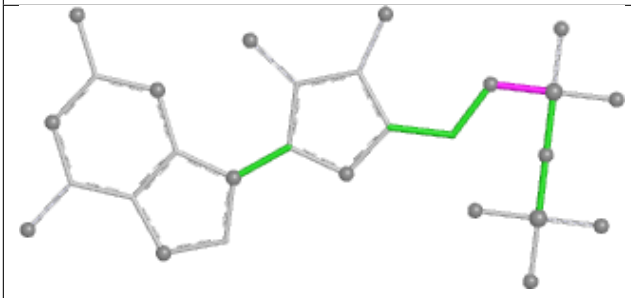
Ligand GDP PF 502



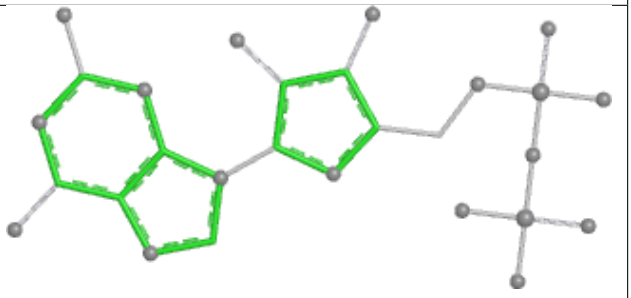
Bond lengths



Bond angles

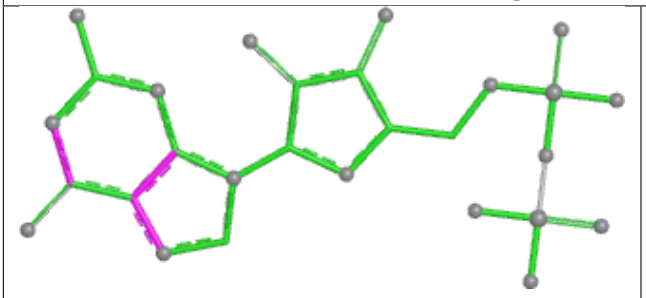


Torsions

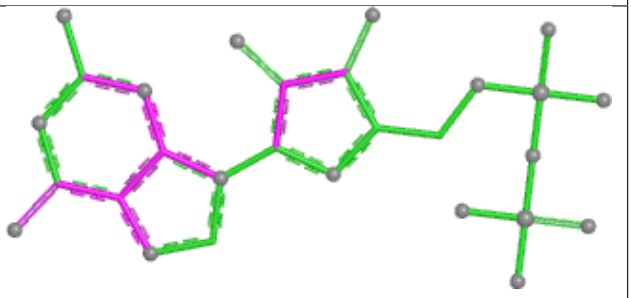


Rings

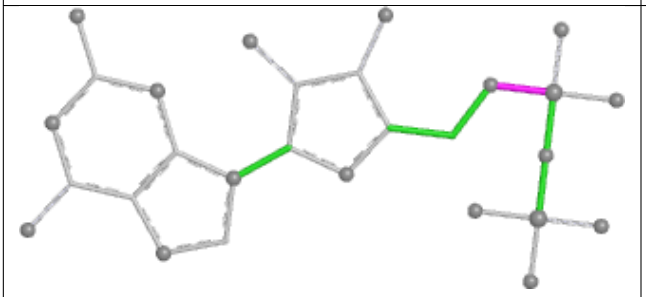
Ligand GDP MJ 502



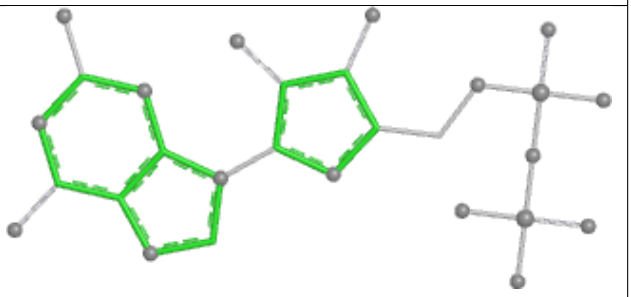
Bond lengths



Bond angles

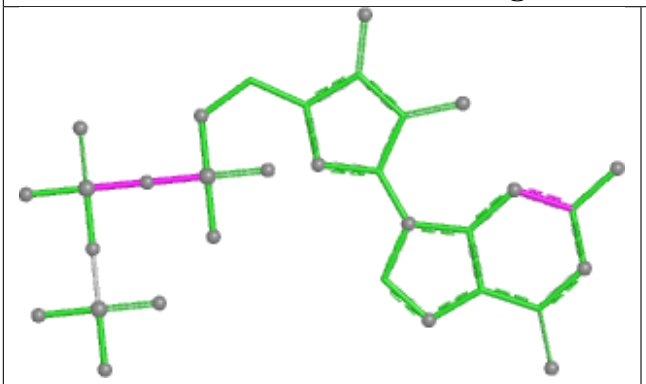


Torsions

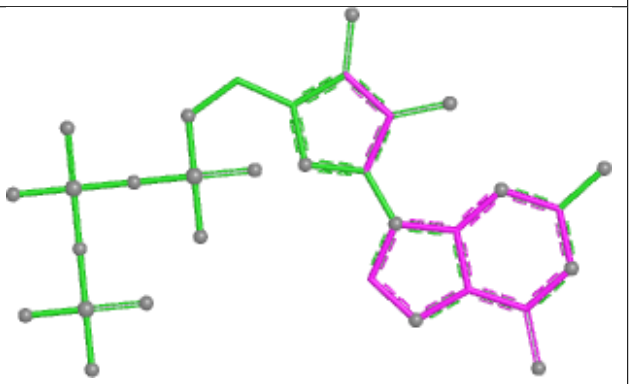


Rings

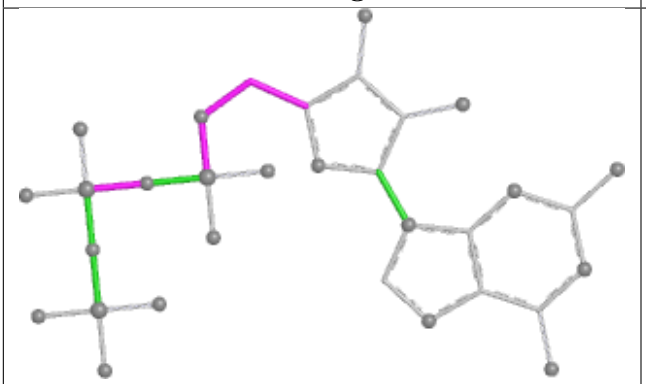
Ligand GTP RG 501



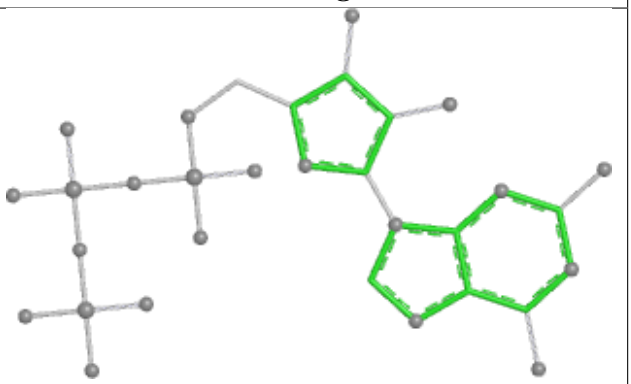
Bond lengths



Bond angles

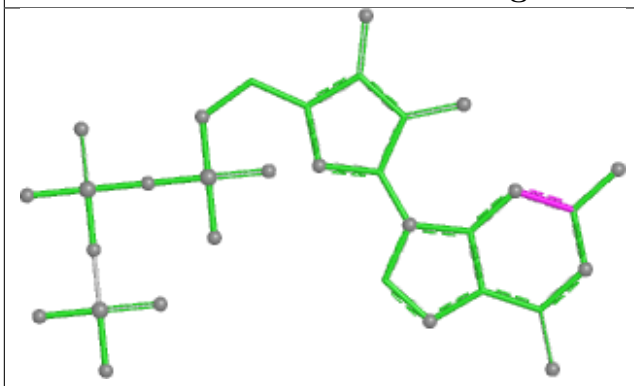


Torsions

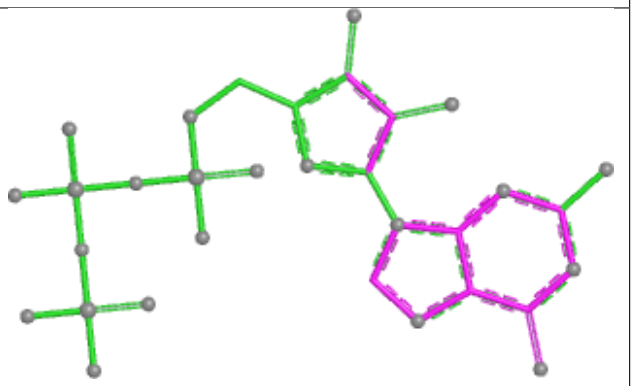


Rings

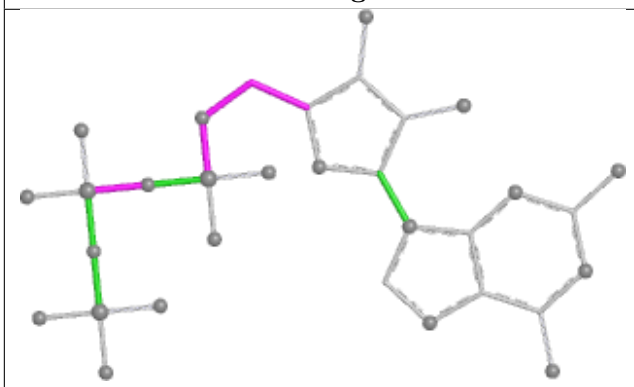
Ligand GTP TK 501



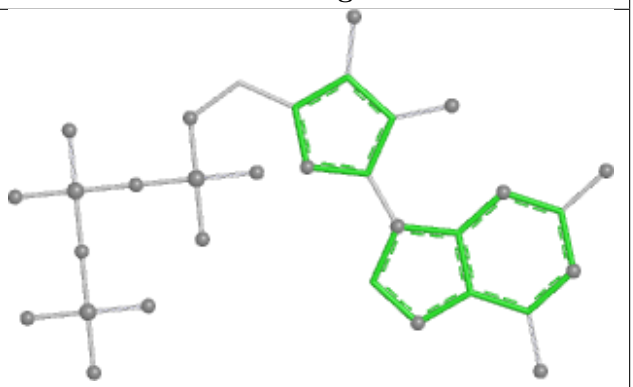
Bond lengths



Bond angles

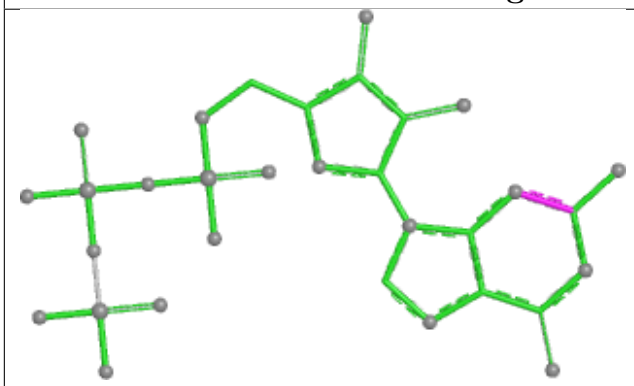


Torsions

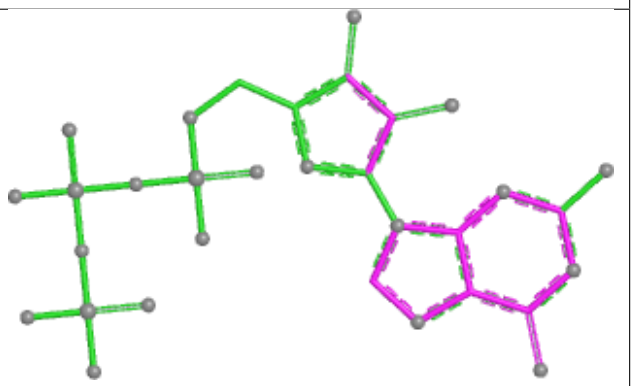


Rings

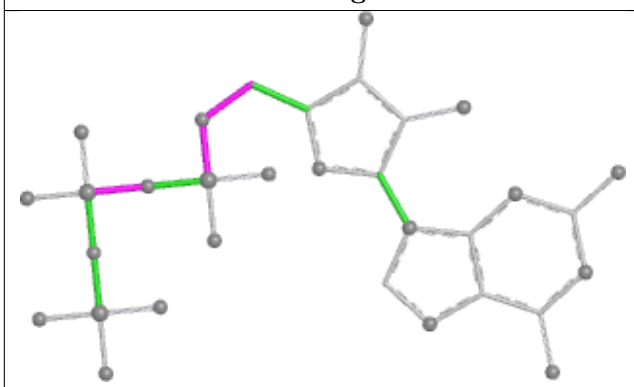
Ligand GTP CM 501



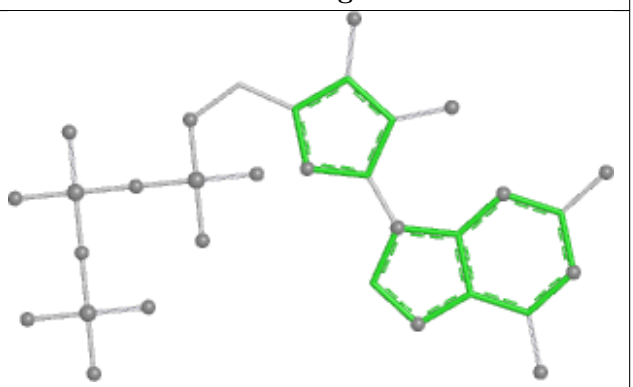
Bond lengths



Bond angles

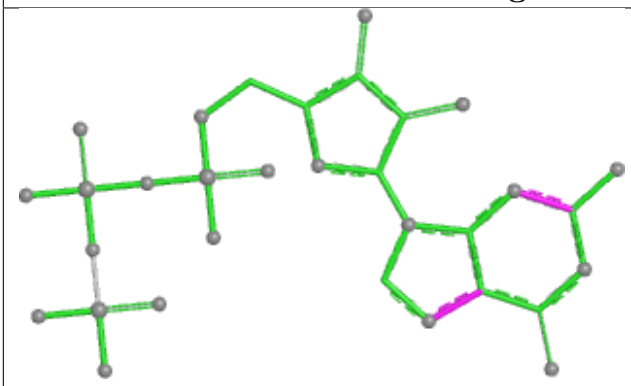


Torsions

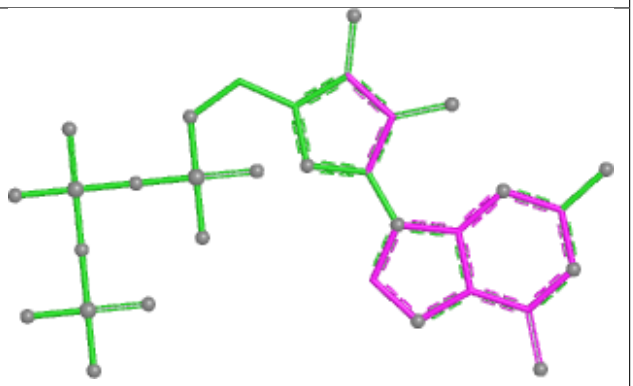


Rings

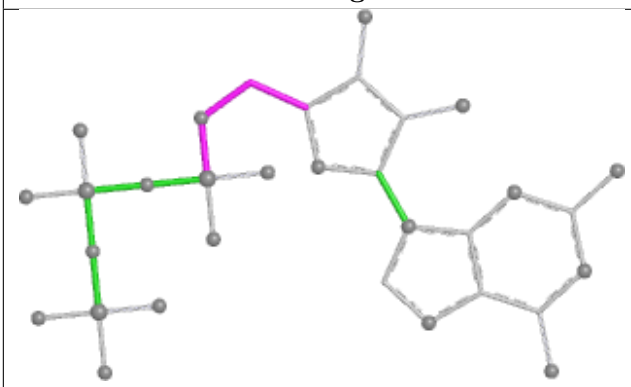
Ligand GTP CK 501



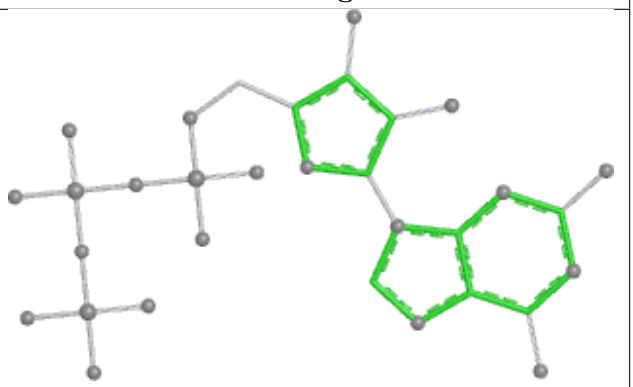
Bond lengths



Bond angles

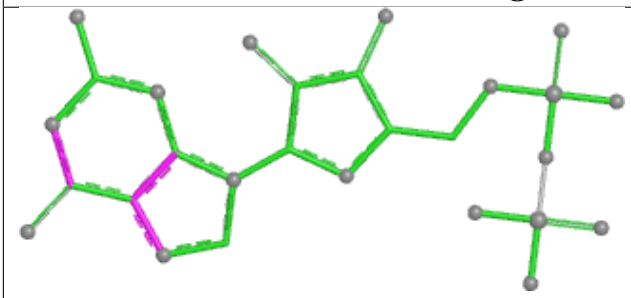


Torsions

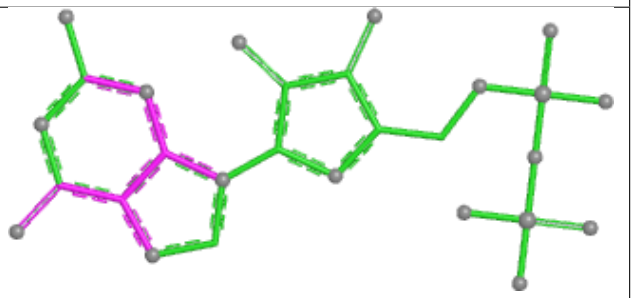


Rings

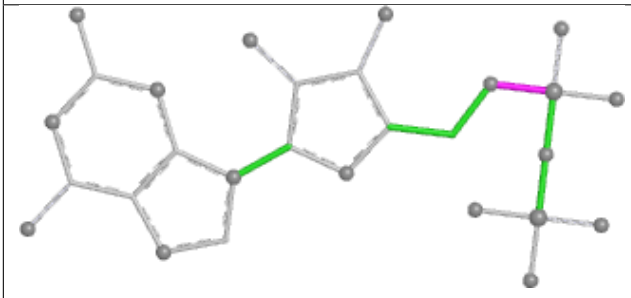
Ligand GDP EH 502



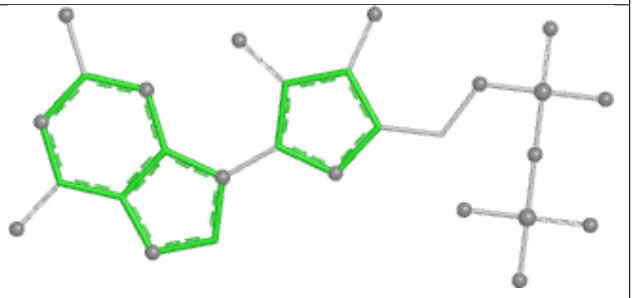
Bond lengths



Bond angles

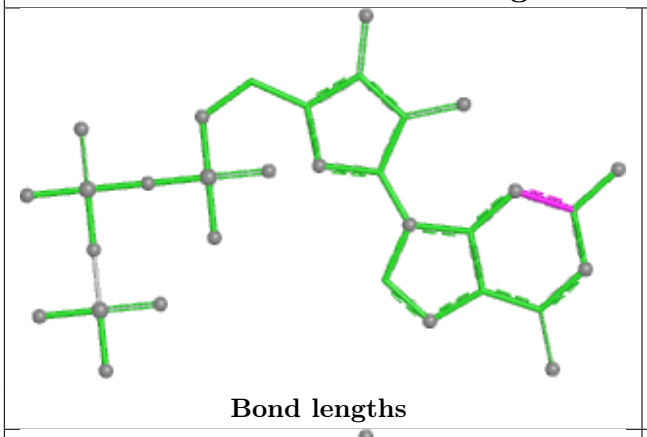


Torsions

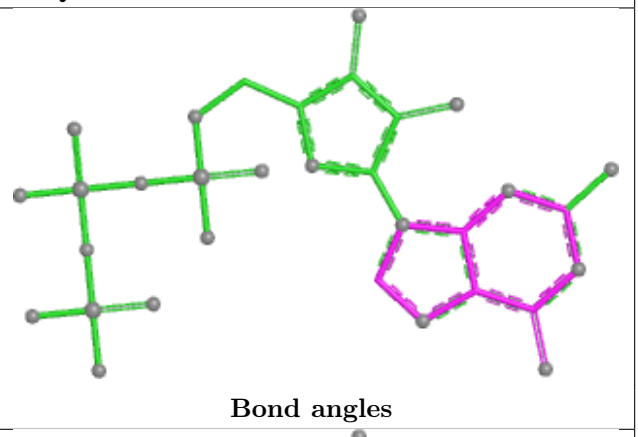


Rings

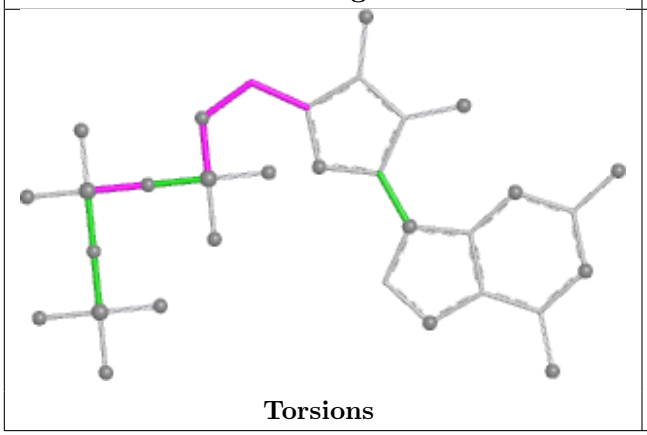
Ligand GTP QC 501



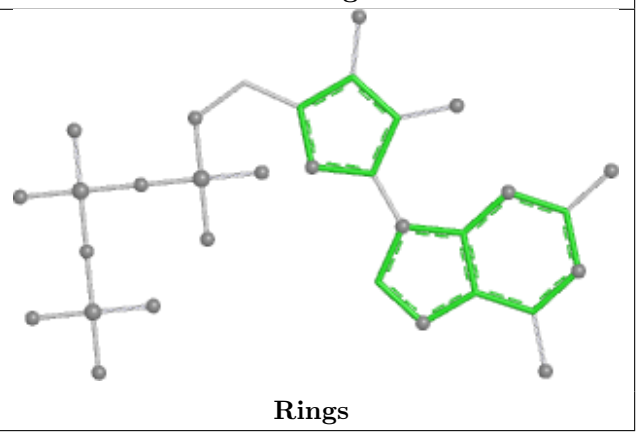
Bond lengths



Bond angles

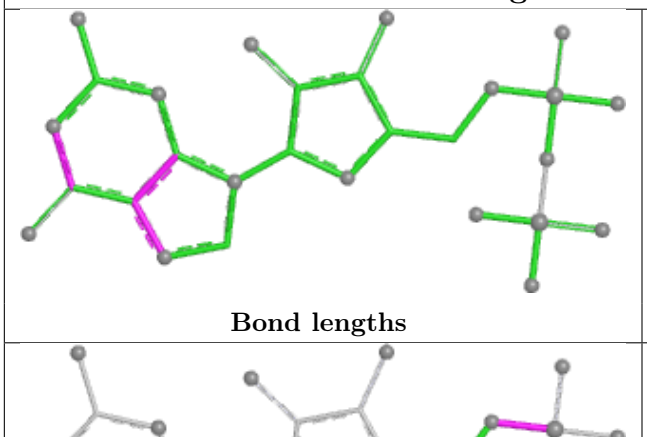


Torsions

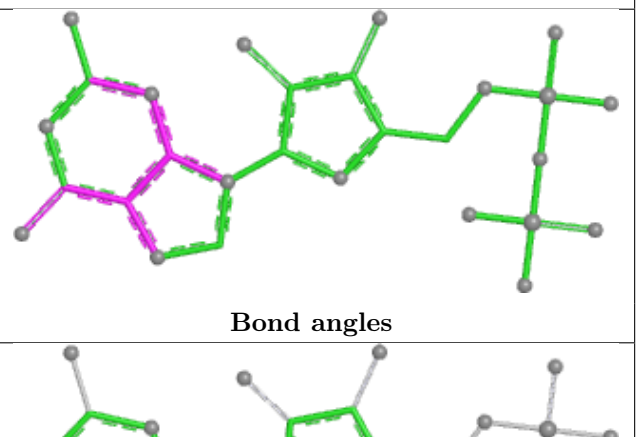


Rings

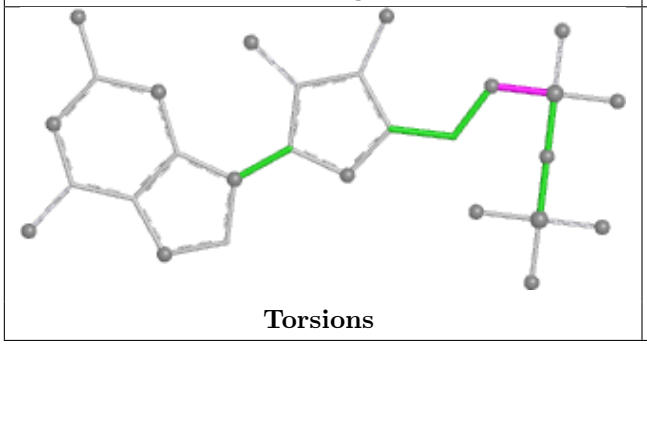
Ligand GDP EN 502



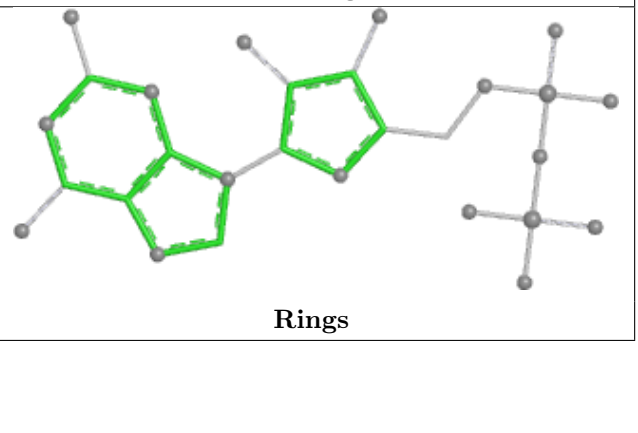
Bond lengths



Bond angles

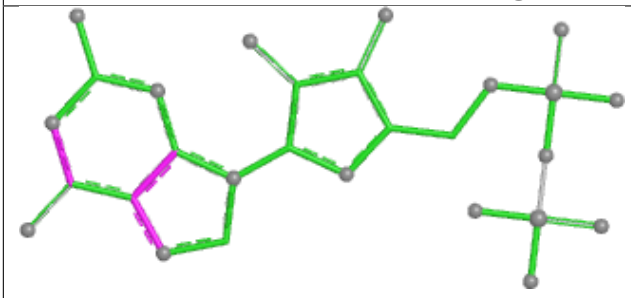


Torsions

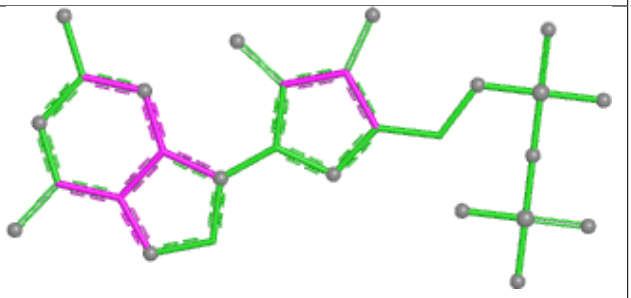


Rings

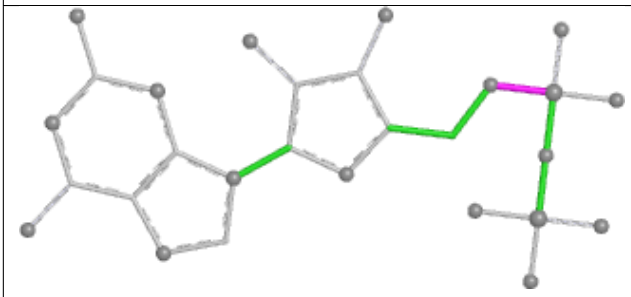
Ligand GDP DL 502



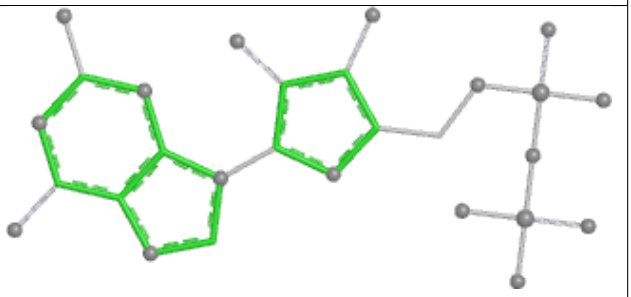
Bond lengths



Bond angles

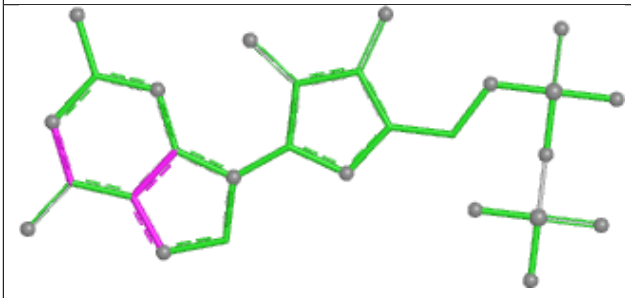


Torsions

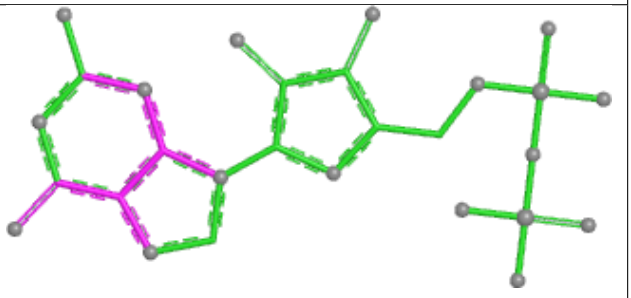


Rings

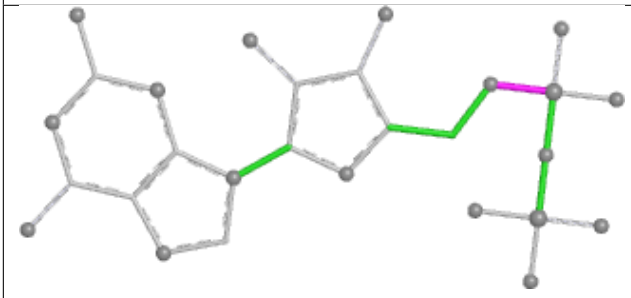
Ligand GDP SH 502



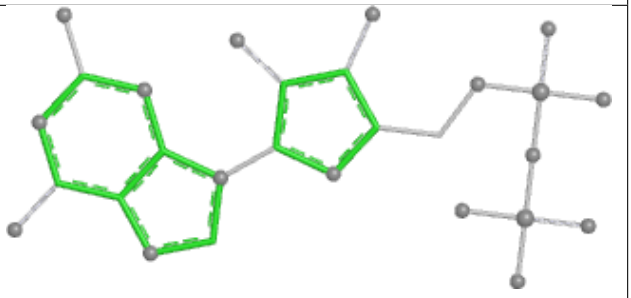
Bond lengths



Bond angles

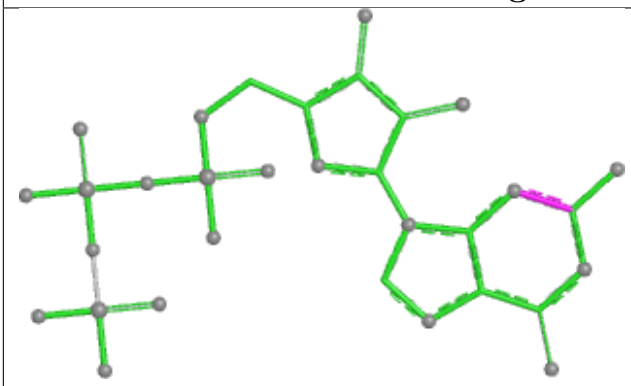


Torsions

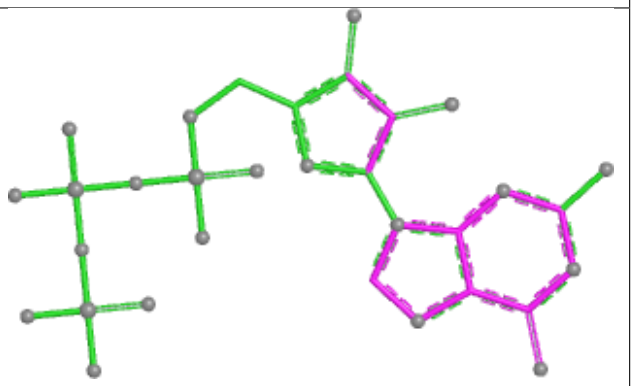


Rings

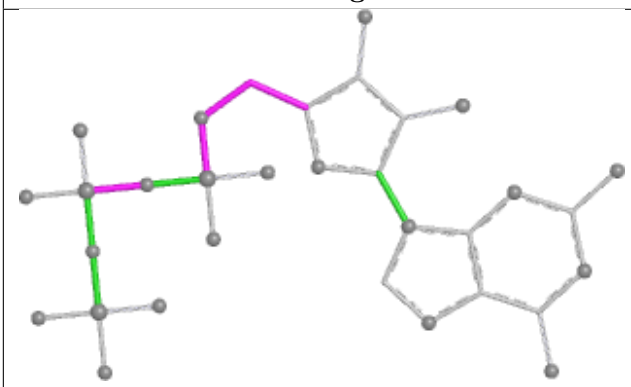
Ligand GTP OA 501



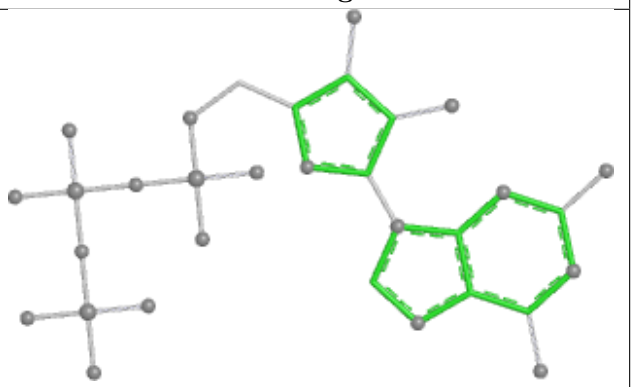
Bond lengths



Bond angles

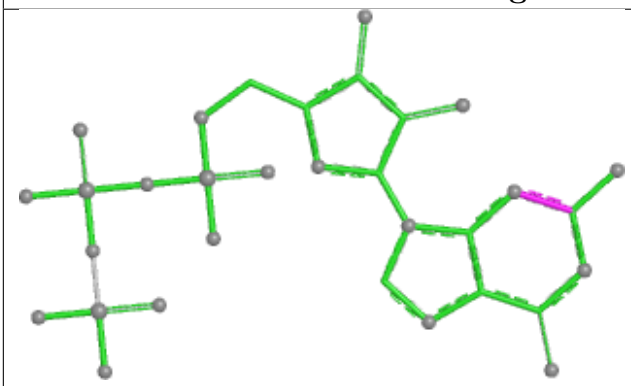


Torsions

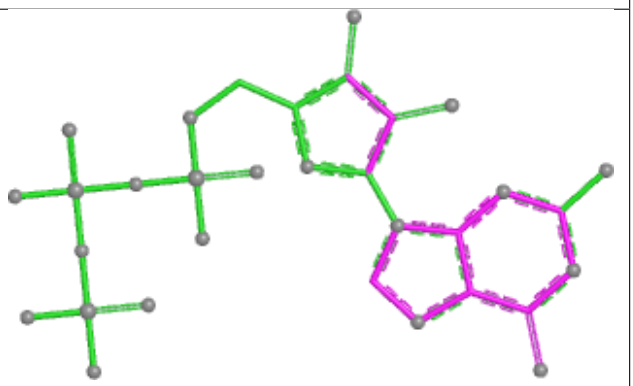


Rings

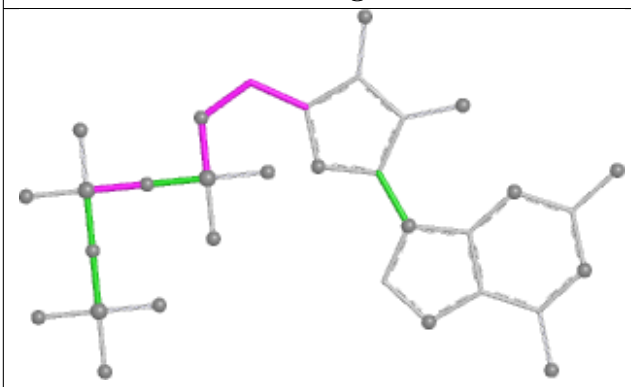
Ligand GTP RO 501



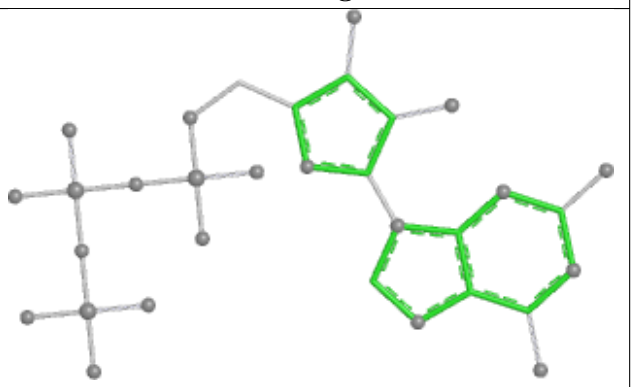
Bond lengths



Bond angles

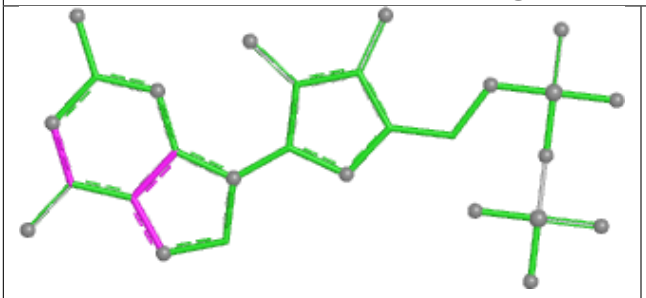


Torsions

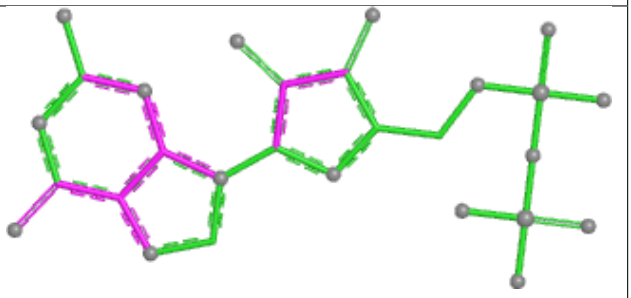


Rings

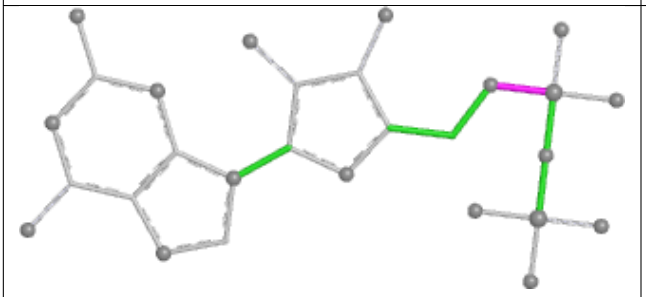
Ligand GDP UL 502



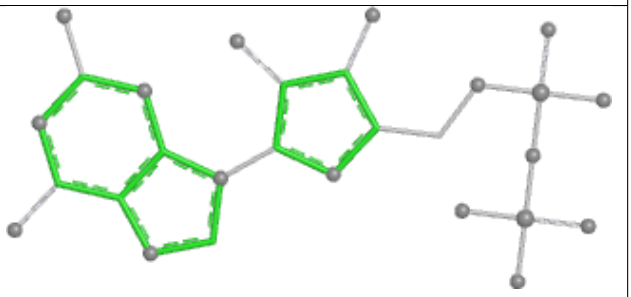
Bond lengths



Bond angles

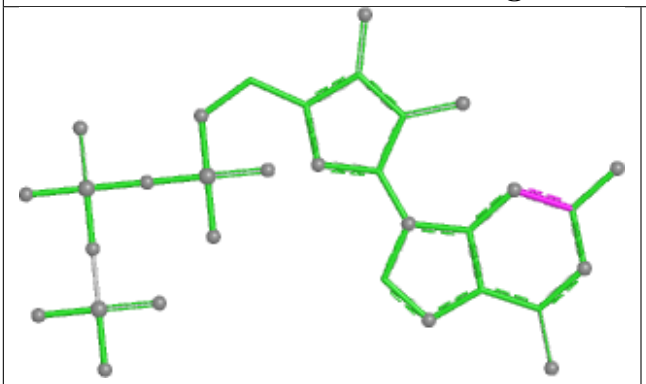


Torsions

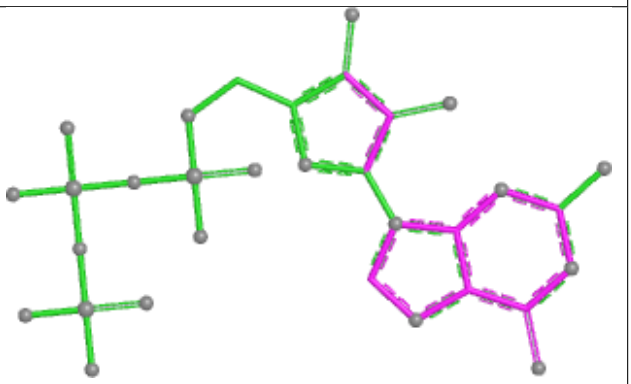


Rings

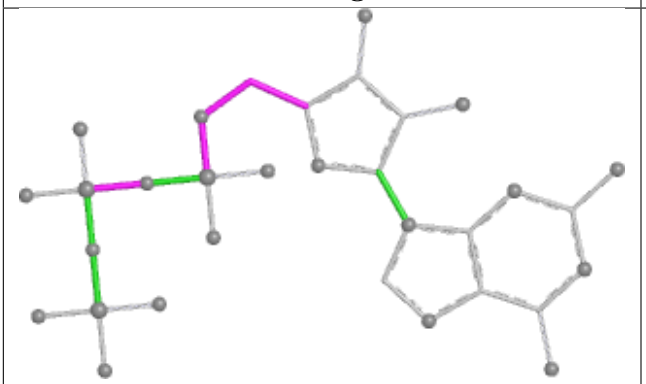
Ligand GTP WA 501



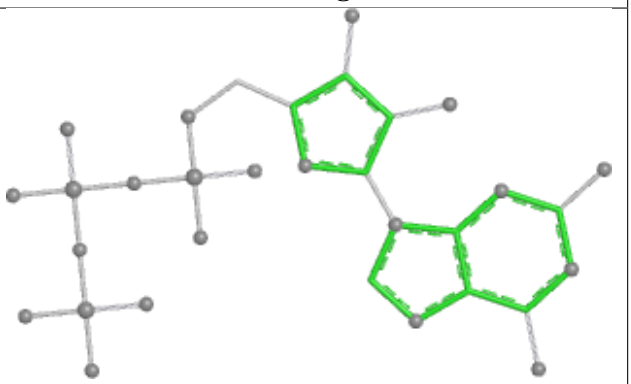
Bond lengths



Bond angles

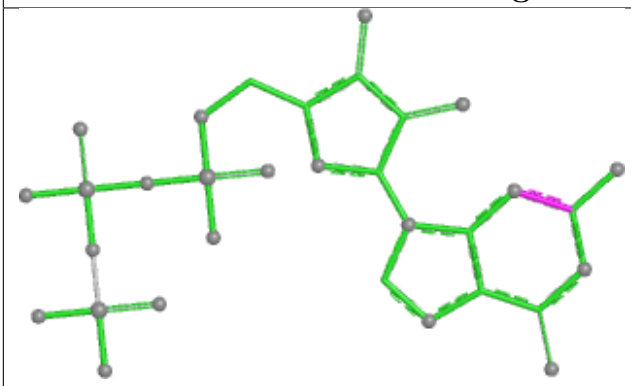


Torsions

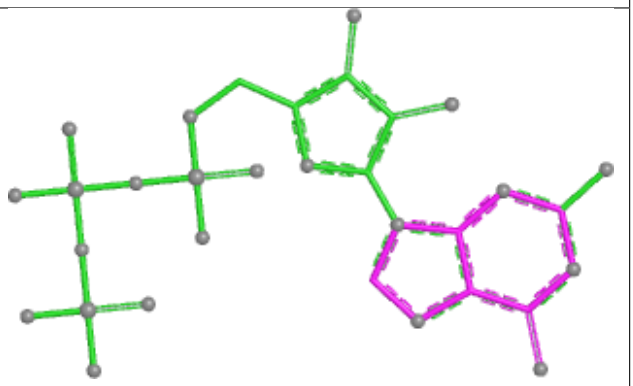


Rings

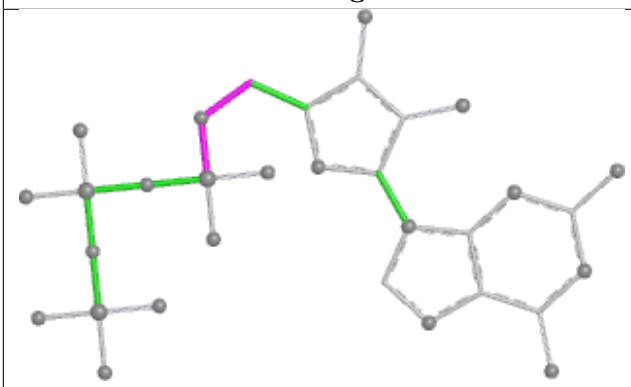
Ligand GTP JK 501



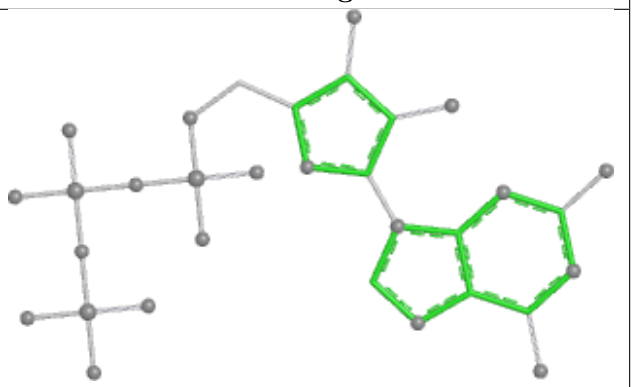
Bond lengths



Bond angles

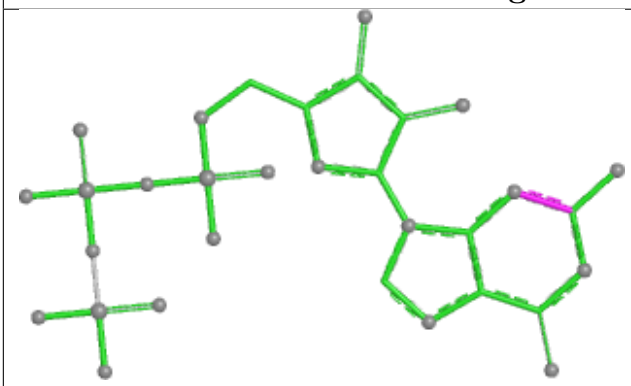


Torsions

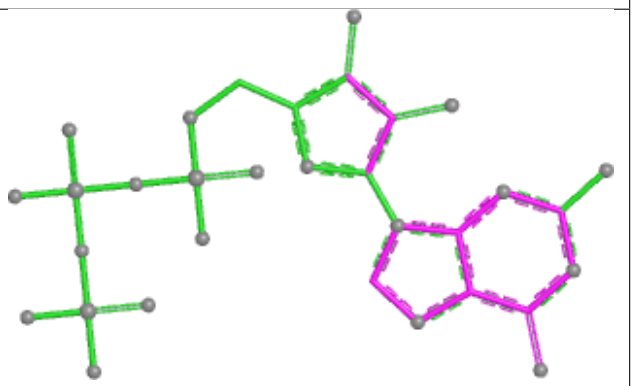


Rings

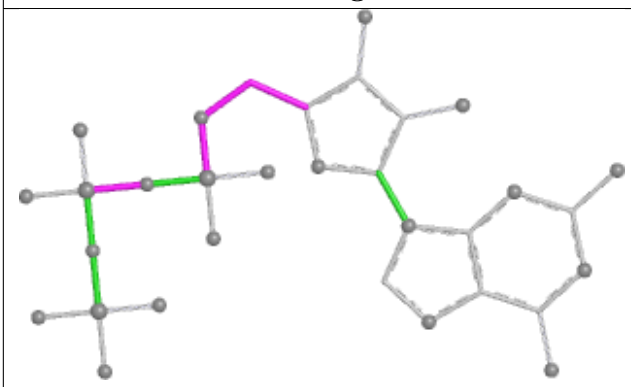
Ligand GTP AA 501



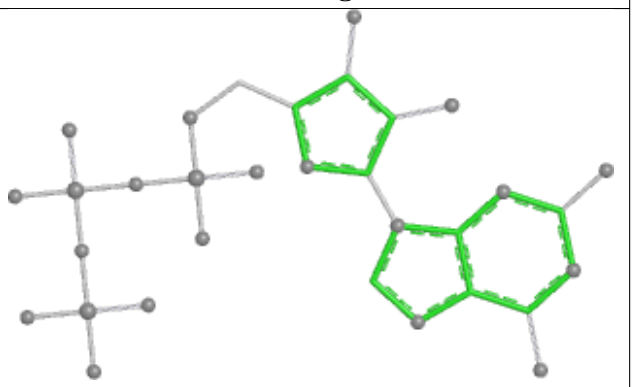
Bond lengths



Bond angles

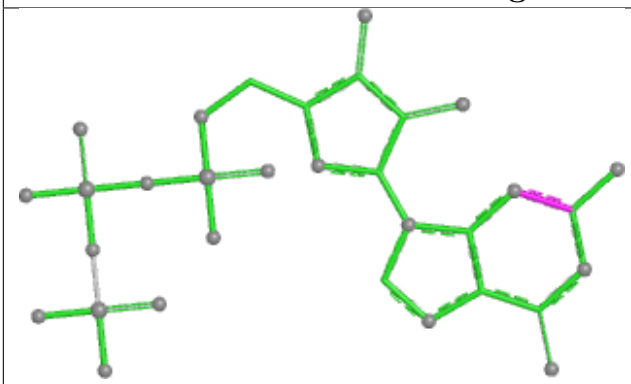


Torsions

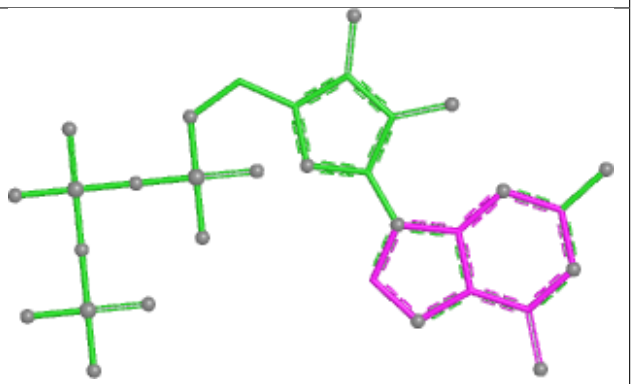


Rings

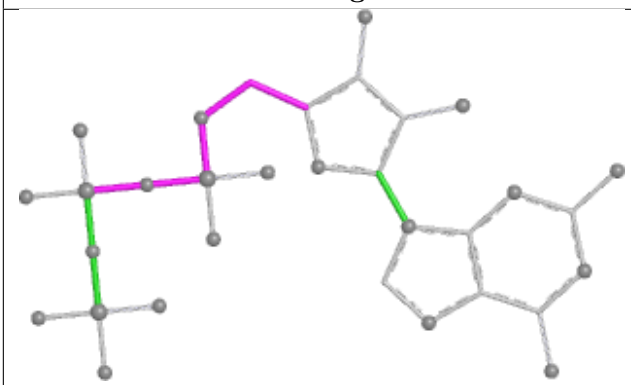
Ligand GTP HC 501



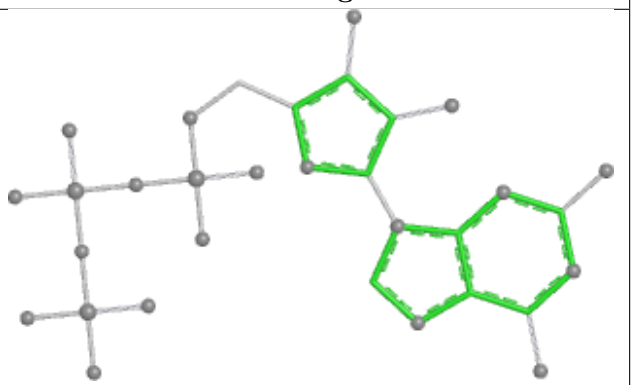
Bond lengths



Bond angles

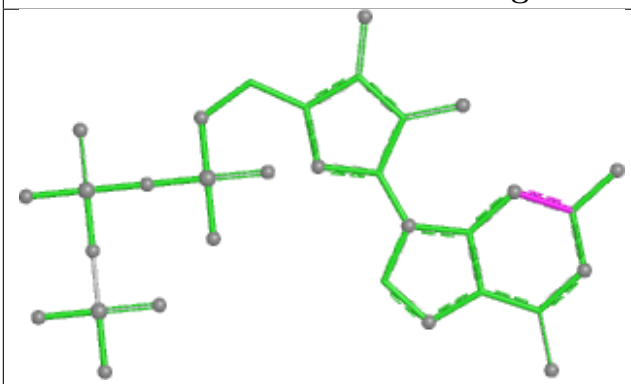


Torsions

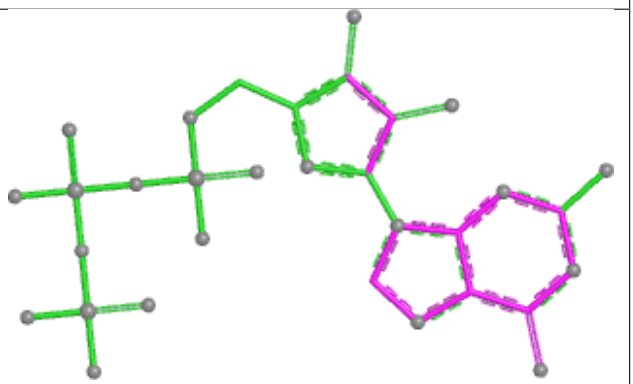


Rings

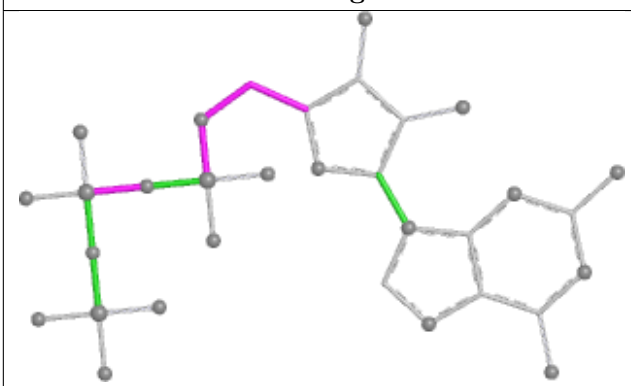
Ligand GTP TE 501



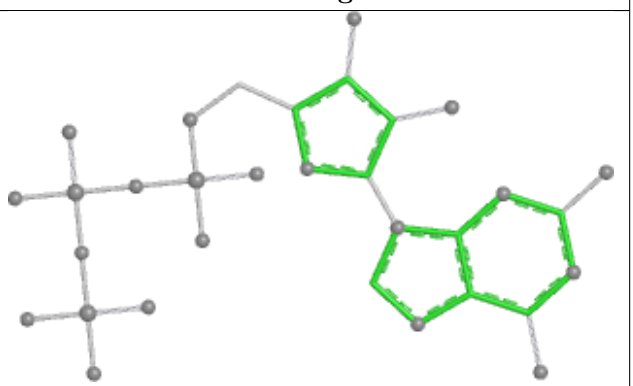
Bond lengths



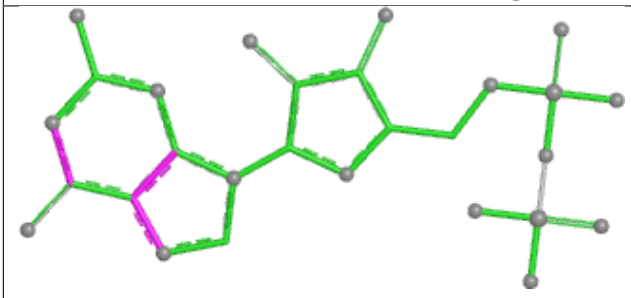
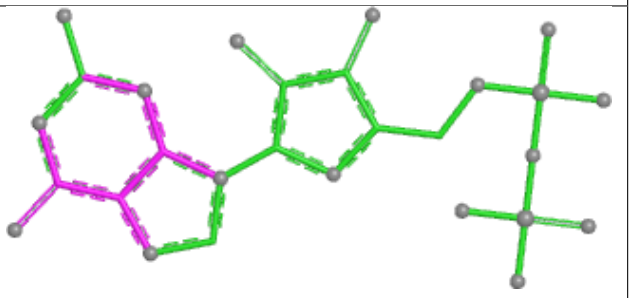
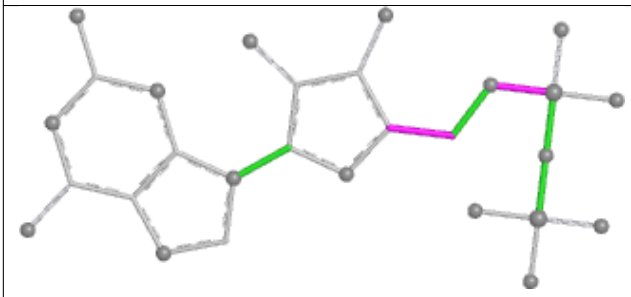
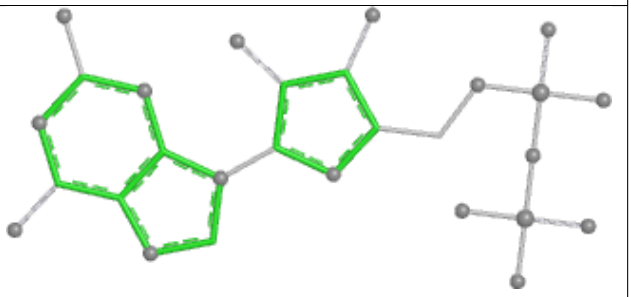
Bond angles

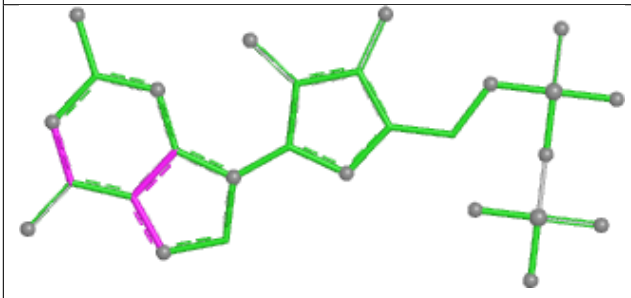
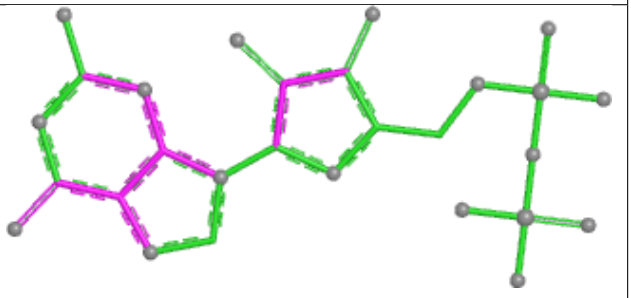
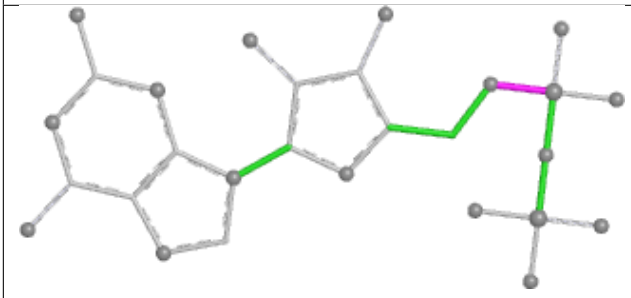
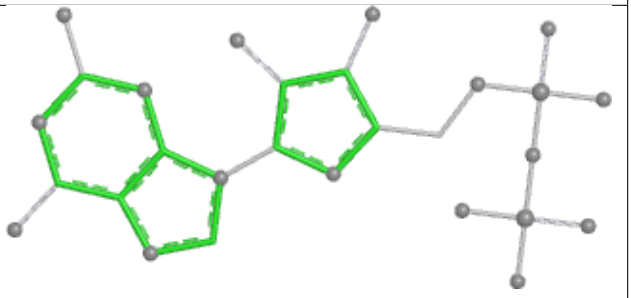


Torsions

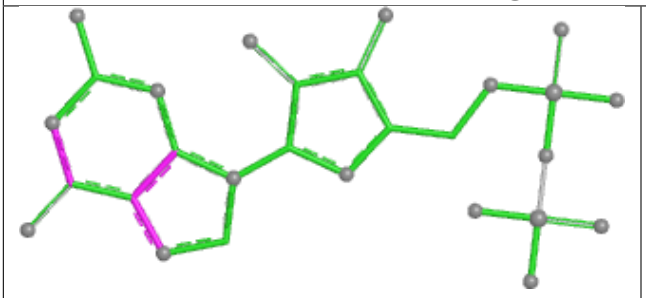


Rings

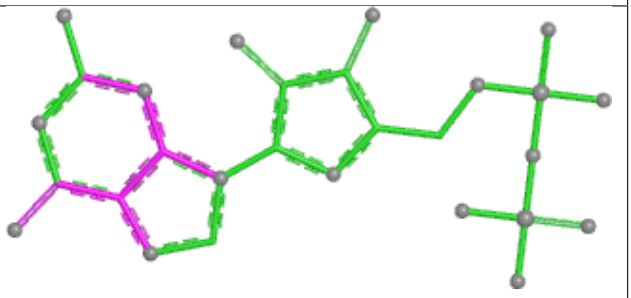
Ligand GDP OD 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP QF 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

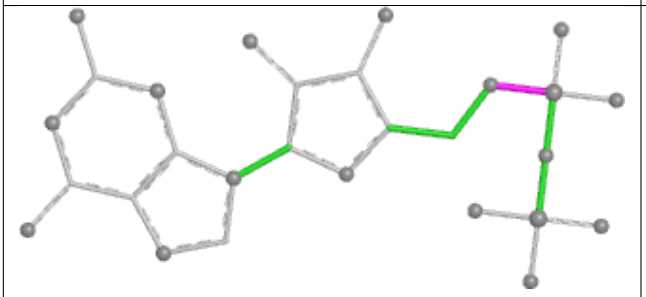
Ligand GDP KN 502



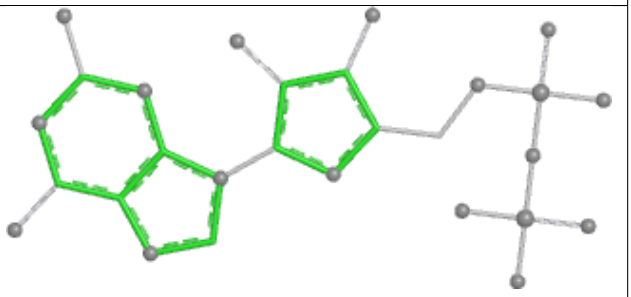
Bond lengths



Bond angles

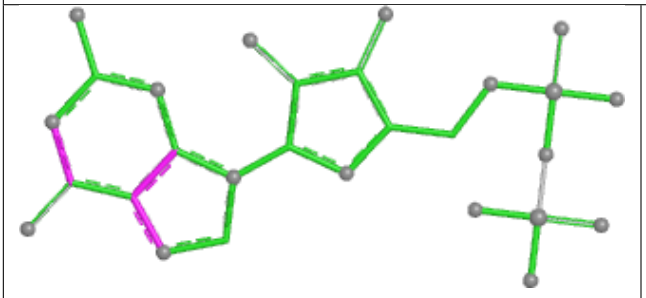


Torsions

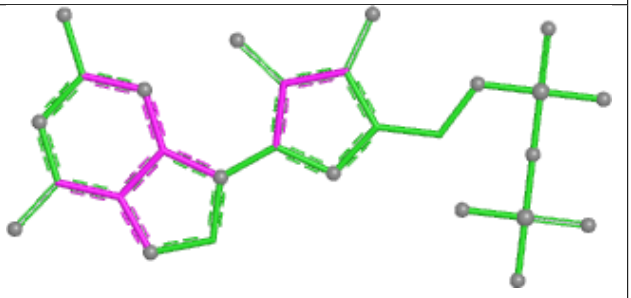


Rings

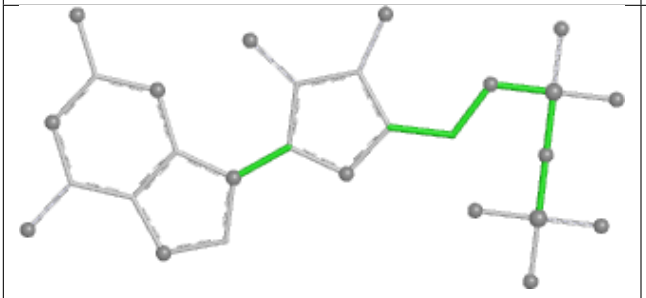
Ligand GDP PL 502



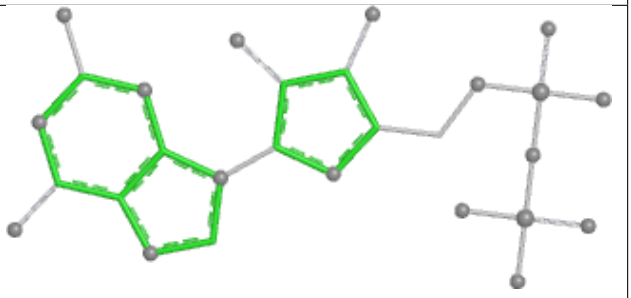
Bond lengths



Bond angles

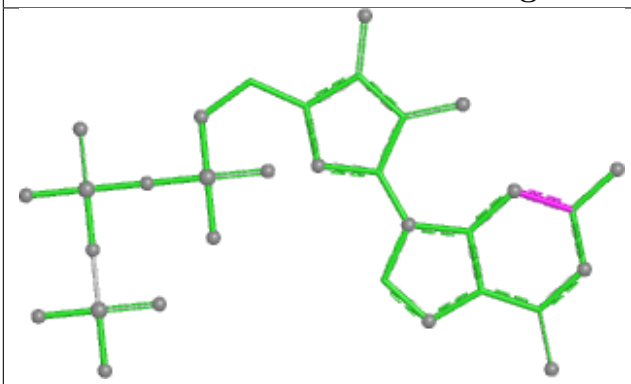


Torsions

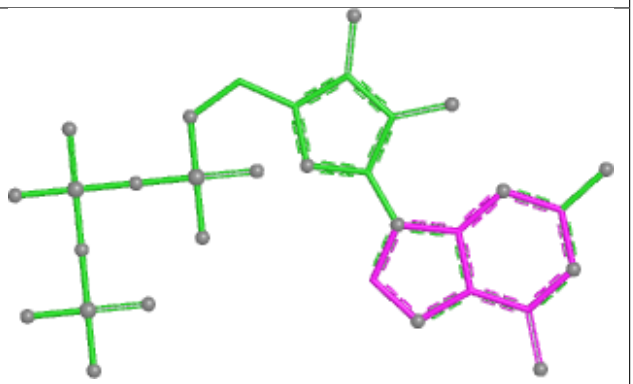


Rings

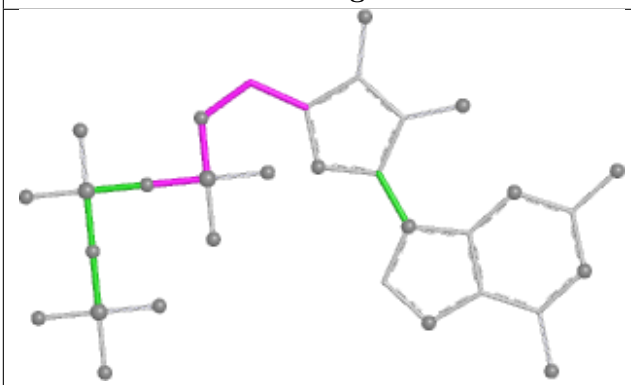
Ligand GTP JI 501



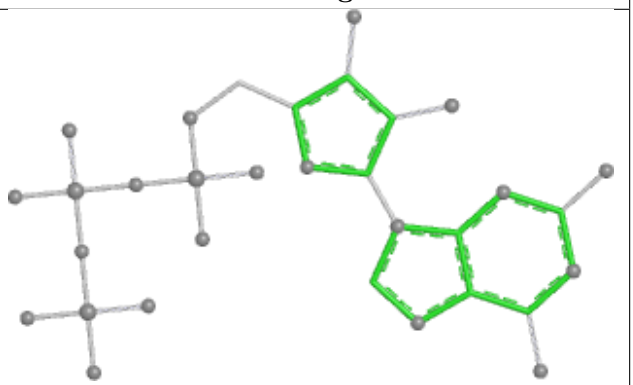
Bond lengths



Bond angles

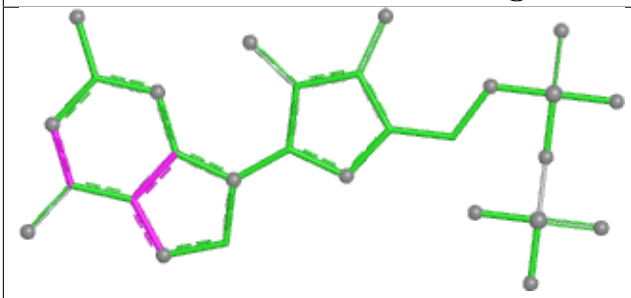


Torsions

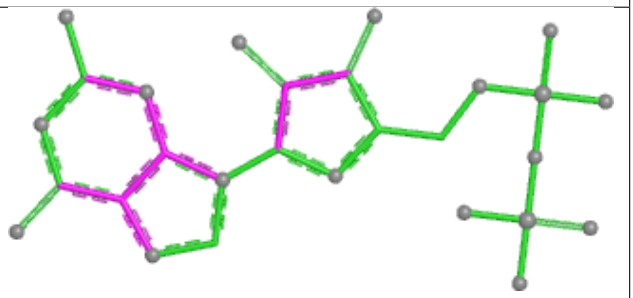


Rings

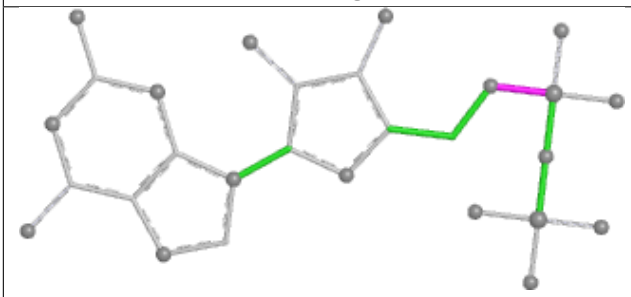
Ligand GDP PH 502



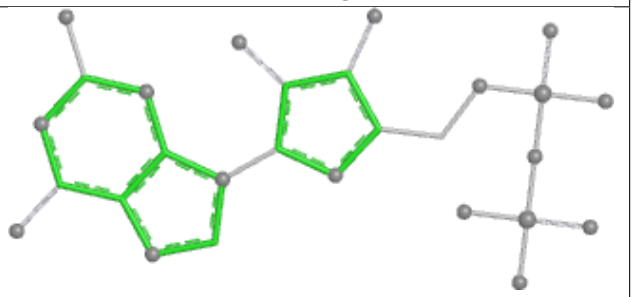
Bond lengths



Bond angles

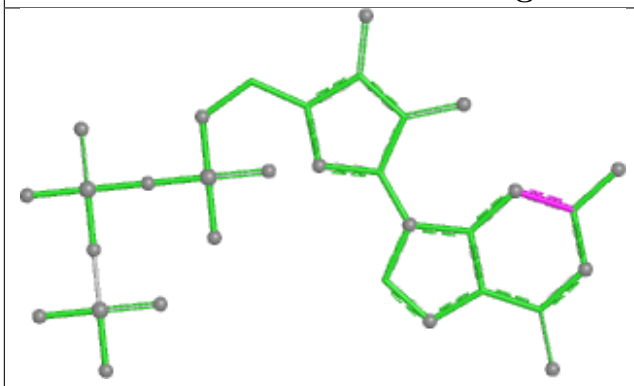


Torsions

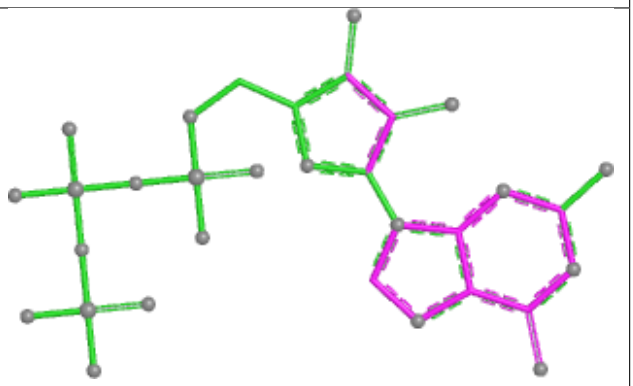


Rings

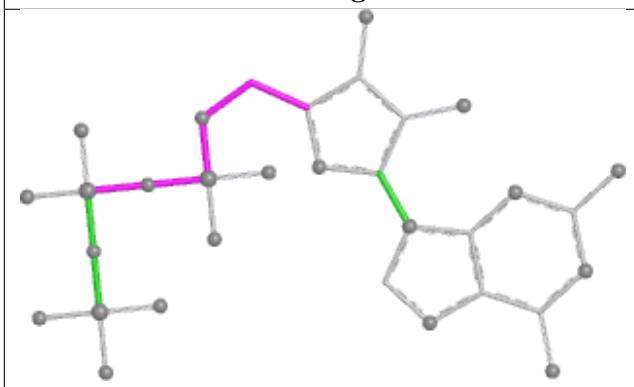
Ligand GTP IG 501



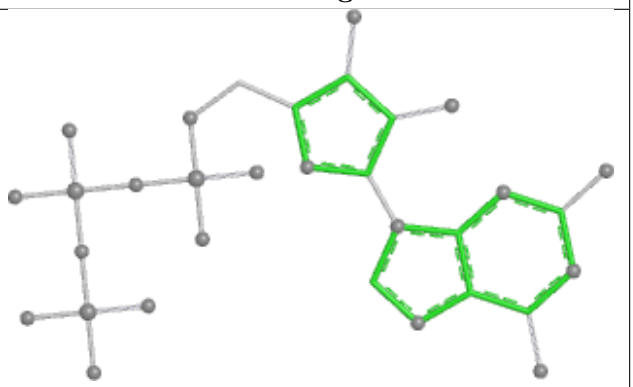
Bond lengths



Bond angles

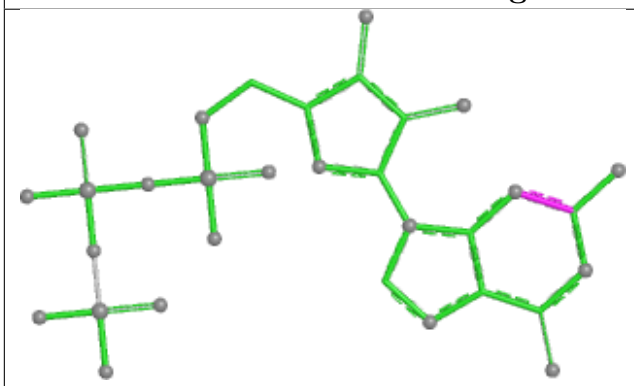


Torsions

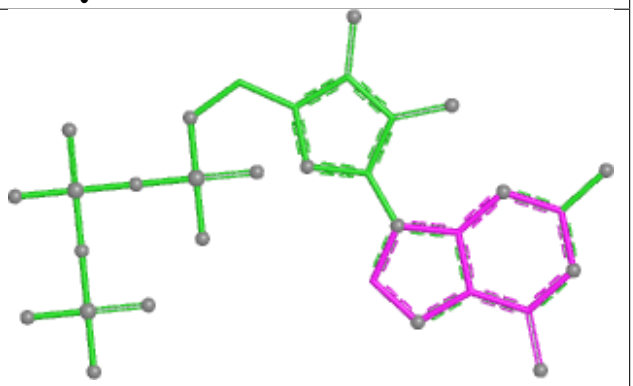


Rings

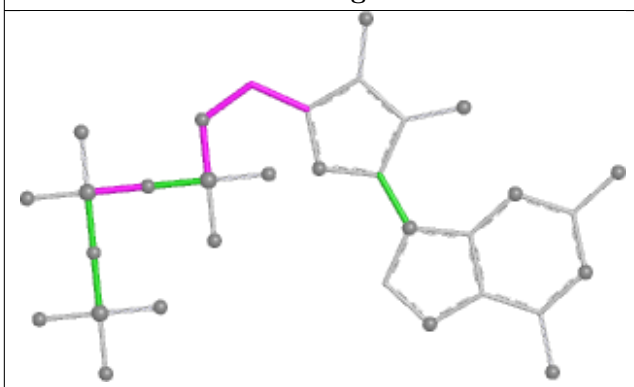
Ligand GTP DQ 501



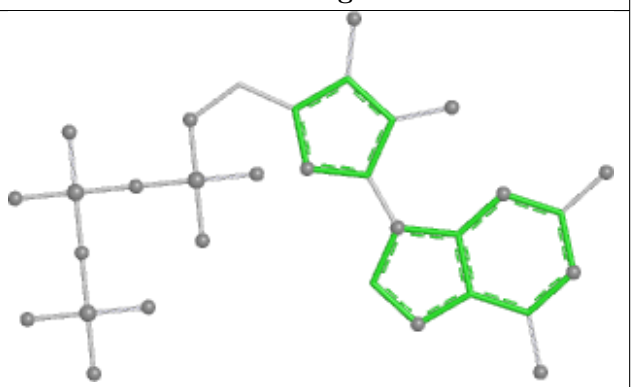
Bond lengths



Bond angles

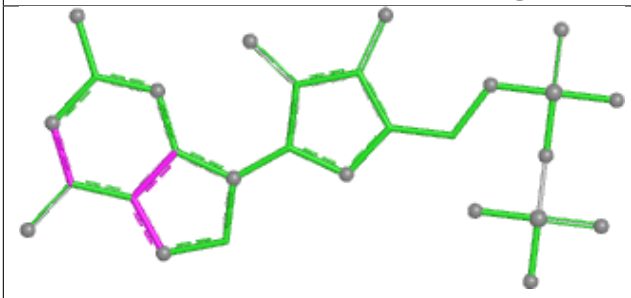


Torsions

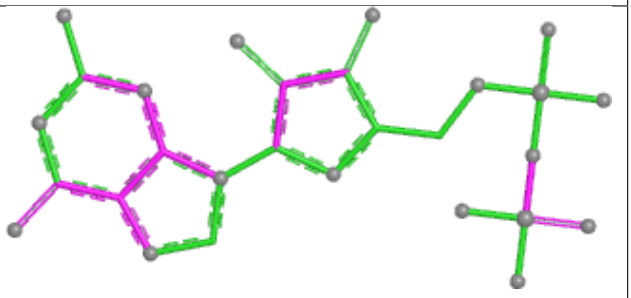


Rings

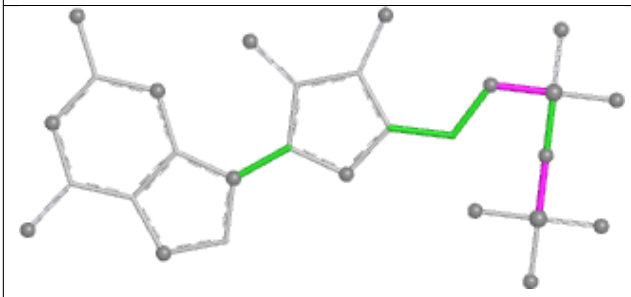
Ligand GDP GJ 502



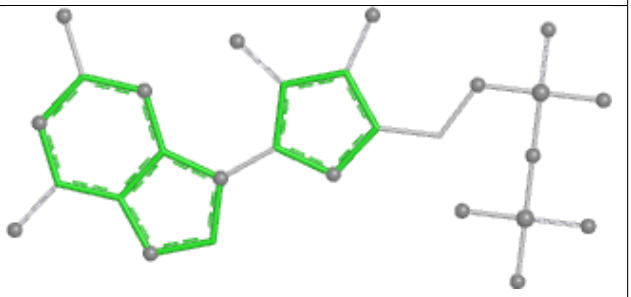
Bond lengths



Bond angles

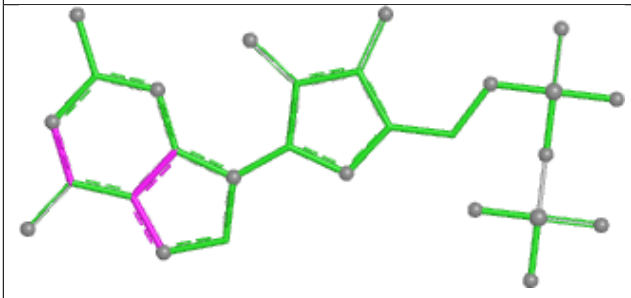


Torsions

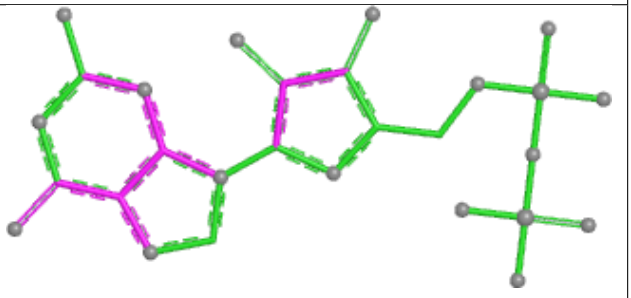


Rings

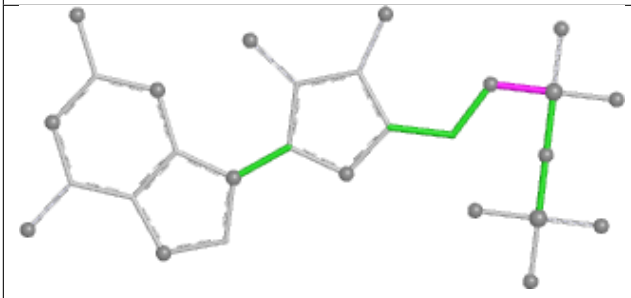
Ligand GDP SB 502



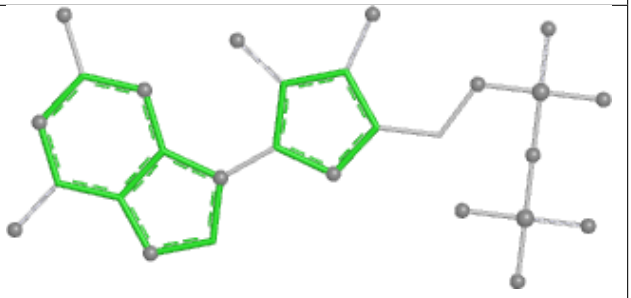
Bond lengths



Bond angles

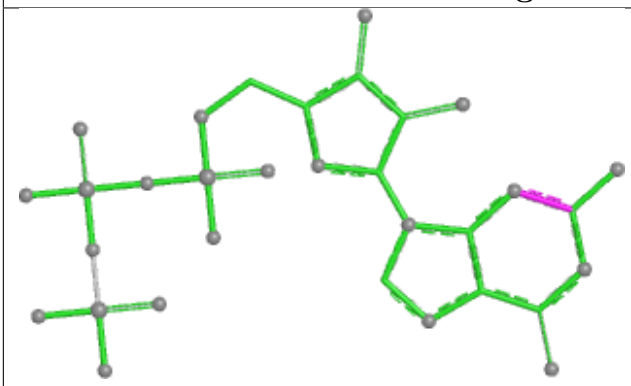


Torsions

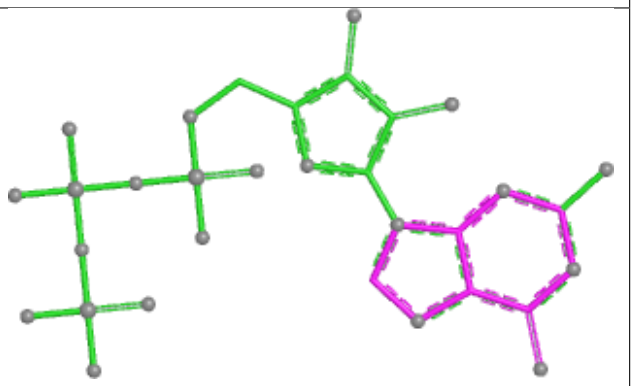


Rings

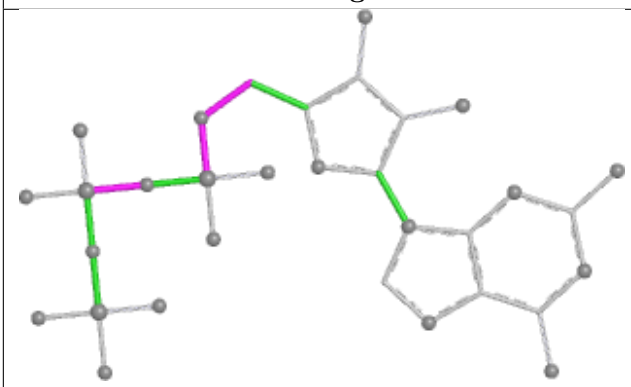
Ligand GTP CI 501



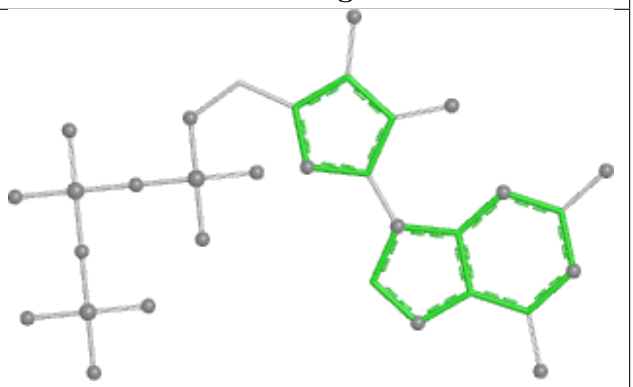
Bond lengths



Bond angles

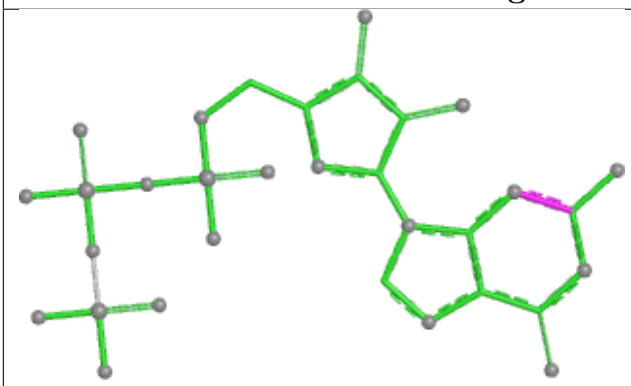


Torsions

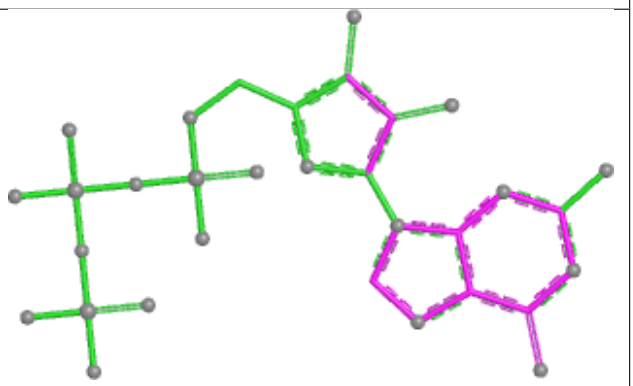


Rings

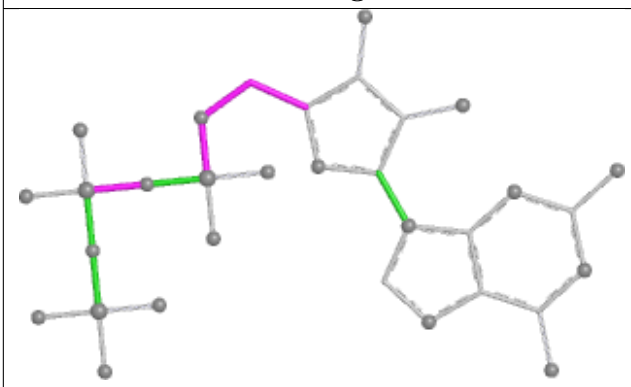
Ligand GTP GA 501



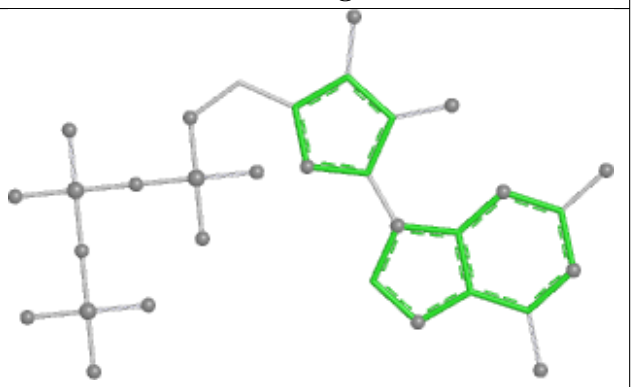
Bond lengths



Bond angles

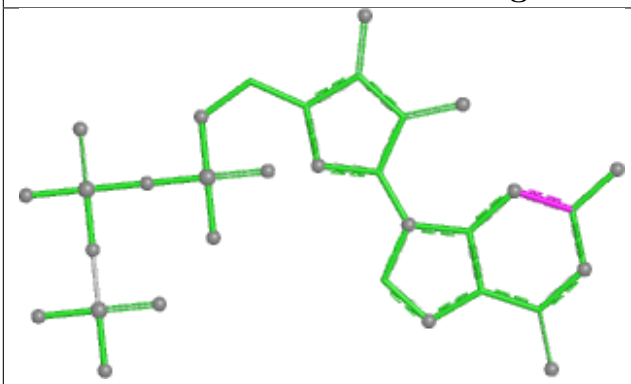


Torsions

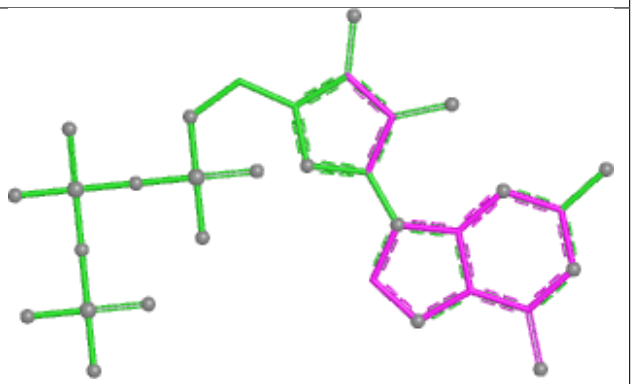


Rings

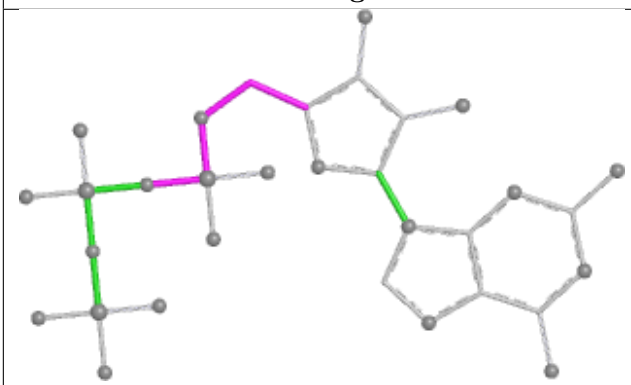
Ligand GTP HE 501



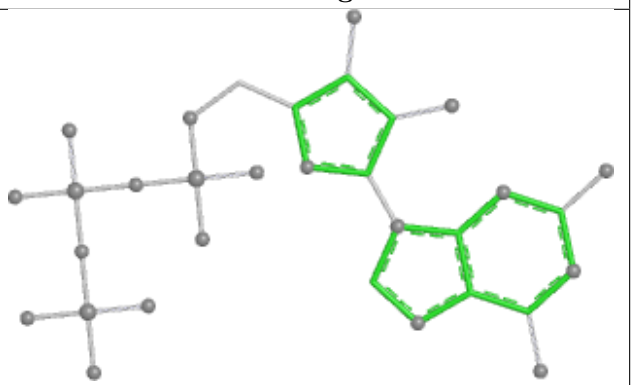
Bond lengths



Bond angles

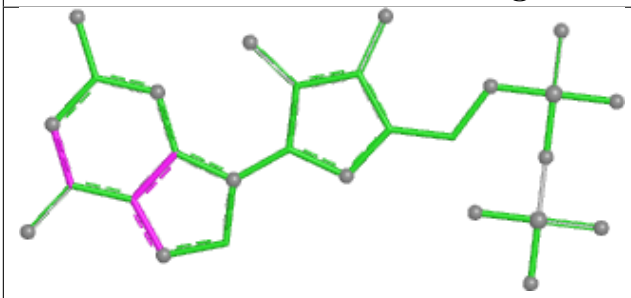


Torsions

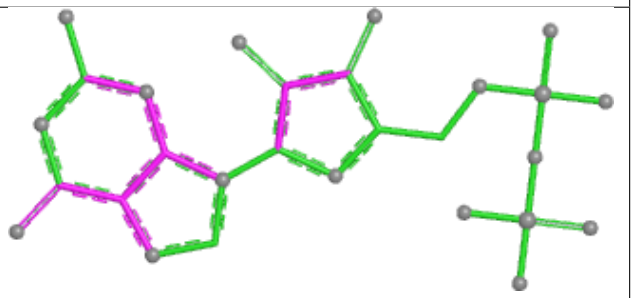


Rings

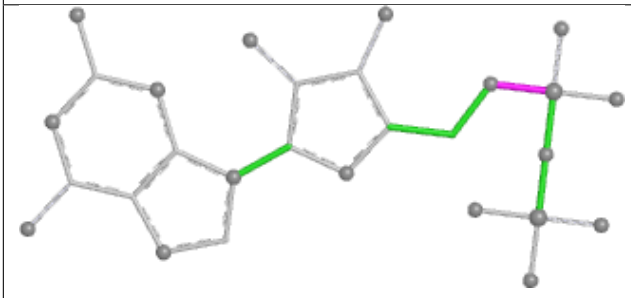
Ligand GDP KJ 502



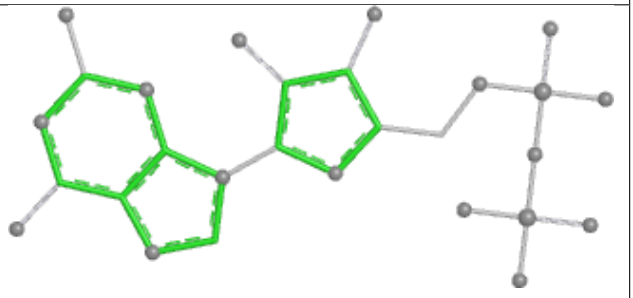
Bond lengths



Bond angles

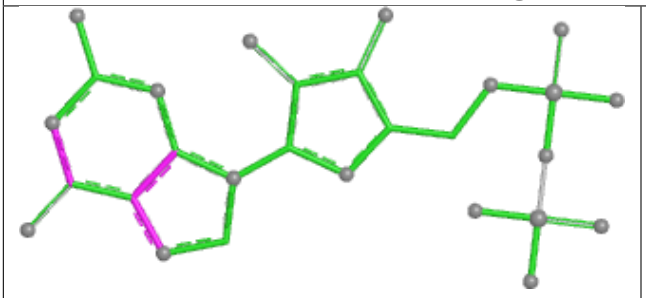


Torsions

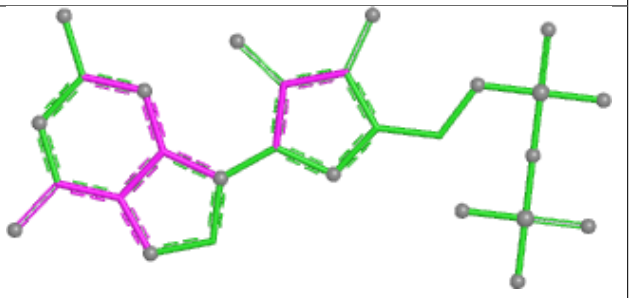


Rings

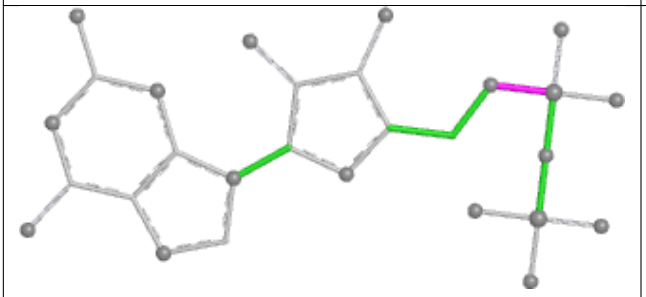
Ligand GDP TF 502



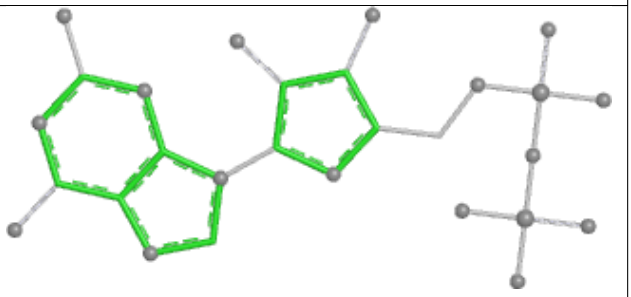
Bond lengths



Bond angles

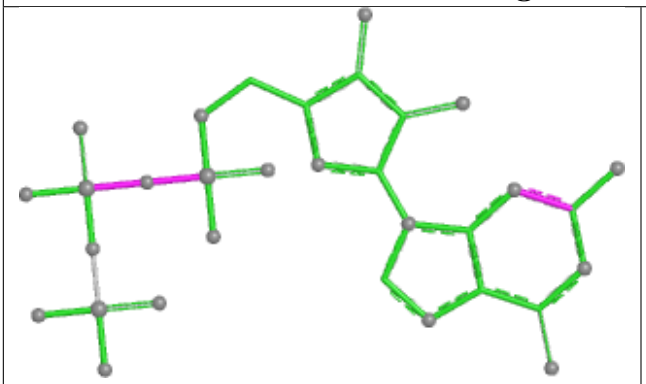


Torsions

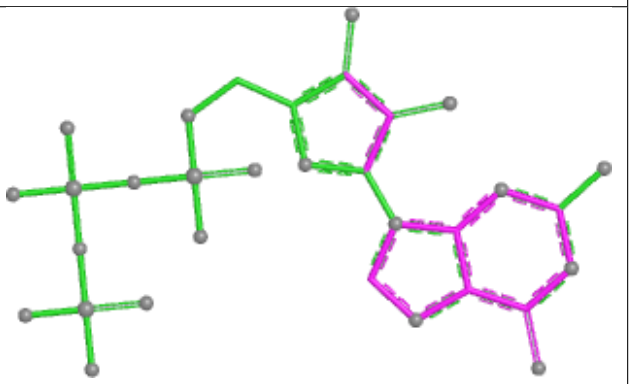


Rings

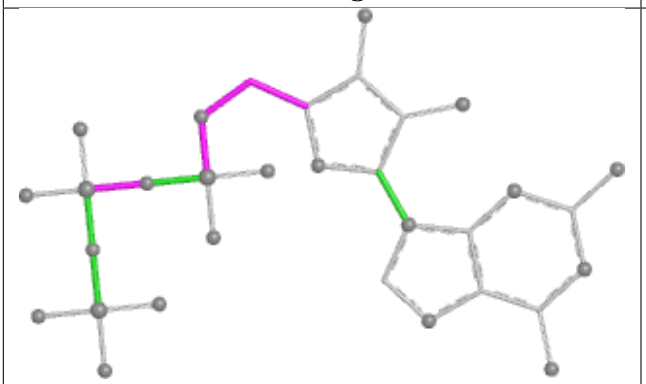
Ligand GTP VI 501



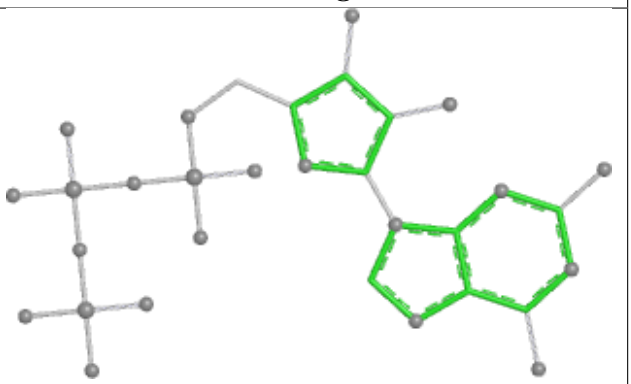
Bond lengths



Bond angles

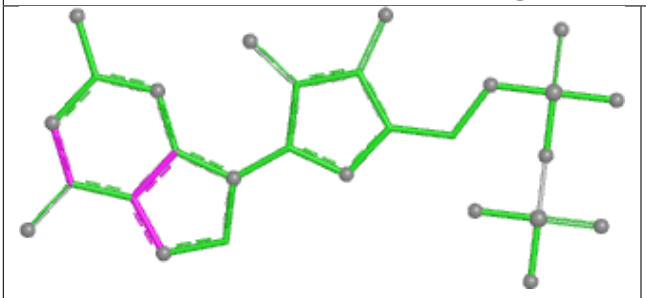


Torsions

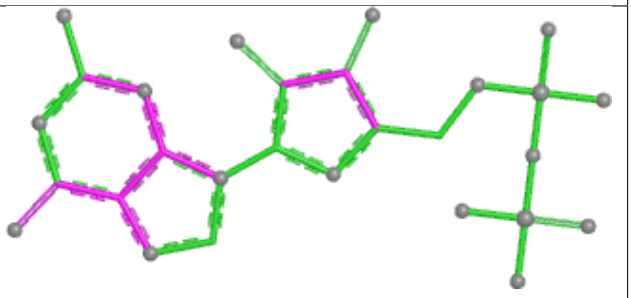


Rings

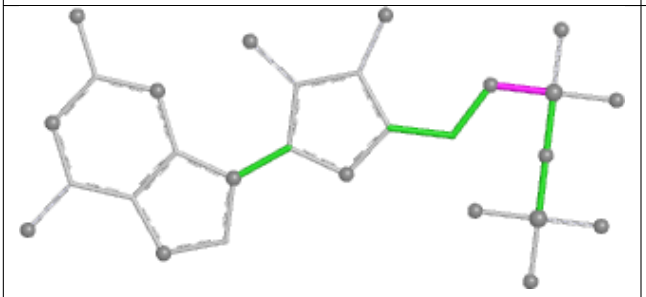
Ligand GDP LP 502



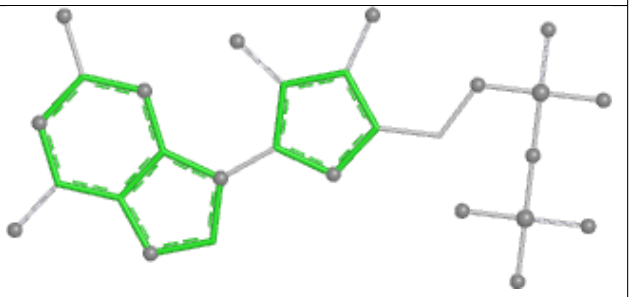
Bond lengths



Bond angles

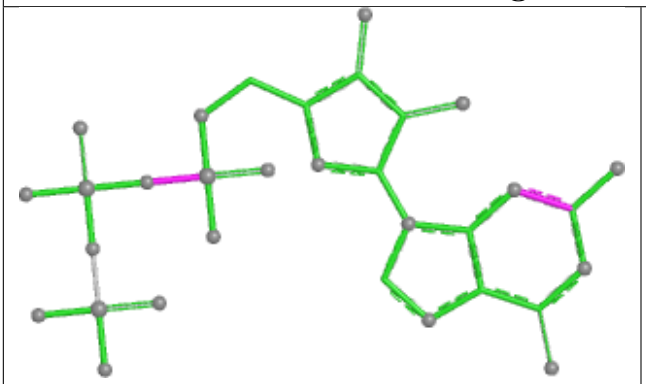


Torsions

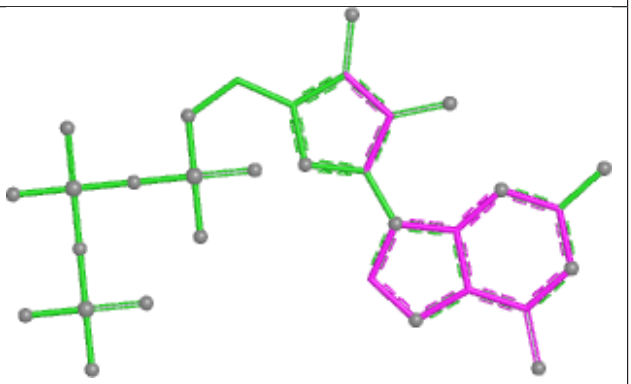


Rings

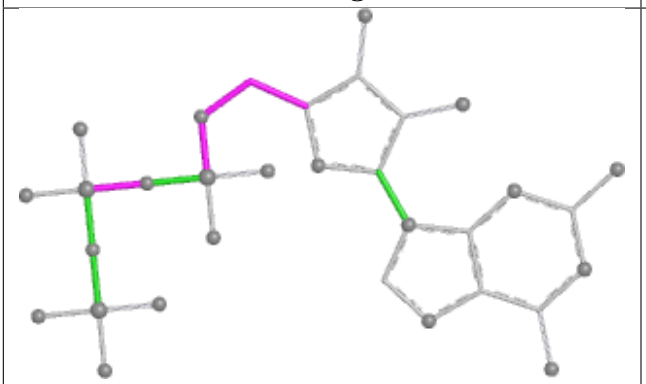
Ligand GTP RC 501



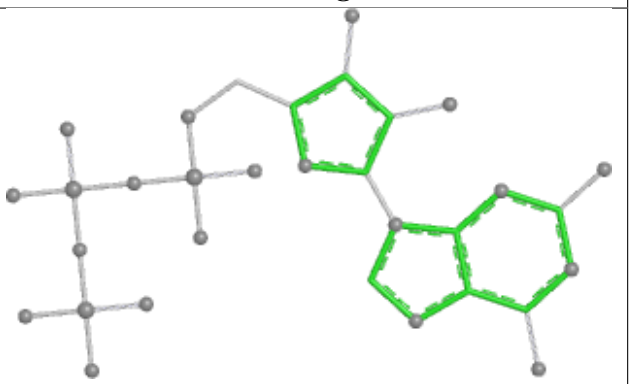
Bond lengths



Bond angles

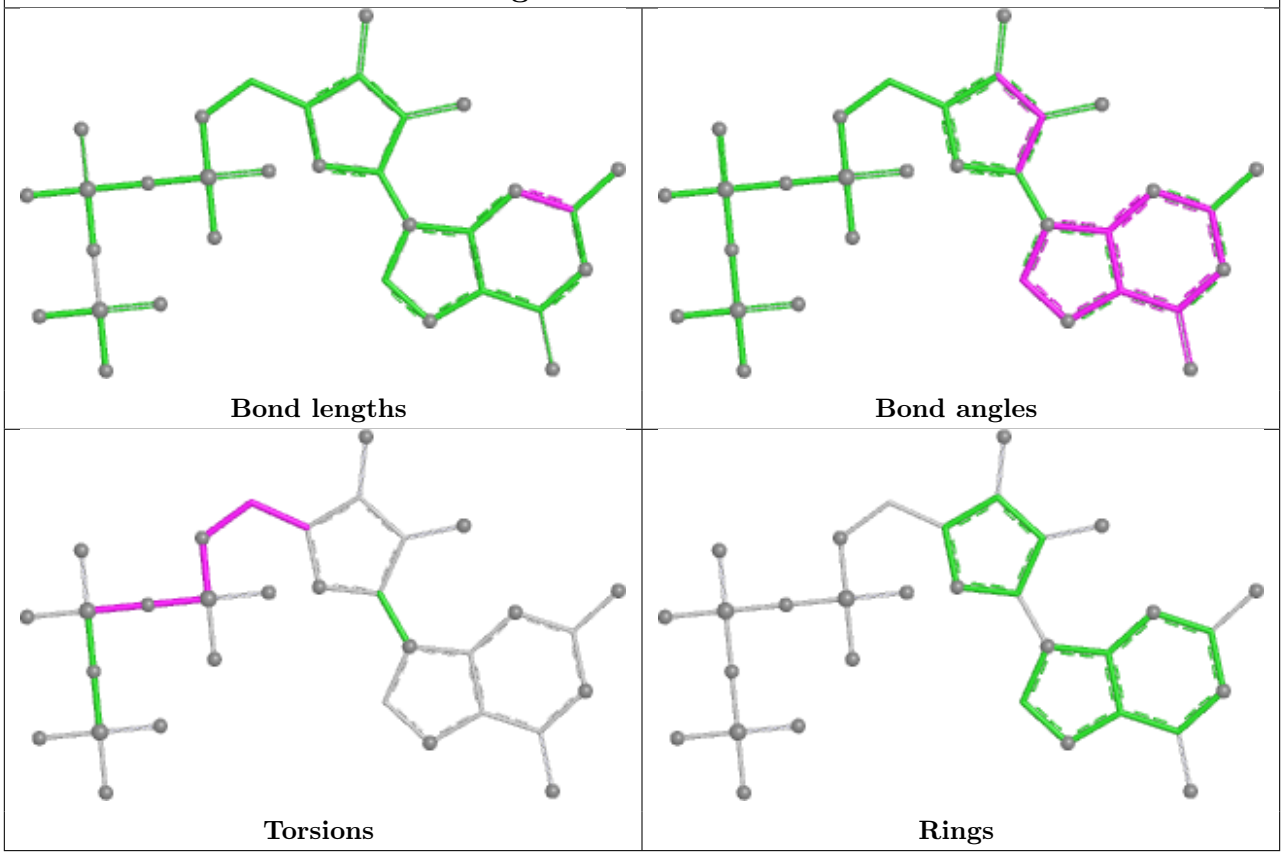


Torsions

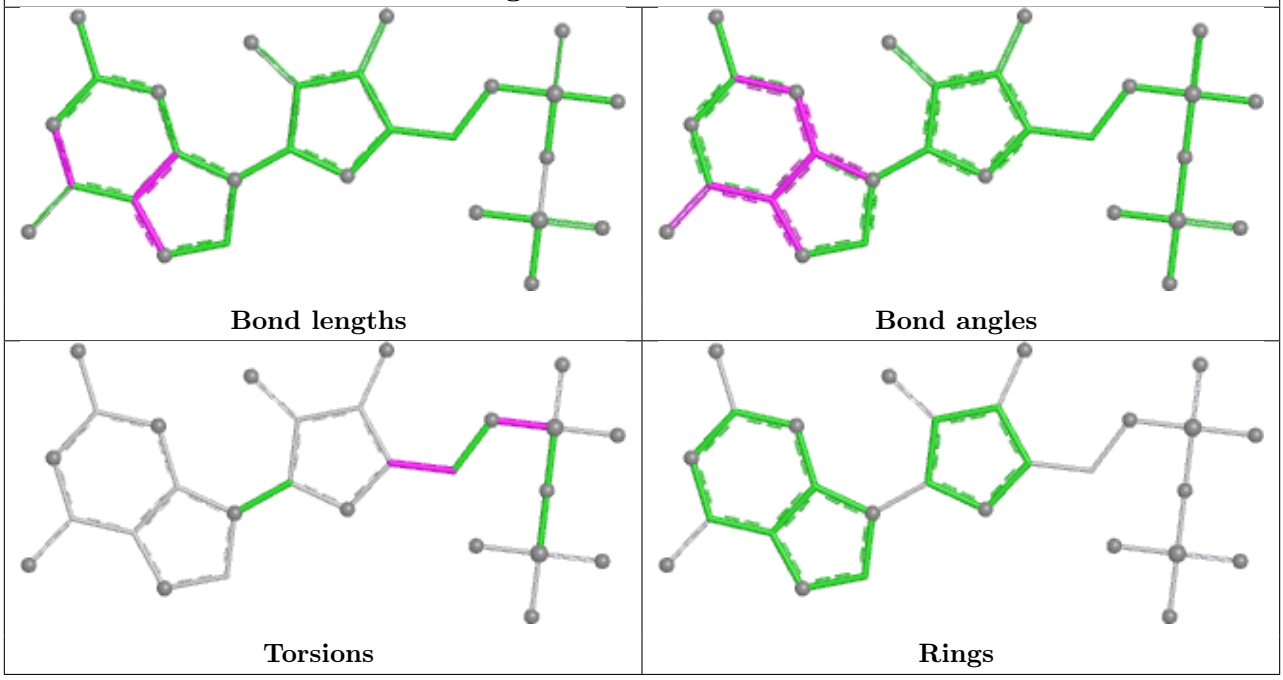


Rings

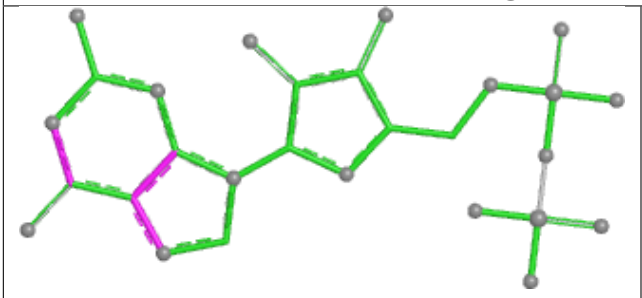
Ligand GTP OE 501



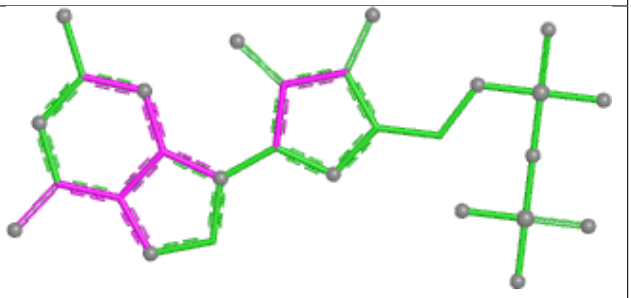
Ligand GDP MD 502



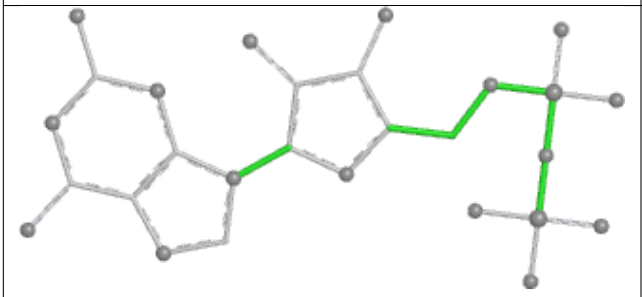
Ligand GDP WN 502



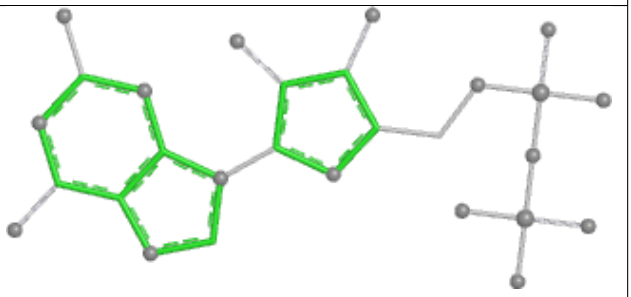
Bond lengths



Bond angles

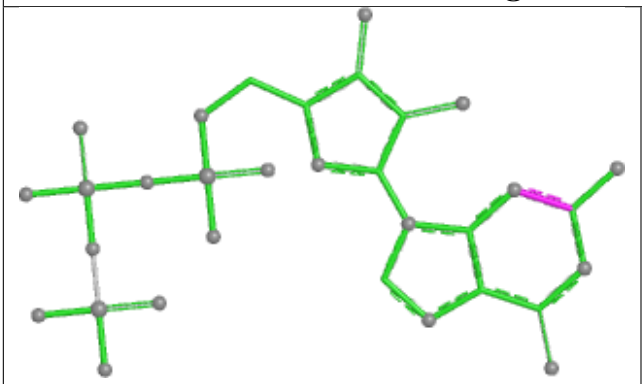


Torsions

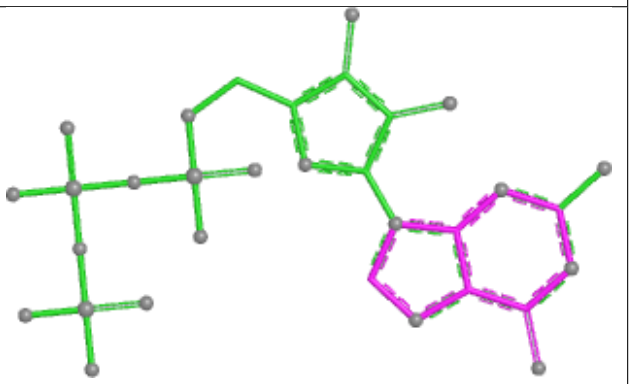


Rings

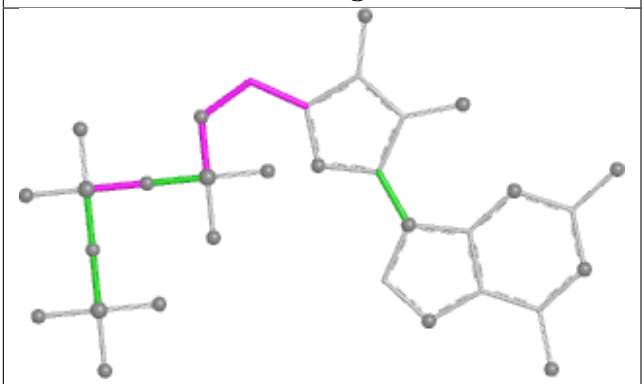
Ligand GTP MK 501



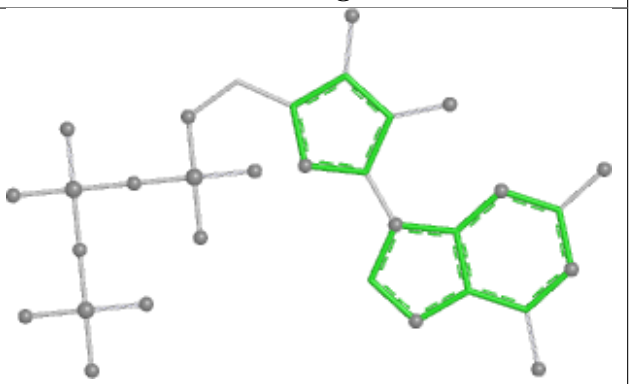
Bond lengths



Bond angles

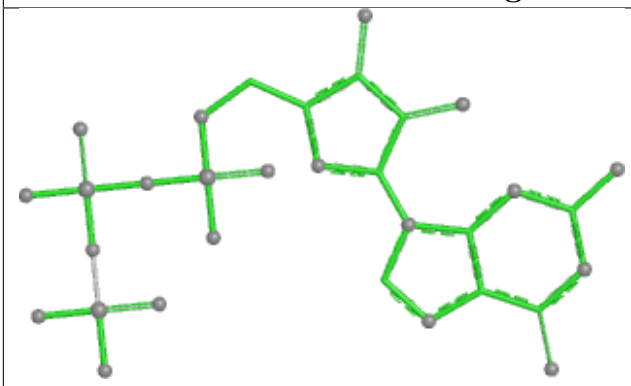


Torsions

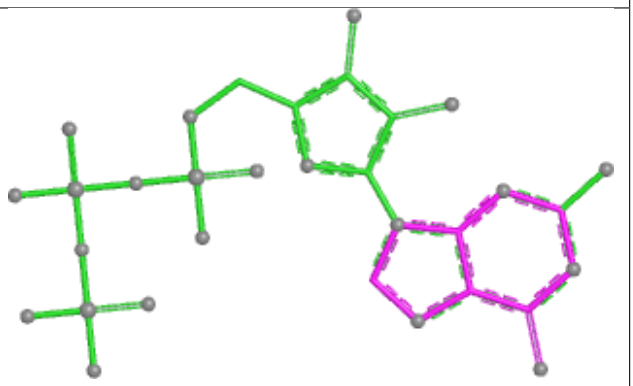


Rings

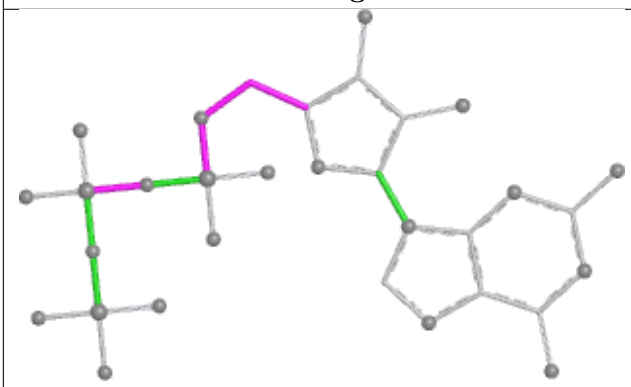
Ligand GTP NM 501



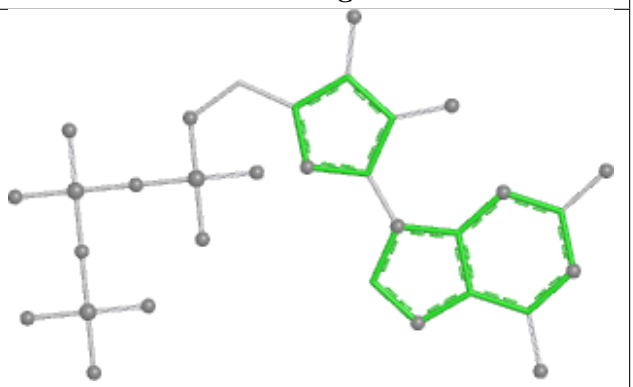
Bond lengths



Bond angles

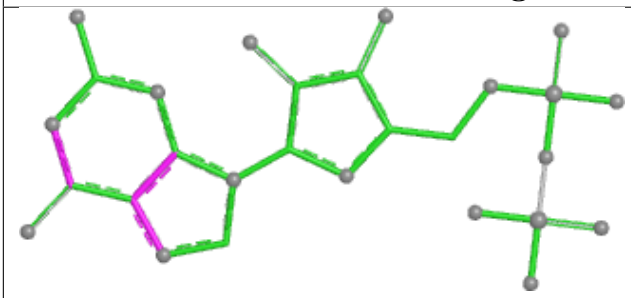


Torsions

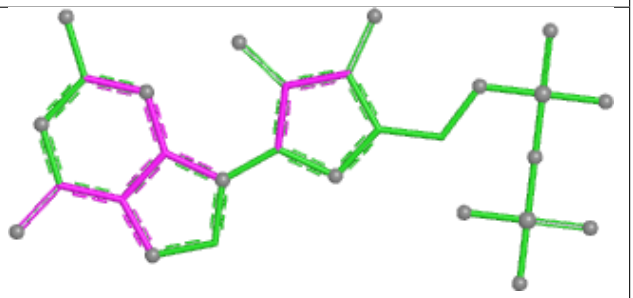


Rings

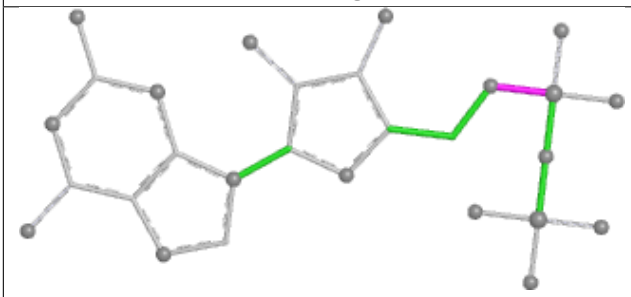
Ligand GDP VL 502



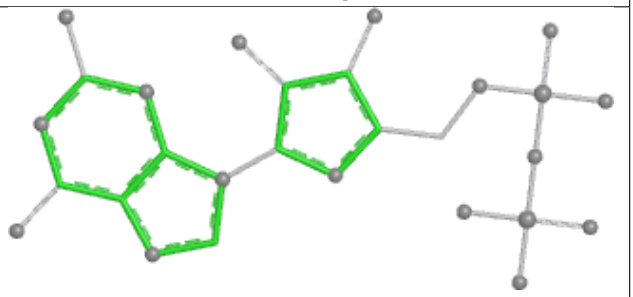
Bond lengths



Bond angles

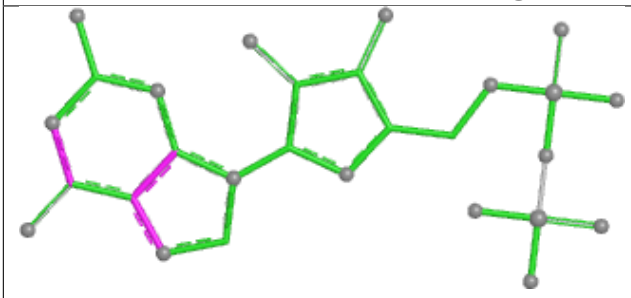


Torsions

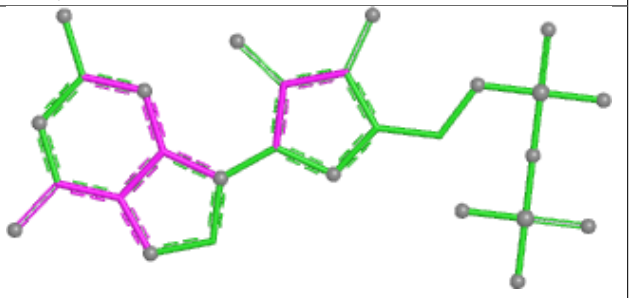


Rings

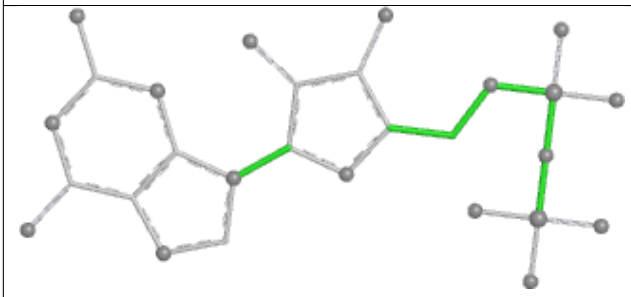
Ligand GDP QL 502



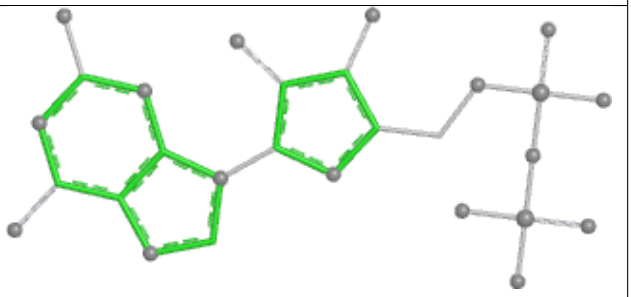
Bond lengths



Bond angles

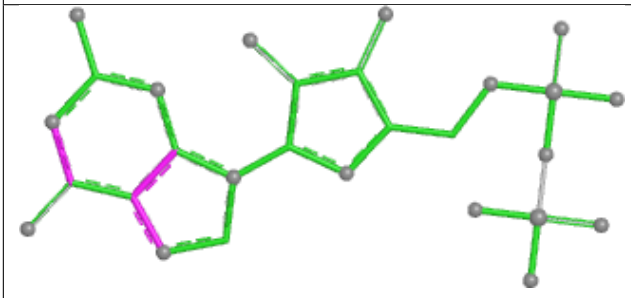


Torsions

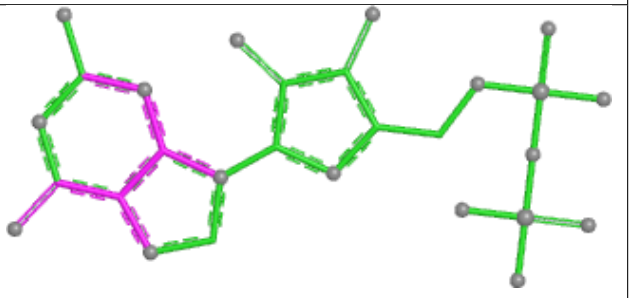


Rings

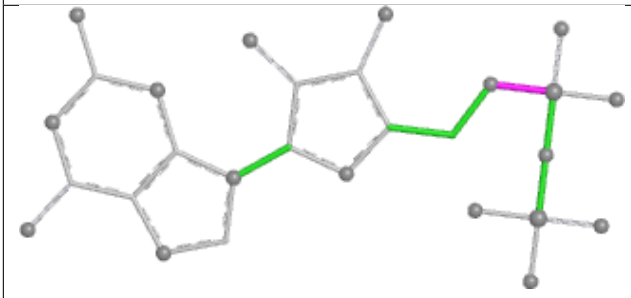
Ligand GDP HD 502



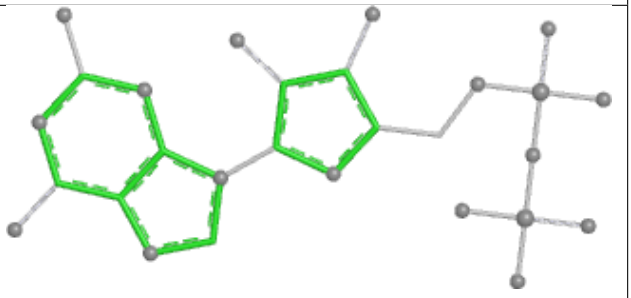
Bond lengths



Bond angles

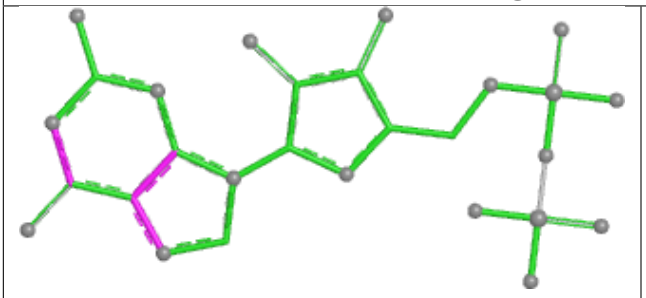


Torsions

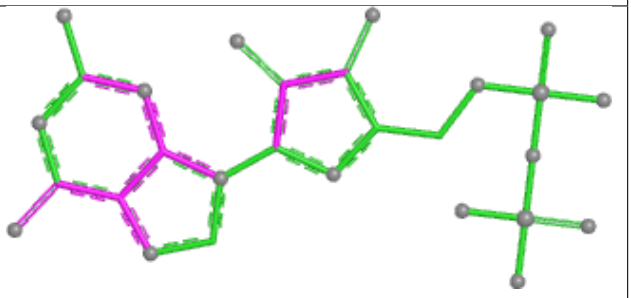


Rings

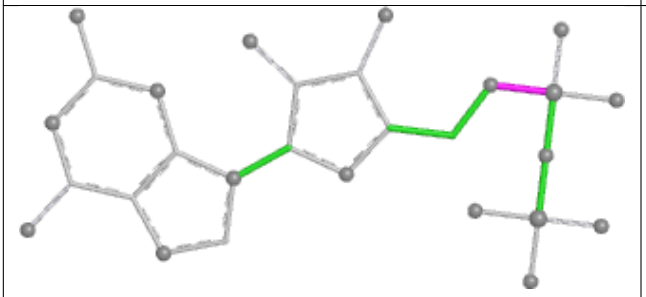
Ligand GDP FN 502



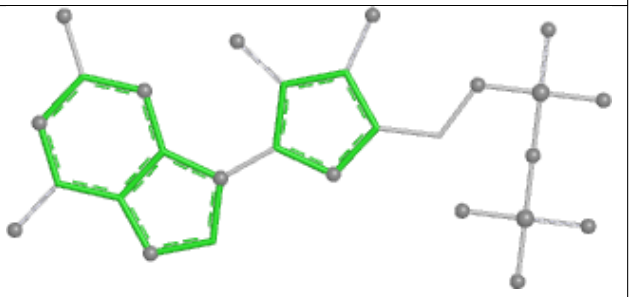
Bond lengths



Bond angles

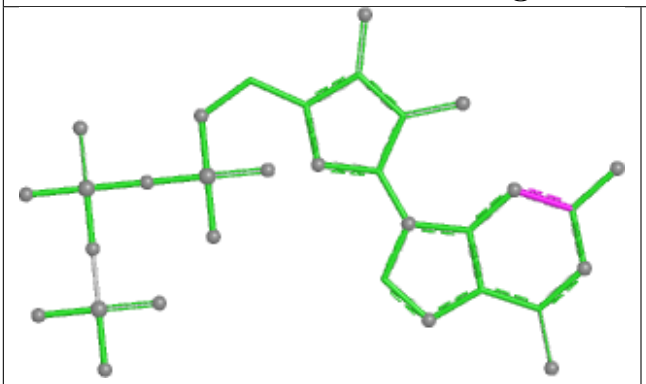


Torsions

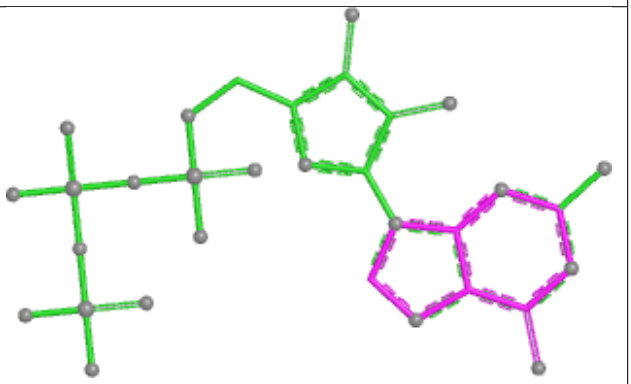


Rings

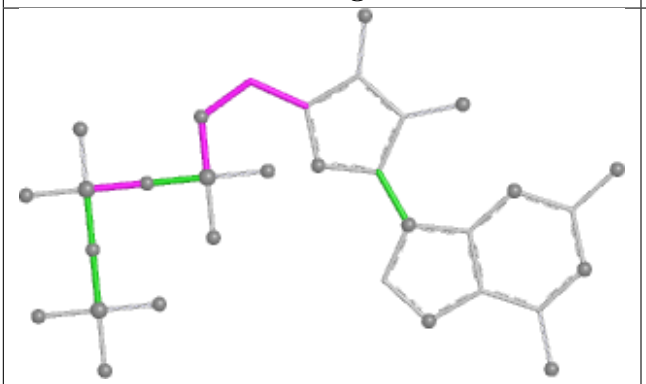
Ligand GTP IM 501



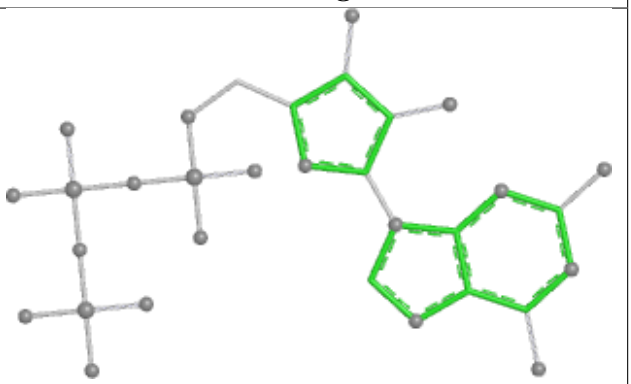
Bond lengths



Bond angles

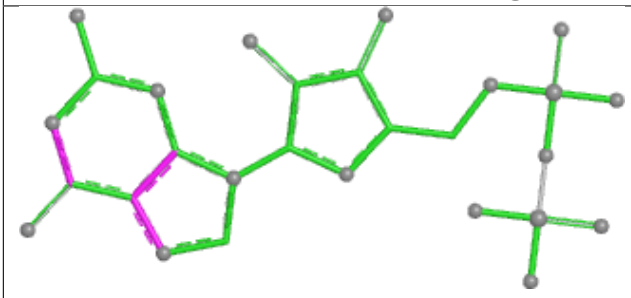


Torsions

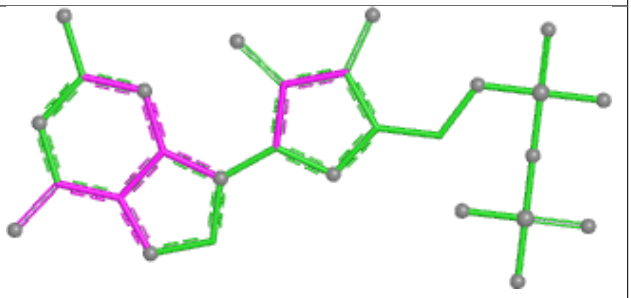


Rings

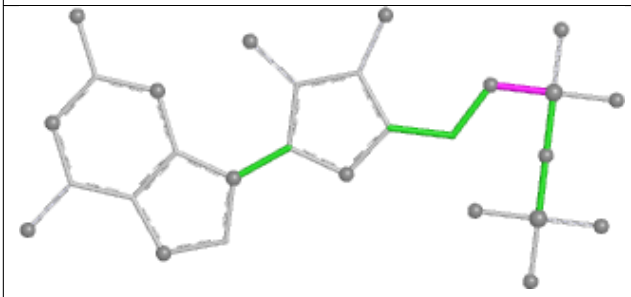
Ligand GDP ND 502



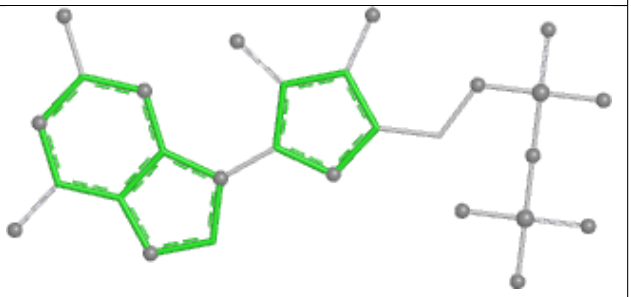
Bond lengths



Bond angles

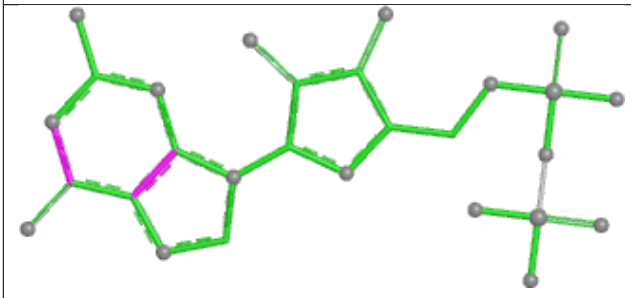


Torsions

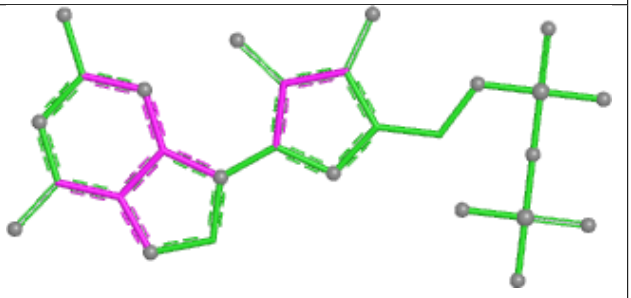


Rings

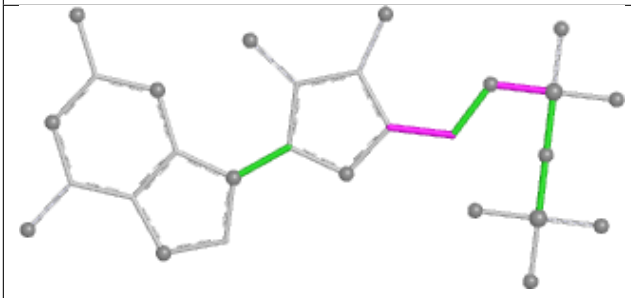
Ligand GDP OB 502



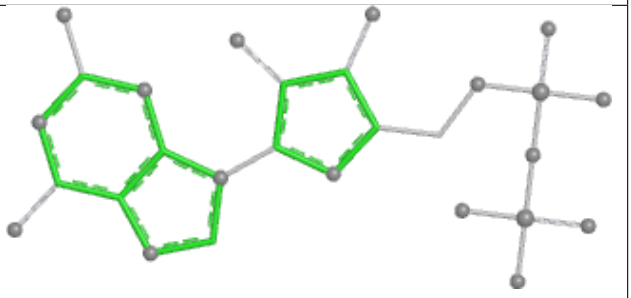
Bond lengths



Bond angles

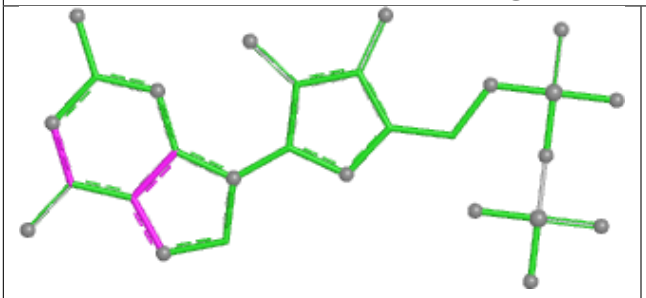


Torsions

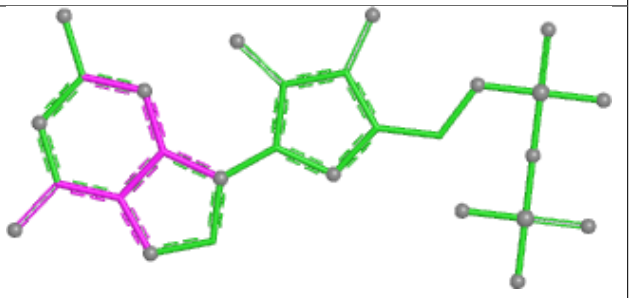


Rings

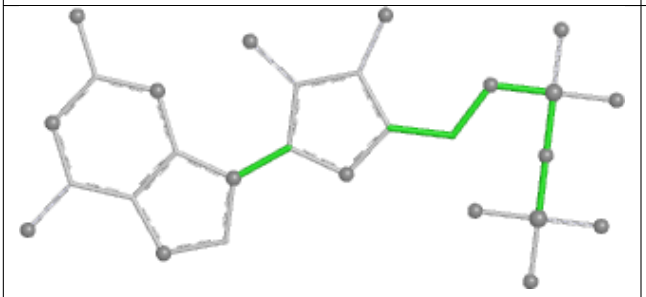
Ligand GDP CH 502



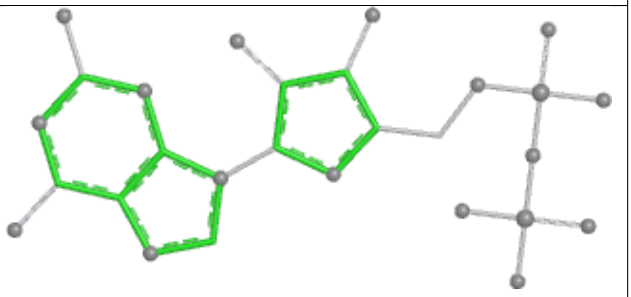
Bond lengths



Bond angles

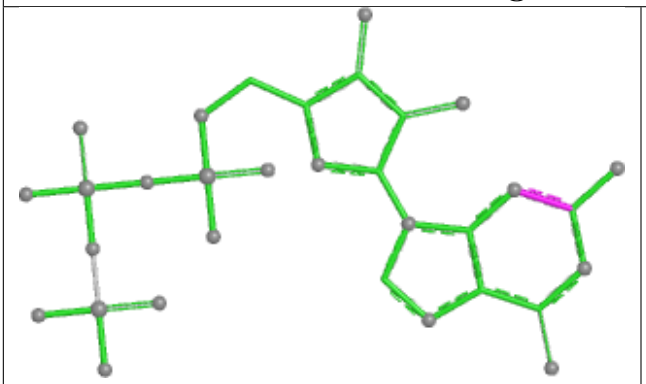


Torsions

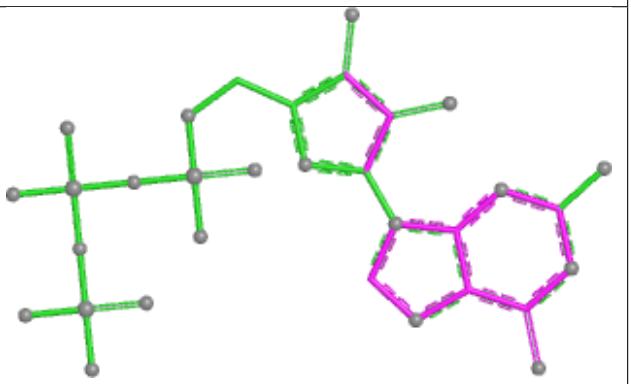


Rings

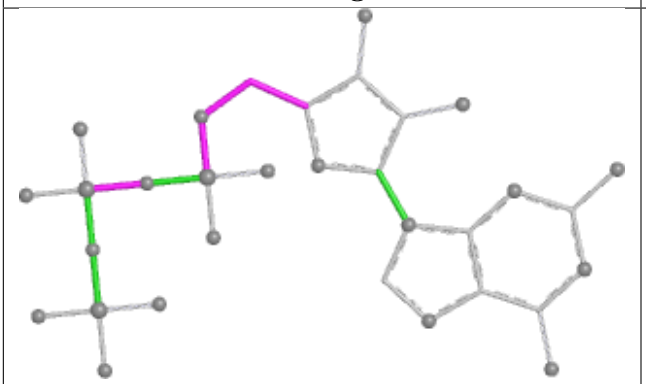
Ligand GTP OG 501



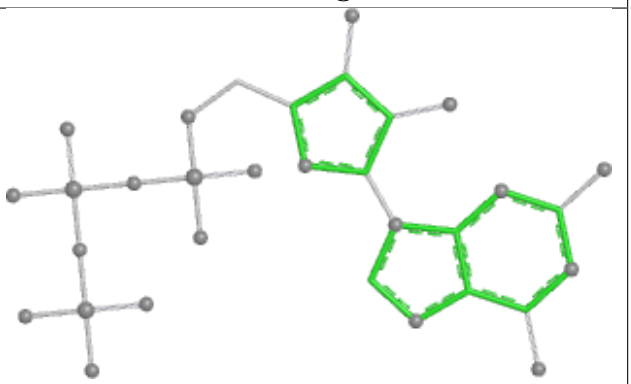
Bond lengths



Bond angles

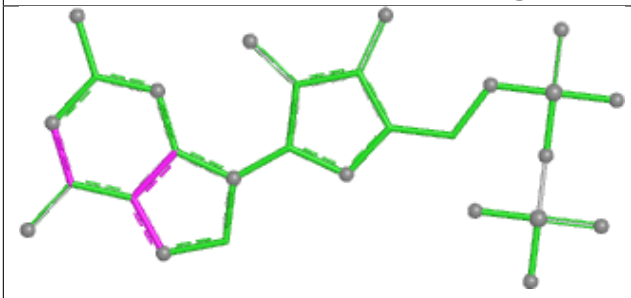


Torsions

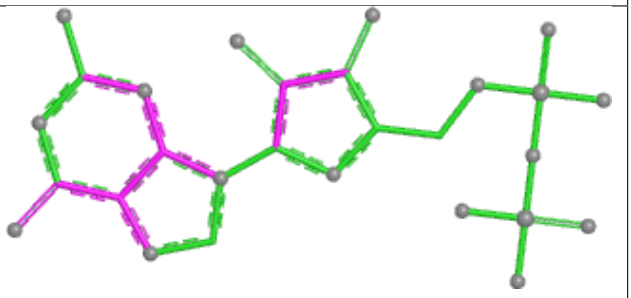


Rings

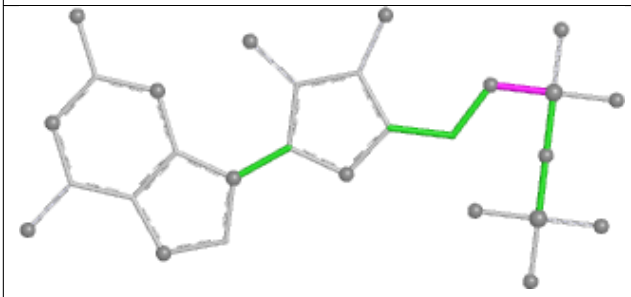
Ligand GDP SD 502



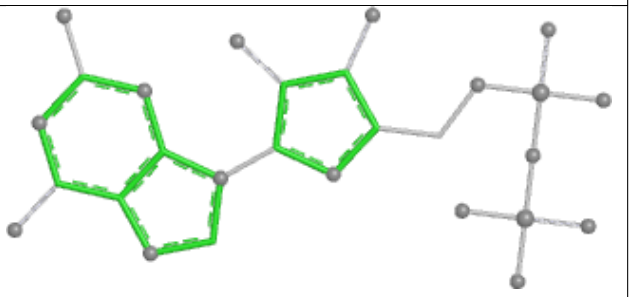
Bond lengths



Bond angles

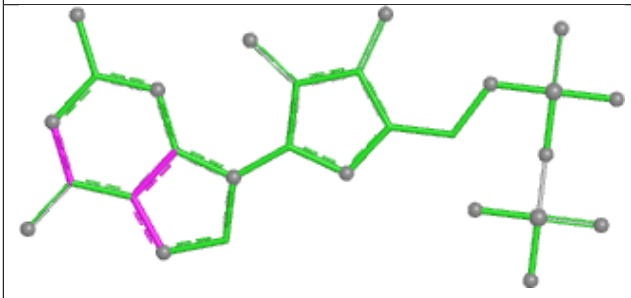


Torsions

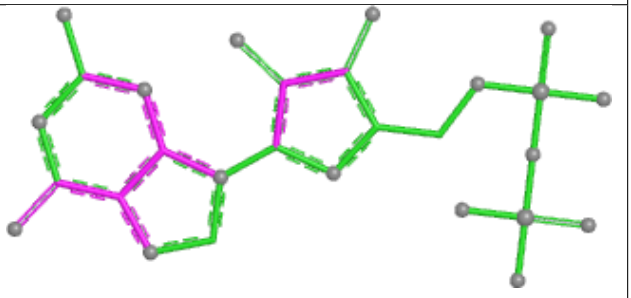


Rings

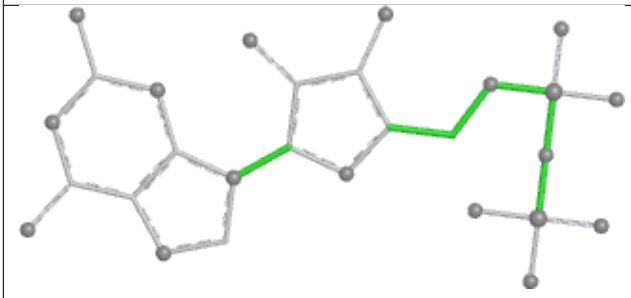
Ligand GDP AB 502



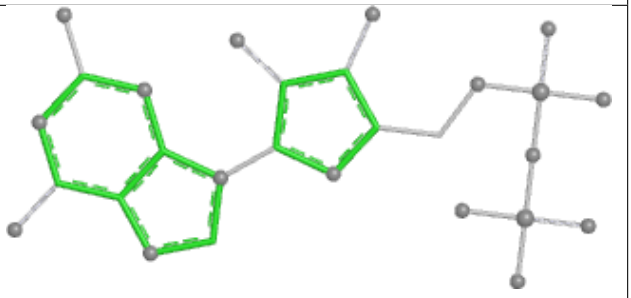
Bond lengths



Bond angles

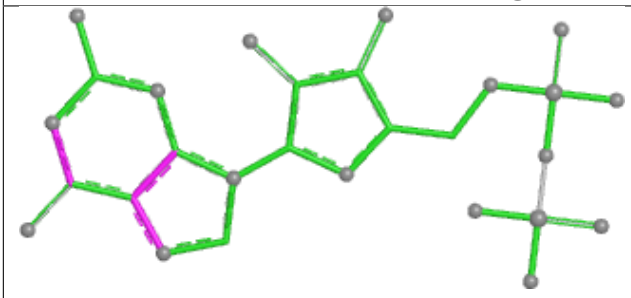


Torsions

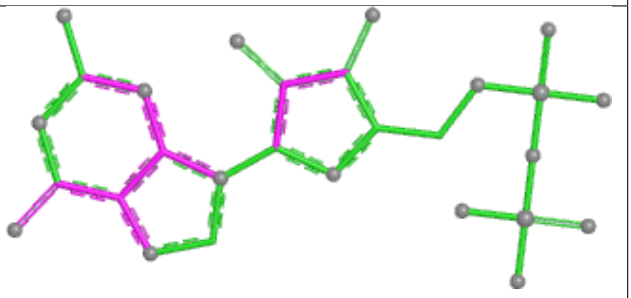


Rings

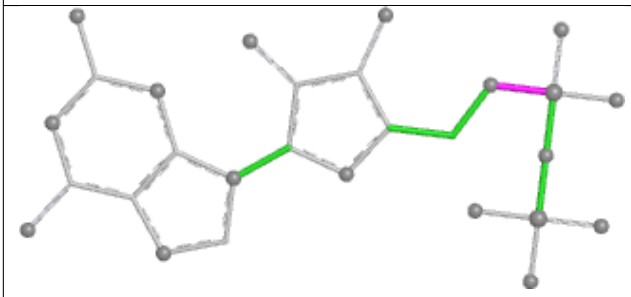
Ligand GDP FH 502



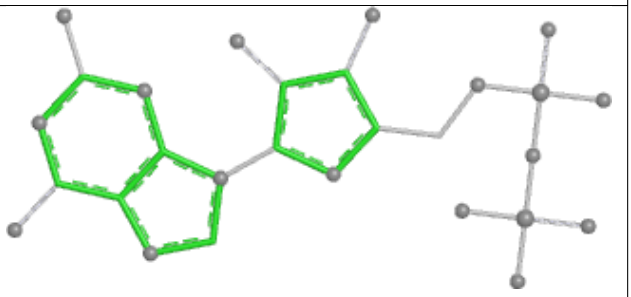
Bond lengths



Bond angles

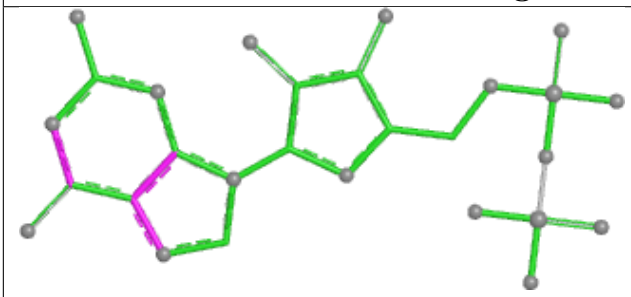


Torsions

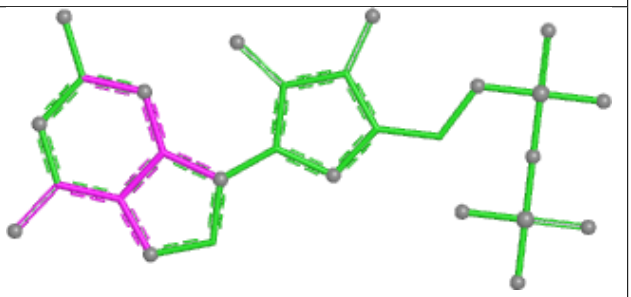


Rings

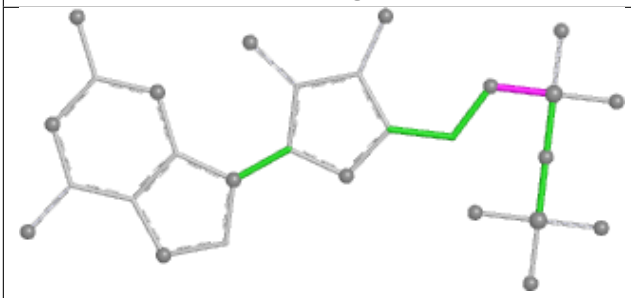
Ligand GDP EJ 502



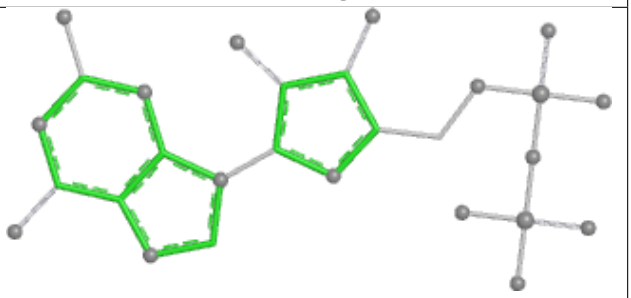
Bond lengths



Bond angles

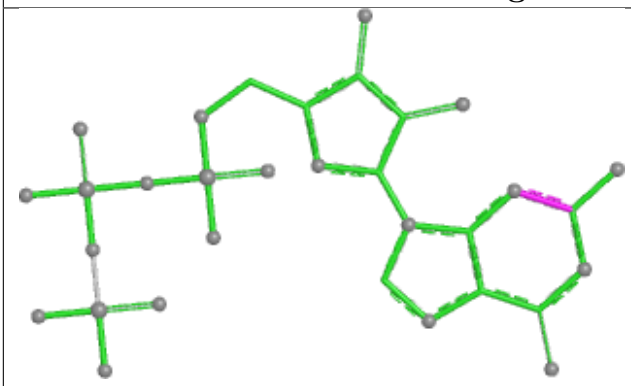


Torsions

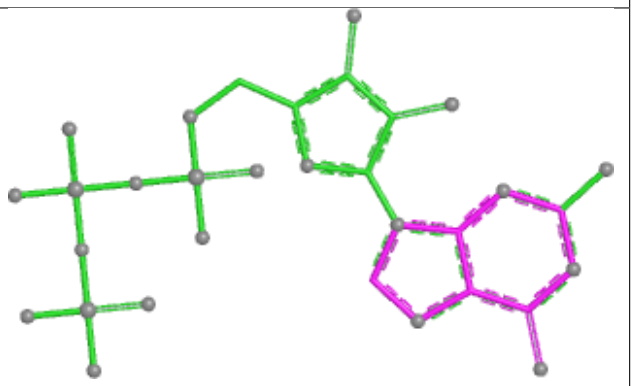


Rings

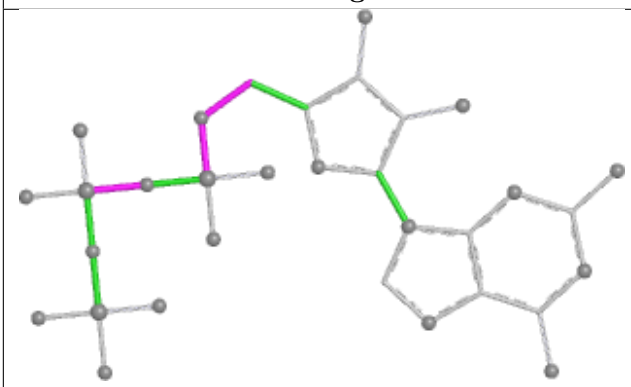
Ligand GTP AK 501



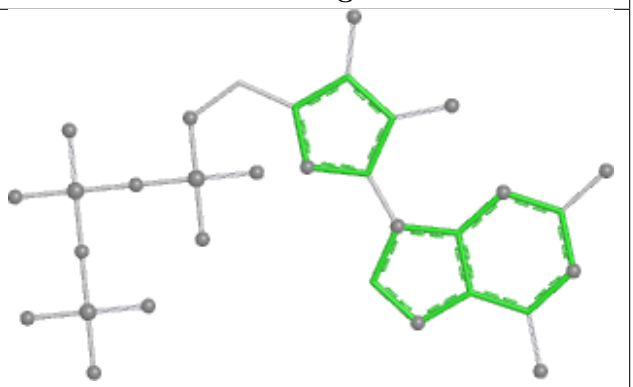
Bond lengths



Bond angles

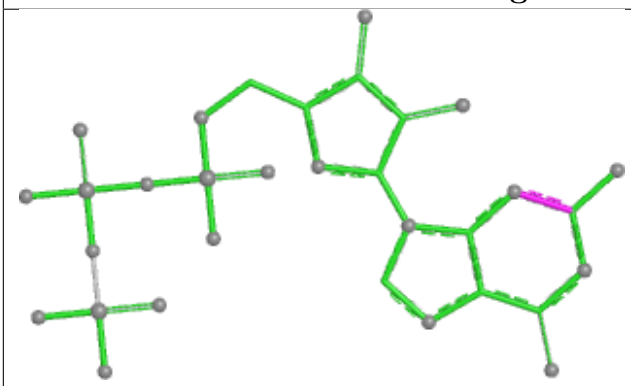


Torsions

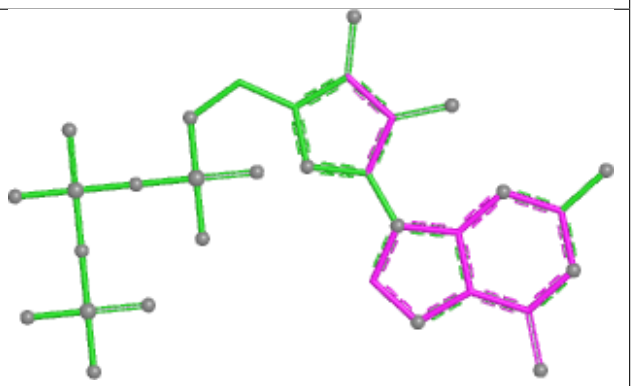


Rings

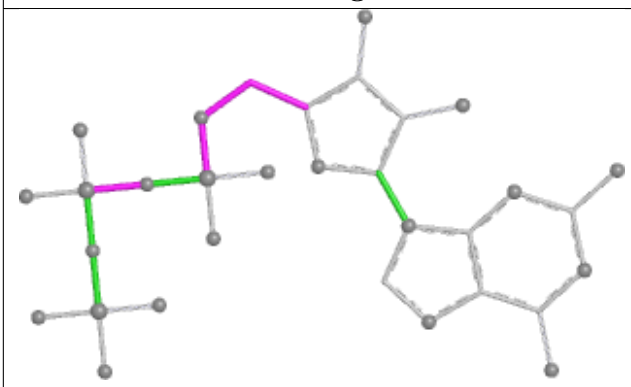
Ligand GTP BC 501



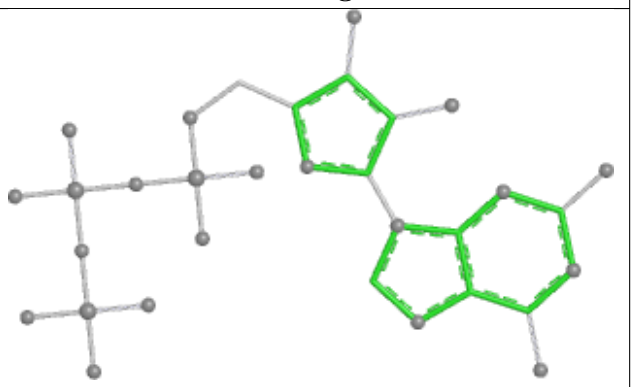
Bond lengths



Bond angles

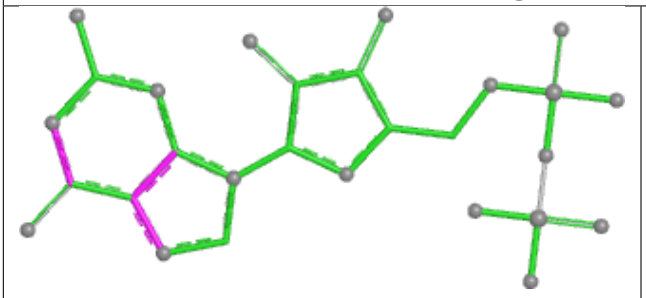


Torsions

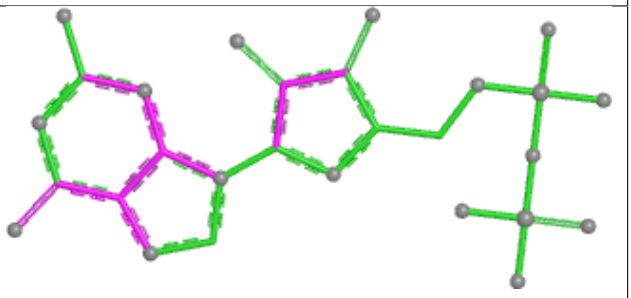


Rings

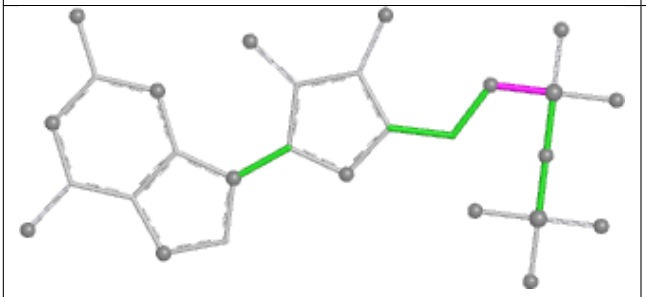
Ligand GDP SN 502



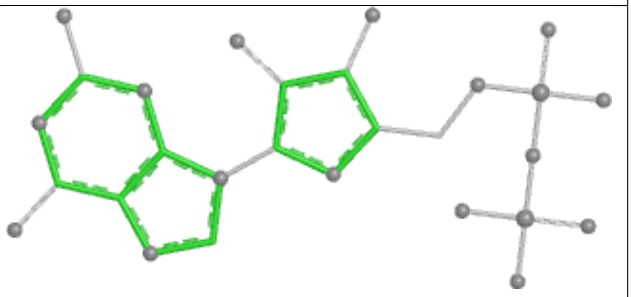
Bond lengths



Bond angles

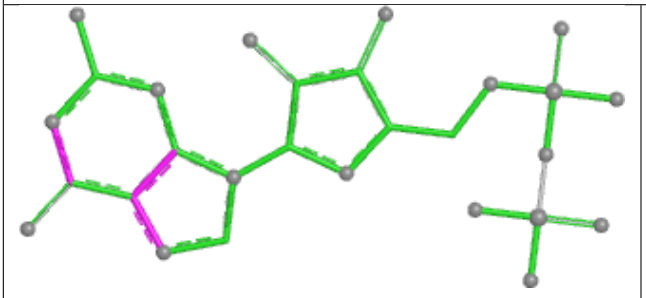


Torsions

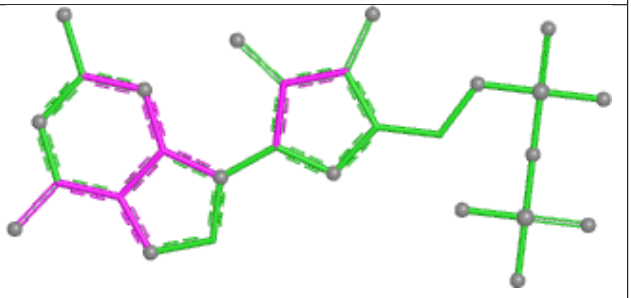


Rings

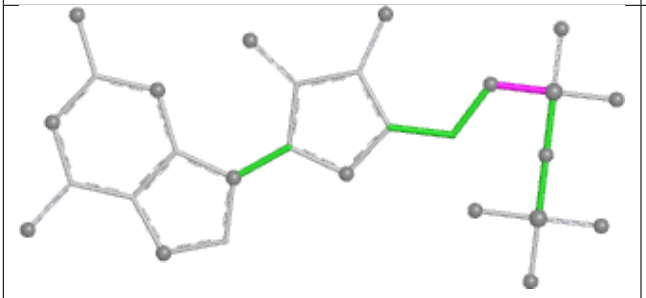
Ligand GDP WL 502



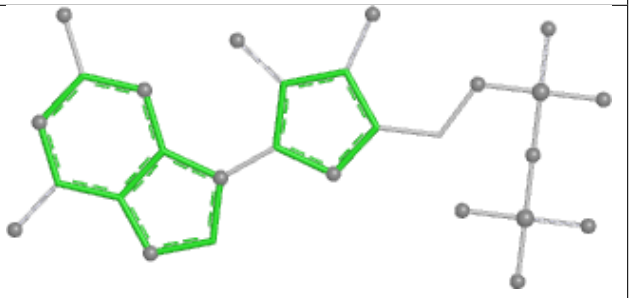
Bond lengths



Bond angles

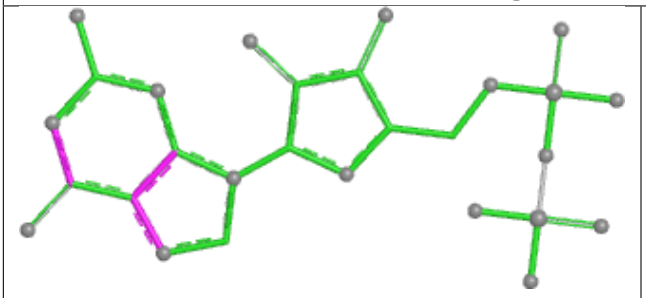


Torsions

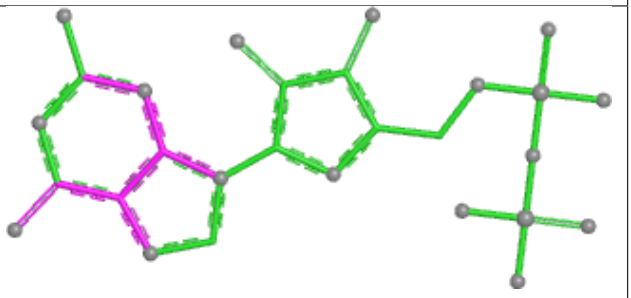


Rings

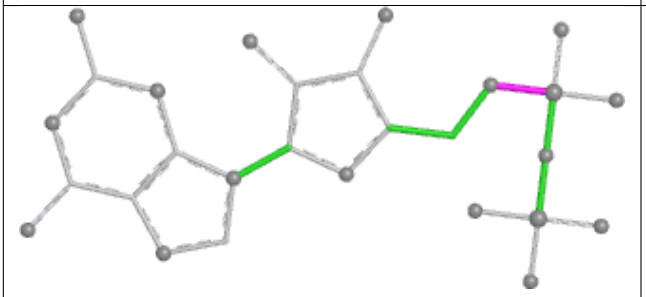
Ligand GDP CD 502



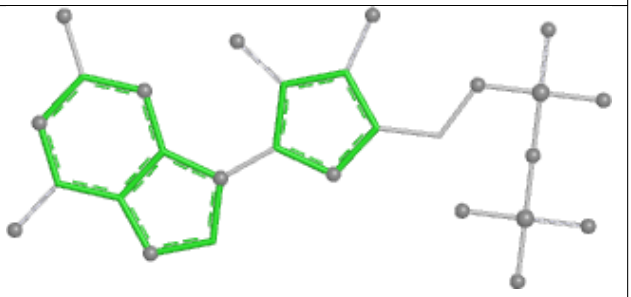
Bond lengths



Bond angles

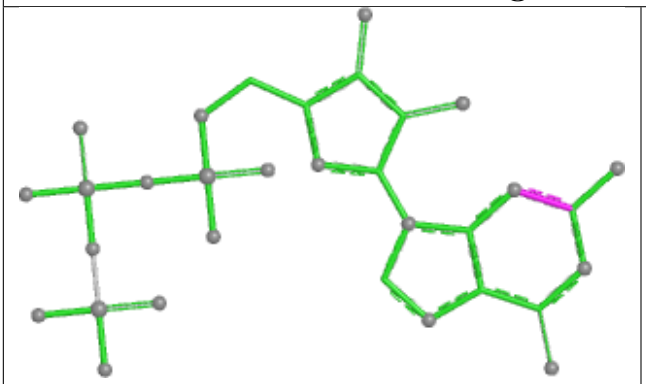


Torsions

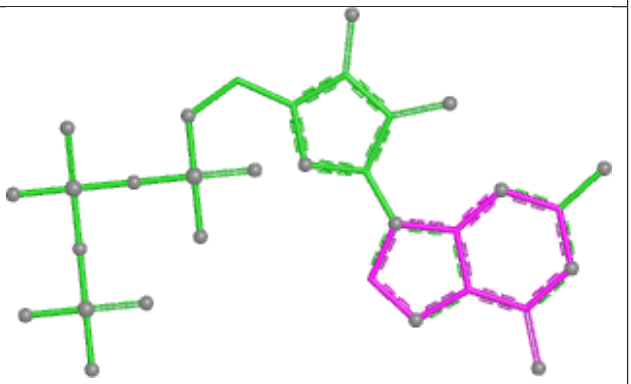


Rings

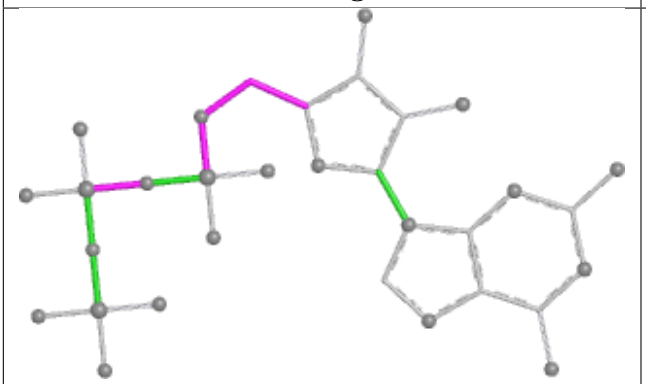
Ligand GTP VO 501



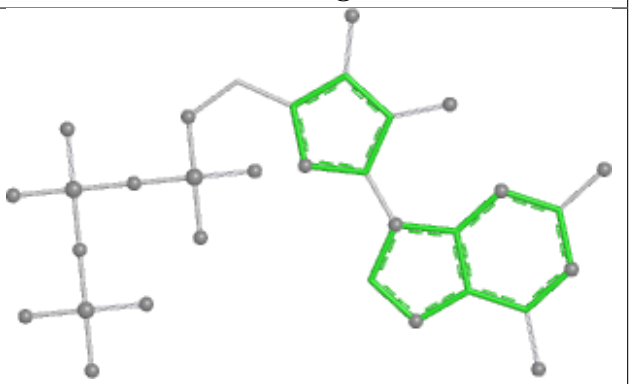
Bond lengths



Bond angles

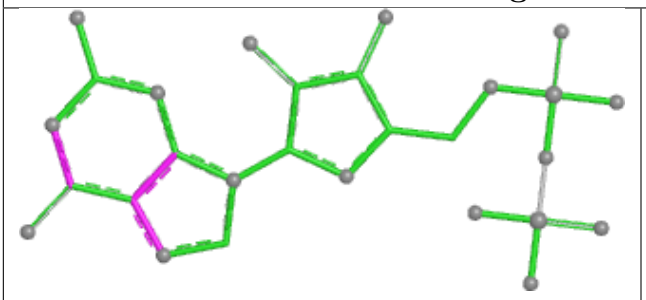


Torsions

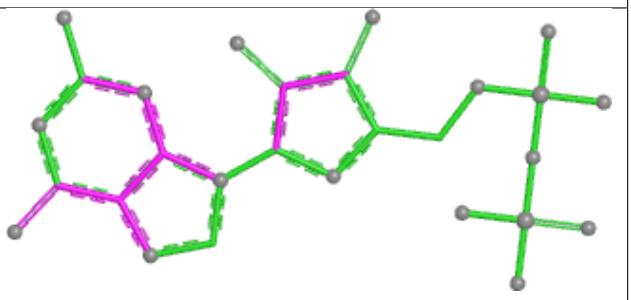


Rings

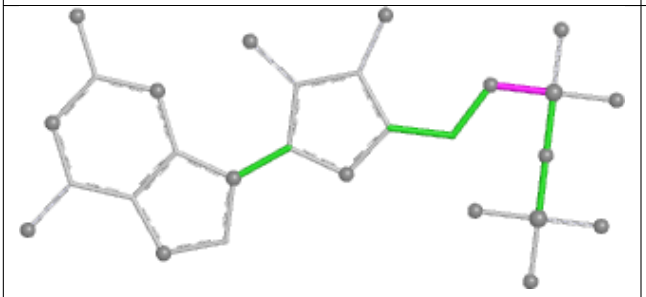
Ligand GDP RF 502



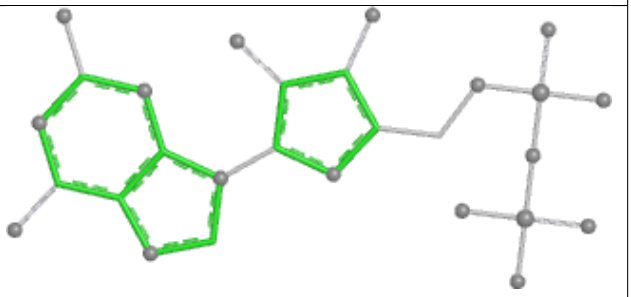
Bond lengths



Bond angles

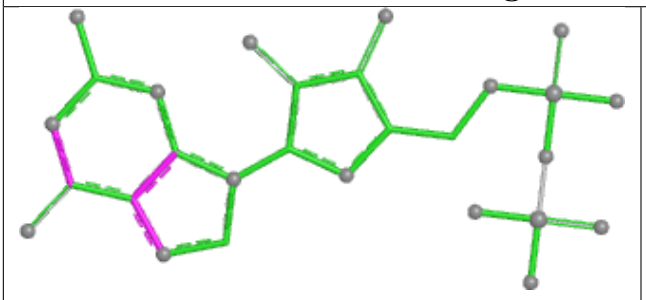


Torsions

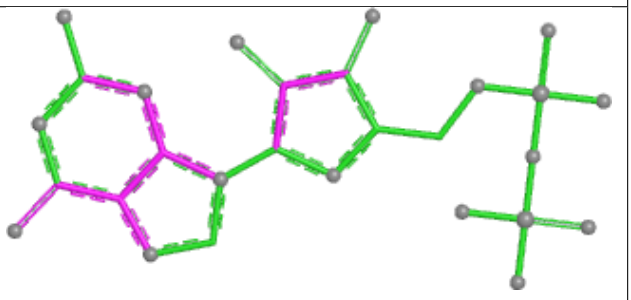


Rings

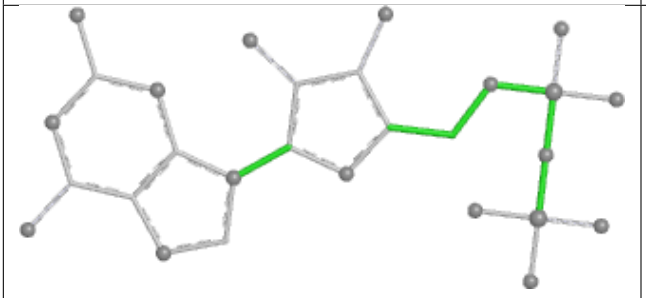
Ligand GDP WB 502



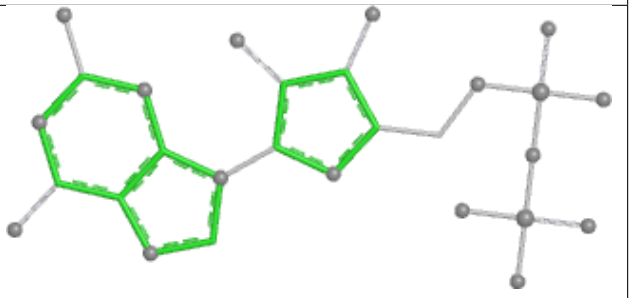
Bond lengths



Bond angles

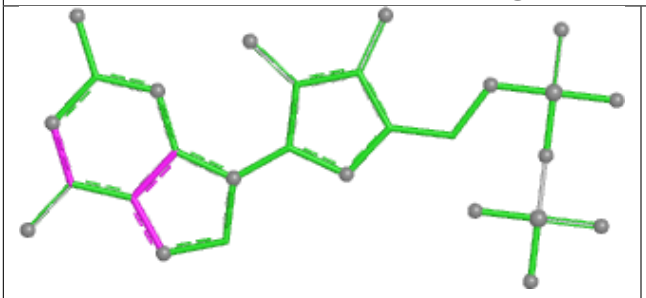


Torsions

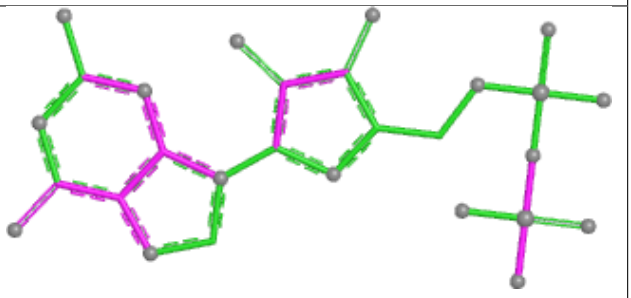


Rings

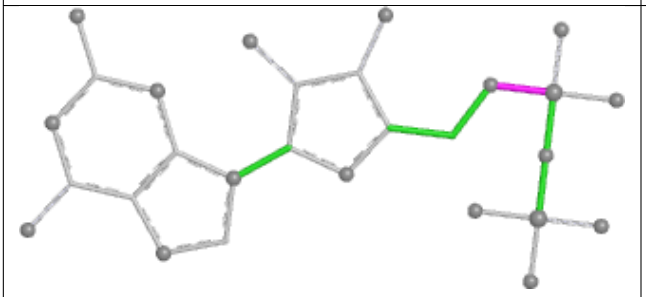
Ligand GDP TB 502



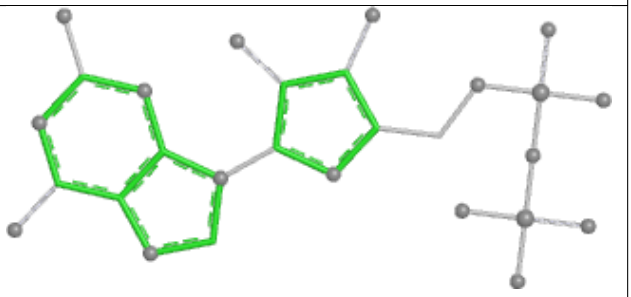
Bond lengths



Bond angles

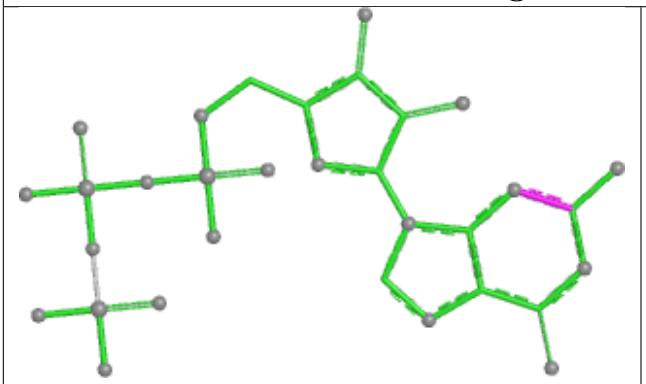


Torsions

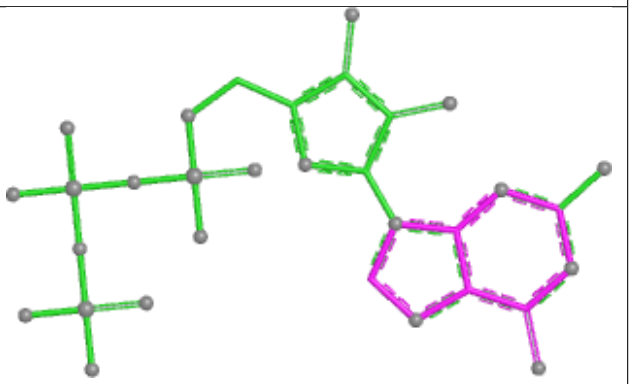


Rings

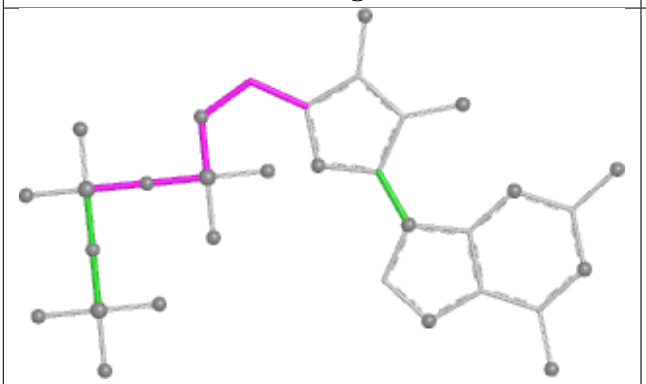
Ligand GTP GO 501



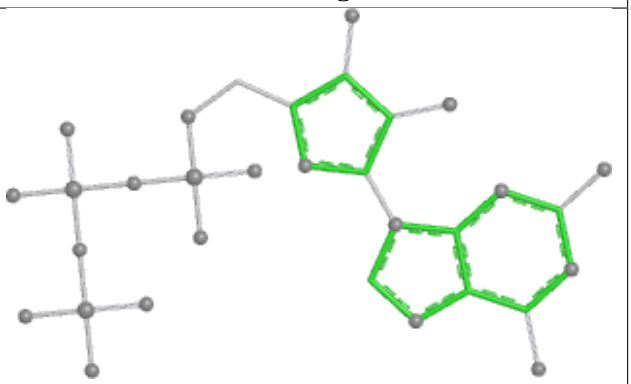
Bond lengths



Bond angles

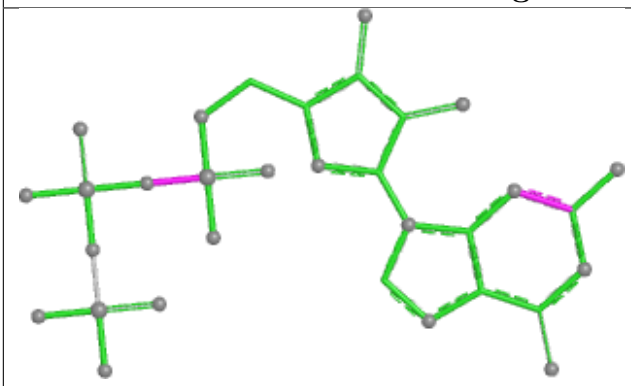


Torsions

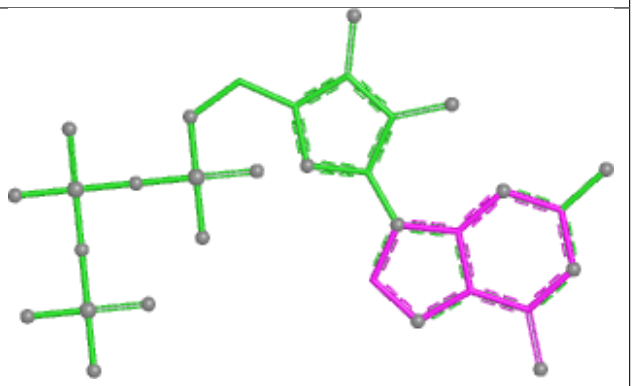


Rings

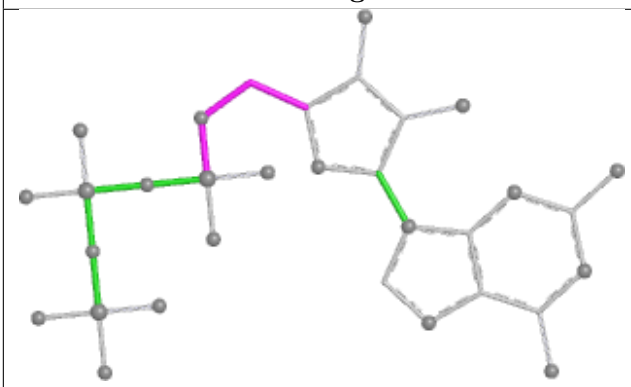
Ligand GTP JG 501



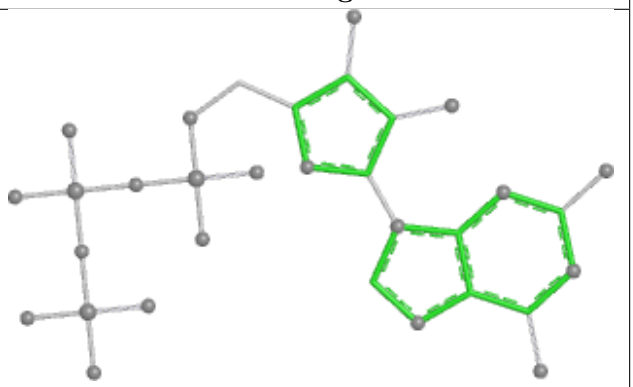
Bond lengths



Bond angles

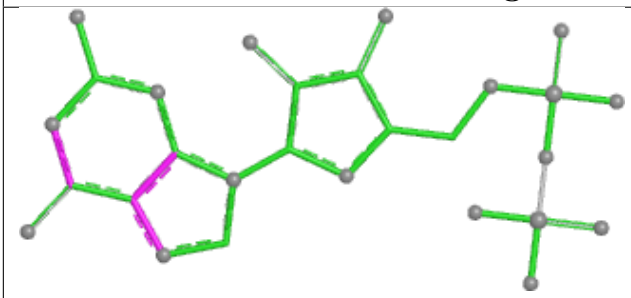


Torsions

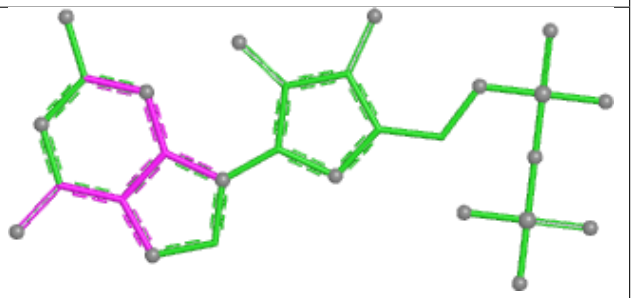


Rings

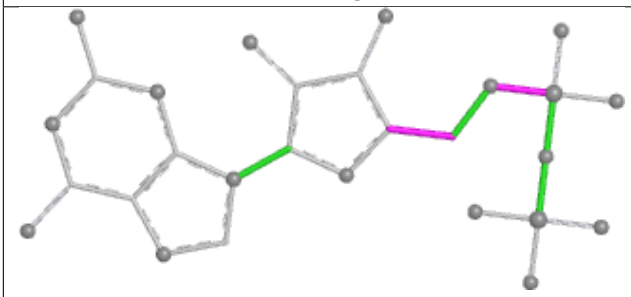
Ligand GDP MH 502



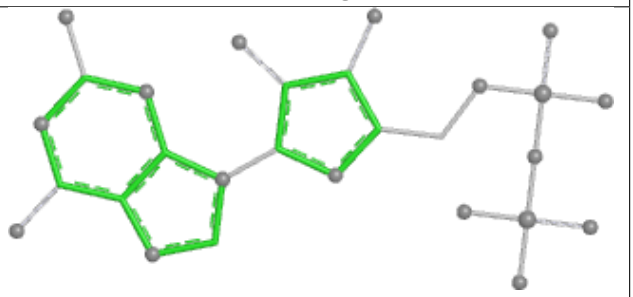
Bond lengths



Bond angles

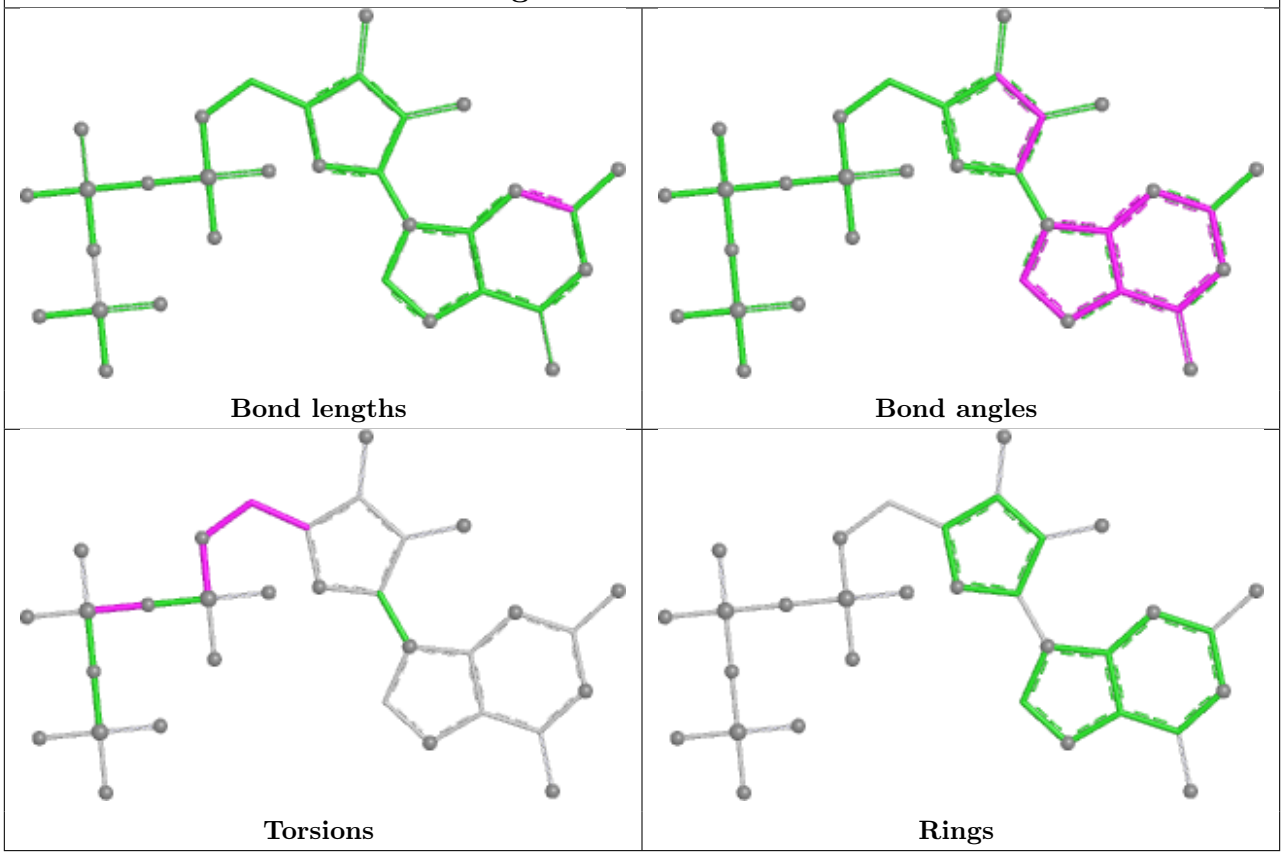


Torsions

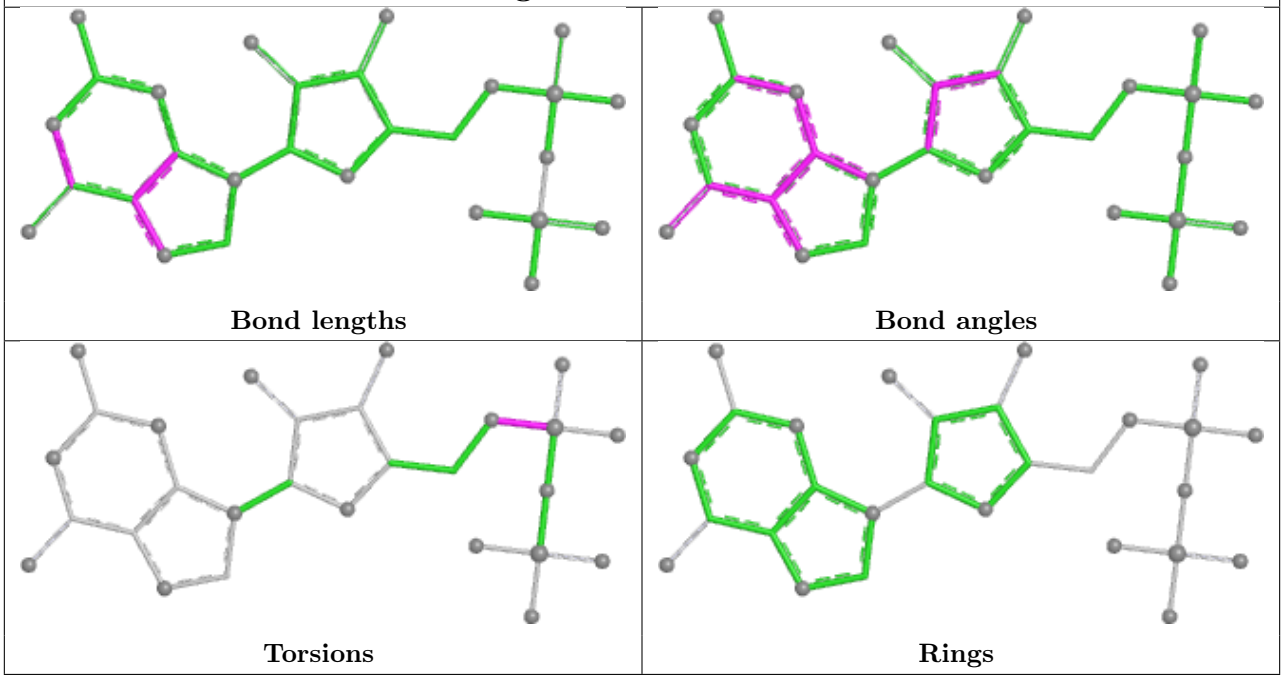


Rings

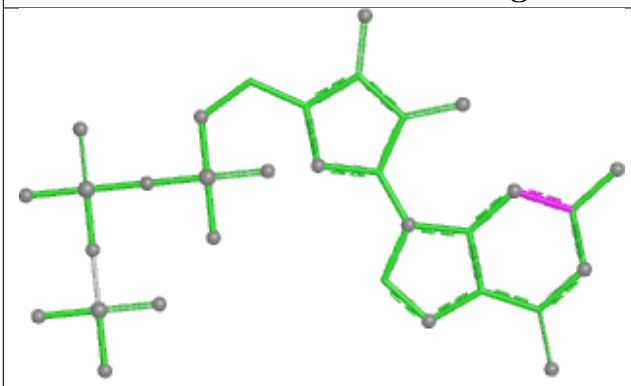
Ligand GTP VE 501



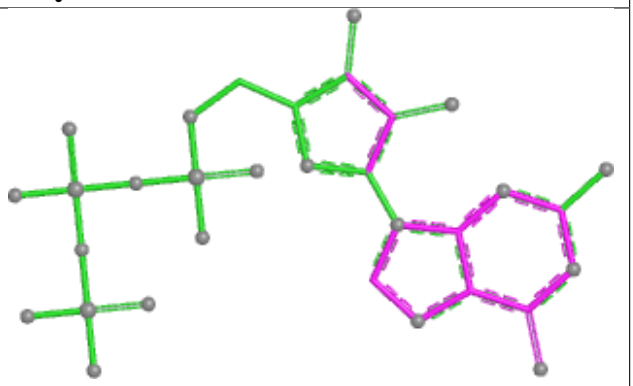
Ligand GDP SL 502



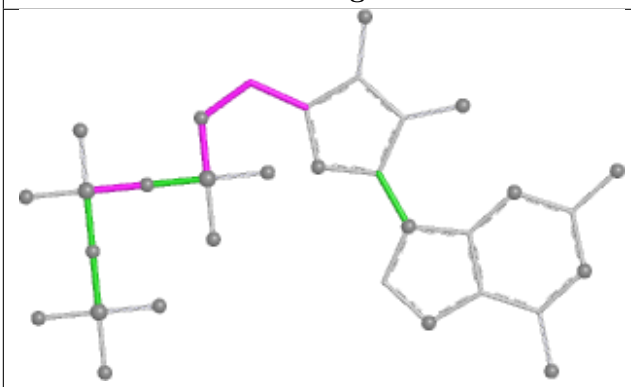
Ligand GTP QE 501



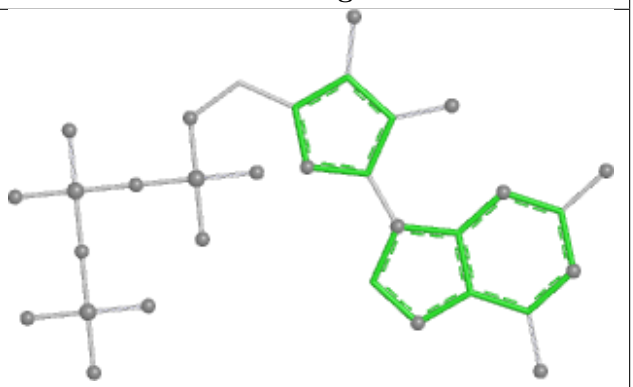
Bond lengths



Bond angles

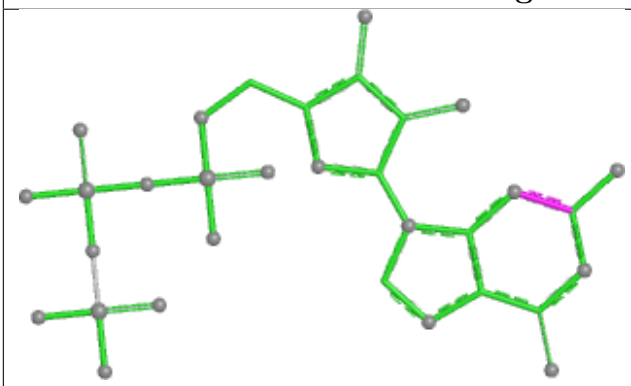


Torsions

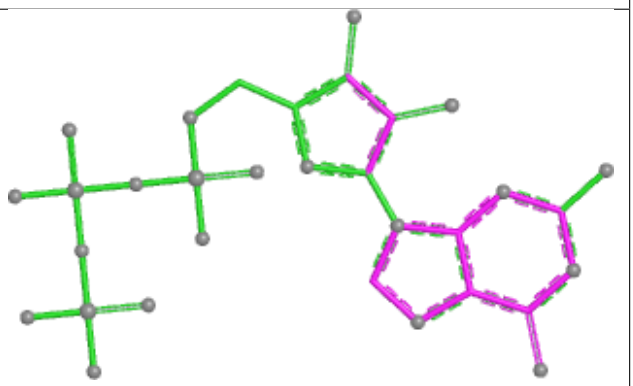


Rings

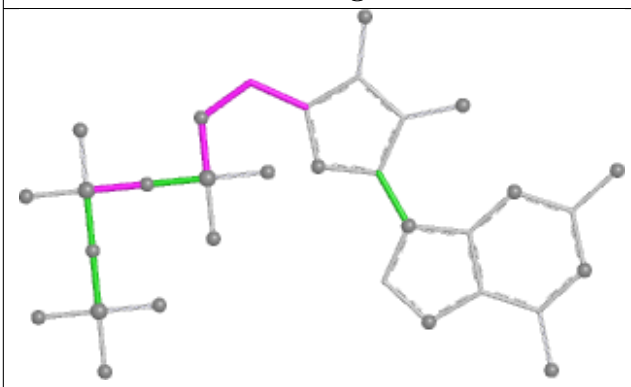
Ligand GTP IA 501



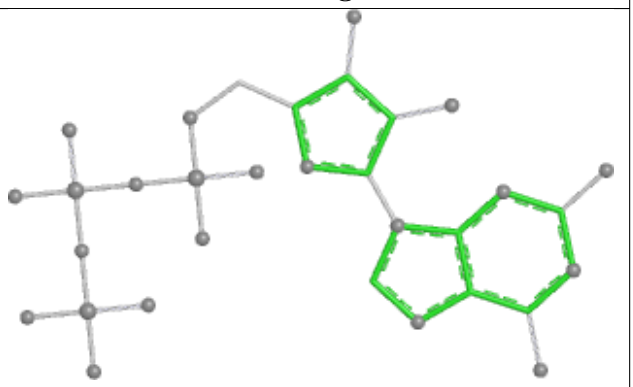
Bond lengths



Bond angles

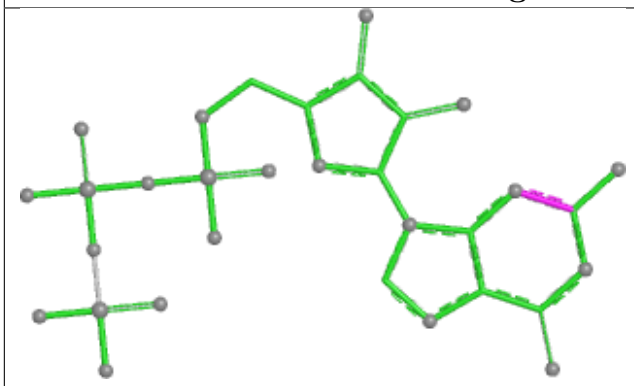


Torsions

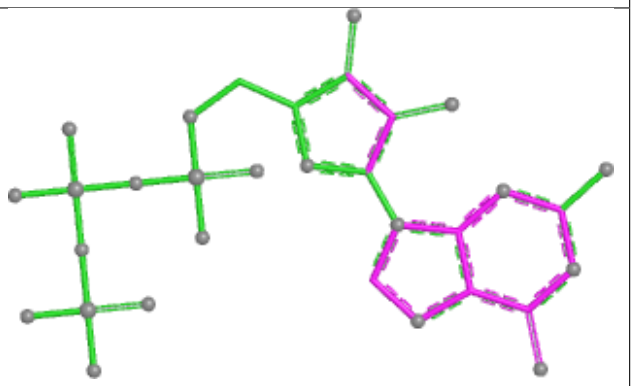


Rings

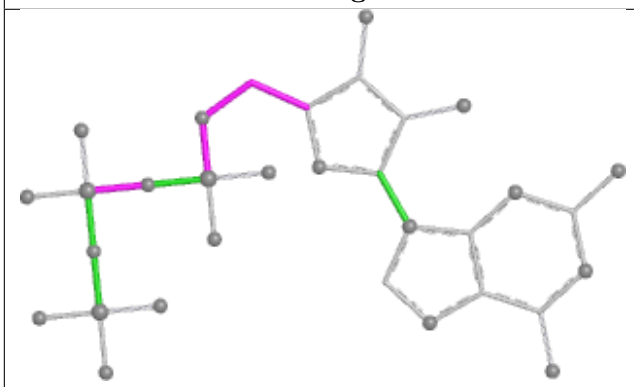
Ligand GTP NA 501



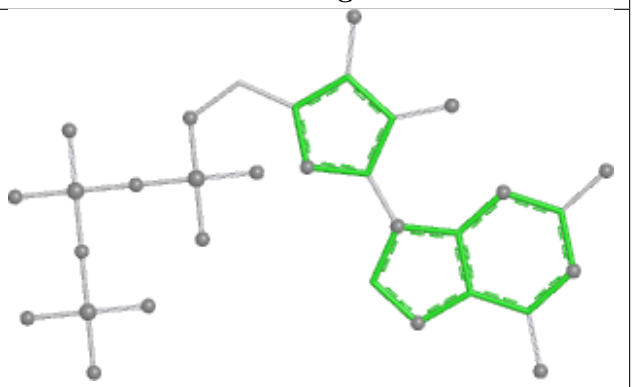
Bond lengths



Bond angles

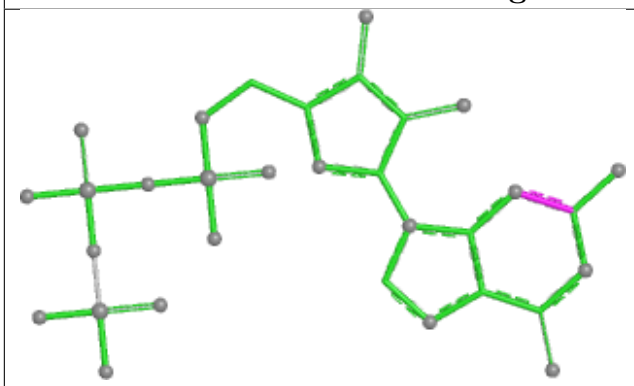


Torsions

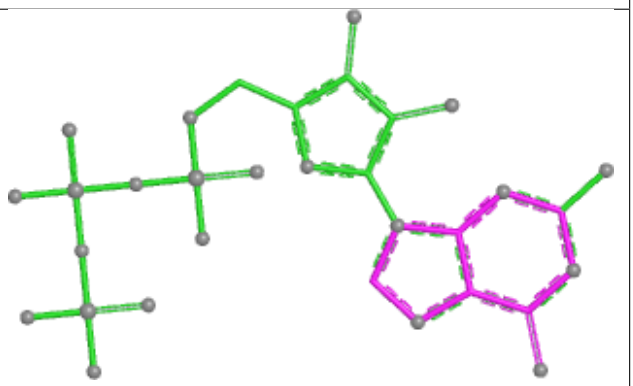


Rings

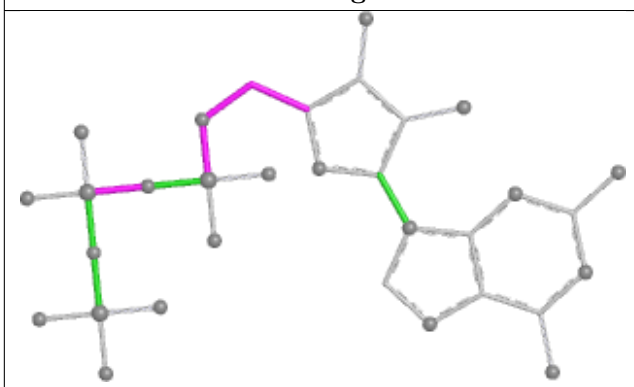
Ligand GTP VK 501



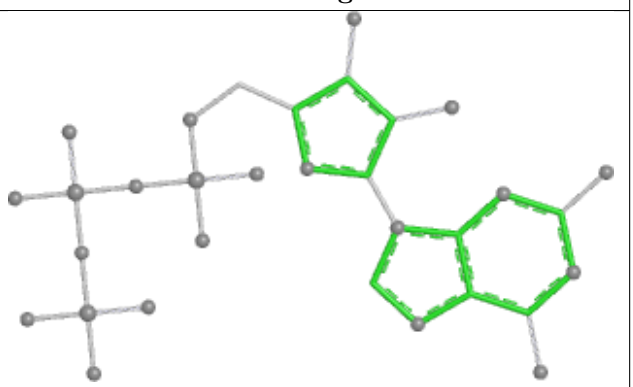
Bond lengths



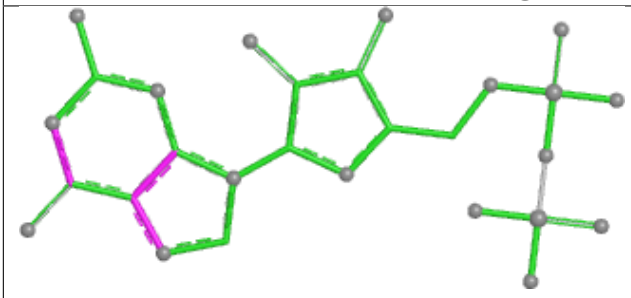
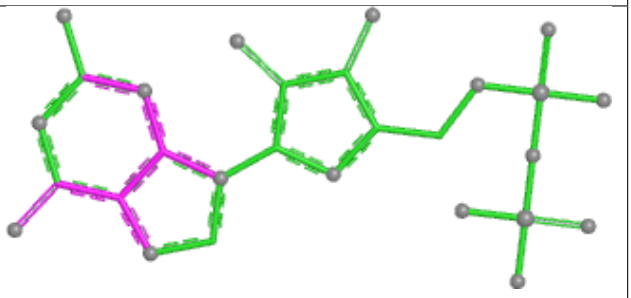
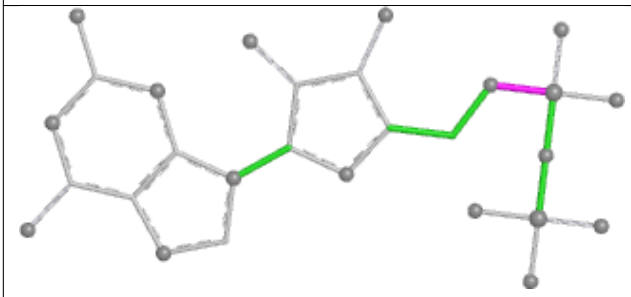
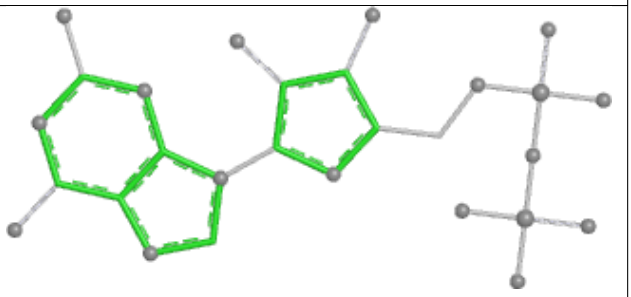
Bond angles

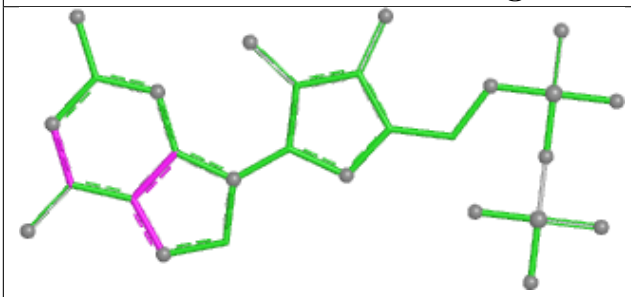
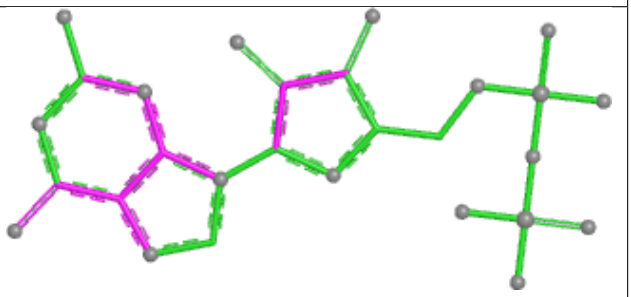
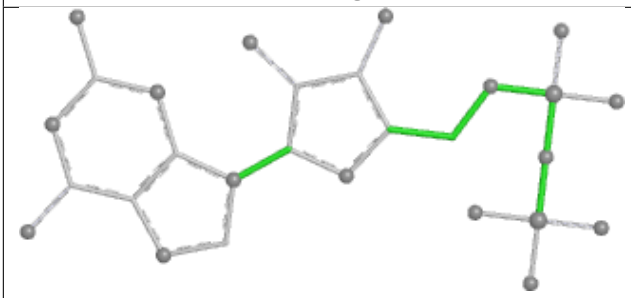
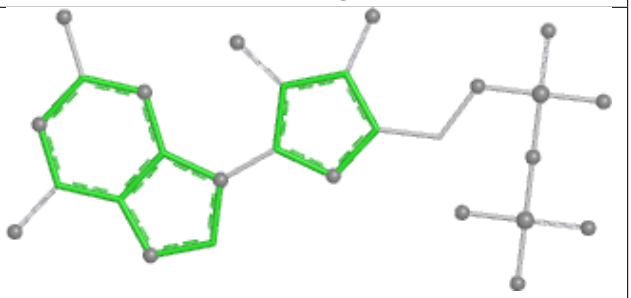


Torsions



Rings

Ligand GDP IF 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP HN 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

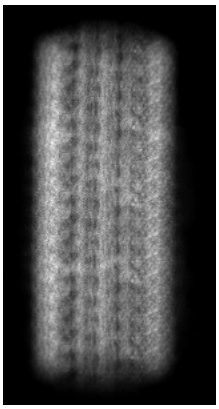
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35823. These allow visual inspection of the internal detail of the map and identification of artifacts.

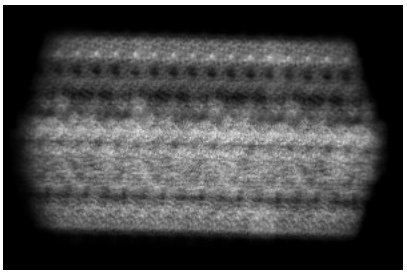
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

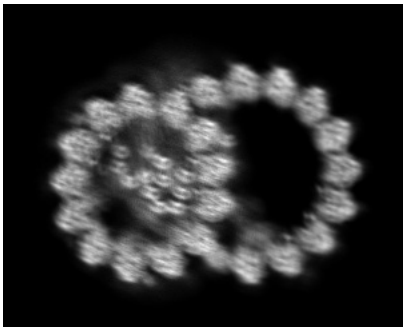
6.1.1 Primary map



X



Y

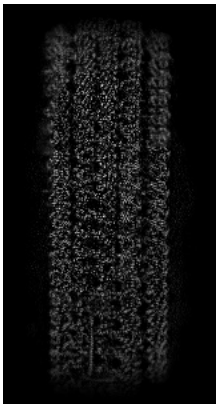


Z

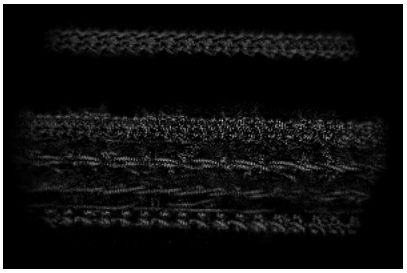
The images above show the map projected in three orthogonal directions.

6.2 Central slices

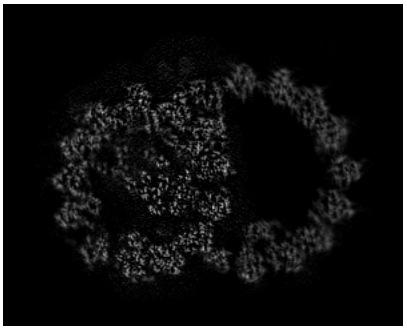
6.2.1 Primary map



X Index: 265



Y Index: 213

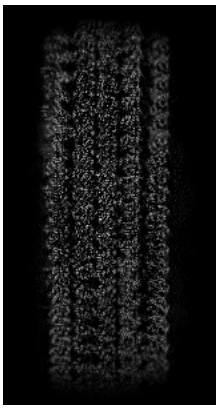


Z Index: 400

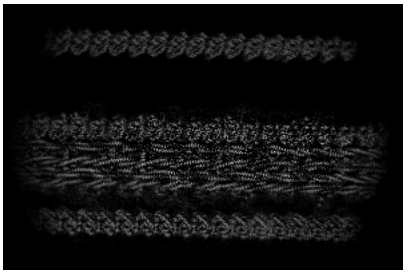
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

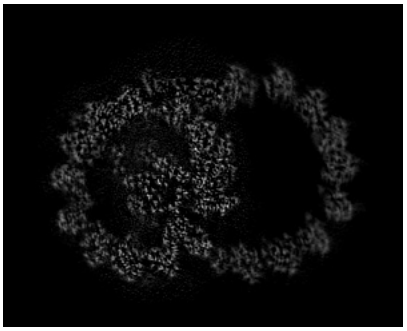
6.3.1 Primary map



X Index: 270



Y Index: 196

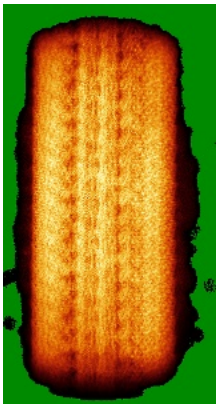


Z Index: 448

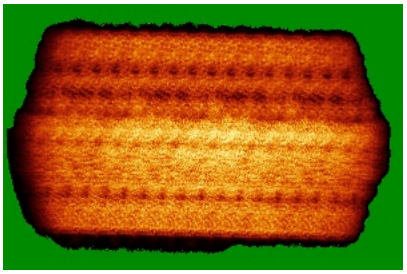
The images above show the largest variance slices of the map in three orthogonal directions.

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

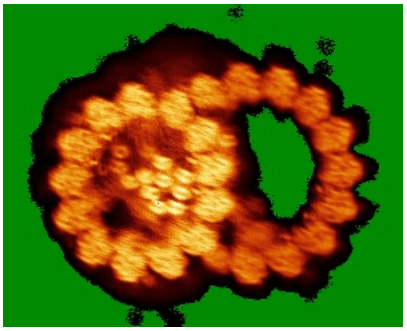
6.4.1 Primary map



X



Y



Z

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.

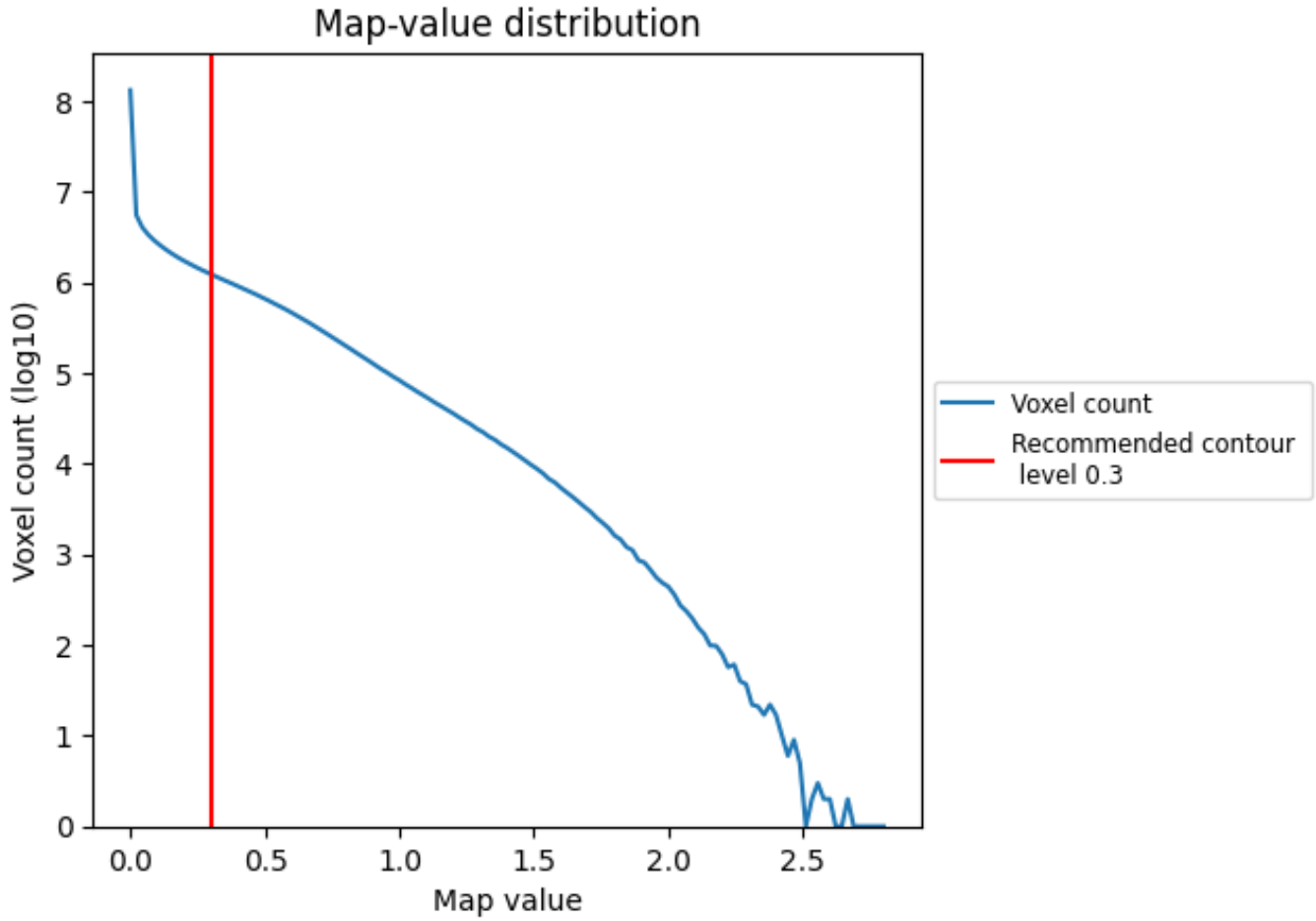
6.6 Mask visualisation (i)

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

7 Map analysis

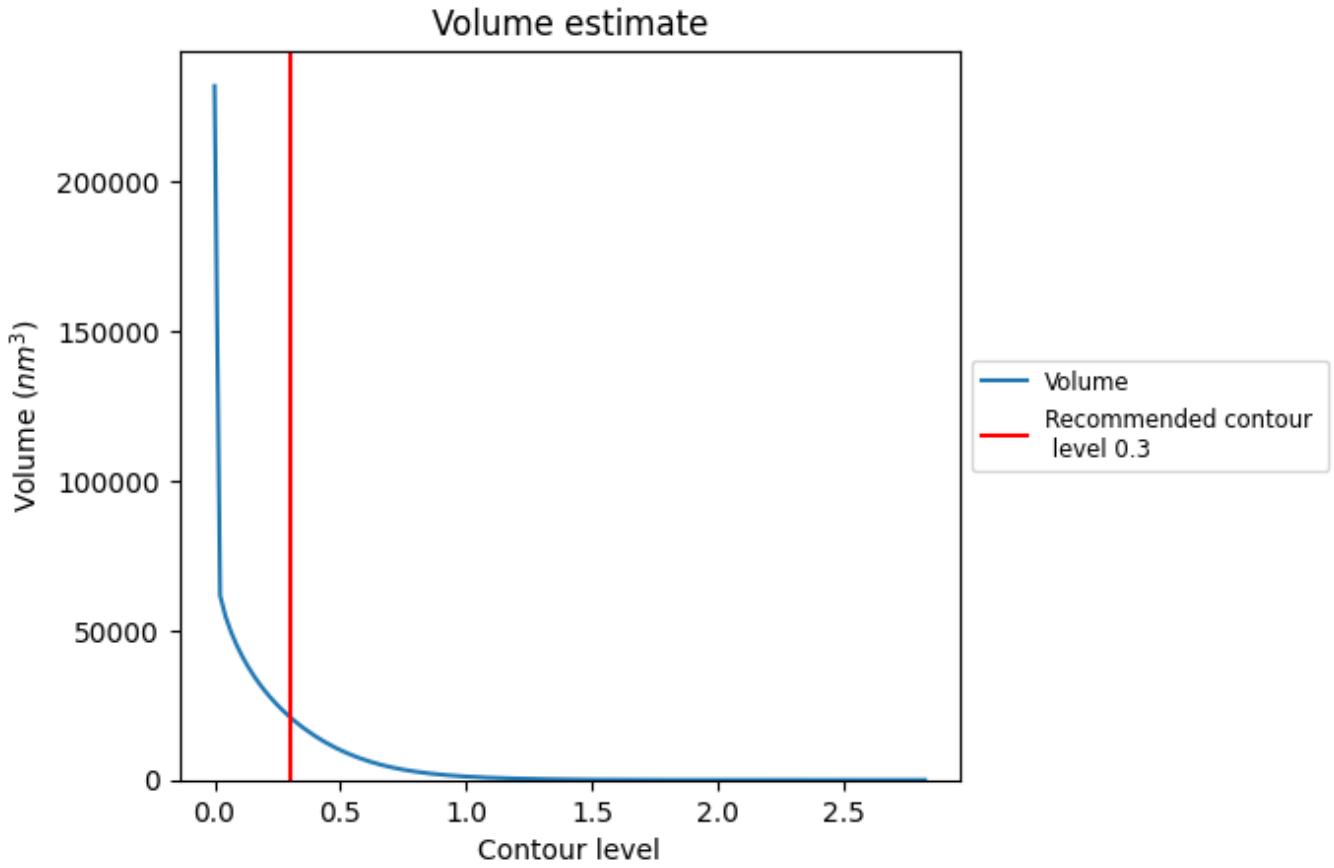
This section contains the results of statistical analysis of the map.

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 21016 nm^3; this corresponds to an approximate mass of 18985 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

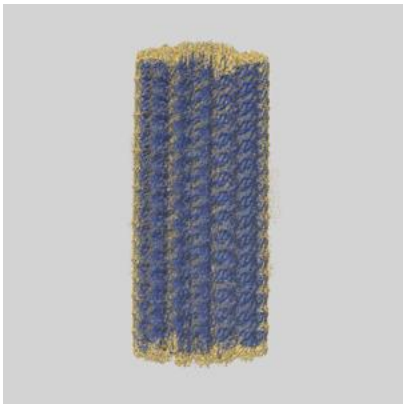
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

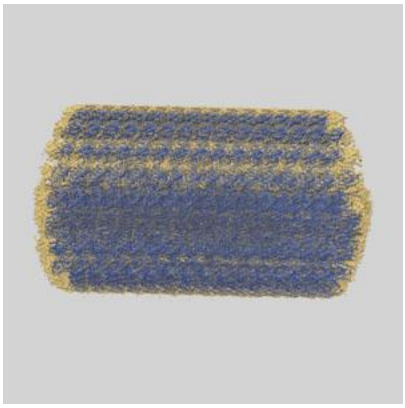
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35823 and PDB model 8IYJ. Per-residue inclusion information can be found in section 3 on page 85.

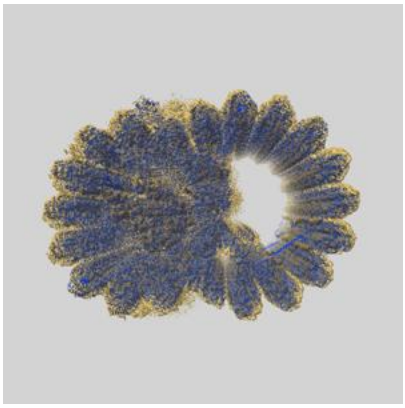
9.1 Map-model overlay



X



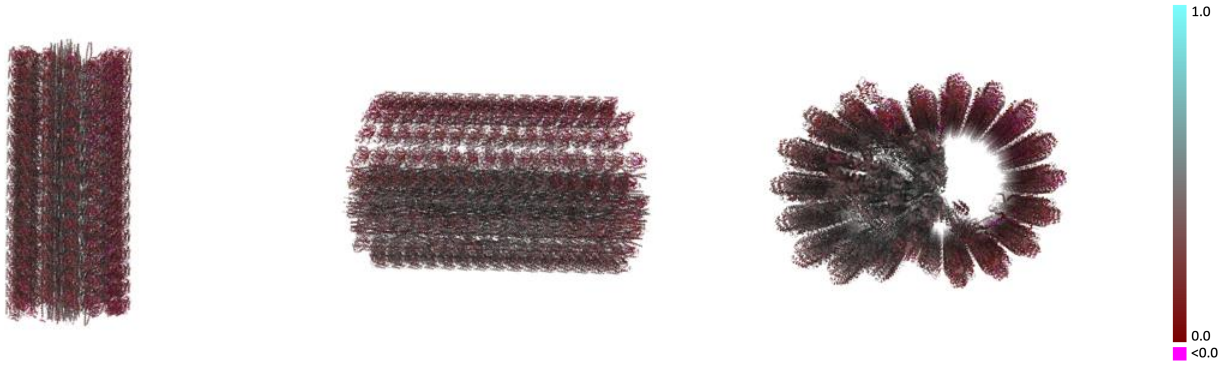
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



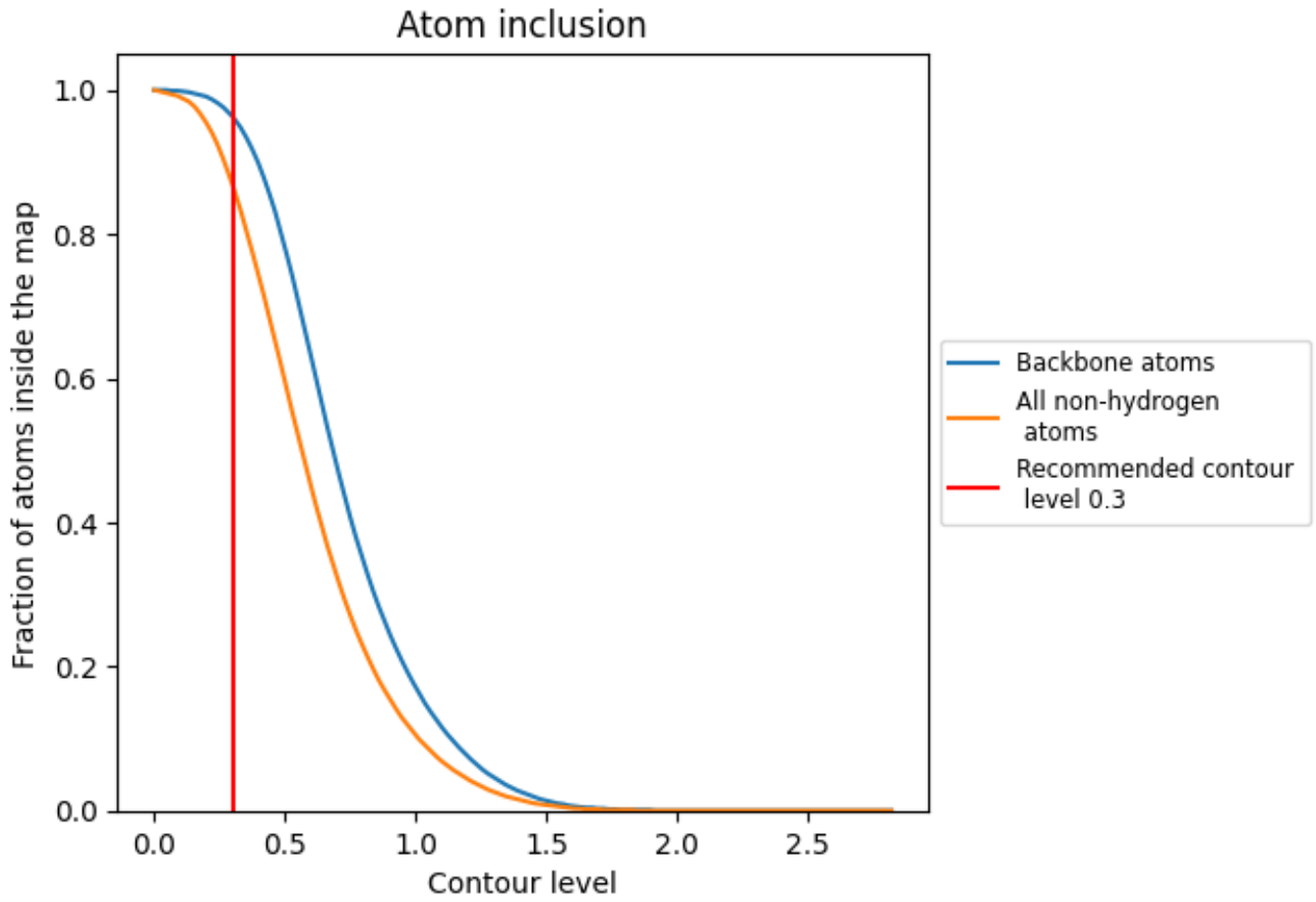
X Y Z

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

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 87% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.3500
0	0.7450	0.3730
1	0.8190	0.3730
2	0.8610	0.4040
3	0.7760	0.3250
4	0.7930	0.3380
5	0.8770	0.3650
6	0.8500	0.3880
7	0.8190	0.3740
8	0.9100	0.4350
A	0.7950	0.3460
A0	0.8820	0.4010
A1	0.8990	0.4490
A2	0.9230	0.4990
A3	0.9280	0.5010
A4	0.9010	0.4480
A5	0.8410	0.3840
AA	0.8650	0.2940
AB	0.9190	0.3730
AC	0.9390	0.4340
AD	0.9280	0.4460
AE	0.9290	0.4640
AF	0.9250	0.4520
AG	0.9500	0.4610
AH	0.9330	0.4700
AI	0.9300	0.4800
AJ	0.9220	0.4670
AK	0.9270	0.4730
AL	0.9370	0.4510
AM	0.9220	0.4350
AN	0.9420	0.3990
AO	0.9110	0.3680
AP	0.8850	0.3590
B	0.7980	0.3430
B0	0.8720	0.3970

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B1	0.8860	0.4460
B2	0.9190	0.4950
B3	0.9200	0.4960
B4	0.8860	0.4550
B5	0.7900	0.3900
BB	0.9060	0.3690
BC	0.9180	0.3980
BD	0.9420	0.4120
BE	0.9140	0.4070
BF	0.9410	0.4480
BG	0.9530	0.4550
BH	0.9520	0.4650
BI	0.9580	0.4700
BJ	0.9440	0.4530
BK	0.9540	0.4640
BL	0.9250	0.4330
BM	0.9190	0.4170
BN	0.9380	0.3890
BO	0.8930	0.3780
BP	0.8510	0.3330
C	0.8290	0.3600
C0	0.8950	0.4070
C1	0.9270	0.4750
C2	0.9450	0.5030
C3	0.9300	0.4910
C4	0.8790	0.4090
C5	0.8230	0.3570
C6	0.6400	0.3920
CB	0.8430	0.3530
CC	0.8710	0.3850
CD	0.9060	0.3980
CE	0.9270	0.3920
CF	0.9470	0.4340
CG	0.9510	0.4460
CH	0.9550	0.4760
CI	0.9490	0.4640
CJ	0.9520	0.4680
CK	0.9480	0.4730
CL	0.9360	0.4330
CM	0.9200	0.4070
CN	0.9170	0.3490
CO	0.8580	0.3660

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CP	0.8390	0.3480
CQ	0.7210	0.3190
D	0.7960	0.4060
D0	0.8360	0.4130
D1	0.8890	0.4600
D2	0.9110	0.4910
D3	0.9250	0.4970
D4	0.8580	0.4260
D5	0.8620	0.4030
DB	0.7410	0.3540
DC	0.8540	0.3470
DD	0.8990	0.3840
DE	0.9230	0.4050
DF	0.9730	0.3680
DG	0.9570	0.3880
DH	0.9490	0.4210
DI	0.9320	0.3990
DJ	0.9520	0.4460
DK	0.9470	0.4320
DL	0.9430	0.4110
DM	0.9360	0.3780
DN	0.9080	0.3820
DO	0.8770	0.3710
DP	0.8510	0.3670
DQ	0.7420	0.3270
E	0.9300	0.4530
EA	0.8070	0.3620
EB	0.8810	0.3930
EC	0.8840	0.4030
ED	0.9430	0.3720
EE	0.9300	0.3360
EF	0.9240	0.3970
EG	0.9340	0.4070
EH	0.9360	0.4180
EI	0.9290	0.4120
EJ	0.9370	0.4070
EK	0.9320	0.3920
EL	0.8850	0.3760
EM	0.8300	0.3300
EN	0.8540	0.3670
EO	0.7560	0.3380
F	0.6990	0.3720

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
FA	0.8130	0.3330
FB	0.8760	0.3630
FC	0.9030	0.3740
FD	0.9410	0.3690
FE	0.9640	0.3360
FF	0.9340	0.3820
FG	0.9060	0.3640
FH	0.9120	0.3890
FI	0.9100	0.3910
FJ	0.9110	0.3900
FK	0.9180	0.3920
FL	0.9250	0.3760
FM	0.8840	0.3570
FN	0.8930	0.3560
FO	0.8540	0.3220
G	0.7720	0.3440
GA	0.7870	0.3120
GB	0.8800	0.3270
GC	0.8600	0.3130
GD	0.8880	0.3340
GE	0.9080	0.3400
GF	0.9190	0.3590
GG	0.9200	0.3500
GH	0.9210	0.3660
GI	0.9000	0.3640
GJ	0.9360	0.3790
GK	0.9310	0.3780
GL	0.9270	0.3870
GM	0.9090	0.3910
GN	0.9080	0.3980
GO	0.8720	0.3720
H	0.8750	0.4220
HA	0.7880	0.2800
HB	0.8590	0.3120
HC	0.8520	0.3050
HD	0.8810	0.3330
HE	0.8950	0.3530
HF	0.9350	0.3900
HG	0.9200	0.4050
HH	0.9480	0.4210
HI	0.9340	0.4020
HJ	0.9090	0.3320

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
HK	0.9160	0.3590
HL	0.9090	0.3550
HM	0.8930	0.3700
HN	0.9100	0.3950
HO	0.8800	0.3640
HP	0.8350	0.3240
I	0.9050	0.4550
I1	0.8500	0.3640
IA	0.8200	0.2520
IB	0.8380	0.2660
IC	0.8470	0.3060
ID	0.8650	0.3260
IE	0.9100	0.3640
IF	0.9220	0.3980
IG	0.9010	0.3990
IH	0.9140	0.4050
II	0.9190	0.4110
IJ	0.9420	0.3800
IK	0.9110	0.3600
IL	0.9140	0.3590
IM	0.8890	0.3740
IN	0.8950	0.3970
IO	0.8930	0.3800
IP	0.8520	0.3420
J	0.9580	0.4510
J1	0.8120	0.3530
J2	0.7990	0.3460
J3	0.8590	0.3460
J4	0.8080	0.3100
J5	0.6680	0.2790
JB	0.8110	0.2140
JC	0.8560	0.2420
JD	0.8700	0.2980
JE	0.8660	0.3150
JF	0.9030	0.3500
JG	0.9050	0.3770
JH	0.9150	0.4000
JI	0.9140	0.3950
JJ	0.9220	0.4140
JK	0.9310	0.4010
JL	0.9040	0.3780
JM	0.8920	0.3820

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
JN	0.8860	0.3780
JO	0.8880	0.3950
JP	0.8710	0.3890
JQ	0.8460	0.3210
K	0.9290	0.4750
K1	0.3040	0.2490
K2	0.1240	0.1370
K3	0.7560	0.3790
KA	0.8940	0.3650
KB	0.8960	0.4290
KC	0.9030	0.4370
KD	0.9150	0.4460
KE	0.9210	0.4410
KF	0.9410	0.4520
KG	0.9510	0.4420
KH	0.9490	0.4410
KI	0.9080	0.4350
KJ	0.9020	0.4320
KK	0.9360	0.4160
KL	0.9320	0.4090
KM	0.8980	0.3950
KN	0.8820	0.3740
KO	0.8700	0.3620
KP	0.7800	0.3260
L	0.9540	0.4910
L1	0.3750	0.2720
LA	0.9200	0.4160
LB	0.9230	0.4720
LC	0.9320	0.4940
LD	0.9330	0.4980
LE	0.9270	0.4890
LF	0.9340	0.4820
LG	0.9460	0.4830
LH	0.9350	0.4990
LI	0.9270	0.4890
LJ	0.9330	0.4930
LK	0.9250	0.4710
LL	0.9440	0.4410
LM	0.9150	0.4160
LN	0.8880	0.4080
LO	0.8720	0.3930
LP	0.8770	0.3690

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
M	0.9390	0.4690
M1	0.8740	0.4260
M2	0.9280	0.4820
M3	0.8930	0.4850
M4	0.9420	0.4580
MA	0.9250	0.3880
MB	0.9250	0.4490
MC	0.9190	0.4800
MD	0.9270	0.4940
ME	0.9160	0.4910
MF	0.9310	0.4910
MG	0.9410	0.4970
MH	0.9430	0.5050
MI	0.9290	0.4960
MJ	0.9340	0.4990
MK	0.9110	0.4850
ML	0.9270	0.4700
MM	0.9220	0.4380
MN	0.9100	0.4100
MO	0.8830	0.3890
MP	0.8770	0.3620
N	0.8580	0.4250
N1	0.7580	0.3370
N2	0.8480	0.4170
NA	0.8040	0.2160
NB	0.8590	0.2490
NC	0.8320	0.2390
ND	0.8590	0.2560
NE	0.8990	0.2590
NF	0.8930	0.3440
NG	0.8770	0.3570
NH	0.8800	0.3590
NI	0.8820	0.3340
NJ	0.8630	0.3150
NK	0.8590	0.3210
NL	0.8630	0.3260
NM	0.8370	0.3240
NN	0.8550	0.2990
NO	0.8520	0.2840
NP	0.8130	0.2410
O	0.8340	0.3660
O1	0.8260	0.4270

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O2	0.8570	0.4650
O3	0.8790	0.4850
O4	0.8290	0.4220
O5	0.8840	0.4290
O6	0.8270	0.4090
O7	0.7630	0.3860
O8	0.8410	0.4300
O9	0.8720	0.4380
OA	0.6500	0.1890
OB	0.7760	0.2220
OC	0.7920	0.2310
OD	0.8330	0.2400
OE	0.8370	0.2330
OF	0.8870	0.2420
OG	0.8930	0.2530
OH	0.9030	0.2590
OI	0.8780	0.2460
OJ	0.8710	0.2450
OK	0.8730	0.2460
OL	0.8920	0.2470
OM	0.8590	0.2560
ON	0.8320	0.2420
OO	0.8050	0.2380
OP	0.7350	0.2020
P	0.8590	0.4530
P1	0.7340	0.3020
P2	0.8260	0.3510
P3	0.7070	0.3900
P4	0.8340	0.4410
P5	0.8210	0.4500
P6	0.8680	0.4310
P7	0.6220	0.3510
P8	0.8710	0.4750
P9	0.8010	0.3540
PB	0.8240	0.1820
PC	0.8430	0.1930
PD	0.8690	0.2200
PE	0.8960	0.2040
PF	0.8830	0.2140
PG	0.8680	0.2230
PH	0.8840	0.2450
PI	0.8800	0.2420

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
PJ	0.8850	0.2420
PK	0.8730	0.2380
PL	0.9120	0.2280
PM	0.8850	0.2250
PN	0.8880	0.2170
PO	0.8520	0.2080
PP	0.7940	0.1750
Q	0.7590	0.3850
Q1	0.8530	0.4350
Q2	0.8780	0.4680
Q3	0.8610	0.4650
Q4	0.8150	0.4100
Q5	0.7470	0.3710
QB	0.6730	0.1560
QC	0.7690	0.1760
QD	0.8170	0.2060
QE	0.8750	0.1810
QF	0.8640	0.1940
QG	0.8360	0.2040
QH	0.8650	0.2280
QI	0.8470	0.2240
QJ	0.8660	0.2370
QK	0.8590	0.2260
QL	0.8810	0.2140
QM	0.8380	0.2120
QN	0.8140	0.2100
QO	0.7980	0.2020
QP	0.6950	0.1720
R	0.8810	0.4430
R0	0.8700	0.3790
R1	0.9040	0.4620
R2	0.9220	0.4960
R3	0.9260	0.4670
R4	0.8520	0.3830
R5	0.8110	0.3690
RC	0.8530	0.1870
RD	0.8990	0.2130
RE	0.9030	0.2030
RF	0.9070	0.1920
RG	0.8840	0.1840
RH	0.9070	0.2250
RI	0.8940	0.2210

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
RJ	0.9150	0.2360
RK	0.9030	0.2260
RL	0.9190	0.2180
RM	0.8990	0.2140
RN	0.9000	0.2170
RO	0.8680	0.2050
RP	0.7710	0.1710
S	0.8470	0.4180
S0	0.8060	0.3660
S1	0.9270	0.4420
S2	0.9350	0.4630
S3	0.9250	0.4420
S4	0.8740	0.4030
S5	0.8590	0.4150
S6	0.9190	0.4870
S7	0.9020	0.4740
S8	0.9220	0.4490
S9	0.8440	0.3670
SA	0.7240	0.2080
SB	0.8390	0.2370
SC	0.8500	0.2410
SD	0.9010	0.2200
SE	0.8460	0.2170
SF	0.8770	0.2460
SG	0.8640	0.2570
SH	0.8890	0.2710
SI	0.8700	0.2680
SJ	0.8850	0.2430
SK	0.8830	0.2540
SL	0.8670	0.2600
SM	0.8260	0.2480
SN	0.7240	0.2130
T	0.8320	0.4090
T0	0.8040	0.3560
T1	0.8710	0.3820
T2	0.9220	0.4490
T3	0.9180	0.4580
T4	0.9040	0.4270
T5	0.7980	0.3550
TA	0.7380	0.2280
TB	0.8190	0.2650
TC	0.8450	0.2660

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
TD	0.9110	0.2560
TE	0.8590	0.2250
TF	0.8680	0.2620
TG	0.8700	0.2800
TH	0.8760	0.2890
TI	0.8540	0.2840
TJ	0.8660	0.2690
TK	0.8960	0.2720
TL	0.8610	0.2840
TM	0.8500	0.2720
TN	0.7700	0.2330
U	0.8880	0.4560
U0	0.8070	0.3730
U1	0.9130	0.4170
U2	0.9180	0.4390
U3	0.8930	0.3860
U4	0.7930	0.3300
U5	0.6360	0.3010
U6	0.7690	0.3130
U7	0.8590	0.3930
U8	0.7320	0.3290
U9	0.6040	0.2760
UA	0.7360	0.2330
UB	0.8440	0.2530
UC	0.8430	0.2650
UD	0.8920	0.2410
UE	0.8580	0.2150
UF	0.8660	0.2480
UG	0.8640	0.2610
UH	0.8800	0.2710
UI	0.8780	0.2700
UJ	0.8590	0.2480
UK	0.8780	0.2360
UL	0.8060	0.2420
UM	0.7860	0.2460
UN	0.7390	0.2150
UO	0.6310	0.1830
V	0.8930	0.4570
V0	0.2680	0.2490
V1	0.6600	0.3050
V2	0.8200	0.3290
V3	0.6700	0.2920

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
V4	0.5980	0.2690
V5	0.7330	0.3060
V6	0.8660	0.3570
V7	0.8460	0.3410
V8	0.7510	0.3320
V9	0.7430	0.3340
VA	0.7630	0.2010
VB	0.8560	0.2300
VC	0.8590	0.2530
VD	0.9000	0.2570
VE	0.8690	0.2550
VF	0.8590	0.2750
VG	0.8500	0.2910
VH	0.8860	0.3030
VI	0.8650	0.2990
VJ	0.8680	0.2870
VK	0.8870	0.2760
VL	0.8870	0.2760
VM	0.8490	0.2710
VN	0.8290	0.2370
VO	0.7700	0.2270
W	0.8300	0.4350
W0	0.3180	0.1640
W2	0.6400	0.3100
W4	0.8310	0.4070
W5	0.8800	0.4200
W6	0.8760	0.4340
W7	0.7690	0.3340
WA	0.7630	0.2440
WB	0.8580	0.2860
WC	0.8550	0.3090
WD	0.9140	0.3140
WE	0.9030	0.2940
WF	0.9100	0.3180
WG	0.8940	0.3360
WH	0.9190	0.3590
WI	0.8880	0.3430
WJ	0.9150	0.3410
WK	0.9000	0.3270
WL	0.9310	0.3210
WM	0.8720	0.3150
WN	0.8850	0.3020

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
WO	0.8350	0.2800
WP	0.7660	0.2230
X	0.9030	0.4400
X0	0.7600	0.4530
X1	0.7070	0.3740
X2	0.7720	0.4480
X3	0.7500	0.4150
X4	0.8110	0.4380
X5	0.7700	0.3840
X6	0.7830	0.3710
X7	0.4670	0.2840
X8	0.4050	0.1970
XA	0.7370	0.3240
XB	0.9040	0.3860
XC	0.9740	0.3550
XD	0.9560	0.4080
XE	0.9500	0.4290
XF	0.9450	0.4270
XG	0.9430	0.4000
XH	0.9190	0.3820
Y	0.8980	0.4550
Y0	0.8170	0.3290
Y1	0.8540	0.3580
Y2	0.8790	0.3210
Y3	0.7040	0.2240
Y4	0.7680	0.3150
Y5	0.6860	0.2970
YA	0.7140	0.3380
YB	0.8500	0.3800
YC	0.7350	0.3030
YD	0.9020	0.4210
YE	0.8340	0.3980
YF	0.9020	0.3830
YG	0.8000	0.3630
YH	0.7570	0.3130
Z	0.8110	0.3990
Z1	0.8040	0.4030
Z2	0.7830	0.4180
Z3	0.9100	0.4100
Z4	0.8900	0.4100
Z5	0.8200	0.3610
a	0.5800	0.2430

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a1	0.8360	0.4130
a2	0.9120	0.4490
a3	0.9160	0.4710
a4	0.8200	0.3810
a6	0.5760	0.2710
b	0.4820	0.2450
b1	0.8640	0.3380
b2	0.8880	0.4280
b3	0.9300	0.4380
b4	0.8990	0.3900
b5	0.8220	0.3460
c	0.5560	0.2370
d	0.4670	0.2280
e	0.8750	0.3360
f	0.8700	0.3610
g	0.8630	0.3400
h	0.8200	0.3530
h1	0.9130	0.4070
h2	0.9060	0.4390
h3	0.8960	0.4440
h4	0.8470	0.3780
i	0.8750	0.3950
i1	0.9330	0.3980
i2	0.8110	0.3250
i3	0.7840	0.3450
i4	0.8250	0.2940
j	0.8740	0.4100
j1	0.8270	0.3630
k	0.8450	0.3420
l	0.9480	0.4940
m	0.9580	0.4950
n	0.9480	0.4780
o	0.4630	0.2030
p	0.5340	0.2370
q	0.8580	0.4050
r	0.8490	0.4290
s	0.8670	0.4030
y	0.8330	0.3600