Full wwPDB EM Validation Report ⓘ

Dec 13, 2022 – 05:15 PM EST

PDB ID	:	7UNG
EMDB ID	:	EMD-26624
Title	:	48-nm repeat of the human respiratory doublet microtubule
Authors	:	Gui, M.; Croft, J.T.; Zabeo, D.; Acharya, V.; Kollman, J.M.; Burgoyne, T.; Hoog, J.L.; Brown, A.
Deposited on	:	2022-04-11
Resolution	:	3.60 Å(reported)

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

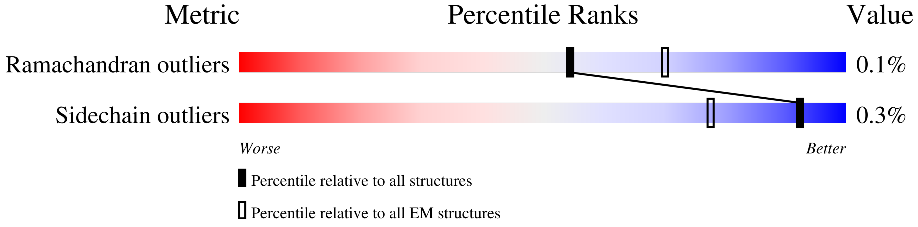
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

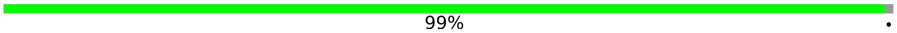
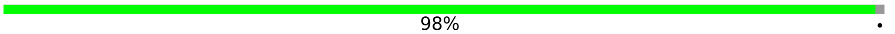
The reported resolution of this entry is 3.60 Å.

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



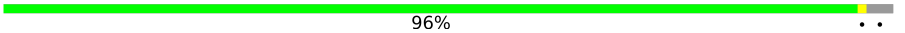
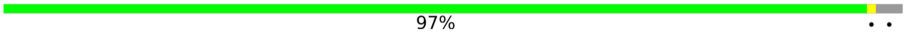
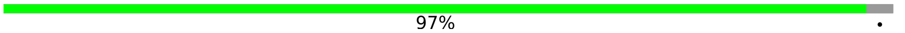
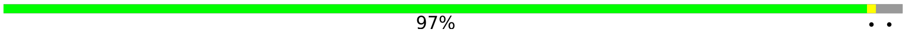
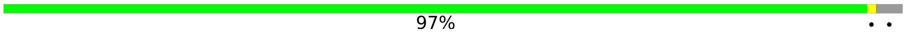
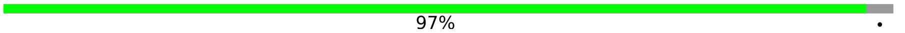
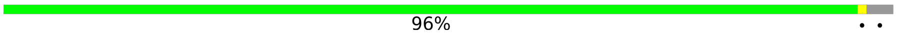
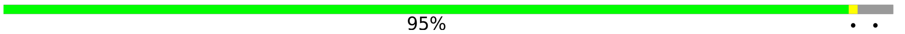
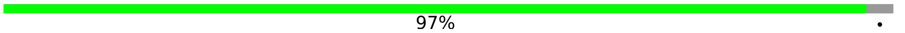
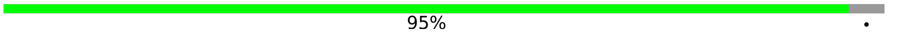
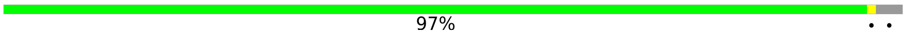
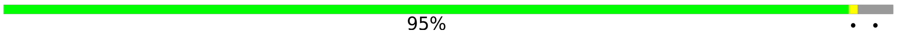
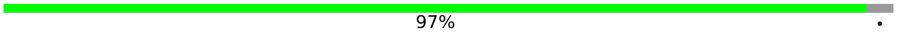
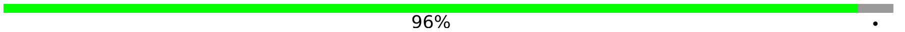
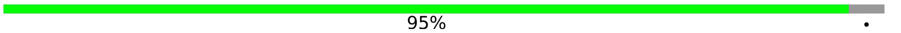
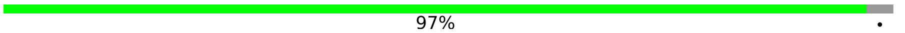
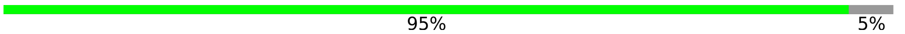
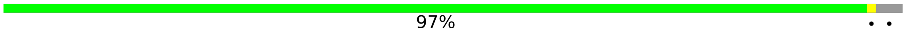
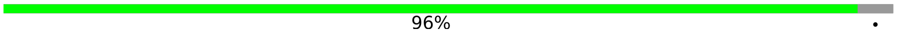
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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%

Mol	Chain	Length	Quality of chain
1	0	229	
1	7	229	
2	1	833	
2	2	833	
3	3	514	
3	4	514	
4	5	376	
4	6	376	
5	8	194	
5	9	194	

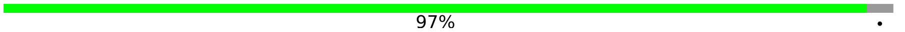
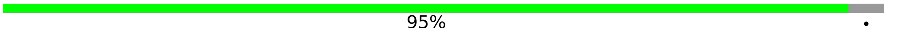
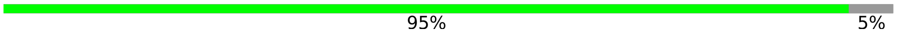
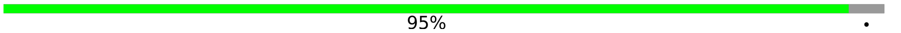
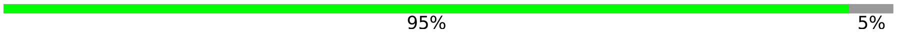
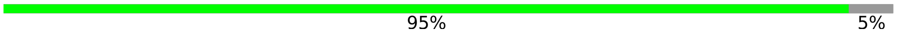
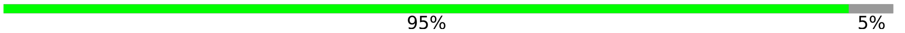
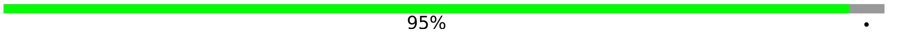
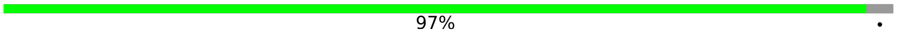
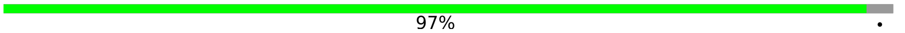
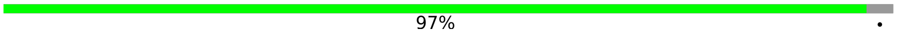
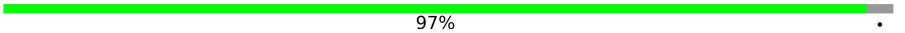
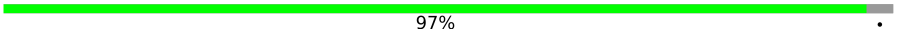
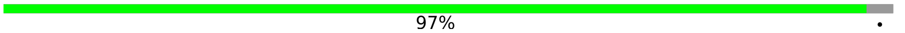
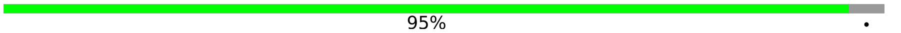
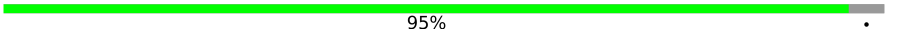
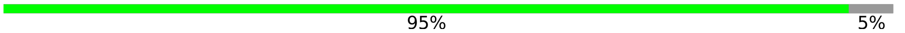
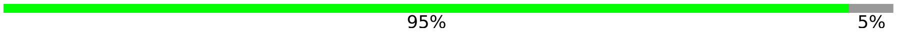
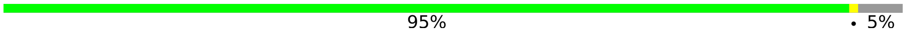
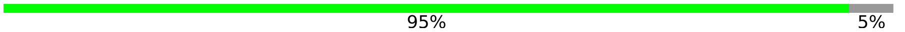
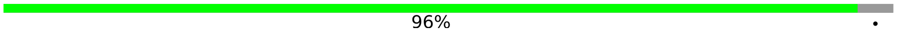
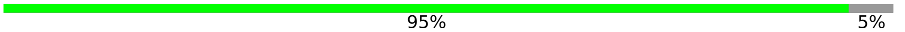
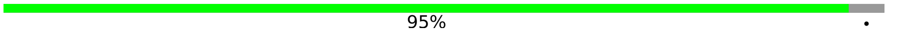
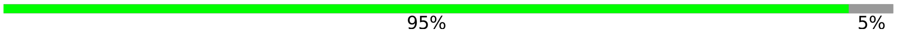
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	A	101	
7	A0	418	
7	A1	418	
7	A2	418	
7	A3	418	
7	A4	418	
8	AA	451	
8	AC	451	
8	AE	451	
8	AG	451	
8	AI	451	
8	AK	451	
8	AM	451	
8	BA	451	
8	BC	451	
8	BE	451	
8	BG	451	
8	BI	451	
8	BK	451	
8	BM	451	
8	CA	451	
8	CC	451	
8	CE	451	
8	CG	451	
8	CI	451	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	CK	451	
8	CM	451	
8	DA	451	
8	DC	451	
8	DE	451	
8	DG	451	
8	DI	451	
8	DK	451	
8	DM	451	
8	EC	451	
8	EE	451	
8	EG	451	
8	EI	451	
8	EK	451	
8	EM	451	
8	FC	451	
8	FE	451	
8	FG	451	
8	FI	451	
8	FK	451	
8	FM	451	
8	GC	451	
8	GE	451	
8	GG	451	
8	GI	451	

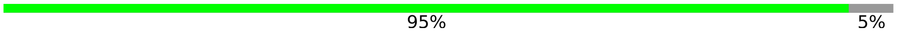
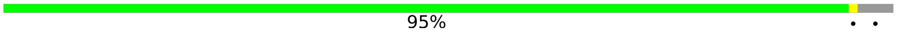
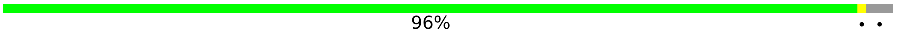
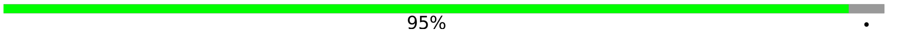
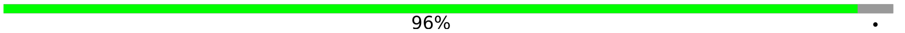
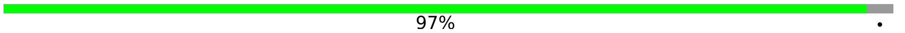
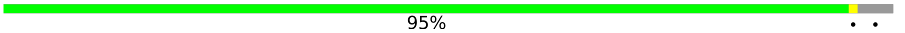
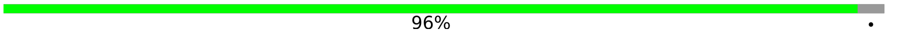
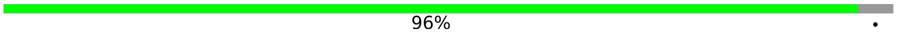
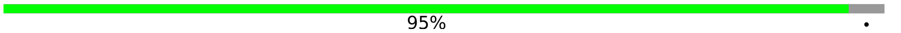
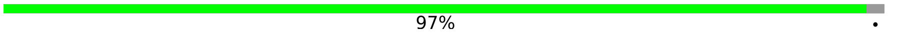
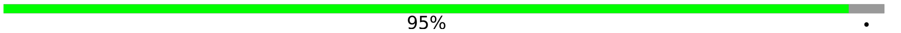
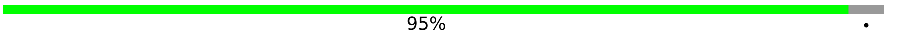
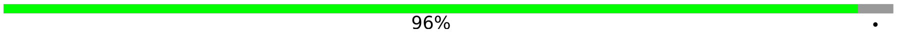
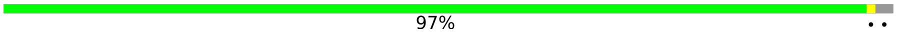
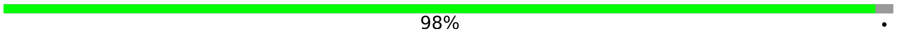
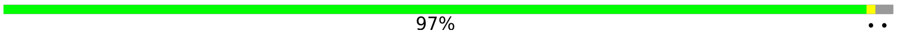
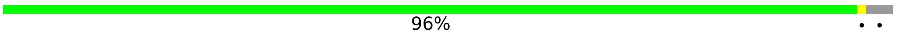
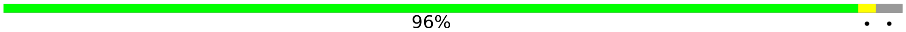
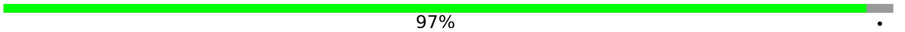
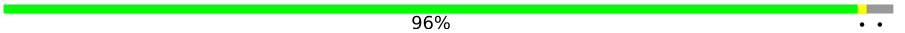
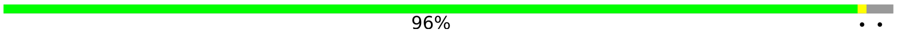
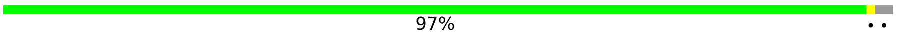
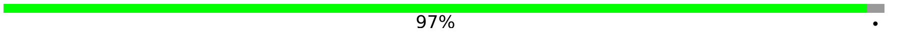
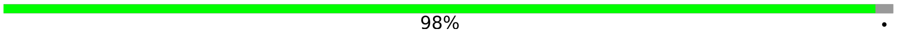
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	GK	451	95% •
8	GM	451	96% •
8	HC	451	95% • •
8	HE	451	96% •
8	HG	451	95% •
8	HI	451	95% •
8	HK	451	95% •
8	HM	451	95% •
8	HO	451	86% • 14%
8	IC	451	95% • •
8	IE	451	96% •
8	IG	451	97% •
8	II	451	96% •
8	IK	451	97% •
8	IM	451	96% •
8	IO	451	95% •
8	JC	451	97% •
8	JE	451	95% 5%
8	JG	451	95% 5%
8	JI	451	95% 5%
8	JK	451	95% • •
8	JM	451	95% 5%
8	KC	451	96% •
8	KE	451	95% •
8	KG	451	96% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	KI	451	
8	KK	451	
8	KM	451	
8	KO	451	
8	LC	451	
8	LE	451	
8	LG	451	
8	LI	451	
8	LK	451	
8	LM	451	
8	MC	451	
8	ME	451	
8	MG	451	
8	MI	451	
8	MK	451	
8	MM	451	
8	NC	451	
8	NE	451	
8	NG	451	
8	NI	451	
8	NK	451	
8	NM	451	
8	OC	451	
8	OE	451	
8	OG	451	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	OI	451	98% •
8	OK	451	97% •
8	OM	451	97% •
8	OO	451	94% 6%
8	PC	451	97% •
8	PE	451	97% •
8	PG	451	97% •
8	PI	451	97% •
8	PK	451	97% • •
8	PM	451	97% •
8	PO	451	97% •
8	QC	451	97% •
8	QE	451	98% •
8	QG	451	97% • •
8	QI	451	97% •
8	QK	451	97% •
8	QM	451	97% • •
8	QO	451	98% •
8	RC	451	90% • 9%
8	RE	451	95% 5%
8	RG	451	96% •
8	RI	451	97% •
8	RK	451	97% •
8	RM	451	97% •
8	RO	451	97% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	SE	451	95% 5%
8	SG	451	95% 5%
8	SI	451	95% •
8	SK	451	94% • •
8	SM	451	95% •
8	SO	451	95% •
8	TE	451	95% 5%
8	TG	451	95% 5%
8	TI	451	96% •
8	TK	451	95% 5%
8	TM	451	95% • •
8	TO	451	95% 5%
8	UE	451	95% •
8	UG	451	95% •
8	UI	451	95% • •
8	UK	451	95% •
8	UM	451	95% •
8	UO	451	95% •
8	VE	451	97% •
8	VG	451	95% • •
8	VI	451	97% •
8	VK	451	95% •
8	VM	451	97% • •
8	VO	451	96% •
8	WE	451	96% • •

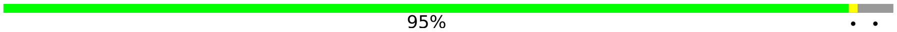
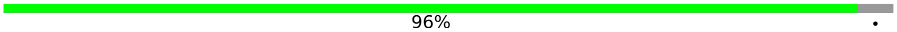
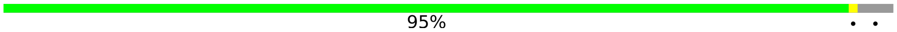
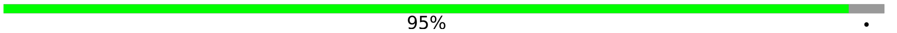
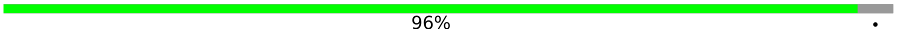
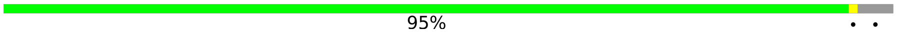
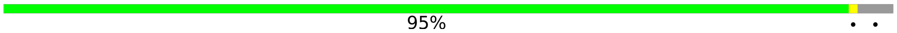
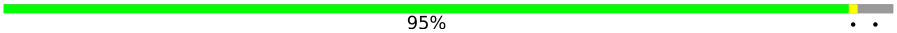
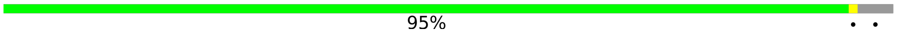
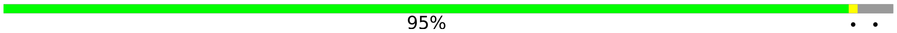
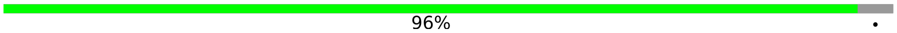
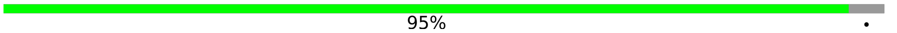
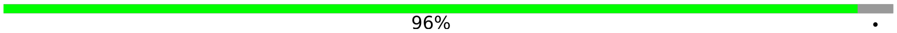
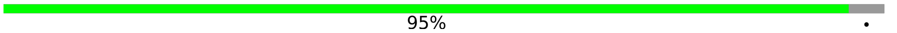
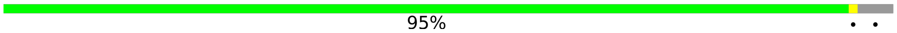
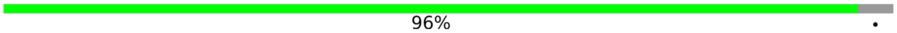
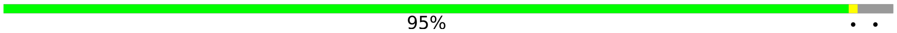
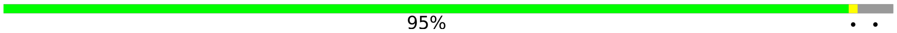
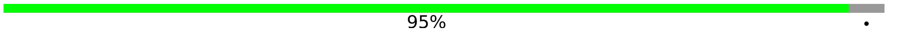
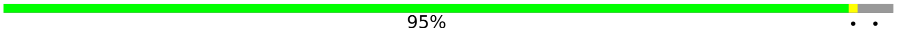
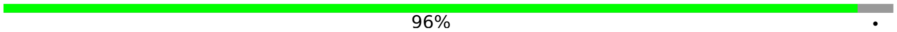
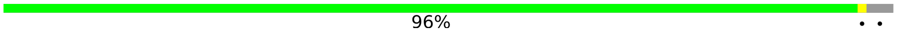
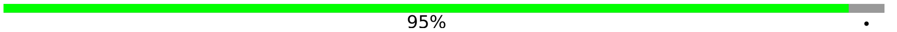
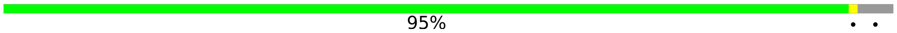
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	WG	451	95% 5%
8	WI	451	97% •
8	WK	451	95% 5%
8	WM	451	96% • •
8	WO	451	96% •
9	AB	445	98% • •
9	AD	445	98% •
9	AF	445	97% • •
9	AH	445	97% • •
9	AJ	445	97% • •
9	AL	445	98% • •
9	BB	445	96% •
9	BD	445	95% • •
9	BF	445	95% • •
9	BH	445	95% •
9	BJ	445	95% • •
9	BL	445	96% •
9	CB	445	96% • •
9	CD	445	96% •
9	CF	445	95% •
9	CH	445	96% •
9	CJ	445	95% •
9	CL	445	96% •
9	DB	445	95% • •
9	DD	445	95% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	DF	445	
9	DH	445	
9	DJ	445	
9	DL	445	
9	EB	445	
9	ED	445	
9	EF	445	
9	EH	445	
9	EJ	445	
9	EL	445	
9	EN	445	
9	FB	445	
9	FD	445	
9	FF	445	
9	FH	445	
9	FJ	445	
9	FL	445	
9	FN	445	
9	GB	445	
9	GD	445	
9	GF	445	
9	GH	445	
9	GJ	445	
9	GL	445	
9	GN	445	

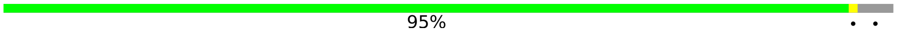
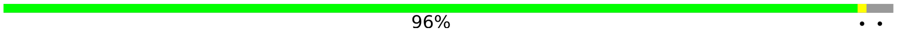
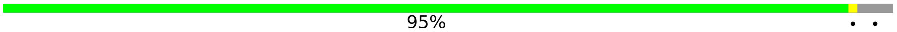
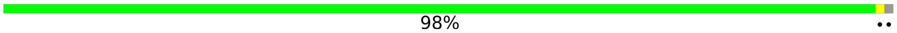
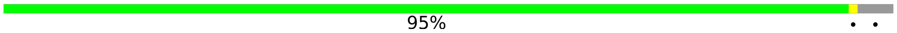
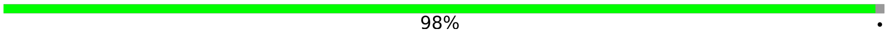
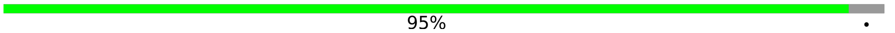
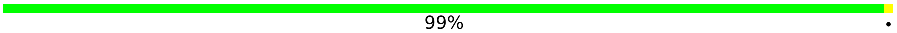
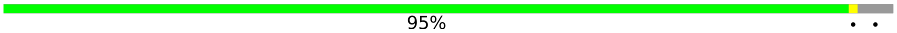
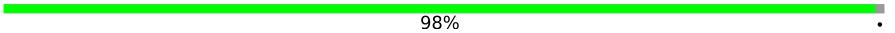
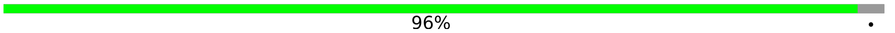
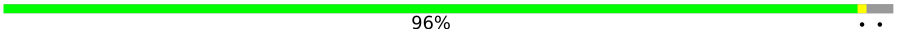
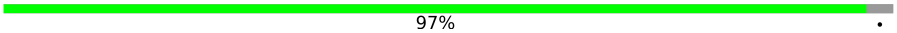
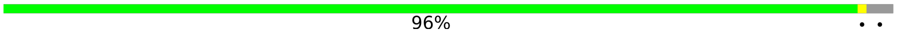
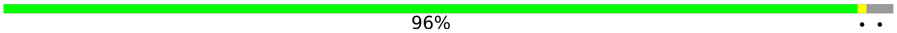
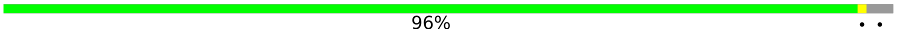
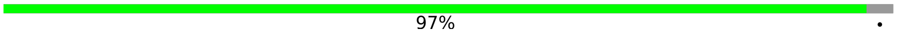
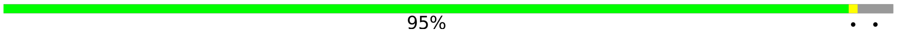
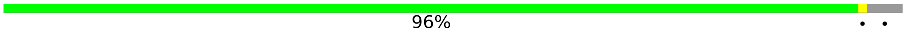
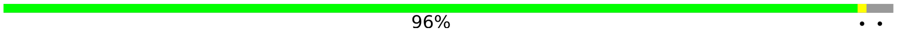
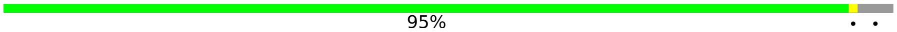
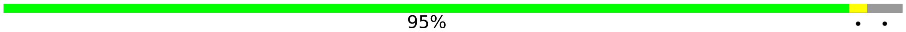
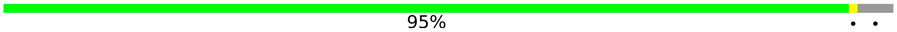
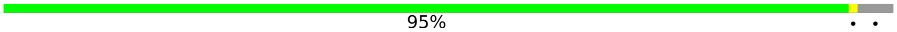
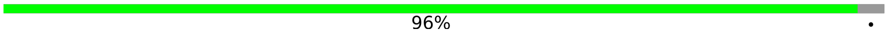
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	HB	445	94% • •
9	HD	445	95% • •
9	HF	445	96% •
9	HH	445	95% •
9	HJ	445	95% • •
9	HL	445	94% • •
9	HN	445	94% • •
9	IB	445	91% 9%
9	ID	445	95% •
9	IF	445	96% • •
9	IH	445	95% •
9	IJ	445	96% •
9	IL	445	95% •
9	IN	445	95% • •
9	JB	445	95% • •
9	JD	445	96% •
9	JF	445	95% • •
9	JH	445	95% •
9	JJ	445	95% • •
9	JL	445	95% • •
9	JN	445	95% • •
9	KB	445	92% • 7%
9	KD	445	96% • •
9	KF	445	95% • •
9	KH	445	96% • •

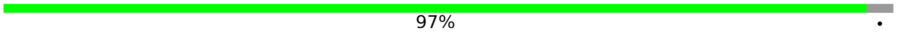
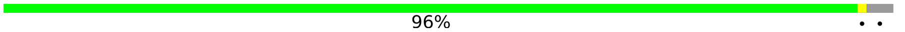
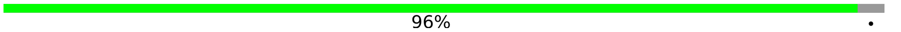
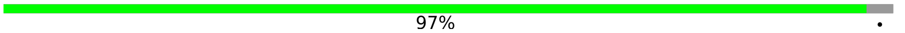
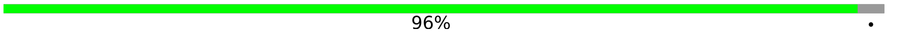
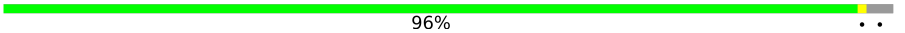
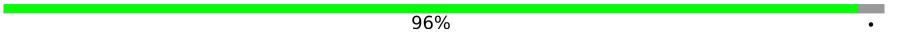
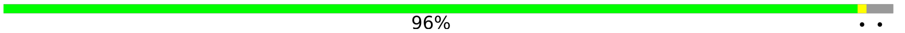
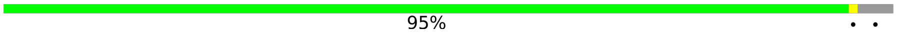
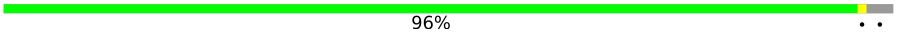
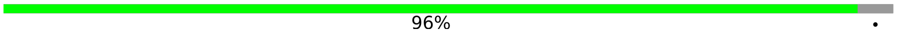
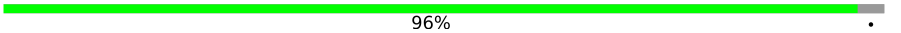
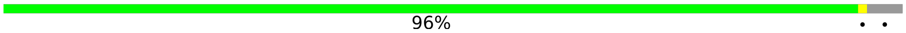
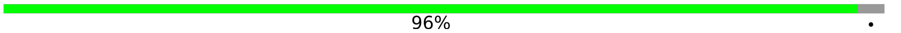
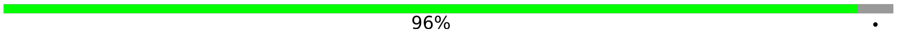
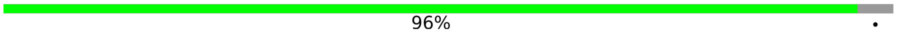
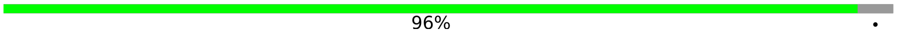
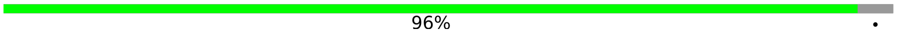
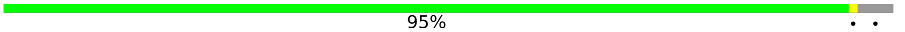
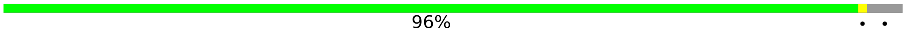
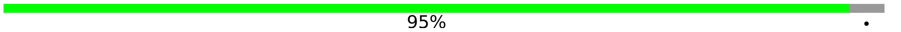
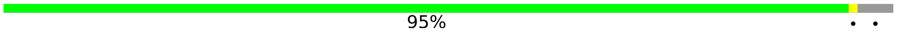
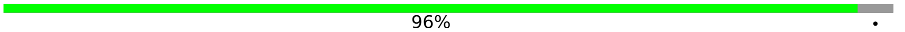
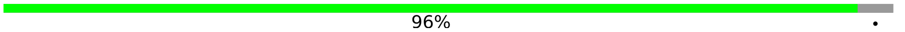
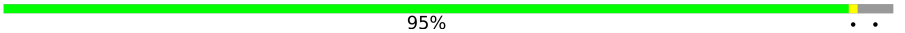
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	KJ	445	 95%
9	KL	445	 96%
9	KN	445	 95%
9	LB	445	 98%
9	LD	445	 95%
9	LF	445	 98%
9	LH	445	 95%
9	LJ	445	 99%
9	LL	445	 95%
9	LN	445	 98%
9	MB	445	 96%
9	MD	445	 96%
9	MF	445	 97%
9	MH	445	 96%
9	MJ	445	 96%
9	ML	445	 96%
9	MN	445	 97%
9	NB	445	 95%
9	ND	445	 96%
9	NF	445	 96%
9	NH	445	 95%
9	NJ	445	 95%
9	NL	445	 95%
9	NN	445	 95%
9	OB	445	 96%

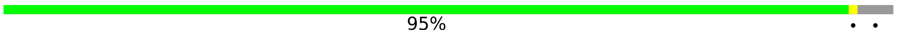
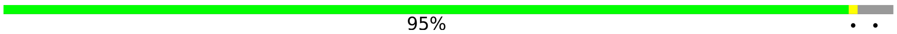
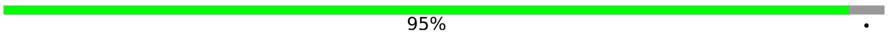
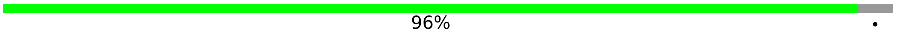
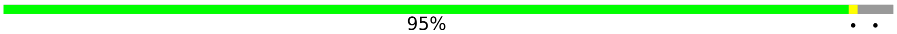
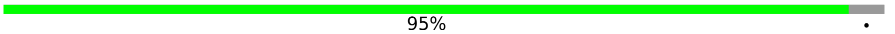
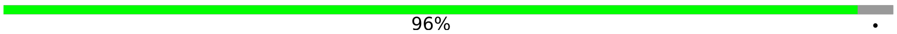
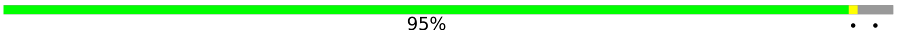
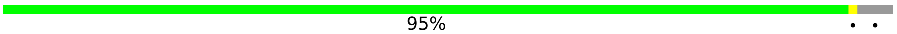
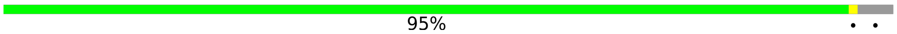
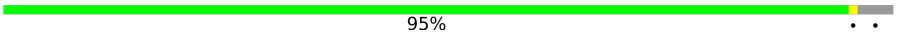
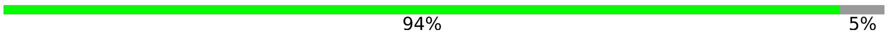
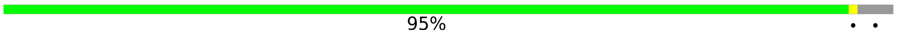
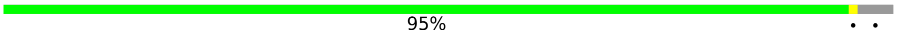
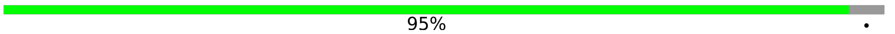
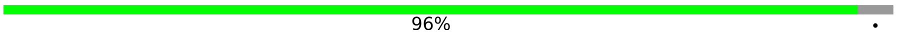
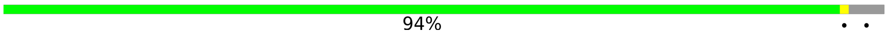
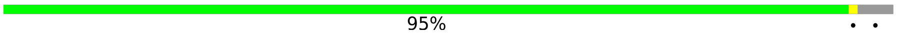
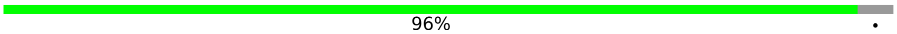
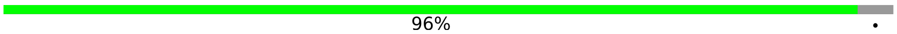
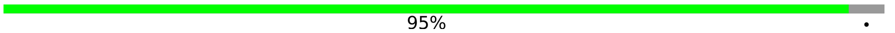
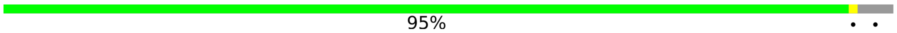
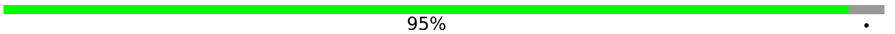
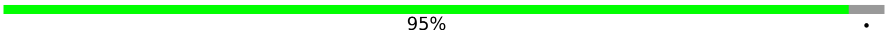
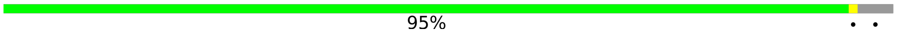
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	OD	445	 97% •
9	OF	445	 96% • •
9	OH	445	 96% •
9	OJ	445	 97% •
9	OL	445	 96% •
9	ON	445	 96% • •
9	PD	445	 96% •
9	PF	445	 96% • •
9	PH	445	 95% • •
9	PJ	445	 96% • •
9	PL	445	 96% •
9	PN	445	 96% •
9	QD	445	 96% • •
9	QF	445	 96% •
9	QH	445	 96% •
9	QJ	445	 96% •
9	QL	445	 96% •
9	QN	445	 96% •
9	RD	445	 95% • •
9	RF	445	 96% • •
9	RH	445	 95% •
9	RJ	445	 95% • •
9	RL	445	 96% •
9	RN	445	 96% •
9	SD	445	 95% • •

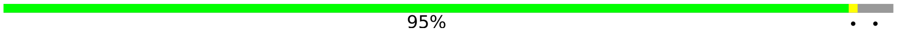
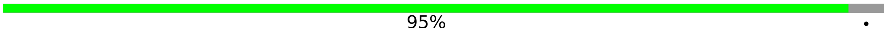
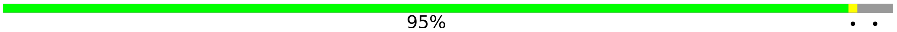
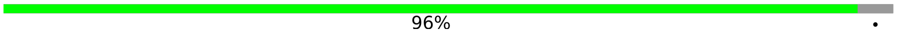
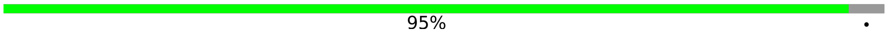
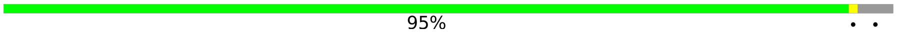
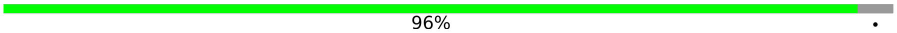
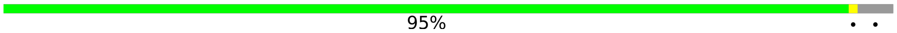
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	SF	445	
9	SH	445	
9	SJ	445	
9	SL	445	
9	SN	445	
9	TD	445	
9	TF	445	
9	TH	445	
9	TJ	445	
9	TL	445	
9	TN	445	
9	TP	445	
9	UD	445	
9	UF	445	
9	UH	445	
9	UJ	445	
9	UL	445	
9	UN	445	
9	UP	445	
9	VD	445	
9	VF	445	
9	VH	445	
9	VJ	445	
9	VL	445	
9	VN	445	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	VP	445	
9	WD	445	
9	WF	445	
9	WH	445	
9	WJ	445	
9	WL	445	
9	WN	445	
9	WP	445	
10	B	495	
10	C	495	
11	B0	430	
11	B1	430	
11	B2	430	
11	B3	430	
11	B4	430	
11	B5	430	
11	B6	430	
11	B7	430	
11	B8	430	
11	B9	430	
12	C0	490	
12	C1	490	
12	C2	490	
12	C3	490	
12	C4	490	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	D	485	
14	D0	435	
14	D1	435	
14	D2	435	
14	D3	435	
14	D5	435	
14	D6	435	
14	D7	435	
14	D8	435	
15	E	301	
15	F	301	
16	F0	222	
16	F1	222	
16	F2	222	
16	F3	222	
16	F4	222	
16	F5	222	
16	F6	222	
16	F7	222	
16	F8	222	
16	G0	222	
16	G1	222	
16	G2	222	
16	G3	222	
16	G4	222	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	G5	222	 70% 30%
16	G6	222	 70% 29%
16	G7	222	 72% 28%
16	G8	222	 70% 30%
16	H0	222	 70% 29%
16	H1	222	 72% 28%
16	H2	222	 70% 30%
17	G	121	 76% • 22%
18	H	275	 29% 71%
18	I	275	 53% 47%
18	J	275	 53% 47%
18	K	275	 52% • 47%
18	L	275	 52% 47%
18	M	275	 52% 47%
18	N	275	 52% • 47%
19	I1	150	 58% • 41%
20	J1	284	 29% 71%
20	J2	284	 79% • 20%
20	J3	284	 79% • 20%
20	J4	284	 71% • 28%
20	J5	284	 23% 77%
21	K1	134	 82% • 17%
22	L1	147	 86% 14%
22	L2	147	 61% • 39%
23	M1	201	 51% 49%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
23	M2	201	50% 50%
23	M3	201	50% 49%
23	M4	201	50% 49%
24	O	382	7% 93%
24	P	382	96% • •
24	Q	382	10% 90%
24	R	382	57% 43%
24	S	382	43% 57%
25	T	640	75% 24%
25	U	640	76% 24%
25	V	640	76% 24%
26	W	749	81% • 18%
26	X	749	93% • 6%
26	Y	749	93% • 6%
26	Z	749	68% • 32%
27	XA	193	96% •
27	XB	193	96% • •
27	XC	193	96% • •
27	XD	193	96% • •
27	XE	193	95% • •
27	XF	193	96% •
27	XG	193	96% •
28	YB	257	86% 14%
28	YC	257	86% 14%
28	YD	257	85% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	YE	257	86% 14%
28	YF	257	85% 14%
28	YG	257	86% 14%
29	a	551	31% 68%
29	b	551	61% 39%
29	c	551	51% 48%
29	d	551	39% 60%
30	e	620	98% •
30	f	620	98% •
30	g	620	98% •
31	h	256	57% 43%
31	i	256	97% •
31	j	256	96% •
31	k	256	98% •
32	l	177	66% 34%
32	m	177	66% • 34%
32	n	177	66% • 34%
33	o	552	72% • 27%
33	o1	552	7% 93%
33	p	552	28% 71%
34	q	169	66% 34%
34	r	169	66% 34%
34	s	169	66% 34%
35	y	136	46% 54%
35	z	136	82% 18%

2 Entry composition ⓘ

There are 38 unique types of molecules in this entry. The entry contains 1265783 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 Protein CFAP95.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	52	418	265	75	77	1	0	0
1	7	146	1197	757	206	230	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	272	2226	1407	388	424	7	0	0
2	2	446	3607	2298	629	667	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	297	2514	1539	476	489	10	0	0
3	4	215	1837	1120	349	358	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	371	2943	1873	506	543	21	0	0
4	6	371	2943	1873	506	543	21	0	0

- Molecule 5 is a protein called Protein CFAP107.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	8	168	Total C N O S 1414 909 251 251 3	0	0
5	9	48	Total C N O S 411 261 71 78 1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	191	PHE	LEU	conflict	UNP Q8N1D5
9	191	PHE	LEU	conflict	UNP Q8N1D5

- Molecule 6 is a protein called Protein CFAP141.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	A	50	Total C N O S 423 269 75 76 3	0	0

- Molecule 7 is a protein called Tektin-1.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	A0	220	Total C N O S 1771 1102 325 335 9	0	0
7	A1	391	Total C N O S 3185 1978 576 619 12	0	0
7	A2	391	Total C N O S 3185 1978 576 619 12	0	0
7	A3	333	Total C N O S 2715 1688 485 532 10	0	0
7	A4	35	Total C N O 294 183 59 52	0	0

- Molecule 8 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	AA	439	Total C N O S 3429 2170 583 654 22	0	0
8	AC	439	Total C N O S 3429 2170 583 654 22	0	0
8	AE	439	Total C N O S 3429 2170 583 654 22	0	0
8	AG	439	Total C N O S 3429 2170 583 654 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	AK	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	AM	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	BA	432	Total 3383	C 2143	N 575	O 643	S 22	0	0
8	BC	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	BE	432	Total 3383	C 2143	N 575	O 643	S 22	0	0
8	BG	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	BI	432	Total 3383	C 2143	N 575	O 643	S 22	0	0
8	BK	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	BM	433	Total 3387	C 2145	N 576	O 644	S 22	0	0
8	CA	432	Total 3385	C 2144	N 575	O 644	S 22	0	0
8	CC	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	CE	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	CG	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	CI	431	Total 3377	C 2140	N 574	O 641	S 22	0	0
8	CK	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	CM	431	Total 3377	C 2140	N 574	O 641	S 22	0	0
8	DA	383	Total 2978	C 1887	N 504	O 567	S 20	0	0
8	DC	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	DE	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	DG	430	Total 3371	C 2137	N 573	O 639	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DI	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	DK	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	DM	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	EC	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	EE	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	EG	438	Total 3423	C 2167	N 582	O 652	S 22	0	0
8	EI	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	EK	438	Total 3423	C 2167	N 582	O 652	S 22	0	0
8	EM	438	Total 3423	C 2167	N 582	O 652	S 22	0	0
8	FC	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	FE	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	FG	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	FI	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	FK	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	FM	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	GC	435	Total 3409	C 2158	N 579	O 650	S 22	0	0
8	GE	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	GG	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	GI	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	GK	432	Total 3385	C 2144	N 575	O 644	S 22	0	0
8	GM	434	Total 3402	C 2154	N 578	O 648	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
8	HC	431	Total C N O S 3379 2141 574 642 22	0	0
8	HE	432	Total C N O S 3385 2144 575 644 22	0	0
8	HG	432	Total C N O S 3385 2144 575 644 22	0	0
8	HI	432	Total C N O S 3385 2144 575 644 22	0	0
8	HK	431	Total C N O S 3377 2140 574 641 22	0	0
8	HM	431	Total C N O S 3379 2141 574 642 22	0	0
8	HO	389	Total C N O S 3058 1935 520 582 21	0	0
8	IC	433	Total C N O S 3393 2148 576 647 22	0	0
8	IE	431	Total C N O S 3379 2141 574 642 22	0	0
8	IG	439	Total C N O S 3429 2170 583 654 22	0	0
8	II	432	Total C N O S 3385 2144 575 644 22	0	0
8	IK	439	Total C N O S 3429 2170 583 654 22	0	0
8	IM	431	Total C N O S 3379 2141 574 642 22	0	0
8	IO	431	Total C N O S 3377 2140 574 641 22	0	0
8	JC	439	Total C N O S 3429 2170 583 654 22	0	0
8	JE	430	Total C N O S 3371 2137 573 639 22	0	0
8	JG	430	Total C N O S 3371 2137 573 639 22	0	0
8	JI	430	Total C N O S 3371 2137 573 639 22	0	0
8	JK	431	Total C N O S 3377 2140 574 641 22	0	0
8	JM	430	Total C N O S 3371 2137 573 639 22	0	0
8	KC	433	Total C N O S 3390 2148 576 644 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
8	KE	432	Total C N O S 3385 2144 575 644 22	0	0
8	KG	433	Total C N O S 3390 2148 576 644 22	0	0
8	KI	430	Total C N O S 3373 2138 573 640 22	0	0
8	KK	433	Total C N O S 3390 2148 576 644 22	0	0
8	KM	438	Total C N O S 3423 2167 582 652 22	0	0
8	KO	432	Total C N O S 3383 2143 575 643 22	0	0
8	LC	433	Total C N O S 3389 2146 576 645 22	0	0
8	LE	439	Total C N O S 3429 2170 583 654 22	0	0
8	LG	434	Total C N O S 3397 2150 577 648 22	0	0
8	LI	436	Total C N O S 3410 2158 580 650 22	0	0
8	LK	433	Total C N O S 3390 2148 576 644 22	0	0
8	LM	431	Total C N O S 3379 2141 574 642 22	0	0
8	MC	440	Total C N O S 3436 2175 584 655 22	0	0
8	ME	432	Total C N O S 3386 2146 575 643 22	0	0
8	MG	432	Total C N O S 3384 2145 575 642 22	0	0
8	MI	433	Total C N O S 3392 2149 576 645 22	0	0
8	MK	440	Total C N O S 3436 2175 584 655 22	0	0
8	MM	440	Total C N O S 3436 2175 584 655 22	0	0
8	NC	440	Total C N O S 3436 2175 584 655 22	0	0
8	NE	439	Total C N O S 3429 2170 583 654 22	0	0
8	NG	439	Total C N O S 3429 2170 583 654 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	NI	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	NK	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	NM	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	OC	441	Total 3445	C 2180	N 585	O 658	S 22	0	0
8	OE	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	OG	441	Total 3445	C 2180	N 585	O 658	S 22	0	0
8	OI	441	Total 3445	C 2180	N 585	O 658	S 22	0	0
8	OK	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	OM	441	Total 3445	C 2180	N 585	O 658	S 22	0	0
8	OO	422	Total 3309	C 2092	N 563	O 632	S 22	0	0
8	PC	441	Total 3445	C 2180	N 585	O 658	S 22	0	0
8	PE	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	PG	441	Total 3445	C 2180	N 585	O 658	S 22	0	0
8	PI	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	PK	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	PM	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	PO	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	QC	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	QE	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	QG	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	QI	440	Total 3436	C 2175	N 584	O 655	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	QK	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	QM	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	QO	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	RC	411	Total 3209	C 2029	N 547	O 612	S 21	0	0
8	RE	430	Total 3371	C 2137	N 573	O 639	S 22	0	0
8	RG	432	Total 3384	C 2145	N 575	O 642	S 22	0	0
8	RI	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	RK	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	RM	440	Total 3436	C 2175	N 584	O 655	S 22	0	0
8	RO	439	Total 3429	C 2170	N 583	O 654	S 22	0	0
8	SE	429	Total 3365	C 2134	N 572	O 637	S 22	0	0
8	SG	430	Total 3373	C 2138	N 573	O 640	S 22	0	0
8	SI	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	SK	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	SM	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	SO	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	TE	429	Total 3365	C 2134	N 572	O 637	S 22	0	0
8	TG	430	Total 3373	C 2138	N 573	O 640	S 22	0	0
8	TI	431	Total 3379	C 2141	N 574	O 642	S 22	0	0
8	TK	429	Total 3365	C 2134	N 572	O 637	S 22	0	0
8	TM	431	Total 3379	C 2141	N 574	O 642	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
8	TO	429	Total C N O S 3365 2134 572 637 22	0	0
8	UE	431	Total C N O S 3379 2141 574 642 22	0	0
8	UG	432	Total C N O S 3385 2144 575 644 22	0	0
8	UI	432	Total C N O S 3385 2144 575 644 22	0	0
8	UK	431	Total C N O S 3379 2141 574 642 22	0	0
8	UM	431	Total C N O S 3379 2141 574 642 22	0	0
8	UO	431	Total C N O S 3379 2141 574 642 22	0	0
8	VE	439	Total C N O S 3429 2170 583 654 22	0	0
8	VG	433	Total C N O S 3393 2148 576 647 22	0	0
8	VI	439	Total C N O S 3429 2170 583 654 22	0	0
8	VK	431	Total C N O S 3379 2141 574 642 22	0	0
8	VM	439	Total C N O S 3429 2170 583 654 22	0	0
8	VO	431	Total C N O S 3379 2141 574 642 22	0	0
8	WE	439	Total C N O S 3429 2170 583 654 22	0	0
8	WG	430	Total C N O S 3371 2137 573 639 22	0	0
8	WI	438	Total C N O S 3423 2167 582 652 22	0	0
8	WK	430	Total C N O S 3371 2137 573 639 22	0	0
8	WM	439	Total C N O S 3429 2170 583 654 22	0	0
8	WO	431	Total C N O S 3379 2141 574 642 22	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
9	AB	437	Total C N O S 3433 2155 585 667 26	0	0
9	AD	437	Total C N O S 3433 2155 585 667 26	0	0
9	AF	437	Total C N O S 3433 2155 585 667 26	0	0
9	AH	437	Total C N O S 3433 2155 585 667 26	0	0
9	AJ	437	Total C N O S 3433 2155 585 667 26	0	0
9	AL	437	Total C N O S 3433 2155 585 667 26	0	0
9	BB	427	Total C N O S 3356 2109 575 646 26	0	0
9	BD	426	Total C N O S 3348 2105 574 643 26	0	0
9	BF	427	Total C N O S 3356 2109 575 646 26	0	0
9	BH	426	Total C N O S 3348 2105 574 643 26	0	0
9	BJ	430	Total C N O S 3373 2119 578 650 26	0	0
9	BL	426	Total C N O S 3348 2105 574 643 26	0	0
9	CB	428	Total C N O S 3361 2112 576 647 26	0	0
9	CD	426	Total C N O S 3348 2105 574 643 26	0	0
9	CF	427	Total C N O S 3356 2109 575 646 26	0	0
9	CH	426	Total C N O S 3348 2105 574 643 26	0	0
9	CJ	427	Total C N O S 3356 2109 575 646 26	0	0
9	CL	426	Total C N O S 3348 2105 574 643 26	0	0
9	DB	426	Total C N O S 3348 2105 574 643 26	0	0
9	DD	426	Total C N O S 3348 2105 574 643 26	0	0
9	DF	426	Total C N O S 3348 2105 574 643 26	0	0
9	DH	426	Total C N O S 3348 2105 574 643 26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
9	DJ	426	Total C N O S 3348 2105 574 643 26	0	0
9	DL	426	Total C N O S 3348 2105 574 643 26	0	0
9	EB	426	Total C N O S 3348 2105 574 643 26	0	0
9	ED	426	Total C N O S 3348 2105 574 643 26	0	0
9	EF	426	Total C N O S 3348 2105 574 643 26	0	0
9	EH	426	Total C N O S 3348 2105 574 643 26	0	0
9	EJ	426	Total C N O S 3348 2105 574 643 26	0	0
9	EL	426	Total C N O S 3348 2105 574 643 26	0	0
9	EN	428	Total C N O S 3361 2112 576 647 26	0	0
9	FB	426	Total C N O S 3348 2105 574 643 26	0	0
9	FD	426	Total C N O S 3348 2105 574 643 26	0	0
9	FF	426	Total C N O S 3348 2105 574 643 26	0	0
9	FH	426	Total C N O S 3348 2105 574 643 26	0	0
9	FJ	426	Total C N O S 3348 2105 574 643 26	0	0
9	FL	426	Total C N O S 3348 2105 574 643 26	0	0
9	FN	427	Total C N O S 3356 2109 575 646 26	0	0
9	GB	410	Total C N O S 3208 2016 548 619 25	0	0
9	GD	426	Total C N O S 3348 2105 574 643 26	0	0
9	GF	427	Total C N O S 3356 2109 575 646 26	0	0
9	GH	426	Total C N O S 3348 2105 574 643 26	0	0
9	GJ	430	Total C N O S 3373 2119 578 650 26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
9	GL	426	Total C N O S 3348 2105 574 643 26	0	0
9	GN	426	Total C N O S 3348 2105 574 643 26	0	0
9	HB	427	Total C N O S 3356 2109 575 646 26	0	0
9	HD	426	Total C N O S 3348 2105 574 643 26	0	0
9	HF	427	Total C N O S 3356 2109 575 646 26	0	0
9	HH	426	Total C N O S 3348 2105 574 643 26	0	0
9	HJ	428	Total C N O S 3361 2112 576 647 26	0	0
9	HL	426	Total C N O S 3348 2105 574 643 26	0	0
9	HN	425	Total C N O S 3339 2100 572 641 26	0	0
9	IB	407	Total C N O S 3197 2010 544 618 25	0	0
9	ID	426	Total C N O S 3348 2105 574 643 26	0	0
9	IF	428	Total C N O S 3361 2112 576 647 26	0	0
9	IH	426	Total C N O S 3348 2105 574 643 26	0	0
9	IJ	429	Total C N O S 3368 2116 577 649 26	0	0
9	IL	426	Total C N O S 3348 2105 574 643 26	0	0
9	IN	427	Total C N O S 3356 2109 575 646 26	0	0
9	JB	426	Total C N O S 3348 2105 574 643 26	0	0
9	JD	426	Total C N O S 3348 2105 574 643 26	0	0
9	JF	427	Total C N O S 3356 2109 575 646 26	0	0
9	JH	426	Total C N O S 3348 2105 574 643 26	0	0
9	JJ	426	Total C N O S 3348 2105 574 643 26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	JL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	JN	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	KB	412	Total 3222	C 2021	N 550	O 625	S 26	0	0
9	KD	431	Total 3382	C 2124	N 579	O 653	S 26	0	0
9	KF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	KH	431	Total 3382	C 2124	N 579	O 653	S 26	0	0
9	KJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	KL	431	Total 3382	C 2124	N 579	O 653	S 26	0	0
9	KN	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	LB	440	Total 3456	C 2168	N 588	O 674	S 26	0	0
9	LD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	LF	439	Total 3451	C 2165	N 587	O 673	S 26	0	0
9	LH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	LJ	443	Total 3483	C 2183	N 591	O 683	S 26	0	0
9	LL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	LN	440	Total 3456	C 2168	N 588	O 674	S 26	0	0
9	MB	430	Total 3373	C 2119	N 578	O 650	S 26	0	0
9	MD	432	Total 3391	C 2129	N 580	O 656	S 26	0	0
9	MF	431	Total 3382	C 2124	N 579	O 653	S 26	0	0
9	MH	432	Total 3391	C 2129	N 580	O 656	S 26	0	0
9	MJ	432	Total 3391	C 2129	N 580	O 656	S 26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
9	ML	432	Total C N O S 3391 2129 580 656 26	0	0
9	MN	430	Total C N O S 3373 2119 578 650 26	0	0
9	NB	428	Total C N O S 3361 2112 576 647 26	0	0
9	ND	428	Total C N O S 3361 2112 576 647 26	0	0
9	NF	430	Total C N O S 3373 2119 578 650 26	0	0
9	NH	428	Total C N O S 3361 2112 576 647 26	0	0
9	NJ	429	Total C N O S 3368 2116 577 649 26	0	0
9	NL	428	Total C N O S 3361 2112 576 647 26	0	0
9	NN	428	Total C N O S 3361 2112 576 647 26	0	0
9	OB	431	Total C N O S 3382 2124 579 653 26	0	0
9	OD	430	Total C N O S 3373 2119 578 650 26	0	0
9	OF	432	Total C N O S 3391 2129 580 656 26	0	0
9	OH	430	Total C N O S 3373 2119 578 650 26	0	0
9	OJ	432	Total C N O S 3391 2129 580 656 26	0	0
9	OL	430	Total C N O S 3373 2119 578 650 26	0	0
9	ON	431	Total C N O S 3382 2124 579 653 26	0	0
9	PD	430	Total C N O S 3373 2119 578 650 26	0	0
9	PF	432	Total C N O S 3391 2129 580 656 26	0	0
9	PH	426	Total C N O S 3348 2105 574 643 26	0	0
9	PJ	430	Total C N O S 3373 2119 578 650 26	0	0
9	PL	429	Total C N O S 3368 2116 577 649 26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	PN	430	Total 3373	C 2119	N 578	O 650	S 26	0	0
9	QD	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	QF	430	Total 3373	C 2119	N 578	O 650	S 26	0	0
9	QH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	QJ	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
9	QL	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	QN	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	RD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	RF	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
9	RH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	RJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	RL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	RN	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	SD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	SF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	SH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	SJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	SL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	SN	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	TD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	TF	427	Total 3356	C 2109	N 575	O 646	S 26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
9	TH	426	Total C N O S 3348 2105 574 643 26	0	0
9	TJ	426	Total C N O S 3348 2105 574 643 26	0	0
9	TL	426	Total C N O S 3348 2105 574 643 26	0	0
9	TN	426	Total C N O S 3348 2105 574 643 26	0	0
9	TP	421	Total C N O S 3302 2074 567 635 26	0	0
9	UD	426	Total C N O S 3348 2105 574 643 26	0	0
9	UF	427	Total C N O S 3356 2109 575 646 26	0	0
9	UH	426	Total C N O S 3348 2105 574 643 26	0	0
9	UJ	427	Total C N O S 3356 2109 575 646 26	0	0
9	UL	426	Total C N O S 3348 2105 574 643 26	0	0
9	UN	427	Total C N O S 3356 2109 575 646 26	0	0
9	UP	427	Total C N O S 3356 2109 575 646 26	0	0
9	VD	426	Total C N O S 3348 2105 574 643 26	0	0
9	VF	427	Total C N O S 3356 2109 575 646 26	0	0
9	VH	426	Total C N O S 3348 2105 574 643 26	0	0
9	VJ	427	Total C N O S 3356 2109 575 646 26	0	0
9	VL	426	Total C N O S 3348 2105 574 643 26	0	0
9	VN	427	Total C N O S 3356 2109 575 646 26	0	0
9	VP	427	Total C N O S 3356 2109 575 646 26	0	0
9	WD	426	Total C N O S 3348 2105 574 643 26	0	0
9	WF	426	Total C N O S 3348 2105 574 643 26	0	0

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms	AltConf	Trace
10	B	180	Total C N O S 1507 921 287 289 10	0	0
10	C	356	Total C N O S 3062 1903 551 592 16	0	0

- Molecule 11 is a protein called Tektin-2.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	B0	193	Total C N O S 1574 958 294 315 7	0	0
11	B1	392	Total C N O S 3187 1956 586 630 15	0	0
11	B2	391	Total C N O S 3180 1951 585 629 15	0	0
11	B3	354	Total C N O S 2868 1760 521 572 15	0	0
11	B4	51	Total C N O S 412 255 76 80 1	0	0
11	B5	51	Total C N O 254 152 51 51	0	0
11	B6	354	Total C N O 1766 1058 354 354	0	0
11	B7	391	Total C N O 1951 1169 391 391	0	0
11	B8	392	Total C N O 1956 1172 392 392	0	0
11	B9	193	Total C N O 962 576 193 193	0	0

- Molecule 12 is a protein called Tektin-3.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	C0	33	Total C N O 285 171 54 60	0	0
12	C1	336	Total C N O S 2732 1683 495 541 13	0	0
12	C2	393	Total C N O S 3199 1968 584 632 15	0	0
12	C3	394	Total C N O S 3210 1974 588 633 15	0	0
12	C4	219	Total C N O S 1786 1111 321 341 13	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
13	D	179	Total C N O S 1459 919 260 271 9	0	0

- Molecule 14 is a protein called Tektin-4.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	D0	266	Total C N O S 2180 1326 409 432 13	0	0
14	D1	396	Total C N O S 3256 1989 616 632 19	0	0
14	D2	398	Total C N O S 3275 2000 620 636 19	0	0
14	D3	317	Total C N O S 2603 1596 492 498 17	0	0
14	D5	317	Total C N O 1583 948 317 318	0	0
14	D6	398	Total C N O 1987 1190 398 399	0	0
14	D7	396	Total C N O 1976 1184 396 396	0	0
14	D8	266	Total C N O 1327 794 266 267	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
15	E	277	Total C N O S 2227 1403 397 415 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
15	F	277	Total C N O S 2227 1403 397 415 12	0	0

- Molecule 16 is a protein called Sperm acrosome-associated protein 9.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	F0	157	Total C N O S 1263 788 225 240 10	0	0
16	F1	160	Total C N O S 1289 805 231 243 10	0	0
16	F2	156	Total C N O 776 464 156 156	0	0
16	F3	157	Total C N O S 1263 788 225 240 10	0	0
16	F4	160	Total C N O S 1289 805 231 243 10	0	0
16	F5	156	Total C N O 776 464 156 156	0	0
16	F6	157	Total C N O S 1263 788 225 240 10	0	0
16	F7	160	Total C N O S 1289 805 231 243 10	0	0
16	F8	156	Total C N O 776 464 156 156	0	0
16	G0	159	Total C N O S 1278 799 227 242 10	0	0
16	G1	158	Total C N O S 1271 794 226 241 10	0	0
16	G2	156	Total C N O 776 464 156 156	0	0
16	G3	157	Total C N O S 1263 788 225 240 10	0	0
16	G4	160	Total C N O S 1289 805 231 243 10	0	0
16	G5	156	Total C N O 776 464 156 156	0	0
16	G6	157	Total C N O S 1263 788 225 240 10	0	0
16	G7	160	Total C N O S 1289 805 231 243 10	0	0
16	G8	156	Total C N O 776 464 156 156	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H0	157	1263	788	225	240	10	0	0
16	H1	160	1289	805	231	243	10	0	0
16	H2	156	776	464	156	156		0	0

- Molecule 17 is a protein called Uncharacterized protein C15orf65.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	G	94	750	478	127	139	6	0	0

- Molecule 18 is a protein called Protein FAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	H	80	619	405	108	103	3	0	0
18	I	145	1080	698	187	189	6	0	0
18	J	146	1085	701	188	190	6	0	0
18	K	145	1080	698	187	189	6	0	0
18	L	145	1080	698	187	189	6	0	0
18	M	145	1080	698	187	189	6	0	0
18	N	146	1085	701	188	190	6	0	0

- Molecule 19 is a protein called UPF0686 protein C11orf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I1	89	763	481	135	143	4	0	0

- Molecule 20 is a protein called Isoform 2 of Cilia- and flagella-associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J1	81	704	448	135	119	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
20	J2	226	Total C N O S 1849 1169 349 323 8	0	0
20	J3	226	Total C N O S 1849 1169 349 323 8	0	0
20	J4	205	Total C N O S 1674 1064 313 290 7	0	0
20	J5	65	Total C N O S 514 324 94 93 3	0	0

- Molecule 21 is a protein called Protein FAM183A.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	K1	111	Total C N O S 945 594 179 170 2	0	0

- Molecule 22 is a protein called Uncharacterized protein C5orf49.

Mol	Chain	Residues	Atoms	AltConf	Trace
22	L1	127	Total C N O S 1045 659 195 190 1	0	0
22	L2	90	Total C N O S 746 469 139 137 1	0	0

- Molecule 23 is a protein called Protein FAM166C.

Mol	Chain	Residues	Atoms	AltConf	Trace
23	M1	102	Total C N O S 825 526 147 148 4	0	0
23	M2	101	Total C N O S 818 521 146 147 4	0	0
23	M3	102	Total C N O S 825 526 147 148 4	0	0
23	M4	102	Total C N O S 825 526 147 148 4	0	0

- Molecule 24 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms	AltConf	Trace
24	O	25	Total C N O S 212 129 51 31 1	0	0
24	P	368	Total C N O S 3089 1886 608 584 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	40	327	203	56	67	1	0	0
24	R	219	1816	1105	354	348	9	0	0
24	S	165	1387	852	269	263	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	T	484	3984	2570	666	734	14	0	0
25	U	485	3992	2576	667	735	14	0	0
25	V	485	3992	2576	667	735	14	0	0

- Molecule 26 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	W	614	5064	3269	845	926	24	0	0
26	X	701	5797	3742	964	1063	28	0	0
26	Y	701	5797	3742	964	1063	28	0	0
26	Z	510	4239	2739	702	776	22	0	0

- Molecule 27 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	XA	186	1549	998	270	274	7	0	0
27	XB	186	1549	998	270	274	7	0	0
27	XC	186	1549	998	270	274	7	0	0
27	XD	186	1549	998	270	274	7	0	0
27	XE	186	1549	998	270	274	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	XF	186	1549	998	270	274	7	0	0
27	XG	186	1549	998	270	274	7	0	0

- Molecule 28 is a protein called Parkin coregulated gene protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	YB	220	1771	1147	301	314	9	0	0
28	YC	220	1771	1147	301	314	9	0	0
28	YD	220	1771	1147	301	314	9	0	0
28	YE	220	1771	1147	301	314	9	0	0
28	YF	220	1771	1147	301	314	9	0	0
28	YG	220	1771	1147	301	314	9	0	0

- Molecule 29 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	174	1467	898	279	280	10	0	0
29	b	334	2878	1734	571	560	13	0	0
29	c	284	2419	1475	454	472	18	0	0
29	d	218	1858	1126	373	353	6	0	0

- Molecule 30 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	610	4717	2978	827	882	30	0	0
30	f	610	4717	2978	827	882	30	0	0
30	g	610	4717	2978	827	882	30	0	0

- Molecule 31 is a protein called Enkurin.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	h	146	Total C N O S 1210 766 213 227 4	0	0
31	i	250	Total C N O S 2023 1290 350 373 10	0	0
31	j	248	Total C N O S 2010 1283 348 370 9	0	0
31	k	250	Total C N O S 2023 1290 350 373 10	0	0

- Molecule 32 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms	AltConf	Trace
32	l	117	Total C N O S 908 577 159 168 4	0	0
32	m	117	Total C N O S 908 577 159 168 4	0	0
32	n	117	Total C N O S 908 577 159 168 4	0	0

- Molecule 33 is a protein called Protein CFAP210.

Mol	Chain	Residues	Atoms	AltConf	Trace
33	o	404	Total C N O S 3471 2149 654 653 15	0	0
33	o1	36	Total C N O S 301 185 60 55 1	0	0
33	p	158	Total C N O S 1285 809 229 243 4	0	0

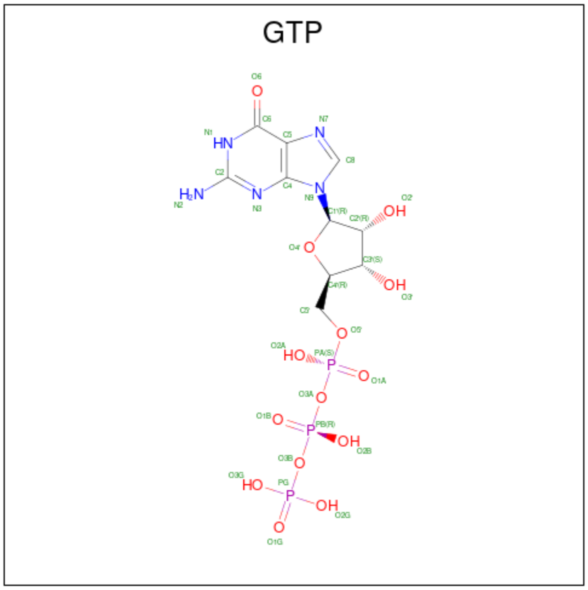
- Molecule 34 is a protein called Protein CFAP276.

Mol	Chain	Residues	Atoms	AltConf	Trace
34	q	112	Total C N O S 906 568 166 171 1	0	0
34	r	112	Total C N O S 906 568 166 171 1	0	0
34	s	112	Total C N O S 906 568 166 171 1	0	0

- Molecule 35 is a protein called UPF0691 protein C9orf116.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	y	63	Total 498	C 312	N 88	O 94	S 4	0	0
35	z	111	Total 891	C 559	N 163	O 165	S 4	0	0

- Molecule 36 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
36	AA	1	Total 32	C 10	N 5	O 14	P 3	0
36	AC	1	Total 32	C 10	N 5	O 14	P 3	0
36	AE	1	Total 32	C 10	N 5	O 14	P 3	0
36	AG	1	Total 32	C 10	N 5	O 14	P 3	0
36	AI	1	Total 32	C 10	N 5	O 14	P 3	0
36	AK	1	Total 32	C 10	N 5	O 14	P 3	0
36	AM	1	Total 32	C 10	N 5	O 14	P 3	0
36	BA	1	Total 32	C 10	N 5	O 14	P 3	0
36	BC	1	Total 32	C 10	N 5	O 14	P 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
36	BE	1	Total C N O P 32 10 5 14 3	0
36	BG	1	Total C N O P 32 10 5 14 3	0
36	BI	1	Total C N O P 32 10 5 14 3	0
36	BK	1	Total C N O P 32 10 5 14 3	0
36	BM	1	Total C N O P 32 10 5 14 3	0
36	CA	1	Total C N O P 32 10 5 14 3	0
36	CC	1	Total C N O P 32 10 5 14 3	0
36	CE	1	Total C N O P 32 10 5 14 3	0
36	CG	1	Total C N O P 32 10 5 14 3	0
36	CI	1	Total C N O P 32 10 5 14 3	0
36	CK	1	Total C N O P 32 10 5 14 3	0
36	CM	1	Total C N O P 32 10 5 14 3	0
36	DA	1	Total C N O P 32 10 5 14 3	0
36	DC	1	Total C N O P 32 10 5 14 3	0
36	DE	1	Total C N O P 32 10 5 14 3	0
36	DG	1	Total C N O P 32 10 5 14 3	0
36	DI	1	Total C N O P 32 10 5 14 3	0
36	DK	1	Total C N O P 32 10 5 14 3	0
36	DM	1	Total C N O P 32 10 5 14 3	0
36	EC	1	Total C N O P 32 10 5 14 3	0
36	EE	1	Total C N O P 32 10 5 14 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
36	EG	1	Total C N O P 32 10 5 14 3	0
36	EI	1	Total C N O P 32 10 5 14 3	0
36	EK	1	Total C N O P 32 10 5 14 3	0
36	EM	1	Total C N O P 32 10 5 14 3	0
36	FC	1	Total C N O P 32 10 5 14 3	0
36	FE	1	Total C N O P 32 10 5 14 3	0
36	FG	1	Total C N O P 32 10 5 14 3	0
36	FI	1	Total C N O P 32 10 5 14 3	0
36	FK	1	Total C N O P 32 10 5 14 3	0
36	FM	1	Total C N O P 32 10 5 14 3	0
36	GC	1	Total C N O P 32 10 5 14 3	0
36	GE	1	Total C N O P 32 10 5 14 3	0
36	GG	1	Total C N O P 32 10 5 14 3	0
36	GI	1	Total C N O P 32 10 5 14 3	0
36	GK	1	Total C N O P 32 10 5 14 3	0
36	GM	1	Total C N O P 32 10 5 14 3	0
36	HC	1	Total C N O P 32 10 5 14 3	0
36	HE	1	Total C N O P 32 10 5 14 3	0
36	HG	1	Total C N O P 32 10 5 14 3	0
36	HI	1	Total C N O P 32 10 5 14 3	0
36	HK	1	Total C N O P 32 10 5 14 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
36	HM	1	Total 32	C 10	N 5	O 14	P 3	0
36	HO	1	Total 32	C 10	N 5	O 14	P 3	0
36	IC	1	Total 32	C 10	N 5	O 14	P 3	0
36	IE	1	Total 32	C 10	N 5	O 14	P 3	0
36	IG	1	Total 32	C 10	N 5	O 14	P 3	0
36	II	1	Total 32	C 10	N 5	O 14	P 3	0
36	IK	1	Total 32	C 10	N 5	O 14	P 3	0
36	IM	1	Total 32	C 10	N 5	O 14	P 3	0
36	IO	1	Total 32	C 10	N 5	O 14	P 3	0
36	JC	1	Total 32	C 10	N 5	O 14	P 3	0
36	JE	1	Total 32	C 10	N 5	O 14	P 3	0
36	JG	1	Total 32	C 10	N 5	O 14	P 3	0
36	JI	1	Total 32	C 10	N 5	O 14	P 3	0
36	JK	1	Total 32	C 10	N 5	O 14	P 3	0
36	JM	1	Total 32	C 10	N 5	O 14	P 3	0
36	KC	1	Total 32	C 10	N 5	O 14	P 3	0
36	KE	1	Total 32	C 10	N 5	O 14	P 3	0
36	KG	1	Total 32	C 10	N 5	O 14	P 3	0
36	KI	1	Total 32	C 10	N 5	O 14	P 3	0
36	KK	1	Total 32	C 10	N 5	O 14	P 3	0
36	KM	1	Total 32	C 10	N 5	O 14	P 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
36	KO	1	Total 32	C 10	N 5	O 14	P 3	0
36	LC	1	Total 32	C 10	N 5	O 14	P 3	0
36	LE	1	Total 32	C 10	N 5	O 14	P 3	0
36	LG	1	Total 32	C 10	N 5	O 14	P 3	0
36	LI	1	Total 32	C 10	N 5	O 14	P 3	0
36	LK	1	Total 32	C 10	N 5	O 14	P 3	0
36	LM	1	Total 32	C 10	N 5	O 14	P 3	0
36	MC	1	Total 32	C 10	N 5	O 14	P 3	0
36	ME	1	Total 32	C 10	N 5	O 14	P 3	0
36	MG	1	Total 32	C 10	N 5	O 14	P 3	0
36	MI	1	Total 32	C 10	N 5	O 14	P 3	0
36	MK	1	Total 32	C 10	N 5	O 14	P 3	0
36	MM	1	Total 32	C 10	N 5	O 14	P 3	0
36	NC	1	Total 32	C 10	N 5	O 14	P 3	0
36	NE	1	Total 32	C 10	N 5	O 14	P 3	0
36	NG	1	Total 32	C 10	N 5	O 14	P 3	0
36	NI	1	Total 32	C 10	N 5	O 14	P 3	0
36	NK	1	Total 32	C 10	N 5	O 14	P 3	0
36	NM	1	Total 32	C 10	N 5	O 14	P 3	0
36	OC	1	Total 32	C 10	N 5	O 14	P 3	0
36	OE	1	Total 32	C 10	N 5	O 14	P 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
36	OG	1	Total C N O P 32 10 5 14 3	0
36	OI	1	Total C N O P 32 10 5 14 3	0
36	OK	1	Total C N O P 32 10 5 14 3	0
36	OM	1	Total C N O P 32 10 5 14 3	0
36	OO	1	Total C N O P 32 10 5 14 3	0
36	PC	1	Total C N O P 32 10 5 14 3	0
36	PE	1	Total C N O P 32 10 5 14 3	0
36	PG	1	Total C N O P 32 10 5 14 3	0
36	PI	1	Total C N O P 32 10 5 14 3	0
36	PK	1	Total C N O P 32 10 5 14 3	0
36	PM	1	Total C N O P 32 10 5 14 3	0
36	PO	1	Total C N O P 32 10 5 14 3	0
36	QC	1	Total C N O P 32 10 5 14 3	0
36	QE	1	Total C N O P 32 10 5 14 3	0
36	QG	1	Total C N O P 32 10 5 14 3	0
36	QI	1	Total C N O P 32 10 5 14 3	0
36	QK	1	Total C N O P 32 10 5 14 3	0
36	QM	1	Total C N O P 32 10 5 14 3	0
36	QO	1	Total C N O P 32 10 5 14 3	0
36	RC	1	Total C N O P 32 10 5 14 3	0
36	RE	1	Total C N O P 32 10 5 14 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
36	RG	1	Total 32	C 10	N 5	O 14	P 3	0
36	RI	1	Total 32	C 10	N 5	O 14	P 3	0
36	RK	1	Total 32	C 10	N 5	O 14	P 3	0
36	RM	1	Total 32	C 10	N 5	O 14	P 3	0
36	RO	1	Total 32	C 10	N 5	O 14	P 3	0
36	SE	1	Total 32	C 10	N 5	O 14	P 3	0
36	SG	1	Total 32	C 10	N 5	O 14	P 3	0
36	SI	1	Total 32	C 10	N 5	O 14	P 3	0
36	SK	1	Total 32	C 10	N 5	O 14	P 3	0
36	SM	1	Total 32	C 10	N 5	O 14	P 3	0
36	SO	1	Total 32	C 10	N 5	O 14	P 3	0
36	TE	1	Total 32	C 10	N 5	O 14	P 3	0
36	TG	1	Total 32	C 10	N 5	O 14	P 3	0
36	TI	1	Total 32	C 10	N 5	O 14	P 3	0
36	TK	1	Total 32	C 10	N 5	O 14	P 3	0
36	TM	1	Total 32	C 10	N 5	O 14	P 3	0
36	TO	1	Total 32	C 10	N 5	O 14	P 3	0
36	UE	1	Total 32	C 10	N 5	O 14	P 3	0
36	UG	1	Total 32	C 10	N 5	O 14	P 3	0
36	UI	1	Total 32	C 10	N 5	O 14	P 3	0
36	UK	1	Total 32	C 10	N 5	O 14	P 3	0

Continued on next page...

Continued from previous page...

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

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	AA	1	Total 1	Mg 1	0
37	AC	1	Total 1	Mg 1	0
37	AE	1	Total 1	Mg 1	0
37	AG	1	Total 1	Mg 1	0
37	AI	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
37	AK	1	Total Mg 1 1	0
37	AM	1	Total Mg 1 1	0
37	BA	1	Total Mg 1 1	0
37	BC	1	Total Mg 1 1	0
37	BE	1	Total Mg 1 1	0
37	BG	1	Total Mg 1 1	0
37	BI	1	Total Mg 1 1	0
37	BK	1	Total Mg 1 1	0
37	BM	1	Total Mg 1 1	0
37	CA	1	Total Mg 1 1	0
37	CC	1	Total Mg 1 1	0
37	CE	1	Total Mg 1 1	0
37	CG	1	Total Mg 1 1	0
37	CI	1	Total Mg 1 1	0
37	CK	1	Total Mg 1 1	0
37	CM	1	Total Mg 1 1	0
37	DA	1	Total Mg 1 1	0
37	DC	1	Total Mg 1 1	0
37	DE	1	Total Mg 1 1	0
37	DG	1	Total Mg 1 1	0
37	DI	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
37	DK	1	Total Mg 1 1	0
37	DM	1	Total Mg 1 1	0
37	EC	1	Total Mg 1 1	0
37	EE	1	Total Mg 1 1	0
37	EG	1	Total Mg 1 1	0
37	EI	1	Total Mg 1 1	0
37	EK	1	Total Mg 1 1	0
37	EM	1	Total Mg 1 1	0
37	FC	1	Total Mg 1 1	0
37	FE	1	Total Mg 1 1	0
37	FG	1	Total Mg 1 1	0
37	FI	1	Total Mg 1 1	0
37	FK	1	Total Mg 1 1	0
37	FM	1	Total Mg 1 1	0
37	GC	1	Total Mg 1 1	0
37	GE	1	Total Mg 1 1	0
37	GG	1	Total Mg 1 1	0
37	GI	1	Total Mg 1 1	0
37	GK	1	Total Mg 1 1	0
37	GM	1	Total Mg 1 1	0
37	HC	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
37	HE	1	Total Mg 1 1	0
37	HG	1	Total Mg 1 1	0
37	HI	1	Total Mg 1 1	0
37	HK	1	Total Mg 1 1	0
37	HM	1	Total Mg 1 1	0
37	HO	1	Total Mg 1 1	0
37	IC	1	Total Mg 1 1	0
37	IE	1	Total Mg 1 1	0
37	IG	1	Total Mg 1 1	0
37	II	1	Total Mg 1 1	0
37	IK	1	Total Mg 1 1	0
37	IM	1	Total Mg 1 1	0
37	IO	1	Total Mg 1 1	0
37	JC	1	Total Mg 1 1	0
37	JE	1	Total Mg 1 1	0
37	JG	1	Total Mg 1 1	0
37	JI	1	Total Mg 1 1	0
37	JK	1	Total Mg 1 1	0
37	JM	1	Total Mg 1 1	0
37	KC	1	Total Mg 1 1	0
37	KE	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
37	KG	1	Total Mg 1 1	0
37	KI	1	Total Mg 1 1	0
37	KK	1	Total Mg 1 1	0
37	KM	1	Total Mg 1 1	0
37	KO	1	Total Mg 1 1	0
37	LC	1	Total Mg 1 1	0
37	LE	1	Total Mg 1 1	0
37	LG	1	Total Mg 1 1	0
37	LI	1	Total Mg 1 1	0
37	LK	1	Total Mg 1 1	0
37	LM	1	Total Mg 1 1	0
37	MC	1	Total Mg 1 1	0
37	ME	1	Total Mg 1 1	0
37	MG	1	Total Mg 1 1	0
37	MI	1	Total Mg 1 1	0
37	MK	1	Total Mg 1 1	0
37	MM	1	Total Mg 1 1	0
37	NC	1	Total Mg 1 1	0
37	NE	1	Total Mg 1 1	0
37	NG	1	Total Mg 1 1	0
37	NI	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
37	NK	1	Total Mg 1 1	0
37	NM	1	Total Mg 1 1	0
37	OC	1	Total Mg 1 1	0
37	OE	1	Total Mg 1 1	0
37	OG	1	Total Mg 1 1	0
37	OI	1	Total Mg 1 1	0
37	OK	1	Total Mg 1 1	0
37	OM	1	Total Mg 1 1	0
37	OO	1	Total Mg 1 1	0
37	PC	1	Total Mg 1 1	0
37	PE	1	Total Mg 1 1	0
37	PG	1	Total Mg 1 1	0
37	PI	1	Total Mg 1 1	0
37	PK	1	Total Mg 1 1	0
37	PM	1	Total Mg 1 1	0
37	PO	1	Total Mg 1 1	0
37	QC	1	Total Mg 1 1	0
37	QE	1	Total Mg 1 1	0
37	QG	1	Total Mg 1 1	0
37	QI	1	Total Mg 1 1	0
37	QK	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

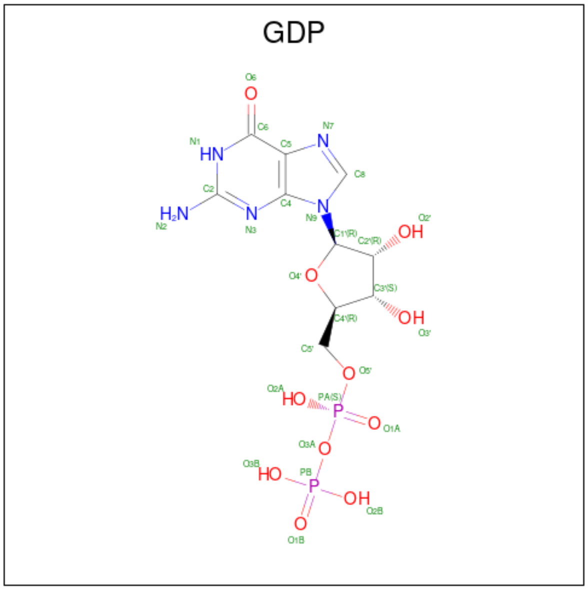
Mol	Chain	Residues	Atoms	AltConf
37	QM	1	Total Mg 1 1	0
37	QO	1	Total Mg 1 1	0
37	RC	1	Total Mg 1 1	0
37	RE	1	Total Mg 1 1	0
37	RG	1	Total Mg 1 1	0
37	RI	1	Total Mg 1 1	0
37	RK	1	Total Mg 1 1	0
37	RM	1	Total Mg 1 1	0
37	RO	1	Total Mg 1 1	0
37	SE	1	Total Mg 1 1	0
37	SG	1	Total Mg 1 1	0
37	SI	1	Total Mg 1 1	0
37	SK	1	Total Mg 1 1	0
37	SM	1	Total Mg 1 1	0
37	SO	1	Total Mg 1 1	0
37	TE	1	Total Mg 1 1	0
37	TG	1	Total Mg 1 1	0
37	TI	1	Total Mg 1 1	0
37	TK	1	Total Mg 1 1	0
37	TM	1	Total Mg 1 1	0
37	TO	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
37	UE	1	Total Mg 1 1	0
37	UG	1	Total Mg 1 1	0
37	UI	1	Total Mg 1 1	0
37	UK	1	Total Mg 1 1	0
37	UM	1	Total Mg 1 1	0
37	UO	1	Total Mg 1 1	0
37	VE	1	Total Mg 1 1	0
37	VG	1	Total Mg 1 1	0
37	VI	1	Total Mg 1 1	0
37	VK	1	Total Mg 1 1	0
37	VM	1	Total Mg 1 1	0
37	VO	1	Total Mg 1 1	0
37	WE	1	Total Mg 1 1	0
37	WG	1	Total Mg 1 1	0
37	WI	1	Total Mg 1 1	0
37	WK	1	Total Mg 1 1	0
37	WM	1	Total Mg 1 1	0
37	WO	1	Total Mg 1 1	0

- Molecule 38 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
38	CF	1	Total C N O P 28 10 5 11 2	0
38	CH	1	Total C N O P 28 10 5 11 2	0
38	CJ	1	Total C N O P 28 10 5 11 2	0
38	CL	1	Total C N O P 28 10 5 11 2	0
38	DB	1	Total C N O P 28 10 5 11 2	0
38	DD	1	Total C N O P 28 10 5 11 2	0
38	DF	1	Total C N O P 28 10 5 11 2	0
38	DH	1	Total C N O P 28 10 5 11 2	0
38	DJ	1	Total C N O P 28 10 5 11 2	0
38	DL	1	Total C N O P 28 10 5 11 2	0
38	EB	1	Total C N O P 28 10 5 11 2	0
38	ED	1	Total C N O P 28 10 5 11 2	0
38	EF	1	Total C N O P 28 10 5 11 2	0
38	EH	1	Total C N O P 28 10 5 11 2	0
38	EJ	1	Total C N O P 28 10 5 11 2	0
38	EL	1	Total C N O P 28 10 5 11 2	0
38	EN	1	Total C N O P 28 10 5 11 2	0
38	FB	1	Total C N O P 28 10 5 11 2	0
38	FD	1	Total C N O P 28 10 5 11 2	0
38	FF	1	Total C N O P 28 10 5 11 2	0
38	FH	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
38	FJ	1	Total C N O P 28 10 5 11 2	0
38	FL	1	Total C N O P 28 10 5 11 2	0
38	FN	1	Total C N O P 28 10 5 11 2	0
38	GB	1	Total C N O P 28 10 5 11 2	0
38	GD	1	Total C N O P 28 10 5 11 2	0
38	GF	1	Total C N O P 28 10 5 11 2	0
38	GH	1	Total C N O P 28 10 5 11 2	0
38	GJ	1	Total C N O P 28 10 5 11 2	0
38	GL	1	Total C N O P 28 10 5 11 2	0
38	GN	1	Total C N O P 28 10 5 11 2	0
38	HB	1	Total C N O P 28 10 5 11 2	0
38	HD	1	Total C N O P 28 10 5 11 2	0
38	HF	1	Total C N O P 28 10 5 11 2	0
38	HH	1	Total C N O P 28 10 5 11 2	0
38	HJ	1	Total C N O P 28 10 5 11 2	0
38	HL	1	Total C N O P 28 10 5 11 2	0
38	HN	1	Total C N O P 28 10 5 11 2	0
38	IB	1	Total C N O P 28 10 5 11 2	0
38	ID	1	Total C N O P 28 10 5 11 2	0
38	IF	1	Total C N O P 28 10 5 11 2	0
38	IH	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
38	IJ	1	Total 28	C 10	N 5	O 11	P 2	0
38	IL	1	Total 28	C 10	N 5	O 11	P 2	0
38	IN	1	Total 28	C 10	N 5	O 11	P 2	0
38	JB	1	Total 28	C 10	N 5	O 11	P 2	0
38	JD	1	Total 28	C 10	N 5	O 11	P 2	0
38	JF	1	Total 28	C 10	N 5	O 11	P 2	0
38	JH	1	Total 28	C 10	N 5	O 11	P 2	0
38	JJ	1	Total 28	C 10	N 5	O 11	P 2	0
38	JL	1	Total 28	C 10	N 5	O 11	P 2	0
38	JN	1	Total 28	C 10	N 5	O 11	P 2	0
38	KB	1	Total 28	C 10	N 5	O 11	P 2	0
38	KD	1	Total 28	C 10	N 5	O 11	P 2	0
38	KF	1	Total 28	C 10	N 5	O 11	P 2	0
38	KH	1	Total 28	C 10	N 5	O 11	P 2	0
38	KJ	1	Total 28	C 10	N 5	O 11	P 2	0
38	KL	1	Total 28	C 10	N 5	O 11	P 2	0
38	KN	1	Total 28	C 10	N 5	O 11	P 2	0
38	LB	1	Total 28	C 10	N 5	O 11	P 2	0
38	LD	1	Total 28	C 10	N 5	O 11	P 2	0
38	LF	1	Total 28	C 10	N 5	O 11	P 2	0
38	LH	1	Total 28	C 10	N 5	O 11	P 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
38	LJ	1	Total C N O P 28 10 5 11 2	0
38	LL	1	Total C N O P 28 10 5 11 2	0
38	LN	1	Total C N O P 28 10 5 11 2	0
38	MB	1	Total C N O P 28 10 5 11 2	0
38	MD	1	Total C N O P 28 10 5 11 2	0
38	MF	1	Total C N O P 28 10 5 11 2	0
38	MH	1	Total C N O P 28 10 5 11 2	0
38	MJ	1	Total C N O P 28 10 5 11 2	0
38	ML	1	Total C N O P 28 10 5 11 2	0
38	MN	1	Total C N O P 28 10 5 11 2	0
38	NB	1	Total C N O P 28 10 5 11 2	0
38	ND	1	Total C N O P 28 10 5 11 2	0
38	NF	1	Total C N O P 28 10 5 11 2	0
38	NH	1	Total C N O P 28 10 5 11 2	0
38	NJ	1	Total C N O P 28 10 5 11 2	0
38	NL	1	Total C N O P 28 10 5 11 2	0
38	NN	1	Total C N O P 28 10 5 11 2	0
38	OB	1	Total C N O P 28 10 5 11 2	0
38	OD	1	Total C N O P 28 10 5 11 2	0
38	OF	1	Total C N O P 28 10 5 11 2	0
38	OH	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
38	OJ	1	Total C N O P 28 10 5 11 2	0
38	OL	1	Total C N O P 28 10 5 11 2	0
38	ON	1	Total C N O P 28 10 5 11 2	0
38	PD	1	Total C N O P 28 10 5 11 2	0
38	PF	1	Total C N O P 28 10 5 11 2	0
38	PH	1	Total C N O P 28 10 5 11 2	0
38	PJ	1	Total C N O P 28 10 5 11 2	0
38	PL	1	Total C N O P 28 10 5 11 2	0
38	PN	1	Total C N O P 28 10 5 11 2	0
38	QD	1	Total C N O P 28 10 5 11 2	0
38	QF	1	Total C N O P 28 10 5 11 2	0
38	QH	1	Total C N O P 28 10 5 11 2	0
38	QJ	1	Total C N O P 28 10 5 11 2	0
38	QL	1	Total C N O P 28 10 5 11 2	0
38	QN	1	Total C N O P 28 10 5 11 2	0
38	RD	1	Total C N O P 28 10 5 11 2	0
38	RF	1	Total C N O P 28 10 5 11 2	0
38	RH	1	Total C N O P 28 10 5 11 2	0
38	RJ	1	Total C N O P 28 10 5 11 2	0
38	RL	1	Total C N O P 28 10 5 11 2	0
38	RN	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
38	SD	1	Total C N O P 28 10 5 11 2	0
38	SF	1	Total C N O P 28 10 5 11 2	0
38	SH	1	Total C N O P 28 10 5 11 2	0
38	SJ	1	Total C N O P 28 10 5 11 2	0
38	SL	1	Total C N O P 28 10 5 11 2	0
38	SN	1	Total C N O P 28 10 5 11 2	0
38	TD	1	Total C N O P 28 10 5 11 2	0
38	TF	1	Total C N O P 28 10 5 11 2	0
38	TH	1	Total C N O P 28 10 5 11 2	0
38	TJ	1	Total C N O P 28 10 5 11 2	0
38	TL	1	Total C N O P 28 10 5 11 2	0
38	TN	1	Total C N O P 28 10 5 11 2	0
38	TP	1	Total C N O P 28 10 5 11 2	0
38	UD	1	Total C N O P 28 10 5 11 2	0
38	UF	1	Total C N O P 28 10 5 11 2	0
38	UH	1	Total C N O P 28 10 5 11 2	0
38	UJ	1	Total C N O P 28 10 5 11 2	0
38	UL	1	Total C N O P 28 10 5 11 2	0
38	UN	1	Total C N O P 28 10 5 11 2	0
38	UP	1	Total C N O P 28 10 5 11 2	0
38	VD	1	Total C N O P 28 10 5 11 2	0

Continued on next page...

Continued from previous page...

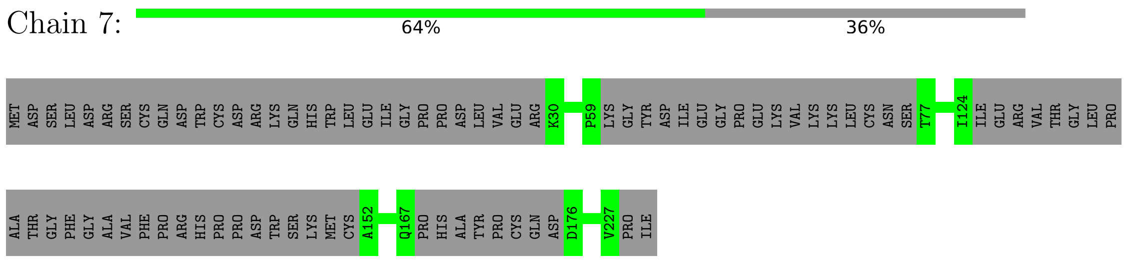
Mol	Chain	Residues	Atoms					AltConf
38	VF	1	Total 28	C 10	N 5	O 11	P 2	0
38	VH	1	Total 28	C 10	N 5	O 11	P 2	0
38	VJ	1	Total 28	C 10	N 5	O 11	P 2	0
38	VL	1	Total 28	C 10	N 5	O 11	P 2	0
38	VN	1	Total 28	C 10	N 5	O 11	P 2	0
38	VP	1	Total 28	C 10	N 5	O 11	P 2	0
38	WD	1	Total 28	C 10	N 5	O 11	P 2	0
38	WF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

3 Residue-property plots ⓘ

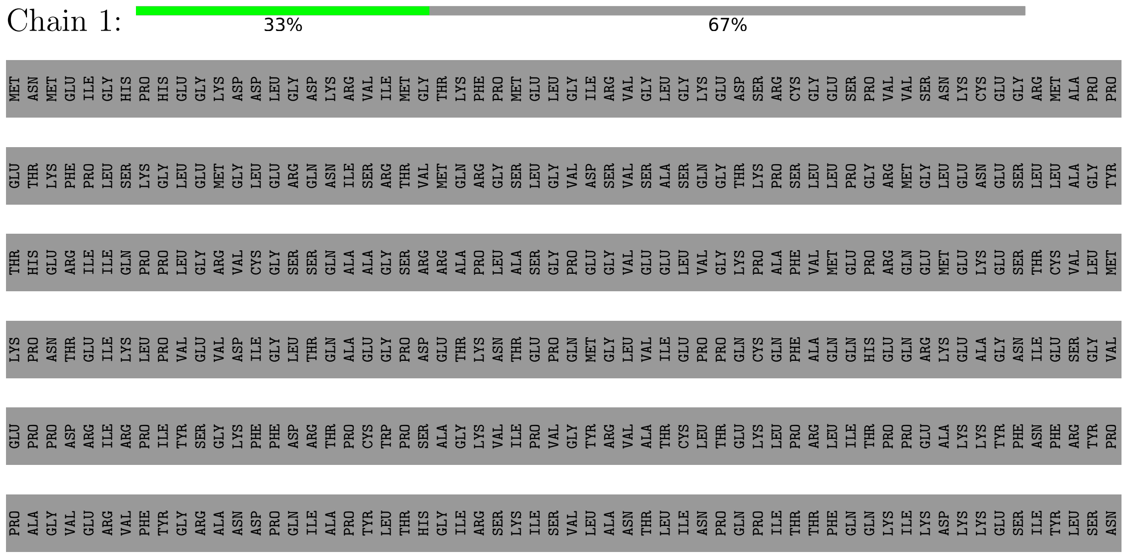
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

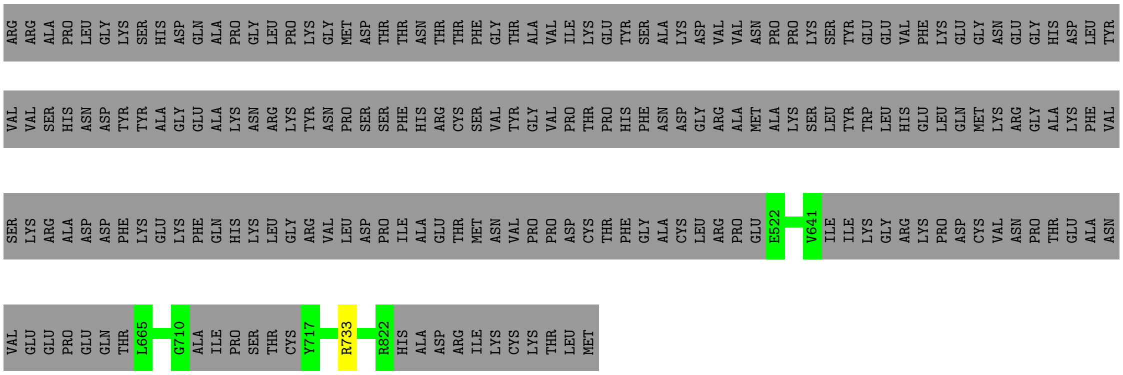
- Molecule 1: Protein CFAP95

- Molecule 1: Protein CFAP95



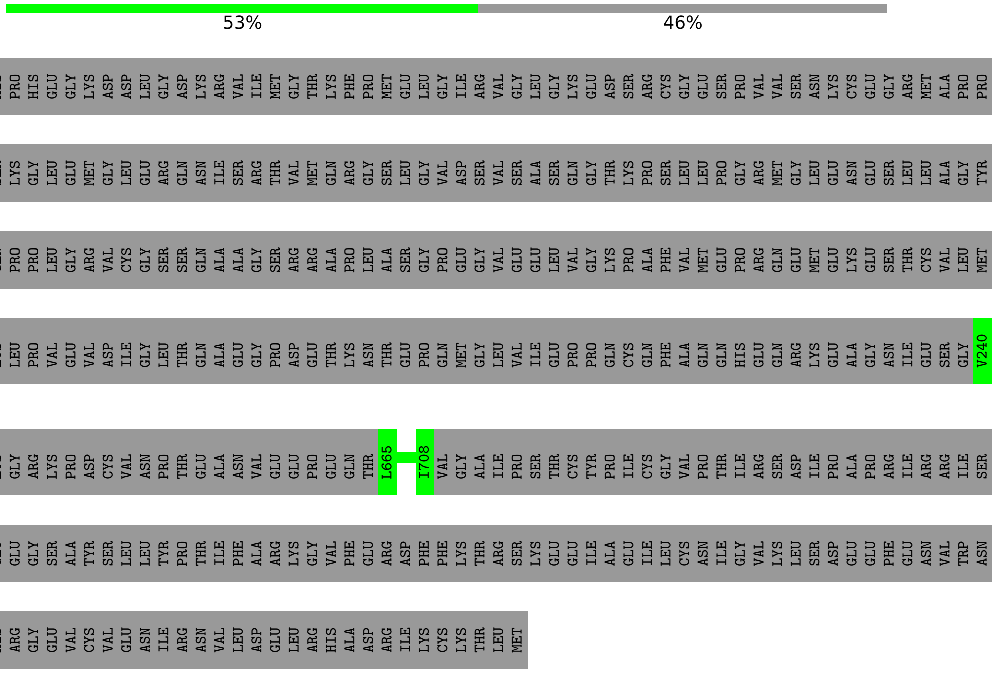
- Molecule 2: EF-hand domain-containing family member B





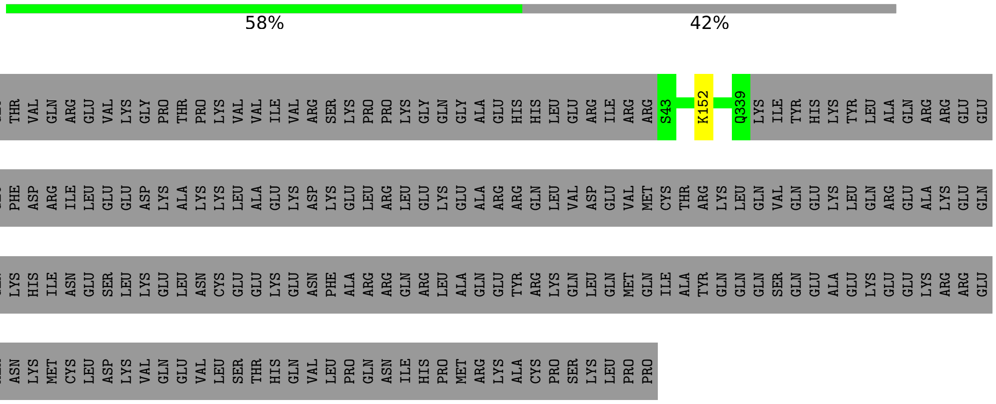
- Molecule 2: EF-hand domain-containing family member B

Chain 2:

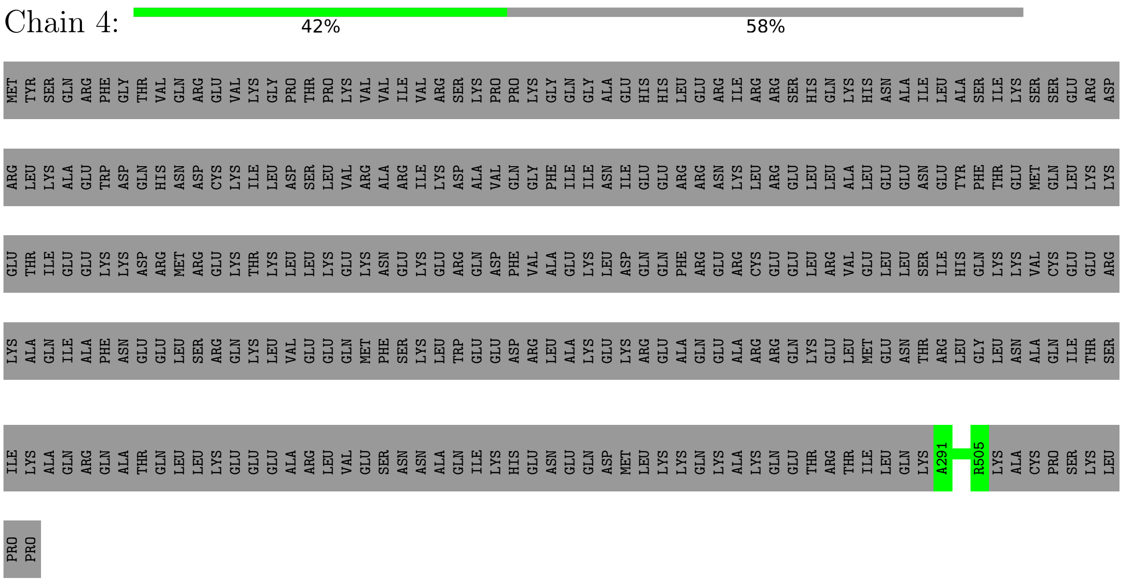


- Molecule 3: Cilia- and flagella-associated protein 53

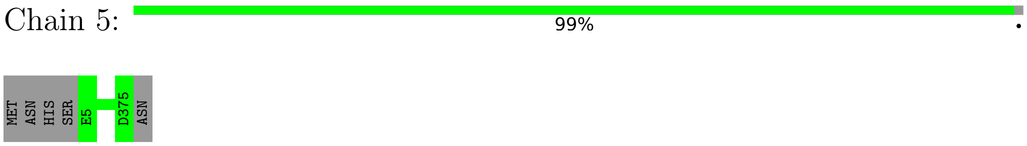
Chain 3:



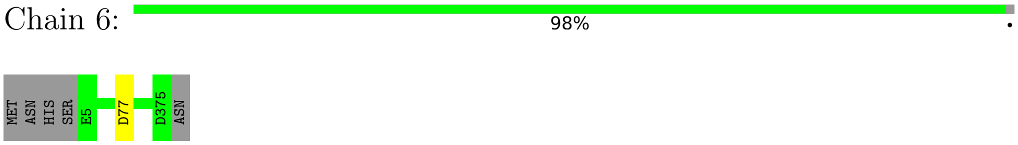
- Molecule 3: Cilia- and flagella-associated protein 53



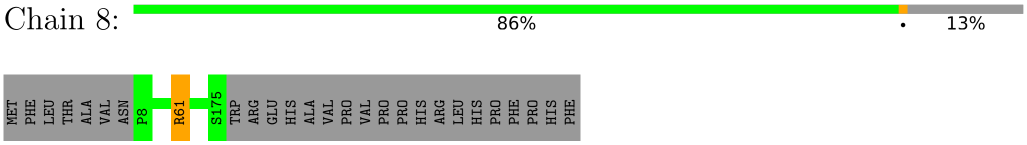
- Molecule 4: Nucleoside diphosphate kinase 7



- Molecule 4: Nucleoside diphosphate kinase 7

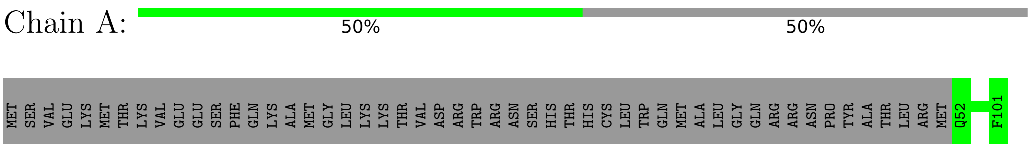


- Molecule 5: Protein CFAP107

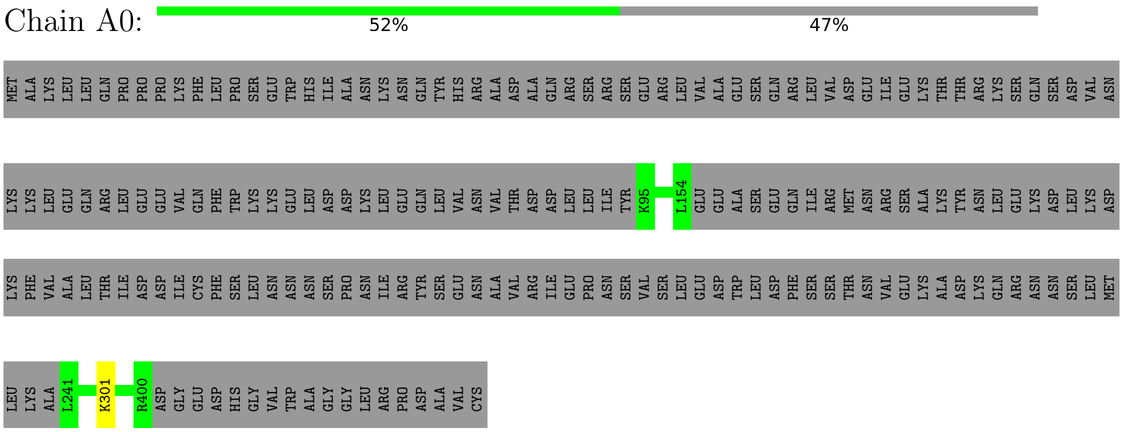


- Molecule 5: Protein CFAP107

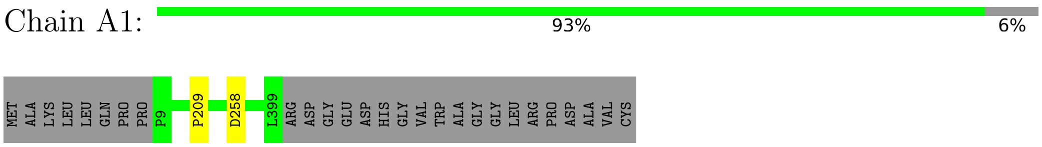
- Molecule 6: Protein CFAP141



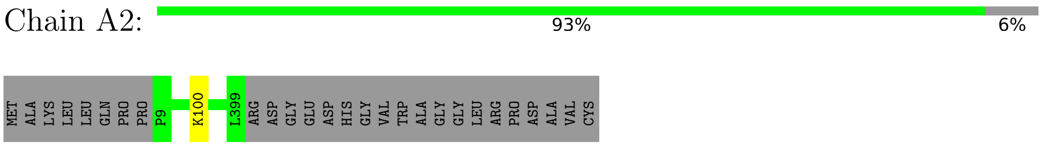
- Molecule 7: Tektin-1



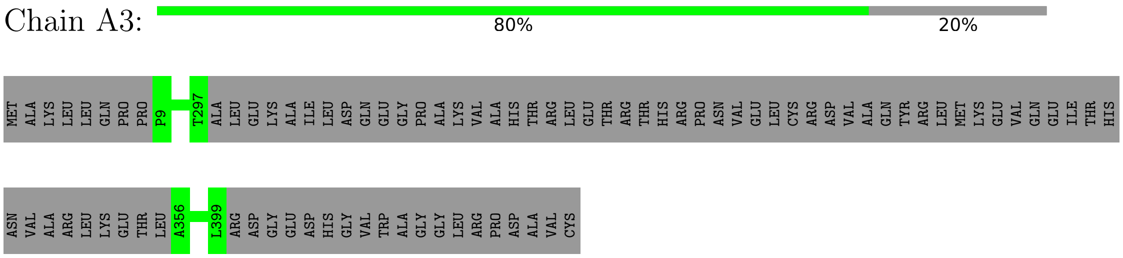
- Molecule 7: Tektin-1



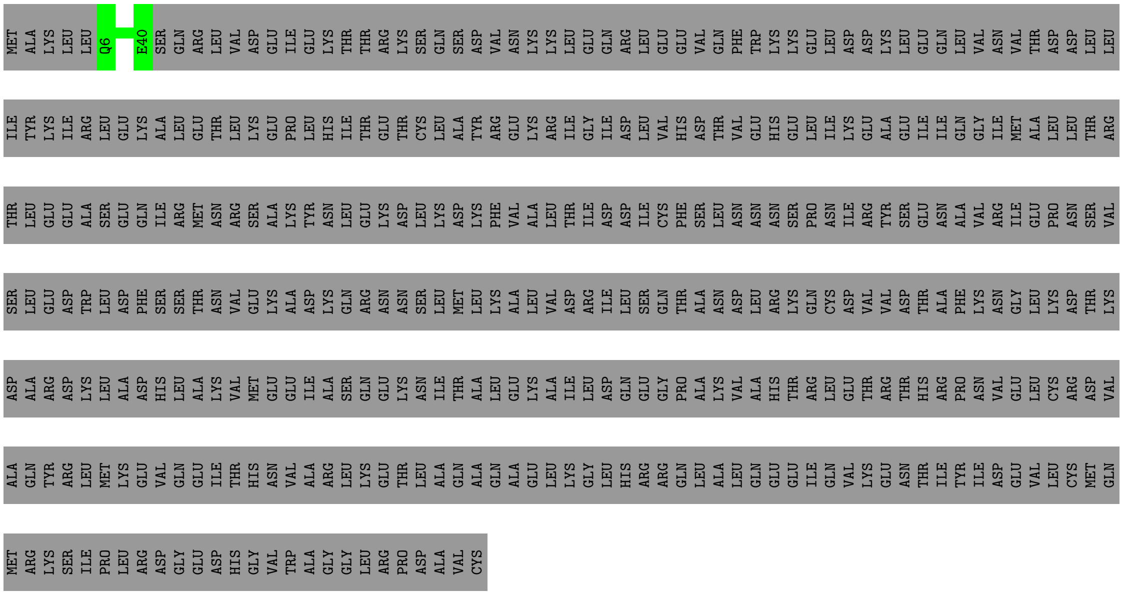
- Molecule 7: Tektin-1



- Molecule 7: Tektin-1

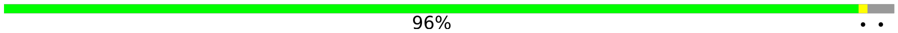


- Molecule 7: Tektin-1



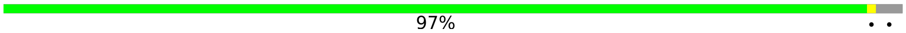
- Molecule 8: Tubulin alpha-1A chain

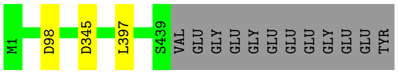
Chain AA:



- Molecule 8: Tubulin alpha-1A chain

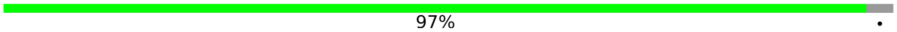
Chain AC:

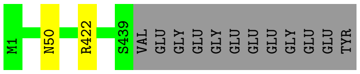




- Molecule 8: Tubulin alpha-1A chain

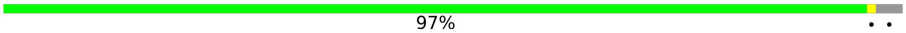
Chain AE:

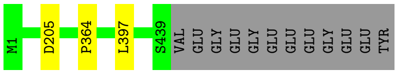




- Molecule 8: Tubulin alpha-1A chain

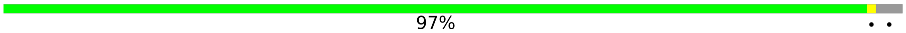
Chain AG:





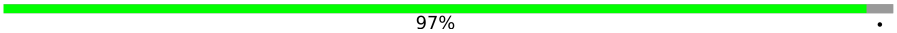
- Molecule 8: Tubulin alpha-1A chain

Chain AI:



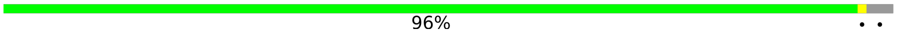
- Molecule 8: Tubulin alpha-1A chain

Chain AK:



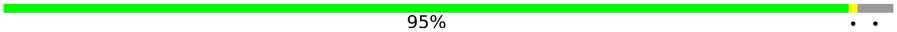
- Molecule 8: Tubulin alpha-1A chain

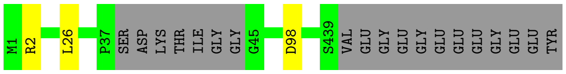
Chain AM:



- Molecule 8: Tubulin alpha-1A chain

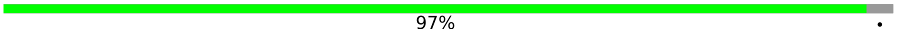
Chain BA:

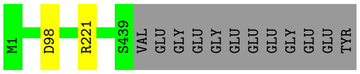




- Molecule 8: Tubulin alpha-1A chain

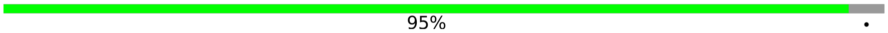
Chain BC:

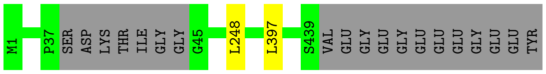




- Molecule 8: Tubulin alpha-1A chain

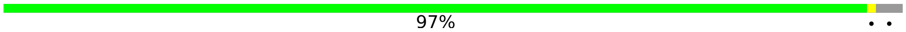
Chain BE:

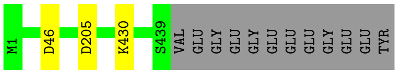




- Molecule 8: Tubulin alpha-1A chain

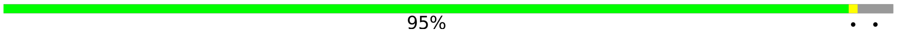
Chain BG:

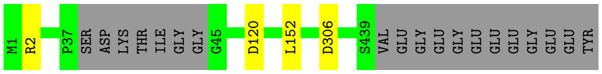




- Molecule 8: Tubulin alpha-1A chain

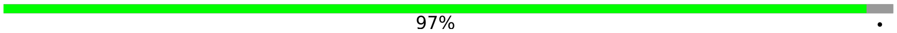
Chain BI:





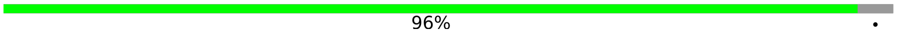
- Molecule 8: Tubulin alpha-1A chain

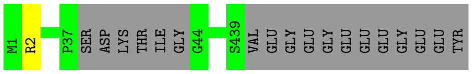
Chain BK:



- Molecule 8: Tubulin alpha-1A chain

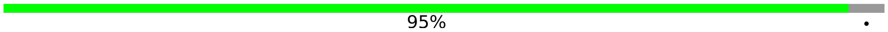
Chain BM:

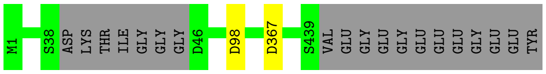




- Molecule 8: Tubulin alpha-1A chain

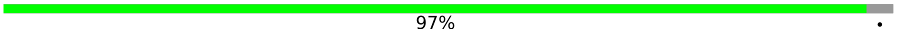
Chain CA:





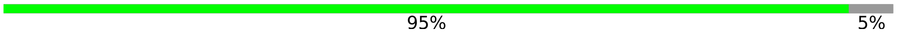
- Molecule 8: Tubulin alpha-1A chain

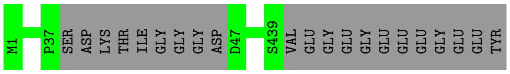
Chain CC:



- Molecule 8: Tubulin alpha-1A chain

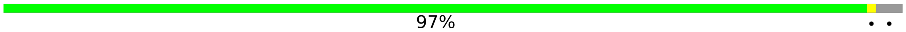
Chain CE:





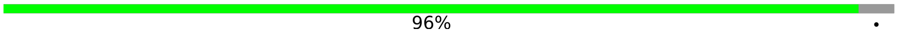
- Molecule 8: Tubulin alpha-1A chain

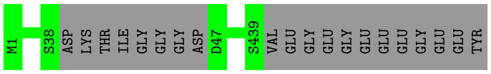
Chain CG:



- Molecule 8: Tubulin alpha-1A chain

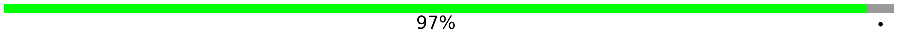
Chain CI:





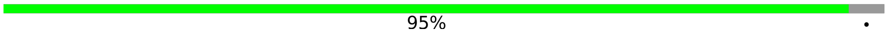
- Molecule 8: Tubulin alpha-1A chain

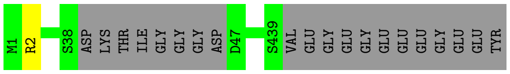
Chain CK:



- Molecule 8: Tubulin alpha-1A chain

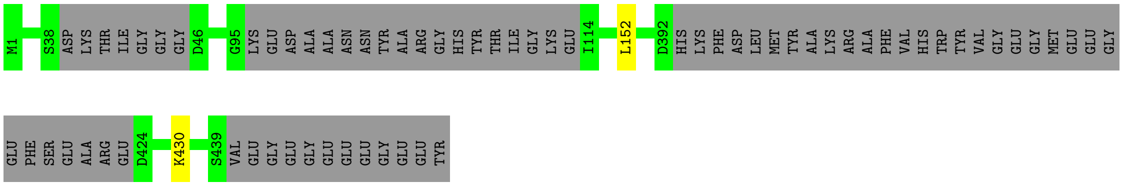
Chain CM:





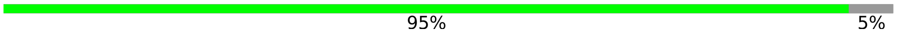
- Molecule 8: Tubulin alpha-1A chain

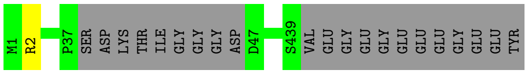
Chain DA:



- Molecule 8: Tubulin alpha-1A chain

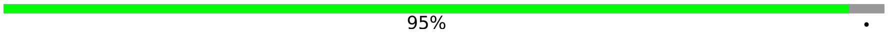
Chain DC:

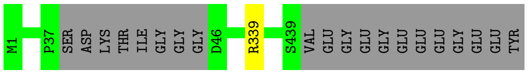




- Molecule 8: Tubulin alpha-1A chain

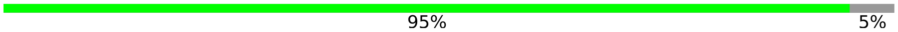
Chain DE:

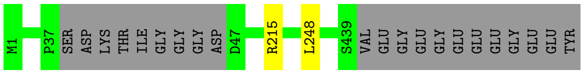




- Molecule 8: Tubulin alpha-1A chain

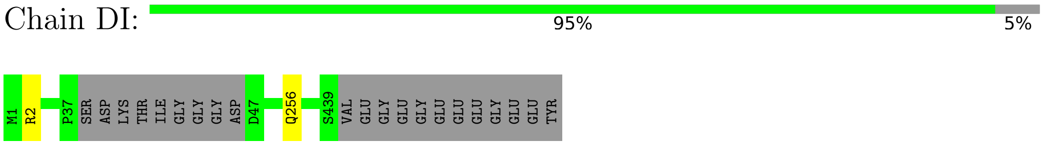
Chain DG:





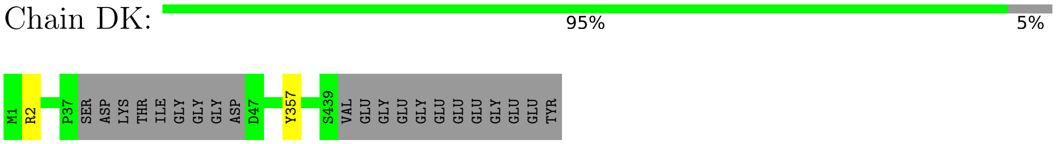
- Molecule 8: Tubulin alpha-1A chain

Chain DI:



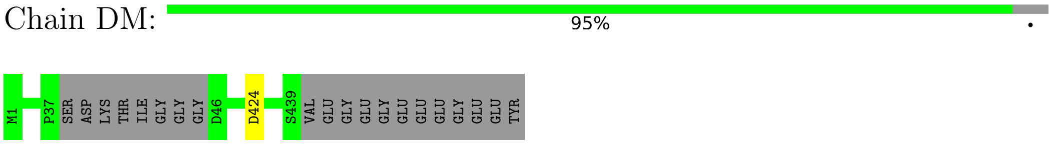
- Molecule 8: Tubulin alpha-1A chain

Chain DK:



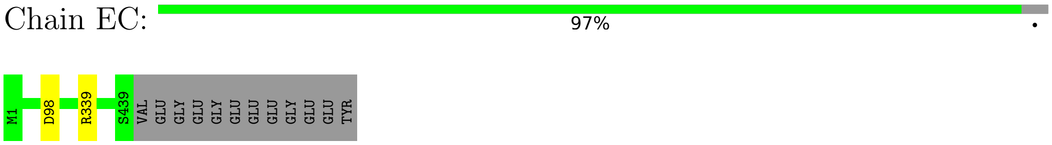
- Molecule 8: Tubulin alpha-1A chain

Chain DM:



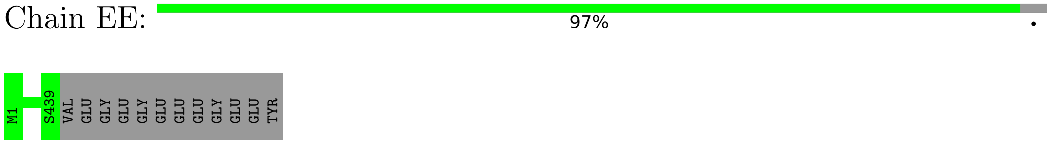
- Molecule 8: Tubulin alpha-1A chain

Chain EC:



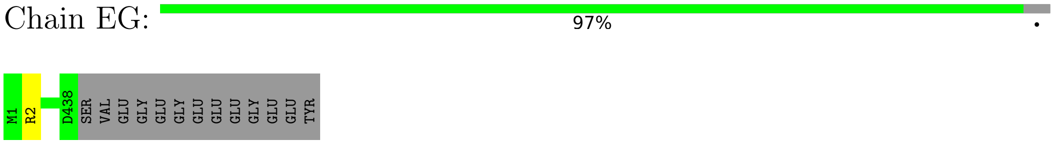
- Molecule 8: Tubulin alpha-1A chain

Chain EE:



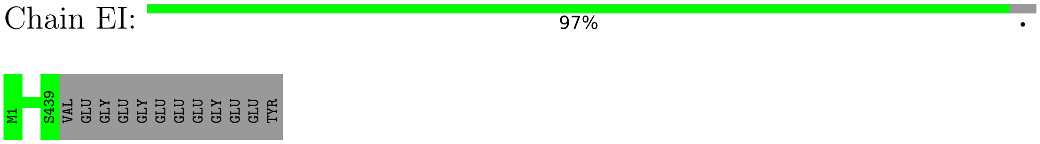
- Molecule 8: Tubulin alpha-1A chain

Chain EG:



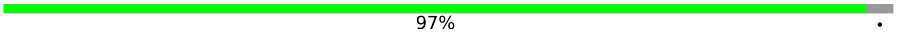
- Molecule 8: Tubulin alpha-1A chain

Chain EI:



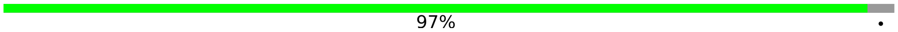
- Molecule 8: Tubulin alpha-1A chain

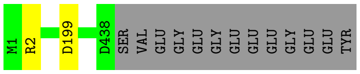
Chain EK:



- Molecule 8: Tubulin alpha-1A chain

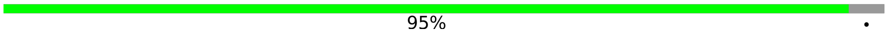
Chain EM:

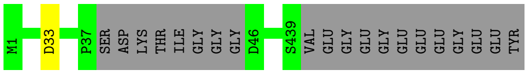




- Molecule 8: Tubulin alpha-1A chain

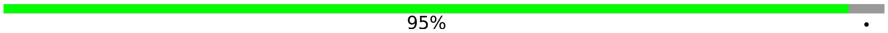
Chain FC:

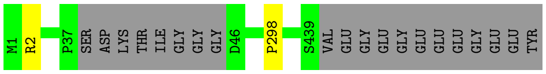




- Molecule 8: Tubulin alpha-1A chain

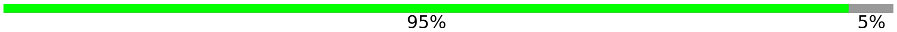
Chain FE:

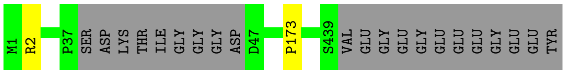




- Molecule 8: Tubulin alpha-1A chain

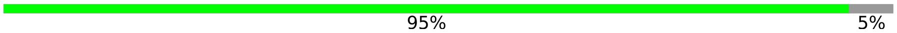
Chain FG:

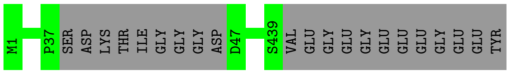




- Molecule 8: Tubulin alpha-1A chain

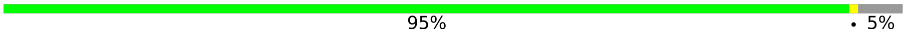
Chain FI:

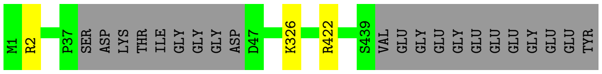




- Molecule 8: Tubulin alpha-1A chain

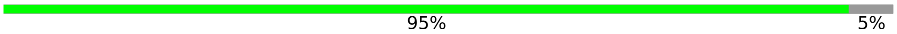
Chain FK:

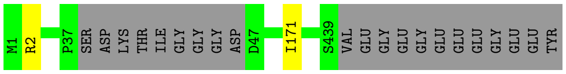




- Molecule 8: Tubulin alpha-1A chain

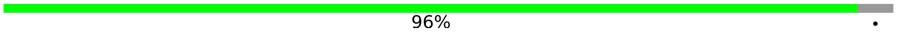
Chain FM:

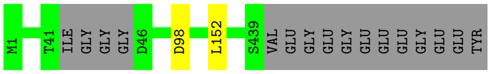




- Molecule 8: Tubulin alpha-1A chain

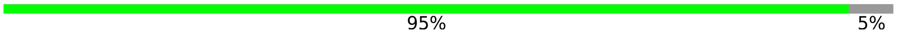
Chain GC:

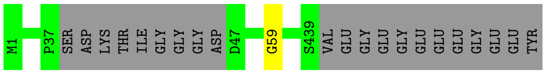




- Molecule 8: Tubulin alpha-1A chain

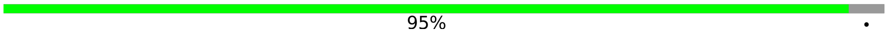
Chain GE:

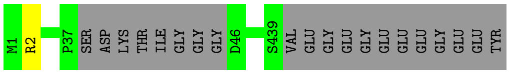




- Molecule 8: Tubulin alpha-1A chain

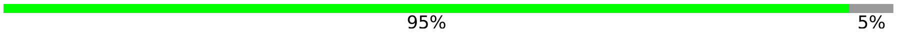
Chain GG:

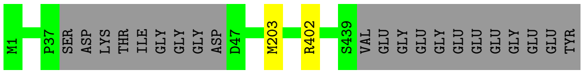




- Molecule 8: Tubulin alpha-1A chain

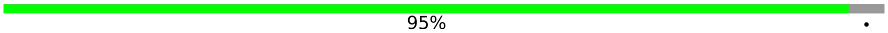
Chain GI:

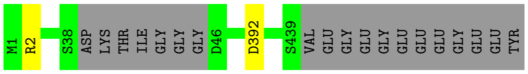




- Molecule 8: Tubulin alpha-1A chain

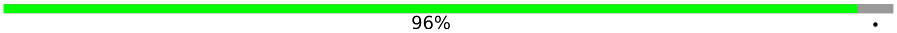
Chain GK:

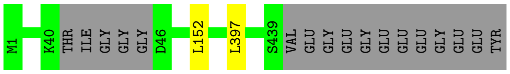




- Molecule 8: Tubulin alpha-1A chain

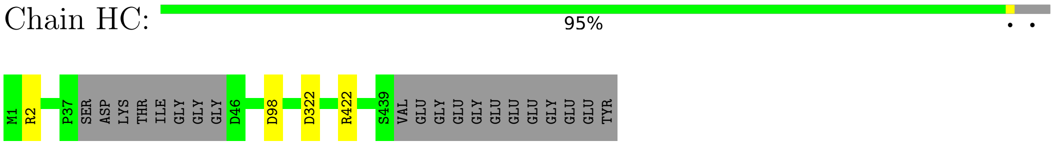
Chain GM:





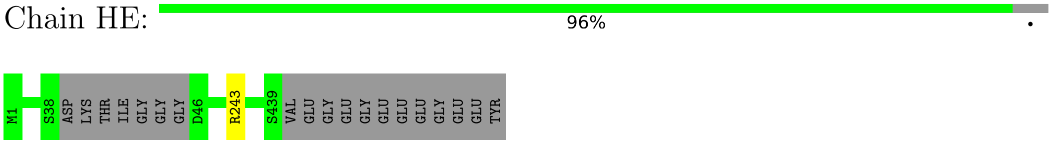
- Molecule 8: Tubulin alpha-1A chain

Chain HC:



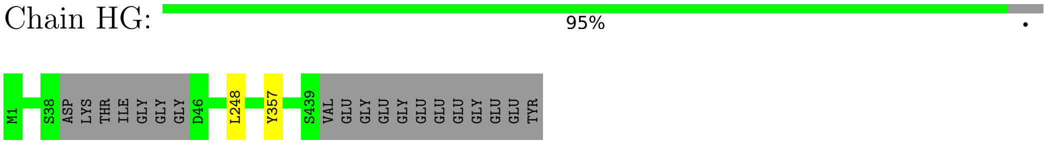
- Molecule 8: Tubulin alpha-1A chain

Chain HE:



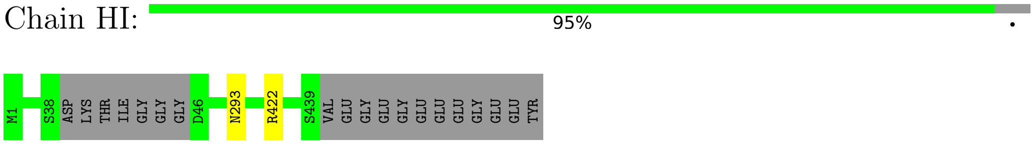
- Molecule 8: Tubulin alpha-1A chain

Chain HG:



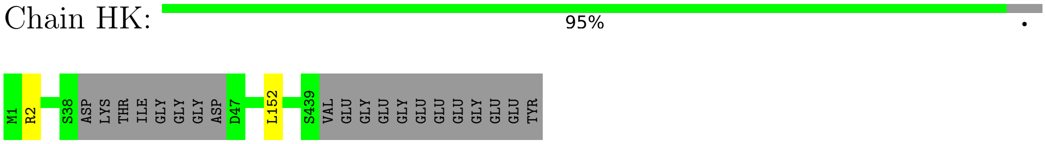
- Molecule 8: Tubulin alpha-1A chain

Chain HI:



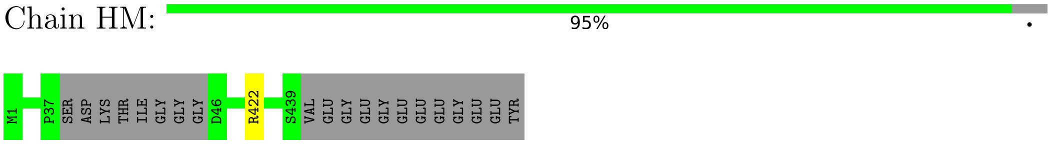
- Molecule 8: Tubulin alpha-1A chain

Chain HK:



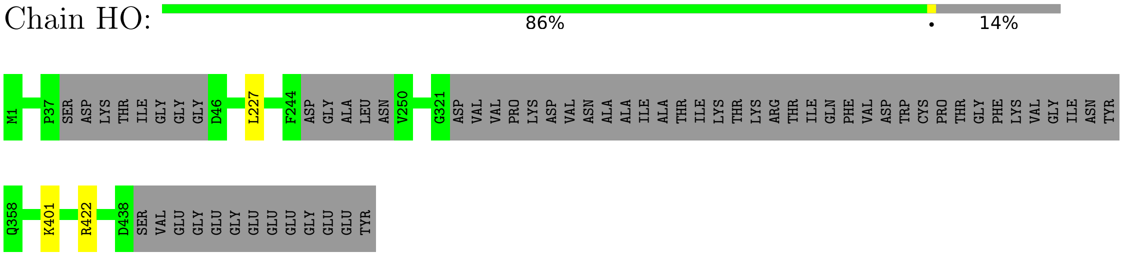
- Molecule 8: Tubulin alpha-1A chain

Chain HM:



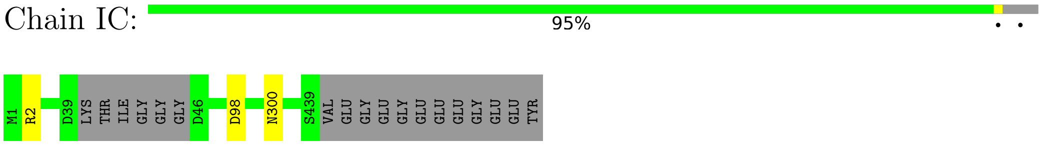
- Molecule 8: Tubulin alpha-1A chain

Chain HO:



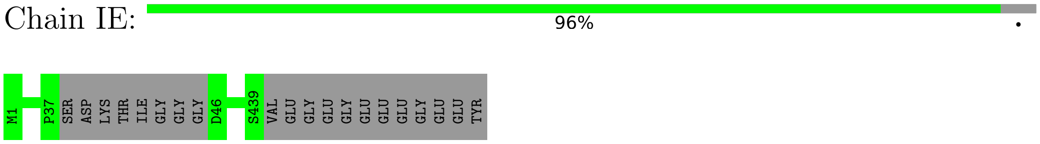
- Molecule 8: Tubulin alpha-1A chain

Chain IC:



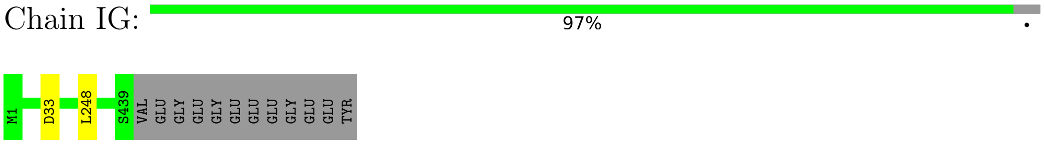
- Molecule 8: Tubulin alpha-1A chain

Chain IE:



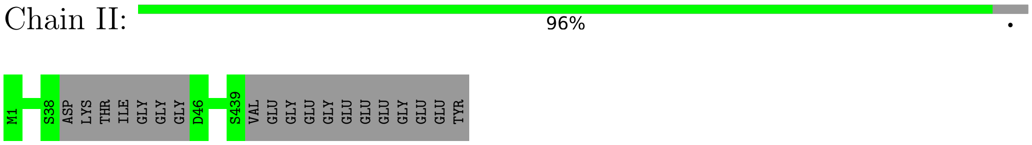
- Molecule 8: Tubulin alpha-1A chain

Chain IG:



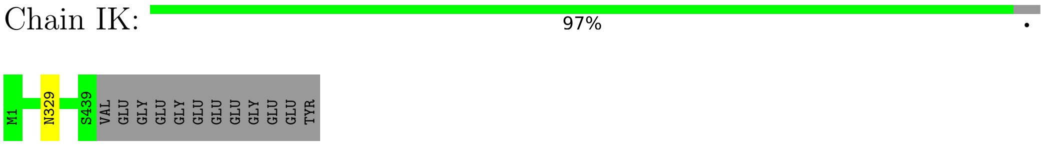
- Molecule 8: Tubulin alpha-1A chain

Chain II:



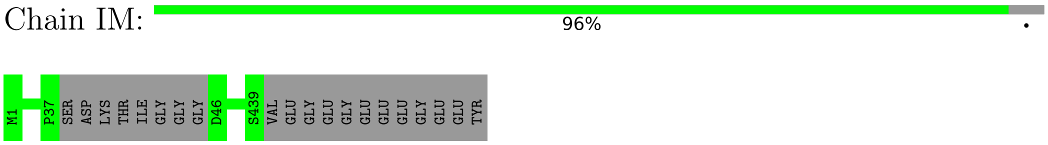
- Molecule 8: Tubulin alpha-1A chain

Chain IK:



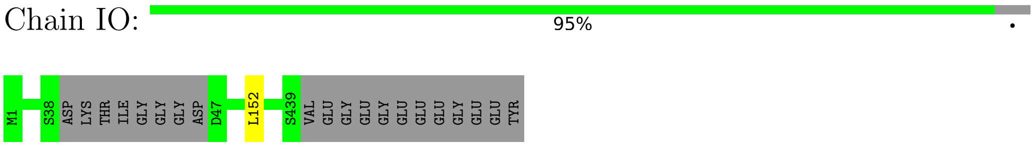
- Molecule 8: Tubulin alpha-1A chain

Chain IM:



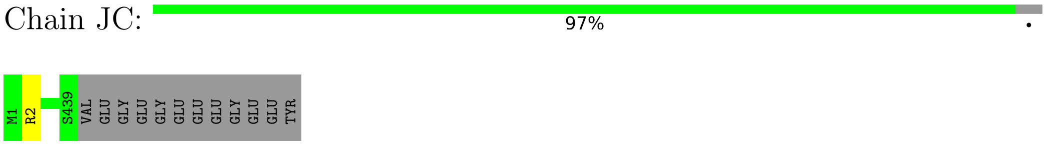
- Molecule 8: Tubulin alpha-1A chain

Chain IO:



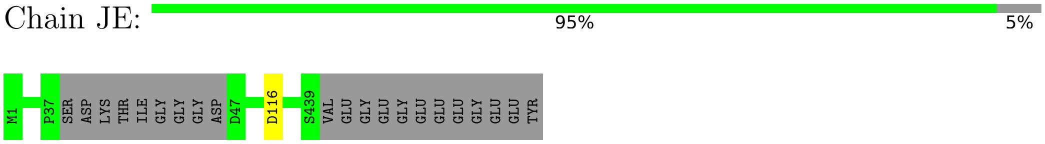
- Molecule 8: Tubulin alpha-1A chain

Chain JC:



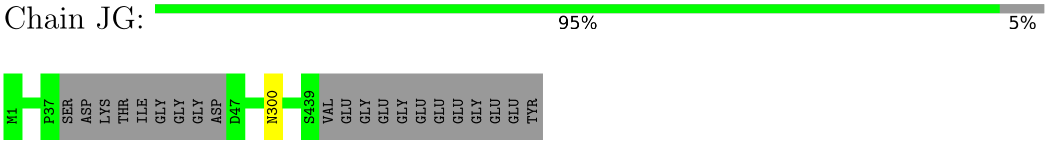
- Molecule 8: Tubulin alpha-1A chain

Chain JE:



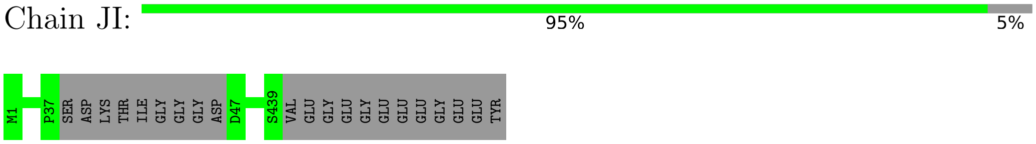
- Molecule 8: Tubulin alpha-1A chain

Chain JG:



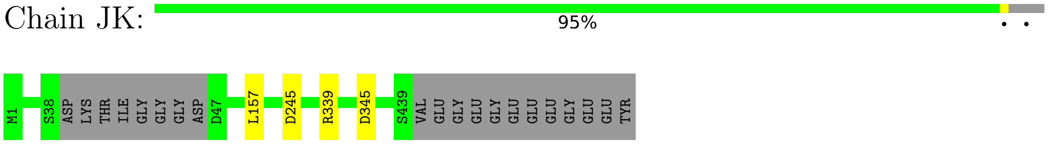
- Molecule 8: Tubulin alpha-1A chain

Chain JI:



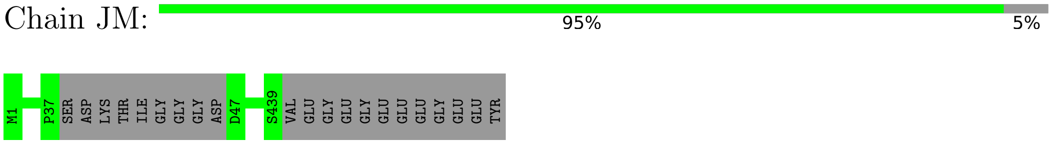
- Molecule 8: Tubulin alpha-1A chain

Chain JK:



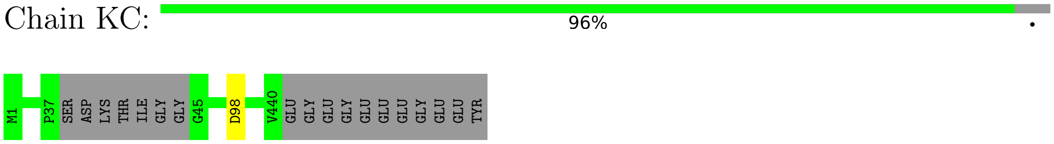
- Molecule 8: Tubulin alpha-1A chain

Chain JM:



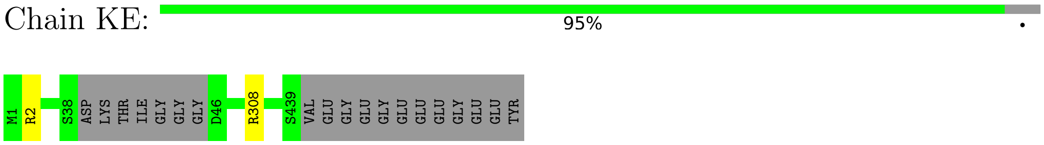
- Molecule 8: Tubulin alpha-1A chain

Chain KC:



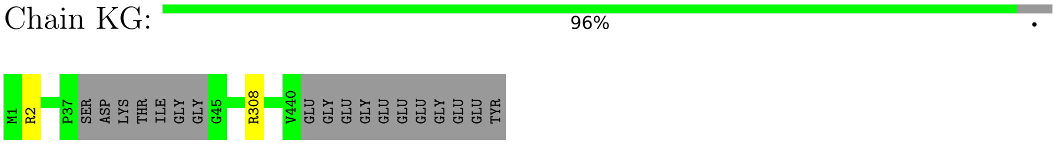
- Molecule 8: Tubulin alpha-1A chain

Chain KE:



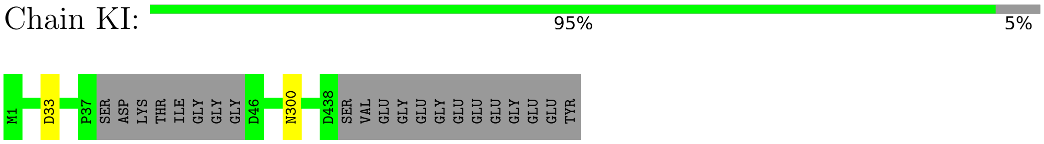
- Molecule 8: Tubulin alpha-1A chain

Chain KG:



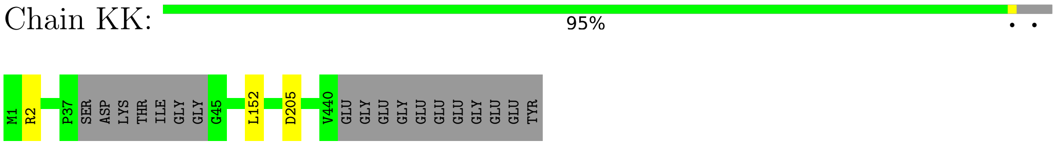
- Molecule 8: Tubulin alpha-1A chain

Chain KI:



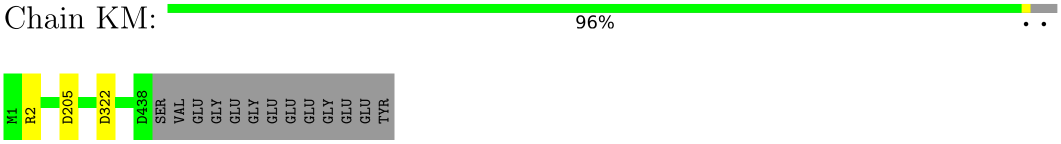
- Molecule 8: Tubulin alpha-1A chain

Chain KK:



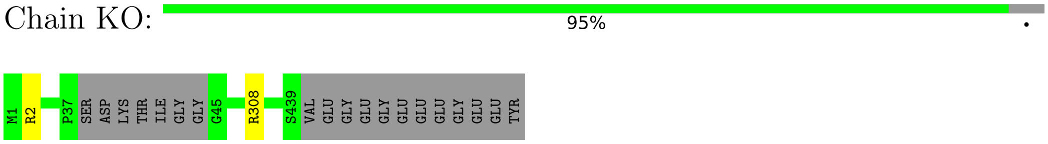
- Molecule 8: Tubulin alpha-1A chain

Chain KM:



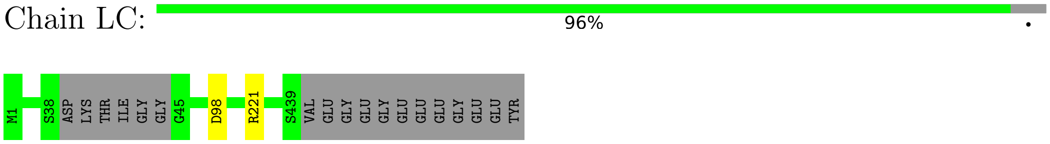
- Molecule 8: Tubulin alpha-1A chain

Chain KO:



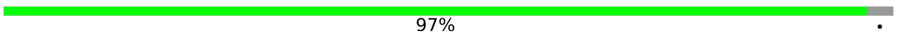
- Molecule 8: Tubulin alpha-1A chain

Chain LC:



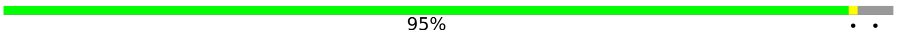
- Molecule 8: Tubulin alpha-1A chain

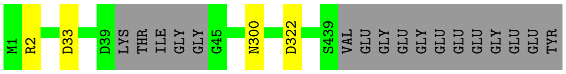
Chain LE:



- Molecule 8: Tubulin alpha-1A chain

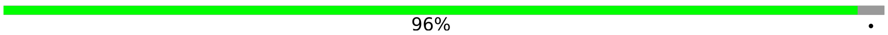
Chain LG:

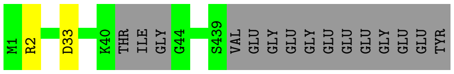




- Molecule 8: Tubulin alpha-1A chain

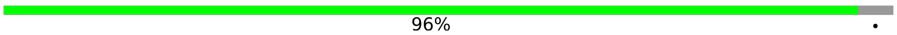
Chain LI:

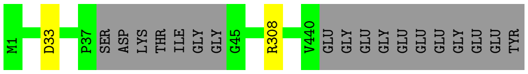




- Molecule 8: Tubulin alpha-1A chain

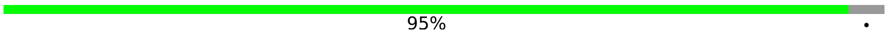
Chain LK:

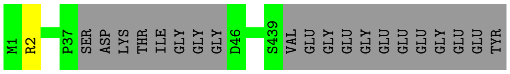




- Molecule 8: Tubulin alpha-1A chain

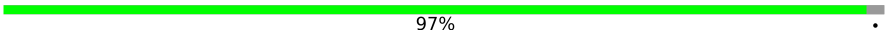
Chain LM:





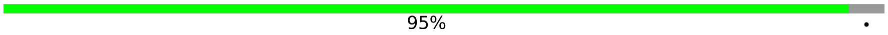
- Molecule 8: Tubulin alpha-1A chain

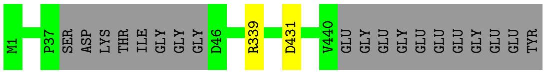
Chain MC:



- Molecule 8: Tubulin alpha-1A chain

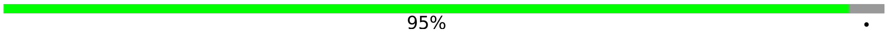
Chain ME:

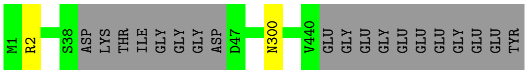




- Molecule 8: Tubulin alpha-1A chain

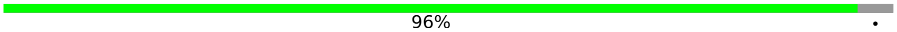
Chain MG:

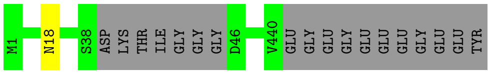




- Molecule 8: Tubulin alpha-1A chain

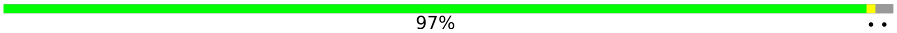
Chain MI:





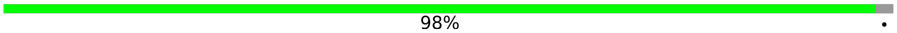
- Molecule 8: Tubulin alpha-1A chain

Chain MK:



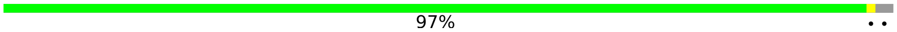
- Molecule 8: Tubulin alpha-1A chain

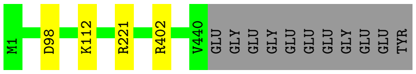
Chain MM:



- Molecule 8: Tubulin alpha-1A chain

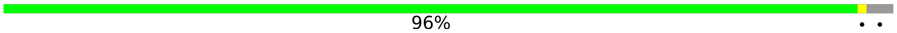
Chain NC:

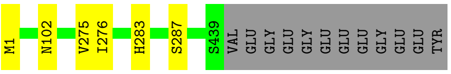




- Molecule 8: Tubulin alpha-1A chain

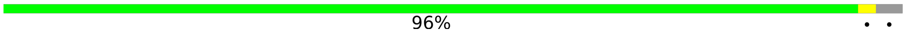
Chain NE:

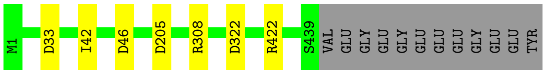




- Molecule 8: Tubulin alpha-1A chain

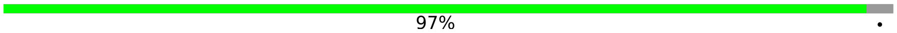
Chain NG:





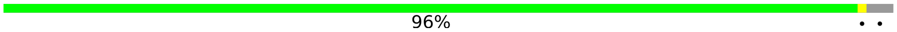
- Molecule 8: Tubulin alpha-1A chain

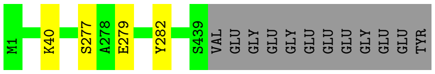
Chain NI:



- Molecule 8: Tubulin alpha-1A chain

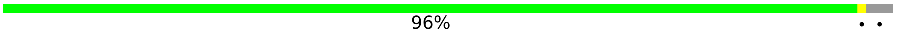
Chain NK:

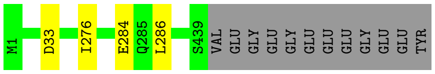




- Molecule 8: Tubulin alpha-1A chain

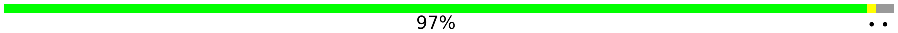
Chain NM:

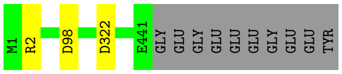




- Molecule 8: Tubulin alpha-1A chain

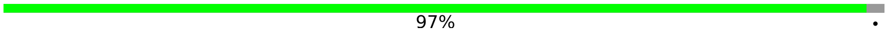
Chain OC:





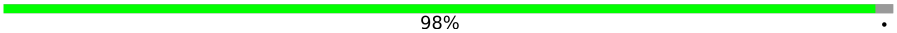
- Molecule 8: Tubulin alpha-1A chain

Chain OE:



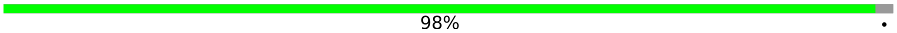
- Molecule 8: Tubulin alpha-1A chain

Chain OG:



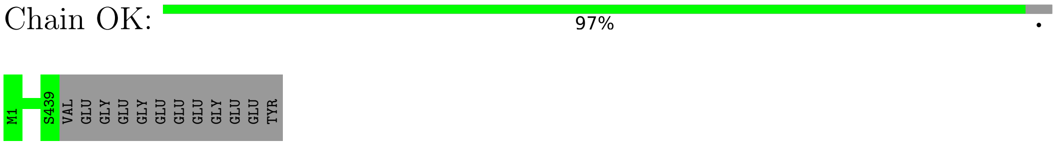
- Molecule 8: Tubulin alpha-1A chain

Chain OI:



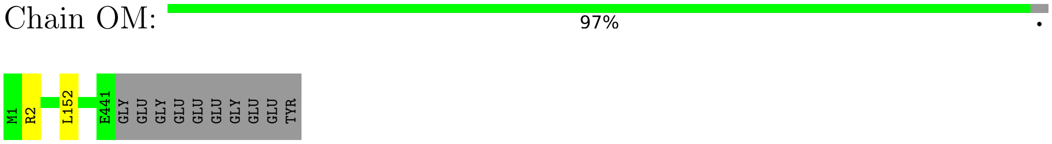
- Molecule 8: Tubulin alpha-1A chain

Chain OK:



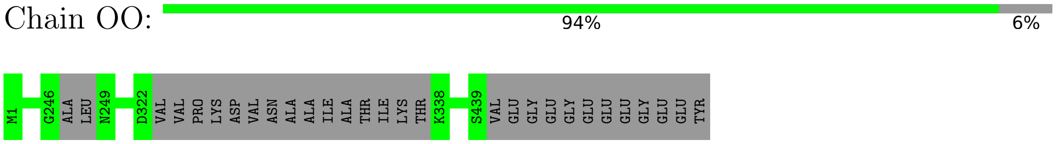
- Molecule 8: Tubulin alpha-1A chain

Chain OM:



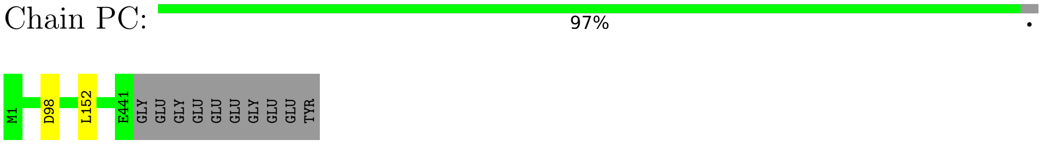
- Molecule 8: Tubulin alpha-1A chain

Chain OO:



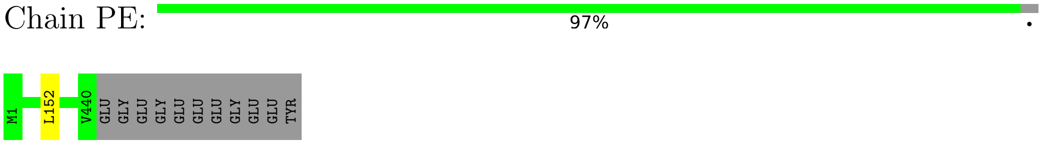
- Molecule 8: Tubulin alpha-1A chain

Chain PC:



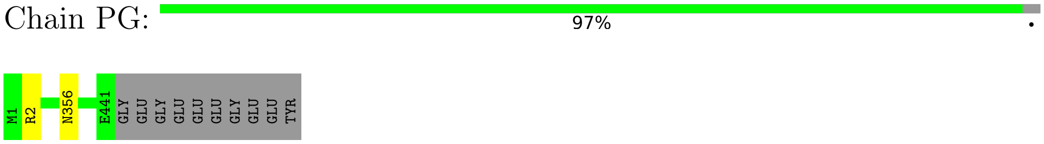
- Molecule 8: Tubulin alpha-1A chain

Chain PE:



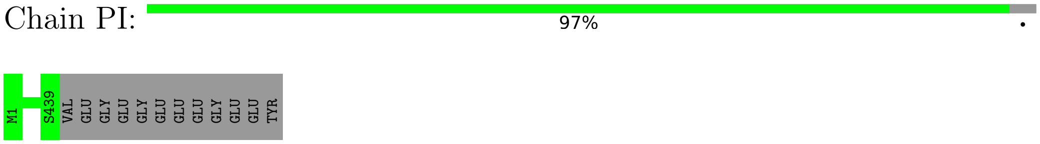
- Molecule 8: Tubulin alpha-1A chain

Chain PG:



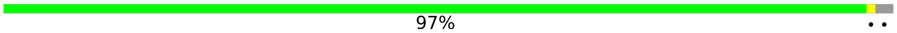
- Molecule 8: Tubulin alpha-1A chain

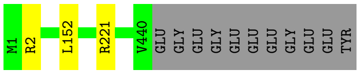
Chain PI:



- Molecule 8: Tubulin alpha-1A chain

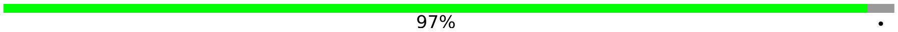
Chain PK:





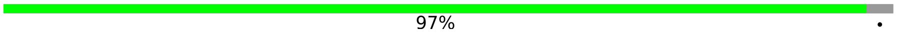
- Molecule 8: Tubulin alpha-1A chain

Chain PM:



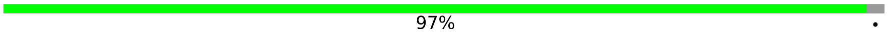
- Molecule 8: Tubulin alpha-1A chain

Chain PO:



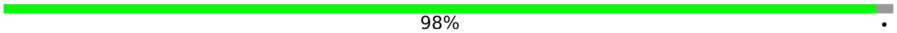
- Molecule 8: Tubulin alpha-1A chain

Chain QC:



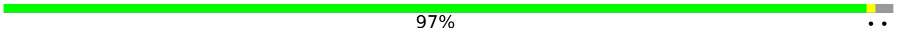
- Molecule 8: Tubulin alpha-1A chain

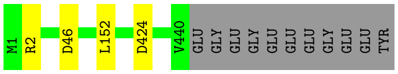
Chain QE:



- Molecule 8: Tubulin alpha-1A chain

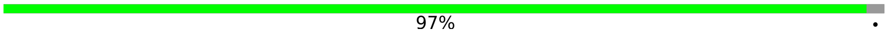
Chain QG:



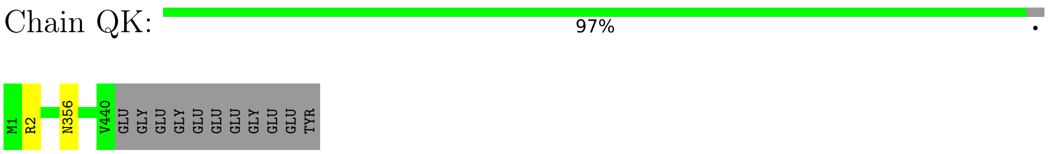


- Molecule 8: Tubulin alpha-1A chain

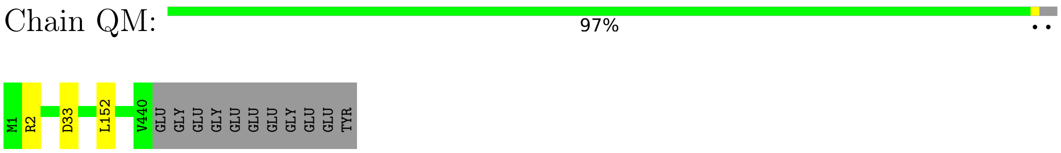
Chain QI:



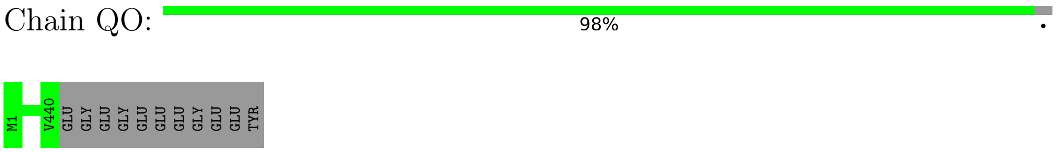
- Molecule 8: Tubulin alpha-1A chain



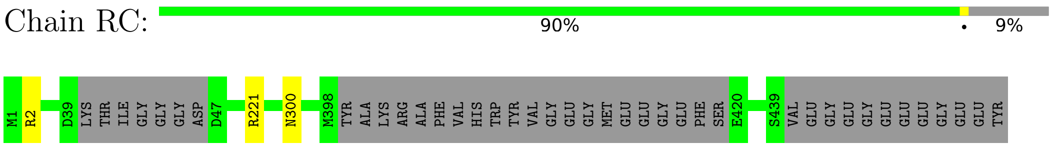
- Molecule 8: Tubulin alpha-1A chain



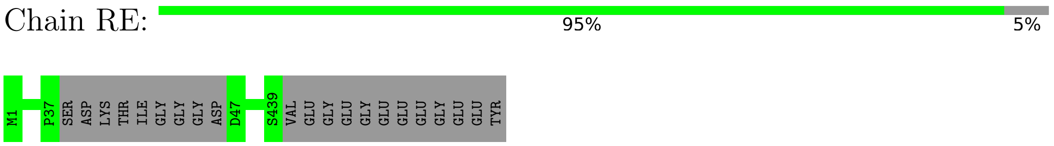
- Molecule 8: Tubulin alpha-1A chain



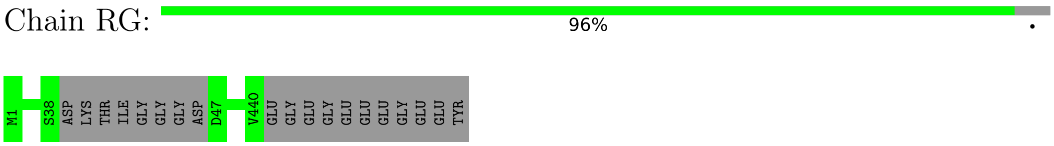
- Molecule 8: Tubulin alpha-1A chain



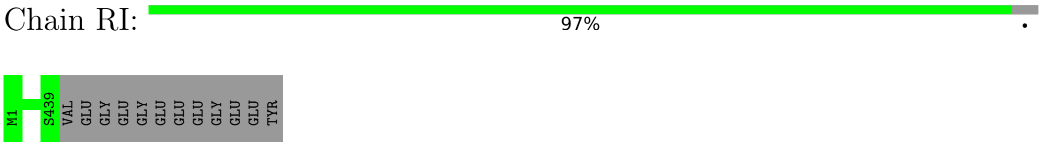
- Molecule 8: Tubulin alpha-1A chain



- Molecule 8: Tubulin alpha-1A chain

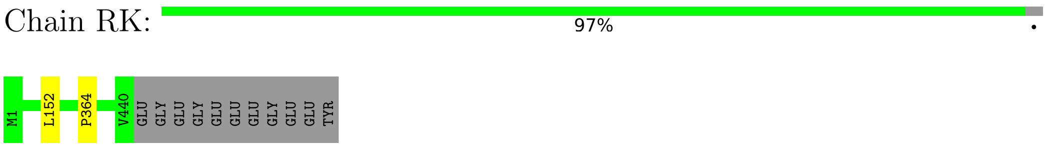


- Molecule 8: Tubulin alpha-1A chain



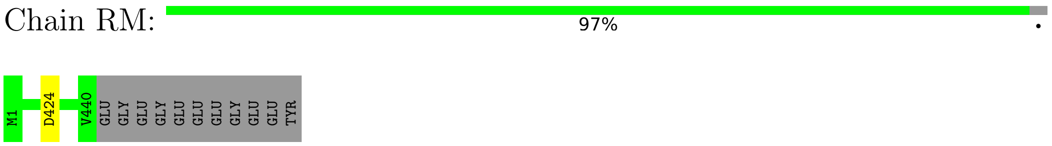
- Molecule 8: Tubulin alpha-1A chain

Chain RK:



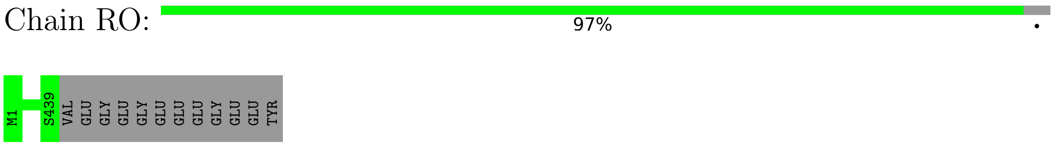
- Molecule 8: Tubulin alpha-1A chain

Chain RM:



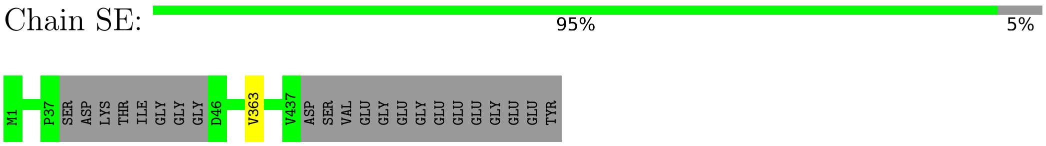
- Molecule 8: Tubulin alpha-1A chain

Chain RO:



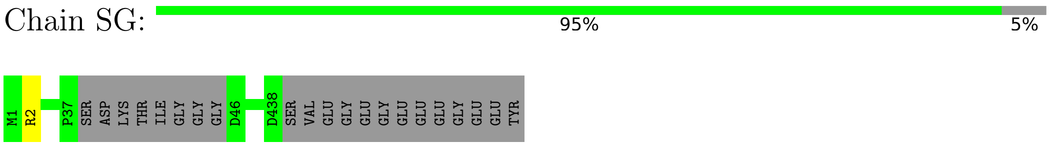
- Molecule 8: Tubulin alpha-1A chain

Chain SE:



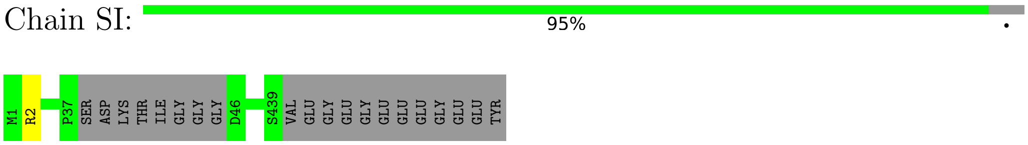
- Molecule 8: Tubulin alpha-1A chain

Chain SG:



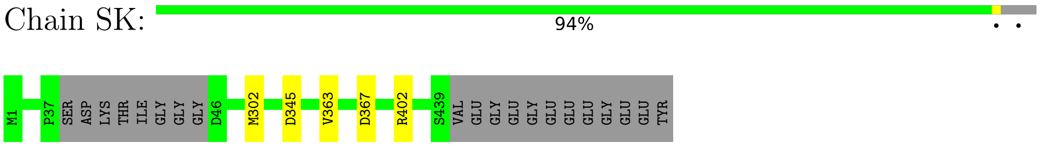
- Molecule 8: Tubulin alpha-1A chain

Chain SI:



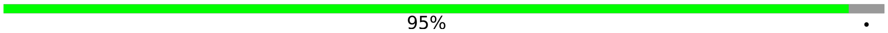
- Molecule 8: Tubulin alpha-1A chain

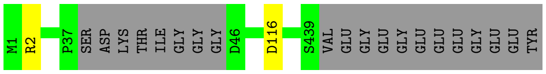
Chain SK:



- Molecule 8: Tubulin alpha-1A chain

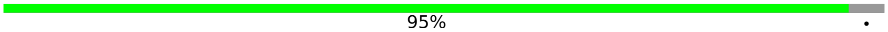
Chain SM:

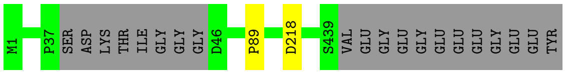




- Molecule 8: Tubulin alpha-1A chain

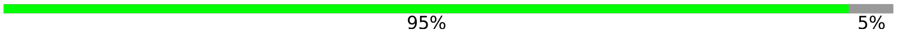
Chain SO:

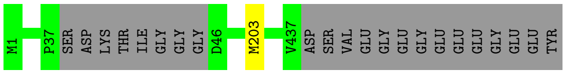




- Molecule 8: Tubulin alpha-1A chain

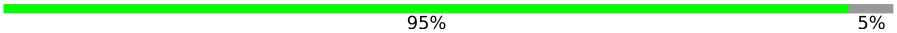
Chain TE:

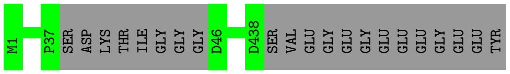




- Molecule 8: Tubulin alpha-1A chain

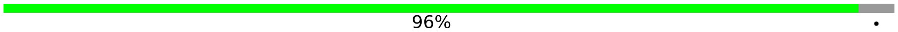
Chain TG:

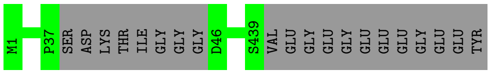




- Molecule 8: Tubulin alpha-1A chain

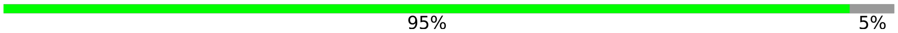
Chain TI:

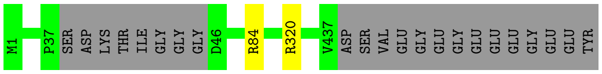




- Molecule 8: Tubulin alpha-1A chain

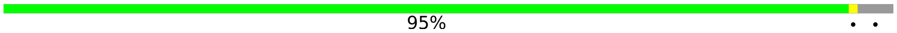
Chain TK:

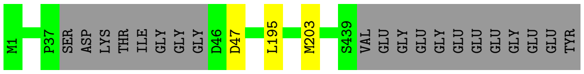




- Molecule 8: Tubulin alpha-1A chain

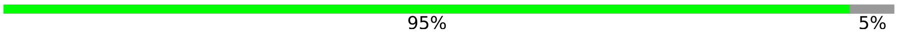
Chain TM:

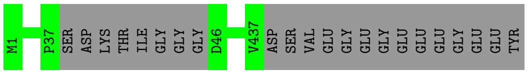




- Molecule 8: Tubulin alpha-1A chain

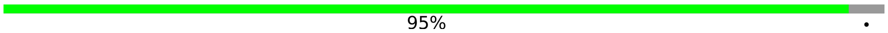
Chain TO:

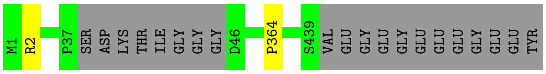




- Molecule 8: Tubulin alpha-1A chain

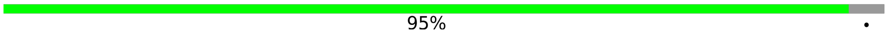
Chain UE:

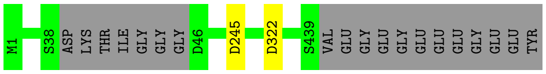




- Molecule 8: Tubulin alpha-1A chain

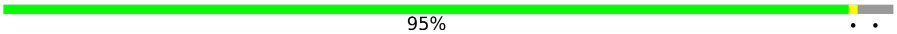
Chain UG:

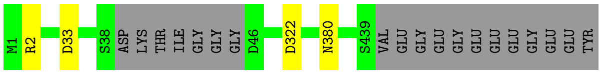




- Molecule 8: Tubulin alpha-1A chain

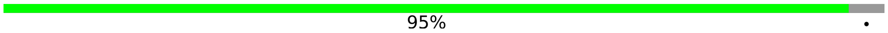
Chain UI:

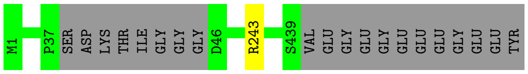




- Molecule 8: Tubulin alpha-1A chain

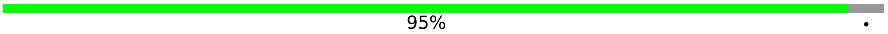
Chain UK:

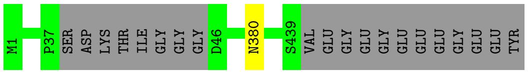




- Molecule 8: Tubulin alpha-1A chain

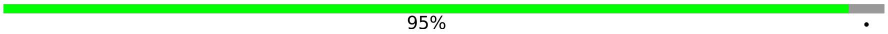
Chain UM:

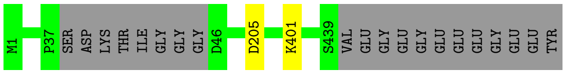




- Molecule 8: Tubulin alpha-1A chain

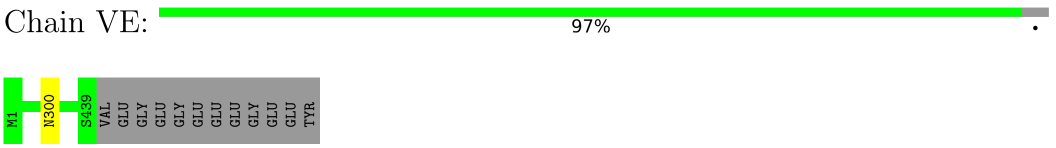
Chain UO:





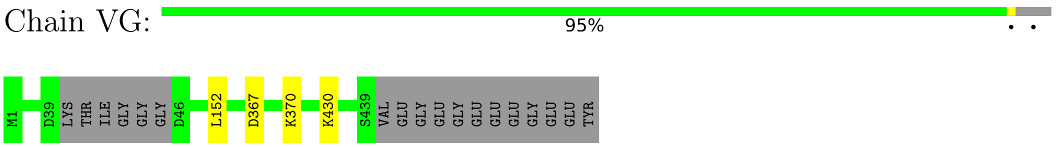
- Molecule 8: Tubulin alpha-1A chain

Chain VE:



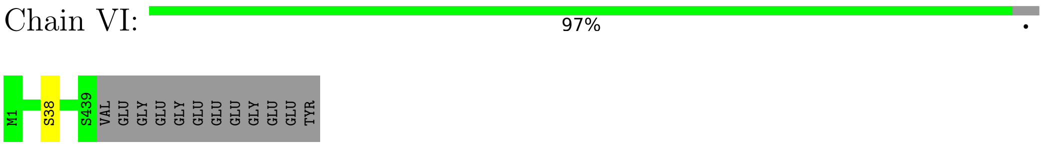
- Molecule 8: Tubulin alpha-1A chain

Chain VG:



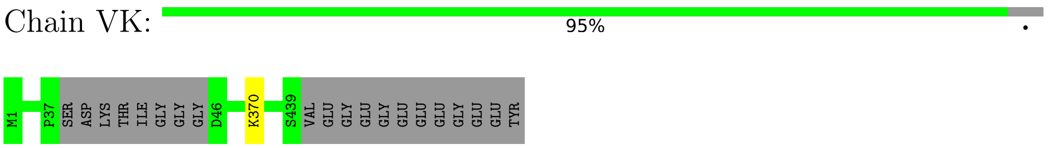
- Molecule 8: Tubulin alpha-1A chain

Chain VI:



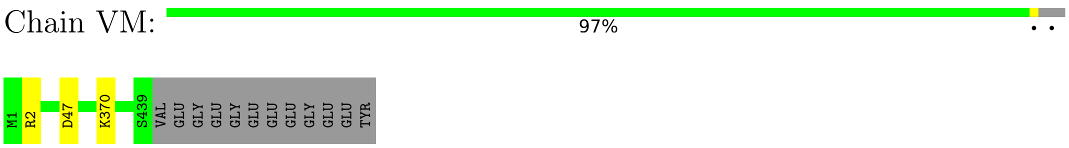
- Molecule 8: Tubulin alpha-1A chain

Chain VK:



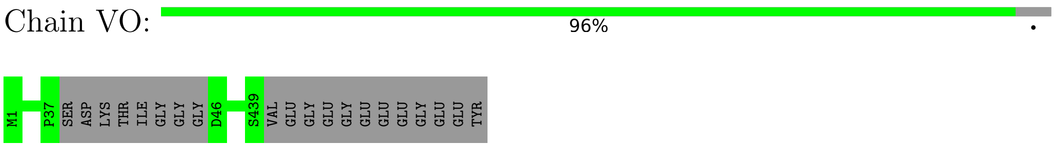
- Molecule 8: Tubulin alpha-1A chain

Chain VM:



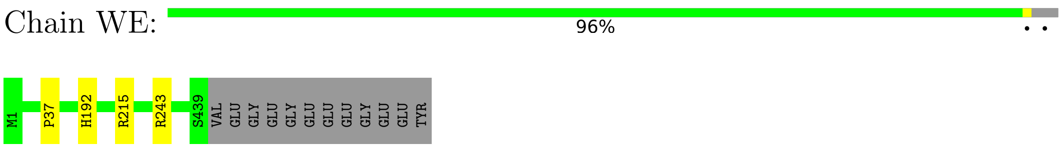
- Molecule 8: Tubulin alpha-1A chain

Chain VO:



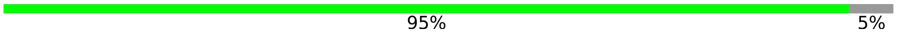
- Molecule 8: Tubulin alpha-1A chain

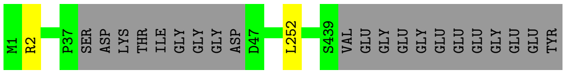
Chain WE:



- Molecule 8: Tubulin alpha-1A chain

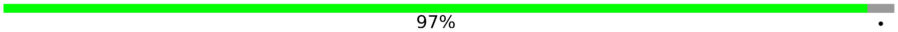
Chain WG:





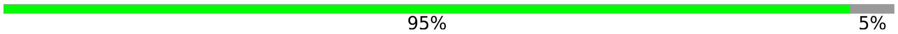
- Molecule 8: Tubulin alpha-1A chain

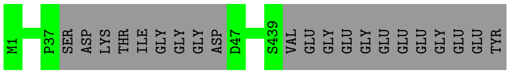
Chain WI:



- Molecule 8: Tubulin alpha-1A chain

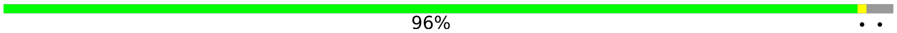
Chain WK:





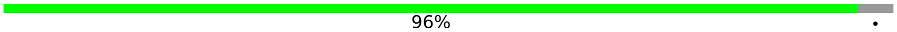
- Molecule 8: Tubulin alpha-1A chain

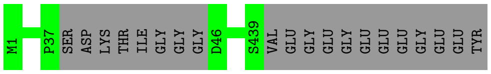
Chain WM:



- Molecule 8: Tubulin alpha-1A chain

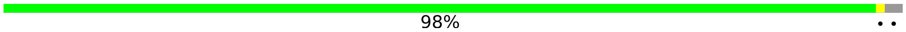
Chain WO:

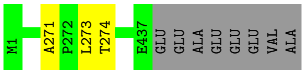




- Molecule 9: Tubulin beta-4B chain

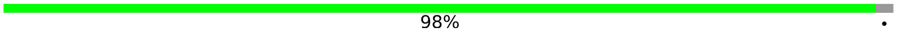
Chain AB:

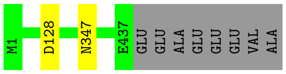




- Molecule 9: Tubulin beta-4B chain

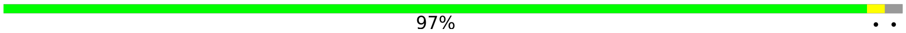
Chain AD:

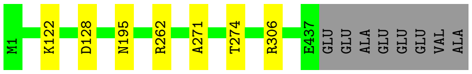




- Molecule 9: Tubulin beta-4B chain

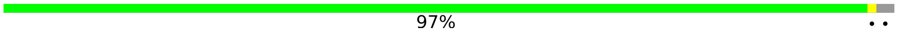
Chain AF:

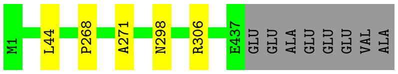




- Molecule 9: Tubulin beta-4B chain

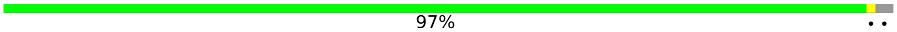
Chain AH:





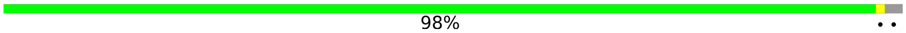
- Molecule 9: Tubulin beta-4B chain

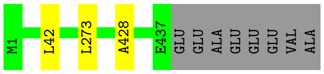
Chain AJ:



- Molecule 9: Tubulin beta-4B chain

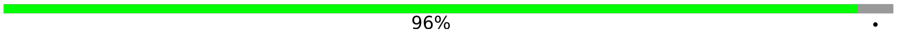
Chain AL:





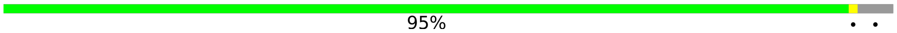
- Molecule 9: Tubulin beta-4B chain

Chain BB:



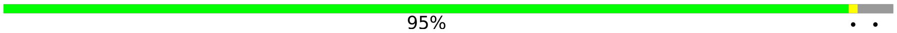
- Molecule 9: Tubulin beta-4B chain

Chain BD:



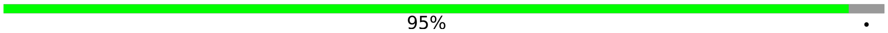
- Molecule 9: Tubulin beta-4B chain

Chain BF:



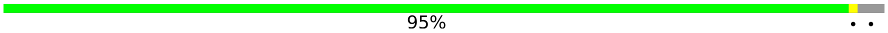
- Molecule 9: Tubulin beta-4B chain

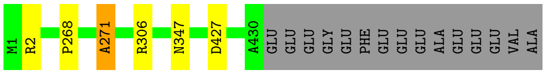
Chain BH:



- Molecule 9: Tubulin beta-4B chain

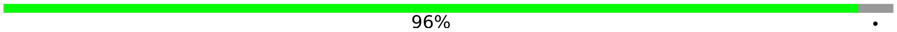
Chain BJ:





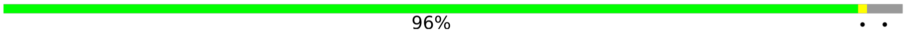
- Molecule 9: Tubulin beta-4B chain

Chain BL:



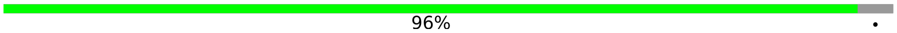
- Molecule 9: Tubulin beta-4B chain

Chain CB:



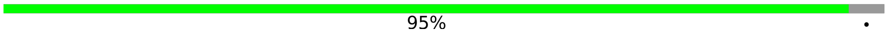
- Molecule 9: Tubulin beta-4B chain

Chain CD:



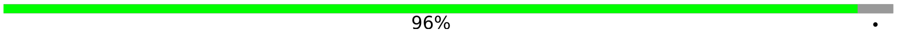
- Molecule 9: Tubulin beta-4B chain

Chain CF:



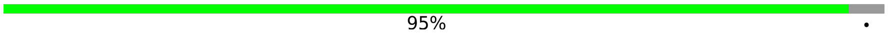
- Molecule 9: Tubulin beta-4B chain

Chain CH:



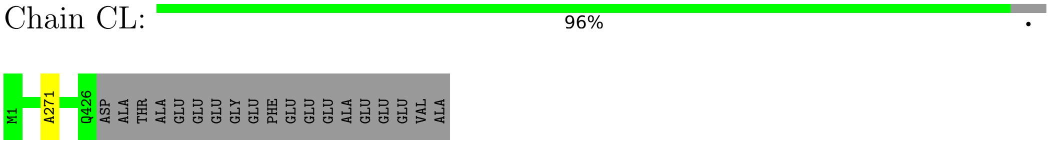
- Molecule 9: Tubulin beta-4B chain

Chain CJ:



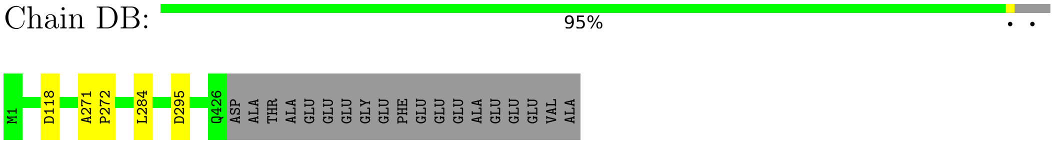
- Molecule 9: Tubulin beta-4B chain

Chain CL:



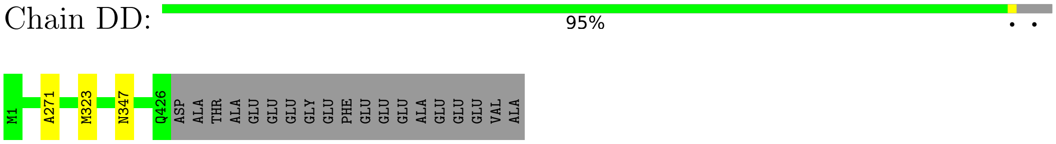
- Molecule 9: Tubulin beta-4B chain

Chain DB:



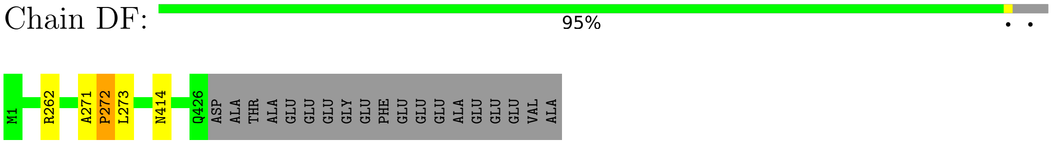
- Molecule 9: Tubulin beta-4B chain

Chain DD:



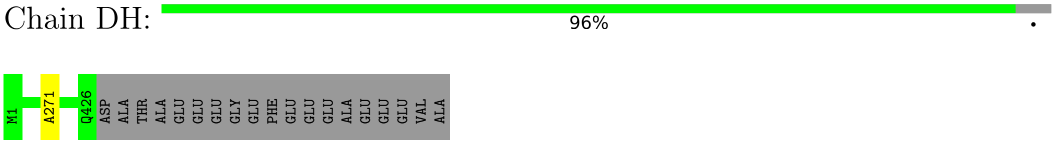
- Molecule 9: Tubulin beta-4B chain

Chain DF:



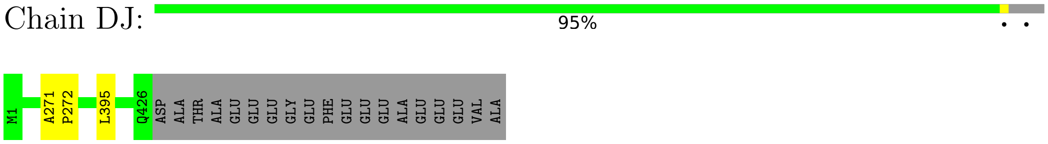
- Molecule 9: Tubulin beta-4B chain

Chain DH:



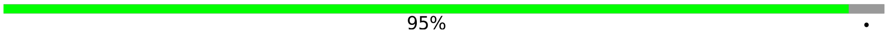
- Molecule 9: Tubulin beta-4B chain

Chain DJ:



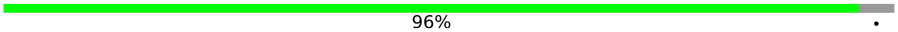
- Molecule 9: Tubulin beta-4B chain

Chain DL:



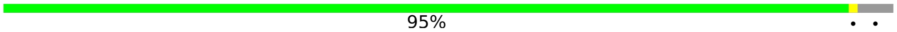
- Molecule 9: Tubulin beta-4B chain

Chain EB:



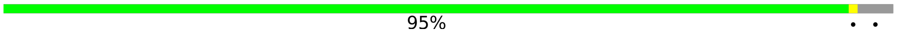
- Molecule 9: Tubulin beta-4B chain

Chain ED:



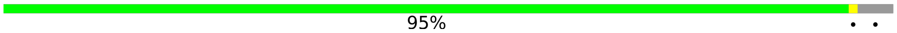
- Molecule 9: Tubulin beta-4B chain

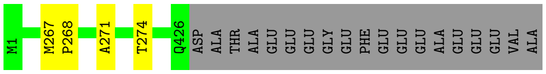
Chain EF:



- Molecule 9: Tubulin beta-4B chain

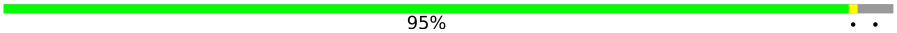
Chain EH:





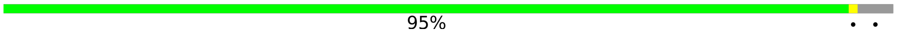
- Molecule 9: Tubulin beta-4B chain

Chain EJ:



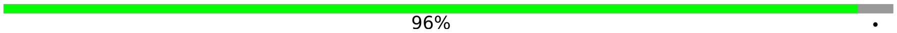
- Molecule 9: Tubulin beta-4B chain

Chain EL:



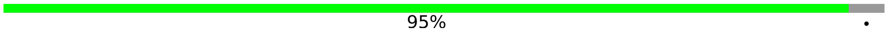
- Molecule 9: Tubulin beta-4B chain

Chain EN:



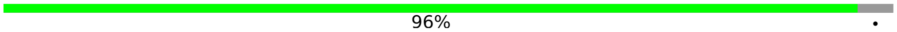
- Molecule 9: Tubulin beta-4B chain

Chain FB:



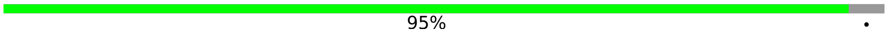
- Molecule 9: Tubulin beta-4B chain

Chain FD:



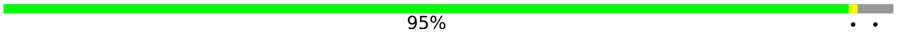
- Molecule 9: Tubulin beta-4B chain

Chain FF:



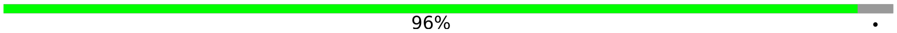
- Molecule 9: Tubulin beta-4B chain

Chain FH:



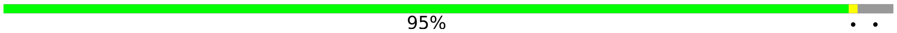
- Molecule 9: Tubulin beta-4B chain

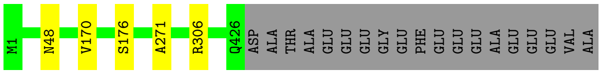
Chain FJ:



- Molecule 9: Tubulin beta-4B chain

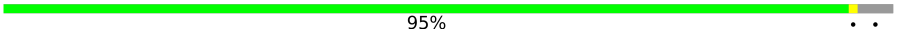
Chain FL:





- Molecule 9: Tubulin beta-4B chain

Chain FN:

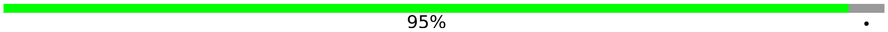


- Molecule 9: Tubulin beta-4B chain

Chain GB:

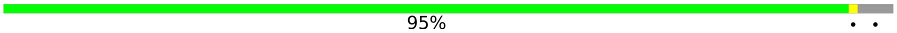
- Molecule 9: Tubulin beta-4B chain

Chain GD:



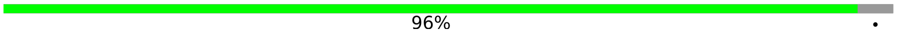
- Molecule 9: Tubulin beta-4B chain

Chain GF:



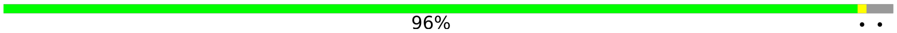
- Molecule 9: Tubulin beta-4B chain

Chain GH:



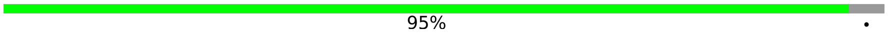
- Molecule 9: Tubulin beta-4B chain

Chain GJ:



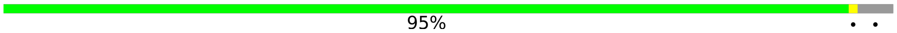
- Molecule 9: Tubulin beta-4B chain

Chain GL:



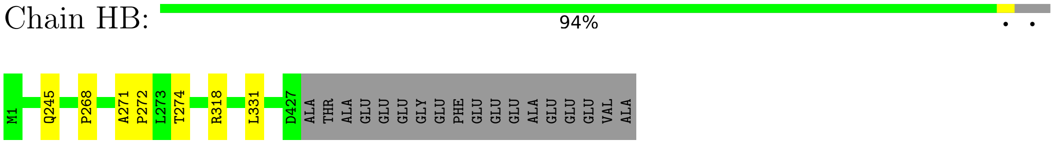
- Molecule 9: Tubulin beta-4B chain

Chain GN:



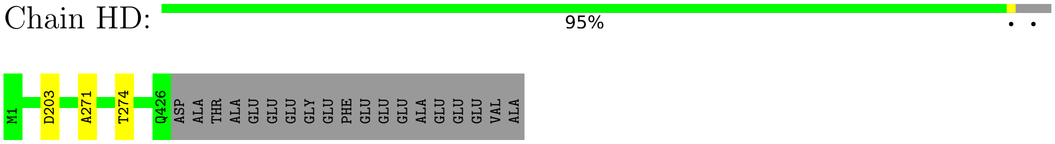
- Molecule 9: Tubulin beta-4B chain

Chain HB:



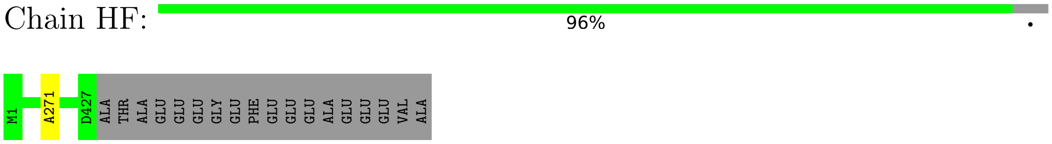
- Molecule 9: Tubulin beta-4B chain

Chain HD:



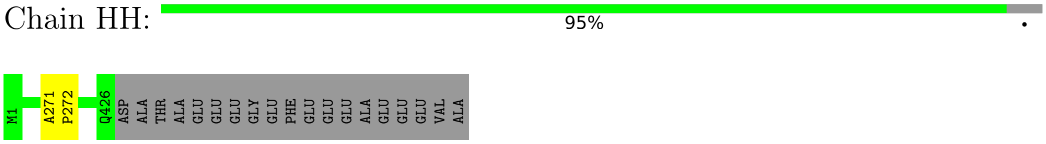
- Molecule 9: Tubulin beta-4B chain

Chain HF:



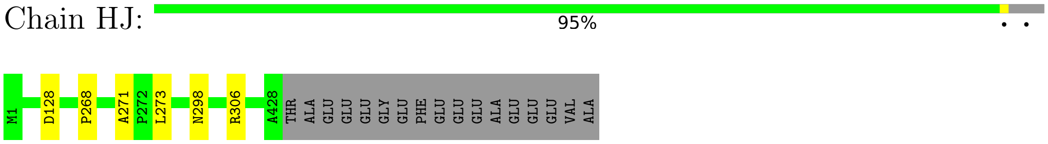
- Molecule 9: Tubulin beta-4B chain

Chain HH:



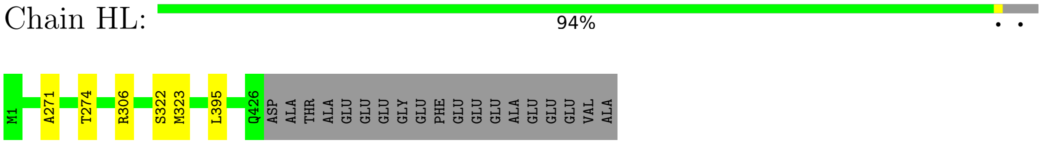
- Molecule 9: Tubulin beta-4B chain

Chain HJ:



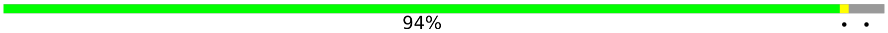
- Molecule 9: Tubulin beta-4B chain

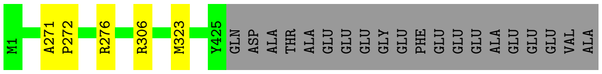
Chain HL:



- Molecule 9: Tubulin beta-4B chain

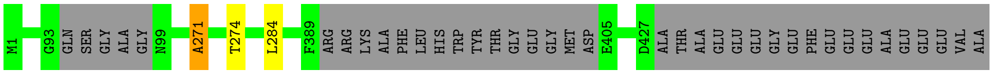
Chain HN:





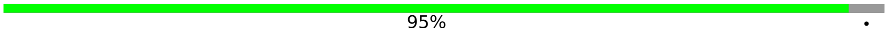
- Molecule 9: Tubulin beta-4B chain

Chain IB:



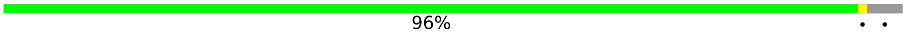
- Molecule 9: Tubulin beta-4B chain

Chain ID:



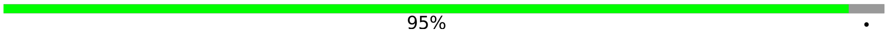
- Molecule 9: Tubulin beta-4B chain

Chain IF:



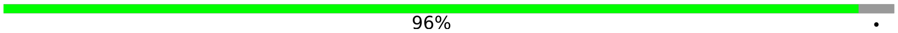
- Molecule 9: Tubulin beta-4B chain

Chain IH:



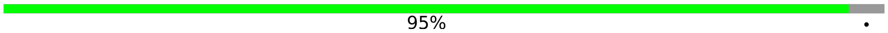
- Molecule 9: Tubulin beta-4B chain

Chain IJ:



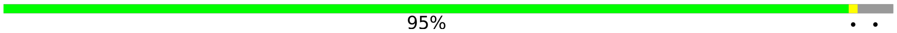
- Molecule 9: Tubulin beta-4B chain

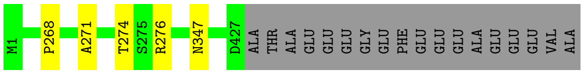
Chain IL:



- Molecule 9: Tubulin beta-4B chain

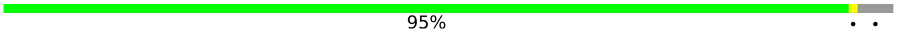
Chain IN:





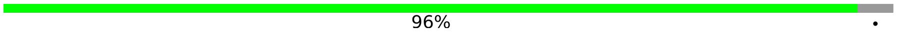
- Molecule 9: Tubulin beta-4B chain

Chain JB:



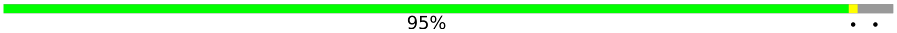
- Molecule 9: Tubulin beta-4B chain

Chain JD:



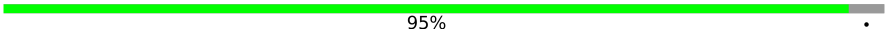
- Molecule 9: Tubulin beta-4B chain

Chain JF:



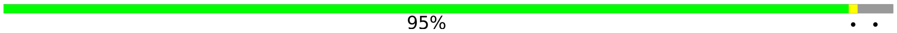
- Molecule 9: Tubulin beta-4B chain

Chain JH:



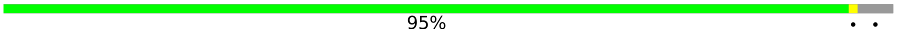
- Molecule 9: Tubulin beta-4B chain

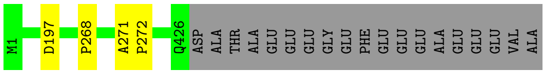
Chain JJ:



- Molecule 9: Tubulin beta-4B chain

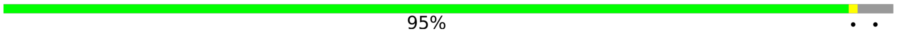
Chain JL:





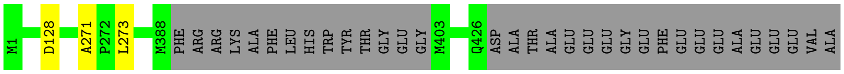
- Molecule 9: Tubulin beta-4B chain

Chain JN:



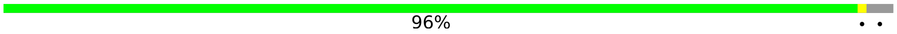
- Molecule 9: Tubulin beta-4B chain

Chain KB:



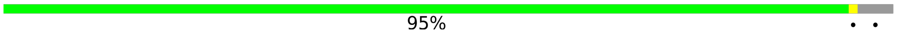
- Molecule 9: Tubulin beta-4B chain

Chain KD:



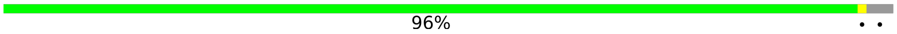
- Molecule 9: Tubulin beta-4B chain

Chain KF:



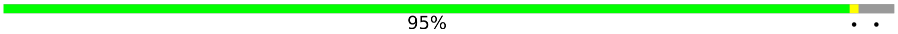
- Molecule 9: Tubulin beta-4B chain

Chain KH:



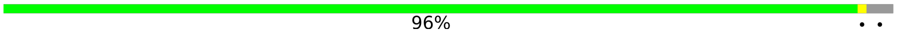
- Molecule 9: Tubulin beta-4B chain

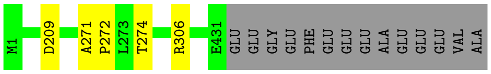
Chain KJ:



- Molecule 9: Tubulin beta-4B chain

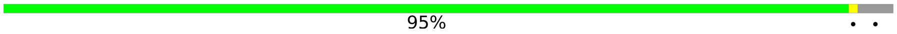
Chain KL:





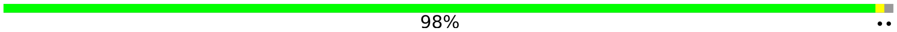
- Molecule 9: Tubulin beta-4B chain

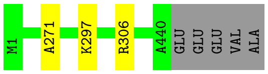
Chain KN:



- Molecule 9: Tubulin beta-4B chain

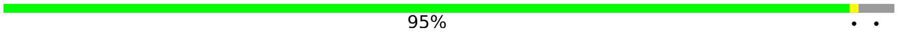
Chain LB:





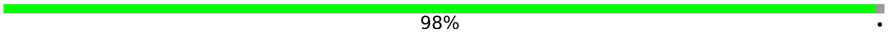
- Molecule 9: Tubulin beta-4B chain

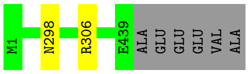
Chain LD:



- Molecule 9: Tubulin beta-4B chain

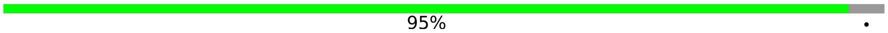
Chain LF:





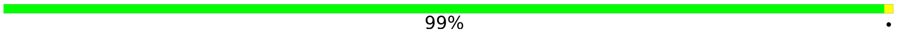
- Molecule 9: Tubulin beta-4B chain

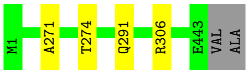
Chain LH:



- Molecule 9: Tubulin beta-4B chain

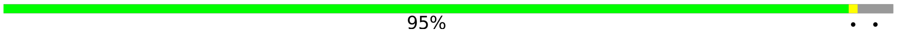
Chain LJ:

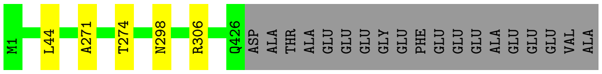




- Molecule 9: Tubulin beta-4B chain

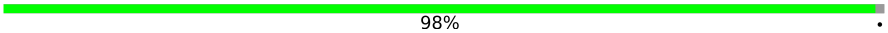
Chain LL:

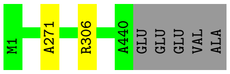




- Molecule 9: Tubulin beta-4B chain

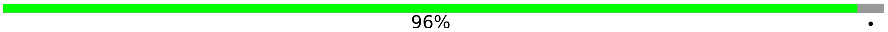
Chain LN:





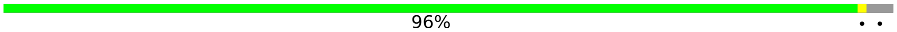
- Molecule 9: Tubulin beta-4B chain

Chain MB:



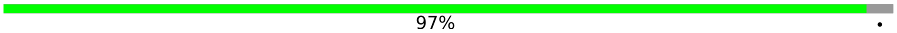
- Molecule 9: Tubulin beta-4B chain

Chain MD:



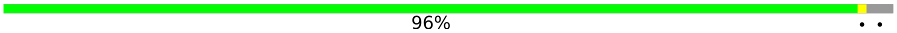
- Molecule 9: Tubulin beta-4B chain

Chain MF:



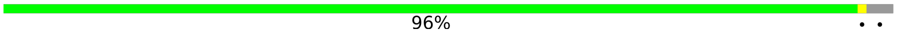
- Molecule 9: Tubulin beta-4B chain

Chain MH:



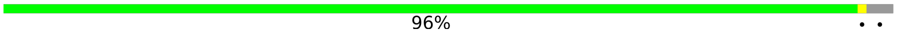
- Molecule 9: Tubulin beta-4B chain

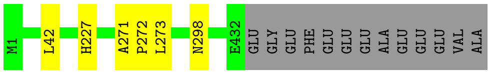
Chain MJ:



- Molecule 9: Tubulin beta-4B chain

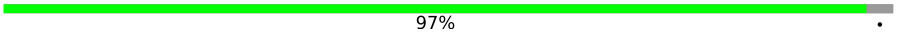
Chain ML:





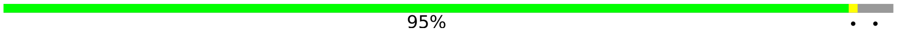
- Molecule 9: Tubulin beta-4B chain

Chain MN:



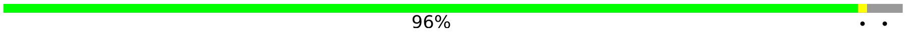
- Molecule 9: Tubulin beta-4B chain

Chain NB:



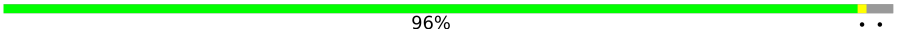
- Molecule 9: Tubulin beta-4B chain

Chain ND:



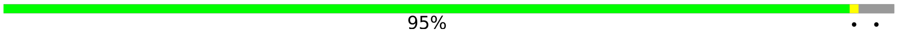
- Molecule 9: Tubulin beta-4B chain

Chain NF:



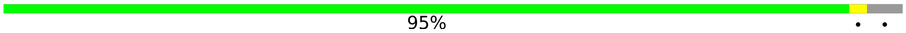
- Molecule 9: Tubulin beta-4B chain

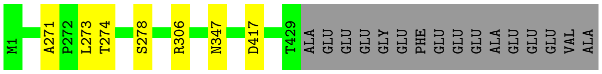
Chain NH:



- Molecule 9: Tubulin beta-4B chain

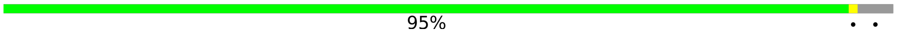
Chain NJ:

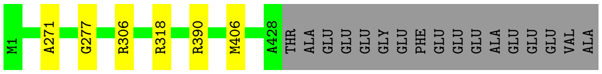




- Molecule 9: Tubulin beta-4B chain

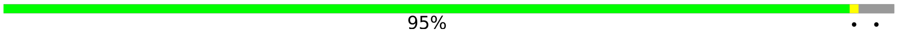
Chain NL:

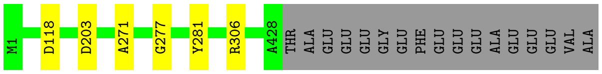




- Molecule 9: Tubulin beta-4B chain

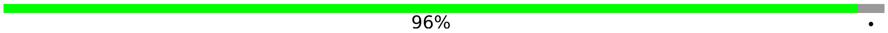
Chain NN:

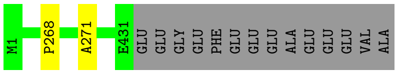




- Molecule 9: Tubulin beta-4B chain

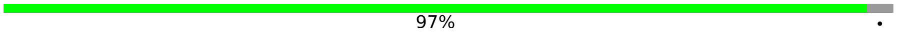
Chain OB:





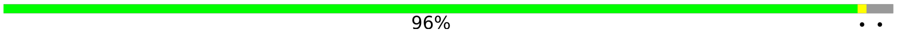
- Molecule 9: Tubulin beta-4B chain

Chain OD:



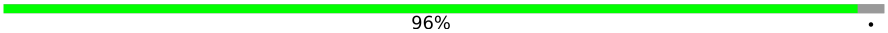
- Molecule 9: Tubulin beta-4B chain

Chain OF:



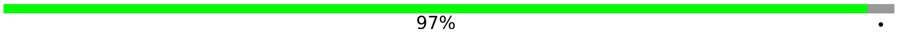
- Molecule 9: Tubulin beta-4B chain

Chain OH:



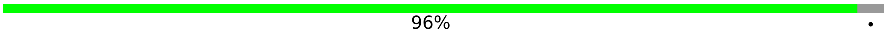
- Molecule 9: Tubulin beta-4B chain

Chain OJ:



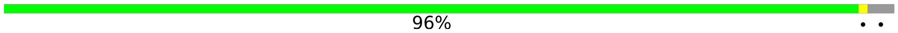
- Molecule 9: Tubulin beta-4B chain

Chain OL:



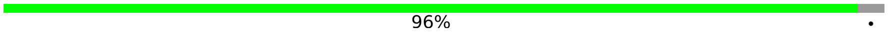
- Molecule 9: Tubulin beta-4B chain

Chain ON:



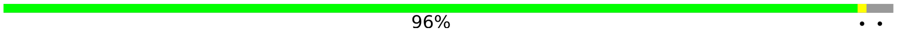
- Molecule 9: Tubulin beta-4B chain

Chain PD:



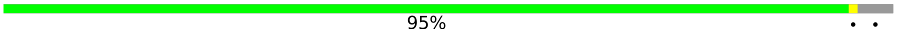
- Molecule 9: Tubulin beta-4B chain

Chain PF:



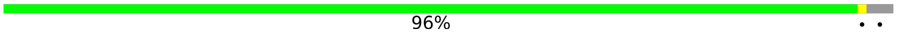
- Molecule 9: Tubulin beta-4B chain

Chain PH:



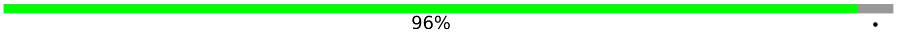
- Molecule 9: Tubulin beta-4B chain

Chain PJ:



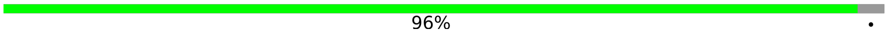
- Molecule 9: Tubulin beta-4B chain

Chain PL:



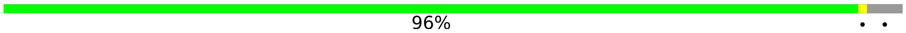
- Molecule 9: Tubulin beta-4B chain

Chain PN:



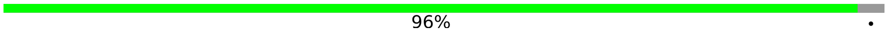
- Molecule 9: Tubulin beta-4B chain

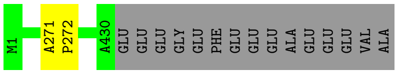
Chain QD:



- Molecule 9: Tubulin beta-4B chain

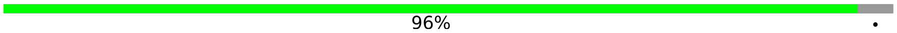
Chain QF:





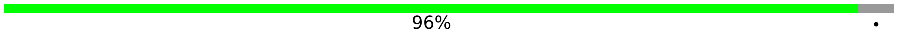
- Molecule 9: Tubulin beta-4B chain

Chain QH:



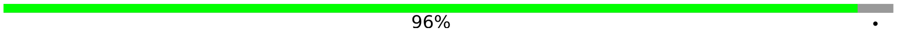
- Molecule 9: Tubulin beta-4B chain

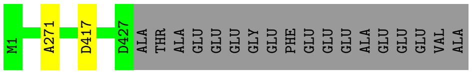
Chain QJ:



- Molecule 9: Tubulin beta-4B chain

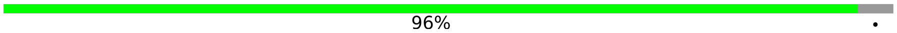
Chain QL:





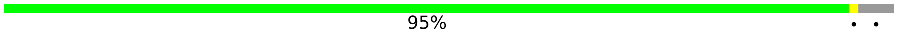
- Molecule 9: Tubulin beta-4B chain

Chain QN:



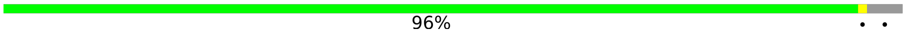
- Molecule 9: Tubulin beta-4B chain

Chain RD:



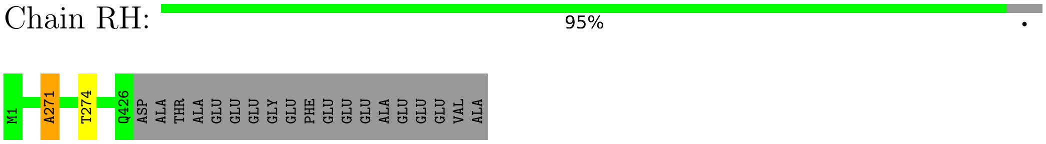
- Molecule 9: Tubulin beta-4B chain

Chain RF:



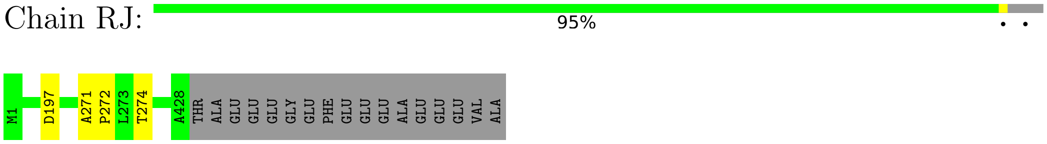
- Molecule 9: Tubulin beta-4B chain

Chain RH:



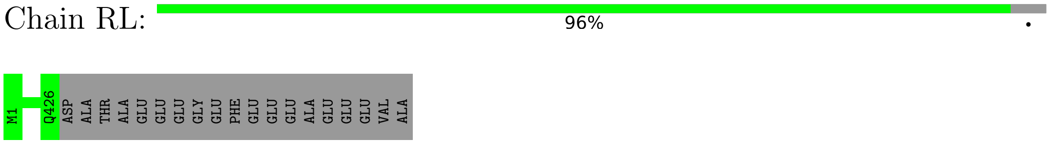
- Molecule 9: Tubulin beta-4B chain

Chain RJ:



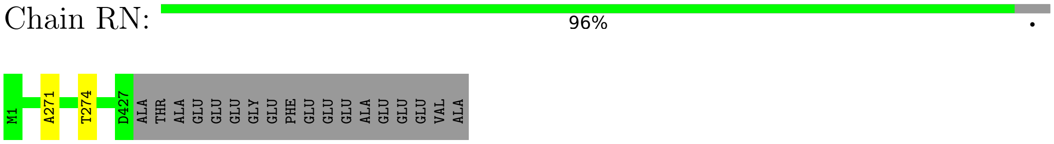
- Molecule 9: Tubulin beta-4B chain

Chain RL:



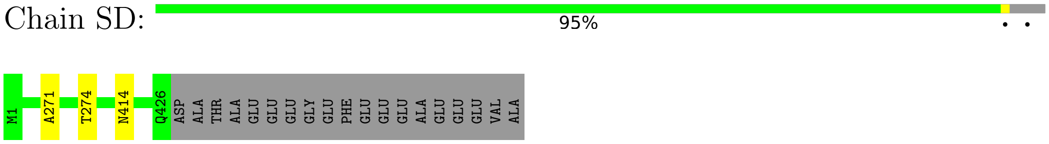
- Molecule 9: Tubulin beta-4B chain

Chain RN:



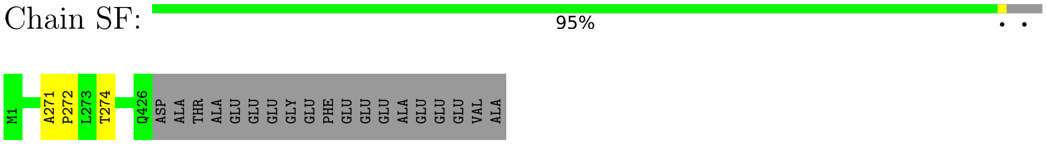
- Molecule 9: Tubulin beta-4B chain

Chain SD:



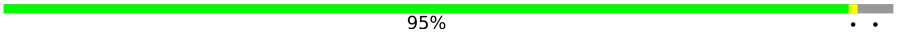
- Molecule 9: Tubulin beta-4B chain

Chain SF:



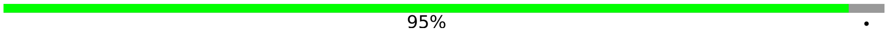
- Molecule 9: Tubulin beta-4B chain

Chain SH:



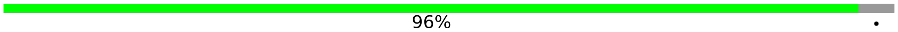
- Molecule 9: Tubulin beta-4B chain

Chain SJ:



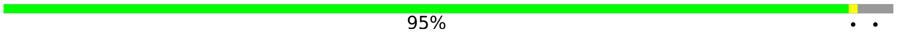
- Molecule 9: Tubulin beta-4B chain

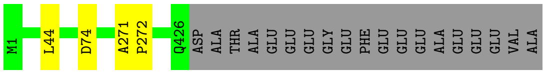
Chain SL:



- Molecule 9: Tubulin beta-4B chain

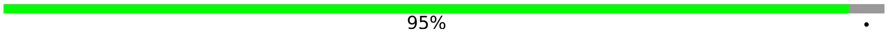
Chain SN:





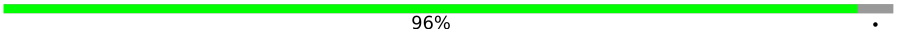
- Molecule 9: Tubulin beta-4B chain

Chain TD:



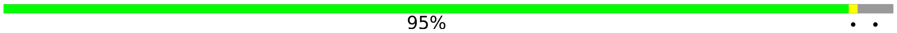
- Molecule 9: Tubulin beta-4B chain

Chain TF:



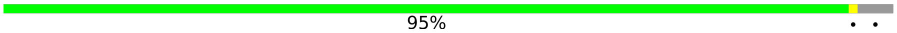
- Molecule 9: Tubulin beta-4B chain

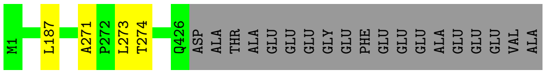
Chain TH:



- Molecule 9: Tubulin beta-4B chain

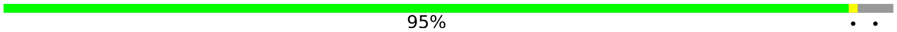
Chain TJ:

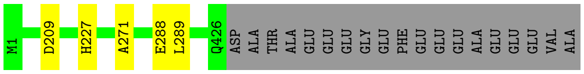




- Molecule 9: Tubulin beta-4B chain

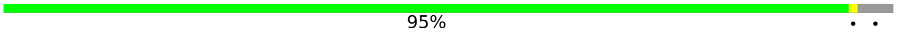
Chain TL:





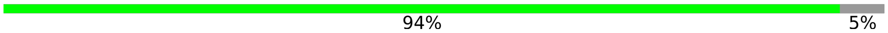
- Molecule 9: Tubulin beta-4B chain

Chain TN:



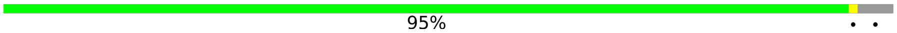
- Molecule 9: Tubulin beta-4B chain

Chain TP:



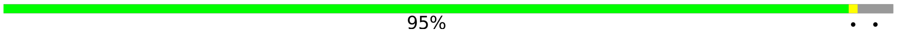
- Molecule 9: Tubulin beta-4B chain

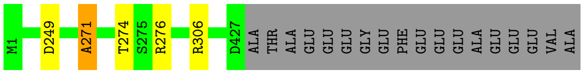
Chain UD:



- Molecule 9: Tubulin beta-4B chain

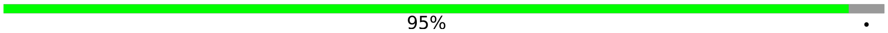
Chain UF:





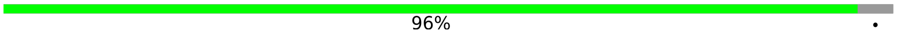
- Molecule 9: Tubulin beta-4B chain

Chain UH:



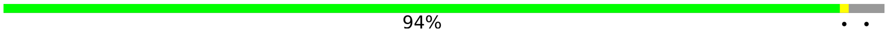
- Molecule 9: Tubulin beta-4B chain

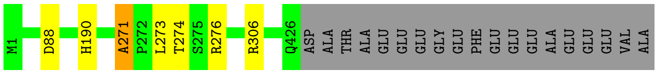
Chain UJ:



- Molecule 9: Tubulin beta-4B chain

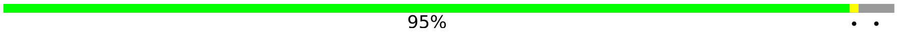
Chain UL:





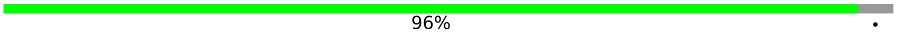
- Molecule 9: Tubulin beta-4B chain

Chain UN:



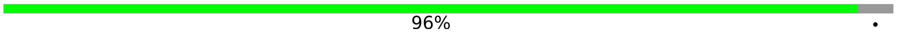
- Molecule 9: Tubulin beta-4B chain

Chain UP:



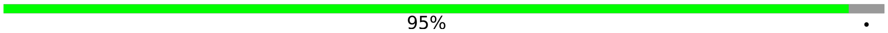
- Molecule 9: Tubulin beta-4B chain

Chain VD:



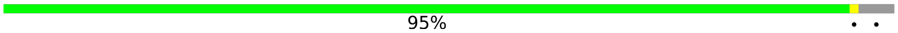
- Molecule 9: Tubulin beta-4B chain

Chain VF:



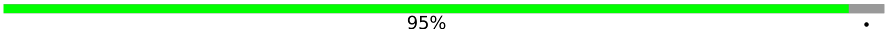
- Molecule 9: Tubulin beta-4B chain

Chain VH:



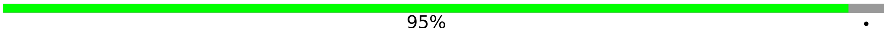
- Molecule 9: Tubulin beta-4B chain

Chain VJ:



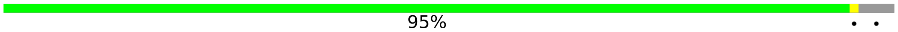
- Molecule 9: Tubulin beta-4B chain

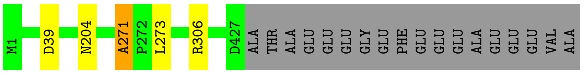
Chain VL:



- Molecule 9: Tubulin beta-4B chain

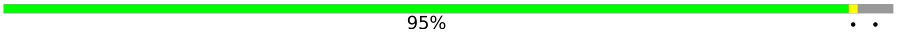
Chain VN:





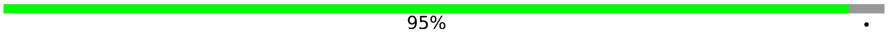
- Molecule 9: Tubulin beta-4B chain

Chain VP:



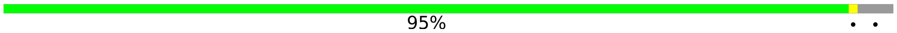
- Molecule 9: Tubulin beta-4B chain

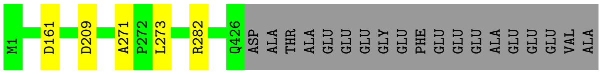
Chain WD:



- Molecule 9: Tubulin beta-4B chain

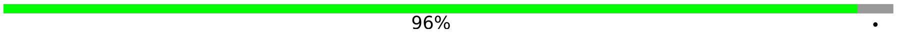
Chain WF:





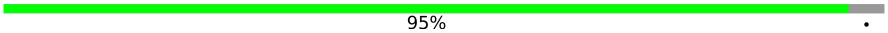
- Molecule 9: Tubulin beta-4B chain

Chain WH:

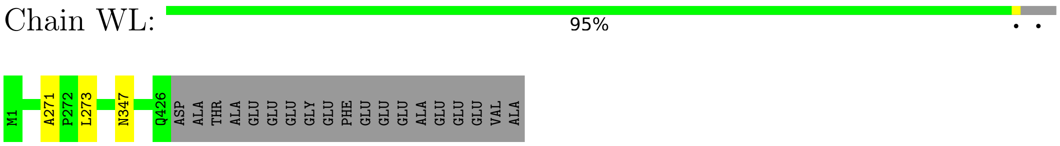


- Molecule 9: Tubulin beta-4B chain

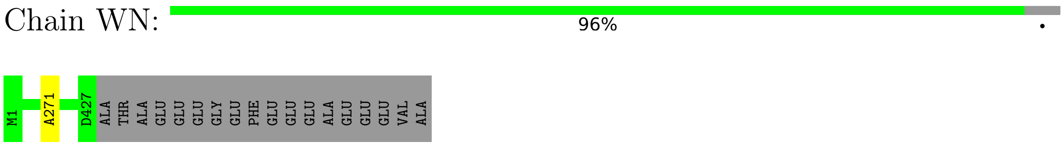
Chain WJ:



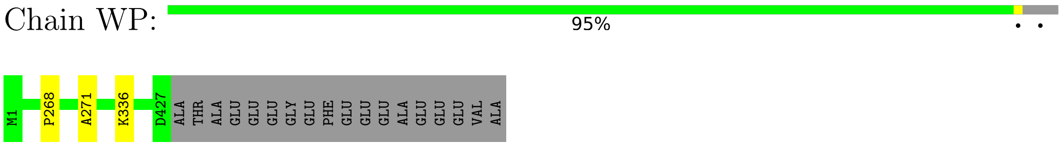
- Molecule 9: Tubulin beta-4B chain



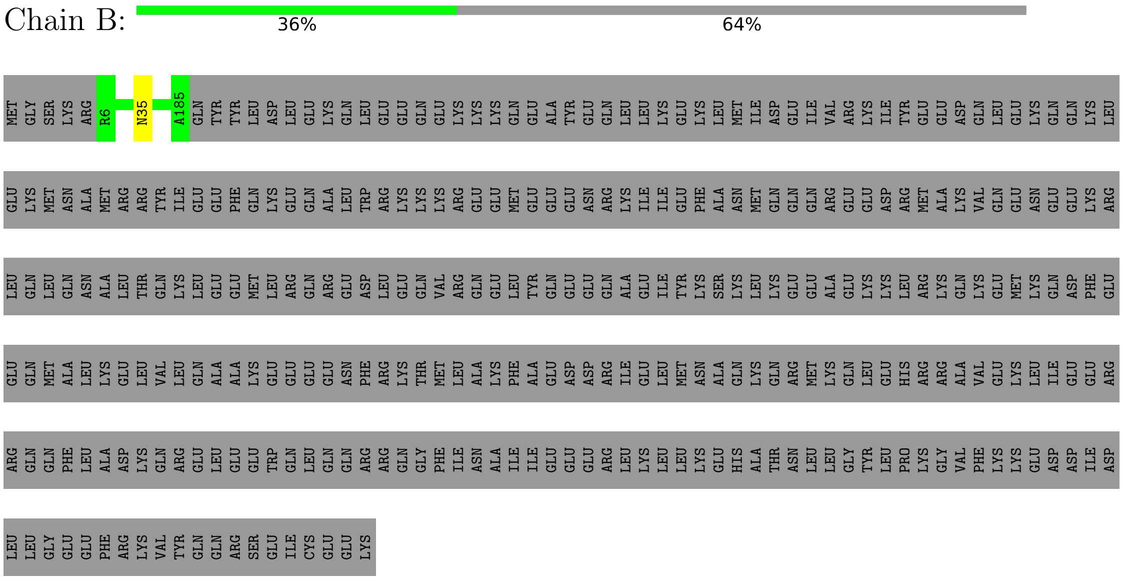
- Molecule 9: Tubulin beta-4B chain



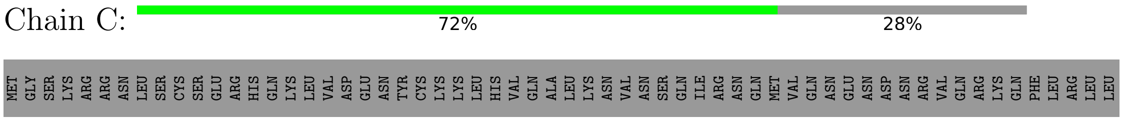
- Molecule 9: Tubulin beta-4B chain

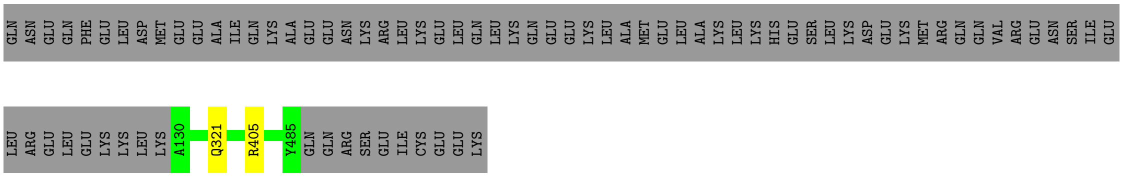


- Molecule 10: Meiosis-specific nuclear structural protein 1



- Molecule 10: Meiosis-specific nuclear structural protein 1



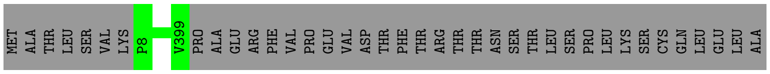


- Molecule 11: Tektin-2

Chain B0:

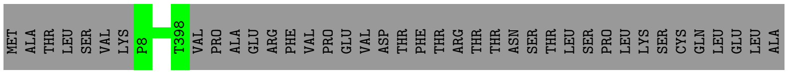
- Molecule 11: Tektin-2

Chain B1:



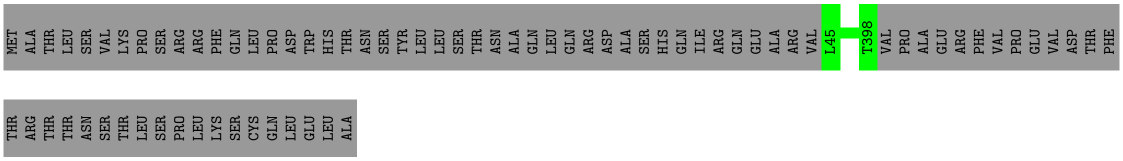
- Molecule 11: Tektin-2

Chain B2:



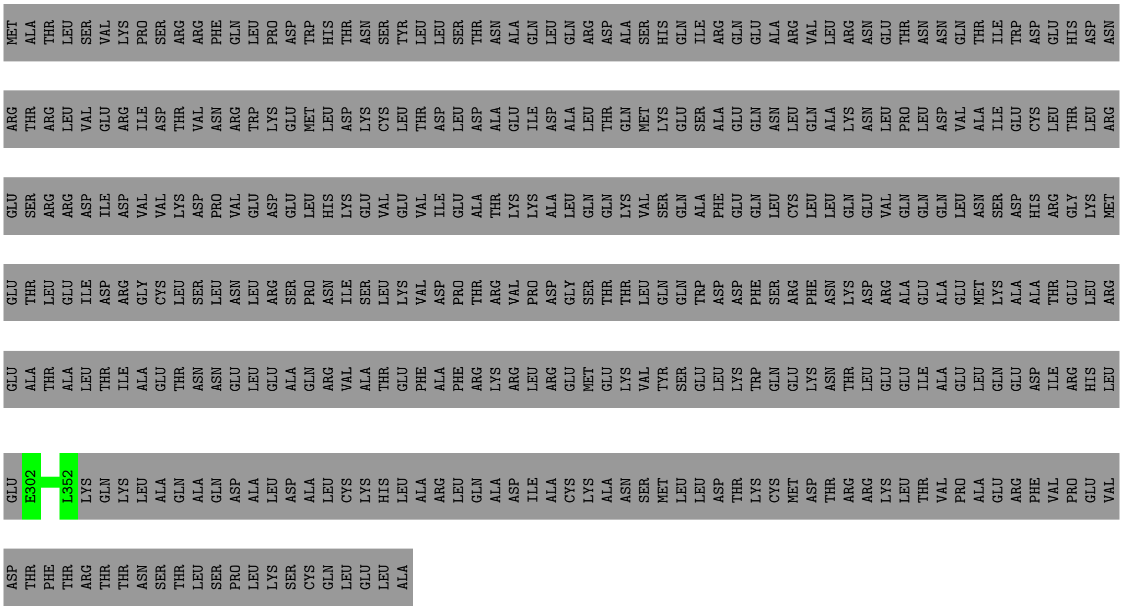
- Molecule 11: Tektin-2

Chain B3:



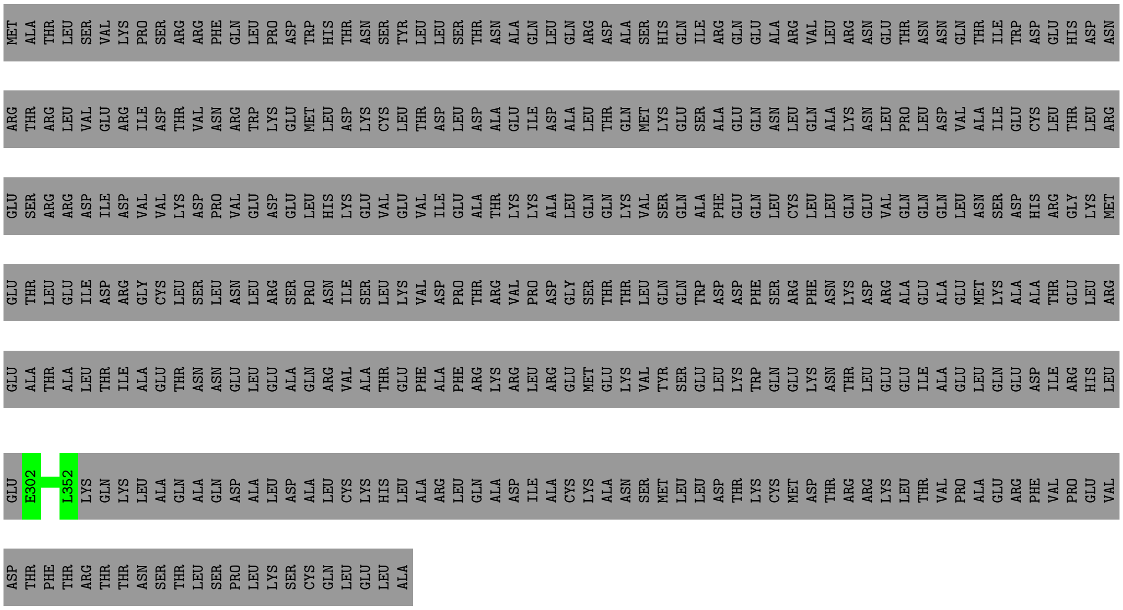
- Molecule 11: Tektin-2

Chain B4:



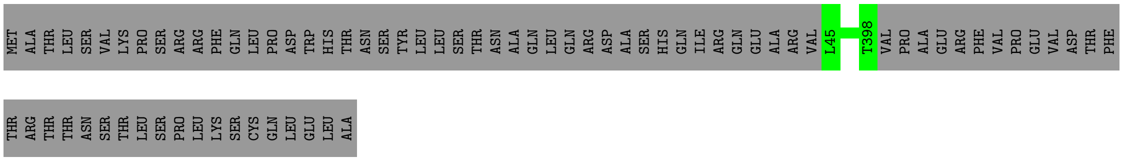
- Molecule 11: Tektin-2

Chain B5:



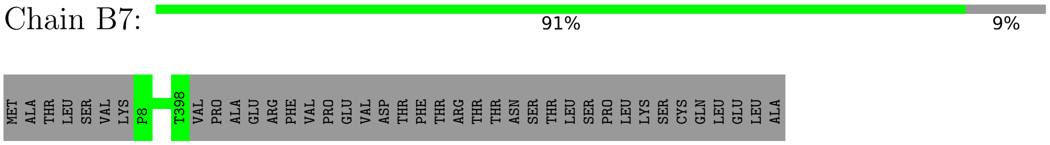
- Molecule 11: Tektin-2

Chain B6:



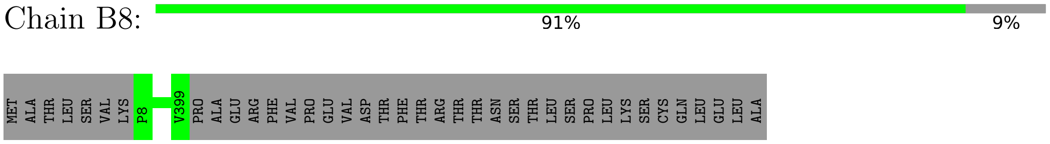
- Molecule 11: Tektin-2

Chain B7:



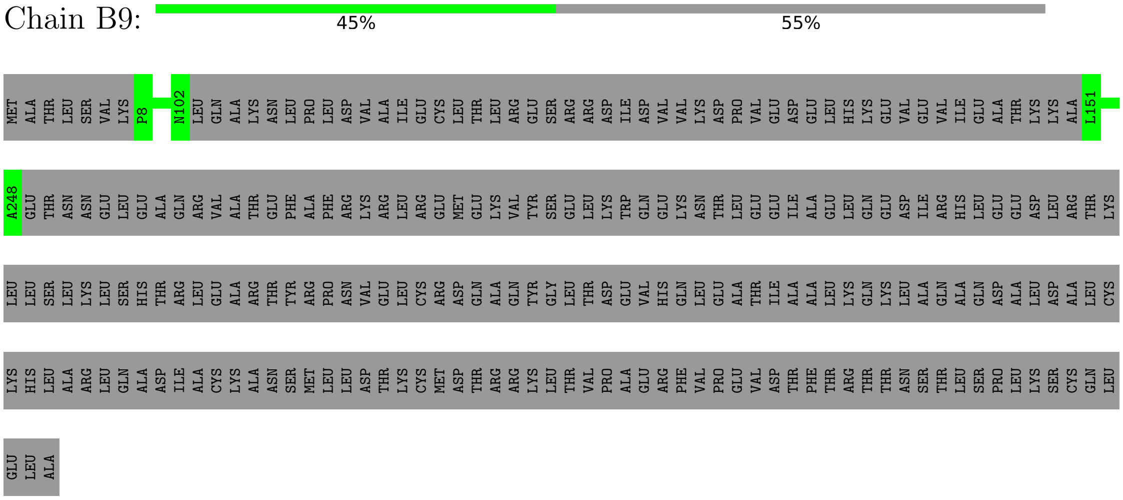
- Molecule 11: Tektin-2

Chain B8:



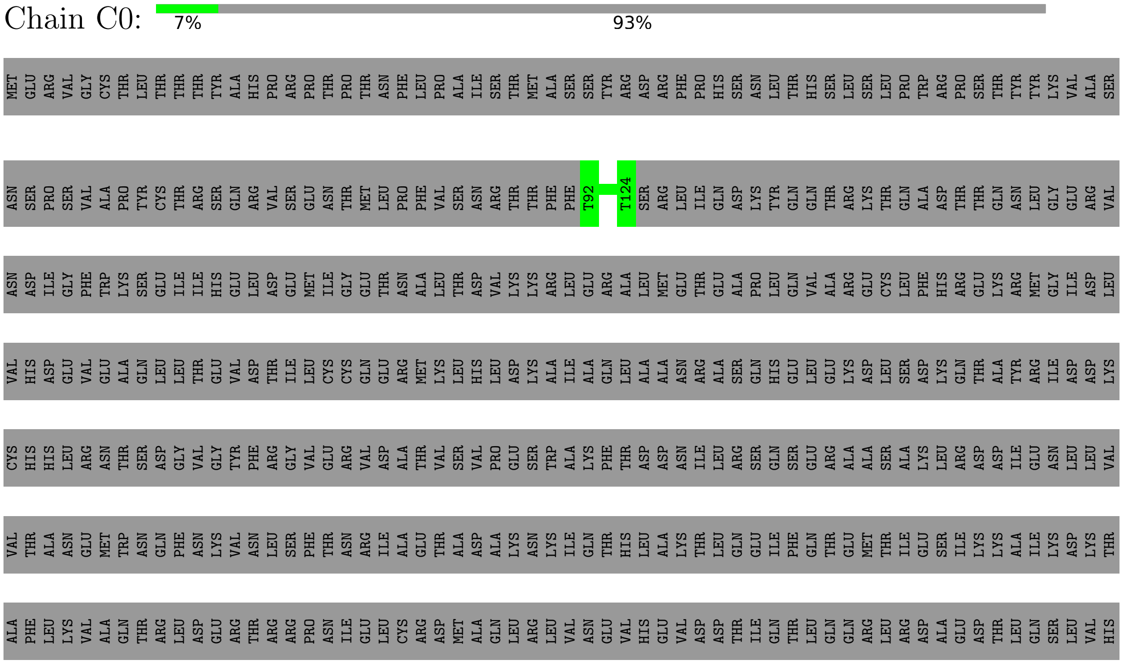
- Molecule 11: Tektin-2

Chain B9:



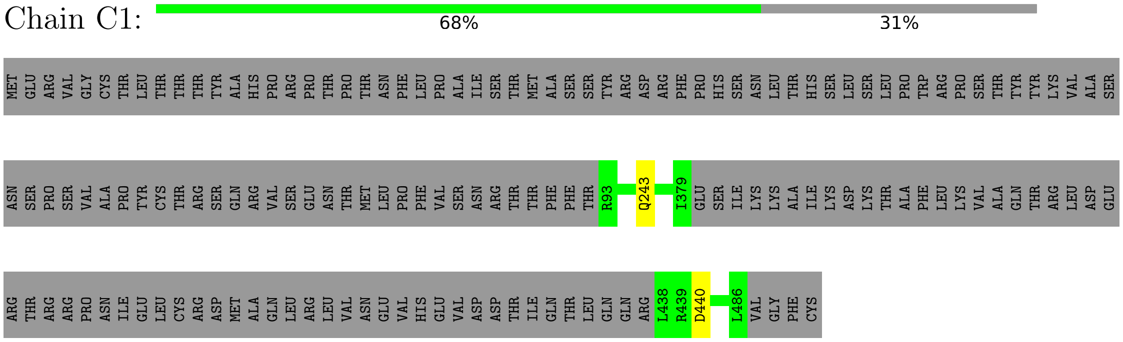
- Molecule 12: Tektin-3

Chain C0:



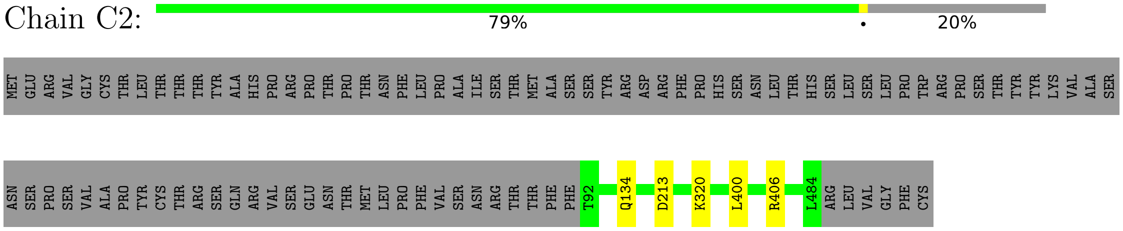
- Molecule 12: Tektin-3

Chain C1:



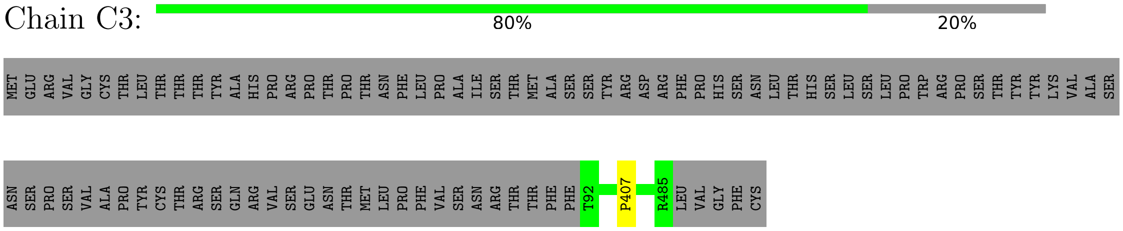
- Molecule 12: Tektin-3

Chain C2:



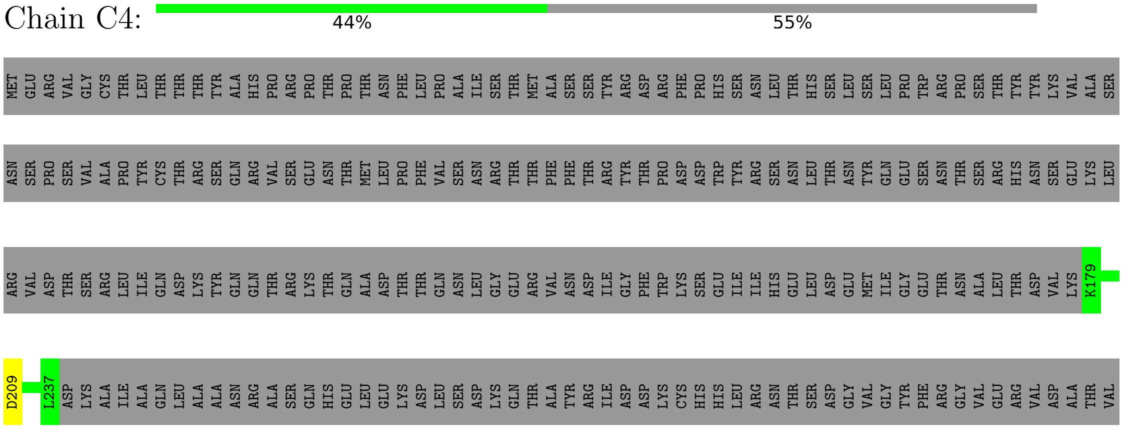
- Molecule 12: Tektin-3

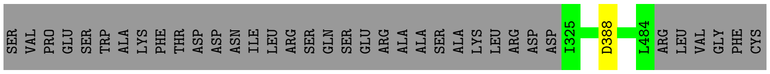
Chain C3:



- Molecule 12: Tektin-3

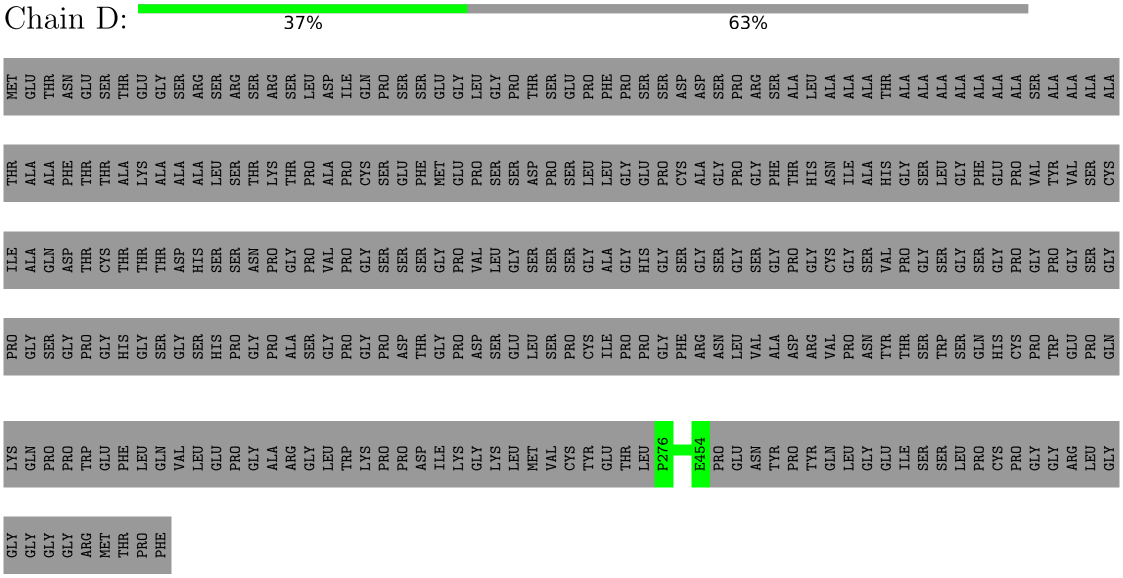
Chain C4:





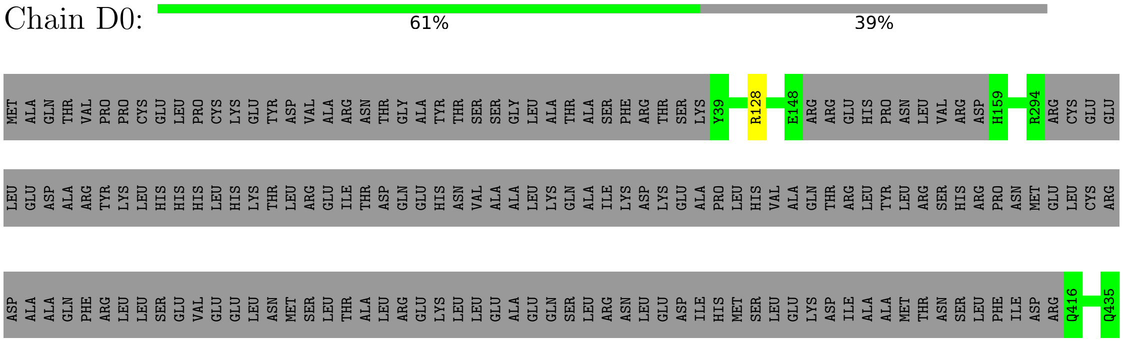
- Molecule 13: Sperm-associated antigen 8

Chain D:



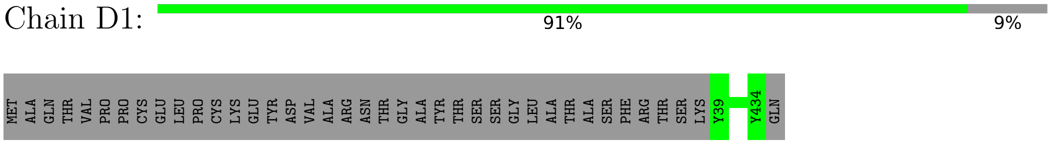
- Molecule 14: Tektin-4

Chain D0:



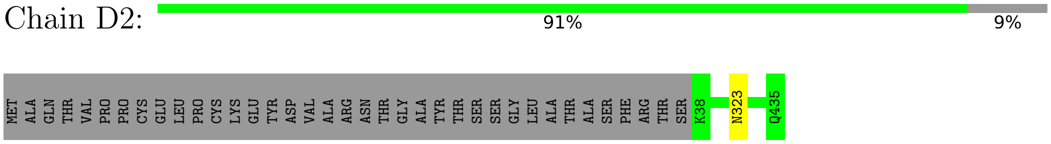
- Molecule 14: Tektin-4

Chain D1:



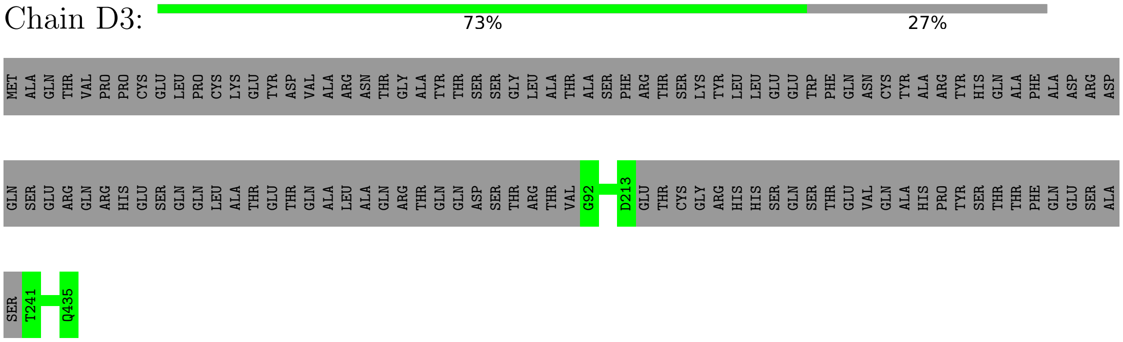
- Molecule 14: Tektin-4

Chain D2:



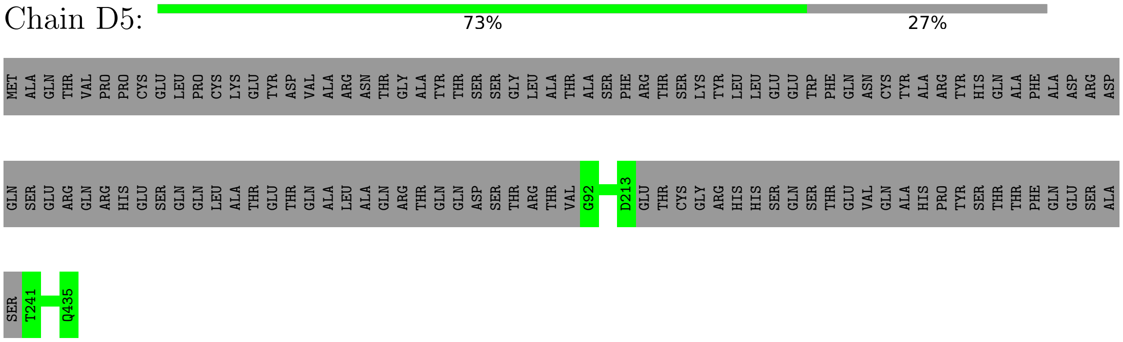
- Molecule 14: Tektin-4

Chain D3:



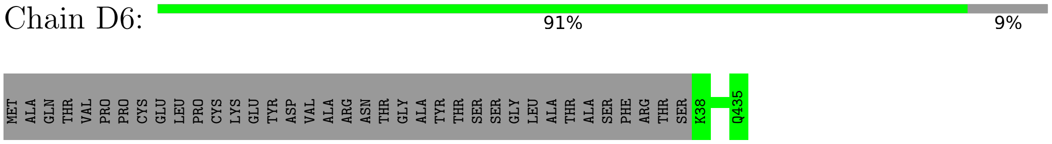
- Molecule 14: Tektin-4

Chain D5:



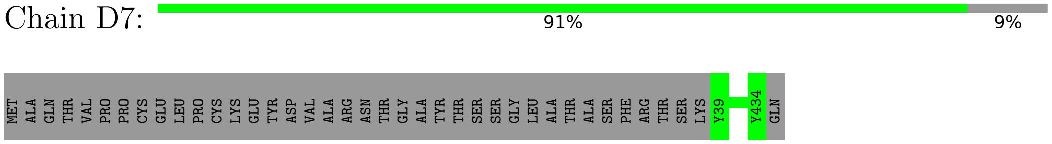
- Molecule 14: Tektin-4

Chain D6:



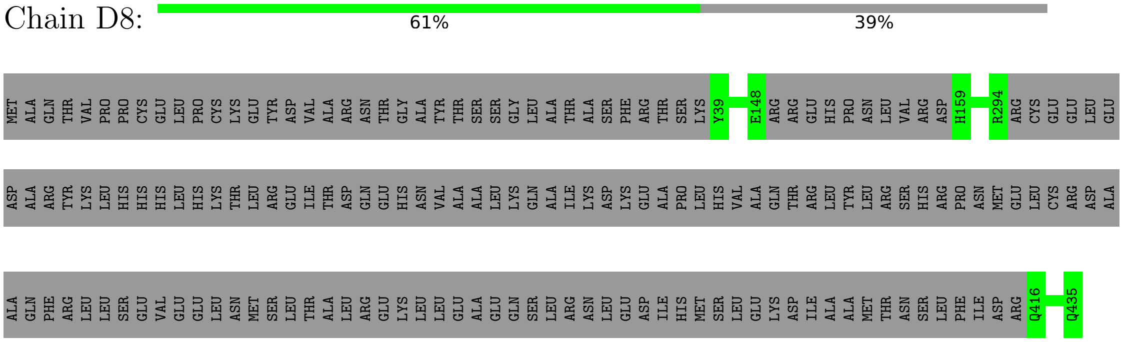
- Molecule 14: Tektin-4

Chain D7:



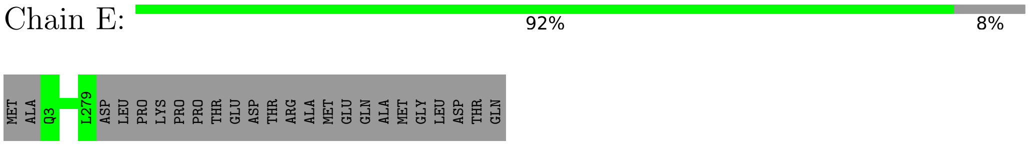
- Molecule 14: Tektin-4

Chain D8:



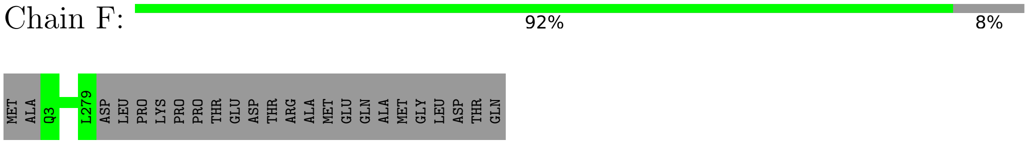
- Molecule 15: Cilia- and flagella-associated protein 161

Chain E:



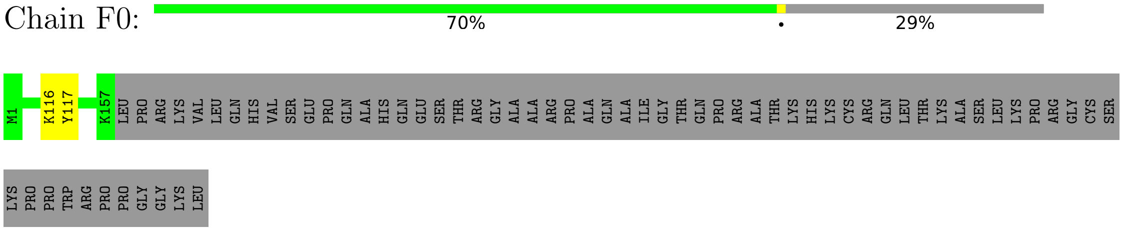
- Molecule 15: Cilia- and flagella-associated protein 161

Chain F:



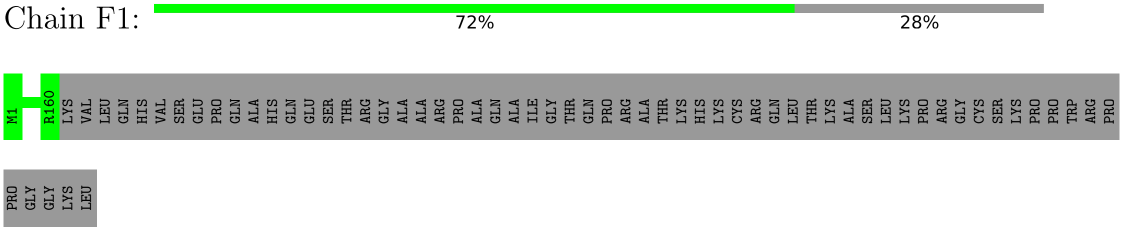
- Molecule 16: Sperm acrosome-associated protein 9

Chain F0:



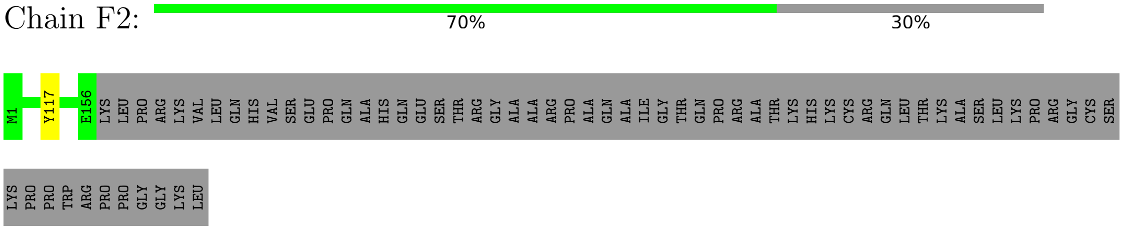
- Molecule 16: Sperm acrosome-associated protein 9

Chain F1:



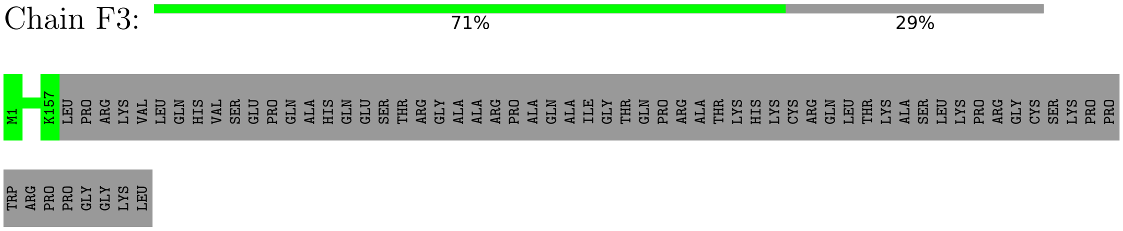
- Molecule 16: Sperm acrosome-associated protein 9

Chain F2:



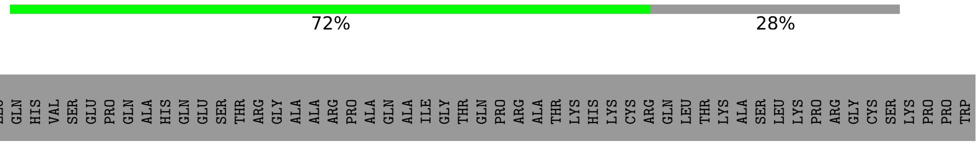
- Molecule 16: Sperm acrosome-associated protein 9

Chain F3:



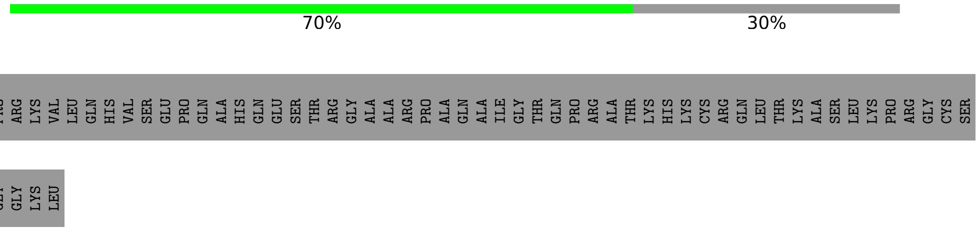
- Molecule 16: Sperm acrosome-associated protein 9

Chain F4:



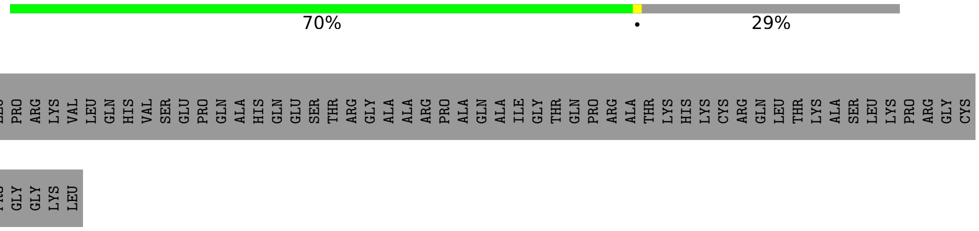
- Molecule 16: Sperm acrosome-associated protein 9

Chain F5:



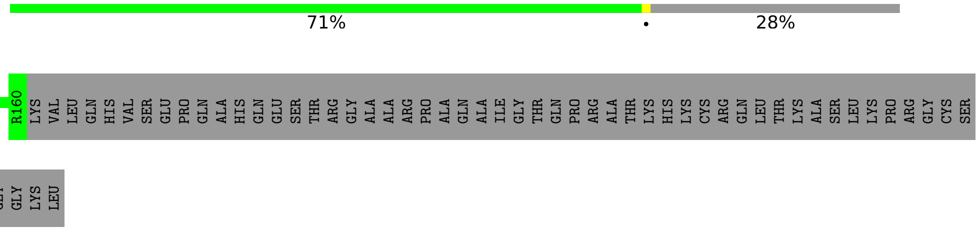
- Molecule 16: Sperm acrosome-associated protein 9

Chain F6:



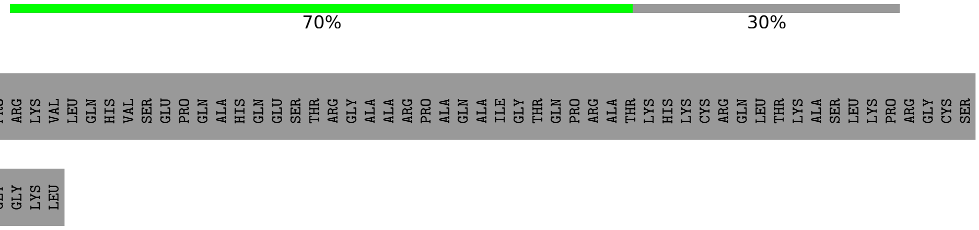
- Molecule 16: Sperm acrosome-associated protein 9

Chain F7:



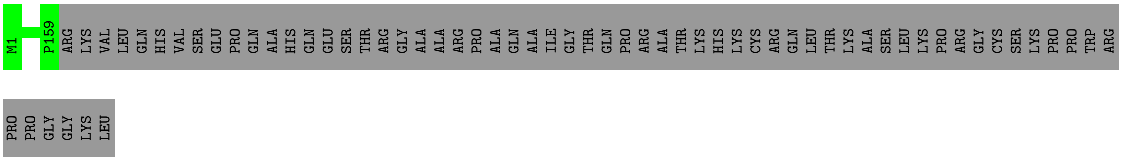
- Molecule 16: Sperm acrosome-associated protein 9

Chain F8:



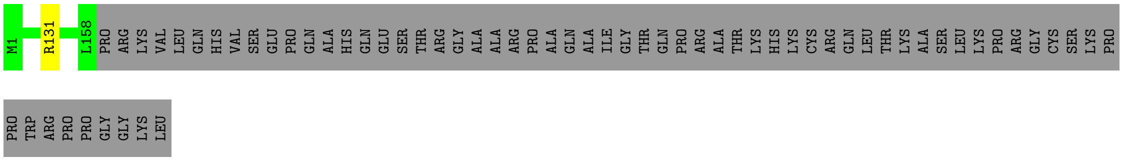
- Molecule 16: Sperm acrosome-associated protein 9

Chain G0:



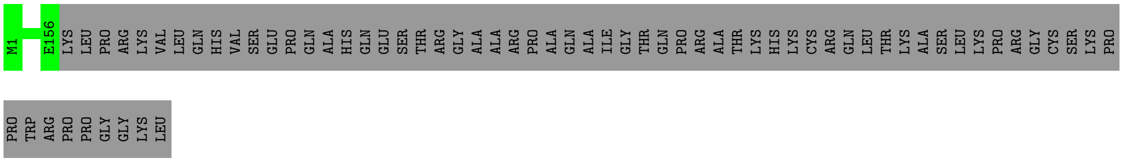
- Molecule 16: Sperm acrosome-associated protein 9

Chain G1:



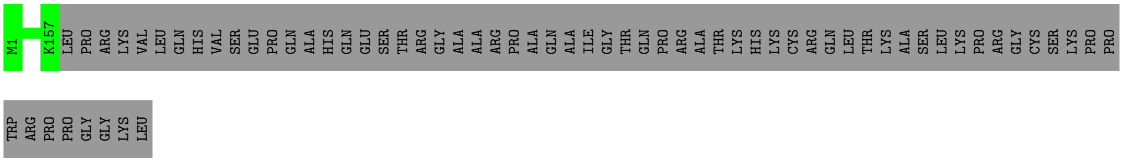
- Molecule 16: Sperm acrosome-associated protein 9

Chain G2:



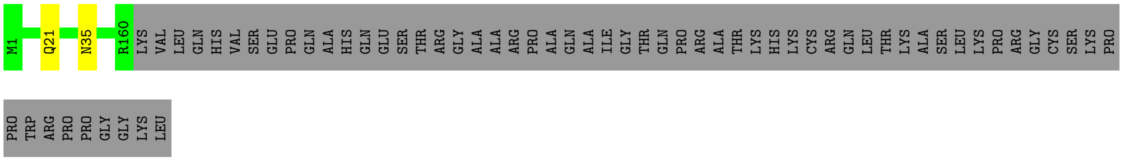
- Molecule 16: Sperm acrosome-associated protein 9

Chain G3:



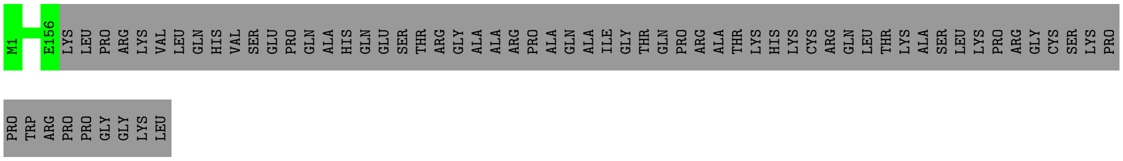
- Molecule 16: Sperm acrosome-associated protein 9

Chain G4:



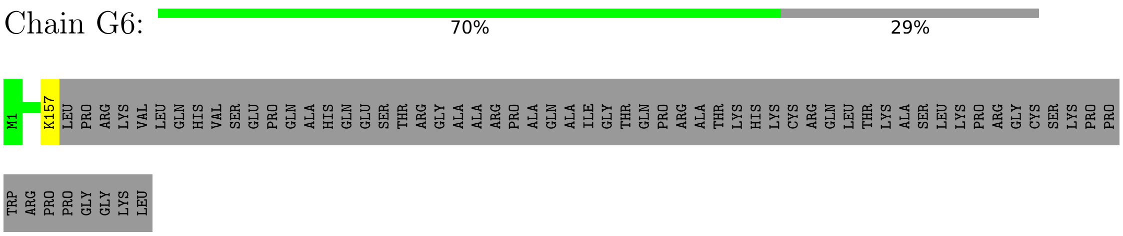
- Molecule 16: Sperm acrosome-associated protein 9

Chain G5:



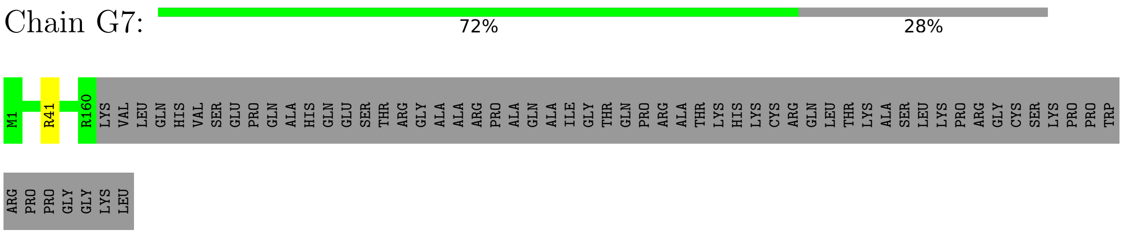
- Molecule 16: Sperm acrosome-associated protein 9

Chain G6:



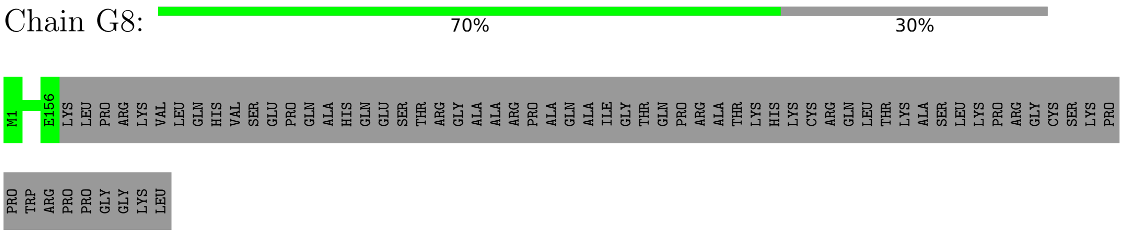
- Molecule 16: Sperm acrosome-associated protein 9

Chain G7:



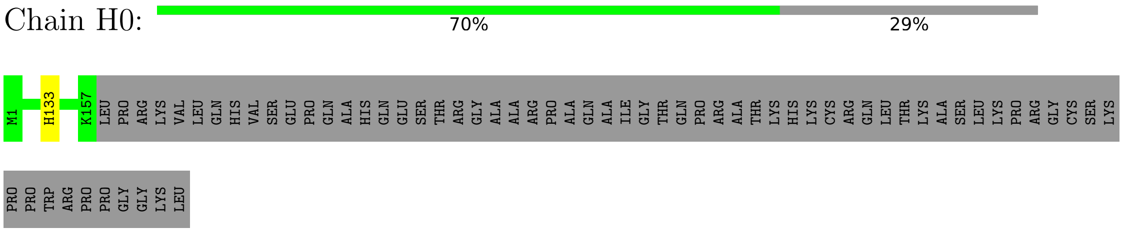
- Molecule 16: Sperm acrosome-associated protein 9

Chain G8:



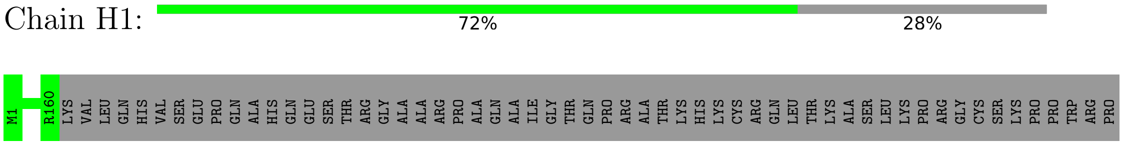
- Molecule 16: Sperm acrosome-associated protein 9

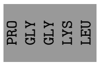
Chain H0:



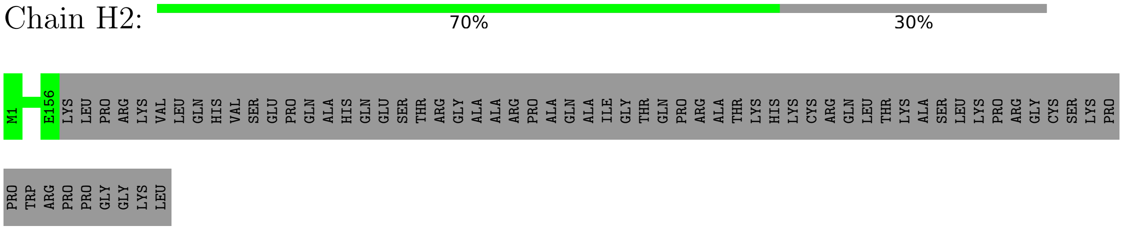
- Molecule 16: Sperm acrosome-associated protein 9

Chain H1:

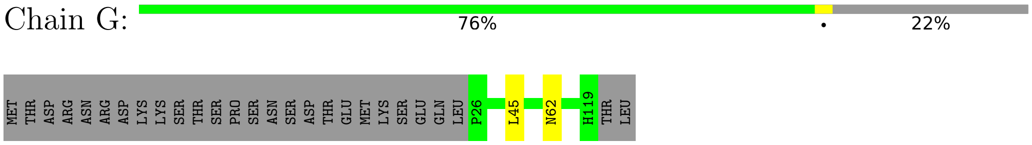




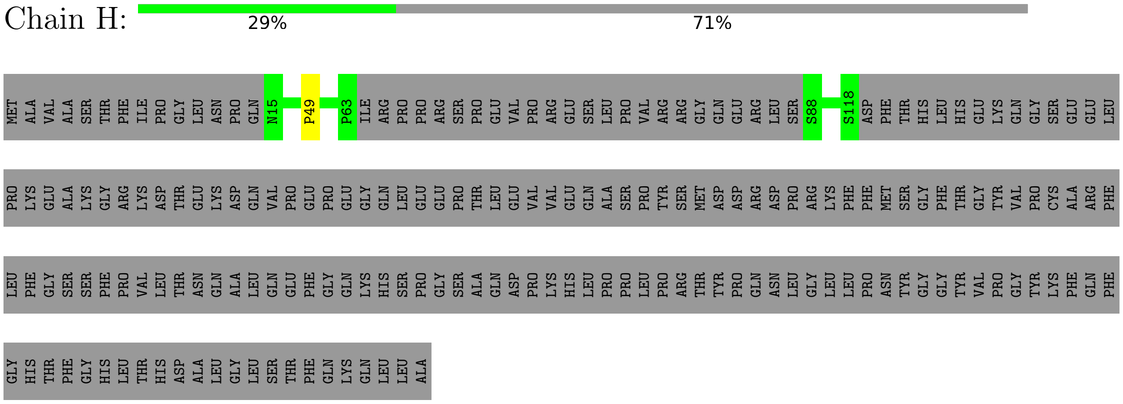
- Molecule 16: Sperm acrosome-associated protein 9



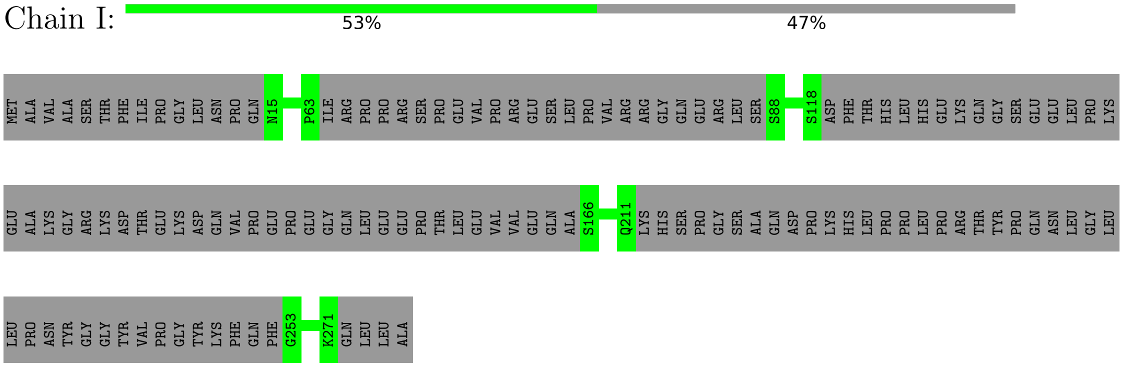
- Molecule 17: Uncharacterized protein C15orf65



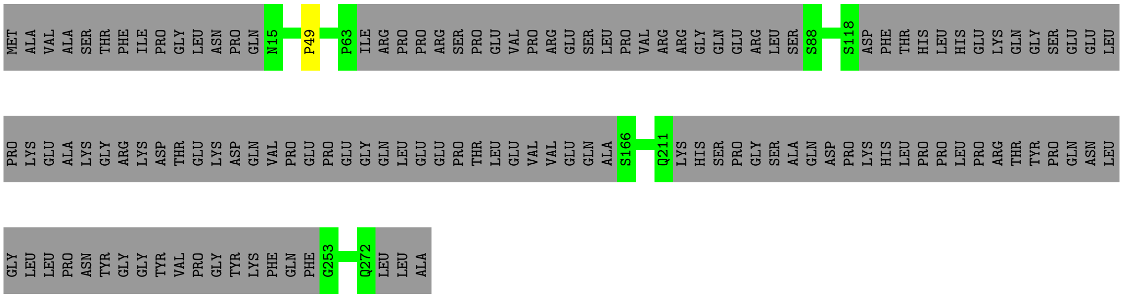
- Molecule 18: Protein FAM166B



- Molecule 18: Protein FAM166B

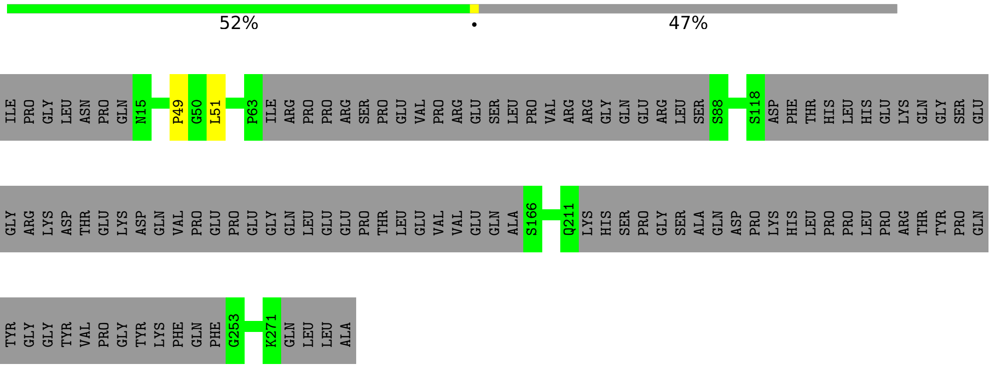


- Molecule 18: Protein FAM166B



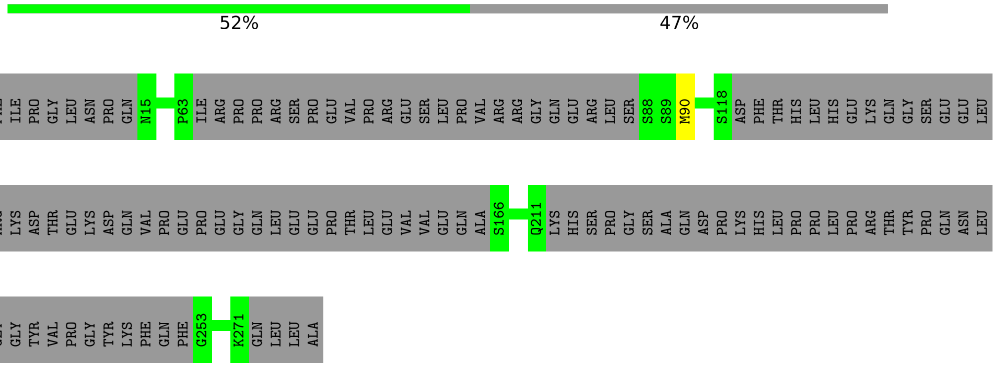
- Molecule 18: Protein FAM166B

Chain K:



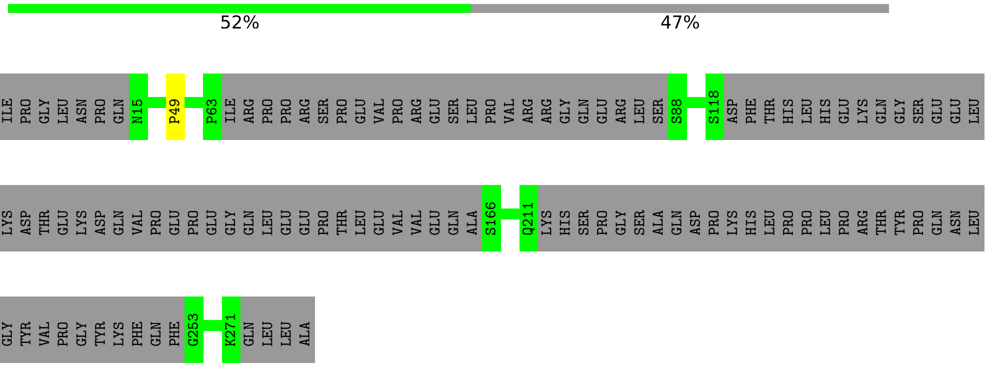
- Molecule 18: Protein FAM166B

Chain L:

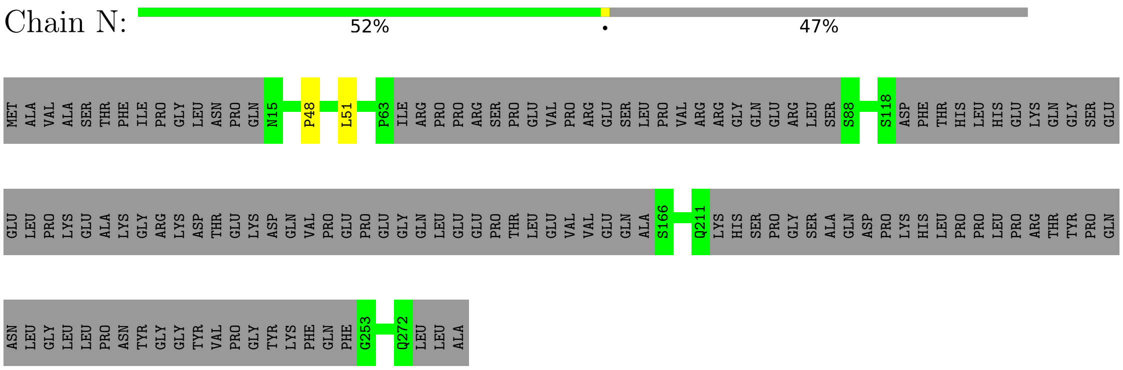


- Molecule 18: Protein FAM166B

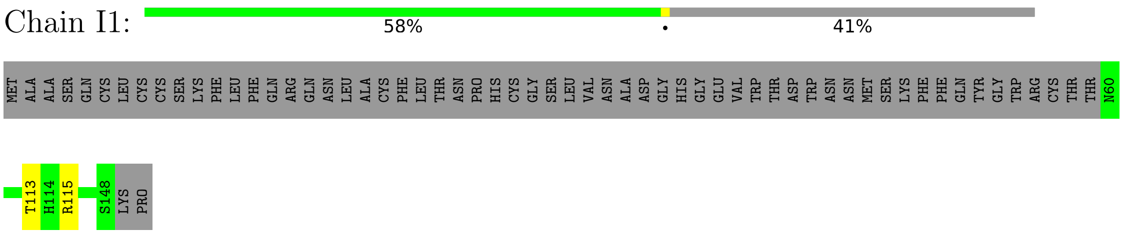
Chain M:



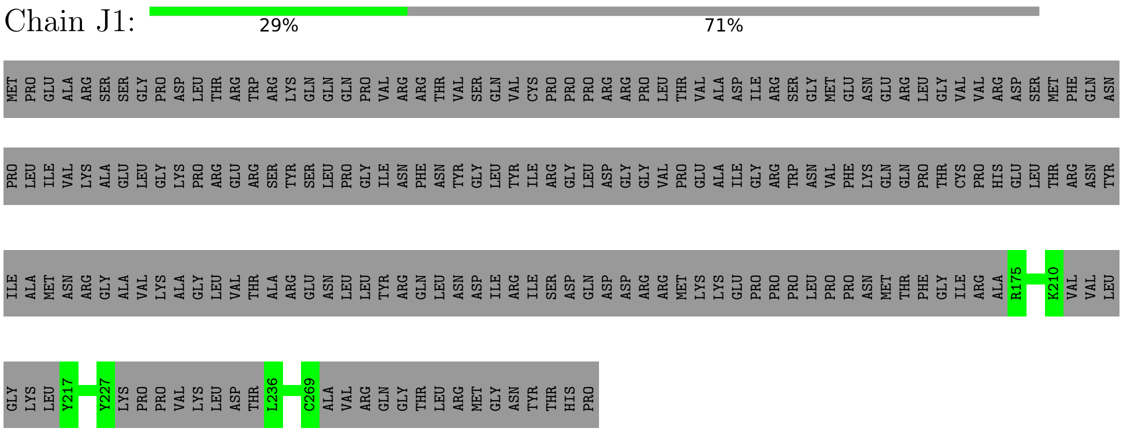
- Molecule 18: Protein FAM166B



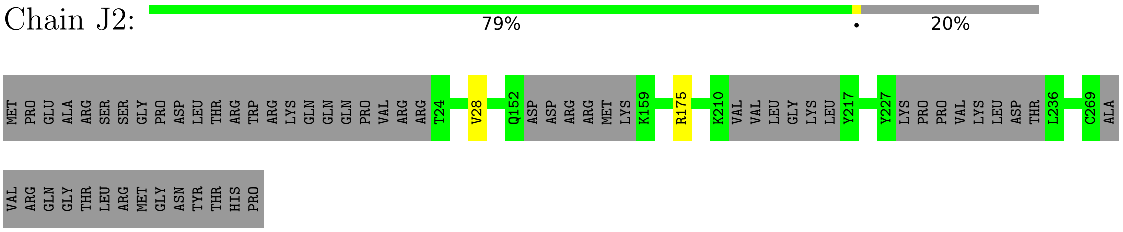
- Molecule 19: UPF0686 protein C11orf1



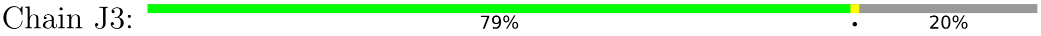
- Molecule 20: Isoform 2 of Cilia- and flagella-associated protein 77

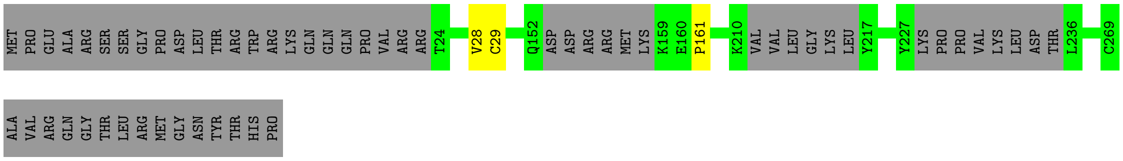


- Molecule 20: Isoform 2 of Cilia- and flagella-associated protein 77



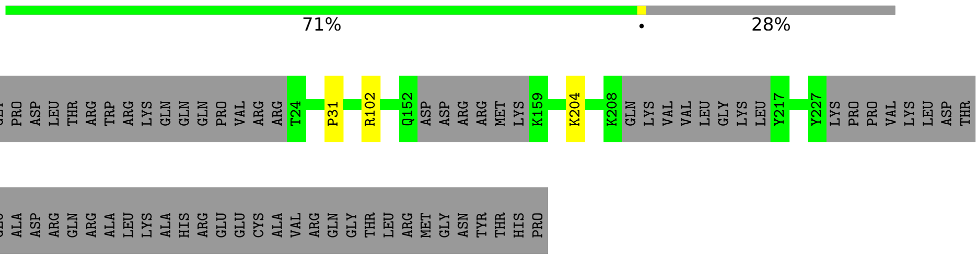
- Molecule 20: Isoform 2 of Cilia- and flagella-associated protein 77





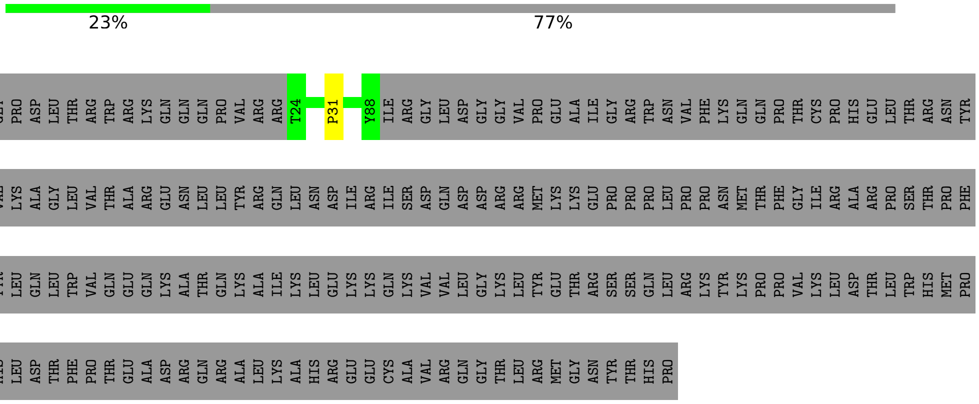
- Molecule 20: Isoform 2 of Cilia- and flagella-associated protein 77

Chain J4:



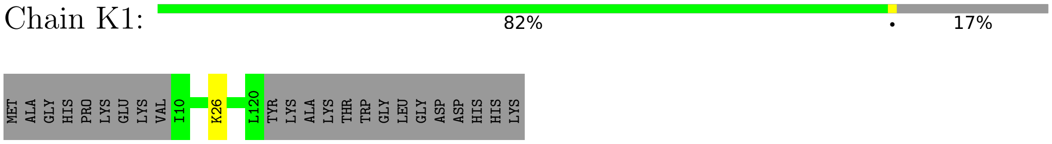
- Molecule 20: Isoform 2 of Cilia- and flagella-associated protein 77

Chain J5:



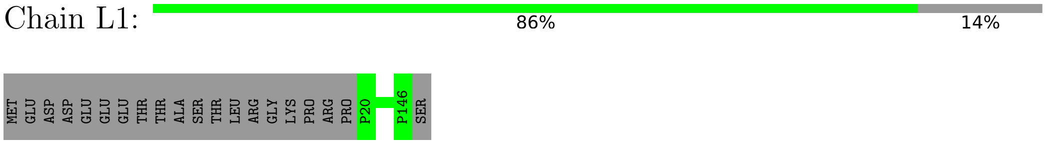
- Molecule 21: Protein FAM183A

Chain K1:



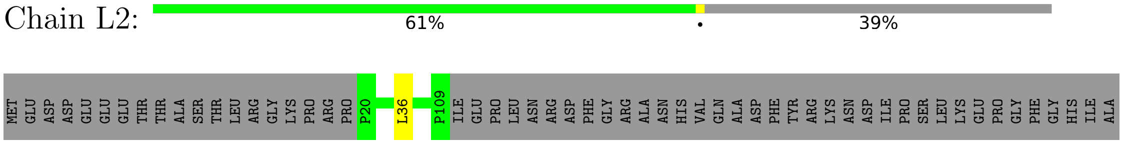
- Molecule 22: Uncharacterized protein C5orf49

Chain L1:



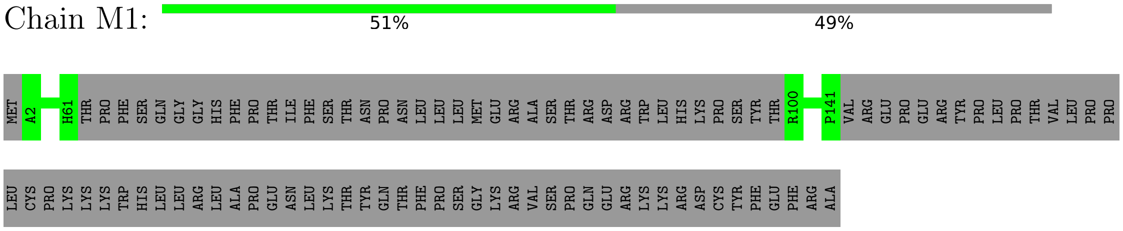
- Molecule 22: Uncharacterized protein C5orf49

Chain L2:



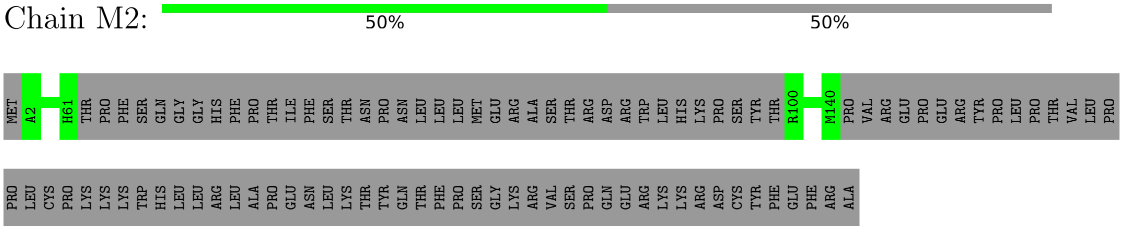
- Molecule 23: Protein FAM166C

Chain M1:



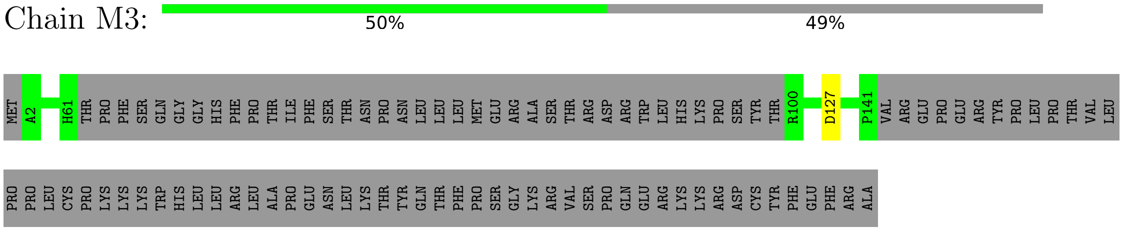
- Molecule 23: Protein FAM166C

Chain M2:



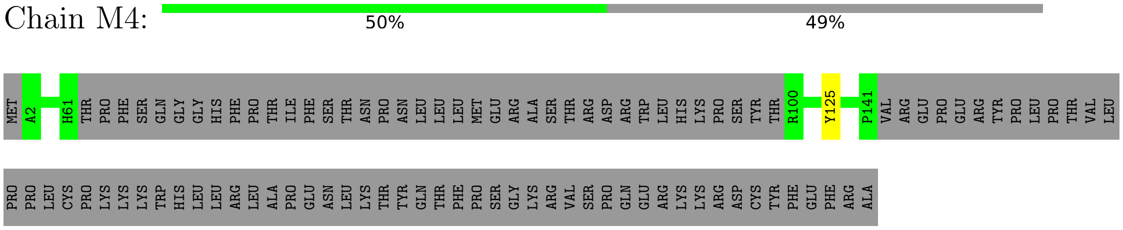
- Molecule 23: Protein FAM166C

Chain M3:



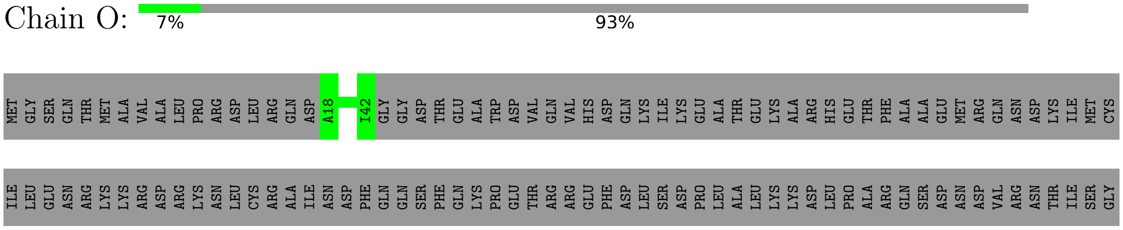
- Molecule 23: Protein FAM166C

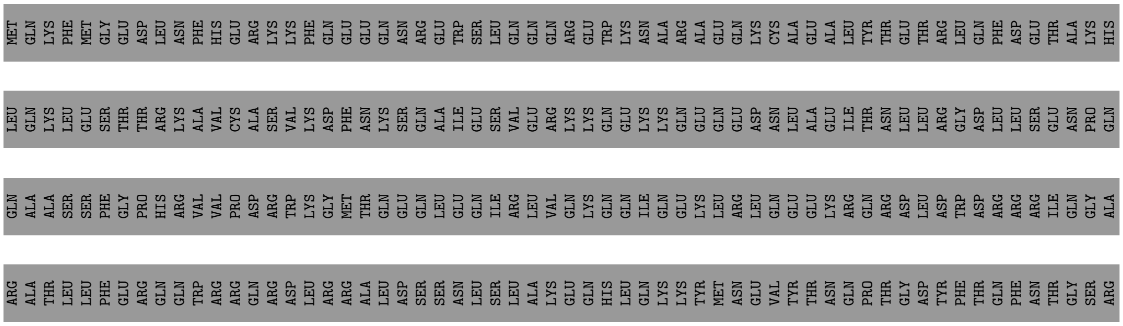
Chain M4:



- Molecule 24: RIB43A-like with coiled-coils protein 2

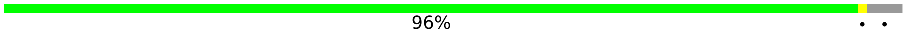
Chain O:





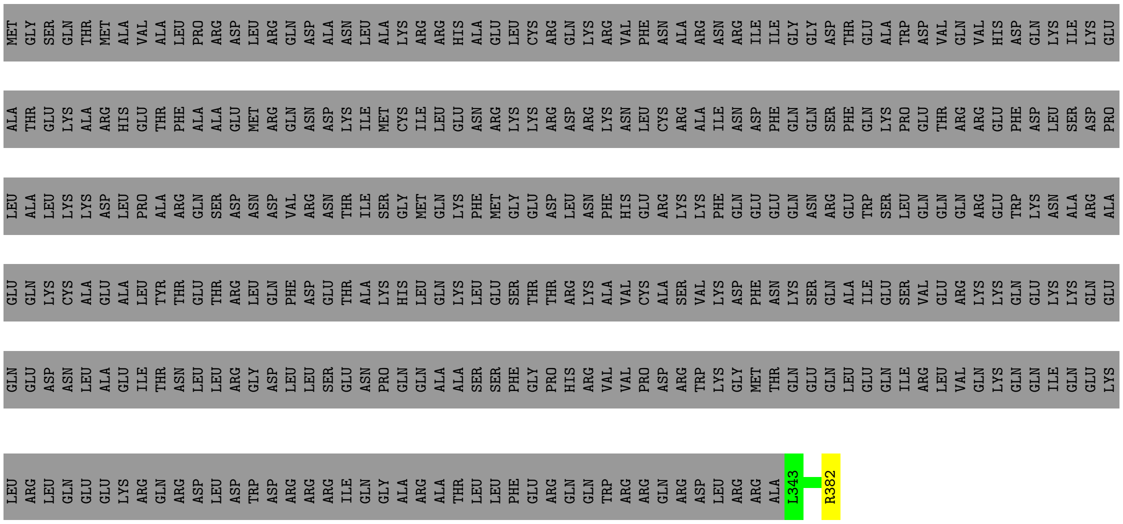
- Molecule 24: RIB43A-like with coiled-coils protein 2

Chain P:



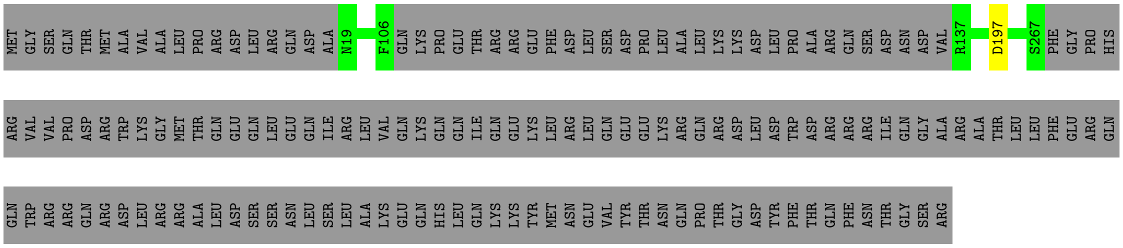
- Molecule 24: RIB43A-like with coiled-coils protein 2

Chain Q:



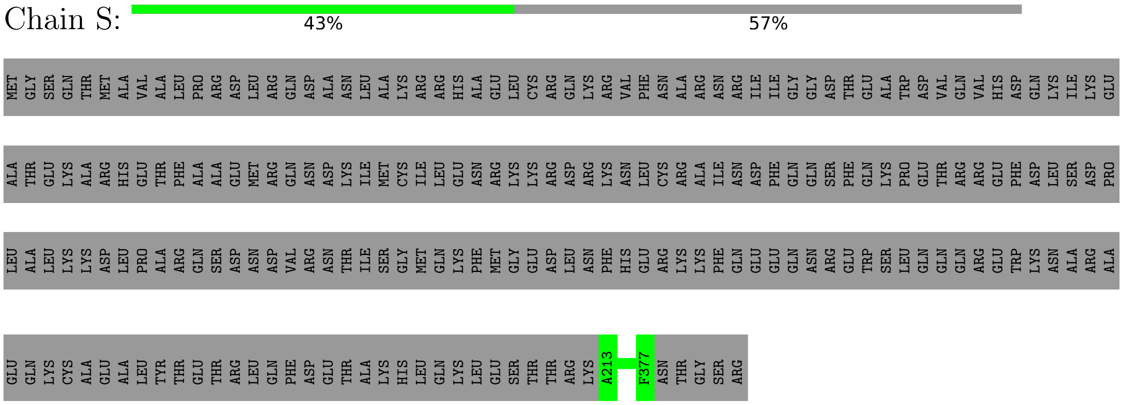
- Molecule 24: RIB43A-like with coiled-coils protein 2

Chain R:



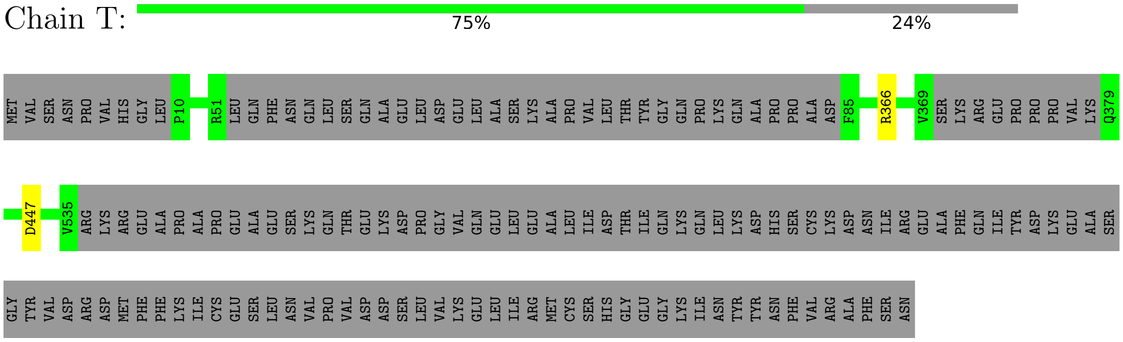
- Molecule 24: RIB43A-like with coiled-coils protein 2

Chain S:



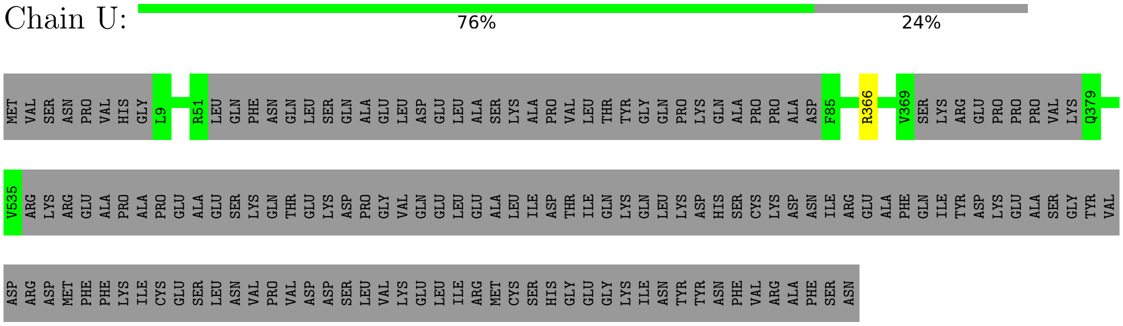
- Molecule 25: EF-hand domain-containing protein 1

Chain T:



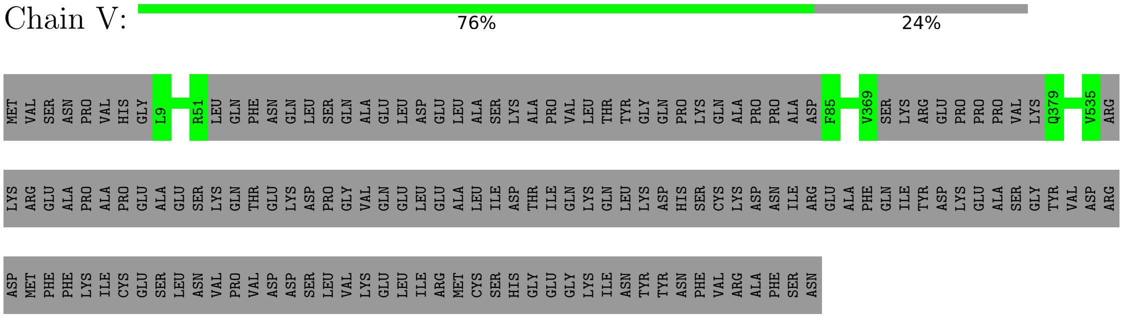
- Molecule 25: EF-hand domain-containing protein 1

Chain U:



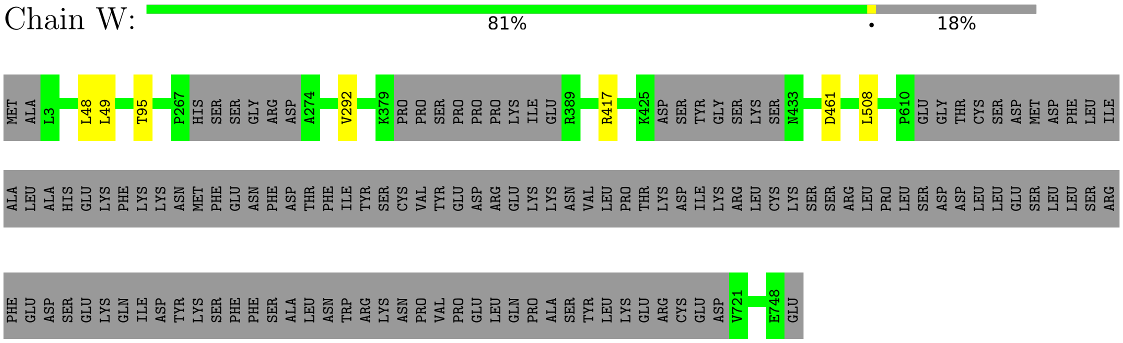
- Molecule 25: EF-hand domain-containing protein 1

Chain V:



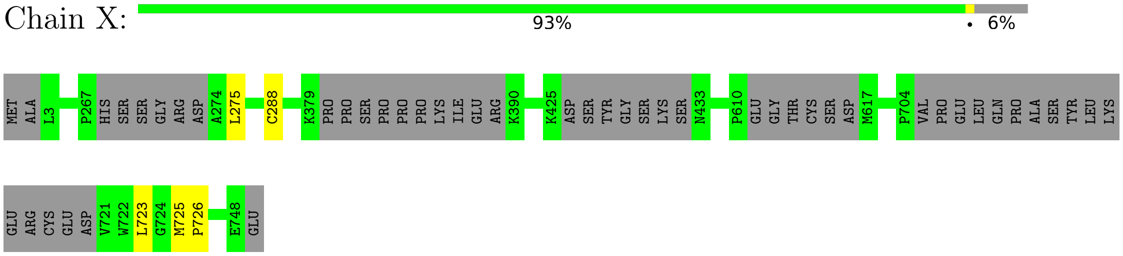
- Molecule 26: EF-hand domain-containing family member C2

Chain W:



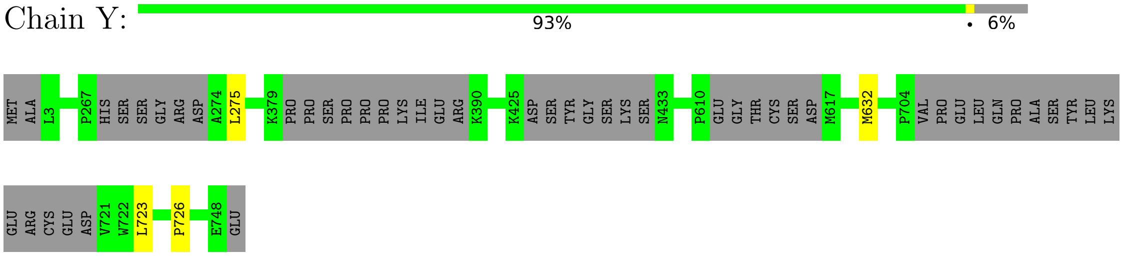
- Molecule 26: EF-hand domain-containing family member C2

Chain X:



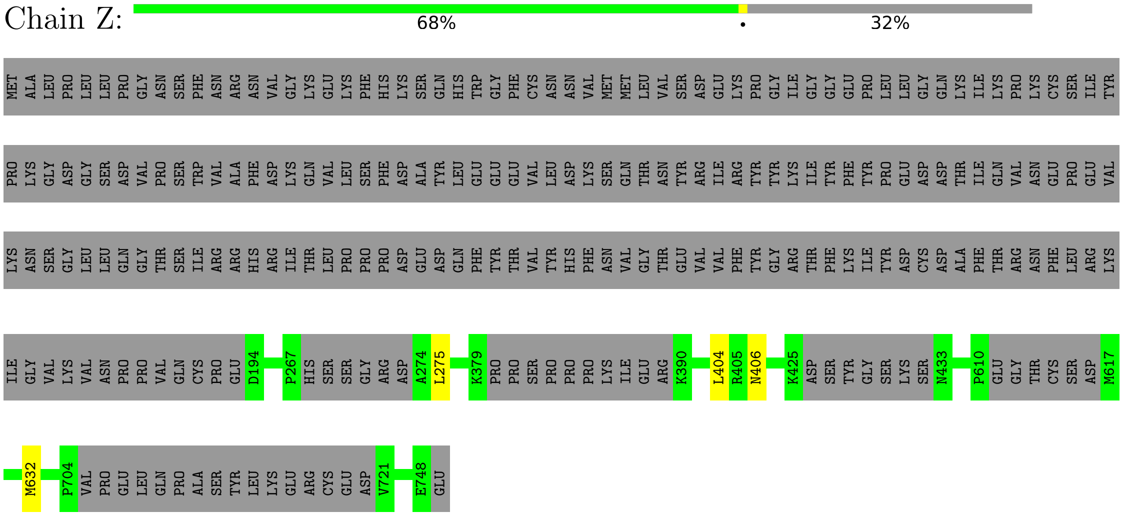
- Molecule 26: EF-hand domain-containing family member C2

Chain Y:



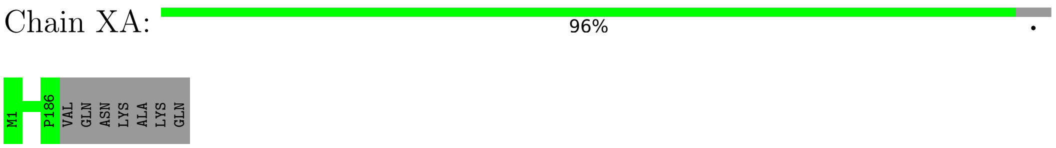
- Molecule 26: EF-hand domain-containing family member C2

Chain Z:



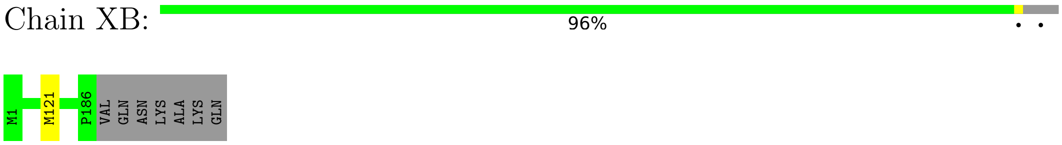
- Molecule 27: Cilia- and flagella-associated protein 20

Chain XA:



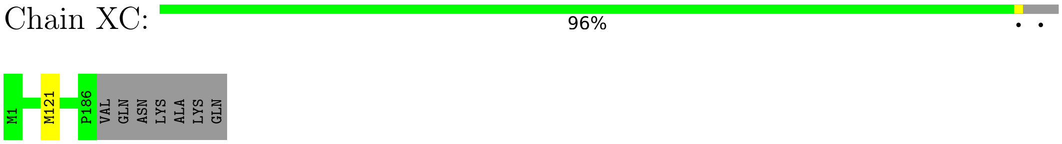
- Molecule 27: Cilia- and flagella-associated protein 20

Chain XB:



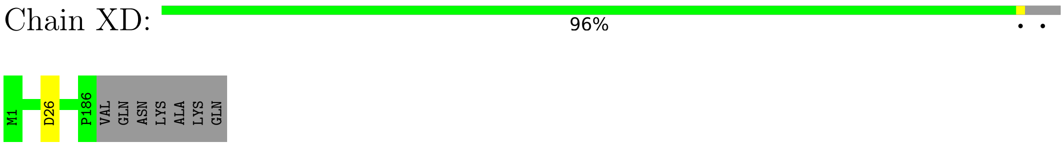
- Molecule 27: Cilia- and flagella-associated protein 20

Chain XC:



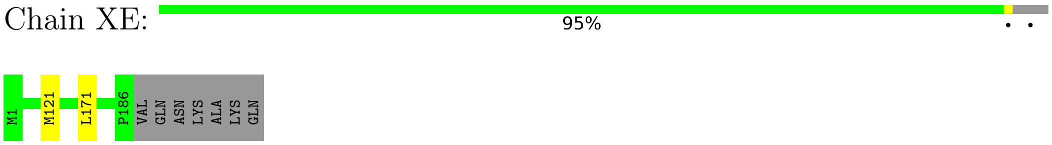
- Molecule 27: Cilia- and flagella-associated protein 20

Chain XD:



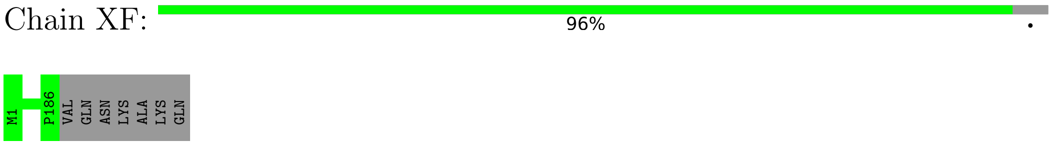
- Molecule 27: Cilia- and flagella-associated protein 20

Chain XE:



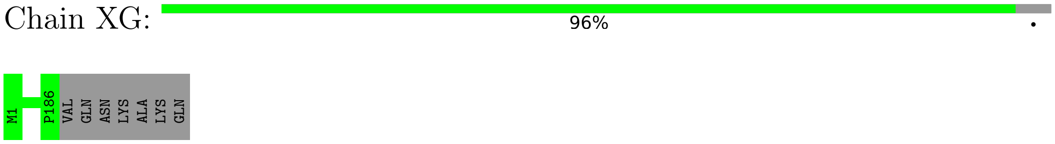
- Molecule 27: Cilia- and flagella-associated protein 20

Chain XF:



- Molecule 27: Cilia- and flagella-associated protein 20

Chain XG:



- Molecule 28: Parkin coregulated gene protein

Chain YB:

- Molecule 28: Parkin coregulated gene protein

Chain YC:

- Molecule 28: Parkin coregulated gene protein

Chain YD:

- Molecule 28: Parkin coregulated gene protein

Chain YE:

- Molecule 28: Parkin coregulated gene protein

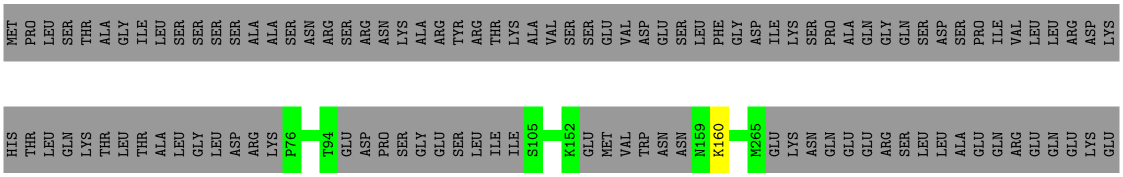
Chain YF:

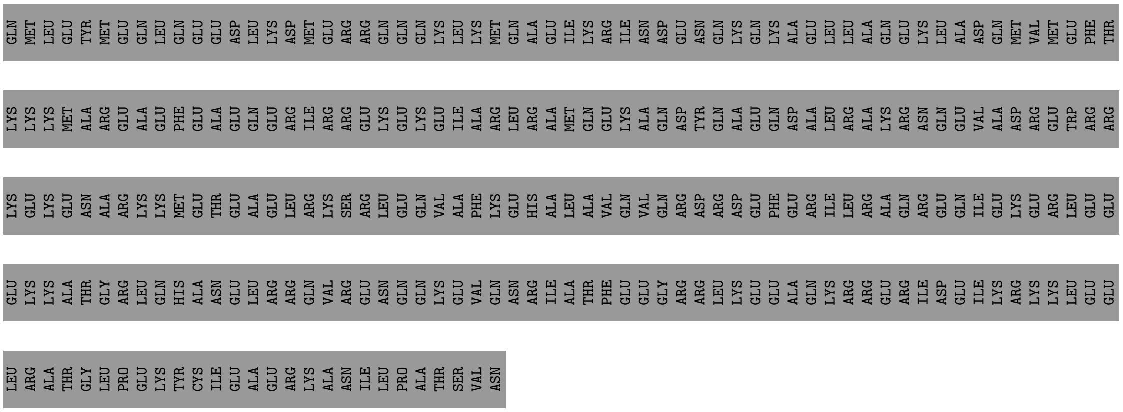
- Molecule 28: Parkin coregulated gene protein

Chain YG:

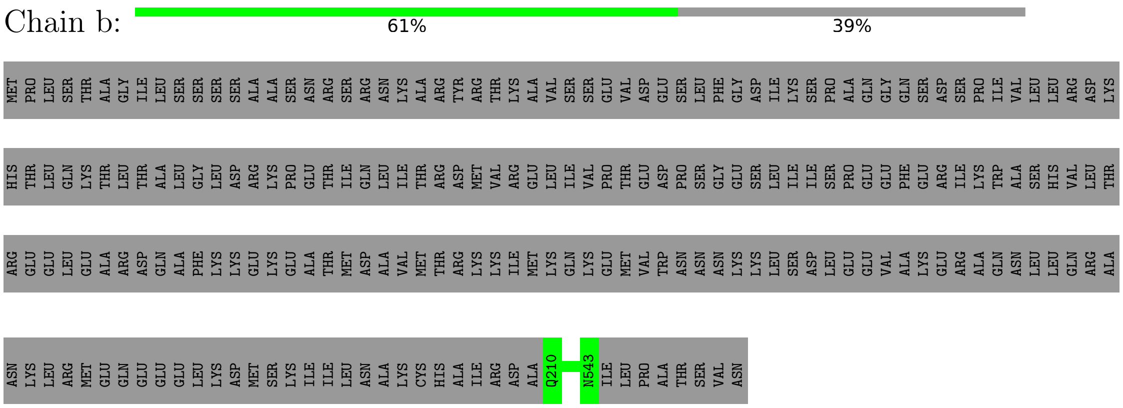
- Molecule 29: Cilia- and flagella-associated protein 45

Chain a:

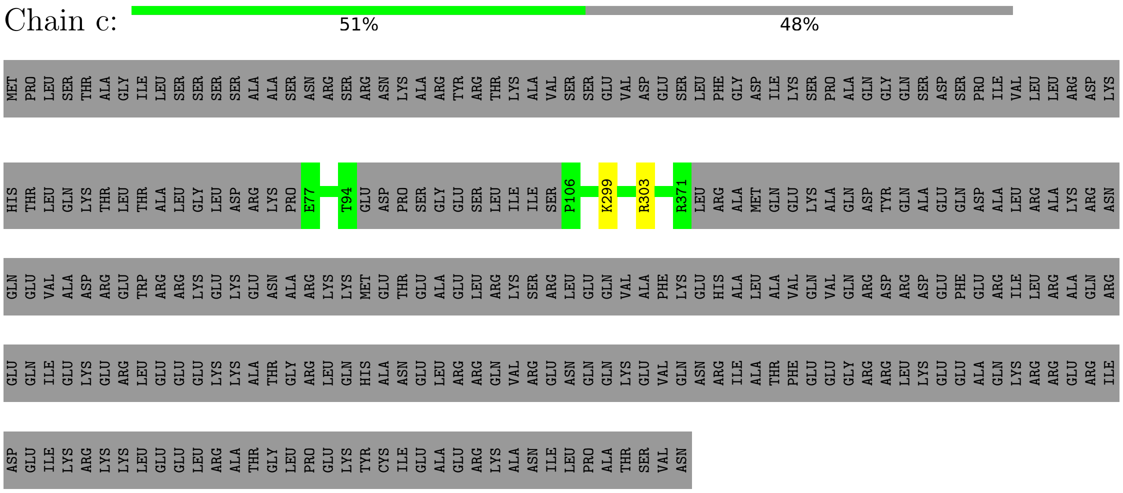




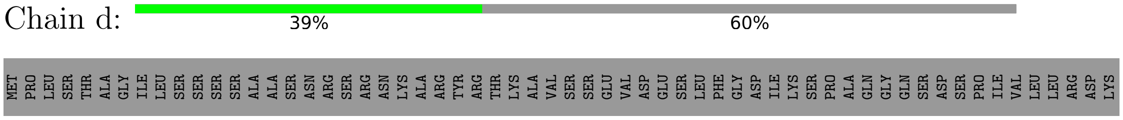
- Molecule 29: Cilia- and flagella-associated protein 45



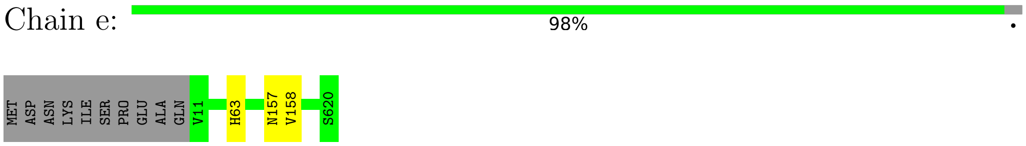
- Molecule 29: Cilia- and flagella-associated protein 45



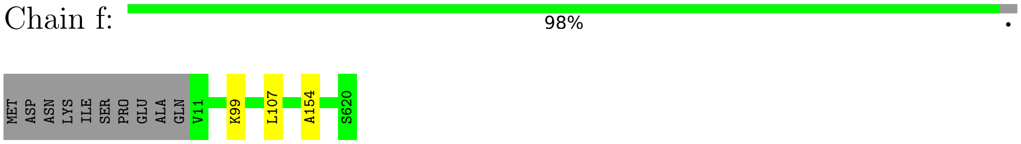
- Molecule 29: Cilia- and flagella-associated protein 45



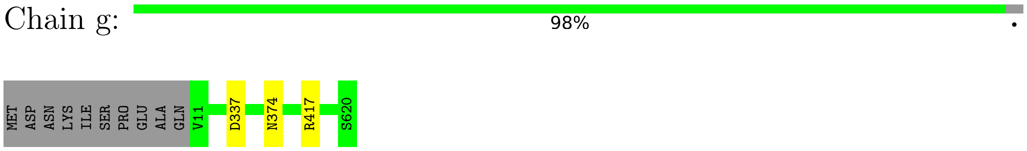
- Molecule 30: Cilia- and flagella-associated protein 52



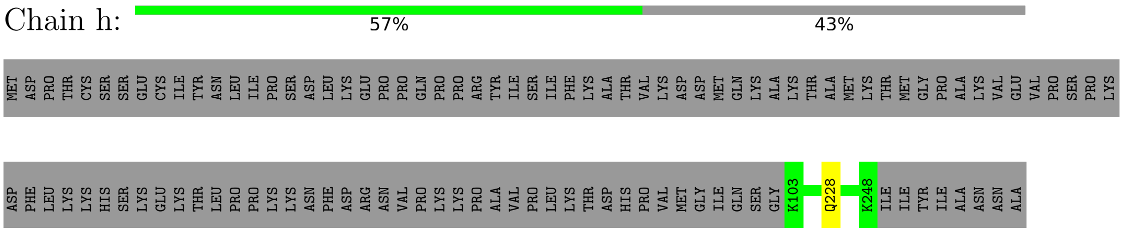
- Molecule 30: Cilia- and flagella-associated protein 52



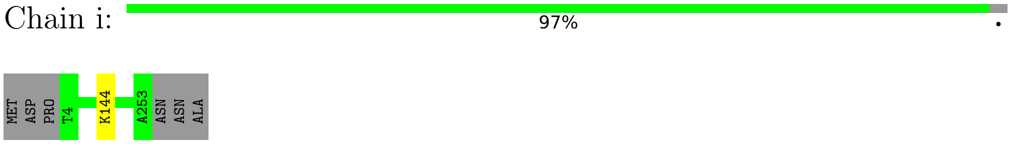
- Molecule 30: Cilia- and flagella-associated protein 52



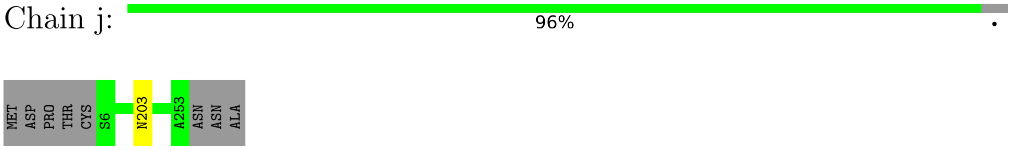
- Molecule 31: Enkurin



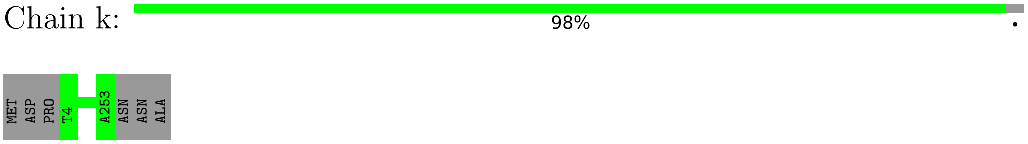
- Molecule 31: Enkurin



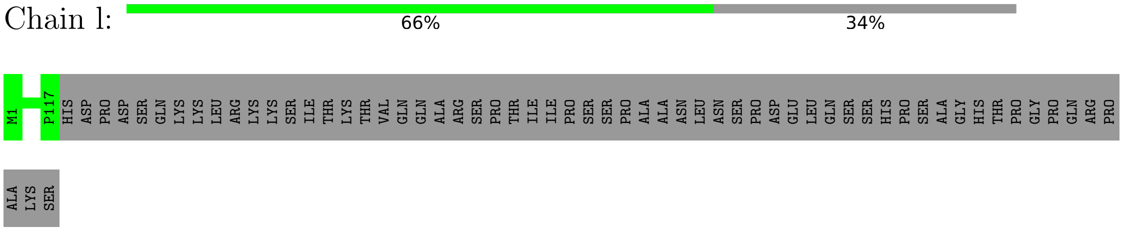
- Molecule 31: Enkurin



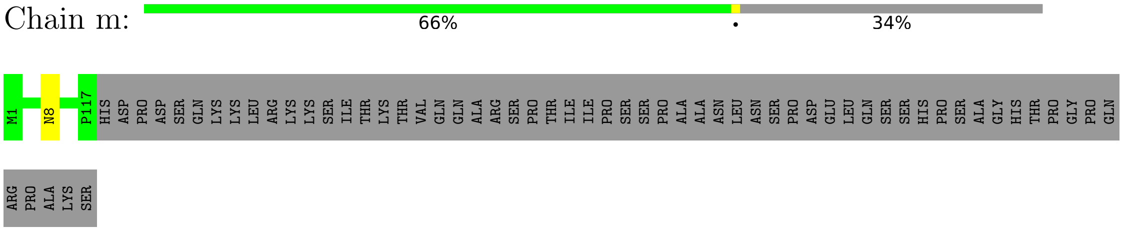
- Molecule 31: Enkurin



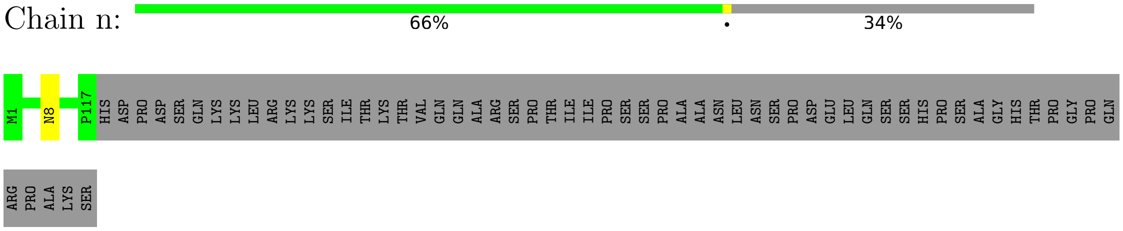
- Molecule 32: Protein Flattop



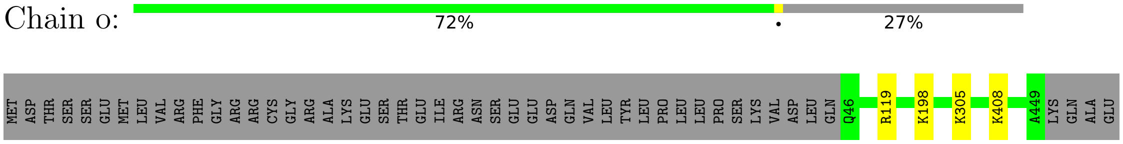
- Molecule 32: Protein Flattop



- Molecule 32: Protein Flattop



- Molecule 33: Protein CFAP210



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

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

- Molecule 33: Protein CFAP210

Chain o1:

MET ASP THR SER SER GLU MET LEU VAL ARG PHE GLY ARG ARG CYS GLY ARG ALA LYS GLU SER THR GLU ILE ARG ASN SER GLU GLU ASP GLN VAL LEU TYR LEU PRO LEU LEU PRO SER LYS VAL ASP LEU GLN Q46 E81 MET HIS LEU ARG SER GLN GLU VAL VAL LYS HIS TRP

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

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

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

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

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

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

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

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

- Molecule 33: Protein CFAP210

Chain p:

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

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

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

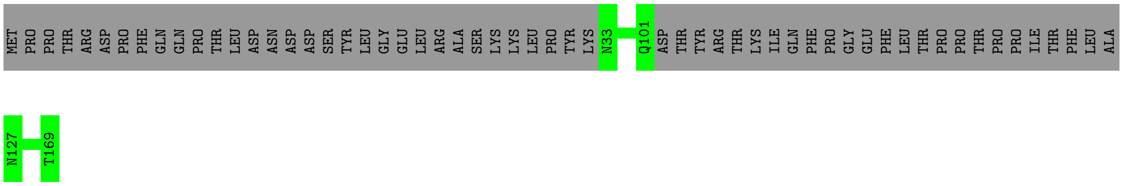
SER ASP LYS LYS TRP GLU GLU GLN LEU LYS LEU ASN ILE GLU LYS ALA PHE LYS GLU GLU GLN GLU LYS ALA GLU LYS ARG HIS ARG GLU ARG VAL ALA LEU ALA LYS ASP HIS LEU LYS GLN ILE LYS GLU HIS GLU GLU GLU GLU GLU ARG ARG LYS LYS TYR GLU GLU LYS ASP ALA

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

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

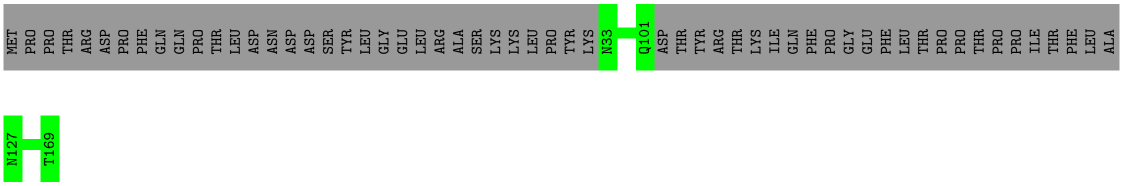
- Molecule 34: Protein CFAP276

Chain q:



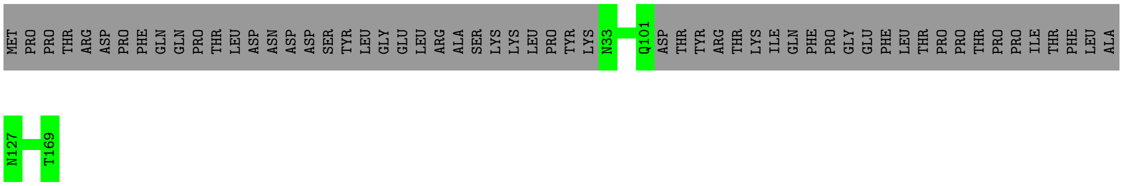
- Molecule 34: Protein CFAP276

Chain r:



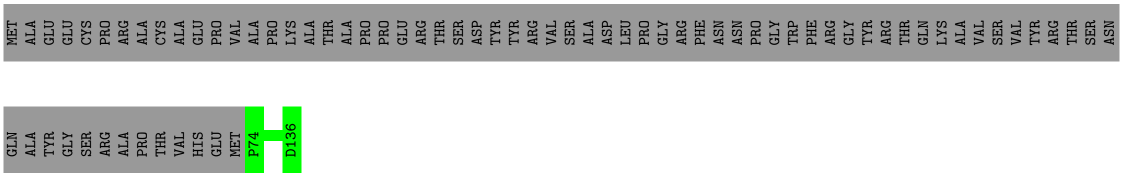
- Molecule 34: Protein CFAP276

Chain s:



- Molecule 35: UPF0691 protein C9orf116

Chain y:



- Molecule 35: UPF0691 protein C9orf116

Chain z:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208558	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 $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP, 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	0.29	0/429	0.64	0/580
1	7	0.28	0/1227	0.59	0/1659
2	1	0.27	0/2265	0.55	0/3049
2	2	0.27	0/3697	0.53	0/4999
3	3	0.33	0/2531	0.58	0/3362
3	4	0.35	0/1851	0.57	0/2456
4	5	0.27	0/3006	0.55	0/4056
4	6	0.28	0/3006	0.54	1/4056 (0.0%)
5	8	0.30	0/1467	0.61	1/1999 (0.1%)
5	9	0.27	0/422	0.57	0/570
6	A	0.29	0/429	0.45	0/571
7	A0	0.29	0/1785	0.53	0/2399
7	A1	0.32	0/3221	0.56	2/4335 (0.0%)
7	A2	0.33	0/3221	0.56	0/4335
7	A3	0.32	0/2744	0.57	0/3689
7	A4	0.31	0/303	0.66	0/410
8	AA	0.28	0/3507	0.52	1/4761 (0.0%)
8	AC	0.29	0/3507	0.55	2/4761 (0.0%)
8	AE	0.28	0/3507	0.55	0/4761
8	AG	0.29	0/3507	0.54	3/4761 (0.1%)
8	AI	0.28	0/3507	0.54	0/4761
8	AK	0.29	0/3507	0.54	0/4761
8	AM	0.28	0/3507	0.53	2/4761 (0.0%)
8	BA	0.27	0/3460	0.55	1/4697 (0.0%)
8	BC	0.26	0/3507	0.52	0/4761
8	BE	0.29	0/3460	0.57	2/4697 (0.0%)
8	BG	0.28	0/3507	0.55	2/4761 (0.0%)
8	BI	0.28	0/3460	0.56	3/4697 (0.1%)
8	BK	0.28	0/3507	0.56	1/4761 (0.0%)
8	BM	0.29	0/3464	0.54	0/4702
8	CA	0.26	0/3462	0.53	1/4700 (0.0%)
8	CC	0.27	0/3507	0.53	0/4761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	CE	0.26	0/3448	0.55	0/4681
8	CG	0.27	0/3507	0.53	2/4761 (0.0%)
8	CI	0.28	0/3454	0.56	0/4689
8	CK	0.28	0/3507	0.57	2/4761 (0.0%)
8	CM	0.29	0/3454	0.55	0/4689
8	DA	0.27	0/3041	0.56	1/4133 (0.0%)
8	DC	0.26	0/3448	0.54	0/4681
8	DE	0.27	0/3456	0.54	0/4692
8	DG	0.27	0/3448	0.54	1/4681 (0.0%)
8	DI	0.27	0/3448	0.55	0/4681
8	DK	0.26	0/3448	0.55	1/4681 (0.0%)
8	DM	0.26	0/3456	0.53	1/4692 (0.0%)
8	EC	0.27	0/3507	0.57	0/4761
8	EE	0.27	0/3507	0.54	0/4761
8	EG	0.27	0/3501	0.56	0/4753
8	EI	0.27	0/3507	0.56	0/4761
8	EK	0.26	0/3501	0.54	0/4753
8	EM	0.27	0/3501	0.58	1/4753 (0.0%)
8	FC	0.26	0/3456	0.54	1/4692 (0.0%)
8	FE	0.28	0/3456	0.57	2/4692 (0.0%)
8	FG	0.28	0/3448	0.56	2/4681 (0.0%)
8	FI	0.27	0/3448	0.56	0/4681
8	FK	0.27	0/3448	0.55	0/4681
8	FM	0.26	0/3448	0.55	1/4681 (0.0%)
8	GC	0.27	0/3486	0.56	1/4732 (0.0%)
8	GE	0.27	0/3448	0.56	1/4681 (0.0%)
8	GG	0.26	0/3456	0.55	0/4692
8	GI	0.27	0/3448	0.55	0/4681
8	GK	0.27	0/3462	0.55	1/4700 (0.0%)
8	GM	0.28	0/3479	0.58	2/4722 (0.0%)
8	HC	0.26	0/3456	0.53	1/4692 (0.0%)
8	HE	0.26	0/3462	0.52	0/4700
8	HG	0.27	0/3462	0.56	2/4700 (0.0%)
8	HI	0.26	0/3462	0.52	0/4700
8	HK	0.28	0/3454	0.55	1/4689 (0.0%)
8	HM	0.28	0/3456	0.54	0/4692
8	HO	0.28	0/3126	0.57	1/4238 (0.0%)
8	IC	0.26	0/3470	0.53	0/4711
8	IE	0.28	0/3456	0.55	0/4692
8	IG	0.26	0/3507	0.54	2/4761 (0.0%)
8	II	0.27	0/3462	0.54	0/4700
8	IK	0.26	0/3507	0.51	0/4761
8	IM	0.29	0/3456	0.56	0/4692

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	IO	0.27	0/3454	0.56	1/4689 (0.0%)
8	JC	0.26	0/3507	0.53	0/4761
8	JE	0.27	0/3448	0.54	1/4681 (0.0%)
8	JG	0.27	0/3448	0.53	0/4681
8	JI	0.27	0/3448	0.54	0/4681
8	JK	0.29	0/3454	0.58	3/4689 (0.1%)
8	JM	0.26	0/3448	0.54	0/4681
8	KC	0.30	0/3467	0.55	0/4707
8	KE	0.28	0/3462	0.53	0/4700
8	KG	0.30	0/3467	0.55	0/4707
8	KI	0.31	0/3450	0.55	1/4684 (0.0%)
8	KK	0.29	0/3467	0.56	2/4707 (0.0%)
8	KM	0.29	0/3501	0.55	2/4753 (0.0%)
8	KO	0.29	0/3460	0.54	0/4697
8	LC	0.29	0/3466	0.54	0/4705
8	LE	0.28	0/3507	0.53	0/4761
8	LG	0.30	0/3474	0.56	2/4716 (0.0%)
8	LI	0.29	0/3487	0.54	1/4732 (0.0%)
8	LK	0.30	0/3467	0.56	1/4707 (0.0%)
8	LM	0.29	0/3456	0.52	0/4692
8	MC	0.28	0/3514	0.55	0/4771
8	ME	0.28	0/3463	0.54	1/4702 (0.0%)
8	MG	0.28	0/3461	0.54	0/4699
8	MI	0.29	0/3469	0.53	0/4710
8	MK	0.28	0/3514	0.55	1/4771 (0.0%)
8	MM	0.30	0/3514	0.54	0/4771
8	NC	0.28	0/3514	0.56	0/4771
8	NE	0.27	0/3507	0.54	0/4761
8	NG	0.27	0/3507	0.58	4/4761 (0.1%)
8	NI	0.27	0/3507	0.55	1/4761 (0.0%)
8	NK	0.26	0/3507	0.54	0/4761
8	NM	0.27	0/3507	0.54	1/4761 (0.0%)
8	OC	0.29	0/3523	0.55	1/4783 (0.0%)
8	OE	0.28	0/3514	0.56	2/4771 (0.0%)
8	OG	0.28	0/3523	0.53	0/4783
8	OI	0.29	0/3523	0.54	0/4783
8	OK	0.26	0/3507	0.52	0/4761
8	OM	0.29	0/3523	0.54	1/4783 (0.0%)
8	OO	0.29	0/3384	0.54	0/4588
8	PC	0.29	0/3523	0.55	1/4783 (0.0%)
8	PE	0.29	0/3514	0.54	1/4771 (0.0%)
8	PG	0.28	0/3523	0.54	0/4783
8	PI	0.27	0/3507	0.51	0/4761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	PK	0.28	0/3514	0.55	1/4771 (0.0%)
8	PM	0.27	0/3507	0.53	0/4761
8	PO	0.27	0/3507	0.53	0/4761
8	QC	0.28	0/3514	0.55	0/4771
8	QE	0.28	0/3514	0.52	0/4771
8	QG	0.28	0/3514	0.55	2/4771 (0.0%)
8	QI	0.28	0/3514	0.54	0/4771
8	QK	0.27	0/3514	0.53	0/4771
8	QM	0.29	0/3514	0.55	2/4771 (0.0%)
8	QO	0.27	0/3514	0.55	0/4771
8	RC	0.28	0/3278	0.55	0/4451
8	RE	0.27	0/3448	0.54	0/4681
8	RG	0.27	0/3461	0.57	0/4699
8	RI	0.27	0/3507	0.55	0/4761
8	RK	0.28	0/3514	0.58	2/4771 (0.0%)
8	RM	0.28	0/3514	0.56	1/4771 (0.0%)
8	RO	0.27	0/3507	0.55	0/4761
8	SE	0.27	0/3442	0.56	0/4673
8	SG	0.27	0/3450	0.54	0/4684
8	SI	0.27	0/3456	0.55	0/4692
8	SK	0.26	0/3456	0.54	2/4692 (0.0%)
8	SM	0.27	0/3456	0.57	1/4692 (0.0%)
8	SO	0.27	0/3456	0.55	2/4692 (0.0%)
8	TE	0.27	0/3442	0.57	0/4673
8	TG	0.28	0/3450	0.58	0/4684
8	TI	0.27	0/3456	0.52	0/4692
8	TK	0.27	0/3442	0.53	0/4673
8	TM	0.27	0/3456	0.55	2/4692 (0.0%)
8	TO	0.28	0/3442	0.58	0/4673
8	UE	0.26	0/3456	0.52	1/4692 (0.0%)
8	UG	0.26	0/3462	0.56	2/4700 (0.0%)
8	UI	0.27	0/3462	0.56	2/4700 (0.0%)
8	UK	0.26	0/3456	0.53	0/4692
8	UM	0.26	0/3456	0.55	0/4692
8	UO	0.26	0/3456	0.54	1/4692 (0.0%)
8	VE	0.26	0/3507	0.54	0/4761
8	VG	0.28	0/3470	0.58	2/4711 (0.0%)
8	VI	0.27	0/3507	0.52	0/4761
8	VK	0.27	0/3456	0.54	0/4692
8	VM	0.27	0/3507	0.53	1/4761 (0.0%)
8	VO	0.26	0/3456	0.53	0/4692
8	WE	0.27	0/3507	0.55	0/4761
8	WG	0.26	0/3448	0.55	1/4681 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	WI	0.27	0/3501	0.55	0/4753
8	WK	0.29	0/3448	0.55	0/4681
8	WM	0.28	0/3507	0.57	2/4761 (0.0%)
8	WO	0.28	0/3456	0.55	0/4692
9	AB	0.30	0/3509	0.58	1/4754 (0.0%)
9	AD	0.30	0/3509	0.60	1/4754 (0.0%)
9	AF	0.31	0/3509	0.58	2/4754 (0.0%)
9	AH	0.30	0/3509	0.58	2/4754 (0.0%)
9	AJ	0.31	0/3509	0.58	1/4754 (0.0%)
9	AL	0.31	0/3509	0.59	1/4754 (0.0%)
9	BB	0.27	0/3431	0.55	0/4649
9	BD	0.28	0/3423	0.55	1/4638 (0.0%)
9	BF	0.28	0/3431	0.55	1/4649 (0.0%)
9	BH	0.29	0/3423	0.57	1/4638 (0.0%)
9	BJ	0.30	0/3448	0.59	2/4673 (0.0%)
9	BL	0.30	0/3423	0.57	1/4638 (0.0%)
9	CB	0.29	0/3436	0.59	2/4656 (0.0%)
9	CD	0.27	0/3423	0.56	0/4638
9	CF	0.29	0/3431	0.57	1/4649 (0.0%)
9	CH	0.28	0/3423	0.57	1/4638 (0.0%)
9	CJ	0.28	0/3431	0.56	1/4649 (0.0%)
9	CL	0.29	0/3423	0.56	0/4638
9	DB	0.27	0/3423	0.59	4/4638 (0.1%)
9	DD	0.28	0/3423	0.60	2/4638 (0.0%)
9	DF	0.29	0/3423	0.59	2/4638 (0.0%)
9	DH	0.28	0/3423	0.61	1/4638 (0.0%)
9	DJ	0.28	0/3423	0.59	2/4638 (0.0%)
9	DL	0.29	0/3423	0.60	3/4638 (0.1%)
9	EB	0.28	0/3423	0.58	1/4638 (0.0%)
9	ED	0.27	0/3423	0.57	1/4638 (0.0%)
9	EF	0.28	0/3423	0.58	1/4638 (0.0%)
9	EH	0.28	0/3423	0.59	3/4638 (0.1%)
9	EJ	0.27	0/3423	0.57	2/4638 (0.0%)
9	EL	0.27	0/3423	0.56	0/4638
9	EN	0.28	0/3436	0.60	1/4656 (0.0%)
9	FB	0.26	0/3423	0.55	0/4638
9	FD	0.27	0/3423	0.58	0/4638
9	FF	0.28	0/3423	0.59	0/4638
9	FH	0.28	0/3423	0.58	1/4638 (0.0%)
9	FJ	0.28	0/3423	0.58	1/4638 (0.0%)
9	FL	0.27	0/3423	0.58	0/4638
9	FN	0.27	0/3431	0.57	1/4649 (0.0%)
9	GB	0.28	0/3277	0.59	1/4441 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	GD	0.28	0/3423	0.55	1/4638 (0.0%)
9	GF	0.27	0/3431	0.58	2/4649 (0.0%)
9	GH	0.28	0/3423	0.58	0/4638
9	GJ	0.29	0/3448	0.60	2/4673 (0.0%)
9	GL	0.28	0/3423	0.58	0/4638
9	GN	0.26	0/3423	0.55	1/4638 (0.0%)
9	HB	0.27	0/3431	0.56	2/4649 (0.0%)
9	HD	0.27	0/3423	0.55	2/4638 (0.0%)
9	HF	0.27	0/3431	0.53	0/4649
9	HH	0.27	0/3423	0.55	1/4638 (0.0%)
9	HJ	0.28	0/3436	0.59	2/4656 (0.0%)
9	HL	0.28	0/3423	0.57	2/4638 (0.0%)
9	HN	0.28	0/3414	0.60	3/4626 (0.1%)
9	IB	0.28	0/3265	0.56	2/4424 (0.0%)
9	ID	0.27	0/3423	0.53	1/4638 (0.0%)
9	IF	0.28	0/3436	0.58	3/4656 (0.1%)
9	IH	0.29	0/3423	0.57	2/4638 (0.0%)
9	IJ	0.28	0/3443	0.56	1/4666 (0.0%)
9	IL	0.28	0/3423	0.56	2/4638 (0.0%)
9	IN	0.28	0/3431	0.57	1/4649 (0.0%)
9	JB	0.27	0/3423	0.55	0/4638
9	JD	0.27	0/3423	0.55	1/4638 (0.0%)
9	JF	0.27	0/3431	0.56	2/4649 (0.0%)
9	JH	0.28	0/3423	0.58	1/4638 (0.0%)
9	JJ	0.27	0/3423	0.54	1/4638 (0.0%)
9	JL	0.29	0/3423	0.60	3/4638 (0.1%)
9	JN	0.29	0/3423	0.60	2/4638 (0.0%)
9	KB	0.29	0/3290	0.56	2/4458 (0.0%)
9	KD	0.31	0/3457	0.57	1/4685 (0.0%)
9	KF	0.28	0/3423	0.55	1/4638 (0.0%)
9	KH	0.32	0/3457	0.58	2/4685 (0.0%)
9	KJ	0.28	0/3423	0.55	1/4638 (0.0%)
9	KL	0.31	0/3457	0.60	2/4685 (0.0%)
9	KN	0.29	0/3423	0.55	3/4638 (0.1%)
9	LB	0.29	0/3532	0.56	1/4785 (0.0%)
9	LD	0.29	0/3423	0.55	1/4638 (0.0%)
9	LF	0.30	0/3527	0.56	0/4778
9	LH	0.29	0/3423	0.55	1/4638 (0.0%)
9	LJ	0.30	0/3559	0.57	1/4821 (0.0%)
9	LL	0.29	0/3423	0.57	2/4638 (0.0%)
9	LN	0.30	0/3532	0.57	1/4785 (0.0%)
9	MB	0.30	0/3448	0.58	1/4673 (0.0%)
9	MD	0.29	0/3466	0.56	2/4697 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	MF	0.28	0/3457	0.56	0/4685
9	MH	0.30	0/3466	0.58	1/4697 (0.0%)
9	MJ	0.28	0/3466	0.56	2/4697 (0.0%)
9	ML	0.30	0/3466	0.61	2/4697 (0.0%)
9	MN	0.28	0/3448	0.56	0/4673
9	NB	0.28	0/3436	0.56	1/4656 (0.0%)
9	ND	0.29	0/3436	0.56	1/4656 (0.0%)
9	NF	0.28	0/3448	0.58	0/4673
9	NH	0.29	0/3436	0.57	1/4656 (0.0%)
9	NJ	0.28	0/3443	0.58	3/4666 (0.1%)
9	NL	0.29	0/3436	0.60	2/4656 (0.0%)
9	NN	0.28	0/3436	0.59	3/4656 (0.1%)
9	OB	0.30	0/3457	0.58	1/4685 (0.0%)
9	OD	0.29	0/3448	0.55	0/4673
9	OF	0.28	0/3466	0.56	2/4697 (0.0%)
9	OH	0.30	0/3448	0.58	1/4673 (0.0%)
9	OJ	0.29	0/3466	0.57	1/4697 (0.0%)
9	OL	0.29	0/3448	0.56	1/4673 (0.0%)
9	ON	0.30	0/3457	0.56	1/4685 (0.0%)
9	PD	0.29	0/3448	0.56	1/4673 (0.0%)
9	PF	0.29	0/3466	0.57	2/4697 (0.0%)
9	PH	0.28	0/3423	0.55	1/4638 (0.0%)
9	PJ	0.28	0/3448	0.56	1/4673 (0.0%)
9	PL	0.29	0/3443	0.56	1/4666 (0.0%)
9	PN	0.30	0/3448	0.57	0/4673
9	QD	0.30	0/3436	0.59	3/4656 (0.1%)
9	QF	0.28	0/3448	0.55	1/4673 (0.0%)
9	QH	0.27	0/3423	0.54	1/4638 (0.0%)
9	QJ	0.28	0/3443	0.55	0/4666
9	QL	0.27	0/3431	0.57	2/4649 (0.0%)
9	QN	0.29	0/3436	0.55	1/4656 (0.0%)
9	RD	0.28	0/3423	0.58	2/4638 (0.0%)
9	RF	0.28	0/3443	0.58	2/4666 (0.0%)
9	RH	0.27	0/3423	0.54	1/4638 (0.0%)
9	RJ	0.28	0/3436	0.58	2/4656 (0.0%)
9	RL	0.27	0/3423	0.56	0/4638
9	RN	0.27	0/3431	0.58	1/4649 (0.0%)
9	SD	0.27	0/3423	0.56	1/4638 (0.0%)
9	SF	0.28	0/3423	0.59	2/4638 (0.0%)
9	SH	0.27	0/3423	0.57	1/4638 (0.0%)
9	SJ	0.27	0/3423	0.57	2/4638 (0.0%)
9	SL	0.28	0/3423	0.59	1/4638 (0.0%)
9	SN	0.28	0/3423	0.58	3/4638 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	TD	0.27	0/3423	0.54	1/4638 (0.0%)
9	TF	0.28	0/3431	0.57	1/4649 (0.0%)
9	TH	0.27	0/3423	0.58	2/4638 (0.0%)
9	TJ	0.27	0/3423	0.57	2/4638 (0.0%)
9	TL	0.27	0/3423	0.59	2/4638 (0.0%)
9	TN	0.28	0/3423	0.58	1/4638 (0.0%)
9	TP	0.26	0/3373	0.57	1/4566 (0.0%)
9	UD	0.27	0/3423	0.54	1/4638 (0.0%)
9	UF	0.27	0/3431	0.55	2/4649 (0.0%)
9	UH	0.26	0/3423	0.54	0/4638
9	UJ	0.27	0/3431	0.54	0/4649
9	UL	0.27	0/3423	0.56	2/4638 (0.0%)
9	UN	0.27	0/3431	0.55	1/4649 (0.0%)
9	UP	0.27	0/3431	0.55	1/4649 (0.0%)
9	VD	0.27	0/3423	0.54	1/4638 (0.0%)
9	VF	0.28	0/3431	0.57	2/4649 (0.0%)
9	VH	0.28	0/3423	0.56	1/4638 (0.0%)
9	VJ	0.28	0/3431	0.56	1/4649 (0.0%)
9	VL	0.27	0/3423	0.55	0/4638
9	VN	0.28	0/3431	0.57	2/4649 (0.0%)
9	VP	0.26	0/3431	0.52	1/4649 (0.0%)
9	WD	0.28	0/3423	0.57	1/4638 (0.0%)
9	WF	0.29	0/3423	0.58	3/4638 (0.1%)
9	WH	0.27	0/3423	0.55	0/4638
9	WJ	0.28	0/3423	0.55	0/4638
9	WL	0.29	0/3423	0.57	1/4638 (0.0%)
9	WN	0.28	0/3431	0.56	1/4649 (0.0%)
9	WP	0.29	0/3431	0.57	1/4649 (0.0%)
10	B	0.32	0/1515	0.53	0/2006
10	C	0.34	0/3089	0.54	0/4093
11	B0	0.30	0/1594	0.54	0/2152
11	B1	0.31	0/3223	0.52	0/4347
11	B2	0.32	0/3216	0.52	0/4337
11	B3	0.31	0/2896	0.53	0/3903
11	B4	0.26	0/416	0.57	0/562
11	B5	0.23	0/253	0.32	0/352
11	B6	0.28	0/1765	0.32	0/2467
11	B7	0.28	0/1950	0.31	0/2726
11	B8	0.29	0/1955	0.31	0/2733
11	B9	0.27	0/960	0.29	0/1339
12	C0	0.32	0/291	0.60	0/395
12	C1	0.31	0/2768	0.56	1/3733 (0.0%)
12	C2	0.30	0/3239	0.57	1/4368 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	C3	0.30	0/3250	0.56	0/4382
12	C4	0.29	0/1803	0.53	2/2426 (0.1%)
13	D	0.28	0/1502	0.61	0/2038
14	D0	0.30	0/2209	0.53	0/2976
14	D1	0.31	0/3303	0.56	0/4452
14	D2	0.33	0/3322	0.56	0/4475
14	D3	0.31	0/2634	0.58	0/3542
14	D5	0.27	0/1581	0.30	0/2207
14	D6	0.28	0/1986	0.31	0/2775
14	D7	0.28	0/1975	0.32	0/2761
14	D8	0.27	0/1324	0.30	0/1845
15	E	0.26	0/2278	0.53	0/3085
15	F	0.25	0/2278	0.53	0/3085
16	F0	0.29	0/1286	0.59	1/1735 (0.1%)
16	F1	0.28	0/1313	0.55	0/1772
16	F2	0.23	0/775	0.35	0/1081
16	F3	0.29	0/1286	0.58	0/1735
16	F4	0.30	0/1313	0.58	1/1772 (0.1%)
16	F5	0.24	0/775	0.35	0/1081
16	F6	0.31	0/1286	0.66	2/1735 (0.1%)
16	F7	0.28	0/1313	0.56	2/1772 (0.1%)
16	F8	0.24	0/775	0.35	0/1081
16	G0	0.30	0/1302	0.58	0/1758
16	G1	0.31	0/1294	0.58	0/1746
16	G2	0.24	0/775	0.35	0/1081
16	G3	0.29	0/1286	0.52	0/1735
16	G4	0.30	0/1313	0.56	1/1772 (0.1%)
16	G5	0.23	0/775	0.34	0/1081
16	G6	0.29	0/1286	0.57	0/1735
16	G7	0.28	0/1313	0.54	0/1772
16	G8	0.23	0/775	0.34	0/1081
16	H0	0.30	0/1286	0.61	0/1735
16	H1	0.32	0/1313	0.58	0/1772
16	H2	0.24	0/775	0.36	0/1081
17	G	0.28	0/775	0.68	1/1058 (0.1%)
18	H	0.28	0/643	0.54	0/881
18	I	0.28	0/1115	0.55	0/1518
18	J	0.28	0/1120	0.58	0/1525
18	K	0.27	0/1115	0.61	0/1518
18	L	0.28	0/1115	0.57	0/1518
18	M	0.27	0/1115	0.53	0/1518
18	N	0.27	0/1120	0.52	0/1525
19	I1	0.28	0/791	0.50	0/1075

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	J1	0.28	0/721	0.58	0/964
20	J2	0.28	0/1892	0.58	0/2553
20	J3	0.32	0/1892	0.63	0/2553
20	J4	0.29	0/1714	0.59	0/2315
20	J5	0.30	0/525	0.66	0/711
21	K1	0.26	0/970	0.62	0/1317
22	L1	0.26	0/1075	0.58	0/1454
22	L2	0.27	0/766	0.63	1/1035 (0.1%)
23	M1	0.31	0/851	0.62	0/1153
23	M2	0.29	0/843	0.58	0/1141
23	M3	0.30	0/851	0.61	1/1153 (0.1%)
23	M4	0.29	0/851	0.57	0/1153
24	O	0.30	0/213	0.73	0/281
24	P	0.30	0/3132	0.54	1/4187 (0.0%)
24	Q	0.31	0/333	0.49	0/448
24	R	0.30	0/1836	0.52	1/2446 (0.0%)
24	S	0.30	0/1406	0.51	0/1883
25	T	0.28	0/4085	0.55	1/5532 (0.0%)
25	U	0.28	0/4093	0.56	0/5544
25	V	0.29	0/4093	0.56	0/5544
26	W	0.28	0/5192	0.59	4/7006 (0.1%)
26	X	0.28	0/5941	0.56	1/8009 (0.0%)
26	Y	0.28	0/5941	0.57	1/8009 (0.0%)
26	Z	0.28	0/4337	0.58	2/5833 (0.0%)
27	XA	0.27	0/1583	0.55	0/2137
27	XB	0.26	0/1583	0.55	0/2137
27	XC	0.26	0/1583	0.55	0/2137
27	XD	0.27	0/1583	0.57	1/2137 (0.0%)
27	XE	0.26	0/1583	0.56	1/2137 (0.0%)
27	XF	0.27	0/1583	0.56	0/2137
27	XG	0.27	0/1583	0.56	0/2137
28	YB	0.27	0/1814	0.53	0/2452
28	YC	0.26	0/1814	0.52	0/2452
28	YD	0.27	0/1814	0.54	1/2452 (0.0%)
28	YE	0.26	0/1814	0.50	0/2452
28	YF	0.28	0/1814	0.55	1/2452 (0.0%)
28	YG	0.28	0/1814	0.55	0/2452
29	a	0.30	0/1473	0.60	0/1951
29	b	0.34	0/2890	0.62	0/3818
29	c	0.31	0/2430	0.60	0/3216
29	d	0.33	0/1869	0.63	1/2472 (0.0%)
30	e	0.27	0/4811	0.58	1/6512 (0.0%)
30	f	0.27	0/4811	0.59	2/6512 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	g	0.27	0/4811	0.60	1/6512 (0.0%)
31	h	0.30	0/1230	0.60	0/1643
31	i	0.26	0/2065	0.49	0/2773
31	j	0.27	0/2052	0.52	0/2755
31	k	0.28	0/2065	0.50	0/2773
32	l	0.26	0/934	0.53	0/1271
32	m	0.28	0/934	0.51	0/1271
32	n	0.26	0/934	0.51	0/1271
33	o	0.32	0/3512	0.54	0/4648
33	o1	0.25	0/304	0.55	0/406
33	p	0.30	0/1309	0.51	0/1754
34	q	0.25	0/930	0.48	0/1259
34	r	0.26	0/930	0.55	0/1259
34	s	0.27	0/930	0.55	0/1259
35	y	0.28	0/510	0.59	0/691
35	z	0.27	0/916	0.60	0/1244
All	All	0.28	0/1283717	0.56	333/1739902 (0.0%)

There are no bond length outliers.

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	CK	32	PRO	CA-N-CD	-10.04	97.44	111.50
8	FG	173	PRO	CA-N-CD	-9.64	98.00	111.50
8	FE	298	PRO	CA-N-CD	-9.59	98.08	111.50
9	HN	271	ALA	C-N-CD	-9.50	99.69	120.60
9	KL	209	ASP	CB-CG-OD1	8.42	125.88	118.30
16	F7	89	GLY	C-N-CA	8.40	142.70	121.70
8	EM	199	ASP	CB-CG-OD2	8.21	125.69	118.30
9	QD	197	ASP	CB-CG-OD1	8.06	125.56	118.30
9	JL	271	ALA	N-CA-C	8.01	132.63	111.00
9	TF	87	PRO	CA-N-CD	-7.98	100.33	111.50
17	G	45	LEU	CA-CB-CG	7.88	133.43	115.30
9	NL	277	GLY	N-CA-C	7.88	132.79	113.10
8	RM	424	ASP	CB-CG-OD2	7.87	125.39	118.30
8	CA	367	ASP	CB-CG-OD2	7.84	125.36	118.30
16	F6	71	ASP	CB-CG-OD1	7.64	125.18	118.30
9	HN	272	PRO	CA-N-CD	-7.56	100.91	111.50
8	ME	431	ASP	CB-CG-OD2	7.56	125.10	118.30
9	DH	271	ALA	N-CA-C	7.51	131.28	111.00
8	OE	345	ASP	CB-CG-OD1	7.47	125.02	118.30
9	HJ	128	ASP	CB-CG-OD1	7.46	125.01	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	DD	271	ALA	N-CA-C	7.38	130.92	111.00
26	W	49	LEU	CA-CB-CG	7.33	132.15	115.30
9	NN	277	GLY	N-CA-C	7.26	131.24	113.10
9	WF	271	ALA	N-CA-C	7.25	130.59	111.00
9	DL	272	PRO	N-CA-C	-7.25	93.25	112.10
9	RJ	271	ALA	N-CA-C	7.23	130.51	111.00
9	AD	128	ASP	CB-CG-OD1	7.20	124.78	118.30
8	NG	46	ASP	CB-CG-OD2	7.20	124.78	118.30
8	RK	152	LEU	CA-CB-CG	7.08	131.58	115.30
9	JD	271	ALA	N-CA-C	7.04	130.01	111.00
8	BK	205	ASP	CB-CG-OD2	7.03	124.63	118.30
8	UG	245	ASP	CB-CG-OD1	7.01	124.61	118.30
9	DL	271	ALA	N-CA-C	6.97	129.81	111.00
9	KB	128	ASP	CB-CG-OD1	6.93	124.54	118.30
9	RN	271	ALA	N-CA-C	6.91	129.65	111.00
8	PK	152	LEU	CA-CB-CG	6.89	131.16	115.30
8	OE	152	LEU	CA-CB-CG	6.87	131.10	115.30
9	QL	271	ALA	N-CA-C	6.85	129.49	111.00
9	JL	197	ASP	CB-CG-OD1	6.83	124.45	118.30
9	LB	271	ALA	N-CA-C	6.83	129.45	111.00
8	JE	116	ASP	CB-CG-OD1	6.82	124.43	118.30
9	DF	271	ALA	N-CA-C	6.79	129.34	111.00
8	JK	245	ASP	CB-CG-OD1	6.78	124.41	118.30
9	IF	327	ASP	CB-CG-OD1	6.78	124.40	118.30
9	OJ	271	ALA	N-CA-C	6.77	129.27	111.00
8	MK	152	LEU	CA-CB-CG	6.73	130.78	115.30
8	DM	424	ASP	CB-CG-OD1	6.72	124.35	118.30
9	AF	128	ASP	CB-CG-OD2	6.68	124.31	118.30
8	QM	33	ASP	CB-CG-OD1	6.68	124.31	118.30
9	JN	271	ALA	N-CA-C	6.67	129.02	111.00
8	LG	322	ASP	CB-CG-OD2	6.66	124.30	118.30
8	KM	205	ASP	CB-CG-OD1	6.63	124.27	118.30
9	WL	271	ALA	N-CA-C	6.63	128.90	111.00
9	RD	271	ALA	N-CA-C	6.61	128.86	111.00
9	OB	271	ALA	N-CA-C	6.60	128.83	111.00
9	DF	272	PRO	N-CA-C	-6.58	94.98	112.10
9	ED	161	ASP	CB-CG-OD2	6.58	124.22	118.30
26	W	461	ASP	CB-CG-OD1	6.58	124.22	118.30
9	NB	271	ALA	N-CA-C	6.55	128.69	111.00
8	VG	152	LEU	CA-CB-CG	6.55	130.36	115.30
9	BJ	271	ALA	N-CA-C	6.54	128.67	111.00
9	BL	271	ALA	N-CA-C	6.54	128.65	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SJ	271	ALA	N-CA-C	6.53	128.62	111.00
8	PC	152	LEU	CA-CB-CG	6.52	130.30	115.30
25	T	447	ASP	CB-CG-OD2	6.52	124.17	118.30
9	ON	271	ALA	N-CA-C	6.52	128.59	111.00
8	AC	345	ASP	CB-CG-OD2	6.51	124.16	118.30
9	UL	271	ALA	N-CA-C	6.51	128.57	111.00
9	KJ	271	ALA	N-CA-C	6.50	128.55	111.00
8	KM	322	ASP	CB-CG-OD2	6.49	124.14	118.30
9	SL	271	ALA	N-CA-C	6.48	128.49	111.00
9	WD	271	ALA	N-CA-C	6.47	128.46	111.00
9	IH	271	ALA	N-CA-C	6.46	128.44	111.00
9	ML	271	ALA	N-CA-C	6.44	128.39	111.00
9	GJ	271	ALA	N-CA-C	6.42	128.35	111.00
9	WP	271	ALA	N-CA-C	6.42	128.34	111.00
9	PD	271	ALA	N-CA-C	6.42	128.32	111.00
9	BD	271	ALA	N-CA-C	6.41	128.32	111.00
8	FE	298	PRO	N-CD-CG	-6.41	93.59	103.20
8	QG	152	LEU	CA-CB-CG	6.40	130.02	115.30
9	IB	271	ALA	N-CA-C	6.38	128.24	111.00
8	JK	345	ASP	CB-CG-OD1	6.38	124.04	118.30
9	PH	209	ASP	CB-CG-OD1	6.37	124.03	118.30
16	F6	146	ASP	CB-CG-OD1	6.36	124.02	118.30
9	JF	268	PRO	N-CA-C	6.35	128.62	112.10
9	EB	271	ALA	N-CA-C	6.35	128.15	111.00
9	MJ	271	ALA	N-CA-C	6.35	128.15	111.00
26	Z	404	LEU	CA-CB-CG	6.35	129.90	115.30
30	f	154	ALA	N-CA-C	6.34	128.12	111.00
8	BI	120	ASP	CB-CG-OD2	6.32	123.99	118.30
26	Y	275	LEU	CA-CB-CG	6.32	129.83	115.30
9	LL	271	ALA	N-CA-C	6.32	128.05	111.00
9	GD	271	ALA	N-CA-C	6.31	128.05	111.00
9	DJ	271	ALA	N-CA-C	6.31	128.03	111.00
9	MB	271	ALA	N-CA-C	6.30	128.01	111.00
9	NJ	271	ALA	N-CA-C	6.29	127.99	111.00
8	TM	47	ASP	CB-CG-OD1	6.29	123.96	118.30
9	AB	271	ALA	N-CA-C	6.28	127.96	111.00
9	KL	271	ALA	N-CA-C	6.28	127.95	111.00
8	NG	205	ASP	CB-CG-OD1	6.26	123.93	118.30
9	CJ	271	ALA	N-CA-C	6.25	127.89	111.00
8	DA	152	LEU	CA-CB-CG	6.25	129.68	115.30
9	KF	271	ALA	N-CA-C	6.25	127.88	111.00
9	VF	203	ASP	CB-CG-OD2	6.25	123.92	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	QM	152	LEU	CA-CB-CG	6.24	129.65	115.30
8	LG	33	ASP	CB-CG-OD1	6.23	123.90	118.30
8	GC	152	LEU	CA-CB-CG	6.22	129.60	115.30
24	R	197	ASP	CB-CG-OD1	6.22	123.89	118.30
9	PF	271	ALA	N-CA-C	6.21	127.77	111.00
8	HK	152	LEU	CA-CB-CG	6.20	129.57	115.30
9	HH	271	ALA	N-CA-C	6.20	127.73	111.00
9	OH	271	ALA	N-CA-C	6.19	127.72	111.00
9	HD	203	ASP	CB-CG-OD2	6.18	123.86	118.30
9	SN	74	ASP	CB-CG-OD2	6.16	123.85	118.30
9	EJ	271	ALA	N-CA-C	6.14	127.59	111.00
8	GE	59	GLY	N-CA-C	6.13	128.44	113.10
8	OM	152	LEU	CA-CB-CG	6.13	129.39	115.30
26	W	48	LEU	CA-CB-CG	6.12	129.38	115.30
8	BE	397	LEU	CA-CB-CG	6.12	129.38	115.30
9	ML	42	LEU	CA-CB-CG	6.11	129.35	115.30
9	OF	271	ALA	N-CA-C	6.10	127.48	111.00
9	LD	271	ALA	N-CA-C	6.08	127.41	111.00
9	KN	41	ASP	CB-CG-OD1	6.07	123.77	118.30
9	UP	203	ASP	CB-CG-OD2	6.07	123.77	118.30
9	JH	271	ALA	N-CA-C	6.06	127.36	111.00
9	DB	271	ALA	N-CA-C	6.06	127.36	111.00
8	QG	424	ASP	CB-CG-OD1	6.05	123.75	118.30
9	EH	267	MET	CA-CB-CG	6.05	123.59	113.30
8	AG	205	ASP	CB-CG-OD1	6.04	123.74	118.30
8	HG	357	TYR	C-N-CA	-6.03	106.61	121.70
8	HO	227	LEU	CA-CB-CG	6.02	129.15	115.30
9	VP	271	ALA	N-CA-C	6.02	127.26	111.00
9	KH	161	ASP	CB-CG-OD1	6.01	123.71	118.30
8	UI	33	ASP	CB-CG-OD1	6.01	123.71	118.30
9	EF	271	ALA	N-CA-C	6.00	127.21	111.00
9	QD	271	ALA	N-CA-C	6.00	127.20	111.00
8	HC	322	ASP	CB-CG-OD2	5.99	123.69	118.30
23	M3	127	ASP	CB-CG-OD1	5.98	123.68	118.30
8	NM	33	ASP	CB-CG-OD1	5.98	123.68	118.30
9	IJ	271	ALA	N-CA-C	5.96	127.11	111.00
9	LJ	271	ALA	N-CA-C	5.96	127.09	111.00
9	DL	274	THR	N-CA-C	-5.96	94.92	111.00
9	TD	271	ALA	N-CA-C	5.96	127.08	111.00
9	LL	44	LEU	CA-CB-CG	5.92	128.92	115.30
9	RJ	197	ASP	CB-CG-OD1	5.92	123.63	118.30
9	UN	271	ALA	N-CA-C	5.91	126.95	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	UD	271	ALA	N-CA-C	5.90	126.94	111.00
9	OL	271	ALA	N-CA-C	5.90	126.94	111.00
12	C1	440	ASP	CB-CG-OD2	5.88	123.59	118.30
8	GK	392	ASP	CB-CG-OD2	5.88	123.59	118.30
9	QL	417	ASP	CB-CG-OD1	5.87	123.58	118.30
9	JJ	271	ALA	N-CA-C	5.87	126.84	111.00
9	UF	271	ALA	N-CA-C	5.86	126.82	111.00
30	f	107	LEU	CA-CB-CG	5.86	128.77	115.30
8	WM	152	LEU	CA-CB-CG	5.85	128.76	115.30
9	VJ	271	ALA	N-CA-C	5.85	126.79	111.00
8	CG	248	LEU	CA-CB-CG	5.83	128.71	115.30
9	ND	271	ALA	N-CA-C	5.82	126.70	111.00
8	KK	152	LEU	CA-CB-CG	5.81	128.67	115.30
8	FG	173	PRO	N-CD-CG	-5.81	94.48	103.20
9	NN	203	ASP	CB-CG-OD2	5.79	123.52	118.30
8	NG	33	ASP	CB-CG-OD1	5.79	123.51	118.30
9	HJ	271	ALA	N-CA-C	5.79	126.64	111.00
9	UL	88	ASP	CB-CG-OD1	5.78	123.50	118.30
9	GN	271	ALA	N-CA-C	5.77	126.58	111.00
9	SH	271	ALA	N-CA-C	5.77	126.58	111.00
16	F0	116	LYS	C-N-CA	5.77	136.12	121.70
7	A1	258	ASP	CB-CG-OD1	5.75	123.48	118.30
8	NG	322	ASP	CB-CG-OD2	5.74	123.47	118.30
8	BI	152	LEU	CA-CB-CG	5.74	128.50	115.30
9	TH	271	ALA	N-CA-C	5.73	126.48	111.00
9	HL	395	LEU	CA-CB-CG	5.72	128.46	115.30
9	CB	271	ALA	N-CA-C	5.72	126.44	111.00
9	DB	118	ASP	CB-CG-OD1	5.71	123.44	118.30
8	UO	205	ASP	CB-CG-OD2	5.71	123.44	118.30
9	RF	271	ALA	N-CA-C	5.70	126.39	111.00
8	VM	47	ASP	CB-CG-OD2	5.69	123.42	118.30
9	PJ	271	ALA	N-CA-C	5.69	126.37	111.00
9	IF	271	ALA	N-CA-C	5.68	126.35	111.00
9	ID	271	ALA	N-CA-C	5.68	126.33	111.00
26	X	275	LEU	CA-CB-CG	5.67	128.35	115.30
28	YD	209	ASP	CB-CG-OD2	5.67	123.41	118.30
8	WG	252	LEU	CA-CB-CG	5.67	128.34	115.30
8	AM	218	ASP	CB-CG-OD1	5.66	123.40	118.30
9	RH	271	ALA	N-CA-C	5.66	126.29	111.00
8	AG	397	LEU	CA-CB-CG	5.66	128.32	115.30
9	AH	271	ALA	N-CA-C	5.66	126.28	111.00
8	BG	205	ASP	CB-CG-OD2	5.66	123.39	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	SM	116	ASP	CB-CG-OD1	5.66	123.39	118.30
8	SO	218	ASP	CB-CG-OD1	5.66	123.39	118.30
9	TL	209	ASP	CB-CG-OD1	5.66	123.39	118.30
8	GM	152	LEU	CA-CB-CG	5.64	128.28	115.30
8	UI	322	ASP	CB-CG-OD1	5.62	123.36	118.30
9	MJ	44	LEU	CA-CB-CG	5.62	128.22	115.30
30	g	337	ASP	CB-CG-OD1	5.59	123.33	118.30
9	SF	272	PRO	N-CA-C	-5.59	97.56	112.10
9	SN	271	ALA	N-CA-C	5.59	126.09	111.00
9	MD	271	ALA	N-CA-C	5.58	126.07	111.00
9	JF	271	ALA	N-CA-C	5.57	126.05	111.00
9	HN	323	MET	CA-CB-CG	5.57	122.77	113.30
8	FM	171	ILE	C-N-CA	5.56	135.60	121.70
8	BI	306	ASP	CB-CG-OD2	5.56	123.30	118.30
8	VG	367	ASP	CB-CG-OD1	5.56	123.30	118.30
9	HB	271	ALA	N-CA-C	5.56	126.01	111.00
9	CF	271	ALA	N-CA-C	5.55	125.99	111.00
8	NI	195	LEU	CA-CB-CG	5.55	128.06	115.30
9	HD	271	ALA	N-CA-C	5.55	125.97	111.00
9	IB	284	LEU	CA-CB-CG	5.54	128.04	115.30
27	XE	171	LEU	CA-CB-CG	5.54	128.04	115.30
9	GF	240	LEU	CA-CB-CG	5.53	128.03	115.30
9	VN	271	ALA	N-CA-C	5.52	125.90	111.00
9	RF	233	MET	CA-CB-CG	5.51	122.68	113.30
8	RK	364	PRO	CA-N-CD	-5.51	103.78	111.50
8	DK	357	TYR	C-N-CA	-5.51	107.92	121.70
9	PF	417	ASP	CB-CG-OD1	5.50	123.25	118.30
9	IL	42	LEU	CA-CB-CG	5.50	127.95	115.30
9	GJ	269	GLY	N-CA-C	-5.50	99.35	113.10
9	NJ	417	ASP	CB-CG-OD1	5.50	123.25	118.30
12	C4	209	ASP	CB-CG-OD1	5.50	123.25	118.30
9	IH	41	ASP	CB-CG-OD2	5.49	123.24	118.30
8	KI	33	ASP	CB-CG-OD1	5.48	123.23	118.30
22	L2	36	LEU	CA-CB-CG	5.48	127.90	115.30
8	SO	89	PRO	CA-N-CD	-5.46	103.86	111.50
9	JN	118	ASP	CB-CG-OD1	5.45	123.21	118.30
9	QN	271	ALA	N-CA-C	5.45	125.72	111.00
9	AH	44	LEU	CA-CB-CG	5.45	127.83	115.30
9	BJ	427	ASP	CB-CG-OD1	5.44	123.20	118.30
9	QD	112	LEU	CA-CB-CG	5.43	127.80	115.30
9	QH	118	ASP	CB-CG-OD1	5.43	123.19	118.30
27	XD	26	ASP	CB-CG-OD1	5.43	123.19	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	IN	271	ALA	N-CA-C	5.42	125.65	111.00
9	TP	271	ALA	N-CA-C	5.42	125.62	111.00
9	MH	26	ASP	CB-CG-OD2	5.40	123.16	118.30
9	TL	271	ALA	N-CA-C	5.39	125.56	111.00
7	A1	209	PRO	C-N-CA	5.39	135.17	121.70
24	P	275	PRO	C-N-CA	5.39	135.17	121.70
9	WF	209	ASP	CB-CG-OD2	5.38	123.14	118.30
9	LN	271	ALA	N-CA-C	5.38	125.52	111.00
8	CK	32	PRO	N-CD-CG	-5.38	95.14	103.20
28	YF	104	ASP	CB-CG-OD2	5.38	123.14	118.30
9	SD	271	ALA	N-CA-C	5.37	125.50	111.00
9	SF	271	ALA	N-CA-C	5.37	125.49	111.00
9	WF	161	ASP	CB-CG-OD1	5.37	123.13	118.30
8	BG	46	ASP	CB-CG-OD1	5.36	123.13	118.30
26	Z	275	LEU	CA-CB-CG	5.36	127.64	115.30
9	MD	128	ASP	CB-CG-OD1	5.36	123.12	118.30
8	LI	33	ASP	CB-CG-OD2	5.35	123.12	118.30
16	F4	89	GLY	C-N-CA	5.35	135.08	121.70
9	KH	271	ALA	N-CA-C	5.35	125.43	111.00
8	BA	26	LEU	CA-CB-CG	5.34	127.59	115.30
9	QF	271	ALA	N-CA-C	5.34	125.42	111.00
9	TJ	271	ALA	N-CA-C	5.34	125.41	111.00
9	PL	271	ALA	N-CA-C	5.33	125.40	111.00
8	WM	171	ILE	C-N-CA	5.33	135.02	121.70
12	C2	400	LEU	CA-CB-CG	5.33	127.55	115.30
9	OF	377	LEU	CA-CB-CG	5.32	127.54	115.30
12	C4	388	ASP	CB-CG-OD2	5.32	123.09	118.30
8	UG	322	ASP	CB-CG-OD1	5.31	123.08	118.30
9	AJ	417	ASP	CB-CG-OD2	5.31	123.08	118.30
8	IG	33	ASP	CB-CG-OD1	5.30	123.07	118.30
5	8	61	ARG	N-CA-C	5.30	125.30	111.00
8	AM	397	LEU	CA-CB-CG	5.29	127.47	115.30
9	EH	268	PRO	N-CA-C	5.28	125.83	112.10
9	NL	271	ALA	N-CA-C	5.28	125.26	111.00
9	TN	271	ALA	N-CA-C	5.27	125.24	111.00
9	DJ	395	LEU	CA-CB-CG	5.27	127.42	115.30
9	EH	271	ALA	N-CA-C	5.27	125.22	111.00
9	DB	284	LEU	CA-CB-CG	5.26	127.40	115.30
9	SJ	272	PRO	N-CA-C	-5.26	98.43	112.10
8	IG	248	LEU	CA-CB-CG	5.26	127.39	115.30
9	CH	271	ALA	N-CA-C	5.25	125.19	111.00
9	HB	331	LEU	CA-CB-CG	5.25	127.38	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CB	284	LEU	CA-CB-CG	5.25	127.37	115.30
9	DB	295	ASP	CB-CG-OD2	5.23	123.01	118.30
26	W	508	LEU	CA-CB-CG	5.23	127.32	115.30
8	AC	397	LEU	CA-CB-CG	5.22	127.31	115.30
8	JK	157	LEU	CA-CB-CG	5.22	127.30	115.30
9	EN	284	LEU	CA-CB-CG	5.21	127.30	115.30
8	GM	397	LEU	CA-CB-CG	5.21	127.30	115.30
9	FJ	271	ALA	N-CA-C	5.21	125.07	111.00
16	F7	96	LEU	CB-CG-CD1	-5.19	102.17	111.00
9	IL	271	ALA	N-CA-C	5.18	125.00	111.00
30	e	157	ASN	C-N-CA	5.18	134.66	121.70
9	RD	135	LEU	CA-CB-CG	5.18	127.22	115.30
8	SK	345	ASP	CB-CG-OD1	5.18	122.96	118.30
9	GF	271	ALA	N-CA-C	5.17	124.96	111.00
9	TJ	187	LEU	CA-CB-CG	5.17	127.18	115.30
8	IO	152	LEU	CA-CB-CG	5.17	127.18	115.30
8	PE	152	LEU	CA-CB-CG	5.16	127.16	115.30
9	UF	249	ASP	CB-CG-OD2	5.16	122.94	118.30
9	FN	271	ALA	N-CA-C	5.16	124.92	111.00
9	NH	203	ASP	CB-CG-OD1	5.15	122.94	118.30
8	TM	195	LEU	CA-CB-CG	5.15	127.14	115.30
9	BH	271	ALA	N-CA-C	5.15	124.89	111.00
8	DG	248	LEU	CA-CB-CG	5.15	127.14	115.30
8	AA	218	ASP	CB-CG-OD1	5.13	122.92	118.30
9	VN	39	ASP	CB-CG-OD1	5.13	122.92	118.30
8	OC	322	ASP	CB-CG-OD2	5.13	122.92	118.30
8	UE	364	PRO	CA-N-CD	-5.13	104.32	111.50
9	JL	268	PRO	N-CA-C	5.12	125.42	112.10
9	SN	44	LEU	CA-CB-CG	5.12	127.08	115.30
4	6	77	ASP	CB-CG-OD2	5.12	122.91	118.30
8	SK	302	MET	CA-CB-CG	5.12	122.00	113.30
8	HG	248	LEU	CA-CB-CG	5.11	127.06	115.30
9	BF	271	ALA	N-CA-C	5.11	124.79	111.00
9	VD	271	ALA	N-CA-C	5.10	124.76	111.00
8	CG	364	PRO	CA-N-CD	-5.09	104.37	111.50
8	BE	248	LEU	CA-CB-CG	5.09	127.01	115.30
16	G4	21	GLN	CA-CB-CG	5.09	124.59	113.40
9	VF	271	ALA	N-CA-C	5.08	124.73	111.00
9	KD	271	ALA	N-CA-C	5.08	124.72	111.00
9	NN	118	ASP	CB-CG-OD2	5.08	122.88	118.30
9	WN	271	ALA	N-CA-C	5.08	124.73	111.00
9	LH	271	ALA	N-CA-C	5.08	124.72	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	GB	271	ALA	N-CA-C	5.08	124.71	111.00
9	DD	323	MET	CA-CB-CG	5.07	121.92	113.30
8	FC	33	ASP	CB-CG-OD1	5.07	122.86	118.30
29	d	462	LEU	CA-CB-CG	5.07	126.95	115.30
8	AG	364	PRO	CA-N-CD	-5.06	104.41	111.50
9	AL	42	LEU	CA-CB-CG	5.06	126.95	115.30
9	EJ	272	PRO	N-CA-C	-5.04	99.00	112.10
9	KN	271	ALA	N-CA-C	5.04	124.61	111.00
9	NJ	278	SER	N-CA-C	5.04	124.60	111.00
9	TH	42	LEU	CA-CB-CG	5.04	126.88	115.30
9	VH	271	ALA	N-CA-C	5.03	124.57	111.00
8	LK	33	ASP	CB-CG-OD2	5.02	122.82	118.30
9	HL	271	ALA	N-CA-C	5.02	124.56	111.00
8	KK	205	ASP	CB-CG-OD1	5.02	122.82	118.30
9	KN	377	LEU	CA-CB-CG	5.02	126.84	115.30
9	IF	327	ASP	CB-CG-OD2	-5.01	113.79	118.30
9	FH	271	ALA	N-CA-C	5.01	124.52	111.00
9	AF	271	ALA	N-CA-C	5.00	124.51	111.00
9	KB	271	ALA	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	50/229 (22%)	44 (88%)	6 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	138/229 (60%)	127 (92%)	11 (8%)	0	100	100
2	1	266/833 (32%)	259 (97%)	7 (3%)	0	100	100
2	2	442/833 (53%)	436 (99%)	6 (1%)	0	100	100
3	3	295/514 (57%)	292 (99%)	3 (1%)	0	100	100
3	4	213/514 (41%)	213 (100%)	0	0	100	100
4	5	369/376 (98%)	358 (97%)	11 (3%)	0	100	100
4	6	369/376 (98%)	361 (98%)	8 (2%)	0	100	100
5	8	166/194 (86%)	151 (91%)	15 (9%)	0	100	100
5	9	46/194 (24%)	41 (89%)	5 (11%)	0	100	100
6	A	48/101 (48%)	48 (100%)	0	0	100	100
7	A0	216/418 (52%)	215 (100%)	1 (0%)	0	100	100
7	A1	389/418 (93%)	383 (98%)	6 (2%)	0	100	100
7	A2	389/418 (93%)	382 (98%)	7 (2%)	0	100	100
7	A3	329/418 (79%)	324 (98%)	5 (2%)	0	100	100
7	A4	33/418 (8%)	32 (97%)	1 (3%)	0	100	100
8	AA	437/451 (97%)	428 (98%)	8 (2%)	1 (0%)	47	79
8	AC	437/451 (97%)	425 (97%)	11 (2%)	1 (0%)	47	79
8	AE	437/451 (97%)	426 (98%)	11 (2%)	0	100	100
8	AG	437/451 (97%)	425 (97%)	12 (3%)	0	100	100
8	AI	437/451 (97%)	424 (97%)	12 (3%)	1 (0%)	47	79
8	AK	437/451 (97%)	428 (98%)	9 (2%)	0	100	100
8	AM	437/451 (97%)	424 (97%)	13 (3%)	0	100	100
8	BA	428/451 (95%)	414 (97%)	13 (3%)	1 (0%)	47	79
8	BC	437/451 (97%)	425 (97%)	11 (2%)	1 (0%)	47	79
8	BE	428/451 (95%)	416 (97%)	12 (3%)	0	100	100
8	BG	437/451 (97%)	420 (96%)	17 (4%)	0	100	100
8	BI	428/451 (95%)	415 (97%)	13 (3%)	0	100	100
8	BK	437/451 (97%)	420 (96%)	17 (4%)	0	100	100
8	BM	429/451 (95%)	419 (98%)	10 (2%)	0	100	100
8	CA	428/451 (95%)	418 (98%)	9 (2%)	1 (0%)	47	79
8	CC	437/451 (97%)	423 (97%)	13 (3%)	1 (0%)	47	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CE	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
8	CG	437/451 (97%)	418 (96%)	19 (4%)	0	100	100
8	CI	427/451 (95%)	412 (96%)	15 (4%)	0	100	100
8	CK	437/451 (97%)	425 (97%)	12 (3%)	0	100	100
8	CM	427/451 (95%)	414 (97%)	13 (3%)	0	100	100
8	DA	375/451 (83%)	364 (97%)	11 (3%)	0	100	100
8	DC	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
8	DE	427/451 (95%)	418 (98%)	9 (2%)	0	100	100
8	DG	426/451 (94%)	410 (96%)	16 (4%)	0	100	100
8	DI	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
8	DK	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
8	DM	427/451 (95%)	418 (98%)	9 (2%)	0	100	100
8	EC	437/451 (97%)	423 (97%)	13 (3%)	1 (0%)	47	79
8	EE	437/451 (97%)	426 (98%)	11 (2%)	0	100	100
8	EG	436/451 (97%)	412 (94%)	24 (6%)	0	100	100
8	EI	437/451 (97%)	418 (96%)	19 (4%)	0	100	100
8	EK	436/451 (97%)	420 (96%)	16 (4%)	0	100	100
8	EM	436/451 (97%)	419 (96%)	17 (4%)	0	100	100
8	FC	427/451 (95%)	416 (97%)	11 (3%)	0	100	100
8	FE	427/451 (95%)	413 (97%)	14 (3%)	0	100	100
8	FG	426/451 (94%)	410 (96%)	16 (4%)	0	100	100
8	FI	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
8	FK	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
8	FM	426/451 (94%)	410 (96%)	16 (4%)	0	100	100
8	GC	431/451 (96%)	420 (97%)	10 (2%)	1 (0%)	47	79
8	GE	426/451 (94%)	420 (99%)	6 (1%)	0	100	100
8	GG	427/451 (95%)	414 (97%)	13 (3%)	0	100	100
8	GI	426/451 (94%)	419 (98%)	7 (2%)	0	100	100
8	GK	428/451 (95%)	422 (99%)	6 (1%)	0	100	100
8	GM	430/451 (95%)	417 (97%)	13 (3%)	0	100	100
8	HC	427/451 (95%)	414 (97%)	12 (3%)	1 (0%)	47	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	HE	428/451 (95%)	420 (98%)	8 (2%)	0	100	100
8	HG	428/451 (95%)	414 (97%)	14 (3%)	0	100	100
8	HI	428/451 (95%)	419 (98%)	9 (2%)	0	100	100
8	HK	427/451 (95%)	416 (97%)	11 (3%)	0	100	100
8	HM	427/451 (95%)	417 (98%)	10 (2%)	0	100	100
8	HO	381/451 (84%)	369 (97%)	12 (3%)	0	100	100
8	IC	429/451 (95%)	422 (98%)	6 (1%)	1 (0%)	47	79
8	IE	427/451 (95%)	413 (97%)	14 (3%)	0	100	100
8	IG	437/451 (97%)	423 (97%)	14 (3%)	0	100	100
8	II	428/451 (95%)	416 (97%)	12 (3%)	0	100	100
8	IK	437/451 (97%)	427 (98%)	10 (2%)	0	100	100
8	IM	427/451 (95%)	414 (97%)	13 (3%)	0	100	100
8	IO	427/451 (95%)	413 (97%)	14 (3%)	0	100	100
8	JC	437/451 (97%)	423 (97%)	14 (3%)	0	100	100
8	JE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
8	JG	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
8	JI	426/451 (94%)	410 (96%)	16 (4%)	0	100	100
8	JK	427/451 (95%)	411 (96%)	16 (4%)	0	100	100
8	JM	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
8	KC	429/451 (95%)	418 (97%)	10 (2%)	1 (0%)	47	79
8	KE	428/451 (95%)	415 (97%)	13 (3%)	0	100	100
8	KG	429/451 (95%)	417 (97%)	12 (3%)	0	100	100
8	KI	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
8	KK	429/451 (95%)	419 (98%)	10 (2%)	0	100	100
8	KM	436/451 (97%)	421 (97%)	15 (3%)	0	100	100
8	KO	428/451 (95%)	413 (96%)	15 (4%)	0	100	100
8	LC	429/451 (95%)	418 (97%)	10 (2%)	1 (0%)	47	79
8	LE	437/451 (97%)	422 (97%)	15 (3%)	0	100	100
8	LG	430/451 (95%)	417 (97%)	13 (3%)	0	100	100
8	LI	432/451 (96%)	420 (97%)	12 (3%)	0	100	100
8	LK	429/451 (95%)	420 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	LM	427/451 (95%)	418 (98%)	9 (2%)	0	100	100
8	MC	438/451 (97%)	426 (97%)	11 (2%)	1 (0%)	47	79
8	ME	428/451 (95%)	411 (96%)	17 (4%)	0	100	100
8	MG	428/451 (95%)	417 (97%)	11 (3%)	0	100	100
8	MI	429/451 (95%)	418 (97%)	11 (3%)	0	100	100
8	MK	438/451 (97%)	428 (98%)	10 (2%)	0	100	100
8	MM	438/451 (97%)	420 (96%)	18 (4%)	0	100	100
8	NC	438/451 (97%)	423 (97%)	14 (3%)	1 (0%)	47	79
8	NE	437/451 (97%)	424 (97%)	13 (3%)	0	100	100
8	NG	437/451 (97%)	424 (97%)	12 (3%)	1 (0%)	47	79
8	NI	437/451 (97%)	427 (98%)	10 (2%)	0	100	100
8	NK	437/451 (97%)	429 (98%)	8 (2%)	0	100	100
8	NM	437/451 (97%)	424 (97%)	13 (3%)	0	100	100
8	OC	439/451 (97%)	428 (98%)	10 (2%)	1 (0%)	47	79
8	OE	438/451 (97%)	427 (98%)	11 (2%)	0	100	100
8	OG	439/451 (97%)	424 (97%)	15 (3%)	0	100	100
8	OI	439/451 (97%)	429 (98%)	10 (2%)	0	100	100
8	OK	437/451 (97%)	428 (98%)	9 (2%)	0	100	100
8	OM	439/451 (97%)	425 (97%)	14 (3%)	0	100	100
8	OO	416/451 (92%)	402 (97%)	14 (3%)	0	100	100
8	PC	439/451 (97%)	426 (97%)	12 (3%)	1 (0%)	47	79
8	PE	438/451 (97%)	425 (97%)	13 (3%)	0	100	100
8	PG	439/451 (97%)	420 (96%)	19 (4%)	0	100	100
8	PI	437/451 (97%)	424 (97%)	13 (3%)	0	100	100
8	PK	438/451 (97%)	426 (97%)	12 (3%)	0	100	100
8	PM	437/451 (97%)	423 (97%)	14 (3%)	0	100	100
8	PO	437/451 (97%)	425 (97%)	12 (3%)	0	100	100
8	QC	438/451 (97%)	420 (96%)	17 (4%)	1 (0%)	47	79
8	QE	438/451 (97%)	424 (97%)	14 (3%)	0	100	100
8	QG	438/451 (97%)	420 (96%)	17 (4%)	1 (0%)	47	79
8	QI	438/451 (97%)	422 (96%)	16 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	QK	438/451 (97%)	425 (97%)	13 (3%)	0	100	100
8	QM	438/451 (97%)	425 (97%)	13 (3%)	0	100	100
8	QO	438/451 (97%)	418 (95%)	20 (5%)	0	100	100
8	RC	405/451 (90%)	389 (96%)	16 (4%)	0	100	100
8	RE	426/451 (94%)	418 (98%)	8 (2%)	0	100	100
8	RG	428/451 (95%)	410 (96%)	18 (4%)	0	100	100
8	RI	437/451 (97%)	417 (95%)	20 (5%)	0	100	100
8	RK	438/451 (97%)	427 (98%)	11 (2%)	0	100	100
8	RM	438/451 (97%)	421 (96%)	17 (4%)	0	100	100
8	RO	437/451 (97%)	420 (96%)	17 (4%)	0	100	100
8	SE	425/451 (94%)	415 (98%)	10 (2%)	0	100	100
8	SG	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
8	SI	427/451 (95%)	410 (96%)	17 (4%)	0	100	100
8	SK	427/451 (95%)	417 (98%)	10 (2%)	0	100	100
8	SM	427/451 (95%)	413 (97%)	14 (3%)	0	100	100
8	SO	427/451 (95%)	418 (98%)	9 (2%)	0	100	100
8	TE	425/451 (94%)	414 (97%)	11 (3%)	0	100	100
8	TG	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
8	TI	427/451 (95%)	417 (98%)	10 (2%)	0	100	100
8	TK	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
8	TM	427/451 (95%)	413 (97%)	14 (3%)	0	100	100
8	TO	425/451 (94%)	413 (97%)	12 (3%)	0	100	100
8	UE	427/451 (95%)	413 (97%)	14 (3%)	0	100	100
8	UG	428/451 (95%)	417 (97%)	11 (3%)	0	100	100
8	UI	428/451 (95%)	415 (97%)	13 (3%)	0	100	100
8	UK	427/451 (95%)	418 (98%)	9 (2%)	0	100	100
8	UM	427/451 (95%)	417 (98%)	10 (2%)	0	100	100
8	UO	427/451 (95%)	416 (97%)	11 (3%)	0	100	100
8	VE	437/451 (97%)	420 (96%)	17 (4%)	0	100	100
8	VG	429/451 (95%)	413 (96%)	16 (4%)	0	100	100
8	VI	437/451 (97%)	423 (97%)	13 (3%)	1 (0%)	47	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	VK	427/451 (95%)	419 (98%)	8 (2%)	0	100	100
8	VM	437/451 (97%)	428 (98%)	9 (2%)	0	100	100
8	VO	427/451 (95%)	418 (98%)	9 (2%)	0	100	100
8	WE	437/451 (97%)	423 (97%)	13 (3%)	1 (0%)	47	79
8	WG	426/451 (94%)	410 (96%)	16 (4%)	0	100	100
8	WI	436/451 (97%)	420 (96%)	16 (4%)	0	100	100
8	WK	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
8	WM	437/451 (97%)	415 (95%)	22 (5%)	0	100	100
8	WO	427/451 (95%)	408 (96%)	19 (4%)	0	100	100
9	AB	435/445 (98%)	418 (96%)	17 (4%)	0	100	100
9	AD	435/445 (98%)	419 (96%)	16 (4%)	0	100	100
9	AF	435/445 (98%)	415 (95%)	20 (5%)	0	100	100
9	AH	435/445 (98%)	417 (96%)	17 (4%)	1 (0%)	47	79
9	AJ	435/445 (98%)	418 (96%)	16 (4%)	1 (0%)	47	79
9	AL	435/445 (98%)	410 (94%)	24 (6%)	1 (0%)	47	79
9	BB	425/445 (96%)	405 (95%)	20 (5%)	0	100	100
9	BD	424/445 (95%)	410 (97%)	14 (3%)	0	100	100
9	BF	425/445 (96%)	409 (96%)	16 (4%)	0	100	100
9	BH	424/445 (95%)	404 (95%)	20 (5%)	0	100	100
9	BJ	428/445 (96%)	413 (96%)	13 (3%)	2 (0%)	29	68
9	BL	424/445 (95%)	408 (96%)	15 (4%)	1 (0%)	47	79
9	CB	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
9	CD	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	CF	425/445 (96%)	410 (96%)	14 (3%)	1 (0%)	47	79
9	CH	424/445 (95%)	406 (96%)	17 (4%)	1 (0%)	47	79
9	CJ	425/445 (96%)	407 (96%)	16 (4%)	2 (0%)	29	68
9	CL	424/445 (95%)	410 (97%)	13 (3%)	1 (0%)	47	79
9	DB	424/445 (95%)	406 (96%)	17 (4%)	1 (0%)	47	79
9	DD	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	DF	424/445 (95%)	407 (96%)	16 (4%)	1 (0%)	47	79
9	DH	424/445 (95%)	396 (93%)	28 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	DJ	424/445 (95%)	403 (95%)	20 (5%)	1 (0%)	47	79
9	DL	424/445 (95%)	397 (94%)	26 (6%)	1 (0%)	47	79
9	EB	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
9	ED	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
9	EF	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
9	EH	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	EJ	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
9	EL	424/445 (95%)	411 (97%)	12 (3%)	1 (0%)	47	79
9	EN	426/445 (96%)	417 (98%)	9 (2%)	0	100	100
9	FB	424/445 (95%)	407 (96%)	17 (4%)	0	100	100
9	FD	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	FF	424/445 (95%)	410 (97%)	13 (3%)	1 (0%)	47	79
9	FH	424/445 (95%)	407 (96%)	17 (4%)	0	100	100
9	FJ	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
9	FL	424/445 (95%)	405 (96%)	17 (4%)	2 (0%)	29	68
9	FN	425/445 (96%)	416 (98%)	9 (2%)	0	100	100
9	GB	406/445 (91%)	396 (98%)	10 (2%)	0	100	100
9	GD	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	GF	425/445 (96%)	406 (96%)	19 (4%)	0	100	100
9	GH	424/445 (95%)	406 (96%)	18 (4%)	0	100	100
9	GJ	428/445 (96%)	408 (95%)	19 (4%)	1 (0%)	47	79
9	GL	424/445 (95%)	403 (95%)	21 (5%)	0	100	100
9	GN	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
9	HB	425/445 (96%)	408 (96%)	15 (4%)	2 (0%)	29	68
9	HD	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	HF	425/445 (96%)	405 (95%)	19 (4%)	1 (0%)	47	79
9	HH	424/445 (95%)	406 (96%)	17 (4%)	1 (0%)	47	79
9	HJ	426/445 (96%)	411 (96%)	14 (3%)	1 (0%)	47	79
9	HL	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	HN	423/445 (95%)	407 (96%)	16 (4%)	0	100	100
9	IB	401/445 (90%)	385 (96%)	15 (4%)	1 (0%)	47	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	ID	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
9	IF	426/445 (96%)	408 (96%)	18 (4%)	0	100	100
9	IH	424/445 (95%)	404 (95%)	19 (4%)	1 (0%)	47	79
9	IJ	427/445 (96%)	410 (96%)	17 (4%)	0	100	100
9	IL	424/445 (95%)	403 (95%)	21 (5%)	0	100	100
9	IN	425/445 (96%)	406 (96%)	18 (4%)	1 (0%)	47	79
9	JB	424/445 (95%)	406 (96%)	18 (4%)	0	100	100
9	JD	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	JF	425/445 (96%)	409 (96%)	15 (4%)	1 (0%)	47	79
9	JH	424/445 (95%)	402 (95%)	22 (5%)	0	100	100
9	JJ	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	JL	424/445 (95%)	401 (95%)	22 (5%)	1 (0%)	47	79
9	JN	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
9	KB	408/445 (92%)	392 (96%)	16 (4%)	0	100	100
9	KD	429/445 (96%)	415 (97%)	14 (3%)	0	100	100
9	KF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
9	KH	429/445 (96%)	416 (97%)	13 (3%)	0	100	100
9	KJ	424/445 (95%)	410 (97%)	14 (3%)	0	100	100
9	KL	429/445 (96%)	410 (96%)	18 (4%)	1 (0%)	47	79
9	KN	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
9	LB	438/445 (98%)	423 (97%)	15 (3%)	0	100	100
9	LD	424/445 (95%)	410 (97%)	14 (3%)	0	100	100
9	LF	437/445 (98%)	418 (96%)	19 (4%)	0	100	100
9	LH	424/445 (95%)	403 (95%)	21 (5%)	0	100	100
9	LJ	441/445 (99%)	424 (96%)	17 (4%)	0	100	100
9	LL	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	LN	438/445 (98%)	421 (96%)	17 (4%)	0	100	100
9	MB	428/445 (96%)	414 (97%)	14 (3%)	0	100	100
9	MD	430/445 (97%)	416 (97%)	13 (3%)	1 (0%)	47	79
9	MF	429/445 (96%)	414 (96%)	15 (4%)	0	100	100
9	MH	430/445 (97%)	415 (96%)	14 (3%)	1 (0%)	47	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	MJ	430/445 (97%)	418 (97%)	12 (3%)	0	100	100
9	ML	430/445 (97%)	414 (96%)	15 (4%)	1 (0%)	47	79
9	MN	428/445 (96%)	411 (96%)	17 (4%)	0	100	100
9	NB	426/445 (96%)	410 (96%)	15 (4%)	1 (0%)	47	79
9	ND	426/445 (96%)	411 (96%)	15 (4%)	0	100	100
9	NF	428/445 (96%)	406 (95%)	22 (5%)	0	100	100
9	NH	426/445 (96%)	404 (95%)	21 (5%)	1 (0%)	47	79
9	NJ	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
9	NL	426/445 (96%)	404 (95%)	22 (5%)	0	100	100
9	NN	426/445 (96%)	404 (95%)	21 (5%)	1 (0%)	47	79
9	OB	429/445 (96%)	412 (96%)	16 (4%)	1 (0%)	47	79
9	OD	428/445 (96%)	412 (96%)	16 (4%)	0	100	100
9	OF	430/445 (97%)	413 (96%)	17 (4%)	0	100	100
9	OH	428/445 (96%)	409 (96%)	19 (4%)	0	100	100
9	OJ	430/445 (97%)	415 (96%)	15 (4%)	0	100	100
9	OL	428/445 (96%)	408 (95%)	18 (4%)	2 (0%)	29	68
9	ON	429/445 (96%)	414 (96%)	14 (3%)	1 (0%)	47	79
9	PD	428/445 (96%)	410 (96%)	16 (4%)	2 (0%)	29	68
9	PF	430/445 (97%)	411 (96%)	18 (4%)	1 (0%)	47	79
9	PH	424/445 (95%)	404 (95%)	20 (5%)	0	100	100
9	PJ	428/445 (96%)	414 (97%)	13 (3%)	1 (0%)	47	79
9	PL	427/445 (96%)	407 (95%)	20 (5%)	0	100	100
9	PN	428/445 (96%)	404 (94%)	24 (6%)	0	100	100
9	QD	426/445 (96%)	407 (96%)	19 (4%)	0	100	100
9	QF	428/445 (96%)	411 (96%)	16 (4%)	1 (0%)	47	79
9	QH	424/445 (95%)	410 (97%)	14 (3%)	0	100	100
9	QJ	427/445 (96%)	408 (96%)	19 (4%)	0	100	100
9	QL	425/445 (96%)	414 (97%)	11 (3%)	0	100	100
9	QN	426/445 (96%)	408 (96%)	18 (4%)	0	100	100
9	RD	424/445 (95%)	410 (97%)	14 (3%)	0	100	100
9	RF	427/445 (96%)	410 (96%)	17 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	RH	424/445 (95%)	406 (96%)	17 (4%)	1 (0%)	47	79
9	RJ	426/445 (96%)	408 (96%)	17 (4%)	1 (0%)	47	79
9	RL	424/445 (95%)	407 (96%)	17 (4%)	0	100	100
9	RN	425/445 (96%)	409 (96%)	16 (4%)	0	100	100
9	SD	424/445 (95%)	410 (97%)	14 (3%)	0	100	100
9	SF	424/445 (95%)	406 (96%)	18 (4%)	0	100	100
9	SH	424/445 (95%)	412 (97%)	12 (3%)	0	100	100
9	SJ	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
9	SL	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	SN	424/445 (95%)	408 (96%)	15 (4%)	1 (0%)	47	79
9	TD	424/445 (95%)	413 (97%)	11 (3%)	0	100	100
9	TF	425/445 (96%)	403 (95%)	22 (5%)	0	100	100
9	TH	424/445 (95%)	407 (96%)	17 (4%)	0	100	100
9	TJ	424/445 (95%)	407 (96%)	17 (4%)	0	100	100
9	TL	424/445 (95%)	400 (94%)	24 (6%)	0	100	100
9	TN	424/445 (95%)	402 (95%)	22 (5%)	0	100	100
9	TP	417/445 (94%)	402 (96%)	15 (4%)	0	100	100
9	UD	424/445 (95%)	410 (97%)	14 (3%)	0	100	100
9	UF	425/445 (96%)	411 (97%)	13 (3%)	1 (0%)	47	79
9	UH	424/445 (95%)	413 (97%)	11 (3%)	0	100	100
9	UJ	425/445 (96%)	407 (96%)	18 (4%)	0	100	100
9	UL	424/445 (95%)	411 (97%)	12 (3%)	1 (0%)	47	79
9	UN	425/445 (96%)	407 (96%)	17 (4%)	1 (0%)	47	79
9	UP	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
9	VD	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
9	VF	425/445 (96%)	404 (95%)	20 (5%)	1 (0%)	47	79
9	VH	424/445 (95%)	408 (96%)	16 (4%)	0	100	100
9	VJ	425/445 (96%)	408 (96%)	16 (4%)	1 (0%)	47	79
9	VL	424/445 (95%)	408 (96%)	15 (4%)	1 (0%)	47	79
9	VN	425/445 (96%)	406 (96%)	18 (4%)	1 (0%)	47	79
9	VP	425/445 (96%)	411 (97%)	14 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	WD	424/445 (95%)	412 (97%)	11 (3%)	1 (0%)	47	79
9	WF	424/445 (95%)	407 (96%)	17 (4%)	0	100	100
9	WH	424/445 (95%)	401 (95%)	23 (5%)	0	100	100
9	WJ	424/445 (95%)	401 (95%)	23 (5%)	0	100	100
9	WL	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
9	WN	425/445 (96%)	401 (94%)	24 (6%)	0	100	100
9	WP	425/445 (96%)	405 (95%)	19 (4%)	1 (0%)	47	79
10	B	178/495 (36%)	177 (99%)	1 (1%)	0	100	100
10	C	354/495 (72%)	352 (99%)	2 (1%)	0	100	100
11	B0	189/430 (44%)	188 (100%)	1 (0%)	0	100	100
11	B1	390/430 (91%)	383 (98%)	7 (2%)	0	100	100
11	B2	389/430 (90%)	381 (98%)	8 (2%)	0	100	100
11	B3	352/430 (82%)	343 (97%)	9 (3%)	0	100	100
11	B4	49/430 (11%)	47 (96%)	2 (4%)	0	100	100
11	B5	49/430 (11%)	47 (96%)	2 (4%)	0	100	100
11	B6	352/430 (82%)	348 (99%)	4 (1%)	0	100	100
11	B7	389/430 (90%)	385 (99%)	4 (1%)	0	100	100
11	B8	390/430 (91%)	385 (99%)	5 (1%)	0	100	100
11	B9	189/430 (44%)	189 (100%)	0	0	100	100
12	C0	31/490 (6%)	30 (97%)	1 (3%)	0	100	100
12	C1	332/490 (68%)	326 (98%)	6 (2%)	0	100	100
12	C2	391/490 (80%)	385 (98%)	5 (1%)	1 (0%)	41	75
12	C3	392/490 (80%)	379 (97%)	12 (3%)	1 (0%)	41	75
12	C4	215/490 (44%)	211 (98%)	4 (2%)	0	100	100
13	D	177/485 (36%)	165 (93%)	12 (7%)	0	100	100
14	D0	260/435 (60%)	256 (98%)	4 (2%)	0	100	100
14	D1	394/435 (91%)	389 (99%)	5 (1%)	0	100	100
14	D2	396/435 (91%)	391 (99%)	5 (1%)	0	100	100
14	D3	313/435 (72%)	308 (98%)	5 (2%)	0	100	100
14	D5	313/435 (72%)	309 (99%)	4 (1%)	0	100	100
14	D6	396/435 (91%)	390 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	D7	394/435 (91%)	383 (97%)	11 (3%)	0	100	100
14	D8	260/435 (60%)	257 (99%)	3 (1%)	0	100	100
15	E	275/301 (91%)	265 (96%)	10 (4%)	0	100	100
15	F	275/301 (91%)	267 (97%)	8 (3%)	0	100	100
16	F0	155/222 (70%)	150 (97%)	4 (3%)	1 (1%)	25	64
16	F1	158/222 (71%)	152 (96%)	6 (4%)	0	100	100
16	F2	154/222 (69%)	150 (97%)	3 (2%)	1 (1%)	25	64
16	F3	155/222 (70%)	150 (97%)	5 (3%)	0	100	100
16	F4	158/222 (71%)	155 (98%)	3 (2%)	0	100	100
16	F5	154/222 (69%)	150 (97%)	3 (2%)	1 (1%)	25	64
16	F6	155/222 (70%)	148 (96%)	7 (4%)	0	100	100
16	F7	158/222 (71%)	150 (95%)	8 (5%)	0	100	100
16	F8	154/222 (69%)	150 (97%)	3 (2%)	1 (1%)	25	64
16	G0	157/222 (71%)	150 (96%)	7 (4%)	0	100	100
16	G1	156/222 (70%)	148 (95%)	8 (5%)	0	100	100
16	G2	154/222 (69%)	149 (97%)	5 (3%)	0	100	100
16	G3	155/222 (70%)	150 (97%)	5 (3%)	0	100	100
16	G4	158/222 (71%)	150 (95%)	8 (5%)	0	100	100
16	G5	154/222 (69%)	151 (98%)	3 (2%)	0	100	100
16	G6	155/222 (70%)	150 (97%)	5 (3%)	0	100	100
16	G7	158/222 (71%)	149 (94%)	9 (6%)	0	100	100
16	G8	154/222 (69%)	149 (97%)	5 (3%)	0	100	100
16	H0	155/222 (70%)	151 (97%)	3 (2%)	1 (1%)	25	64
16	H1	158/222 (71%)	153 (97%)	5 (3%)	0	100	100
16	H2	154/222 (69%)	149 (97%)	5 (3%)	0	100	100
17	G	92/121 (76%)	88 (96%)	4 (4%)	0	100	100
18	H	76/275 (28%)	72 (95%)	3 (4%)	1 (1%)	12	50
18	I	137/275 (50%)	131 (96%)	6 (4%)	0	100	100
18	J	138/275 (50%)	131 (95%)	6 (4%)	1 (1%)	22	61
18	K	137/275 (50%)	134 (98%)	2 (2%)	1 (1%)	22	61
18	L	137/275 (50%)	131 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	M	137/275 (50%)	131 (96%)	5 (4%)	1 (1%)	22	61
18	N	138/275 (50%)	130 (94%)	7 (5%)	1 (1%)	22	61
19	I1	87/150 (58%)	85 (98%)	2 (2%)	0	100	100
20	J1	75/284 (26%)	72 (96%)	3 (4%)	0	100	100
20	J2	218/284 (77%)	209 (96%)	8 (4%)	1 (0%)	29	68
20	J3	218/284 (77%)	208 (95%)	8 (4%)	2 (1%)	17	57
20	J4	197/284 (69%)	186 (94%)	10 (5%)	1 (0%)	29	68
20	J5	63/284 (22%)	58 (92%)	4 (6%)	1 (2%)	9	46
21	K1	109/134 (81%)	100 (92%)	9 (8%)	0	100	100
22	L1	125/147 (85%)	116 (93%)	9 (7%)	0	100	100
22	L2	88/147 (60%)	83 (94%)	5 (6%)	0	100	100
23	M1	98/201 (49%)	94 (96%)	4 (4%)	0	100	100
23	M2	97/201 (48%)	94 (97%)	3 (3%)	0	100	100
23	M3	98/201 (49%)	95 (97%)	3 (3%)	0	100	100
23	M4	98/201 (49%)	95 (97%)	3 (3%)	0	100	100
24	O	23/382 (6%)	23 (100%)	0	0	100	100
24	P	366/382 (96%)	359 (98%)	6 (2%)	1 (0%)	41	75
24	Q	38/382 (10%)	37 (97%)	1 (3%)	0	100	100
24	R	215/382 (56%)	215 (100%)	0	0	100	100
24	S	163/382 (43%)	161 (99%)	2 (1%)	0	100	100
25	T	478/640 (75%)	447 (94%)	31 (6%)	0	100	100
25	U	479/640 (75%)	451 (94%)	28 (6%)	0	100	100
25	V	479/640 (75%)	454 (95%)	25 (5%)	0	100	100
26	W	604/749 (81%)	571 (94%)	32 (5%)	1 (0%)	47	79
26	X	689/749 (92%)	638 (93%)	49 (7%)	2 (0%)	41	75
26	Y	689/749 (92%)	642 (93%)	46 (7%)	1 (0%)	51	83
26	Z	498/749 (66%)	468 (94%)	30 (6%)	0	100	100
27	XA	184/193 (95%)	178 (97%)	6 (3%)	0	100	100
27	XB	184/193 (95%)	177 (96%)	7 (4%)	0	100	100
27	XC	184/193 (95%)	178 (97%)	6 (3%)	0	100	100
27	XD	184/193 (95%)	178 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	XE	184/193 (95%)	175 (95%)	9 (5%)	0	100	100
27	XF	184/193 (95%)	174 (95%)	10 (5%)	0	100	100
27	XG	184/193 (95%)	177 (96%)	7 (4%)	0	100	100
28	YB	218/257 (85%)	212 (97%)	6 (3%)	0	100	100
28	YC	218/257 (85%)	213 (98%)	5 (2%)	0	100	100
28	YD	218/257 (85%)	210 (96%)	8 (4%)	0	100	100
28	YE	218/257 (85%)	215 (99%)	3 (1%)	0	100	100
28	YF	218/257 (85%)	215 (99%)	3 (1%)	0	100	100
28	YG	218/257 (85%)	211 (97%)	7 (3%)	0	100	100
29	a	168/551 (30%)	167 (99%)	1 (1%)	0	100	100
29	b	332/551 (60%)	332 (100%)	0	0	100	100
29	c	280/551 (51%)	277 (99%)	3 (1%)	0	100	100
29	d	216/551 (39%)	216 (100%)	0	0	100	100
30	e	608/620 (98%)	582 (96%)	24 (4%)	2 (0%)	41	75
30	f	608/620 (98%)	583 (96%)	25 (4%)	0	100	100
30	g	608/620 (98%)	582 (96%)	26 (4%)	0	100	100
31	h	144/256 (56%)	142 (99%)	2 (1%)	0	100	100
31	i	248/256 (97%)	242 (98%)	5 (2%)	1 (0%)	34	71
31	j	246/256 (96%)	244 (99%)	2 (1%)	0	100	100
31	k	248/256 (97%)	244 (98%)	4 (2%)	0	100	100
32	l	115/177 (65%)	110 (96%)	5 (4%)	0	100	100
32	m	115/177 (65%)	112 (97%)	2 (2%)	1 (1%)	17	57
32	n	115/177 (65%)	111 (96%)	3 (3%)	1 (1%)	17	57
33	o	402/552 (73%)	400 (100%)	2 (0%)	0	100	100
33	o1	34/552 (6%)	33 (97%)	1 (3%)	0	100	100
33	p	156/552 (28%)	153 (98%)	3 (2%)	0	100	100
34	q	108/169 (64%)	102 (94%)	6 (6%)	0	100	100
34	r	108/169 (64%)	98 (91%)	10 (9%)	0	100	100
34	s	108/169 (64%)	103 (95%)	5 (5%)	0	100	100
35	y	61/136 (45%)	59 (97%)	2 (3%)	0	100	100
35	z	109/136 (80%)	104 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	159406/181357 (88%)	153891 (96%)	5408 (3%)	107 (0%)	54	83

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AC	98	ASP
8	BC	98	ASP
12	C2	213	ASP
12	C3	407	PRO
9	DF	272	PRO
9	DL	272	PRO
9	EL	272	PRO
16	F0	117	TYR
16	F2	117	TYR
16	F8	117	TYR
8	GC	98	ASP
18	H	49	PRO
18	J	49	PRO
20	J4	31	PRO
20	J5	31	PRO
18	K	49	PRO
8	KC	98	ASP
8	LC	98	ASP
18	M	49	PRO
8	MC	98	ASP
8	OC	98	ASP
8	PC	98	ASP
8	WE	37	PRO
26	Y	726	PRO
30	e	158	VAL
8	AI	40	LYS
9	AJ	271	ALA
8	EC	98	ASP
9	FL	176	SER
8	HC	98	ASP
8	IC	98	ASP
20	J3	161	PRO
8	NC	98	ASP
8	NG	42	ILE
24	P	276	ASP
8	AA	97	GLU
8	BA	98	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	CC	98	ASP
16	F5	117	TYR
16	H0	133	HIS
9	JL	272	PRO
9	OB	268	PRO
8	QG	46	ASP
9	SN	272	PRO
26	X	726	PRO
9	NN	271	ALA
9	WD	268	PRO
31	i	144	LYS
32	n	8	ASN
9	AL	428	ALA
20	J3	28	VAL
9	ML	272	PRO
18	N	48	PRO
9	RH	271	ALA
8	VI	38	SER
26	W	292	VAL
30	e	63	HIS
32	m	8	ASN
8	CA	98	ASP
9	DB	272	PRO
20	J2	28	VAL
9	NB	268	PRO
9	PJ	272	PRO
8	QC	98	ASP
9	RJ	272	PRO
9	VF	271	ALA
9	CL	271	ALA
9	FF	271	ALA
9	HH	272	PRO
9	PF	268	PRO
9	UF	271	ALA
9	BJ	268	PRO
9	CJ	271	ALA
9	CJ	272	PRO
9	GJ	271	ALA
9	HJ	268	PRO
9	IH	271	ALA
9	PD	268	PRO
9	UL	271	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	VL	271	ALA
9	WP	268	PRO
9	BJ	271	ALA
9	CF	271	ALA
9	DJ	272	PRO
9	FL	271	ALA
9	HB	268	PRO
9	IB	271	ALA
9	MD	272	PRO
9	MH	271	ALA
9	OL	271	ALA
9	OL	272	PRO
9	ON	268	PRO
9	QF	272	PRO
9	UN	271	ALA
9	VJ	271	ALA
9	AH	268	PRO
9	BL	271	ALA
9	HF	271	ALA
9	JF	272	PRO
9	KL	272	PRO
9	NH	271	ALA
9	PD	271	ALA
26	X	288	CYS
9	CH	271	ALA
9	HB	272	PRO
9	IN	268	PRO
9	VN	271	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/209 (22%)	47 (100%)	0	100	100
1	7	135/209 (65%)	135 (100%)	0	100	100
2	1	243/724 (34%)	242 (100%)	1 (0%)	91	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	392/724 (54%)	391 (100%)	1 (0%)	92	97
3	3	274/470 (58%)	273 (100%)	1 (0%)	91	97
3	4	197/470 (42%)	197 (100%)	0	100	100
4	5	315/320 (98%)	315 (100%)	0	100	100
4	6	315/320 (98%)	315 (100%)	0	100	100
5	8	157/181 (87%)	156 (99%)	1 (1%)	86	94
5	9	47/181 (26%)	47 (100%)	0	100	100
6	A	44/90 (49%)	44 (100%)	0	100	100
7	A0	195/376 (52%)	194 (100%)	1 (0%)	88	95
7	A1	356/376 (95%)	356 (100%)	0	100	100
7	A2	356/376 (95%)	355 (100%)	1 (0%)	92	97
7	A3	305/376 (81%)	305 (100%)	0	100	100
7	A4	31/376 (8%)	31 (100%)	0	100	100
8	AA	369/378 (98%)	367 (100%)	2 (0%)	88	95
8	AC	369/378 (98%)	369 (100%)	0	100	100
8	AE	369/378 (98%)	367 (100%)	2 (0%)	88	95
8	AG	369/378 (98%)	369 (100%)	0	100	100
8	AI	369/378 (98%)	367 (100%)	2 (0%)	88	95
8	AK	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	AM	369/378 (98%)	367 (100%)	2 (0%)	88	95
8	BA	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	BC	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	BE	364/378 (96%)	364 (100%)	0	100	100
8	BG	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	BI	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	BK	369/378 (98%)	369 (100%)	0	100	100
8	BM	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	CA	365/378 (97%)	365 (100%)	0	100	100
8	CC	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	CE	363/378 (96%)	363 (100%)	0	100	100
8	CG	369/378 (98%)	368 (100%)	1 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	364/378 (96%)	364 (100%)	0	100	100
8	CK	369/378 (98%)	369 (100%)	0	100	100
8	CM	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	DA	327/378 (86%)	326 (100%)	1 (0%)	92	97
8	DC	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	DE	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	DG	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	DI	363/378 (96%)	361 (99%)	2 (1%)	86	94
8	DK	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	DM	364/378 (96%)	364 (100%)	0	100	100
8	EC	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	EE	369/378 (98%)	369 (100%)	0	100	100
8	EG	368/378 (97%)	367 (100%)	1 (0%)	92	97
8	EI	369/378 (98%)	369 (100%)	0	100	100
8	EK	368/378 (97%)	368 (100%)	0	100	100
8	EM	368/378 (97%)	367 (100%)	1 (0%)	92	97
8	FC	364/378 (96%)	364 (100%)	0	100	100
8	FE	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	FG	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	FI	363/378 (96%)	363 (100%)	0	100	100
8	FK	363/378 (96%)	360 (99%)	3 (1%)	81	91
8	FM	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	GC	368/378 (97%)	368 (100%)	0	100	100
8	GE	363/378 (96%)	363 (100%)	0	100	100
8	GG	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	GI	363/378 (96%)	361 (99%)	2 (1%)	86	94
8	GK	365/378 (97%)	364 (100%)	1 (0%)	92	97
8	GM	367/378 (97%)	367 (100%)	0	100	100
8	HC	364/378 (96%)	362 (100%)	2 (0%)	88	95
8	HE	365/378 (97%)	364 (100%)	1 (0%)	92	97
8	HG	365/378 (97%)	365 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	HI	365/378 (97%)	363 (100%)	2 (0%)	88	95
8	HK	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	HM	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	HO	329/378 (87%)	327 (99%)	2 (1%)	86	94
8	IC	366/378 (97%)	364 (100%)	2 (0%)	88	95
8	IE	364/378 (96%)	364 (100%)	0	100	100
8	IG	369/378 (98%)	369 (100%)	0	100	100
8	II	365/378 (97%)	365 (100%)	0	100	100
8	IK	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	IM	364/378 (96%)	364 (100%)	0	100	100
8	IO	364/378 (96%)	364 (100%)	0	100	100
8	JC	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	JE	363/378 (96%)	363 (100%)	0	100	100
8	JG	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	JI	363/378 (96%)	363 (100%)	0	100	100
8	JK	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	JM	363/378 (96%)	363 (100%)	0	100	100
8	KC	365/378 (97%)	365 (100%)	0	100	100
8	KE	365/378 (97%)	363 (100%)	2 (0%)	88	95
8	KG	365/378 (97%)	363 (100%)	2 (0%)	88	95
8	KI	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	KK	365/378 (97%)	364 (100%)	1 (0%)	92	97
8	KM	368/378 (97%)	367 (100%)	1 (0%)	92	97
8	KO	364/378 (96%)	362 (100%)	2 (0%)	88	95
8	LC	365/378 (97%)	364 (100%)	1 (0%)	92	97
8	LE	369/378 (98%)	369 (100%)	0	100	100
8	LG	366/378 (97%)	364 (100%)	2 (0%)	88	95
8	LI	367/378 (97%)	366 (100%)	1 (0%)	92	97
8	LK	365/378 (97%)	364 (100%)	1 (0%)	92	97
8	LM	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	MC	370/378 (98%)	370 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	ME	365/378 (97%)	364 (100%)	1 (0%)	92	97
8	MG	365/378 (97%)	363 (100%)	2 (0%)	88	95
8	MI	366/378 (97%)	365 (100%)	1 (0%)	92	97
8	MK	370/378 (98%)	368 (100%)	2 (0%)	88	95
8	MM	370/378 (98%)	370 (100%)	0	100	100
8	NC	370/378 (98%)	367 (99%)	3 (1%)	81	91
8	NE	369/378 (98%)	363 (98%)	6 (2%)	62	83
8	NG	369/378 (98%)	367 (100%)	2 (0%)	88	95
8	NI	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	NK	369/378 (98%)	365 (99%)	4 (1%)	73	88
8	NM	369/378 (98%)	366 (99%)	3 (1%)	81	91
8	OC	371/378 (98%)	370 (100%)	1 (0%)	92	97
8	OE	370/378 (98%)	370 (100%)	0	100	100
8	OG	371/378 (98%)	370 (100%)	1 (0%)	92	97
8	OI	371/378 (98%)	370 (100%)	1 (0%)	92	97
8	OK	369/378 (98%)	369 (100%)	0	100	100
8	OM	371/378 (98%)	370 (100%)	1 (0%)	92	97
8	OO	356/378 (94%)	356 (100%)	0	100	100
8	PC	371/378 (98%)	371 (100%)	0	100	100
8	PE	370/378 (98%)	370 (100%)	0	100	100
8	PG	371/378 (98%)	369 (100%)	2 (0%)	88	95
8	PI	369/378 (98%)	369 (100%)	0	100	100
8	PK	370/378 (98%)	368 (100%)	2 (0%)	88	95
8	PM	369/378 (98%)	369 (100%)	0	100	100
8	PO	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	QC	370/378 (98%)	370 (100%)	0	100	100
8	QE	370/378 (98%)	370 (100%)	0	100	100
8	QG	370/378 (98%)	369 (100%)	1 (0%)	92	97
8	QI	370/378 (98%)	369 (100%)	1 (0%)	92	97
8	QK	370/378 (98%)	368 (100%)	2 (0%)	88	95
8	QM	370/378 (98%)	369 (100%)	1 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QO	370/378 (98%)	370 (100%)	0	100	100
8	RC	349/378 (92%)	346 (99%)	3 (1%)	78	90
8	RE	363/378 (96%)	363 (100%)	0	100	100
8	RG	365/378 (97%)	365 (100%)	0	100	100
8	RI	369/378 (98%)	369 (100%)	0	100	100
8	RK	370/378 (98%)	370 (100%)	0	100	100
8	RM	370/378 (98%)	370 (100%)	0	100	100
8	RO	369/378 (98%)	369 (100%)	0	100	100
8	SE	362/378 (96%)	361 (100%)	1 (0%)	92	97
8	SG	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	SI	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	SK	364/378 (96%)	361 (99%)	3 (1%)	81	91
8	SM	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	SO	364/378 (96%)	364 (100%)	0	100	100
8	TE	362/378 (96%)	361 (100%)	1 (0%)	92	97
8	TG	363/378 (96%)	363 (100%)	0	100	100
8	TI	364/378 (96%)	364 (100%)	0	100	100
8	TK	362/378 (96%)	360 (99%)	2 (1%)	86	94
8	TM	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	TO	362/378 (96%)	362 (100%)	0	100	100
8	UE	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	UG	365/378 (97%)	365 (100%)	0	100	100
8	UI	365/378 (97%)	363 (100%)	2 (0%)	88	95
8	UK	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	UM	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	UO	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	VE	369/378 (98%)	368 (100%)	1 (0%)	92	97
8	VG	366/378 (97%)	364 (100%)	2 (0%)	88	95
8	VI	369/378 (98%)	369 (100%)	0	100	100
8	VK	364/378 (96%)	363 (100%)	1 (0%)	92	97
8	VM	369/378 (98%)	367 (100%)	2 (0%)	88	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	VO	364/378 (96%)	364 (100%)	0	100	100
8	WE	369/378 (98%)	366 (99%)	3 (1%)	81	91
8	WG	363/378 (96%)	362 (100%)	1 (0%)	92	97
8	WI	368/378 (97%)	367 (100%)	1 (0%)	92	97
8	WK	363/378 (96%)	363 (100%)	0	100	100
8	WM	369/378 (98%)	367 (100%)	2 (0%)	88	95
8	WO	364/378 (96%)	364 (100%)	0	100	100
9	AB	374/380 (98%)	372 (100%)	2 (0%)	88	95
9	AD	374/380 (98%)	373 (100%)	1 (0%)	92	97
9	AF	374/380 (98%)	369 (99%)	5 (1%)	69	86
9	AH	374/380 (98%)	372 (100%)	2 (0%)	88	95
9	AJ	374/380 (98%)	372 (100%)	2 (0%)	88	95
9	AL	374/380 (98%)	373 (100%)	1 (0%)	92	97
9	BB	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	BD	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	BF	367/380 (97%)	365 (100%)	2 (0%)	88	95
9	BH	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	BJ	368/380 (97%)	365 (99%)	3 (1%)	81	91
9	BL	366/380 (96%)	366 (100%)	0	100	100
9	CB	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	CD	366/380 (96%)	366 (100%)	0	100	100
9	CF	367/380 (97%)	365 (100%)	2 (0%)	88	95
9	CH	366/380 (96%)	366 (100%)	0	100	100
9	CJ	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	CL	366/380 (96%)	366 (100%)	0	100	100
9	DB	366/380 (96%)	366 (100%)	0	100	100
9	DD	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	DF	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	DH	366/380 (96%)	366 (100%)	0	100	100
9	DJ	366/380 (96%)	366 (100%)	0	100	100
9	DL	366/380 (96%)	365 (100%)	1 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	EB	366/380 (96%)	366 (100%)	0	100	100
9	ED	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	EF	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	EH	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	EJ	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	EL	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	EN	367/380 (97%)	367 (100%)	0	100	100
9	FB	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	FD	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	FF	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	FH	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	FJ	366/380 (96%)	366 (100%)	0	100	100
9	FL	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	FN	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	GB	353/380 (93%)	351 (99%)	2 (1%)	86	94
9	GD	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	GF	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	GH	366/380 (96%)	366 (100%)	0	100	100
9	GJ	368/380 (97%)	365 (99%)	3 (1%)	81	91
9	GL	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	GN	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	HB	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	HD	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	HF	367/380 (97%)	367 (100%)	0	100	100
9	HH	366/380 (96%)	366 (100%)	0	100	100
9	HJ	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	HL	366/380 (96%)	362 (99%)	4 (1%)	73	88
9	HN	365/380 (96%)	363 (100%)	2 (0%)	88	95
9	IB	353/380 (93%)	352 (100%)	1 (0%)	92	97
9	ID	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	IF	367/380 (97%)	366 (100%)	1 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	IH	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	IJ	368/380 (97%)	367 (100%)	1 (0%)	92	97
9	IL	366/380 (96%)	366 (100%)	0	100	100
9	IN	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	JB	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	JD	366/380 (96%)	366 (100%)	0	100	100
9	JF	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	JH	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	JJ	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	JL	366/380 (96%)	366 (100%)	0	100	100
9	JN	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	KB	355/380 (93%)	354 (100%)	1 (0%)	92	97
9	KD	369/380 (97%)	367 (100%)	2 (0%)	88	95
9	KF	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	KH	369/380 (97%)	368 (100%)	1 (0%)	92	97
9	KJ	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	KL	369/380 (97%)	367 (100%)	2 (0%)	88	95
9	KN	366/380 (96%)	366 (100%)	0	100	100
9	LB	376/380 (99%)	374 (100%)	2 (0%)	88	95
9	LD	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	LF	376/380 (99%)	374 (100%)	2 (0%)	88	95
9	LH	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	LJ	379/380 (100%)	376 (99%)	3 (1%)	81	91
9	LL	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	LN	376/380 (99%)	375 (100%)	1 (0%)	92	97
9	MB	368/380 (97%)	368 (100%)	0	100	100
9	MD	370/380 (97%)	369 (100%)	1 (0%)	92	97
9	MF	369/380 (97%)	368 (100%)	1 (0%)	92	97
9	MH	370/380 (97%)	369 (100%)	1 (0%)	92	97
9	MJ	370/380 (97%)	369 (100%)	1 (0%)	92	97
9	ML	370/380 (97%)	367 (99%)	3 (1%)	81	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	MN	368/380 (97%)	368 (100%)	0	100	100
9	NB	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	ND	367/380 (97%)	365 (100%)	2 (0%)	88	95
9	NF	368/380 (97%)	364 (99%)	4 (1%)	73	88
9	NH	367/380 (97%)	365 (100%)	2 (0%)	88	95
9	NJ	368/380 (97%)	364 (99%)	4 (1%)	73	88
9	NL	367/380 (97%)	363 (99%)	4 (1%)	73	88
9	NN	367/380 (97%)	365 (100%)	2 (0%)	88	95
9	OB	369/380 (97%)	369 (100%)	0	100	100
9	OD	368/380 (97%)	368 (100%)	0	100	100
9	OF	370/380 (97%)	369 (100%)	1 (0%)	92	97
9	OH	368/380 (97%)	368 (100%)	0	100	100
9	OJ	370/380 (97%)	369 (100%)	1 (0%)	92	97
9	OL	368/380 (97%)	367 (100%)	1 (0%)	92	97
9	ON	369/380 (97%)	368 (100%)	1 (0%)	92	97
9	PD	368/380 (97%)	368 (100%)	0	100	100
9	PF	370/380 (97%)	370 (100%)	0	100	100
9	PH	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	PJ	368/380 (97%)	367 (100%)	1 (0%)	92	97
9	PL	368/380 (97%)	367 (100%)	1 (0%)	92	97
9	PN	368/380 (97%)	367 (100%)	1 (0%)	92	97
9	QD	367/380 (97%)	367 (100%)	0	100	100
9	QF	368/380 (97%)	368 (100%)	0	100	100
9	QH	366/380 (96%)	366 (100%)	0	100	100
9	QJ	368/380 (97%)	366 (100%)	2 (0%)	88	95
9	QL	367/380 (97%)	367 (100%)	0	100	100
9	QN	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	RD	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	RF	368/380 (97%)	367 (100%)	1 (0%)	92	97
9	RH	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	RJ	367/380 (97%)	366 (100%)	1 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	RL	366/380 (96%)	366 (100%)	0	100	100
9	RN	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	SD	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	SF	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	SH	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	SJ	366/380 (96%)	366 (100%)	0	100	100
9	SL	366/380 (96%)	366 (100%)	0	100	100
9	SN	366/380 (96%)	366 (100%)	0	100	100
9	TD	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	TF	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	TH	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	TJ	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	TL	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	TN	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	TP	361/380 (95%)	360 (100%)	1 (0%)	92	97
9	UD	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	UF	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	UH	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	UJ	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	UL	366/380 (96%)	361 (99%)	5 (1%)	67	85
9	UN	367/380 (97%)	363 (99%)	4 (1%)	73	88
9	UP	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	VD	366/380 (96%)	366 (100%)	0	100	100
9	VF	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	VH	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	VJ	367/380 (97%)	365 (100%)	2 (0%)	88	95
9	VL	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	VN	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	VP	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	WD	366/380 (96%)	366 (100%)	0	100	100
9	WF	366/380 (96%)	364 (100%)	2 (0%)	88	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	WH	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	WJ	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	WL	366/380 (96%)	364 (100%)	2 (0%)	88	95
9	WN	367/380 (97%)	367 (100%)	0	100	100
9	WP	367/380 (97%)	366 (100%)	1 (0%)	92	97
10	B	163/455 (36%)	162 (99%)	1 (1%)	86	94
10	C	322/455 (71%)	320 (99%)	2 (1%)	86	94
11	B0	176/388 (45%)	175 (99%)	1 (1%)	86	94
11	B1	353/388 (91%)	353 (100%)	0	100	100
11	B2	352/388 (91%)	352 (100%)	0	100	100
11	B3	318/388 (82%)	318 (100%)	0	100	100
11	B4	45/388 (12%)	45 (100%)	0	100	100
12	C0	33/446 (7%)	33 (100%)	0	100	100
12	C1	303/446 (68%)	302 (100%)	1 (0%)	92	97
12	C2	356/446 (80%)	353 (99%)	3 (1%)	81	91
12	C3	357/446 (80%)	357 (100%)	0	100	100
12	C4	201/446 (45%)	201 (100%)	0	100	100
13	D	163/393 (42%)	163 (100%)	0	100	100
14	D0	237/387 (61%)	236 (100%)	1 (0%)	91	97
14	D1	355/387 (92%)	355 (100%)	0	100	100
14	D2	357/387 (92%)	356 (100%)	1 (0%)	92	97
14	D3	285/387 (74%)	285 (100%)	0	100	100
15	E	246/266 (92%)	246 (100%)	0	100	100
15	F	246/266 (92%)	246 (100%)	0	100	100
16	F0	146/199 (73%)	146 (100%)	0	100	100
16	F1	149/199 (75%)	149 (100%)	0	100	100
16	F3	146/199 (73%)	146 (100%)	0	100	100
16	F4	149/199 (75%)	149 (100%)	0	100	100
16	F6	146/199 (73%)	146 (100%)	0	100	100
16	F7	149/199 (75%)	148 (99%)	1 (1%)	84	93
16	G0	148/199 (74%)	148 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	G1	147/199 (74%)	146 (99%)	1 (1%)	84	93
16	G3	146/199 (73%)	146 (100%)	0	100	100
16	G4	149/199 (75%)	148 (99%)	1 (1%)	84	93
16	G6	146/199 (73%)	145 (99%)	1 (1%)	84	93
16	G7	149/199 (75%)	148 (99%)	1 (1%)	84	93
16	H0	146/199 (73%)	146 (100%)	0	100	100
16	H1	149/199 (75%)	149 (100%)	0	100	100
17	G	88/115 (76%)	87 (99%)	1 (1%)	73	88
18	H	66/235 (28%)	66 (100%)	0	100	100
18	I	106/235 (45%)	106 (100%)	0	100	100
18	J	106/235 (45%)	106 (100%)	0	100	100
18	K	106/235 (45%)	105 (99%)	1 (1%)	78	90
18	L	106/235 (45%)	105 (99%)	1 (1%)	78	90
18	M	106/235 (45%)	106 (100%)	0	100	100
18	N	106/235 (45%)	105 (99%)	1 (1%)	78	90
19	I1	86/139 (62%)	84 (98%)	2 (2%)	50	76
20	J1	75/252 (30%)	75 (100%)	0	100	100
20	J2	200/252 (79%)	199 (100%)	1 (0%)	88	95
20	J3	200/252 (79%)	199 (100%)	1 (0%)	88	95
20	J4	182/252 (72%)	180 (99%)	2 (1%)	73	88
20	J5	58/252 (23%)	58 (100%)	0	100	100
21	K1	105/123 (85%)	104 (99%)	1 (1%)	76	88
22	L1	113/131 (86%)	113 (100%)	0	100	100
22	L2	82/131 (63%)	82 (100%)	0	100	100
23	M1	87/180 (48%)	87 (100%)	0	100	100
23	M2	86/180 (48%)	86 (100%)	0	100	100
23	M3	87/180 (48%)	87 (100%)	0	100	100
23	M4	87/180 (48%)	86 (99%)	1 (1%)	73	88
24	O	21/342 (6%)	21 (100%)	0	100	100
24	P	331/342 (97%)	331 (100%)	0	100	100
24	Q	37/342 (11%)	36 (97%)	1 (3%)	44	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	R	194/342 (57%)	194 (100%)	0	100	100
24	S	150/342 (44%)	150 (100%)	0	100	100
25	T	439/577 (76%)	438 (100%)	1 (0%)	93	98
25	U	440/577 (76%)	439 (100%)	1 (0%)	93	98
25	V	440/577 (76%)	440 (100%)	0	100	100
26	W	561/688 (82%)	559 (100%)	2 (0%)	91	97
26	X	645/688 (94%)	643 (100%)	2 (0%)	92	97
26	Y	645/688 (94%)	643 (100%)	2 (0%)	92	97
26	Z	471/688 (68%)	469 (100%)	2 (0%)	91	97
27	XA	174/180 (97%)	174 (100%)	0	100	100
27	XB	174/180 (97%)	173 (99%)	1 (1%)	86	94
27	XC	174/180 (97%)	173 (99%)	1 (1%)	86	94
27	XD	174/180 (97%)	174 (100%)	0	100	100
27	XE	174/180 (97%)	173 (99%)	1 (1%)	86	94
27	XF	174/180 (97%)	174 (100%)	0	100	100
27	XG	174/180 (97%)	174 (100%)	0	100	100
28	YB	192/227 (85%)	192 (100%)	0	100	100
28	YC	192/227 (85%)	192 (100%)	0	100	100
28	YD	192/227 (85%)	192 (100%)	0	100	100
28	YE	192/227 (85%)	192 (100%)	0	100	100
28	YF	192/227 (85%)	192 (100%)	0	100	100
28	YG	192/227 (85%)	192 (100%)	0	100	100
29	a	162/495 (33%)	161 (99%)	1 (1%)	86	94
29	b	302/495 (61%)	302 (100%)	0	100	100
29	c	263/495 (53%)	261 (99%)	2 (1%)	81	91
29	d	189/495 (38%)	188 (100%)	1 (0%)	88	95
30	e	514/523 (98%)	514 (100%)	0	100	100
30	f	514/523 (98%)	513 (100%)	1 (0%)	93	98
30	g	514/523 (98%)	512 (100%)	2 (0%)	91	97
31	h	133/233 (57%)	132 (99%)	1 (1%)	81	91
31	i	228/233 (98%)	228 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	j	226/233 (97%)	225 (100%)	1 (0%)	91	97
31	k	228/233 (98%)	228 (100%)	0	100	100
32	l	100/153 (65%)	100 (100%)	0	100	100
32	m	100/153 (65%)	100 (100%)	0	100	100
32	n	100/153 (65%)	100 (100%)	0	100	100
33	o	366/495 (74%)	362 (99%)	4 (1%)	73	88
33	o1	32/495 (6%)	32 (100%)	0	100	100
33	p	134/495 (27%)	132 (98%)	2 (2%)	65	84
34	q	100/153 (65%)	100 (100%)	0	100	100
34	r	100/153 (65%)	100 (100%)	0	100	100
34	s	100/153 (65%)	100 (100%)	0	100	100
35	y	58/117 (50%)	58 (100%)	0	100	100
35	z	98/117 (84%)	98 (100%)	0	100	100
All	All	134531/150776 (89%)	134112 (100%)	419 (0%)	92	97

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	733	ARG
2	2	463	LYS
3	3	152	LYS
5	8	61	ARG
7	A0	301	LYS
7	A2	100	LYS
8	AA	2	ARG
8	AA	221	ARG
9	AB	273	LEU
9	AB	274	THR
9	AD	347	ASN
8	AE	50	ASN
8	AE	422	ARG
9	AF	122	LYS
9	AF	195	ASN
9	AF	262	ARG
9	AF	274	THR
9	AF	306	ARG
9	AH	298	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	AH	306	ARG
8	AI	2	ARG
8	AI	422	ARG
9	AJ	274	THR
9	AJ	306	ARG
8	AK	2	ARG
9	AL	273	LEU
8	AM	2	ARG
8	AM	326	LYS
10	B	35	ASN
11	B0	20	ASN
8	BA	2	ARG
9	BB	347	ASN
8	BC	221	ARG
9	BD	274	THR
9	BD	347	ASN
9	BF	190	HIS
9	BF	274	THR
8	BG	430	LYS
9	BH	306	ARG
8	BI	2	ARG
9	BJ	2	ARG
9	BJ	306	ARG
9	BJ	347	ASN
8	BM	2	ARG
10	C	321	GLN
10	C	405	ARG
12	C1	243	GLN
12	C2	134	GLN
12	C2	320	LYS
12	C2	406	ARG
9	CB	274	THR
8	CC	2	ARG
9	CF	274	THR
9	CF	306	ARG
8	CG	2	ARG
9	CJ	274	THR
8	CM	2	ARG
14	D0	128	ARG
14	D2	323	ASN
8	DA	430	LYS
8	DC	2	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	DD	347	ASN
8	DE	339	ARG
9	DF	262	ARG
9	DF	273	LEU
9	DF	414	ASN
8	DG	215	ARG
8	DI	2	ARG
8	DI	256	GLN
8	DK	2	ARG
9	DL	274	THR
8	EC	339	ARG
9	ED	292	GLN
9	ED	323	MET
9	EF	273	LEU
9	EF	298	ASN
9	EF	306	ARG
8	EG	2	ARG
9	EH	274	THR
9	EJ	251	ARG
9	EL	213	ARG
9	EL	306	ARG
8	EM	2	ARG
16	F7	87	HIS
9	FB	268	PRO
9	FB	298	ASN
9	FD	273	LEU
8	FE	2	ARG
9	FF	2	ARG
8	FG	2	ARG
9	FH	274	THR
9	FH	280	GLN
9	FH	337	ASN
8	FK	2	ARG
8	FK	326	LYS
8	FK	422	ARG
9	FL	48	ASN
9	FL	170	VAL
9	FL	306	ARG
8	FM	2	ARG
9	FN	273	LEU
9	FN	274	THR
9	FN	306	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	G	62	ASN
16	G1	131	ARG
16	G4	35	ASN
16	G6	157	LYS
16	G7	41	ARG
9	GB	273	LEU
9	GB	276	ARG
9	GD	321	MET
9	GF	274	THR
8	GG	2	ARG
8	GI	203	MET
8	GI	402	ARG
9	GJ	273	LEU
9	GJ	274	THR
9	GJ	279	GLN
8	GK	2	ARG
9	GL	337	ASN
9	GL	390	ARG
9	GN	256	ASN
9	GN	273	LEU
9	HB	245	GLN
9	HB	274	THR
9	HB	318	ARG
8	HC	2	ARG
8	HC	422	ARG
9	HD	274	THR
8	HE	243	ARG
8	HI	293	ASN
8	HI	422	ARG
9	HJ	273	LEU
9	HJ	298	ASN
9	HJ	306	ARG
8	HK	2	ARG
9	HL	274	THR
9	HL	306	ARG
9	HL	322	SER
9	HL	323	MET
8	HM	422	ARG
9	HN	276	ARG
9	HN	306	ARG
8	HO	401	LYS
8	HO	422	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	I1	113	THR
19	I1	115	ARG
9	IB	274	THR
8	IC	2	ARG
8	IC	300	ASN
9	ID	274	THR
9	IF	273	LEU
9	IH	291	GLN
9	IJ	274	THR
8	IK	329	ASN
9	IN	274	THR
9	IN	276	ARG
9	IN	347	ASN
20	J2	175	ARG
20	J3	29	CYS
20	J4	102	ARG
20	J4	204	LYS
9	JB	131	GLN
9	JB	306	ARG
9	JB	347	ASN
8	JC	2	ARG
9	JF	274	THR
8	JG	300	ASN
9	JH	276	ARG
9	JJ	274	THR
9	JJ	306	ARG
8	JK	339	ARG
9	JN	298	ASN
18	K	51	LEU
21	K1	26	LYS
9	KB	273	LEU
9	KD	273	LEU
9	KD	274	THR
8	KE	2	ARG
8	KE	308	ARG
9	KF	273	LEU
9	KF	306	ARG
9	KF	414	ASN
8	KG	2	ARG
8	KG	308	ARG
9	KH	306	ARG
8	KI	300	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	KJ	274	THR
9	KJ	306	ARG
8	KK	2	ARG
9	KL	274	THR
9	KL	306	ARG
8	KM	2	ARG
8	KO	2	ARG
8	KO	308	ARG
18	L	90	MET
9	LB	297	LYS
9	LB	306	ARG
8	LC	221	ARG
9	LD	274	THR
9	LD	298	ASN
9	LF	298	ASN
9	LF	306	ARG
8	LG	2	ARG
8	LG	300	ASN
9	LH	306	ARG
8	LI	2	ARG
9	LJ	274	THR
9	LJ	291	GLN
9	LJ	306	ARG
8	LK	308	ARG
9	LL	274	THR
9	LL	298	ASN
9	LL	306	ARG
8	LM	2	ARG
9	LN	306	ARG
23	M4	125	TYR
9	MD	298	ASN
8	ME	339	ARG
9	MF	306	ARG
8	MG	2	ARG
8	MG	300	ASN
9	MH	298	ASN
8	MI	18	ASN
9	MJ	227	HIS
8	MK	1	MET
8	MK	84	ARG
9	ML	227	HIS
9	ML	273	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	ML	298	ASN
18	N	51	LEU
9	NB	274	THR
9	NB	282	ARG
9	NB	285	THR
8	NC	112	LYS
8	NC	221	ARG
8	NC	402	ARG
9	ND	274	THR
9	ND	285	THR
8	NE	1	MET
8	NE	102	ASN
8	NE	275	VAL
8	NE	276	ILE
8	NE	283	HIS
8	NE	287	SER
9	NF	253	LEU
9	NF	273	LEU
9	NF	284	LEU
9	NF	306	ARG
8	NG	308	ARG
8	NG	422	ARG
9	NH	306	ARG
9	NH	318	ARG
8	NI	2	ARG
9	NJ	273	LEU
9	NJ	274	THR
9	NJ	306	ARG
9	NJ	347	ASN
8	NK	40	LYS
8	NK	277	SER
8	NK	279	GLU
8	NK	282	TYR
9	NL	306	ARG
9	NL	318	ARG
9	NL	390	ARG
9	NL	406	MET
8	NM	276	ILE
8	NM	284	GLU
8	NM	286	LEU
9	NN	281	TYR
9	NN	306	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	OC	2	ARG
9	OF	274	THR
8	OG	300	ASN
8	OI	300	ASN
9	OJ	274	THR
9	OL	274	THR
8	OM	2	ARG
9	ON	274	THR
8	PG	2	ARG
8	PG	356	ASN
9	PH	274	THR
9	PH	306	ARG
9	PH	347	ASN
9	PJ	273	LEU
8	PK	2	ARG
8	PK	221	ARG
9	PL	306	ARG
9	PN	274	THR
8	PO	430	LYS
24	Q	382	ARG
8	QG	2	ARG
8	QI	2	ARG
9	QJ	273	LEU
9	QJ	274	THR
8	QK	2	ARG
8	QK	356	ASN
8	QM	2	ARG
9	QN	247	ASN
8	RC	2	ARG
8	RC	221	ARG
8	RC	300	ASN
9	RD	83	GLN
9	RF	274	THR
9	RH	274	THR
9	RJ	274	THR
9	RN	274	THR
9	SD	274	THR
9	SD	414	ASN
8	SE	363	VAL
9	SF	274	THR
8	SG	2	ARG
9	SH	298	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	SH	306	ARG
8	SI	2	ARG
8	SK	363	VAL
8	SK	367	ASP
8	SK	402	ARG
8	SM	2	ARG
25	T	366	ARG
9	TD	390	ARG
8	TE	203	MET
9	TF	325	GLU
9	TH	195	ASN
9	TJ	273	LEU
9	TJ	274	THR
8	TK	84	ARG
8	TK	320	ARG
9	TL	227	HIS
9	TL	288	GLU
9	TL	289	LEU
8	TM	203	MET
9	TN	273	LEU
9	TN	306	ARG
9	TP	274	THR
25	U	366	ARG
9	UD	274	THR
9	UD	276	ARG
8	UE	2	ARG
9	UF	274	THR
9	UF	276	ARG
9	UF	306	ARG
9	UH	174	LYS
9	UH	306	ARG
8	UI	2	ARG
8	UI	380	ASN
9	UJ	273	LEU
8	UK	243	ARG
9	UL	190	HIS
9	UL	273	LEU
9	UL	274	THR
9	UL	276	ARG
9	UL	306	ARG
8	UM	380	ASN
9	UN	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	UN	273	LEU
9	UN	274	THR
9	UN	306	ARG
8	UO	401	LYS
9	UP	306	ARG
8	VE	300	ASN
9	VF	274	THR
8	VG	370	LYS
8	VG	430	LYS
9	VH	274	THR
9	VH	306	ARG
9	VJ	273	LEU
9	VJ	274	THR
8	VK	370	LYS
9	VL	306	ARG
8	VM	2	ARG
8	VM	370	LYS
9	VN	204	ASN
9	VN	273	LEU
9	VN	306	ARG
9	VP	273	LEU
9	VP	274	THR
9	VP	306	ARG
26	W	95	THR
26	W	417	ARG
8	WE	192	HIS
8	WE	215	ARG
8	WE	243	ARG
9	WF	273	LEU
9	WF	282	ARG
8	WG	2	ARG
9	WH	379	LYS
8	WI	18	ASN
9	WJ	99	ASN
9	WJ	274	THR
9	WL	273	LEU
9	WL	347	ASN
8	WM	2	ARG
8	WM	221	ARG
9	WP	336	LYS
26	X	723	LEU
26	X	725	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	XB	121	MET
27	XC	121	MET
27	XE	121	MET
26	Y	632	MET
26	Y	723	LEU
26	Z	406	ASN
26	Z	632	MET
29	a	160	LYS
29	c	299	LYS
29	c	303	ARG
29	d	504	LYS
30	f	99	LYS
30	g	374	ASN
30	g	417	ARG
31	h	228	GLN
31	j	203	ASN
33	o	119	ARG
33	o	198	LYS
33	o	305	LYS
33	o	408	LYS
33	p	395	ARG
33	p	420	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (252) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	604	GLN
3	3	173	GLN
5	8	103	ASN
6	A	90	ASN
7	A0	369	GLN
7	A2	224	ASN
7	A3	251	ASN
9	AD	165	ASN
9	AD	347	ASN
8	AI	11	GLN
9	AL	256	ASN
8	AM	11	GLN
8	AM	101	ASN
11	B0	20	ASN
11	B2	31	GLN
11	B3	369	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	BB	195	ASN
9	BB	347	ASN
9	BD	100	ASN
9	BJ	298	ASN
9	BL	134	GLN
8	CA	88	HIS
8	CC	258	ASN
9	CD	99	ASN
8	CE	101	ASN
9	CJ	204	ASN
9	CL	256	ASN
9	CL	414	ASN
8	CM	101	ASN
14	D2	71	GLN
14	D2	323	ASN
8	DC	258	ASN
9	DD	256	ASN
9	DD	298	ASN
9	DF	14	ASN
9	DF	298	ASN
9	DF	414	ASN
8	DG	101	ASN
8	DI	285	GLN
9	DL	99	ASN
9	DL	165	ASN
9	DL	292	GLN
8	DM	285	GLN
9	ED	131	GLN
9	EF	8	GLN
8	EG	258	ASN
9	EH	298	ASN
8	EI	293	ASN
9	FD	15	GLN
8	FE	11	GLN
8	FE	91	GLN
8	FE	380	ASN
9	FF	247	ASN
9	FH	14	ASN
9	FH	195	ASN
9	FH	414	ASN
8	FI	11	GLN
8	FI	18	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	FI	380	ASN
8	FK	380	ASN
9	FL	375	GLN
17	G	62	ASN
16	G0	35	ASN
9	GB	14	ASN
8	GC	11	GLN
9	GD	6	HIS
9	GD	11	GLN
9	GD	280	GLN
9	GF	6	HIS
9	GF	11	GLN
9	GF	134	GLN
9	GF	245	GLN
9	GF	291	GLN
8	GI	226	ASN
8	GI	329	ASN
9	GJ	292	GLN
9	GJ	298	ASN
9	GL	226	ASN
9	GL	334	GLN
9	GL	337	ASN
16	H0	133	HIS
9	HB	298	ASN
8	HC	128	GLN
9	HD	245	GLN
9	HF	11	GLN
9	HJ	298	ASN
9	HL	247	ASN
9	IB	298	ASN
8	IE	285	GLN
9	IH	256	ASN
9	IH	291	GLN
8	II	101	ASN
8	II	216	ASN
9	IJ	334	GLN
8	IK	216	ASN
9	IL	347	ASN
8	IM	11	GLN
8	IM	85	GLN
9	IN	291	GLN
9	JD	348	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	JE	101	ASN
9	JF	375	GLN
8	JG	258	ASN
8	JI	11	GLN
9	JJ	347	ASN
9	JJ	348	ASN
8	JK	258	ASN
9	JL	6	HIS
9	JL	279	GLN
9	JL	298	ASN
9	JL	348	ASN
9	JL	423	GLN
8	JM	101	ASN
9	JN	99	ASN
9	JN	414	ASN
21	K1	18	GLN
21	K1	36	GLN
9	KD	256	ASN
8	KE	11	GLN
8	KE	101	ASN
9	KF	414	ASN
8	KG	356	ASN
9	KH	99	ASN
8	KM	393	HIS
8	KO	101	ASN
8	LC	11	GLN
9	LD	99	ASN
9	LD	247	ASN
8	LE	11	GLN
8	LE	226	ASN
9	LF	191	GLN
9	LH	347	ASN
8	LK	11	GLN
9	MB	8	GLN
8	MC	300	ASN
8	ME	11	GLN
8	MG	258	ASN
9	MH	99	ASN
9	MH	307	HIS
8	MI	11	GLN
8	MI	216	ASN
8	MI	300	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	MJ	8	GLN
9	MJ	298	ASN
8	MK	11	GLN
8	MM	11	GLN
9	MN	8	GLN
8	NE	226	ASN
9	NF	256	ASN
9	NF	279	GLN
9	NF	280	GLN
9	NF	334	GLN
8	NG	101	ASN
9	NJ	279	GLN
9	NL	348	ASN
9	NN	6	HIS
9	NN	94	GLN
9	NN	134	GLN
9	NN	280	GLN
9	OH	332	ASN
9	OH	334	GLN
9	OJ	137	HIS
9	OJ	334	GLN
8	OK	226	ASN
8	OO	256	GLN
24	P	107	GLN
8	PC	258	ASN
8	PI	133	GLN
8	PO	283	HIS
9	QD	8	GLN
9	QD	134	GLN
9	QF	6	HIS
9	QF	8	GLN
8	QG	258	ASN
8	QG	356	ASN
9	QH	8	GLN
8	QI	301	GLN
9	QN	245	GLN
24	R	52	GLN
8	RC	258	ASN
9	RD	264	HIS
9	RD	291	GLN
9	RF	99	ASN
9	RF	134	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	RG	11	GLN
8	RG	285	GLN
8	RI	133	GLN
8	RI	283	HIS
9	RL	134	GLN
9	RL	375	GLN
9	RN	256	ASN
8	RO	18	ASN
8	SG	380	ASN
9	SH	298	ASN
8	SM	285	GLN
9	SN	247	ASN
8	SO	35	GLN
8	SO	61	HIS
9	TD	256	ASN
9	TD	375	GLN
9	TD	426	GLN
8	TE	300	ASN
9	TF	256	ASN
8	TK	372	GLN
9	TL	292	GLN
8	TM	226	ASN
9	TN	414	ASN
8	TO	11	GLN
9	TP	298	ASN
9	UD	375	GLN
8	UE	216	ASN
9	UF	414	ASN
9	UH	190	HIS
9	UH	292	GLN
8	UI	372	GLN
9	UJ	43	GLN
9	UN	100	ASN
9	UN	334	GLN
9	UN	347	ASN
8	UO	102	ASN
9	UP	14	ASN
9	UP	292	GLN
9	VF	298	ASN
9	VH	247	ASN
9	VJ	298	ASN
9	VJ	334	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	VK	128	GLN
9	VL	256	ASN
9	VL	347	ASN
8	VM	15	GLN
8	VM	128	GLN
8	VO	186	ASN
9	VP	292	GLN
8	WE	11	GLN
9	WF	334	GLN
8	WG	283	HIS
9	WH	204	ASN
9	WJ	298	ASN
9	WL	137	HIS
8	WM	285	GLN
9	WN	298	ASN
8	WO	329	ASN
27	XA	92	GLN
27	XB	131	GLN
27	XD	33	HIS
27	XG	7	GLN
27	XG	33	HIS
27	XG	53	ASN
28	YG	204	ASN
30	e	33	HIS
30	g	33	HIS
31	h	109	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 451 ligands modelled in this entry, 149 are monoatomic - leaving 302 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	GTP	PO	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
36	GTP	KE	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.63	7 (21%)
36	GTP	KO	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.67	7 (21%)
38	GDP	PL	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	DM	501	37	26,34,34	1.10	2 (7%)	32,54,54	1.68	6 (18%)
38	GDP	AB	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.41	4 (13%)
36	GTP	RK	501	37	26,34,34	1.20	2 (7%)	32,54,54	1.67	7 (21%)
36	GTP	TG	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.61	7 (21%)
38	GDP	DH	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.29	4 (13%)
38	GDP	BD	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	GF	502	-	24,30,30	0.92	1 (4%)	30,47,47	1.29	4 (13%)
38	GDP	DL	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.29	4 (13%)
36	GTP	QO	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.64	7 (21%)
38	GDP	WF	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)
36	GTP	II	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.64	7 (21%)
38	GDP	LN	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.38	4 (13%)
36	GTP	IO	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.63	7 (21%)
36	GTP	GI	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.55	7 (21%)
36	GTP	RG	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.58	7 (21%)
38	GDP	MD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
38	GDP	RJ	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	WL	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	AG	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.55	7 (21%)
36	GTP	TO	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.55	7 (21%)
36	GTP	KI	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.62	7 (21%)
38	GDP	TJ	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
38	GDP	WJ	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
38	GDP	BB	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.37	4 (13%)
36	GTP	OI	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.71	6 (18%)
38	GDP	TF	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.29	4 (13%)
38	GDP	TP	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	OM	501	37	26,34,34	1.19	2 (7%)	32,54,54	1.58	7 (21%)
36	GTP	HC	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.51	7 (21%)
38	GDP	IF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	RF	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	5 (16%)
36	GTP	CI	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.66	6 (18%)
36	GTP	DE	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.55	6 (18%)
38	GDP	JJ	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
38	GDP	CB	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.39	4 (13%)
36	GTP	OC	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.70	7 (21%)
38	GDP	DD	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.28	4 (13%)
36	GTP	AA	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.53	7 (21%)
36	GTP	PC	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.59	6 (18%)
36	GTP	HI	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
36	GTP	WG	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.69	6 (18%)
38	GDP	HL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	PJ	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	JN	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
36	GTP	PE	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.56	7 (21%)
36	GTP	HM	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.55	7 (21%)
36	GTP	AI	501	37	26,34,34	1.20	2 (7%)	32,54,54	1.53	7 (21%)
38	GDP	BJ	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.39	4 (13%)
36	GTP	VE	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.62	7 (21%)
36	GTP	WO	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.55	6 (18%)
36	GTP	GM	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.57	6 (18%)
38	GDP	JL	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	WN	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
38	GDP	IB	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	PK	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.50	7 (21%)
38	GDP	UN	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
36	GTP	VO	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.61	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
38	GDP	EH	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)
36	GTP	HG	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
36	GTP	RM	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.59	7 (21%)
38	GDP	JF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
36	GTP	GE	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.53	7 (21%)
36	GTP	CA	501	37	26,34,34	1.12	2 (7%)	32,54,54	1.58	6 (18%)
36	GTP	OK	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.53	6 (18%)
38	GDP	ML	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
38	GDP	SH	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	5 (16%)
38	GDP	UD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	VN	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	KJ	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	SI	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.47	7 (21%)
36	GTP	LM	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.51	7 (21%)
38	GDP	JD	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
36	GTP	KK	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.63	7 (21%)
38	GDP	FN	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	5 (16%)
38	GDP	NH	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	DK	501	37	26,34,34	1.12	2 (7%)	32,54,54	1.69	6 (18%)
36	GTP	AC	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.53	7 (21%)
36	GTP	LI	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.57	7 (21%)
36	GTP	NK	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.58	7 (21%)
38	GDP	KN	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.42	4 (13%)
36	GTP	NI	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.56	7 (21%)
38	GDP	LF	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	MI	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)
38	GDP	BF	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.40	4 (13%)
38	GDP	OF	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	PN	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	SD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	5 (16%)
36	GTP	SK	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.46	7 (21%)
36	GTP	VK	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.63	7 (21%)
38	GDP	SL	502	-	24,30,30	0.92	1 (4%)	30,47,47	1.35	5 (16%)
38	GDP	RD	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	5 (16%)
36	GTP	MG	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.57	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	GTP	SG	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.52	7 (21%)
36	GTP	DA	501	37	26,34,34	1.10	2 (7%)	32,54,54	1.53	6 (18%)
38	GDP	PD	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	VG	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
38	GDP	QD	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	SF	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.25	4 (13%)
36	GTP	EK	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)
36	GTP	IC	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.56	7 (21%)
36	GTP	WE	501	37	26,34,34	1.12	2 (7%)	32,54,54	1.55	6 (18%)
36	GTP	NC	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.59	7 (21%)
38	GDP	WH	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
36	GTP	IG	501	37	26,34,34	1.12	2 (7%)	32,54,54	1.63	6 (18%)
38	GDP	MJ	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	KD	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	TN	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
38	GDP	QL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	MM	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.56	7 (21%)
36	GTP	JC	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.60	6 (18%)
36	GTP	SO	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.49	7 (21%)
38	GDP	GN	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	VH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
38	GDP	DB	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.28	4 (13%)
36	GTP	CE	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.57	7 (21%)
38	GDP	LB	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.37	4 (13%)
36	GTP	RI	501	37	26,34,34	1.19	2 (7%)	32,54,54	1.65	7 (21%)
38	GDP	EN	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
38	GDP	AJ	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.44	4 (13%)
36	GTP	RO	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.54	7 (21%)
36	GTP	IE	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
38	GDP	NF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
38	GDP	FH	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	5 (16%)
38	GDP	IL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	SN	502	-	24,30,30	0.92	1 (4%)	30,47,47	1.34	5 (16%)
38	GDP	GD	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	SM	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.48	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	GTP	GG	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.53	7 (21%)
38	GDP	MB	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.39	4 (13%)
38	GDP	OD	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	4 (13%)
36	GTP	LE	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.63	7 (21%)
36	GTP	BI	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
36	GTP	DG	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.63	6 (18%)
36	GTP	NM	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.52	7 (21%)
38	GDP	HD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	KH	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
36	GTP	SE	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.54	7 (21%)
38	GDP	MF	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
38	GDP	EB	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.32	4 (13%)
36	GTP	IM	501	37	26,34,34	1.12	2 (7%)	32,54,54	1.63	6 (18%)
38	GDP	FF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
36	GTP	JM	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
38	GDP	IN	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	GH	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	BM	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.61	7 (21%)
36	GTP	DC	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.60	6 (18%)
38	GDP	AD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
38	GDP	AF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.40	4 (13%)
38	GDP	MH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
38	GDP	ND	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	QF	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
36	GTP	LG	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
38	GDP	KL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	MK	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.58	7 (21%)
36	GTP	FE	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.54	7 (21%)
38	GDP	RL	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	4 (13%)
36	GTP	TM	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.52	7 (21%)
36	GTP	QC	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.51	7 (21%)
36	GTP	OO	501	37	26,34,34	1.19	2 (7%)	32,54,54	1.65	7 (21%)
38	GDP	RH	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	5 (16%)
38	GDP	VL	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	OG	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.55	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
38	GDP	CF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
36	GTP	MC	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.55	7 (21%)
38	GDP	TH	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
36	GTP	FK	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.42	6 (18%)
36	GTP	TI	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.49	7 (21%)
38	GDP	GB	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	VJ	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
38	GDP	TL	502	-	24,30,30	0.92	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	CM	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.63	7 (21%)
36	GTP	PG	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
38	GDP	AH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.39	4 (13%)
38	GDP	UF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	RC	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.56	7 (21%)
38	GDP	LD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	AL	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.40	4 (13%)
38	GDP	CD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	VP	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	BC	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.61	7 (21%)
36	GTP	PM	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.63	7 (21%)
36	GTP	FI	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.44	6 (18%)
38	GDP	KB	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.39	4 (13%)
38	GDP	WP	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
36	GTP	BA	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
36	GTP	QI	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
36	GTP	AK	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.53	7 (21%)
38	GDP	QJ	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	HJ	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	BE	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.59	7 (21%)
38	GDP	NN	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
36	GTP	QM	501	37	26,34,34	1.19	2 (7%)	32,54,54	1.56	7 (21%)
36	GTP	HO	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.58	7 (21%)
36	GTP	TK	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.56	7 (21%)
38	GDP	DJ	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
36	GTP	ME	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.54	7 (21%)
38	GDP	OB	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.42	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
38	GDP	QN	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	WI	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.64	6 (18%)
38	GDP	NB	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
36	GTP	LC	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.62	7 (21%)
36	GTP	GC	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.49	7 (21%)
36	GTP	QE	501	37	26,34,34	1.20	2 (7%)	32,54,54	1.58	7 (21%)
36	GTP	VM	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.53	7 (21%)
36	GTP	UO	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
36	GTP	NG	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.60	8 (25%)
38	GDP	GL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	IJ	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
38	GDP	EJ	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.26	4 (13%)
36	GTP	BK	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.55	7 (21%)
38	GDP	EF	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	5 (16%)
36	GTP	RE	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.64	7 (21%)
36	GTP	LK	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.62	7 (21%)
38	GDP	ON	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	UJ	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	KM	501	37	26,34,34	1.20	2 (7%)	32,54,54	1.65	7 (21%)
38	GDP	JH	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	IH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
38	GDP	CL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	UH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	UK	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.61	7 (21%)
36	GTP	JG	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
38	GDP	CH	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.30	4 (13%)
38	GDP	ID	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	LH	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
36	GTP	KG	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.63	7 (21%)
36	GTP	EE	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.54	7 (21%)
38	GDP	NJ	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	ED	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	UL	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
36	GTP	JK	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.58	7 (21%)
36	GTP	EC	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.55	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	GDP	VD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
36	GTP	FM	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.47	7 (21%)
38	GDP	NL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
38	GDP	CJ	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
36	GTP	BG	501	37	26,34,34	1.19	2 (7%)	32,54,54	1.58	7 (21%)
36	GTP	EM	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.59	7 (21%)
38	GDP	BH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
36	GTP	CG	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.62	7 (21%)
36	GTP	KC	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.59	7 (21%)
36	GTP	NE	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.58	7 (21%)
36	GTP	AM	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.55	7 (21%)
38	GDP	PF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	UE	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.62	7 (21%)
36	GTP	CK	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.64	7 (21%)
36	GTP	GK	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.53	7 (21%)
38	GDP	UP	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	HB	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	OH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
36	GTP	IK	501	37	26,34,34	1.13	2 (7%)	32,54,54	1.63	7 (21%)
38	GDP	OJ	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.33	4 (13%)
38	GDP	EL	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.25	4 (13%)
36	GTP	JE	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.57	7 (21%)
36	GTP	WM	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.53	6 (18%)
38	GDP	LL	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	VI	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.58	7 (21%)
38	GDP	PH	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	SJ	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.37	5 (16%)
36	GTP	QK	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.52	6 (18%)
38	GDP	HF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	HE	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
38	GDP	BL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
36	GTP	UG	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.62	7 (21%)
36	GTP	FG	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.54	7 (21%)
36	GTP	HK	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
36	GTP	EI	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.58	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
36	GTP	AE	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.57	7 (21%)
36	GTP	PI	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
36	GTP	UM	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.51	7 (21%)
38	GDP	FD	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	5 (16%)
38	GDP	JB	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	4 (13%)
38	GDP	DF	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
38	GDP	FB	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
38	GDP	FJ	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
36	GTP	QG	501	37	26,34,34	1.18	2 (7%)	32,54,54	1.60	7 (21%)
38	GDP	TD	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.36	4 (13%)
38	GDP	MN	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
38	GDP	QH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
38	GDP	HH	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)
38	GDP	RN	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	EG	501	37	26,34,34	1.16	2 (7%)	32,54,54	1.57	7 (21%)
36	GTP	TE	501	37	26,34,34	1.12	2 (7%)	32,54,54	1.56	6 (18%)
36	GTP	WK	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.63	6 (18%)
38	GDP	KF	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
38	GDP	VF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
36	GTP	OE	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.58	7 (21%)
38	GDP	FL	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	5 (16%)
38	GDP	WD	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)
38	GDP	LJ	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.41	4 (13%)
36	GTP	CC	501	37	26,34,34	1.14	2 (7%)	32,54,54	1.64	7 (21%)
38	GDP	GJ	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
36	GTP	UI	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.53	7 (21%)
38	GDP	HN	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
36	GTP	FC	501	37	26,34,34	1.15	2 (7%)	32,54,54	1.50	7 (21%)
38	GDP	OL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
36	GTP	JI	501	37	26,34,34	1.17	2 (7%)	32,54,54	1.67	7 (21%)
36	GTP	DI	501	37	26,34,34	1.11	2 (7%)	32,54,54	1.69	6 (18%)

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
36	GTP	PO	501	37	-	4/18/38/38	0/3/3/3
36	GTP	KE	501	-	-	7/18/38/38	0/3/3/3
36	GTP	KO	501	37	-	7/18/38/38	0/3/3/3
38	GDP	PL	502	-	-	2/12/32/32	0/3/3/3
36	GTP	DM	501	37	-	3/18/38/38	0/3/3/3
38	GDP	AB	502	-	-	1/12/32/32	0/3/3/3
36	GTP	RK	501	37	-	3/18/38/38	0/3/3/3
36	GTP	TG	501	37	-	5/18/38/38	0/3/3/3
38	GDP	DH	502	-	-	2/12/32/32	0/3/3/3
38	GDP	BD	502	-	-	1/12/32/32	0/3/3/3
38	GDP	GF	502	-	-	1/12/32/32	0/3/3/3
38	GDP	DL	502	-	-	1/12/32/32	0/3/3/3
36	GTP	QO	501	37	-	8/18/38/38	0/3/3/3
38	GDP	WF	502	-	-	2/12/32/32	0/3/3/3
36	GTP	II	501	37	-	4/18/38/38	0/3/3/3
38	GDP	LN	502	-	-	4/12/32/32	0/3/3/3
36	GTP	IO	501	37	-	6/18/38/38	0/3/3/3
36	GTP	GI	501	37	-	4/18/38/38	0/3/3/3
36	GTP	RG	501	37	-	3/18/38/38	0/3/3/3
38	GDP	MD	502	-	-	2/12/32/32	0/3/3/3
38	GDP	RJ	502	-	-	1/12/32/32	0/3/3/3
38	GDP	WL	502	-	-	1/12/32/32	0/3/3/3
36	GTP	AG	501	37	-	4/18/38/38	0/3/3/3
36	GTP	TO	501	37	-	4/18/38/38	0/3/3/3
36	GTP	KI	501	-	-	5/18/38/38	0/3/3/3
38	GDP	TJ	502	-	-	3/12/32/32	0/3/3/3
38	GDP	WJ	502	-	-	2/12/32/32	0/3/3/3
38	GDP	BB	502	-	-	1/12/32/32	0/3/3/3
36	GTP	OI	501	-	-	3/18/38/38	0/3/3/3
38	GDP	TF	502	-	-	1/12/32/32	0/3/3/3
38	GDP	TP	502	-	-	1/12/32/32	0/3/3/3
36	GTP	OM	501	37	-	7/18/38/38	0/3/3/3
36	GTP	HC	501	37	-	4/18/38/38	0/3/3/3
38	GDP	IF	502	-	-	2/12/32/32	0/3/3/3
38	GDP	RF	502	-	-	1/12/32/32	0/3/3/3
36	GTP	CI	501	37	-	8/18/38/38	0/3/3/3
36	GTP	DE	501	37	-	3/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	JJ	502	-	-	1/12/32/32	0/3/3/3
38	GDP	CB	502	-	-	2/12/32/32	0/3/3/3
36	GTP	OC	501	37	-	6/18/38/38	0/3/3/3
38	GDP	DD	502	-	-	1/12/32/32	0/3/3/3
36	GTP	AA	501	37	-	4/18/38/38	0/3/3/3
36	GTP	PC	501	37	-	8/18/38/38	0/3/3/3
36	GTP	HI	501	37	-	8/18/38/38	0/3/3/3
36	GTP	WG	501	37	-	7/18/38/38	0/3/3/3
38	GDP	HL	502	-	-	1/12/32/32	0/3/3/3
38	GDP	PJ	502	-	-	2/12/32/32	0/3/3/3
38	GDP	JN	502	-	-	2/12/32/32	0/3/3/3
36	GTP	PE	501	37	-	5/18/38/38	0/3/3/3
36	GTP	HM	501	37	-	4/18/38/38	0/3/3/3
36	GTP	AI	501	37	-	4/18/38/38	0/3/3/3
38	GDP	BJ	502	-	-	4/12/32/32	0/3/3/3
36	GTP	VE	501	37	-	4/18/38/38	0/3/3/3
36	GTP	WO	501	37	-	3/18/38/38	0/3/3/3
36	GTP	GM	501	37	-	5/18/38/38	0/3/3/3
38	GDP	JL	502	-	-	1/12/32/32	0/3/3/3
38	GDP	WN	502	-	-	3/12/32/32	0/3/3/3
38	GDP	IB	502	-	-	1/12/32/32	0/3/3/3
36	GTP	PK	501	37	-	4/18/38/38	0/3/3/3
38	GDP	UN	502	-	-	1/12/32/32	0/3/3/3
36	GTP	VO	501	37	-	4/18/38/38	0/3/3/3
38	GDP	EH	502	-	-	2/12/32/32	0/3/3/3
36	GTP	HG	501	37	-	4/18/38/38	0/3/3/3
36	GTP	RM	501	37	-	6/18/38/38	0/3/3/3
38	GDP	JF	502	-	-	1/12/32/32	0/3/3/3
36	GTP	GE	501	37	-	6/18/38/38	0/3/3/3
36	GTP	CA	501	37	-	4/18/38/38	0/3/3/3
36	GTP	OK	501	37	-	4/18/38/38	0/3/3/3
38	GDP	ML	502	-	-	4/12/32/32	0/3/3/3
38	GDP	SH	502	-	-	4/12/32/32	0/3/3/3
38	GDP	UD	502	-	-	1/12/32/32	0/3/3/3
38	GDP	VN	502	-	-	3/12/32/32	0/3/3/3
38	GDP	KJ	502	-	-	3/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GTP	SI	501	37	-	5/18/38/38	0/3/3/3
36	GTP	LM	501	-	-	5/18/38/38	0/3/3/3
38	GDP	JD	502	-	-	2/12/32/32	0/3/3/3
36	GTP	KK	501	-	-	8/18/38/38	0/3/3/3
38	GDP	FN	502	-	-	0/12/32/32	0/3/3/3
38	GDP	NH	502	-	-	1/12/32/32	0/3/3/3
36	GTP	DK	501	37	-	3/18/38/38	0/3/3/3
36	GTP	AC	501	37	-	4/18/38/38	0/3/3/3
36	GTP	LI	501	37	-	5/18/38/38	0/3/3/3
36	GTP	NK	501	37	-	5/18/38/38	0/3/3/3
38	GDP	KN	502	-	-	3/12/32/32	0/3/3/3
36	GTP	NI	501	37	-	4/18/38/38	0/3/3/3
38	GDP	LF	502	-	-	1/12/32/32	0/3/3/3
36	GTP	MI	501	37	-	5/18/38/38	0/3/3/3
38	GDP	BF	502	-	-	3/12/32/32	0/3/3/3
38	GDP	OF	502	-	-	3/12/32/32	0/3/3/3
38	GDP	PN	502	-	-	3/12/32/32	0/3/3/3
38	GDP	SD	502	-	-	3/12/32/32	0/3/3/3
36	GTP	SK	501	37	-	6/18/38/38	0/3/3/3
36	GTP	VK	501	37	-	5/18/38/38	0/3/3/3
38	GDP	SL	502	-	-	0/12/32/32	0/3/3/3
38	GDP	RD	502	-	-	1/12/32/32	0/3/3/3
36	GTP	MG	501	37	-	5/18/38/38	0/3/3/3
36	GTP	SG	501	37	-	5/18/38/38	0/3/3/3
36	GTP	DA	501	37	-	9/18/38/38	0/3/3/3
38	GDP	PD	502	-	-	4/12/32/32	0/3/3/3
36	GTP	VG	501	37	-	8/18/38/38	0/3/3/3
38	GDP	QD	502	-	-	4/12/32/32	0/3/3/3
38	GDP	SF	502	-	-	0/12/32/32	0/3/3/3
36	GTP	EK	501	37	-	5/18/38/38	0/3/3/3
36	GTP	IC	501	37	-	5/18/38/38	0/3/3/3
36	GTP	WE	501	37	-	5/18/38/38	0/3/3/3
36	GTP	NC	501	37	-	5/18/38/38	0/3/3/3
38	GDP	WH	502	-	-	2/12/32/32	0/3/3/3
36	GTP	IG	501	37	-	7/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	MJ	502	-	-	3/12/32/32	0/3/3/3
38	GDP	KD	502	-	-	2/12/32/32	0/3/3/3
38	GDP	TN	502	-	-	4/12/32/32	0/3/3/3
38	GDP	QL	502	-	-	3/12/32/32	0/3/3/3
36	GTP	MM	501	37	-	5/18/38/38	0/3/3/3
36	GTP	JC	501	37	-	4/18/38/38	0/3/3/3
36	GTP	SO	501	37	-	3/18/38/38	0/3/3/3
38	GDP	GN	502	-	-	1/12/32/32	0/3/3/3
38	GDP	VH	502	-	-	0/12/32/32	0/3/3/3
38	GDP	DB	502	-	-	0/12/32/32	0/3/3/3
36	GTP	CE	501	37	-	4/18/38/38	0/3/3/3
38	GDP	LB	502	-	-	2/12/32/32	0/3/3/3
36	GTP	RI	501	37	-	3/18/38/38	0/3/3/3
38	GDP	EN	502	-	-	1/12/32/32	0/3/3/3
38	GDP	AJ	502	-	-	2/12/32/32	0/3/3/3
36	GTP	RO	501	37	-	5/18/38/38	0/3/3/3
36	GTP	IE	501	37	-	4/18/38/38	0/3/3/3
38	GDP	NF	502	-	-	1/12/32/32	0/3/3/3
38	GDP	FH	502	-	-	3/12/32/32	0/3/3/3
38	GDP	IL	502	-	-	2/12/32/32	0/3/3/3
38	GDP	SN	502	-	-	3/12/32/32	0/3/3/3
38	GDP	GD	502	-	-	3/12/32/32	0/3/3/3
36	GTP	SM	501	37	-	5/18/38/38	0/3/3/3
36	GTP	GG	501	37	-	4/18/38/38	0/3/3/3
38	GDP	MB	502	-	-	1/12/32/32	0/3/3/3
38	GDP	OD	502	-	-	2/12/32/32	0/3/3/3
36	GTP	LE	501	37	-	9/18/38/38	0/3/3/3
36	GTP	BI	501	37	-	4/18/38/38	0/3/3/3
36	GTP	DG	501	37	-	8/18/38/38	0/3/3/3
36	GTP	NM	501	37	-	5/18/38/38	0/3/3/3
38	GDP	HD	502	-	-	1/12/32/32	0/3/3/3
38	GDP	KH	502	-	-	0/12/32/32	0/3/3/3
36	GTP	SE	501	37	-	5/18/38/38	0/3/3/3
38	GDP	MF	502	-	-	1/12/32/32	0/3/3/3
38	GDP	EB	502	-	-	0/12/32/32	0/3/3/3
36	GTP	IM	501	37	-	8/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	FF	502	-	-	2/12/32/32	0/3/3/3
36	GTP	JM	501	37	-	4/18/38/38	0/3/3/3
38	GDP	IN	502	-	-	1/12/32/32	0/3/3/3
38	GDP	GH	502	-	-	1/12/32/32	0/3/3/3
36	GTP	BM	501	37	-	4/18/38/38	0/3/3/3
36	GTP	DC	501	37	-	5/18/38/38	0/3/3/3
38	GDP	AD	502	-	-	1/12/32/32	0/3/3/3
38	GDP	AF	502	-	-	2/12/32/32	0/3/3/3
38	GDP	MH	502	-	-	1/12/32/32	0/3/3/3
38	GDP	ND	502	-	-	0/12/32/32	0/3/3/3
38	GDP	QF	502	-	-	2/12/32/32	0/3/3/3
36	GTP	LG	501	37	-	5/18/38/38	0/3/3/3
38	GDP	KL	502	-	-	1/12/32/32	0/3/3/3
36	GTP	MK	501	37	-	5/18/38/38	0/3/3/3
36	GTP	FE	501	37	-	4/18/38/38	0/3/3/3
38	GDP	RL	502	-	-	0/12/32/32	0/3/3/3
36	GTP	TM	501	37	-	3/18/38/38	0/3/3/3
36	GTP	QC	501	37	-	3/18/38/38	0/3/3/3
36	GTP	OO	501	37	-	7/18/38/38	0/3/3/3
38	GDP	RH	502	-	-	0/12/32/32	0/3/3/3
38	GDP	VL	502	-	-	1/12/32/32	0/3/3/3
36	GTP	OG	501	37	-	5/18/38/38	0/3/3/3
38	GDP	CF	502	-	-	2/12/32/32	0/3/3/3
36	GTP	MC	501	37	-	5/18/38/38	0/3/3/3
38	GDP	TH	502	-	-	3/12/32/32	0/3/3/3
36	GTP	FK	501	37	-	5/18/38/38	0/3/3/3
36	GTP	TI	501	37	-	2/18/38/38	0/3/3/3
38	GDP	GB	502	-	-	3/12/32/32	0/3/3/3
38	GDP	VJ	502	-	-	2/12/32/32	0/3/3/3
38	GDP	TL	502	-	-	4/12/32/32	0/3/3/3
36	GTP	CM	501	37	-	3/18/38/38	0/3/3/3
36	GTP	PG	501	37	-	7/18/38/38	0/3/3/3
38	GDP	AH	502	-	-	1/12/32/32	0/3/3/3
38	GDP	UF	502	-	-	2/12/32/32	0/3/3/3
36	GTP	RC	501	-	-	6/18/38/38	0/3/3/3
38	GDP	LD	502	-	-	4/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	AL	502	-	-	1/12/32/32	0/3/3/3
38	GDP	CD	502	-	-	2/12/32/32	0/3/3/3
38	GDP	VP	502	-	-	1/12/32/32	0/3/3/3
36	GTP	BC	501	37	-	4/18/38/38	0/3/3/3
36	GTP	PM	501	37	-	8/18/38/38	0/3/3/3
36	GTP	FI	501	37	-	6/18/38/38	0/3/3/3
38	GDP	KB	502	-	-	3/12/32/32	0/3/3/3
38	GDP	WP	502	-	-	3/12/32/32	0/3/3/3
36	GTP	BA	501	37	-	5/18/38/38	0/3/3/3
36	GTP	QI	501	37	-	6/18/38/38	0/3/3/3
36	GTP	AK	501	37	-	4/18/38/38	0/3/3/3
38	GDP	QJ	502	-	-	2/12/32/32	0/3/3/3
38	GDP	HJ	502	-	-	1/12/32/32	0/3/3/3
36	GTP	BE	501	37	-	4/18/38/38	0/3/3/3
38	GDP	NN	502	-	-	1/12/32/32	0/3/3/3
36	GTP	QM	501	37	-	8/18/38/38	0/3/3/3
36	GTP	HO	501	37	-	9/18/38/38	0/3/3/3
36	GTP	TK	501	37	-	5/18/38/38	0/3/3/3
38	GDP	DJ	502	-	-	1/12/32/32	0/3/3/3
36	GTP	ME	501	37	-	5/18/38/38	0/3/3/3
38	GDP	OB	502	-	-	4/12/32/32	0/3/3/3
38	GDP	QN	502	-	-	4/12/32/32	0/3/3/3
36	GTP	WI	501	37	-	3/18/38/38	0/3/3/3
38	GDP	NB	502	-	-	1/12/32/32	0/3/3/3
36	GTP	LC	501	37	-	7/18/38/38	0/3/3/3
36	GTP	GC	501	37	-	5/18/38/38	0/3/3/3
36	GTP	QE	501	37	-	9/18/38/38	0/3/3/3
36	GTP	VM	501	37	-	7/18/38/38	0/3/3/3
36	GTP	UO	501	37	-	5/18/38/38	0/3/3/3
36	GTP	NG	501	37	-	5/18/38/38	0/3/3/3
38	GDP	GL	502	-	-	0/12/32/32	0/3/3/3
38	GDP	IJ	502	-	-	1/12/32/32	0/3/3/3
38	GDP	EJ	502	-	-	1/12/32/32	0/3/3/3
36	GTP	BK	501	37	-	5/18/38/38	0/3/3/3
38	GDP	EF	502	-	-	0/12/32/32	0/3/3/3
36	GTP	RE	501	-	-	3/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GTP	LK	501	37	-	6/18/38/38	0/3/3/3
38	GDP	ON	502	-	-	3/12/32/32	0/3/3/3
38	GDP	UJ	502	-	-	3/12/32/32	0/3/3/3
36	GTP	KM	501	37	-	5/18/38/38	0/3/3/3
38	GDP	JH	502	-	-	1/12/32/32	0/3/3/3
38	GDP	IH	502	-	-	2/12/32/32	0/3/3/3
38	GDP	CL	502	-	-	2/12/32/32	0/3/3/3
38	GDP	UH	502	-	-	1/12/32/32	0/3/3/3
36	GTP	UK	501	37	-	3/18/38/38	0/3/3/3
36	GTP	JG	501	37	-	2/18/38/38	0/3/3/3
38	GDP	CH	502	-	-	1/12/32/32	0/3/3/3
38	GDP	ID	502	-	-	2/12/32/32	0/3/3/3
38	GDP	LH	502	-	-	4/12/32/32	0/3/3/3
36	GTP	KG	501	-	-	6/18/38/38	0/3/3/3
36	GTP	EE	501	37	-	5/18/38/38	0/3/3/3
38	GDP	NJ	502	-	-	1/12/32/32	0/3/3/3
38	GDP	ED	502	-	-	3/12/32/32	0/3/3/3
38	GDP	UL	502	-	-	1/12/32/32	0/3/3/3
36	GTP	JK	501	37	-	5/18/38/38	0/3/3/3
36	GTP	EC	501	37	-	5/18/38/38	0/3/3/3
38	GDP	VD	502	-	-	0/12/32/32	0/3/3/3
36	GTP	FM	501	37	-	5/18/38/38	0/3/3/3
38	GDP	NL	502	-	-	1/12/32/32	0/3/3/3
38	GDP	CJ	502	-	-	1/12/32/32	0/3/3/3
36	GTP	BG	501	37	-	5/18/38/38	0/3/3/3
36	GTP	EM	501	37	-	5/18/38/38	0/3/3/3
38	GDP	BH	502	-	-	3/12/32/32	0/3/3/3
36	GTP	CG	501	37	-	6/18/38/38	0/3/3/3
36	GTP	KC	501	37	-	4/18/38/38	0/3/3/3
36	GTP	NE	501	37	-	4/18/38/38	0/3/3/3
36	GTP	AM	501	37	-	4/18/38/38	0/3/3/3
38	GDP	PF	502	-	-	3/12/32/32	0/3/3/3
36	GTP	UE	501	37	-	4/18/38/38	0/3/3/3
36	GTP	CK	501	37	-	10/18/38/38	0/3/3/3
36	GTP	GK	501	37	-	5/18/38/38	0/3/3/3
38	GDP	UP	502	-	-	1/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	HB	502	-	-	1/12/32/32	0/3/3/3
38	GDP	OH	502	-	-	1/12/32/32	0/3/3/3
36	GTP	IK	501	37	-	5/18/38/38	0/3/3/3
38	GDP	OJ	502	-	-	2/12/32/32	0/3/3/3
38	GDP	EL	502	-	-	2/12/32/32	0/3/3/3
36	GTP	JE	501	37	-	2/18/38/38	0/3/3/3
36	GTP	WM	501	37	-	8/18/38/38	0/3/3/3
38	GDP	LL	502	-	-	3/12/32/32	0/3/3/3
36	GTP	VI	501	37	-	6/18/38/38	0/3/3/3
38	GDP	PH	502	-	-	3/12/32/32	0/3/3/3
38	GDP	SJ	502	-	-	0/12/32/32	0/3/3/3
36	GTP	QK	501	37	-	9/18/38/38	0/3/3/3
38	GDP	HF	502	-	-	0/12/32/32	0/3/3/3
36	GTP	HE	501	37	-	4/18/38/38	0/3/3/3
38	GDP	BL	502	-	-	2/12/32/32	0/3/3/3
36	GTP	UG	501	37	-	5/18/38/38	0/3/3/3
36	GTP	FG	501	37	-	5/18/38/38	0/3/3/3
36	GTP	HK	501	37	-	4/18/38/38	0/3/3/3
36	GTP	EI	501	37	-	6/18/38/38	0/3/3/3
36	GTP	AE	501	37	-	3/18/38/38	0/3/3/3
36	GTP	PI	501	37	-	3/18/38/38	0/3/3/3
36	GTP	UM	501	37	-	8/18/38/38	0/3/3/3
38	GDP	FD	502	-	-	4/12/32/32	0/3/3/3
38	GDP	JB	502	-	-	1/12/32/32	0/3/3/3
38	GDP	DF	502	-	-	1/12/32/32	0/3/3/3
38	GDP	FB	502	-	-	1/12/32/32	0/3/3/3
38	GDP	FJ	502	-	-	1/12/32/32	0/3/3/3
36	GTP	QG	501	37	-	6/18/38/38	0/3/3/3
38	GDP	TD	502	-	-	3/12/32/32	0/3/3/3
38	GDP	MN	502	-	-	1/12/32/32	0/3/3/3
38	GDP	QH	502	-	-	4/12/32/32	0/3/3/3
38	GDP	HH	502	-	-	0/12/32/32	0/3/3/3
38	GDP	RN	502	-	-	1/12/32/32	0/3/3/3
36	GTP	EG	501	37	-	5/18/38/38	0/3/3/3
36	GTP	TE	501	37	-	5/18/38/38	0/3/3/3
36	GTP	WK	501	37	-	5/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	KF	502	-	-	3/12/32/32	0/3/3/3
38	GDP	VF	502	-	-	1/12/32/32	0/3/3/3
36	GTP	OE	501	37	-	4/18/38/38	0/3/3/3
38	GDP	FL	502	-	-	3/12/32/32	0/3/3/3
38	GDP	WD	502	-	-	4/12/32/32	0/3/3/3
38	GDP	LJ	502	-	-	3/12/32/32	0/3/3/3
36	GTP	CC	501	37	-	8/18/38/38	0/3/3/3
38	GDP	GJ	502	-	-	4/12/32/32	0/3/3/3
36	GTP	UI	501	37	-	5/18/38/38	0/3/3/3
38	GDP	HN	502	-	-	1/12/32/32	0/3/3/3
36	GTP	FC	501	37	-	5/18/38/38	0/3/3/3
38	GDP	OL	502	-	-	4/12/32/32	0/3/3/3
36	GTP	JI	501	37	-	2/18/38/38	0/3/3/3
36	GTP	DI	501	37	-	3/18/38/38	0/3/3/3

All (451) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	RK	501	GTP	C5-C6	-4.37	1.38	1.47
36	RE	501	GTP	C5-C6	-4.34	1.38	1.47
36	QE	501	GTP	C5-C6	-4.29	1.38	1.47
36	BG	501	GTP	C5-C6	-4.28	1.38	1.47
36	RI	501	GTP	C5-C6	-4.28	1.38	1.47
36	OO	501	GTP	C5-C6	-4.27	1.38	1.47
36	UE	501	GTP	C5-C6	-4.27	1.38	1.47
36	OM	501	GTP	C5-C6	-4.26	1.38	1.47
36	AI	501	GTP	C5-C6	-4.26	1.38	1.47
36	KM	501	GTP	C5-C6	-4.26	1.38	1.47
36	NE	501	GTP	C5-C6	-4.24	1.38	1.47
36	QG	501	GTP	C5-C6	-4.23	1.38	1.47
36	QM	501	GTP	C5-C6	-4.23	1.38	1.47
36	BE	501	GTP	C5-C6	-4.23	1.38	1.47
36	BC	501	GTP	C5-C6	-4.23	1.38	1.47
36	NC	501	GTP	C5-C6	-4.22	1.38	1.47
36	BM	501	GTP	C5-C6	-4.21	1.38	1.47
36	KE	501	GTP	C5-C6	-4.21	1.38	1.47
36	BA	501	GTP	C5-C6	-4.21	1.38	1.47
36	BK	501	GTP	C5-C6	-4.20	1.38	1.47
36	BI	501	GTP	C5-C6	-4.20	1.38	1.47
36	RO	501	GTP	C5-C6	-4.20	1.38	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	KK	501	GTP	C5-C6	-4.20	1.38	1.47
36	QO	501	GTP	C5-C6	-4.19	1.38	1.47
36	FM	501	GTP	C5-C6	-4.18	1.38	1.47
36	SE	501	GTP	C5-C6	-4.18	1.38	1.47
36	KG	501	GTP	C5-C6	-4.17	1.38	1.47
36	NG	501	GTP	C5-C6	-4.17	1.38	1.47
36	SO	501	GTP	C5-C6	-4.17	1.38	1.47
36	SG	501	GTP	C5-C6	-4.17	1.38	1.47
36	MG	501	GTP	C5-C6	-4.17	1.38	1.47
36	FI	501	GTP	C5-C6	-4.17	1.39	1.47
36	KO	501	GTP	C5-C6	-4.16	1.39	1.47
36	GG	501	GTP	C5-C6	-4.16	1.39	1.47
36	AG	501	GTP	C5-C6	-4.16	1.39	1.47
36	PG	501	GTP	C5-C6	-4.16	1.39	1.47
36	OC	501	GTP	C5-C6	-4.15	1.39	1.47
36	MM	501	GTP	C5-C6	-4.15	1.39	1.47
36	EI	501	GTP	C5-C6	-4.15	1.39	1.47
36	QI	501	GTP	C5-C6	-4.15	1.39	1.47
36	SI	501	GTP	C5-C6	-4.15	1.39	1.47
36	QK	501	GTP	C5-C6	-4.15	1.39	1.47
36	LG	501	GTP	C5-C6	-4.15	1.39	1.47
36	RG	501	GTP	C5-C6	-4.14	1.39	1.47
36	VE	501	GTP	C5-C6	-4.14	1.39	1.47
36	MI	501	GTP	C5-C6	-4.14	1.39	1.47
36	JI	501	GTP	C5-C6	-4.14	1.39	1.47
36	LK	501	GTP	C5-C6	-4.14	1.39	1.47
36	KI	501	GTP	C5-C6	-4.14	1.39	1.47
36	LM	501	GTP	C5-C6	-4.14	1.39	1.47
36	QC	501	GTP	C5-C6	-4.14	1.39	1.47
36	LC	501	GTP	C5-C6	-4.14	1.39	1.47
36	JM	501	GTP	C5-C6	-4.13	1.39	1.47
36	FK	501	GTP	C5-C6	-4.13	1.39	1.47
36	AK	501	GTP	C5-C6	-4.13	1.39	1.47
36	SK	501	GTP	C5-C6	-4.13	1.39	1.47
36	LE	501	GTP	C5-C6	-4.13	1.39	1.47
36	AE	501	GTP	C5-C6	-4.13	1.39	1.47
36	OI	501	GTP	C5-C6	-4.13	1.39	1.47
36	PK	501	GTP	C5-C6	-4.13	1.39	1.47
36	LI	501	GTP	C5-C6	-4.13	1.39	1.47
36	SM	501	GTP	C5-C6	-4.13	1.39	1.47
36	HM	501	GTP	C5-C6	-4.13	1.39	1.47
36	NK	501	GTP	C5-C6	-4.13	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	NI	501	GTP	C5-C6	-4.12	1.39	1.47
36	RM	501	GTP	C5-C6	-4.12	1.39	1.47
36	HO	501	GTP	C5-C6	-4.12	1.39	1.47
36	AM	501	GTP	C5-C6	-4.12	1.39	1.47
36	EM	501	GTP	C5-C6	-4.12	1.39	1.47
36	PM	501	GTP	C5-C6	-4.12	1.39	1.47
36	MC	501	GTP	C5-C6	-4.12	1.39	1.47
36	VK	501	GTP	C5-C6	-4.12	1.39	1.47
36	JE	501	GTP	C5-C6	-4.11	1.39	1.47
36	MK	501	GTP	C5-C6	-4.11	1.39	1.47
36	HC	501	GTP	C5-C6	-4.11	1.39	1.47
36	HI	501	GTP	C5-C6	-4.11	1.39	1.47
36	EE	501	GTP	C5-C6	-4.11	1.39	1.47
36	PI	501	GTP	C5-C6	-4.10	1.39	1.47
36	FC	501	GTP	C5-C6	-4.10	1.39	1.47
36	JK	501	GTP	C5-C6	-4.10	1.39	1.47
36	FE	501	GTP	C5-C6	-4.10	1.39	1.47
36	NM	501	GTP	C5-C6	-4.10	1.39	1.47
36	EK	501	GTP	C5-C6	-4.10	1.39	1.47
36	OG	501	GTP	C5-C6	-4.10	1.39	1.47
36	ME	501	GTP	C5-C6	-4.09	1.39	1.47
36	FG	501	GTP	C5-C6	-4.09	1.39	1.47
36	OE	501	GTP	C5-C6	-4.09	1.39	1.47
36	UI	501	GTP	C5-C6	-4.09	1.39	1.47
36	AA	501	GTP	C5-C6	-4.09	1.39	1.47
36	GC	501	GTP	C5-C6	-4.09	1.39	1.47
36	UO	501	GTP	C5-C6	-4.09	1.39	1.47
36	EG	501	GTP	C5-C6	-4.08	1.39	1.47
36	CK	501	GTP	C5-C6	-4.08	1.39	1.47
36	HE	501	GTP	C5-C6	-4.08	1.39	1.47
36	RC	501	GTP	C5-C6	-4.08	1.39	1.47
36	EC	501	GTP	C5-C6	-4.08	1.39	1.47
36	OK	501	GTP	C5-C6	-4.08	1.39	1.47
36	TK	501	GTP	C5-C6	-4.08	1.39	1.47
36	HK	501	GTP	C5-C6	-4.07	1.39	1.47
36	PE	501	GTP	C5-C6	-4.07	1.39	1.47
36	AC	501	GTP	C5-C6	-4.07	1.39	1.47
36	KC	501	GTP	C5-C6	-4.07	1.39	1.47
36	UG	501	GTP	C5-C6	-4.07	1.39	1.47
36	VO	501	GTP	C5-C6	-4.07	1.39	1.47
36	TM	501	GTP	C5-C6	-4.06	1.39	1.47
36	TO	501	GTP	C5-C6	-4.06	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	PO	501	GTP	C5-C6	-4.06	1.39	1.47
36	GE	501	GTP	C5-C6	-4.05	1.39	1.47
36	HG	501	GTP	C5-C6	-4.05	1.39	1.47
36	TI	501	GTP	C5-C6	-4.05	1.39	1.47
36	CC	501	GTP	C5-C6	-4.04	1.39	1.47
36	VG	501	GTP	C5-C6	-4.04	1.39	1.47
36	IO	501	GTP	C5-C6	-4.03	1.39	1.47
36	CM	501	GTP	C5-C6	-4.03	1.39	1.47
36	VI	501	GTP	C5-C6	-4.03	1.39	1.47
36	GI	501	GTP	C5-C6	-4.02	1.39	1.47
36	JG	501	GTP	C5-C6	-4.02	1.39	1.47
36	WM	501	GTP	C5-C6	-4.02	1.39	1.47
36	VM	501	GTP	C5-C6	-4.02	1.39	1.47
36	DG	501	GTP	C5-C6	-4.02	1.39	1.47
36	WI	501	GTP	C5-C6	-4.02	1.39	1.47
36	GK	501	GTP	C5-C6	-4.00	1.39	1.47
36	WK	501	GTP	C5-C6	-4.00	1.39	1.47
36	PC	501	GTP	C5-C6	-4.00	1.39	1.47
36	TG	501	GTP	C5-C6	-4.00	1.39	1.47
36	JC	501	GTP	C5-C6	-3.99	1.39	1.47
36	IK	501	GTP	C5-C6	-3.99	1.39	1.47
36	UK	501	GTP	C5-C6	-3.98	1.39	1.47
36	CA	501	GTP	C5-C6	-3.98	1.39	1.47
36	UM	501	GTP	C5-C6	-3.98	1.39	1.47
36	IE	501	GTP	C5-C6	-3.97	1.39	1.47
36	WO	501	GTP	C5-C6	-3.97	1.39	1.47
36	GM	501	GTP	C5-C6	-3.97	1.39	1.47
36	CI	501	GTP	C5-C6	-3.97	1.39	1.47
36	DE	501	GTP	C5-C6	-3.96	1.39	1.47
36	IC	501	GTP	C5-C6	-3.96	1.39	1.47
36	TE	501	GTP	C5-C6	-3.95	1.39	1.47
36	CE	501	GTP	C5-C6	-3.95	1.39	1.47
36	CG	501	GTP	C5-C6	-3.95	1.39	1.47
36	IG	501	GTP	C5-C6	-3.94	1.39	1.47
36	WG	501	GTP	C5-C6	-3.93	1.39	1.47
36	DK	501	GTP	C5-C6	-3.92	1.39	1.47
36	DA	501	GTP	C5-C6	-3.91	1.39	1.47
36	II	501	GTP	C5-C6	-3.91	1.39	1.47
36	DC	501	GTP	C5-C6	-3.90	1.39	1.47
36	IM	501	GTP	C5-C6	-3.90	1.39	1.47
36	DI	501	GTP	C5-C6	-3.84	1.39	1.47
36	WE	501	GTP	C5-C6	-3.84	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	DM	501	GTP	C5-C6	-3.81	1.39	1.47
38	RN	502	GDP	C6-N1	-2.73	1.33	1.37
38	LF	502	GDP	C6-N1	-2.70	1.33	1.37
38	KJ	502	GDP	C6-N1	-2.69	1.33	1.37
38	DB	502	GDP	C6-N1	-2.69	1.33	1.37
38	QD	502	GDP	C6-N1	-2.68	1.33	1.37
38	EB	502	GDP	C6-N1	-2.67	1.33	1.37
38	RJ	502	GDP	C6-N1	-2.67	1.33	1.37
38	MB	502	GDP	C6-N1	-2.67	1.33	1.37
38	EH	502	GDP	C6-N1	-2.66	1.33	1.37
38	MN	502	GDP	C6-N1	-2.64	1.33	1.37
38	JD	502	GDP	C6-N1	-2.64	1.33	1.37
38	KN	502	GDP	C6-N1	-2.64	1.33	1.37
38	QJ	502	GDP	C6-N1	-2.64	1.33	1.37
38	LJ	502	GDP	C6-N1	-2.63	1.34	1.37
38	OJ	502	GDP	C6-N1	-2.63	1.34	1.37
38	DH	502	GDP	C6-N1	-2.62	1.34	1.37
38	AL	502	GDP	C6-N1	-2.62	1.34	1.37
38	MJ	502	GDP	C6-N1	-2.62	1.34	1.37
38	JH	502	GDP	C6-N1	-2.62	1.34	1.37
38	QF	502	GDP	C6-N1	-2.61	1.34	1.37
38	OD	502	GDP	C6-N1	-2.61	1.34	1.37
38	OB	502	GDP	C6-N1	-2.60	1.34	1.37
38	EL	502	GDP	C6-N1	-2.60	1.34	1.37
38	KB	502	GDP	C6-N1	-2.60	1.34	1.37
38	RL	502	GDP	C6-N1	-2.59	1.34	1.37
38	EJ	502	GDP	C6-N1	-2.59	1.34	1.37
38	QN	502	GDP	C6-N1	-2.59	1.34	1.37
38	KF	502	GDP	C6-N1	-2.58	1.34	1.37
38	EN	502	GDP	C6-N1	-2.58	1.34	1.37
38	MF	502	GDP	C6-N1	-2.58	1.34	1.37
38	ED	502	GDP	C6-N1	-2.57	1.34	1.37
38	RD	502	GDP	C6-N1	-2.57	1.34	1.37
38	RF	502	GDP	C6-N1	-2.57	1.34	1.37
38	FN	502	GDP	C6-N1	-2.57	1.34	1.37
38	JL	502	GDP	C6-N1	-2.56	1.34	1.37
38	RH	502	GDP	C6-N1	-2.56	1.34	1.37
38	AB	502	GDP	C6-N1	-2.56	1.34	1.37
38	FH	502	GDP	C6-N1	-2.56	1.34	1.37
38	FF	502	GDP	C6-N1	-2.56	1.34	1.37
38	HJ	502	GDP	C6-N1	-2.55	1.34	1.37
38	MH	502	GDP	C6-N1	-2.55	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	LH	502	GDP	C6-N1	-2.55	1.34	1.37
38	AJ	502	GDP	C6-N1	-2.55	1.34	1.37
38	VH	502	GDP	C6-N1	-2.55	1.34	1.37
38	SF	502	GDP	C6-N1	-2.55	1.34	1.37
38	LB	502	GDP	C6-N1	-2.54	1.34	1.37
38	JN	502	GDP	C6-N1	-2.54	1.34	1.37
38	SD	502	GDP	C6-N1	-2.54	1.34	1.37
38	JB	502	GDP	C6-N1	-2.54	1.34	1.37
38	GN	502	GDP	C6-N1	-2.54	1.34	1.37
38	KH	502	GDP	C6-N1	-2.54	1.34	1.37
38	DJ	502	GDP	C6-N1	-2.54	1.34	1.37
38	DL	502	GDP	C6-N1	-2.54	1.34	1.37
38	KD	502	GDP	C6-N1	-2.54	1.34	1.37
38	LD	502	GDP	C6-N1	-2.53	1.34	1.37
38	QL	502	GDP	C6-N1	-2.53	1.34	1.37
38	KL	502	GDP	C6-N1	-2.53	1.34	1.37
38	JJ	502	GDP	C6-N1	-2.53	1.34	1.37
38	OF	502	GDP	C6-N1	-2.53	1.34	1.37
38	MD	502	GDP	C6-N1	-2.53	1.34	1.37
38	PL	502	GDP	C6-N1	-2.53	1.34	1.37
38	PH	502	GDP	C6-N1	-2.52	1.34	1.37
38	AF	502	GDP	C6-N1	-2.52	1.34	1.37
38	LL	502	GDP	C6-N1	-2.52	1.34	1.37
38	ML	502	GDP	C6-N1	-2.52	1.34	1.37
38	PD	502	GDP	C6-N1	-2.52	1.34	1.37
38	AH	502	GDP	C6-N1	-2.52	1.34	1.37
38	WJ	502	GDP	C6-N1	-2.52	1.34	1.37
38	NJ	502	GDP	C6-N1	-2.51	1.34	1.37
38	OH	502	GDP	C6-N1	-2.51	1.34	1.37
38	ON	502	GDP	C6-N1	-2.51	1.34	1.37
38	VJ	502	GDP	C6-N1	-2.51	1.34	1.37
38	BH	502	GDP	C6-N1	-2.51	1.34	1.37
38	UJ	502	GDP	C6-N1	-2.51	1.34	1.37
38	SH	502	GDP	C6-N1	-2.51	1.34	1.37
38	WN	502	GDP	C6-N1	-2.51	1.34	1.37
38	UP	502	GDP	C6-N1	-2.51	1.34	1.37
38	FD	502	GDP	C6-N1	-2.51	1.34	1.37
38	SJ	502	GDP	C6-N1	-2.50	1.34	1.37
38	IH	502	GDP	C6-N1	-2.49	1.34	1.37
38	PF	502	GDP	C6-N1	-2.49	1.34	1.37
38	QH	502	GDP	C6-N1	-2.49	1.34	1.37
38	HN	502	GDP	C6-N1	-2.49	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	VL	502	GDP	C6-N1	-2.49	1.34	1.37
38	CJ	502	GDP	C6-N1	-2.49	1.34	1.37
38	PJ	502	GDP	C6-N1	-2.48	1.34	1.37
38	CB	502	GDP	C6-N1	-2.48	1.34	1.37
38	HD	502	GDP	C6-N1	-2.48	1.34	1.37
38	PN	502	GDP	C6-N1	-2.48	1.34	1.37
38	DD	502	GDP	C6-N1	-2.48	1.34	1.37
38	JF	502	GDP	C6-N1	-2.48	1.34	1.37
38	WP	502	GDP	C6-N1	-2.48	1.34	1.37
38	CD	502	GDP	C6-N1	-2.47	1.34	1.37
38	VD	502	GDP	C6-N1	-2.47	1.34	1.37
38	VF	502	GDP	C6-N1	-2.47	1.34	1.37
38	FJ	502	GDP	C6-N1	-2.47	1.34	1.37
38	UD	502	GDP	C6-N1	-2.47	1.34	1.37
38	EF	502	GDP	C6-N1	-2.47	1.34	1.37
38	IF	502	GDP	C6-N1	-2.47	1.34	1.37
38	NN	502	GDP	C6-N1	-2.47	1.34	1.37
38	DF	502	GDP	C6-N1	-2.47	1.34	1.37
38	OL	502	GDP	C6-N1	-2.47	1.34	1.37
38	SN	502	GDP	C6-N1	-2.47	1.34	1.37
38	IJ	502	GDP	C6-N1	-2.46	1.34	1.37
38	AD	502	GDP	C6-N1	-2.46	1.34	1.37
38	VP	502	GDP	C6-N1	-2.46	1.34	1.37
38	LN	502	GDP	C6-N1	-2.46	1.34	1.37
38	WD	502	GDP	C6-N1	-2.46	1.34	1.37
38	UF	502	GDP	C6-N1	-2.45	1.34	1.37
38	UH	502	GDP	C6-N1	-2.45	1.34	1.37
38	SL	502	GDP	C6-N1	-2.44	1.34	1.37
38	CF	502	GDP	C6-N1	-2.43	1.34	1.37
38	NB	502	GDP	C6-N1	-2.43	1.34	1.37
38	IL	502	GDP	C6-N1	-2.43	1.34	1.37
38	TP	502	GDP	C6-N1	-2.43	1.34	1.37
38	WL	502	GDP	C6-N1	-2.43	1.34	1.37
38	HB	502	GDP	C6-N1	-2.43	1.34	1.37
38	NH	502	GDP	C6-N1	-2.43	1.34	1.37
38	FL	502	GDP	C6-N1	-2.43	1.34	1.37
38	UL	502	GDP	C6-N1	-2.43	1.34	1.37
38	BD	502	GDP	C6-N1	-2.42	1.34	1.37
38	NF	502	GDP	C6-N1	-2.42	1.34	1.37
38	ND	502	GDP	C6-N1	-2.42	1.34	1.37
38	BF	502	GDP	C6-N1	-2.42	1.34	1.37
38	GD	502	GDP	C6-N1	-2.42	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	HF	502	GDP	C6-N1	-2.42	1.34	1.37
38	GL	502	GDP	C6-N1	-2.42	1.34	1.37
38	HL	502	GDP	C6-N1	-2.42	1.34	1.37
38	NL	502	GDP	C6-N1	-2.42	1.34	1.37
38	WH	502	GDP	C6-N1	-2.42	1.34	1.37
38	VN	502	GDP	C6-N1	-2.41	1.34	1.37
38	HH	502	GDP	C6-N1	-2.41	1.34	1.37
38	IB	502	GDP	C6-N1	-2.41	1.34	1.37
38	TH	502	GDP	C6-N1	-2.40	1.34	1.37
38	UN	502	GDP	C6-N1	-2.40	1.34	1.37
38	TN	502	GDP	C6-N1	-2.40	1.34	1.37
38	FB	502	GDP	C6-N1	-2.40	1.34	1.37
38	TJ	502	GDP	C6-N1	-2.40	1.34	1.37
38	ID	502	GDP	C6-N1	-2.40	1.34	1.37
38	TF	502	GDP	C6-N1	-2.40	1.34	1.37
38	BL	502	GDP	C6-N1	-2.39	1.34	1.37
38	CL	502	GDP	C6-N1	-2.39	1.34	1.37
38	CH	502	GDP	C6-N1	-2.39	1.34	1.37
38	BB	502	GDP	C6-N1	-2.39	1.34	1.37
38	GB	502	GDP	C6-N1	-2.38	1.34	1.37
38	TD	502	GDP	C6-N1	-2.37	1.34	1.37
38	BJ	502	GDP	C6-N1	-2.37	1.34	1.37
38	GJ	502	GDP	C6-N1	-2.37	1.34	1.37
38	WF	502	GDP	C6-N1	-2.37	1.34	1.37
38	IN	502	GDP	C6-N1	-2.36	1.34	1.37
38	GH	502	GDP	C6-N1	-2.35	1.34	1.37
38	TL	502	GDP	C6-N1	-2.35	1.34	1.37
38	GF	502	GDP	C6-N1	-2.34	1.34	1.37
36	IE	501	GTP	C2-N3	2.26	1.38	1.33
36	DA	501	GTP	C2-N3	2.26	1.38	1.33
36	DC	501	GTP	C2-N3	2.25	1.38	1.33
36	VE	501	GTP	C2-N3	2.25	1.38	1.33
36	DG	501	GTP	C2-N3	2.24	1.38	1.33
36	CK	501	GTP	C2-N3	2.24	1.38	1.33
36	CC	501	GTP	C2-N3	2.24	1.38	1.33
36	PC	501	GTP	C2-N3	2.23	1.38	1.33
36	RC	501	GTP	C2-N3	2.23	1.38	1.33
36	II	501	GTP	C2-N3	2.23	1.38	1.33
36	IC	501	GTP	C2-N3	2.23	1.38	1.33
36	IG	501	GTP	C2-N3	2.22	1.38	1.33
36	CG	501	GTP	C2-N3	2.22	1.38	1.33
36	CE	501	GTP	C2-N3	2.22	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	KK	501	GTP	C2-N3	2.22	1.38	1.33
36	GI	501	GTP	C2-N3	2.21	1.38	1.33
36	EC	501	GTP	C2-N3	2.21	1.38	1.33
36	IM	501	GTP	C2-N3	2.21	1.38	1.33
36	IO	501	GTP	C2-N3	2.21	1.38	1.33
36	HG	501	GTP	C2-N3	2.20	1.38	1.33
36	FC	501	GTP	C2-N3	2.20	1.38	1.33
36	UM	501	GTP	C2-N3	2.20	1.38	1.33
36	VG	501	GTP	C2-N3	2.20	1.38	1.33
36	VI	501	GTP	C2-N3	2.20	1.38	1.33
36	WI	501	GTP	C2-N3	2.20	1.38	1.33
36	HC	501	GTP	C2-N3	2.19	1.38	1.33
36	CM	501	GTP	C2-N3	2.19	1.38	1.33
36	CA	501	GTP	C2-N3	2.19	1.38	1.33
36	LE	501	GTP	C2-N3	2.19	1.38	1.33
36	IK	501	GTP	C2-N3	2.19	1.38	1.33
36	DE	501	GTP	C2-N3	2.19	1.38	1.33
36	LK	501	GTP	C2-N3	2.19	1.38	1.33
36	FE	501	GTP	C2-N3	2.19	1.38	1.33
36	HO	501	GTP	C2-N3	2.18	1.38	1.33
36	PK	501	GTP	C2-N3	2.18	1.38	1.33
36	OK	501	GTP	C2-N3	2.18	1.38	1.33
36	UE	501	GTP	C2-N3	2.18	1.38	1.33
36	VM	501	GTP	C2-N3	2.18	1.38	1.33
36	UG	501	GTP	C2-N3	2.18	1.38	1.33
36	MG	501	GTP	C2-N3	2.18	1.38	1.33
36	KC	501	GTP	C2-N3	2.18	1.38	1.33
36	KG	501	GTP	C2-N3	2.18	1.38	1.33
36	NE	501	GTP	C2-N3	2.17	1.38	1.33
36	NG	501	GTP	C2-N3	2.17	1.38	1.33
36	DI	501	GTP	C2-N3	2.17	1.38	1.33
36	FM	501	GTP	C2-N3	2.17	1.38	1.33
36	WM	501	GTP	C2-N3	2.17	1.38	1.33
36	QK	501	GTP	C2-N3	2.17	1.38	1.33
36	HK	501	GTP	C2-N3	2.17	1.38	1.33
36	HI	501	GTP	C2-N3	2.17	1.38	1.33
36	JK	501	GTP	C2-N3	2.17	1.38	1.33
36	VO	501	GTP	C2-N3	2.17	1.38	1.33
36	SI	501	GTP	C2-N3	2.17	1.38	1.33
36	VK	501	GTP	C2-N3	2.17	1.38	1.33
36	JM	501	GTP	C2-N3	2.16	1.38	1.33
36	JC	501	GTP	C2-N3	2.16	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	SE	501	GTP	C2-N3	2.16	1.38	1.33
36	GC	501	GTP	C2-N3	2.16	1.38	1.33
36	HE	501	GTP	C2-N3	2.16	1.38	1.33
36	HM	501	GTP	C2-N3	2.16	1.38	1.33
36	PE	501	GTP	C2-N3	2.16	1.38	1.33
36	NC	501	GTP	C2-N3	2.16	1.38	1.33
36	UI	501	GTP	C2-N3	2.16	1.38	1.33
36	CI	501	GTP	C2-N3	2.15	1.38	1.33
36	RK	501	GTP	C2-N3	2.15	1.38	1.33
36	BK	501	GTP	C2-N3	2.15	1.38	1.33
36	JE	501	GTP	C2-N3	2.15	1.38	1.33
36	BA	501	GTP	C2-N3	2.15	1.38	1.33
36	FG	501	GTP	C2-N3	2.15	1.38	1.33
36	TK	501	GTP	C2-N3	2.15	1.38	1.33
36	QO	501	GTP	C2-N3	2.14	1.38	1.33
36	PG	501	GTP	C2-N3	2.14	1.38	1.33
36	RO	501	GTP	C2-N3	2.14	1.38	1.33
36	KO	501	GTP	C2-N3	2.14	1.38	1.33
36	MC	501	GTP	C2-N3	2.14	1.38	1.33
36	NK	501	GTP	C2-N3	2.14	1.38	1.33
36	SK	501	GTP	C2-N3	2.14	1.38	1.33
36	EM	501	GTP	C2-N3	2.14	1.38	1.33
36	EG	501	GTP	C2-N3	2.14	1.38	1.33
36	SG	501	GTP	C2-N3	2.14	1.38	1.33
36	BC	501	GTP	C2-N3	2.14	1.38	1.33
36	KM	501	GTP	C2-N3	2.14	1.38	1.33
36	UO	501	GTP	C2-N3	2.14	1.38	1.33
36	WG	501	GTP	C2-N3	2.14	1.38	1.33
36	TM	501	GTP	C2-N3	2.13	1.38	1.33
36	UK	501	GTP	C2-N3	2.13	1.38	1.33
36	GG	501	GTP	C2-N3	2.13	1.38	1.33
36	LG	501	GTP	C2-N3	2.13	1.38	1.33
36	GM	501	GTP	C2-N3	2.13	1.38	1.33
36	ME	501	GTP	C2-N3	2.13	1.38	1.33
36	LI	501	GTP	C2-N3	2.13	1.38	1.33
36	PI	501	GTP	C2-N3	2.13	1.38	1.33
36	EE	501	GTP	C2-N3	2.12	1.38	1.33
36	OG	501	GTP	C2-N3	2.12	1.38	1.33
36	TO	501	GTP	C2-N3	2.12	1.38	1.33
36	RI	501	GTP	C2-N3	2.12	1.38	1.33
36	NI	501	GTP	C2-N3	2.12	1.38	1.33
36	BE	501	GTP	C2-N3	2.12	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	KI	501	GTP	C2-N3	2.12	1.38	1.33
36	JI	501	GTP	C2-N3	2.12	1.38	1.33
36	BM	501	GTP	C2-N3	2.12	1.38	1.33
36	OM	501	GTP	C2-N3	2.12	1.38	1.33
36	LM	501	GTP	C2-N3	2.12	1.38	1.33
36	TG	501	GTP	C2-N3	2.11	1.38	1.33
36	BG	501	GTP	C2-N3	2.11	1.38	1.33
36	QG	501	GTP	C2-N3	2.11	1.38	1.33
36	BI	501	GTP	C2-N3	2.11	1.38	1.33
36	LC	501	GTP	C2-N3	2.11	1.38	1.33
36	RE	501	GTP	C2-N3	2.11	1.38	1.33
36	EK	501	GTP	C2-N3	2.11	1.38	1.33
36	SM	501	GTP	C2-N3	2.11	1.38	1.33
36	FK	501	GTP	C2-N3	2.11	1.38	1.33
36	QM	501	GTP	C2-N3	2.11	1.38	1.33
36	OC	501	GTP	C2-N3	2.10	1.38	1.33
36	TE	501	GTP	C2-N3	2.10	1.38	1.33
36	OE	501	GTP	C2-N3	2.10	1.38	1.33
36	SO	501	GTP	C2-N3	2.10	1.38	1.33
36	MK	501	GTP	C2-N3	2.10	1.38	1.33
36	NM	501	GTP	C2-N3	2.10	1.38	1.33
36	GE	501	GTP	C2-N3	2.10	1.38	1.33
36	KE	501	GTP	C2-N3	2.09	1.38	1.33
36	QC	501	GTP	C2-N3	2.09	1.38	1.33
36	QI	501	GTP	C2-N3	2.09	1.38	1.33
36	AI	501	GTP	C2-N3	2.09	1.38	1.33
36	RG	501	GTP	C2-N3	2.09	1.38	1.33
36	MI	501	GTP	C2-N3	2.09	1.38	1.33
36	AK	501	GTP	C2-N3	2.08	1.38	1.33
36	MM	501	GTP	C2-N3	2.08	1.38	1.33
36	OO	501	GTP	C2-N3	2.08	1.38	1.33
36	WO	501	GTP	C2-N3	2.08	1.38	1.33
36	WE	501	GTP	C2-N3	2.08	1.38	1.33
36	GK	501	GTP	C2-N3	2.08	1.38	1.33
36	PM	501	GTP	C2-N3	2.08	1.38	1.33
36	JG	501	GTP	C2-N3	2.07	1.38	1.33
36	QE	501	GTP	C2-N3	2.07	1.38	1.33
36	PO	501	GTP	C2-N3	2.07	1.38	1.33
36	WK	501	GTP	C2-N3	2.05	1.38	1.33
36	AE	501	GTP	C2-N3	2.05	1.38	1.33
36	OI	501	GTP	C2-N3	2.05	1.38	1.33
36	RM	501	GTP	C2-N3	2.05	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	EI	501	GTP	C2-N3	2.05	1.38	1.33
36	DM	501	GTP	C2-N3	2.05	1.38	1.33
36	AG	501	GTP	C2-N3	2.05	1.38	1.33
36	TI	501	GTP	C2-N3	2.05	1.38	1.33
36	AM	501	GTP	C2-N3	2.04	1.38	1.33
36	AA	501	GTP	C2-N3	2.04	1.38	1.33
36	AC	501	GTP	C2-N3	2.03	1.38	1.33
36	FI	501	GTP	C2-N3	2.02	1.38	1.33
36	DK	501	GTP	C2-N3	2.02	1.38	1.33

All (1643) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	AB	502	GDP	PA-O3A-PB	-4.58	117.11	132.83
38	AJ	502	GDP	PA-O3A-PB	-4.56	117.17	132.83
38	OB	502	GDP	PA-O3A-PB	-4.54	117.26	132.83
36	DM	501	GTP	PB-O3B-PG	-4.49	117.42	132.83
38	AF	502	GDP	PA-O3A-PB	-4.47	117.50	132.83
36	OI	501	GTP	PB-O3B-PG	-4.38	117.79	132.83
38	LJ	502	GDP	PA-O3A-PB	-4.35	117.89	132.83
38	NL	502	GDP	PA-O3A-PB	-4.33	117.98	132.83
38	KF	502	GDP	PA-O3A-PB	-4.31	118.03	132.83
36	CI	501	GTP	PB-O3B-PG	-4.31	118.05	132.83
38	AD	502	GDP	PA-O3A-PB	-4.30	118.07	132.83
38	BF	502	GDP	PA-O3A-PB	-4.30	118.08	132.83
36	PI	501	GTP	PB-O3B-PG	-4.28	118.13	132.83
38	QN	502	GDP	PA-O3A-PB	-4.28	118.14	132.83
38	BL	502	GDP	PA-O3A-PB	-4.27	118.17	132.83
38	KN	502	GDP	PA-O3A-PB	-4.27	118.19	132.83
38	LN	502	GDP	PA-O3A-PB	-4.25	118.25	132.83
36	WG	501	GTP	PB-O3B-PG	-4.24	118.29	132.83
38	BH	502	GDP	PA-O3A-PB	-4.22	118.34	132.83
38	NH	502	GDP	PA-O3A-PB	-4.22	118.35	132.83
38	QD	502	GDP	PA-O3A-PB	-4.21	118.39	132.83
38	BJ	502	GDP	PA-O3A-PB	-4.17	118.50	132.83
38	NB	502	GDP	PA-O3A-PB	-4.17	118.51	132.83
36	OC	501	GTP	PB-O3B-PG	-4.17	118.52	132.83
38	NN	502	GDP	PA-O3A-PB	-4.17	118.52	132.83
38	CB	502	GDP	PA-O3A-PB	-4.16	118.56	132.83
38	BB	502	GDP	PA-O3A-PB	-4.16	118.57	132.83
38	PD	502	GDP	PA-O3A-PB	-4.14	118.63	132.83
36	IG	501	GTP	PB-O3B-PG	-4.13	118.64	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	HB	502	GDP	PA-O3A-PB	-4.13	118.64	132.83
38	KB	502	GDP	PA-O3A-PB	-4.13	118.64	132.83
38	AH	502	GDP	PA-O3A-PB	-4.13	118.65	132.83
38	NF	502	GDP	PA-O3A-PB	-4.13	118.65	132.83
38	OF	502	GDP	PA-O3A-PB	-4.13	118.66	132.83
38	OD	502	GDP	PA-O3A-PB	-4.12	118.67	132.83
38	UJ	502	GDP	PA-O3A-PB	-4.12	118.70	132.83
38	LL	502	GDP	PA-O3A-PB	-4.11	118.71	132.83
36	IM	501	GTP	PA-O3A-PB	-4.11	118.72	132.83
36	HI	501	GTP	PB-O3B-PG	-4.11	118.73	132.83
38	QJ	502	GDP	PA-O3A-PB	-4.11	118.74	132.83
36	CC	501	GTP	PB-O3B-PG	-4.10	118.74	132.83
38	LB	502	GDP	PA-O3A-PB	-4.10	118.74	132.83
38	PH	502	GDP	PA-O3A-PB	-4.10	118.77	132.83
38	MN	502	GDP	PA-O3A-PB	-4.10	118.77	132.83
36	WG	501	GTP	PA-O3A-PB	-4.09	118.78	132.83
36	DI	501	GTP	PB-O3B-PG	-4.09	118.79	132.83
38	OH	502	GDP	PA-O3A-PB	-4.09	118.80	132.83
38	AL	502	GDP	PA-O3A-PB	-4.08	118.82	132.83
38	PJ	502	GDP	PA-O3A-PB	-4.07	118.84	132.83
38	ON	502	GDP	PA-O3A-PB	-4.07	118.85	132.83
38	NJ	502	GDP	PA-O3A-PB	-4.06	118.90	132.83
36	DK	501	GTP	PA-O3A-PB	-4.05	118.91	132.83
38	IJ	502	GDP	PA-O3A-PB	-4.05	118.91	132.83
36	OC	501	GTP	PA-O3A-PB	-4.05	118.92	132.83
36	JG	501	GTP	PB-O3B-PG	-4.04	118.95	132.83
38	OL	502	GDP	PA-O3A-PB	-4.04	118.96	132.83
38	KL	502	GDP	PA-O3A-PB	-4.04	118.97	132.83
38	HL	502	GDP	PA-O3A-PB	-4.03	118.98	132.83
38	VJ	502	GDP	PA-O3A-PB	-4.03	119.00	132.83
36	WK	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
36	OO	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
38	LD	502	GDP	PA-O3A-PB	-4.02	119.03	132.83
36	DI	501	GTP	PA-O3A-PB	-4.02	119.03	132.83
38	BD	502	GDP	PA-O3A-PB	-4.01	119.06	132.83
38	HD	502	GDP	PA-O3A-PB	-4.01	119.06	132.83
38	HJ	502	GDP	PA-O3A-PB	-3.99	119.12	132.83
38	OJ	502	GDP	PA-O3A-PB	-3.99	119.13	132.83
36	II	501	GTP	PB-O3B-PG	-3.99	119.14	132.83
36	JI	501	GTP	PB-O3B-PG	-3.98	119.16	132.83
38	PL	502	GDP	PA-O3A-PB	-3.98	119.17	132.83
36	IK	501	GTP	PB-O3B-PG	-3.98	119.19	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	QL	502	GDP	PA-O3A-PB	-3.97	119.19	132.83
38	UF	502	GDP	PA-O3A-PB	-3.97	119.20	132.83
38	KJ	502	GDP	PA-O3A-PB	-3.97	119.21	132.83
38	VN	502	GDP	PA-O3A-PB	-3.97	119.22	132.83
36	QE	501	GTP	PB-O3B-PG	-3.95	119.29	132.83
38	LF	502	GDP	PA-O3A-PB	-3.94	119.29	132.83
36	DC	501	GTP	PB-O3B-PG	-3.94	119.30	132.83
38	CJ	502	GDP	PA-O3A-PB	-3.94	119.32	132.83
38	VP	502	GDP	PA-O3A-PB	-3.93	119.33	132.83
38	MB	502	GDP	PA-O3A-PB	-3.93	119.33	132.83
38	ND	502	GDP	PA-O3A-PB	-3.93	119.34	132.83
36	OI	501	GTP	PA-O3A-PB	-3.93	119.35	132.83
38	IL	502	GDP	PA-O3A-PB	-3.93	119.35	132.83
38	QF	502	GDP	PA-O3A-PB	-3.92	119.36	132.83
38	HF	502	GDP	PA-O3A-PB	-3.92	119.36	132.83
38	PN	502	GDP	PA-O3A-PB	-3.91	119.39	132.83
38	WL	502	GDP	PA-O3A-PB	-3.91	119.40	132.83
38	VL	502	GDP	PA-O3A-PB	-3.91	119.40	132.83
38	ID	502	GDP	PA-O3A-PB	-3.91	119.40	132.83
36	HI	501	GTP	PA-O3A-PB	-3.91	119.41	132.83
38	UN	502	GDP	PA-O3A-PB	-3.90	119.43	132.83
38	IN	502	GDP	PA-O3A-PB	-3.90	119.44	132.83
36	RE	501	GTP	PB-O3B-PG	-3.90	119.45	132.83
38	JH	502	GDP	PA-O3A-PB	-3.90	119.45	132.83
36	KO	501	GTP	PB-O3B-PG	-3.89	119.49	132.83
38	PF	502	GDP	PA-O3A-PB	-3.88	119.51	132.83
38	QH	502	GDP	PA-O3A-PB	-3.87	119.53	132.83
36	UE	501	GTP	PB-O3B-PG	-3.87	119.56	132.83
36	QG	501	GTP	PB-O3B-PG	-3.86	119.59	132.83
36	DK	501	GTP	PB-O3B-PG	-3.86	119.59	132.83
38	UH	502	GDP	PA-O3A-PB	-3.85	119.60	132.83
36	PM	501	GTP	PB-O3B-PG	-3.85	119.61	132.83
36	QO	501	GTP	PB-O3B-PG	-3.85	119.61	132.83
36	IO	501	GTP	PA-O3A-PB	-3.85	119.63	132.83
38	GH	502	GDP	PA-O3A-PB	-3.84	119.64	132.83
38	JD	502	GDP	PA-O3A-PB	-3.84	119.66	132.83
36	CK	501	GTP	PB-O3B-PG	-3.83	119.68	132.83
38	JL	502	GDP	PA-O3A-PB	-3.83	119.68	132.83
38	UP	502	GDP	PA-O3A-PB	-3.83	119.70	132.83
38	CH	502	GDP	PA-O3A-PB	-3.81	119.75	132.83
38	IB	502	GDP	PA-O3A-PB	-3.81	119.77	132.83
38	WP	502	GDP	PA-O3A-PB	-3.81	119.77	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	KM	501	GTP	PB-O3B-PG	-3.80	119.79	132.83
38	UL	502	GDP	PA-O3A-PB	-3.79	119.83	132.83
36	UG	501	GTP	PA-O3A-PB	-3.78	119.84	132.83
38	IF	502	GDP	PA-O3A-PB	-3.78	119.85	132.83
36	CM	501	GTP	PB-O3B-PG	-3.78	119.85	132.83
36	CI	501	GTP	PA-O3A-PB	-3.78	119.86	132.83
38	IH	502	GDP	PA-O3A-PB	-3.78	119.86	132.83
36	DG	501	GTP	PB-O3B-PG	-3.77	119.87	132.83
36	HK	501	GTP	PB-O3B-PG	-3.77	119.88	132.83
38	VF	502	GDP	PA-O3A-PB	-3.77	119.88	132.83
36	CG	501	GTP	PB-O3B-PG	-3.77	119.89	132.83
38	JB	502	GDP	PA-O3A-PB	-3.77	119.89	132.83
36	PG	501	GTP	PB-O3B-PG	-3.77	119.90	132.83
38	SL	502	GDP	PA-O3A-PB	-3.76	119.91	132.83
38	RD	502	GDP	PA-O3A-PB	-3.76	119.91	132.83
38	CF	502	GDP	PA-O3A-PB	-3.76	119.93	132.83
38	KD	502	GDP	PA-O3A-PB	-3.76	119.94	132.83
36	JM	501	GTP	PB-O3B-PG	-3.76	119.94	132.83
36	UK	501	GTP	PA-O3A-PB	-3.75	119.95	132.83
38	VD	502	GDP	PA-O3A-PB	-3.75	119.97	132.83
38	JJ	502	GDP	PA-O3A-PB	-3.74	119.98	132.83
36	GI	501	GTP	PA-O3A-PB	-3.74	119.99	132.83
36	WI	501	GTP	PB-O3B-PG	-3.74	119.99	132.83
36	QI	501	GTP	PB-O3B-PG	-3.74	120.00	132.83
36	VK	501	GTP	PB-O3B-PG	-3.73	120.01	132.83
36	VG	501	GTP	PB-O3B-PG	-3.73	120.02	132.83
38	CD	502	GDP	PA-O3A-PB	-3.73	120.02	132.83
38	KH	502	GDP	PA-O3A-PB	-3.73	120.02	132.83
38	TD	502	GDP	PA-O3A-PB	-3.73	120.03	132.83
36	HG	501	GTP	PB-O3B-PG	-3.73	120.03	132.83
36	IE	501	GTP	PB-O3B-PG	-3.73	120.03	132.83
36	EC	501	GTP	PB-O3B-PG	-3.73	120.04	132.83
38	DJ	502	GDP	PA-O3A-PB	-3.72	120.06	132.83
38	CL	502	GDP	PA-O3A-PB	-3.72	120.06	132.83
36	DG	501	GTP	PA-O3A-PB	-3.72	120.06	132.83
36	JC	501	GTP	PB-O3B-PG	-3.72	120.07	132.83
38	FB	502	GDP	PA-O3A-PB	-3.72	120.07	132.83
36	UK	501	GTP	PB-O3B-PG	-3.72	120.08	132.83
38	RN	502	GDP	PA-O3A-PB	-3.71	120.10	132.83
36	KK	501	GTP	PB-O3B-PG	-3.71	120.11	132.83
36	TG	501	GTP	PB-O3B-PG	-3.71	120.11	132.83
36	EK	501	GTP	PB-O3B-PG	-3.71	120.11	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	OK	501	GTP	PB-O3B-PG	-3.69	120.15	132.83
36	KG	501	GTP	PB-O3B-PG	-3.69	120.17	132.83
36	EM	501	GTP	PB-O3B-PG	-3.69	120.17	132.83
38	MJ	502	GDP	PA-O3A-PB	-3.69	120.17	132.83
36	IO	501	GTP	PB-O3B-PG	-3.68	120.18	132.83
36	RI	501	GTP	PA-O3A-PB	-3.68	120.21	132.83
36	BM	501	GTP	PA-O3A-PB	-3.68	120.21	132.83
36	HO	501	GTP	PB-O3B-PG	-3.68	120.22	132.83
38	FD	502	GDP	PA-O3A-PB	-3.67	120.25	132.83
38	WF	502	GDP	PA-O3A-PB	-3.66	120.26	132.83
38	TP	502	GDP	PA-O3A-PB	-3.66	120.26	132.83
36	QO	501	GTP	PA-O3A-PB	-3.66	120.27	132.83
36	IM	501	GTP	PB-O3B-PG	-3.66	120.27	132.83
38	WN	502	GDP	PA-O3A-PB	-3.66	120.27	132.83
38	GD	502	GDP	PA-O3A-PB	-3.66	120.28	132.83
36	JK	501	GTP	PB-O3B-PG	-3.65	120.29	132.83
38	HN	502	GDP	PA-O3A-PB	-3.65	120.30	132.83
36	PC	501	GTP	PB-O3B-PG	-3.65	120.30	132.83
36	OM	501	GTP	PB-O3B-PG	-3.65	120.30	132.83
36	JI	501	GTP	PA-O3A-PB	-3.65	120.31	132.83
36	RK	501	GTP	PB-O3B-PG	-3.65	120.31	132.83
36	EE	501	GTP	PB-O3B-PG	-3.65	120.31	132.83
38	GN	502	GDP	PA-O3A-PB	-3.65	120.31	132.83
38	VH	502	GDP	PA-O3A-PB	-3.64	120.33	132.83
38	MF	502	GDP	PA-O3A-PB	-3.64	120.35	132.83
36	NG	501	GTP	PA-O3A-PB	-3.63	120.35	132.83
36	NI	501	GTP	PA-O3A-PB	-3.63	120.36	132.83
36	UG	501	GTP	PB-O3B-PG	-3.63	120.38	132.83
36	VE	501	GTP	PA-O3A-PB	-3.63	120.39	132.83
36	WI	501	GTP	PA-O3A-PB	-3.62	120.39	132.83
36	LE	501	GTP	PB-O3B-PG	-3.62	120.40	132.83
38	MD	502	GDP	PA-O3A-PB	-3.62	120.41	132.83
36	OO	501	GTP	PA-O3A-PB	-3.62	120.41	132.83
38	WJ	502	GDP	PA-O3A-PB	-3.62	120.42	132.83
36	RK	501	GTP	PA-O3A-PB	-3.61	120.43	132.83
38	GB	502	GDP	PA-O3A-PB	-3.61	120.43	132.83
36	CG	501	GTP	PA-O3A-PB	-3.61	120.43	132.83
38	UD	502	GDP	PA-O3A-PB	-3.61	120.44	132.83
36	VO	501	GTP	PB-O3B-PG	-3.61	120.44	132.83
36	QM	501	GTP	PB-O3B-PG	-3.61	120.44	132.83
36	BC	501	GTP	PA-O3A-PB	-3.61	120.45	132.83
36	VO	501	GTP	PA-O3A-PB	-3.60	120.46	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	JF	502	GDP	PA-O3A-PB	-3.60	120.47	132.83
36	UM	501	GTP	PB-O3B-PG	-3.60	120.47	132.83
36	KC	501	GTP	PB-O3B-PG	-3.60	120.48	132.83
36	BA	501	GTP	PB-O3B-PG	-3.60	120.49	132.83
38	DL	502	GDP	PA-O3A-PB	-3.59	120.52	132.83
36	LI	501	GTP	PB-O3B-PG	-3.59	120.52	132.83
36	VI	501	GTP	PB-O3B-PG	-3.58	120.53	132.83
36	KI	501	GTP	PB-O3B-PG	-3.58	120.54	132.83
36	NK	501	GTP	PA-O3A-PB	-3.58	120.54	132.83
38	RF	502	GDP	PA-O3A-PB	-3.58	120.54	132.83
36	VK	501	GTP	PA-O3A-PB	-3.57	120.56	132.83
38	WH	502	GDP	PA-O3A-PB	-3.57	120.58	132.83
36	AK	501	GTP	PA-O3A-PB	-3.57	120.58	132.83
38	HH	502	GDP	PA-O3A-PB	-3.57	120.58	132.83
36	KO	501	GTP	PA-O3A-PB	-3.57	120.58	132.83
36	II	501	GTP	PA-O3A-PB	-3.56	120.60	132.83
36	RG	501	GTP	PB-O3B-PG	-3.56	120.60	132.83
36	EG	501	GTP	C5-C6-N1	3.56	120.24	113.95
36	BG	501	GTP	PA-O3A-PB	-3.56	120.61	132.83
36	VM	501	GTP	PB-O3B-PG	-3.56	120.62	132.83
38	GF	502	GDP	PA-O3A-PB	-3.56	120.62	132.83
36	RM	501	GTP	PB-O3B-PG	-3.55	120.64	132.83
36	HE	501	GTP	PA-O3A-PB	-3.54	120.67	132.83
36	KI	501	GTP	C5-C6-N1	3.54	120.21	113.95
36	LC	501	GTP	PA-O3A-PB	-3.54	120.67	132.83
36	IK	501	GTP	PA-O3A-PB	-3.54	120.69	132.83
36	EG	501	GTP	PB-O3B-PG	-3.54	120.69	132.83
36	QK	501	GTP	PB-O3B-PG	-3.53	120.70	132.83
36	HM	501	GTP	PA-O3A-PB	-3.53	120.71	132.83
36	RI	501	GTP	C5-C6-N1	3.53	120.19	113.95
36	EI	501	GTP	PB-O3B-PG	-3.53	120.72	132.83
36	PO	501	GTP	PB-O3B-PG	-3.53	120.73	132.83
38	DH	502	GDP	PA-O3A-PB	-3.52	120.73	132.83
38	MH	502	GDP	PA-O3A-PB	-3.52	120.73	132.83
36	NC	501	GTP	PA-O3A-PB	-3.52	120.75	132.83
38	TF	502	GDP	PA-O3A-PB	-3.52	120.75	132.83
38	TN	502	GDP	PA-O3A-PB	-3.51	120.77	132.83
36	AI	501	GTP	C5-C6-N1	3.51	120.16	113.95
36	HE	501	GTP	PB-O3B-PG	-3.51	120.77	132.83
36	KG	501	GTP	C5-C6-N1	3.51	120.15	113.95
36	AE	501	GTP	PA-O3A-PB	-3.51	120.78	132.83
36	UO	501	GTP	PB-O3B-PG	-3.51	120.79	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	CA	501	GTP	PB-O3B-PG	-3.51	120.80	132.83
36	LC	501	GTP	PB-O3B-PG	-3.51	120.80	132.83
38	DF	502	GDP	PA-O3A-PB	-3.50	120.81	132.83
36	NC	501	GTP	PB-O3B-PG	-3.50	120.81	132.83
38	GL	502	GDP	PA-O3A-PB	-3.50	120.82	132.83
36	GM	501	GTP	PB-O3B-PG	-3.50	120.82	132.83
36	GM	501	GTP	PA-O3A-PB	-3.50	120.82	132.83
38	SH	502	GDP	PA-O3A-PB	-3.50	120.82	132.83
38	SJ	502	GDP	PA-O3A-PB	-3.50	120.83	132.83
38	GN	502	GDP	C3'-C2'-C1'	3.49	106.24	100.98
36	PO	501	GTP	PA-O3A-PB	-3.49	120.84	132.83
36	LG	501	GTP	PB-O3B-PG	-3.49	120.84	132.83
36	BK	501	GTP	PA-O3A-PB	-3.49	120.84	132.83
36	RI	501	GTP	PB-O3B-PG	-3.49	120.85	132.83
38	ML	502	GDP	PA-O3A-PB	-3.49	120.86	132.83
38	JN	502	GDP	PA-O3A-PB	-3.49	120.87	132.83
36	AG	501	GTP	PA-O3A-PB	-3.48	120.88	132.83
36	UO	501	GTP	PA-O3A-PB	-3.48	120.88	132.83
36	BI	501	GTP	PA-O3A-PB	-3.48	120.89	132.83
36	MI	501	GTP	PA-O3A-PB	-3.48	120.89	132.83
36	KO	501	GTP	C5-C6-N1	3.48	120.09	113.95
36	PM	501	GTP	PA-O3A-PB	-3.47	120.91	132.83
36	KE	501	GTP	C5-C6-N1	3.47	120.08	113.95
36	MC	501	GTP	PB-O3B-PG	-3.47	120.92	132.83
38	TL	502	GDP	PA-O3A-PB	-3.47	120.92	132.83
36	KK	501	GTP	C5-C6-N1	3.47	120.08	113.95
36	EI	501	GTP	C5-C6-N1	3.47	120.08	113.95
38	TP	502	GDP	C3'-C2'-C1'	3.47	106.20	100.98
38	ED	502	GDP	PA-O3A-PB	-3.47	120.93	132.83
36	JG	501	GTP	PA-O3A-PB	-3.47	120.93	132.83
38	GB	502	GDP	C3'-C2'-C1'	3.47	106.19	100.98
36	LK	501	GTP	PB-O3B-PG	-3.46	120.94	132.83
38	EN	502	GDP	PA-O3A-PB	-3.46	120.94	132.83
36	NE	501	GTP	PA-O3A-PB	-3.46	120.95	132.83
36	WK	501	GTP	PA-O3A-PB	-3.46	120.96	132.83
36	RG	501	GTP	C5-C6-N1	3.46	120.06	113.95
38	TH	502	GDP	PA-O3A-PB	-3.46	120.96	132.83
36	LK	501	GTP	C5-C6-N1	3.46	120.06	113.95
36	SE	501	GTP	C5-C6-N1	3.46	120.06	113.95
36	KE	501	GTP	PA-O3A-PB	-3.45	120.97	132.83
36	GG	501	GTP	PA-O3A-PB	-3.45	120.99	132.83
36	KM	501	GTP	C5-C6-N1	3.45	120.04	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	KK	501	GTP	PA-O3A-PB	-3.45	121.00	132.83
36	ME	501	GTP	C5-C6-N1	3.44	120.03	113.95
38	RJ	502	GDP	PA-O3A-PB	-3.44	121.01	132.83
36	KE	501	GTP	PB-O3B-PG	-3.44	121.02	132.83
36	OE	501	GTP	PA-O3A-PB	-3.44	121.02	132.83
36	BE	501	GTP	PA-O3A-PB	-3.44	121.02	132.83
36	TE	501	GTP	PB-O3B-PG	-3.44	121.03	132.83
36	RC	501	GTP	C5-C6-N1	3.43	120.02	113.95
38	GL	502	GDP	C3'-C2'-C1'	3.43	106.15	100.98
36	IE	501	GTP	PA-O3A-PB	-3.43	121.05	132.83
36	EM	501	GTP	C5-C6-N1	3.43	120.01	113.95
36	QO	501	GTP	C5-C6-N1	3.43	120.01	113.95
38	GJ	502	GDP	PA-O3A-PB	-3.43	121.06	132.83
36	QG	501	GTP	C5-C6-N1	3.43	120.00	113.95
36	CM	501	GTP	PA-O3A-PB	-3.43	121.07	132.83
36	LE	501	GTP	C5-C6-N1	3.42	120.00	113.95
36	DE	501	GTP	C5-C6-N1	3.42	119.99	113.95
36	DM	501	GTP	PA-O3A-PB	-3.42	121.08	132.83
36	NE	501	GTP	PB-O3B-PG	-3.42	121.08	132.83
36	RO	501	GTP	PB-O3B-PG	-3.42	121.09	132.83
38	TD	502	GDP	C3'-C2'-C1'	3.42	106.13	100.98
36	GC	501	GTP	C5-C6-N1	3.42	119.99	113.95
36	EE	501	GTP	C5-C6-N1	3.42	119.99	113.95
36	OI	501	GTP	C5-C6-N1	3.42	119.99	113.95
36	AG	501	GTP	C5-C6-N1	3.42	119.99	113.95
36	DG	501	GTP	C5-C6-N1	3.42	119.99	113.95
36	UE	501	GTP	PA-O3A-PB	-3.42	121.10	132.83
36	BA	501	GTP	PA-O3A-PB	-3.42	121.10	132.83
36	SE	501	GTP	PB-O3B-PG	-3.41	121.12	132.83
38	EB	502	GDP	C3'-C2'-C1'	3.41	106.11	100.98
38	IH	502	GDP	C3'-C2'-C1'	3.41	106.11	100.98
36	BM	501	GTP	C5-C6-N1	3.40	119.96	113.95
38	DD	502	GDP	PA-O3A-PB	-3.40	121.15	132.83
36	MM	501	GTP	PA-O3A-PB	-3.40	121.15	132.83
36	TM	501	GTP	PA-O3A-PB	-3.40	121.16	132.83
36	JE	501	GTP	C5-C6-N1	3.40	119.95	113.95
36	TK	501	GTP	PA-O3A-PB	-3.40	121.16	132.83
36	MK	501	GTP	PB-O3B-PG	-3.40	121.16	132.83
36	AE	501	GTP	C5-C6-N1	3.40	119.95	113.95
36	QI	501	GTP	C5-C6-N1	3.40	119.95	113.95
36	LI	501	GTP	C5-C6-N1	3.40	119.95	113.95
36	OO	501	GTP	C5-C6-N1	3.40	119.95	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	OM	501	GTP	C5-C6-N1	3.39	119.95	113.95
38	RN	502	GDP	C3'-C2'-C1'	3.39	106.09	100.98
36	BK	501	GTP	C5-C6-N1	3.39	119.94	113.95
36	QK	501	GTP	C5-C6-N1	3.39	119.94	113.95
36	VE	501	GTP	PB-O3B-PG	-3.39	121.19	132.83
38	NB	502	GDP	C3'-C2'-C1'	3.39	106.08	100.98
36	JM	501	GTP	C5-C6-N1	3.39	119.94	113.95
38	MB	502	GDP	C3'-C2'-C1'	3.39	106.08	100.98
36	AC	501	GTP	PA-O3A-PB	-3.39	121.20	132.83
36	BC	501	GTP	PB-O3B-PG	-3.39	121.21	132.83
38	AJ	502	GDP	C3'-C2'-C1'	3.39	106.08	100.98
36	WO	501	GTP	C5-C6-N1	3.38	119.93	113.95
36	OE	501	GTP	C5-C6-N1	3.38	119.93	113.95
36	PC	501	GTP	C5-C6-N1	3.38	119.93	113.95
38	UD	502	GDP	C3'-C2'-C1'	3.38	106.07	100.98
38	FN	502	GDP	C3'-C2'-C1'	3.38	106.07	100.98
38	FF	502	GDP	C3'-C2'-C1'	3.38	106.06	100.98
36	KC	501	GTP	C5-C6-N1	3.38	119.92	113.95
36	JM	501	GTP	PA-O3A-PB	-3.38	121.24	132.83
36	JI	501	GTP	C5-C6-N1	3.38	119.91	113.95
38	FF	502	GDP	PA-O3A-PB	-3.37	121.25	132.83
36	LM	501	GTP	C5-C6-N1	3.37	119.91	113.95
38	TJ	502	GDP	PA-O3A-PB	-3.37	121.26	132.83
36	NK	501	GTP	PB-O3B-PG	-3.37	121.26	132.83
38	FL	502	GDP	PA-O3A-PB	-3.37	121.26	132.83
36	MI	501	GTP	C5-C6-N1	3.37	119.90	113.95
36	JE	501	GTP	PB-O3B-PG	-3.37	121.27	132.83
36	LG	501	GTP	C5-C6-N1	3.37	119.90	113.95
36	LC	501	GTP	C5-C6-N1	3.37	119.90	113.95
36	MK	501	GTP	C5-C6-N1	3.37	119.90	113.95
36	CK	501	GTP	C5-C6-N1	3.36	119.89	113.95
36	JG	501	GTP	C5-C6-N1	3.36	119.89	113.95
36	MG	501	GTP	PB-O3B-PG	-3.36	121.28	132.83
36	MM	501	GTP	C5-C6-N1	3.36	119.89	113.95
36	EC	501	GTP	C5-C6-N1	3.36	119.89	113.95
36	PO	501	GTP	C5-C6-N1	3.36	119.88	113.95
36	QC	501	GTP	C5-C6-N1	3.36	119.88	113.95
36	RE	501	GTP	C5-C6-N1	3.36	119.88	113.95
38	EH	502	GDP	PA-O3A-PB	-3.36	121.31	132.83
36	RO	501	GTP	C5-C6-N1	3.36	119.88	113.95
36	UM	501	GTP	C5-C6-N1	3.36	119.88	113.95
36	AM	501	GTP	C5-C6-N1	3.36	119.88	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	MG	501	GTP	C5-C6-N1	3.35	119.88	113.95
36	MK	501	GTP	PA-O3A-PB	-3.35	121.32	132.83
38	RJ	502	GDP	C3'-C2'-C1'	3.35	106.02	100.98
36	CA	501	GTP	C5-C6-N1	3.35	119.87	113.95
36	NG	501	GTP	C5-C6-N1	3.35	119.87	113.95
36	BM	501	GTP	PB-O3B-PG	-3.35	121.33	132.83
36	RM	501	GTP	C5-C6-N1	3.35	119.86	113.95
36	OC	501	GTP	C5-C6-N1	3.35	119.86	113.95
36	NI	501	GTP	C5-C6-N1	3.35	119.86	113.95
36	MC	501	GTP	C5-C6-N1	3.35	119.86	113.95
36	DA	501	GTP	PB-O3B-PG	-3.34	121.35	132.83
38	DB	502	GDP	C3'-C2'-C1'	3.34	106.01	100.98
36	PG	501	GTP	C5-C6-N1	3.34	119.86	113.95
38	RL	502	GDP	PA-O3A-PB	-3.34	121.36	132.83
36	TK	501	GTP	PB-O3B-PG	-3.34	121.36	132.83
36	RK	501	GTP	C5-C6-N1	3.34	119.85	113.95
36	OK	501	GTP	C5-C6-N1	3.34	119.85	113.95
36	NM	501	GTP	PA-O3A-PB	-3.34	121.36	132.83
36	AC	501	GTP	C5-C6-N1	3.34	119.85	113.95
36	BC	501	GTP	C5-C6-N1	3.34	119.85	113.95
38	EB	502	GDP	PA-O3A-PB	-3.34	121.37	132.83
36	BA	501	GTP	C5-C6-N1	3.34	119.84	113.95
36	BE	501	GTP	C5-C6-N1	3.34	119.84	113.95
36	AA	501	GTP	C5-C6-N1	3.34	119.84	113.95
36	EK	501	GTP	C5-C6-N1	3.34	119.84	113.95
38	NN	502	GDP	C3'-C2'-C1'	3.33	106.00	100.98
36	TO	501	GTP	PA-O3A-PB	-3.33	121.39	132.83
38	LH	502	GDP	PA-O3A-PB	-3.33	121.39	132.83
38	SN	502	GDP	PA-O3A-PB	-3.33	121.39	132.83
36	IG	501	GTP	PA-O3A-PB	-3.33	121.39	132.83
36	RM	501	GTP	PA-O3A-PB	-3.33	121.40	132.83
36	VG	501	GTP	C5-C6-N1	3.33	119.83	113.95
36	UE	501	GTP	C5-C6-N1	3.33	119.83	113.95
36	QM	501	GTP	C5-C6-N1	3.33	119.83	113.95
38	SD	502	GDP	PA-O3A-PB	-3.33	121.41	132.83
38	SD	502	GDP	C3'-C2'-C1'	3.33	105.98	100.98
38	TL	502	GDP	C3'-C2'-C1'	3.33	105.98	100.98
36	QE	501	GTP	C5-C6-N1	3.33	119.82	113.95
36	TG	501	GTP	PA-O3A-PB	-3.32	121.42	132.83
36	JC	501	GTP	C5-C6-N1	3.32	119.82	113.95
36	WI	501	GTP	C5-C6-N1	3.32	119.82	113.95
36	UO	501	GTP	C5-C6-N1	3.32	119.82	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BG	501	GTP	PB-O3B-PG	-3.32	121.42	132.83
36	TO	501	GTP	C5-C6-N1	3.32	119.82	113.95
36	VE	501	GTP	C5-C6-N1	3.32	119.82	113.95
36	BI	501	GTP	C5-C6-N1	3.32	119.81	113.95
36	OG	501	GTP	C5-C6-N1	3.32	119.81	113.95
36	DC	501	GTP	C5-C6-N1	3.32	119.81	113.95
36	IE	501	GTP	C5-C6-N1	3.32	119.81	113.95
36	CE	501	GTP	C5-C6-N1	3.31	119.81	113.95
36	PK	501	GTP	C5-C6-N1	3.31	119.80	113.95
36	CM	501	GTP	C5-C6-N1	3.31	119.80	113.95
36	HG	501	GTP	C5-C6-N1	3.31	119.80	113.95
36	NC	501	GTP	C5-C6-N1	3.31	119.80	113.95
36	DA	501	GTP	C5-C6-N1	3.31	119.80	113.95
36	JK	501	GTP	C5-C6-N1	3.31	119.79	113.95
36	WM	501	GTP	PB-O3B-PG	-3.31	121.47	132.83
36	NE	501	GTP	C5-C6-N1	3.31	119.79	113.95
36	PI	501	GTP	C5-C6-N1	3.31	119.79	113.95
36	AA	501	GTP	PA-O3A-PB	-3.31	121.48	132.83
38	KN	502	GDP	C3'-C2'-C1'	3.31	105.96	100.98
36	WG	501	GTP	C5-C6-N1	3.30	119.79	113.95
38	BJ	502	GDP	C3'-C2'-C1'	3.30	105.95	100.98
36	WK	501	GTP	C5-C6-N1	3.30	119.78	113.95
36	AK	501	GTP	C5-C6-N1	3.30	119.78	113.95
36	CI	501	GTP	C5-C6-N1	3.30	119.78	113.95
36	AM	501	GTP	PA-O3A-PB	-3.30	121.51	132.83
36	MI	501	GTP	PB-O3B-PG	-3.30	121.51	132.83
36	PE	501	GTP	C5-C6-N1	3.30	119.77	113.95
36	VK	501	GTP	C5-C6-N1	3.30	119.77	113.95
36	FE	501	GTP	C5-C6-N1	3.30	119.77	113.95
36	RE	501	GTP	PA-O3A-PB	-3.30	121.51	132.83
36	FK	501	GTP	C5-C6-N1	3.30	119.77	113.95
36	PM	501	GTP	C5-C6-N1	3.29	119.77	113.95
36	PE	501	GTP	PA-O3A-PB	-3.29	121.53	132.83
38	UH	502	GDP	C3'-C2'-C1'	3.29	105.93	100.98
36	HO	501	GTP	C5-C6-N1	3.29	119.76	113.95
36	UG	501	GTP	C5-C6-N1	3.29	119.76	113.95
36	GI	501	GTP	C5-C6-N1	3.29	119.75	113.95
36	II	501	GTP	C5-C6-N1	3.28	119.75	113.95
36	HK	501	GTP	PA-O3A-PB	-3.28	121.56	132.83
38	GD	502	GDP	C3'-C2'-C1'	3.28	105.92	100.98
36	BE	501	GTP	PB-O3B-PG	-3.28	121.56	132.83
36	BI	501	GTP	PB-O3B-PG	-3.28	121.57	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	IC	501	GTP	PB-O3B-PG	-3.28	121.57	132.83
36	UI	501	GTP	C5-C6-N1	3.28	119.74	113.95
36	QI	501	GTP	PA-O3A-PB	-3.28	121.59	132.83
36	NM	501	GTP	C5-C6-N1	3.27	119.73	113.95
36	IO	501	GTP	C5-C6-N1	3.27	119.73	113.95
38	HN	502	GDP	C3'-C2'-C1'	3.27	105.91	100.98
36	IC	501	GTP	C5-C6-N1	3.27	119.73	113.95
38	FH	502	GDP	PA-O3A-PB	-3.27	121.60	132.83
36	TK	501	GTP	C5-C6-N1	3.27	119.73	113.95
36	TG	501	GTP	C5-C6-N1	3.27	119.73	113.95
36	FC	501	GTP	C5-C6-N1	3.27	119.72	113.95
36	KM	501	GTP	PA-O3A-PB	-3.27	121.62	132.83
36	SO	501	GTP	C5-C6-N1	3.26	119.72	113.95
38	IB	502	GDP	C3'-C2'-C1'	3.26	105.89	100.98
36	CC	501	GTP	C5-C6-N1	3.26	119.71	113.95
38	CB	502	GDP	C3'-C2'-C1'	3.26	105.89	100.98
36	SG	501	GTP	C5-C6-N1	3.26	119.71	113.95
36	FG	501	GTP	C8-N7-C5	3.26	109.20	102.99
38	VJ	502	GDP	C3'-C2'-C1'	3.26	105.88	100.98
36	HI	501	GTP	C5-C6-N1	3.26	119.70	113.95
36	VI	501	GTP	PA-O3A-PB	-3.26	121.65	132.83
38	EL	502	GDP	PA-O3A-PB	-3.26	121.65	132.83
36	GE	501	GTP	C5-C6-N1	3.26	119.70	113.95
36	GE	501	GTP	PB-O3B-PG	-3.26	121.66	132.83
36	WM	501	GTP	C5-C6-N1	3.25	119.70	113.95
36	PG	501	GTP	PA-O3A-PB	-3.25	121.67	132.83
36	VI	501	GTP	C5-C6-N1	3.25	119.69	113.95
38	KB	502	GDP	C3'-C2'-C1'	3.25	105.87	100.98
36	TE	501	GTP	C5-C6-N1	3.25	119.69	113.95
36	DK	501	GTP	C5-C6-N1	3.25	119.69	113.95
36	DE	501	GTP	PB-O3B-PG	-3.25	121.68	132.83
36	CG	501	GTP	C5-C6-N1	3.25	119.69	113.95
38	NF	502	GDP	C3'-C2'-C1'	3.25	105.87	100.98
38	RH	502	GDP	PA-O3A-PB	-3.25	121.69	132.83
36	NK	501	GTP	C5-C6-N1	3.25	119.68	113.95
38	VL	502	GDP	C3'-C2'-C1'	3.25	105.86	100.98
36	DM	501	GTP	C5-C6-N1	3.24	119.68	113.95
36	RC	501	GTP	PB-O3B-PG	-3.24	121.70	132.83
36	DI	501	GTP	C5-C6-N1	3.24	119.68	113.95
38	EJ	502	GDP	PA-O3A-PB	-3.24	121.71	132.83
36	CA	501	GTP	PA-O3A-PB	-3.24	121.71	132.83
36	WO	501	GTP	PA-O3A-PB	-3.24	121.71	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	UK	501	GTP	C5-C6-N1	3.24	119.67	113.95
36	HE	501	GTP	C5-C6-N1	3.24	119.67	113.95
36	FI	501	GTP	PB-O3B-PG	-3.24	121.72	132.83
36	WE	501	GTP	PA-O3A-PB	-3.23	121.73	132.83
36	VM	501	GTP	C5-C6-N1	3.23	119.66	113.95
36	SG	501	GTP	PB-O3B-PG	-3.23	121.74	132.83
38	CJ	502	GDP	C3'-C2'-C1'	3.23	105.84	100.98
36	HM	501	GTP	C5-C6-N1	3.23	119.65	113.95
36	HC	501	GTP	C5-C6-N1	3.23	119.65	113.95
38	HF	502	GDP	C3'-C2'-C1'	3.23	105.84	100.98
36	KI	501	GTP	C2-N1-C6	-3.23	119.16	125.10
36	GK	501	GTP	PA-O3A-PB	-3.23	121.76	132.83
38	IL	502	GDP	C3'-C2'-C1'	3.23	105.83	100.98
36	HG	501	GTP	PA-O3A-PB	-3.22	121.76	132.83
36	SM	501	GTP	C5-C6-N1	3.22	119.64	113.95
36	VO	501	GTP	C5-C6-N1	3.22	119.64	113.95
36	HK	501	GTP	C5-C6-N1	3.22	119.64	113.95
38	EN	502	GDP	C3'-C2'-C1'	3.22	105.83	100.98
36	GK	501	GTP	C5-C6-N1	3.22	119.64	113.95
36	BG	501	GTP	C5-C6-N1	3.21	119.63	113.95
36	FG	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
36	WE	501	GTP	C5-C6-N1	3.21	119.62	113.95
38	RL	502	GDP	C3'-C2'-C1'	3.21	105.81	100.98
36	FM	501	GTP	PB-O3B-PG	-3.21	121.81	132.83
38	AH	502	GDP	C3'-C2'-C1'	3.21	105.81	100.98
38	ND	502	GDP	C3'-C2'-C1'	3.21	105.81	100.98
36	SM	501	GTP	PB-O3B-PG	-3.21	121.82	132.83
38	WD	502	GDP	C3'-C2'-C1'	3.21	105.80	100.98
38	IJ	502	GDP	C3'-C2'-C1'	3.20	105.80	100.98
36	IK	501	GTP	C5-C6-N1	3.20	119.60	113.95
36	WI	501	GTP	C3'-C2'-C1'	3.20	105.80	100.98
38	FB	502	GDP	C3'-C2'-C1'	3.20	105.80	100.98
38	BF	502	GDP	C3'-C2'-C1'	3.20	105.79	100.98
38	JN	502	GDP	C3'-C2'-C1'	3.20	105.79	100.98
36	DA	501	GTP	C8-N7-C5	3.19	109.07	102.99
36	WO	501	GTP	C8-N7-C5	3.19	109.07	102.99
38	IN	502	GDP	C3'-C2'-C1'	3.19	105.78	100.98
38	LJ	502	GDP	C3'-C2'-C1'	3.19	105.78	100.98
36	LE	501	GTP	PA-O3A-PB	-3.19	121.89	132.83
38	JD	502	GDP	C3'-C2'-C1'	3.19	105.78	100.98
36	SI	501	GTP	C5-C6-N1	3.19	119.58	113.95
36	FE	501	GTP	PB-O3B-PG	-3.19	121.90	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	WE	501	GTP	C8-N7-C5	3.18	109.06	102.99
36	IG	501	GTP	C5-C6-N1	3.18	119.58	113.95
36	AI	501	GTP	PA-O3A-PB	-3.18	121.90	132.83
38	NJ	502	GDP	C3'-C2'-C1'	3.18	105.77	100.98
38	UF	502	GDP	C3'-C2'-C1'	3.18	105.77	100.98
38	WL	502	GDP	C3'-C2'-C1'	3.18	105.77	100.98
36	GM	501	GTP	C5-C6-N1	3.18	119.57	113.95
38	JB	502	GDP	C3'-C2'-C1'	3.18	105.76	100.98
38	TH	502	GDP	C3'-C2'-C1'	3.18	105.76	100.98
36	FM	501	GTP	C5-C6-N1	3.18	119.56	113.95
38	CL	502	GDP	C3'-C2'-C1'	3.17	105.76	100.98
36	FE	501	GTP	PA-O3A-PB	-3.17	121.94	132.83
36	FG	501	GTP	PB-O3B-PG	-3.17	121.94	132.83
36	SK	501	GTP	PB-O3B-PG	-3.17	121.94	132.83
36	LE	501	GTP	C2-N1-C6	-3.17	119.26	125.10
36	OE	501	GTP	PB-O3B-PG	-3.17	121.95	132.83
36	TM	501	GTP	C5-C6-N1	3.17	119.55	113.95
36	LK	501	GTP	PA-O3A-PB	-3.17	121.96	132.83
36	CC	501	GTP	PA-O3A-PB	-3.17	121.96	132.83
38	HL	502	GDP	C3'-C2'-C1'	3.16	105.74	100.98
36	DC	501	GTP	PA-O3A-PB	-3.16	121.97	132.83
36	EG	501	GTP	C2-N1-C6	-3.16	119.27	125.10
38	FJ	502	GDP	PA-O3A-PB	-3.16	121.98	132.83
36	II	501	GTP	C3'-C2'-C1'	3.16	105.74	100.98
38	AL	502	GDP	C3'-C2'-C1'	3.16	105.73	100.98
36	GG	501	GTP	C5-C6-N1	3.16	119.53	113.95
36	OG	501	GTP	PB-O3B-PG	-3.16	121.99	132.83
38	BH	502	GDP	C3'-C2'-C1'	3.16	105.73	100.98
36	MM	501	GTP	PB-O3B-PG	-3.16	121.99	132.83
36	IG	501	GTP	C8-N7-C5	3.16	109.00	102.99
38	UL	502	GDP	C3'-C2'-C1'	3.16	105.73	100.98
38	UP	502	GDP	C3'-C2'-C1'	3.16	105.73	100.98
36	KO	501	GTP	C2-N1-C6	-3.16	119.29	125.10
36	WG	501	GTP	C8-N7-C5	3.15	109.00	102.99
36	MG	501	GTP	PA-O3A-PB	-3.15	122.00	132.83
36	CE	501	GTP	PB-O3B-PG	-3.15	122.01	132.83
36	LG	501	GTP	PA-O3A-PB	-3.15	122.01	132.83
38	WD	502	GDP	PA-O3A-PB	-3.15	122.01	132.83
36	IM	501	GTP	C5-C6-N1	3.15	119.52	113.95
36	FI	501	GTP	C5-C6-N1	3.15	119.51	113.95
38	VD	502	GDP	C3'-C2'-C1'	3.15	105.72	100.98
38	VH	502	GDP	C3'-C2'-C1'	3.15	105.71	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	FG	501	GTP	C5-C6-N1	3.14	119.50	113.95
36	KE	501	GTP	C2-N1-C6	-3.14	119.31	125.10
36	DK	501	GTP	C2-N1-C6	-3.14	119.32	125.10
38	VF	502	GDP	C3'-C2'-C1'	3.14	105.70	100.98
36	PE	501	GTP	PB-O3B-PG	-3.13	122.08	132.83
38	FN	502	GDP	PA-O3A-PB	-3.13	122.08	132.83
36	IC	501	GTP	PA-O3A-PB	-3.13	122.08	132.83
36	EK	501	GTP	PA-O3A-PB	-3.13	122.09	132.83
36	KC	501	GTP	PA-O3A-PB	-3.13	122.09	132.83
36	ME	501	GTP	PA-O3A-PB	-3.13	122.10	132.83
36	CE	501	GTP	C8-N7-C5	3.13	108.94	102.99
38	BB	502	GDP	C3'-C2'-C1'	3.12	105.68	100.98
36	WE	501	GTP	PB-O3B-PG	-3.12	122.10	132.83
36	KM	501	GTP	C2-N1-C6	-3.12	119.34	125.10
38	AB	502	GDP	C3'-C2'-C1'	3.12	105.68	100.98
38	GJ	502	GDP	C3'-C2'-C1'	3.12	105.68	100.98
36	LK	501	GTP	C2-N1-C6	-3.12	119.35	125.10
36	DM	501	GTP	C8-N7-C5	3.12	108.93	102.99
36	PK	501	GTP	PB-O3B-PG	-3.12	122.12	132.83
38	NH	502	GDP	C3'-C2'-C1'	3.12	105.67	100.98
38	VP	502	GDP	C3'-C2'-C1'	3.12	105.67	100.98
36	TI	501	GTP	C5-C6-N1	3.12	119.46	113.95
36	IE	501	GTP	C8-N7-C5	3.12	108.93	102.99
36	IK	501	GTP	C8-N7-C5	3.12	108.93	102.99
36	PC	501	GTP	C8-N7-C5	3.12	108.93	102.99
36	AI	501	GTP	C2-N1-C6	-3.12	119.36	125.10
36	KI	501	GTP	PA-O3A-PB	-3.11	122.14	132.83
38	PL	502	GDP	C3'-C2'-C1'	3.11	105.67	100.98
36	SK	501	GTP	C5-C6-N1	3.11	119.45	113.95
38	EF	502	GDP	PA-O3A-PB	-3.11	122.14	132.83
36	CK	501	GTP	C3'-C2'-C1'	3.11	105.67	100.98
38	OB	502	GDP	C3'-C2'-C1'	3.11	105.67	100.98
36	CA	501	GTP	C8-N7-C5	3.11	108.92	102.99
36	CK	501	GTP	C2-N1-C6	-3.11	119.37	125.10
36	IC	501	GTP	C8-N7-C5	3.11	108.91	102.99
38	EF	502	GDP	C3'-C2'-C1'	3.11	105.66	100.98
36	PC	501	GTP	C2-N1-C6	-3.11	119.38	125.10
36	MI	501	GTP	C2-N1-C6	-3.11	119.38	125.10
36	SG	501	GTP	C8-N7-C5	3.11	108.91	102.99
36	SK	501	GTP	C8-N7-C5	3.11	108.91	102.99
36	AM	501	GTP	PB-O3B-PG	-3.10	122.17	132.83
36	QC	501	GTP	C8-N7-C5	3.10	108.90	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	CI	501	GTP	C8-N7-C5	3.10	108.90	102.99
36	KG	501	GTP	C2-N1-C6	-3.10	119.39	125.10
36	KK	501	GTP	C2-N1-C6	-3.10	119.39	125.10
38	FD	502	GDP	C3'-C2'-C1'	3.10	105.64	100.98
38	UN	502	GDP	C3'-C2'-C1'	3.10	105.64	100.98
38	RD	502	GDP	C3'-C2'-C1'	3.10	105.64	100.98
36	IM	501	GTP	C8-N7-C5	3.10	108.89	102.99
36	EI	501	GTP	C2-N1-C6	-3.10	119.40	125.10
36	JI	501	GTP	C3'-C2'-C1'	3.10	105.64	100.98
36	OG	501	GTP	PA-O3A-PB	-3.10	122.20	132.83
38	AD	502	GDP	C3'-C2'-C1'	3.10	105.64	100.98
38	ID	502	GDP	C3'-C2'-C1'	3.09	105.64	100.98
36	RI	501	GTP	C2-N1-C6	-3.09	119.40	125.10
36	CM	501	GTP	C8-N7-C5	3.09	108.88	102.99
36	DK	501	GTP	C3'-C2'-C1'	3.09	105.63	100.98
36	GK	501	GTP	C8-N7-C5	3.09	108.88	102.99
36	PO	501	GTP	C8-N7-C5	3.09	108.88	102.99
36	TE	501	GTP	C8-N7-C5	3.09	108.88	102.99
36	IO	501	GTP	C3'-C2'-C1'	3.09	105.63	100.98
36	ME	501	GTP	C8-N7-C5	3.09	108.87	102.99
38	HH	502	GDP	C3'-C2'-C1'	3.09	105.63	100.98
36	DC	501	GTP	C8-N7-C5	3.09	108.87	102.99
36	PE	501	GTP	C8-N7-C5	3.09	108.87	102.99
38	FJ	502	GDP	C3'-C2'-C1'	3.09	105.62	100.98
36	HC	501	GTP	PA-O3A-PB	-3.09	122.24	132.83
36	LI	501	GTP	C2-N1-C6	-3.08	119.42	125.10
36	JE	501	GTP	C2-N1-C6	-3.08	119.42	125.10
36	II	501	GTP	C8-N7-C5	3.08	108.86	102.99
36	RE	501	GTP	C2-N1-C6	-3.08	119.42	125.10
36	TI	501	GTP	PA-O3A-PB	-3.08	122.26	132.83
36	EM	501	GTP	C2-N1-C6	-3.08	119.43	125.10
36	LM	501	GTP	PA-O3A-PB	-3.08	122.27	132.83
38	CD	502	GDP	C3'-C2'-C1'	3.08	105.61	100.98
36	QG	501	GTP	C3'-C2'-C1'	3.08	105.61	100.98
36	LG	501	GTP	C2-N1-C6	-3.08	119.44	125.10
36	FC	501	GTP	PB-O3B-PG	-3.07	122.28	132.83
36	UI	501	GTP	PB-O3B-PG	-3.07	122.28	132.83
36	WO	501	GTP	PB-O3B-PG	-3.07	122.28	132.83
36	OI	501	GTP	C8-N7-C5	3.07	108.84	102.99
36	DK	501	GTP	C8-N7-C5	3.07	108.84	102.99
36	DE	501	GTP	C2-N1-C6	-3.07	119.44	125.10
36	CM	501	GTP	C2-N1-C6	-3.07	119.44	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	KC	501	GTP	C8-N7-C5	3.07	108.84	102.99
36	WI	501	GTP	C8-N7-C5	3.07	108.84	102.99
36	VG	501	GTP	C8-N7-C5	3.07	108.84	102.99
36	FK	501	GTP	C8-N7-C5	3.07	108.83	102.99
36	JE	501	GTP	PA-O3A-PB	-3.07	122.30	132.83
36	VG	501	GTP	C3'-C2'-C1'	3.07	105.59	100.98
38	NL	502	GDP	C3'-C2'-C1'	3.07	105.59	100.98
36	UM	501	GTP	C2-N1-C6	-3.07	119.45	125.10
38	PF	502	GDP	C3'-C2'-C1'	3.07	105.59	100.98
36	ME	501	GTP	C2-N1-C6	-3.07	119.45	125.10
36	RG	501	GTP	C2-N1-C6	-3.06	119.46	125.10
36	JK	501	GTP	C2-N1-C6	-3.06	119.46	125.10
36	LK	501	GTP	C8-N7-C5	3.06	108.82	102.99
36	HI	501	GTP	C8-N7-C5	3.06	108.82	102.99
36	QO	501	GTP	C2-N1-C6	-3.06	119.47	125.10
36	GK	501	GTP	PB-O3B-PG	-3.06	122.34	132.83
36	LC	501	GTP	C8-N7-C5	3.06	108.81	102.99
36	JM	501	GTP	C2-N1-C6	-3.05	119.48	125.10
36	IG	501	GTP	C3'-C2'-C1'	3.05	105.57	100.98
36	CE	501	GTP	PA-O3A-PB	-3.05	122.35	132.83
36	DM	501	GTP	C3'-C2'-C1'	3.05	105.57	100.98
36	HK	501	GTP	C8-N7-C5	3.05	108.80	102.99
36	DG	501	GTP	C8-N7-C5	3.05	108.80	102.99
36	MC	501	GTP	C8-N7-C5	3.05	108.80	102.99
38	VN	502	GDP	C3'-C2'-C1'	3.05	105.57	100.98
36	AC	501	GTP	C8-N7-C5	3.05	108.80	102.99
36	JG	501	GTP	C3'-C2'-C1'	3.05	105.56	100.98
36	WK	501	GTP	C8-N7-C5	3.05	108.79	102.99
36	HM	501	GTP	C8-N7-C5	3.05	108.79	102.99
36	KC	501	GTP	C2-N1-C6	-3.04	119.49	125.10
36	KG	501	GTP	PA-O3A-PB	-3.04	122.38	132.83
36	OC	501	GTP	C8-N7-C5	3.04	108.79	102.99
36	QE	501	GTP	C2-N1-C6	-3.04	119.49	125.10
36	PI	501	GTP	C3'-C2'-C1'	3.04	105.56	100.98
36	JC	501	GTP	C8-N7-C5	3.04	108.78	102.99
38	BL	502	GDP	C3'-C2'-C1'	3.04	105.56	100.98
36	FE	501	GTP	C8-N7-C5	3.04	108.78	102.99
36	CG	501	GTP	C8-N7-C5	3.04	108.78	102.99
36	CK	501	GTP	C8-N7-C5	3.04	108.78	102.99
36	VI	501	GTP	C8-N7-C5	3.04	108.78	102.99
36	AK	501	GTP	C8-N7-C5	3.04	108.78	102.99
36	LE	501	GTP	C8-N7-C5	3.04	108.78	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	DG	501	GTP	C2-N1-C6	-3.04	119.50	125.10
36	SE	501	GTP	C2-N1-C6	-3.04	119.50	125.10
36	OG	501	GTP	C8-N7-C5	3.04	108.78	102.99
36	RM	501	GTP	C8-N7-C5	3.04	108.78	102.99
36	PM	501	GTP	C8-N7-C5	3.04	108.77	102.99
36	DA	501	GTP	C2-N1-C6	-3.04	119.51	125.10
36	OM	501	GTP	C2-N1-C6	-3.04	119.51	125.10
36	MK	501	GTP	C8-N7-C5	3.04	108.77	102.99
36	KI	501	GTP	C8-N7-C5	3.03	108.77	102.99
36	DE	501	GTP	PA-O3A-PB	-3.03	122.42	132.83
36	FC	501	GTP	C8-N7-C5	3.03	108.77	102.99
36	LI	501	GTP	C8-N7-C5	3.03	108.77	102.99
36	RC	501	GTP	C8-N7-C5	3.03	108.77	102.99
36	OK	501	GTP	C8-N7-C5	3.03	108.77	102.99
36	MM	501	GTP	C8-N7-C5	3.03	108.77	102.99
38	GH	502	GDP	C3'-C2'-C1'	3.03	105.54	100.98
38	MJ	502	GDP	C3'-C2'-C1'	3.03	105.54	100.98
36	AG	501	GTP	C2-N1-C6	-3.03	119.52	125.10
38	SJ	502	GDP	C3'-C2'-C1'	3.03	105.54	100.98
36	HG	501	GTP	C8-N7-C5	3.03	108.76	102.99
36	LG	501	GTP	C8-N7-C5	3.03	108.76	102.99
36	DI	501	GTP	C8-N7-C5	3.03	108.76	102.99
36	GE	501	GTP	PA-O3A-PB	-3.03	122.43	132.83
36	VE	501	GTP	C2-N1-C6	-3.03	119.52	125.10
36	DI	501	GTP	C3'-C2'-C1'	3.03	105.54	100.98
36	MI	501	GTP	C8-N7-C5	3.03	108.76	102.99
38	LF	502	GDP	C3'-C2'-C1'	3.03	105.53	100.98
36	LM	501	GTP	C8-N7-C5	3.03	108.75	102.99
36	JI	501	GTP	C2-N1-C6	-3.02	119.53	125.10
36	EG	501	GTP	C3'-C2'-C1'	3.02	105.53	100.98
36	QI	501	GTP	C8-N7-C5	3.02	108.75	102.99
36	NM	501	GTP	C8-N7-C5	3.02	108.75	102.99
36	AM	501	GTP	C8-N7-C5	3.02	108.75	102.99
36	VK	501	GTP	C8-N7-C5	3.02	108.75	102.99
36	CC	501	GTP	C3'-C2'-C1'	3.02	105.53	100.98
36	JK	501	GTP	PA-O3A-PB	-3.02	122.46	132.83
36	TO	501	GTP	C8-N7-C5	3.02	108.75	102.99
36	JM	501	GTP	C3'-C2'-C1'	3.02	105.53	100.98
36	DE	501	GTP	C8-N7-C5	3.02	108.74	102.99
36	SE	501	GTP	C8-N7-C5	3.02	108.74	102.99
36	SO	501	GTP	C8-N7-C5	3.02	108.74	102.99
38	IF	502	GDP	C3'-C2'-C1'	3.02	105.52	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	WM	501	GTP	C8-N7-C5	3.02	108.74	102.99
36	JG	501	GTP	C2-N1-C6	-3.02	119.54	125.10
36	RC	501	GTP	PA-O3A-PB	-3.02	122.48	132.83
36	DC	501	GTP	C2-N1-C6	-3.02	119.55	125.10
36	OC	501	GTP	C2-N1-C6	-3.02	119.55	125.10
36	IM	501	GTP	C3'-C2'-C1'	3.02	105.52	100.98
36	VM	501	GTP	C8-N7-C5	3.01	108.73	102.99
36	QC	501	GTP	C2-N1-C6	-3.01	119.55	125.10
36	CE	501	GTP	C2-N1-C6	-3.01	119.55	125.10
36	KK	501	GTP	C8-N7-C5	3.01	108.73	102.99
36	TG	501	GTP	C8-N7-C5	3.01	108.73	102.99
36	MK	501	GTP	C2-N1-C6	-3.01	119.55	125.10
36	CC	501	GTP	C8-N7-C5	3.01	108.73	102.99
36	KO	501	GTP	C8-N7-C5	3.01	108.73	102.99
36	PI	501	GTP	C8-N7-C5	3.01	108.72	102.99
36	PE	501	GTP	C2-N1-C6	-3.01	119.56	125.10
36	KM	501	GTP	C8-N7-C5	3.01	108.72	102.99
36	SI	501	GTP	C8-N7-C5	3.01	108.72	102.99
38	ED	502	GDP	C3'-C2'-C1'	3.01	105.51	100.98
36	GC	501	GTP	PA-O3A-PB	-3.01	122.50	132.83
36	NG	501	GTP	PB-O3B-PG	-3.00	122.52	132.83
36	FM	501	GTP	C8-N7-C5	3.00	108.71	102.99
36	CC	501	GTP	C2-N1-C6	-3.00	119.57	125.10
36	JC	501	GTP	C2-N1-C6	-3.00	119.57	125.10
36	QM	501	GTP	C2-N1-C6	-3.00	119.57	125.10
36	QM	501	GTP	PA-O3A-PB	-3.00	122.52	132.83
36	BI	501	GTP	C2-N1-C6	-3.00	119.57	125.10
36	FK	501	GTP	PA-O3A-PB	-3.00	122.53	132.83
36	GM	501	GTP	C8-N7-C5	3.00	108.71	102.99
36	JE	501	GTP	C8-N7-C5	3.00	108.71	102.99
36	RE	501	GTP	C3'-C2'-C1'	3.00	105.49	100.98
38	LB	502	GDP	C3'-C2'-C1'	3.00	105.49	100.98
36	AE	501	GTP	C2-N1-C6	-3.00	119.58	125.10
36	PK	501	GTP	C2-N1-C6	-3.00	119.58	125.10
36	TG	501	GTP	C3'-C2'-C1'	3.00	105.49	100.98
36	EC	501	GTP	C2-N1-C6	-3.00	119.58	125.10
36	AE	501	GTP	C8-N7-C5	3.00	108.70	102.99
36	EC	501	GTP	C8-N7-C5	3.00	108.70	102.99
36	RG	501	GTP	C8-N7-C5	3.00	108.70	102.99
36	TM	501	GTP	C8-N7-C5	3.00	108.70	102.99
36	VK	501	GTP	C2-N1-C6	-3.00	119.58	125.10
36	NK	501	GTP	C8-N7-C5	3.00	108.70	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	QO	501	GTP	C8-N7-C5	3.00	108.70	102.99
38	MN	502	GDP	C3'-C2'-C1'	2.99	105.49	100.98
36	LC	501	GTP	C2-N1-C6	-2.99	119.58	125.10
36	MG	501	GTP	C2-N1-C6	-2.99	119.58	125.10
36	HO	501	GTP	PA-O3A-PB	-2.99	122.55	132.83
36	AA	501	GTP	C8-N7-C5	2.99	108.69	102.99
36	GE	501	GTP	C8-N7-C5	2.99	108.69	102.99
36	HI	501	GTP	C3'-C2'-C1'	2.99	105.48	100.98
38	DB	502	GDP	PA-O3A-PB	-2.99	122.57	132.83
36	QG	501	GTP	C2-N1-C6	-2.99	119.59	125.10
38	QJ	502	GDP	C3'-C2'-C1'	2.99	105.48	100.98
38	SL	502	GDP	C3'-C2'-C1'	2.99	105.48	100.98
36	AG	501	GTP	C8-N7-C5	2.99	108.68	102.99
36	UK	501	GTP	C8-N7-C5	2.99	108.68	102.99
36	WI	501	GTP	C2-N1-C6	-2.99	119.60	125.10
36	RG	501	GTP	C3'-C2'-C1'	2.99	105.47	100.98
38	RF	502	GDP	C3'-C2'-C1'	2.99	105.47	100.98
36	DM	501	GTP	C2-N1-C6	-2.99	119.60	125.10
36	WM	501	GTP	C2-N1-C6	-2.99	119.60	125.10
36	KG	501	GTP	C8-N7-C5	2.99	108.68	102.99
36	QK	501	GTP	C2-N1-C6	-2.99	119.60	125.10
36	SM	501	GTP	C8-N7-C5	2.98	108.67	102.99
36	VO	501	GTP	C8-N7-C5	2.98	108.67	102.99
36	VG	501	GTP	C2-N1-C6	-2.98	119.61	125.10
36	MC	501	GTP	C2-N1-C6	-2.98	119.61	125.10
36	BC	501	GTP	C2-N1-C6	-2.98	119.61	125.10
36	WK	501	GTP	C2-N1-C6	-2.98	119.61	125.10
36	DI	501	GTP	C2-N1-C6	-2.98	119.61	125.10
36	KO	501	GTP	C3'-C2'-C1'	2.98	105.46	100.98
36	OK	501	GTP	C2-N1-C6	-2.98	119.61	125.10
36	HE	501	GTP	C8-N7-C5	2.98	108.66	102.99
36	OE	501	GTP	C8-N7-C5	2.98	108.66	102.99
36	PG	501	GTP	C8-N7-C5	2.98	108.66	102.99
36	IC	501	GTP	C2-N1-C6	-2.98	119.61	125.10
36	WG	501	GTP	C2-N1-C6	-2.98	119.61	125.10
36	FI	501	GTP	C8-N7-C5	2.98	108.66	102.99
36	EE	501	GTP	C8-N7-C5	2.98	108.66	102.99
36	QG	501	GTP	C8-N7-C5	2.98	108.66	102.99
36	QK	501	GTP	C8-N7-C5	2.97	108.66	102.99
36	RC	501	GTP	C2-N1-C6	-2.97	119.62	125.10
36	RO	501	GTP	C8-N7-C5	2.97	108.66	102.99
36	RK	501	GTP	C2-N1-C6	-2.97	119.62	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	GI	501	GTP	C2-N1-C6	-2.97	119.62	125.10
36	HO	501	GTP	C8-N7-C5	2.97	108.65	102.99
36	EE	501	GTP	C2-N1-C6	-2.97	119.62	125.10
38	HD	502	GDP	C3'-C2'-C1'	2.97	105.45	100.98
36	CA	501	GTP	C2-N1-C6	-2.97	119.63	125.10
36	MG	501	GTP	C8-N7-C5	2.97	108.65	102.99
36	TK	501	GTP	C8-N7-C5	2.97	108.65	102.99
36	UG	501	GTP	C8-N7-C5	2.97	108.65	102.99
36	EK	501	GTP	C2-N1-C6	-2.97	119.63	125.10
36	QI	501	GTP	C2-N1-C6	-2.97	119.63	125.10
38	HB	502	GDP	C3'-C2'-C1'	2.97	105.45	100.98
36	AI	501	GTP	C8-N7-C5	2.97	108.64	102.99
36	EM	501	GTP	PA-O3A-PB	-2.97	122.65	132.83
36	MM	501	GTP	C2-N1-C6	-2.97	119.64	125.10
36	DE	501	GTP	C3'-C2'-C1'	2.97	105.44	100.98
38	WH	502	GDP	C3'-C2'-C1'	2.97	105.44	100.98
36	LM	501	GTP	C2-N1-C6	-2.97	119.64	125.10
36	PG	501	GTP	C2-N1-C6	-2.97	119.64	125.10
36	JG	501	GTP	C8-N7-C5	2.96	108.64	102.99
36	PO	501	GTP	C2-N1-C6	-2.96	119.64	125.10
36	NI	501	GTP	C8-N7-C5	2.96	108.63	102.99
38	FH	502	GDP	C3'-C2'-C1'	2.96	105.44	100.98
36	VE	501	GTP	C8-N7-C5	2.96	108.63	102.99
36	IO	501	GTP	C8-N7-C5	2.96	108.63	102.99
36	NE	501	GTP	C8-N7-C5	2.96	108.63	102.99
36	JC	501	GTP	C3'-C2'-C1'	2.96	105.43	100.98
36	KE	501	GTP	C8-N7-C5	2.96	108.63	102.99
36	QM	501	GTP	C8-N7-C5	2.96	108.62	102.99
36	OI	501	GTP	C2-N1-C6	-2.96	119.66	125.10
36	TI	501	GTP	C8-N7-C5	2.95	108.62	102.99
36	UI	501	GTP	PA-O3A-PB	-2.95	122.69	132.83
36	BA	501	GTP	C8-N7-C5	2.95	108.62	102.99
36	SO	501	GTP	C2-N1-C6	-2.95	119.66	125.10
36	BI	501	GTP	C8-N7-C5	2.95	108.61	102.99
36	TO	501	GTP	C2-N1-C6	-2.95	119.66	125.10
38	MF	502	GDP	C3'-C2'-C1'	2.95	105.42	100.98
36	AM	501	GTP	C2-N1-C6	-2.95	119.66	125.10
36	GI	501	GTP	C8-N7-C5	2.95	108.61	102.99
36	OO	501	GTP	C2-N1-C6	-2.95	119.67	125.10
36	EG	501	GTP	C8-N7-C5	2.95	108.60	102.99
36	HC	501	GTP	C8-N7-C5	2.95	108.60	102.99
36	PK	501	GTP	C8-N7-C5	2.94	108.60	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	RO	501	GTP	C2-N1-C6	-2.94	119.68	125.10
36	UE	501	GTP	C2-N1-C6	-2.94	119.68	125.10
36	WO	501	GTP	C2-N1-C6	-2.94	119.68	125.10
36	OI	501	GTP	C3'-C2'-C1'	2.94	105.41	100.98
36	KG	501	GTP	C3'-C2'-C1'	2.94	105.40	100.98
36	OE	501	GTP	C2-N1-C6	-2.94	119.69	125.10
36	IG	501	GTP	C2-N1-C6	-2.94	119.69	125.10
36	TE	501	GTP	C2-N1-C6	-2.94	119.69	125.10
36	ME	501	GTP	PB-O3B-PG	-2.94	122.75	132.83
36	GK	501	GTP	C2-N1-C6	-2.94	119.69	125.10
36	EM	501	GTP	C3'-C2'-C1'	2.94	105.40	100.98
38	PJ	502	GDP	C3'-C2'-C1'	2.94	105.40	100.98
36	GC	501	GTP	C8-N7-C5	2.94	108.58	102.99
36	UO	501	GTP	C8-N7-C5	2.94	108.58	102.99
36	HI	501	GTP	C2-N1-C6	-2.93	119.69	125.10
36	BK	501	GTP	C8-N7-C5	2.93	108.58	102.99
36	IE	501	GTP	C2-N1-C6	-2.93	119.69	125.10
36	NG	501	GTP	C8-N7-C5	2.93	108.58	102.99
36	AA	501	GTP	C2-N1-C6	-2.93	119.70	125.10
36	UO	501	GTP	C2-N1-C6	-2.93	119.70	125.10
36	VG	501	GTP	PA-O3A-PB	-2.93	122.77	132.83
36	SG	501	GTP	C2-N1-C6	-2.93	119.70	125.10
36	BE	501	GTP	C8-N7-C5	2.93	108.57	102.99
36	UG	501	GTP	C2-N1-C6	-2.93	119.70	125.10
36	BC	501	GTP	C3'-C2'-C1'	2.93	105.39	100.98
38	OD	502	GDP	C3'-C2'-C1'	2.93	105.39	100.98
36	CG	501	GTP	C2-N1-C6	-2.93	119.71	125.10
36	OM	501	GTP	C8-N7-C5	2.93	108.56	102.99
36	II	501	GTP	C2-N1-C6	-2.93	119.71	125.10
36	HO	501	GTP	C2-N1-C6	-2.93	119.71	125.10
36	JK	501	GTP	C3'-C2'-C1'	2.93	105.38	100.98
36	UI	501	GTP	C2-N1-C6	-2.92	119.71	125.10
36	TG	501	GTP	C2-N1-C6	-2.92	119.71	125.10
36	AC	501	GTP	C2-N1-C6	-2.92	119.72	125.10
36	OG	501	GTP	C2-N1-C6	-2.92	119.72	125.10
36	BA	501	GTP	C2-N1-C6	-2.92	119.72	125.10
36	NG	501	GTP	C2-N1-C6	-2.92	119.72	125.10
36	SI	501	GTP	C3'-C2'-C1'	2.92	105.38	100.98
38	QL	502	GDP	C3'-C2'-C1'	2.92	105.38	100.98
36	UM	501	GTP	C8-N7-C5	2.92	108.55	102.99
36	VI	501	GTP	C2-N1-C6	-2.92	119.72	125.10
36	KC	501	GTP	C3'-C2'-C1'	2.92	105.37	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	FK	501	GTP	C2-N1-C6	-2.92	119.72	125.10
36	BE	501	GTP	C2-N1-C6	-2.92	119.72	125.10
38	AF	502	GDP	C3'-C2'-C1'	2.92	105.37	100.98
36	RM	501	GTP	C2-N1-C6	-2.92	119.73	125.10
36	JK	501	GTP	C8-N7-C5	2.92	108.55	102.99
36	UI	501	GTP	C8-N7-C5	2.92	108.55	102.99
36	OO	501	GTP	C8-N7-C5	2.92	108.55	102.99
38	DF	502	GDP	C3'-C2'-C1'	2.92	105.37	100.98
36	AK	501	GTP	C2-N1-C6	-2.92	119.73	125.10
38	JJ	502	GDP	C3'-C2'-C1'	2.92	105.37	100.98
36	BM	501	GTP	C2-N1-C6	-2.92	119.73	125.10
36	PM	501	GTP	C2-N1-C6	-2.92	119.73	125.10
36	JC	501	GTP	PA-O3A-PB	-2.91	122.82	132.83
36	DC	501	GTP	C3'-C2'-C1'	2.91	105.37	100.98
36	EI	501	GTP	C8-N7-C5	2.91	108.54	102.99
36	BK	501	GTP	C2-N1-C6	-2.91	119.73	125.10
36	SI	501	GTP	PB-O3B-PG	-2.91	122.83	132.83
36	TK	501	GTP	C2-N1-C6	-2.91	119.73	125.10
36	VM	501	GTP	C3'-C2'-C1'	2.91	105.36	100.98
36	IO	501	GTP	C2-N1-C6	-2.91	119.74	125.10
36	UE	501	GTP	C8-N7-C5	2.91	108.53	102.99
36	HG	501	GTP	C2-N1-C6	-2.91	119.74	125.10
36	PI	501	GTP	C2-N1-C6	-2.91	119.74	125.10
36	JM	501	GTP	C8-N7-C5	2.91	108.53	102.99
36	EI	501	GTP	PA-O3A-PB	-2.91	122.85	132.83
36	TM	501	GTP	PB-O3B-PG	-2.90	122.86	132.83
38	BD	502	GDP	C3'-C2'-C1'	2.90	105.35	100.98
36	JI	501	GTP	C8-N7-C5	2.90	108.52	102.99
36	TE	501	GTP	PA-O3A-PB	-2.90	122.87	132.83
36	QO	501	GTP	C3'-C2'-C1'	2.90	105.35	100.98
36	AE	501	GTP	PB-O3B-PG	-2.90	122.87	132.83
36	VO	501	GTP	C2-N1-C6	-2.90	119.76	125.10
38	PN	502	GDP	C3'-C2'-C1'	2.90	105.34	100.98
36	GE	501	GTP	C2-N1-C6	-2.90	119.76	125.10
36	HM	501	GTP	C2-N1-C6	-2.90	119.76	125.10
36	NE	501	GTP	C2-N1-C6	-2.90	119.76	125.10
36	BC	501	GTP	C8-N7-C5	2.90	108.51	102.99
36	RO	501	GTP	C3'-C2'-C1'	2.90	105.34	100.98
36	GC	501	GTP	C2-N1-C6	-2.90	119.77	125.10
36	NC	501	GTP	C8-N7-C5	2.90	108.51	102.99
36	DA	501	GTP	C3'-C2'-C1'	2.89	105.34	100.98
36	GG	501	GTP	C2-N1-C6	-2.89	119.77	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	NI	501	GTP	C2-N1-C6	-2.89	119.77	125.10
36	IK	501	GTP	C2-N1-C6	-2.89	119.77	125.10
38	GF	502	GDP	C3'-C2'-C1'	2.89	105.33	100.98
36	LG	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
36	BM	501	GTP	C8-N7-C5	2.89	108.50	102.99
36	JE	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
36	EM	501	GTP	C8-N7-C5	2.89	108.50	102.99
36	BG	501	GTP	C2-N1-C6	-2.89	119.78	125.10
38	TJ	502	GDP	C3'-C2'-C1'	2.89	105.33	100.98
36	NC	501	GTP	C2-N1-C6	-2.89	119.78	125.10
36	VE	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
36	NM	501	GTP	C2-N1-C6	-2.89	119.78	125.10
36	HE	501	GTP	C2-N1-C6	-2.89	119.78	125.10
36	VM	501	GTP	C2-N1-C6	-2.89	119.78	125.10
36	TM	501	GTP	C2-N1-C6	-2.88	119.79	125.10
36	EK	501	GTP	C8-N7-C5	2.88	108.48	102.99
36	GG	501	GTP	C8-N7-C5	2.88	108.48	102.99
36	IM	501	GTP	C2-N1-C6	-2.88	119.79	125.10
36	RC	501	GTP	C3'-C2'-C1'	2.88	105.31	100.98
36	GG	501	GTP	C3'-C2'-C1'	2.88	105.31	100.98
36	CI	501	GTP	C2-N1-C6	-2.88	119.80	125.10
36	WE	501	GTP	C2-N1-C6	-2.88	119.80	125.10
36	HO	501	GTP	C3'-C2'-C1'	2.88	105.31	100.98
36	RK	501	GTP	C8-N7-C5	2.88	108.47	102.99
36	HC	501	GTP	C2-N1-C6	-2.87	119.81	125.10
36	NK	501	GTP	C2-N1-C6	-2.87	119.81	125.10
36	HK	501	GTP	C2-N1-C6	-2.87	119.81	125.10
36	SI	501	GTP	C2-N1-C6	-2.87	119.81	125.10
38	KJ	502	GDP	C3'-C2'-C1'	2.87	105.30	100.98
36	OC	501	GTP	C3'-C2'-C1'	2.87	105.30	100.98
36	WK	501	GTP	C3'-C2'-C1'	2.87	105.30	100.98
36	FE	501	GTP	C2-N1-C6	-2.87	119.81	125.10
36	SM	501	GTP	C2-N1-C6	-2.87	119.81	125.10
36	BG	501	GTP	C3'-C2'-C1'	2.87	105.30	100.98
38	JF	502	GDP	C3'-C2'-C1'	2.87	105.30	100.98
36	QE	501	GTP	C8-N7-C5	2.86	108.45	102.99
36	DG	501	GTP	C3'-C2'-C1'	2.86	105.29	100.98
36	QC	501	GTP	PB-O3B-PG	-2.86	123.00	132.83
36	CE	501	GTP	C3'-C2'-C1'	2.86	105.29	100.98
36	KK	501	GTP	C3'-C2'-C1'	2.86	105.29	100.98
36	SE	501	GTP	PA-O3A-PB	-2.86	123.01	132.83
36	FC	501	GTP	C2-N1-C6	-2.86	119.83	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	MC	501	GTP	C3'-C2'-C1'	2.86	105.28	100.98
38	CF	502	GDP	C3'-C2'-C1'	2.86	105.28	100.98
36	BG	501	GTP	C8-N7-C5	2.86	108.44	102.99
36	SO	501	GTP	PA-O3A-PB	-2.86	123.02	132.83
38	MD	502	GDP	C3'-C2'-C1'	2.85	105.28	100.98
36	PK	501	GTP	C3'-C2'-C1'	2.85	105.28	100.98
36	LI	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
36	PC	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
38	OF	502	GDP	C3'-C2'-C1'	2.85	105.27	100.98
38	QN	502	GDP	C3'-C2'-C1'	2.85	105.27	100.98
38	KD	502	GDP	C3'-C2'-C1'	2.85	105.27	100.98
36	EC	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
36	EK	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
36	IK	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
36	HM	501	GTP	PB-O3B-PG	-2.85	123.06	132.83
36	GM	501	GTP	C2-N1-C6	-2.84	119.87	125.10
36	LM	501	GTP	PB-O3B-PG	-2.84	123.09	132.83
36	HC	501	GTP	PB-O3B-PG	-2.84	123.09	132.83
36	OO	501	GTP	C3'-C2'-C1'	2.84	105.25	100.98
36	SK	501	GTP	C2-N1-C6	-2.84	119.88	125.10
36	UK	501	GTP	C2-N1-C6	-2.84	119.88	125.10
36	BI	501	GTP	C3'-C2'-C1'	2.83	105.24	100.98
36	FI	501	GTP	C2-N1-C6	-2.83	119.88	125.10
38	EH	502	GDP	C3'-C2'-C1'	2.83	105.24	100.98
36	RI	501	GTP	C8-N7-C5	2.83	108.38	102.99
38	QF	502	GDP	C3'-C2'-C1'	2.83	105.24	100.98
36	FG	501	GTP	C2-N1-C6	-2.83	119.89	125.10
36	KI	501	GTP	C3'-C2'-C1'	2.82	105.23	100.98
36	EE	501	GTP	C3'-C2'-C1'	2.82	105.23	100.98
38	LN	502	GDP	C3'-C2'-C1'	2.82	105.23	100.98
38	JL	502	GDP	C3'-C2'-C1'	2.82	105.23	100.98
36	RG	501	GTP	PA-O3A-PB	-2.82	123.15	132.83
36	RE	501	GTP	C8-N7-C5	2.82	108.35	102.99
36	SO	501	GTP	PB-O3B-PG	-2.81	123.17	132.83
36	LC	501	GTP	C3'-C2'-C1'	2.81	105.22	100.98
36	PG	501	GTP	C3'-C2'-C1'	2.81	105.22	100.98
38	HJ	502	GDP	C3'-C2'-C1'	2.81	105.21	100.98
36	TI	501	GTP	C3'-C2'-C1'	2.81	105.21	100.98
38	DL	502	GDP	C3'-C2'-C1'	2.81	105.21	100.98
36	TI	501	GTP	PB-O3B-PG	-2.81	123.19	132.83
36	TI	501	GTP	C2-N1-C6	-2.81	119.93	125.10
36	OG	501	GTP	C3'-C2'-C1'	2.80	105.20	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BK	501	GTP	C3'-C2'-C1'	2.80	105.20	100.98
38	TN	502	GDP	C3'-C2'-C1'	2.80	105.20	100.98
38	KF	502	GDP	C3'-C2'-C1'	2.80	105.19	100.98
36	FM	501	GTP	C2-N1-C6	-2.80	119.94	125.10
36	KE	501	GTP	C3'-C2'-C1'	2.80	105.19	100.98
36	CG	501	GTP	C3'-C2'-C1'	2.80	105.19	100.98
36	NC	501	GTP	C3'-C2'-C1'	2.79	105.19	100.98
36	SG	501	GTP	C3'-C2'-C1'	2.79	105.18	100.98
36	VK	501	GTP	C3'-C2'-C1'	2.79	105.18	100.98
36	TM	501	GTP	C3'-C2'-C1'	2.79	105.18	100.98
36	IE	501	GTP	C3'-C2'-C1'	2.79	105.17	100.98
38	SN	502	GDP	C3'-C2'-C1'	2.79	105.17	100.98
36	QG	501	GTP	PA-O3A-PB	-2.79	123.27	132.83
38	KL	502	GDP	C3'-C2'-C1'	2.78	105.17	100.98
36	NM	501	GTP	PB-O3B-PG	-2.78	123.28	132.83
38	WF	502	GDP	C3'-C2'-C1'	2.78	105.16	100.98
36	HC	501	GTP	C3'-C2'-C1'	2.78	105.16	100.98
36	GI	501	GTP	PB-O3B-PG	-2.78	123.30	132.83
36	BE	501	GTP	C3'-C2'-C1'	2.77	105.15	100.98
36	CI	501	GTP	C3'-C2'-C1'	2.77	105.15	100.98
38	QD	502	GDP	C3'-C2'-C1'	2.77	105.14	100.98
36	UG	501	GTP	C3'-C2'-C1'	2.77	105.14	100.98
36	TO	501	GTP	C3'-C2'-C1'	2.77	105.14	100.98
38	DH	502	GDP	C3'-C2'-C1'	2.77	105.14	100.98
38	WP	502	GDP	C3'-C2'-C1'	2.76	105.14	100.98
36	NI	501	GTP	PB-O3B-PG	-2.76	123.34	132.83
36	MG	501	GTP	C3'-C2'-C1'	2.76	105.14	100.98
36	FG	501	GTP	C3'-C2'-C1'	2.76	105.13	100.98
38	UJ	502	GDP	C3'-C2'-C1'	2.76	105.13	100.98
36	HM	501	GTP	C3'-C2'-C1'	2.76	105.13	100.98
36	NG	501	GTP	C3'-C2'-C1'	2.76	105.13	100.98
38	ON	502	GDP	C3'-C2'-C1'	2.75	105.12	100.98
36	AK	501	GTP	C3'-C2'-C1'	2.75	105.12	100.98
36	CM	501	GTP	C3'-C2'-C1'	2.75	105.12	100.98
36	HE	501	GTP	C3'-C2'-C1'	2.75	105.11	100.98
36	SG	501	GTP	PA-O3A-PB	-2.75	123.40	132.83
36	CA	501	GTP	C3'-C2'-C1'	2.75	105.11	100.98
36	RO	501	GTP	PA-O3A-PB	-2.74	123.41	132.83
36	UO	501	GTP	C3'-C2'-C1'	2.74	105.11	100.98
36	OM	501	GTP	PA-O3A-PB	-2.74	123.42	132.83
36	IC	501	GTP	C3'-C2'-C1'	2.74	105.10	100.98
36	KM	501	GTP	C3'-C2'-C1'	2.74	105.10	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BA	501	GTP	C3'-C2'-C1'	2.74	105.10	100.98
36	SM	501	GTP	PA-O3A-PB	-2.73	123.44	132.83
36	QI	501	GTP	C3'-C2'-C1'	2.73	105.09	100.98
38	DD	502	GDP	C3'-C2'-C1'	2.73	105.09	100.98
36	WM	501	GTP	C3'-C2'-C1'	2.73	105.08	100.98
36	RI	501	GTP	C3'-C2'-C1'	2.73	105.08	100.98
38	JH	502	GDP	C3'-C2'-C1'	2.73	105.08	100.98
36	TE	501	GTP	C3'-C2'-C1'	2.72	105.08	100.98
38	SF	502	GDP	PA-O3A-PB	-2.72	123.48	132.83
38	OL	502	GDP	C3'-C2'-C1'	2.72	105.07	100.98
36	CK	501	GTP	PA-O3A-PB	-2.72	123.50	132.83
36	GI	501	GTP	C3'-C2'-C1'	2.72	105.07	100.98
36	PI	501	GTP	PA-O3A-PB	-2.71	123.51	132.83
36	UE	501	GTP	C3'-C2'-C1'	2.71	105.06	100.98
36	HG	501	GTP	C3'-C2'-C1'	2.71	105.05	100.98
36	SK	501	GTP	C3'-C2'-C1'	2.70	105.05	100.98
38	QH	502	GDP	C3'-C2'-C1'	2.70	105.05	100.98
38	TF	502	GDP	C3'-C2'-C1'	2.70	105.05	100.98
36	FC	501	GTP	PA-O3A-PB	-2.70	123.56	132.83
36	SO	501	GTP	C3'-C2'-C1'	2.70	105.04	100.98
36	HK	501	GTP	C3'-C2'-C1'	2.70	105.04	100.98
36	RK	501	GTP	C3'-C2'-C1'	2.69	105.03	100.98
36	UI	501	GTP	C3'-C2'-C1'	2.69	105.03	100.98
38	WN	502	GDP	C3'-C2'-C1'	2.69	105.03	100.98
38	WJ	502	GDP	C3'-C2'-C1'	2.69	105.03	100.98
36	QE	501	GTP	C3'-C2'-C1'	2.69	105.03	100.98
36	NI	501	GTP	C3'-C2'-C1'	2.69	105.03	100.98
36	FC	501	GTP	C3'-C2'-C1'	2.69	105.02	100.98
38	OH	502	GDP	C3'-C2'-C1'	2.69	105.02	100.98
36	WG	501	GTP	C3'-C2'-C1'	2.68	105.02	100.98
38	PH	502	GDP	C3'-C2'-C1'	2.68	105.02	100.98
36	BK	501	GTP	PB-O3B-PG	-2.68	123.62	132.83
36	NE	501	GTP	C3'-C2'-C1'	2.68	105.01	100.98
38	RH	502	GDP	C3'-C2'-C1'	2.68	105.01	100.98
36	VO	501	GTP	C3'-C2'-C1'	2.68	105.01	100.98
36	AE	501	GTP	C3'-C2'-C1'	2.68	105.01	100.98
36	GG	501	GTP	PB-O3B-PG	-2.67	123.65	132.83
36	EI	501	GTP	C3'-C2'-C1'	2.66	104.98	100.98
38	OJ	502	GDP	C3'-C2'-C1'	2.66	104.98	100.98
36	LK	501	GTP	C3'-C2'-C1'	2.66	104.98	100.98
36	VI	501	GTP	C3'-C2'-C1'	2.65	104.97	100.98
36	TO	501	GTP	PB-O3B-PG	-2.65	123.73	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	PD	502	GDP	C3'-C2'-C1'	2.65	104.97	100.98
36	MC	501	GTP	PA-O3A-PB	-2.64	123.78	132.83
36	AC	501	GTP	PB-O3B-PG	-2.64	123.78	132.83
36	GE	501	GTP	C3'-C2'-C1'	2.63	104.94	100.98
36	UK	501	GTP	C3'-C2'-C1'	2.63	104.94	100.98
38	DJ	502	GDP	C3'-C2'-C1'	2.63	104.94	100.98
36	FM	501	GTP	C3'-C2'-C1'	2.63	104.93	100.98
36	AI	501	GTP	C3'-C2'-C1'	2.62	104.93	100.98
36	PE	501	GTP	C3'-C2'-C1'	2.62	104.92	100.98
36	NK	501	GTP	C3'-C2'-C1'	2.62	104.92	100.98
36	GC	501	GTP	C3'-C2'-C1'	2.62	104.92	100.98
36	TK	501	GTP	C3'-C2'-C1'	2.61	104.91	100.98
36	AA	501	GTP	C3'-C2'-C1'	2.61	104.91	100.98
36	NM	501	GTP	C3'-C2'-C1'	2.61	104.91	100.98
36	LI	501	GTP	PA-O3A-PB	-2.61	123.88	132.83
36	AA	501	GTP	PB-O3B-PG	-2.60	123.89	132.83
36	GM	501	GTP	C3'-C2'-C1'	2.60	104.89	100.98
36	MK	501	GTP	C3'-C2'-C1'	2.60	104.89	100.98
36	OE	501	GTP	C3'-C2'-C1'	2.59	104.89	100.98
36	PM	501	GTP	C3'-C2'-C1'	2.59	104.89	100.98
36	QC	501	GTP	C3'-C2'-C1'	2.59	104.88	100.98
36	NG	501	GTP	O3G-PG-O3B	2.59	113.31	104.64
36	AC	501	GTP	C3'-C2'-C1'	2.58	104.87	100.98
36	WO	501	GTP	C3'-C2'-C1'	2.58	104.87	100.98
36	QK	501	GTP	C3'-C2'-C1'	2.58	104.86	100.98
36	QM	501	GTP	C3'-C2'-C1'	2.58	104.86	100.98
36	PC	501	GTP	PA-O3A-PB	-2.58	123.99	132.83
36	BM	501	GTP	C3'-C2'-C1'	2.57	104.85	100.98
36	OK	501	GTP	C3'-C2'-C1'	2.57	104.85	100.98
38	LD	502	GDP	C3'-C2'-C1'	2.57	104.84	100.98
36	LE	501	GTP	C3'-C2'-C1'	2.55	104.82	100.98
36	QE	501	GTP	PA-O3A-PB	-2.55	124.07	132.83
36	GK	501	GTP	C3'-C2'-C1'	2.55	104.82	100.98
38	ML	502	GDP	C3'-C2'-C1'	2.54	104.81	100.98
36	MI	501	GTP	C3'-C2'-C1'	2.54	104.81	100.98
36	RK	501	GTP	O6-C6-C5	-2.54	119.41	124.37
36	AG	501	GTP	C3'-C2'-C1'	2.54	104.80	100.98
36	UM	501	GTP	C3'-C2'-C1'	2.54	104.80	100.98
38	SF	502	GDP	C3'-C2'-C1'	2.53	104.78	100.98
36	RM	501	GTP	C3'-C2'-C1'	2.52	104.77	100.98
38	LL	502	GDP	C5-C6-N1	2.52	118.40	113.95
38	EJ	502	GDP	C3'-C2'-C1'	2.52	104.77	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	AL	502	GDP	C5-C6-N1	2.52	118.40	113.95
36	EC	501	GTP	PA-O3A-PB	-2.51	124.20	132.83
36	OM	501	GTP	C3'-C2'-C1'	2.51	104.76	100.98
36	EG	501	GTP	PA-O3A-PB	-2.50	124.24	132.83
38	LH	502	GDP	C5-C6-N1	2.50	118.37	113.95
38	SH	502	GDP	C3'-C2'-C1'	2.50	104.74	100.98
36	AG	501	GTP	PB-O3B-PG	-2.49	124.27	132.83
36	SE	501	GTP	C3'-C2'-C1'	2.49	104.73	100.98
38	KD	502	GDP	C5-C6-N1	2.48	118.33	113.95
36	FE	501	GTP	C3'-C2'-C1'	2.47	104.70	100.98
38	DB	502	GDP	C5-C6-N1	2.47	118.31	113.95
38	CD	502	GDP	C5-C6-N1	2.47	118.31	113.95
38	OD	502	GDP	C5-C6-N1	2.47	118.31	113.95
38	JN	502	GDP	C5-C6-N1	2.47	118.31	113.95
38	MN	502	GDP	C5-C6-N1	2.46	118.30	113.95
38	WH	502	GDP	C8-N7-C5	2.46	107.67	102.99
38	KH	502	GDP	C5-C6-N1	2.46	118.29	113.95
38	MH	502	GDP	C5-C6-N1	2.45	118.28	113.95
38	MJ	502	GDP	C5-C6-N1	2.45	118.28	113.95
38	OH	502	GDP	C5-C6-N1	2.45	118.28	113.95
38	JH	502	GDP	C5-C6-N1	2.45	118.27	113.95
36	SI	501	GTP	PA-O3A-PB	-2.45	124.43	132.83
38	EB	502	GDP	C5-C6-N1	2.45	118.27	113.95
38	EF	502	GDP	C5-C6-N1	2.44	118.27	113.95
38	IJ	502	GDP	C5-C6-N1	2.44	118.27	113.95
38	LD	502	GDP	C5-C6-N1	2.44	118.27	113.95
38	SN	502	GDP	C5-C6-N1	2.44	118.27	113.95
38	CH	502	GDP	C3'-C2'-C1'	2.44	104.65	100.98
38	WP	502	GDP	C8-N7-C5	2.44	107.64	102.99
38	CH	502	GDP	C5-C6-N1	2.44	118.26	113.95
38	FL	502	GDP	C5-C6-N1	2.44	118.26	113.95
38	WF	502	GDP	C8-N7-C5	2.44	107.64	102.99
36	GC	501	GTP	PB-O3B-PG	-2.43	124.48	132.83
38	KN	502	GDP	C5-C6-N1	2.43	118.25	113.95
36	BA	501	GTP	O6-C6-C5	-2.43	119.62	124.37
38	LN	502	GDP	C5-C6-N1	2.43	118.24	113.95
38	WN	502	GDP	C8-N7-C5	2.43	107.62	102.99
38	DL	502	GDP	C8-N7-C5	2.43	107.61	102.99
36	QC	501	GTP	PA-O3A-PB	-2.43	124.50	132.83
38	AH	502	GDP	C5-C6-N1	2.43	118.23	113.95
38	KB	502	GDP	C5-C6-N1	2.42	118.23	113.95
38	IH	502	GDP	C8-N7-C5	2.42	107.61	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	CH	502	GDP	C8-N7-C5	2.42	107.61	102.99
38	OF	502	GDP	C5-C6-N1	2.42	118.23	113.95
38	DJ	502	GDP	C5-C6-N1	2.42	118.23	113.95
38	LF	502	GDP	C5-C6-N1	2.42	118.22	113.95
38	CJ	502	GDP	C8-N7-C5	2.42	107.59	102.99
38	ML	502	GDP	C5-C6-N1	2.42	118.22	113.95
38	VF	502	GDP	C8-N7-C5	2.42	107.59	102.99
38	CB	502	GDP	C8-N7-C5	2.42	107.59	102.99
36	UE	501	GTP	O6-C6-C5	-2.41	119.66	124.37
38	WD	502	GDP	C8-N7-C5	2.41	107.59	102.99
38	KF	502	GDP	C5-C6-N1	2.41	118.22	113.95
38	PN	502	GDP	C8-N7-C5	2.41	107.59	102.99
36	EE	501	GTP	PA-O3A-PB	-2.41	124.55	132.83
38	CL	502	GDP	C8-N7-C5	2.41	107.58	102.99
38	QJ	502	GDP	C8-N7-C5	2.41	107.58	102.99
38	MD	502	GDP	C5-C6-N1	2.41	118.21	113.95
38	LJ	502	GDP	C5-C6-N1	2.41	118.21	113.95
36	ME	501	GTP	C3'-C2'-C1'	2.41	104.61	100.98
36	PO	501	GTP	C3'-C2'-C1'	2.41	104.61	100.98
38	AJ	502	GDP	C5-C6-N1	2.41	118.20	113.95
38	MB	502	GDP	C5-C6-N1	2.41	118.20	113.95
38	BH	502	GDP	C5-C6-N1	2.41	118.20	113.95
38	HJ	502	GDP	C5-C6-N1	2.41	118.20	113.95
36	BM	501	GTP	O6-C6-C5	-2.41	119.67	124.37
38	HD	502	GDP	C8-N7-C5	2.41	107.57	102.99
36	NE	501	GTP	O6-C6-C5	-2.40	119.67	124.37
38	AF	502	GDP	C5-C6-N1	2.40	118.20	113.95
38	OB	502	GDP	C5-C6-N1	2.40	118.20	113.95
38	VN	502	GDP	C8-N7-C5	2.40	107.57	102.99
38	QN	502	GDP	C8-N7-C5	2.40	107.57	102.99
38	BF	502	GDP	C5-C6-N1	2.40	118.19	113.95
38	NF	502	GDP	C5-C6-N1	2.40	118.19	113.95
38	CD	502	GDP	C8-N7-C5	2.40	107.56	102.99
38	RD	502	GDP	C5-C6-N1	2.40	118.19	113.95
38	DD	502	GDP	C8-N7-C5	2.40	107.56	102.99
38	DF	502	GDP	C8-N7-C5	2.40	107.56	102.99
38	VL	502	GDP	C5-C6-N1	2.40	118.19	113.95
38	HJ	502	GDP	C8-N7-C5	2.40	107.56	102.99
38	IL	502	GDP	C8-N7-C5	2.40	107.56	102.99
38	EH	502	GDP	C5-C6-N1	2.40	118.19	113.95
38	LH	502	GDP	C8-N7-C5	2.40	107.56	102.99
38	AD	502	GDP	C5-C6-N1	2.40	118.18	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	HL	502	GDP	C8-N7-C5	2.40	107.55	102.99
38	VH	502	GDP	C8-N7-C5	2.40	107.55	102.99
36	BI	501	GTP	O6-C6-C5	-2.39	119.69	124.37
38	FN	502	GDP	C5-C6-N1	2.39	118.18	113.95
38	NN	502	GDP	C5-C6-N1	2.39	118.18	113.95
38	PH	502	GDP	C5-C6-N1	2.39	118.18	113.95
38	QJ	502	GDP	C5-C6-N1	2.39	118.18	113.95
38	WN	502	GDP	C5-C6-N1	2.39	118.18	113.95
36	RE	501	GTP	O6-C6-C5	-2.39	119.70	124.37
38	MF	502	GDP	C5-C6-N1	2.39	118.17	113.95
38	VH	502	GDP	C5-C6-N1	2.39	118.17	113.95
38	JB	502	GDP	C5-C6-N1	2.39	118.17	113.95
38	IF	502	GDP	C8-N7-C5	2.39	107.54	102.99
38	KJ	502	GDP	C5-C6-N1	2.39	118.17	113.95
38	AB	502	GDP	C5-C6-N1	2.39	118.17	113.95
38	SJ	502	GDP	C5-C6-N1	2.39	118.17	113.95
38	RN	502	GDP	C5-C6-N1	2.39	118.17	113.95
38	KN	502	GDP	C8-N7-C5	2.39	107.54	102.99
38	ED	502	GDP	C5-C6-N1	2.39	118.16	113.95
38	KL	502	GDP	C5-C6-N1	2.38	118.16	113.95
38	ID	502	GDP	C8-N7-C5	2.38	107.53	102.99
38	SL	502	GDP	C5-C6-N1	2.38	118.16	113.95
38	WJ	502	GDP	C8-N7-C5	2.38	107.53	102.99
38	WL	502	GDP	C8-N7-C5	2.38	107.53	102.99
38	UF	502	GDP	C5-C6-N1	2.38	118.16	113.95
36	PK	501	GTP	PA-O3A-PB	-2.38	124.65	132.83
38	UN	502	GDP	C8-N7-C5	2.38	107.53	102.99
36	AK	501	GTP	PB-O3B-PG	-2.38	124.66	132.83
38	ON	502	GDP	C5-C6-N1	2.38	118.15	113.95
36	BG	501	GTP	O6-C6-C5	-2.38	119.73	124.37
38	JF	502	GDP	C8-N7-C5	2.38	107.52	102.99
38	DH	502	GDP	C8-N7-C5	2.38	107.52	102.99
38	IN	502	GDP	C8-N7-C5	2.38	107.52	102.99
38	PD	502	GDP	C8-N7-C5	2.38	107.52	102.99
38	ND	502	GDP	C5-C6-N1	2.38	118.15	113.95
38	RF	502	GDP	C5-C6-N1	2.37	118.14	113.95
38	LJ	502	GDP	C8-N7-C5	2.37	107.51	102.99
38	CF	502	GDP	C5-C6-N1	2.37	118.14	113.95
38	HD	502	GDP	C5-C6-N1	2.37	118.14	113.95
38	LN	502	GDP	C8-N7-C5	2.37	107.51	102.99
38	LF	502	GDP	C8-N7-C5	2.37	107.51	102.99
38	TJ	502	GDP	C8-N7-C5	2.37	107.51	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	FL	502	GDP	O6-C6-C5	-2.37	119.74	124.37
38	BD	502	GDP	C5-C6-N1	2.37	118.14	113.95
38	PF	502	GDP	C5-C6-N1	2.37	118.14	113.95
38	QL	502	GDP	C5-C6-N1	2.37	118.14	113.95
38	KB	502	GDP	C8-N7-C5	2.37	107.50	102.99
38	OH	502	GDP	C8-N7-C5	2.37	107.50	102.99
38	NB	502	GDP	C5-C6-N1	2.37	118.14	113.95
38	OJ	502	GDP	C5-C6-N1	2.37	118.14	113.95
38	HF	502	GDP	C8-N7-C5	2.37	107.50	102.99
38	CF	502	GDP	C8-N7-C5	2.37	107.50	102.99
38	PL	502	GDP	C5-C6-N1	2.37	118.13	113.95
38	QF	502	GDP	C5-C6-N1	2.37	118.13	113.95
38	VJ	502	GDP	C5-C6-N1	2.37	118.13	113.95
38	LD	502	GDP	C8-N7-C5	2.37	107.50	102.99
38	LB	502	GDP	C5-C6-N1	2.37	118.13	113.95
36	AM	501	GTP	C3'-C2'-C1'	2.37	104.54	100.98
38	GH	502	GDP	C8-N7-C5	2.37	107.50	102.99
38	PJ	502	GDP	C5-C6-N1	2.36	118.13	113.95
38	SH	502	GDP	C5-C6-N1	2.36	118.12	113.95
38	HB	502	GDP	C8-N7-C5	2.36	107.49	102.99
38	NJ	502	GDP	C5-C6-N1	2.36	118.12	113.95
36	BC	501	GTP	O6-C6-C5	-2.36	119.76	124.37
38	CJ	502	GDP	C5-C6-N1	2.36	118.12	113.95
38	BL	502	GDP	C5-C6-N1	2.36	118.12	113.95
38	IH	502	GDP	C5-C6-N1	2.36	118.12	113.95
38	PJ	502	GDP	C8-N7-C5	2.36	107.49	102.99
36	NG	501	GTP	O6-C6-C5	-2.36	119.76	124.37
38	KH	502	GDP	C8-N7-C5	2.36	107.49	102.99
38	VF	502	GDP	C5-C6-N1	2.36	118.12	113.95
38	IJ	502	GDP	C8-N7-C5	2.36	107.48	102.99
38	LH	502	GDP	C3'-C2'-C1'	2.36	104.53	100.98
38	HF	502	GDP	C5-C6-N1	2.36	118.11	113.95
38	WJ	502	GDP	C5-C6-N1	2.36	118.11	113.95
38	TP	502	GDP	C5-C6-N1	2.36	118.11	113.95
38	VP	502	GDP	C8-N7-C5	2.36	107.48	102.99
38	UJ	502	GDP	C8-N7-C5	2.36	107.48	102.99
38	UP	502	GDP	C8-N7-C5	2.36	107.48	102.99
38	RH	502	GDP	C5-C6-N1	2.36	118.11	113.95
38	HN	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	TF	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	NL	502	GDP	C5-C6-N1	2.35	118.11	113.95
38	PD	502	GDP	C5-C6-N1	2.35	118.11	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	PN	502	GDP	C5-C6-N1	2.35	118.11	113.95
38	TH	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	QD	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	VD	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	FD	502	GDP	C5-C6-N1	2.35	118.11	113.95
38	BF	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	VL	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	DB	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	VJ	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	LB	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	PL	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	AL	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	CL	502	GDP	C5-C6-N1	2.35	118.10	113.95
38	ON	502	GDP	C8-N7-C5	2.35	107.47	102.99
38	KJ	502	GDP	C8-N7-C5	2.35	107.47	102.99
36	FM	501	GTP	PA-O3A-PB	-2.35	124.77	132.83
38	OL	502	GDP	C5-C6-N1	2.35	118.10	113.95
38	AF	502	GDP	C8-N7-C5	2.35	107.46	102.99
38	HH	502	GDP	C8-N7-C5	2.35	107.46	102.99
38	UN	502	GDP	C5-C6-N1	2.35	118.10	113.95
38	BB	502	GDP	C5-C6-N1	2.35	118.09	113.95
38	BJ	502	GDP	C5-C6-N1	2.35	118.09	113.95
36	SM	501	GTP	C3'-C2'-C1'	2.35	104.51	100.98
38	JJ	502	GDP	C5-C6-N1	2.34	118.09	113.95
38	UH	502	GDP	C5-C6-N1	2.34	118.09	113.95
38	GL	502	GDP	C8-N7-C5	2.34	107.46	102.99
38	NF	502	GDP	C8-N7-C5	2.34	107.46	102.99
38	WP	502	GDP	C5-C6-N1	2.34	118.09	113.95
38	GN	502	GDP	C8-N7-C5	2.34	107.45	102.99
38	OB	502	GDP	C8-N7-C5	2.34	107.45	102.99
38	FH	502	GDP	C5-C6-N1	2.34	118.09	113.95
38	KH	502	GDP	C3'-C2'-C1'	2.34	104.50	100.98
38	TN	502	GDP	C8-N7-C5	2.34	107.45	102.99
38	RL	502	GDP	C5-C6-N1	2.34	118.08	113.95
38	GJ	502	GDP	C8-N7-C5	2.34	107.45	102.99
38	OJ	502	GDP	C8-N7-C5	2.34	107.45	102.99
36	NC	501	GTP	O6-C6-C5	-2.34	119.80	124.37
38	DJ	502	GDP	C8-N7-C5	2.34	107.44	102.99
38	IB	502	GDP	C8-N7-C5	2.34	107.44	102.99
38	SN	502	GDP	O6-C6-C5	-2.34	119.81	124.37
38	IL	502	GDP	C5-C6-N1	2.34	118.08	113.95
38	ND	502	GDP	C8-N7-C5	2.34	107.44	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	NL	502	GDP	C8-N7-C5	2.34	107.44	102.99
38	QH	502	GDP	C5-C6-N1	2.33	118.08	113.95
38	NH	502	GDP	C8-N7-C5	2.33	107.44	102.99
36	AG	501	GTP	O6-C6-C5	-2.33	119.81	124.37
38	VD	502	GDP	C5-C6-N1	2.33	118.07	113.95
36	AI	501	GTP	O6-C6-C5	-2.33	119.81	124.37
38	EL	502	GDP	C8-N7-C5	2.33	107.43	102.99
38	GD	502	GDP	C8-N7-C5	2.33	107.43	102.99
38	NB	502	GDP	C8-N7-C5	2.33	107.43	102.99
38	DF	502	GDP	C5-C6-N1	2.33	118.07	113.95
38	MH	502	GDP	C3'-C2'-C1'	2.33	104.49	100.98
38	VN	502	GDP	C5-C6-N1	2.33	118.07	113.95
38	PH	502	GDP	C8-N7-C5	2.33	107.43	102.99
38	UL	502	GDP	C5-C6-N1	2.33	118.07	113.95
38	FB	502	GDP	C5-C6-N1	2.33	118.06	113.95
38	MJ	502	GDP	C8-N7-C5	2.33	107.43	102.99
38	UL	502	GDP	C8-N7-C5	2.33	107.42	102.99
38	VP	502	GDP	C5-C6-N1	2.33	118.06	113.95
36	BE	501	GTP	O6-C6-C5	-2.33	119.83	124.37
36	WM	501	GTP	PA-O3A-PB	-2.33	124.84	132.83
38	EJ	502	GDP	C5-C6-N1	2.33	118.06	113.95
38	MH	502	GDP	C8-N7-C5	2.32	107.42	102.99
38	TL	502	GDP	C8-N7-C5	2.32	107.42	102.99
38	OL	502	GDP	C8-N7-C5	2.32	107.42	102.99
38	TD	502	GDP	C8-N7-C5	2.32	107.42	102.99
38	AB	502	GDP	C8-N7-C5	2.32	107.42	102.99
38	SD	502	GDP	C5-C6-N1	2.32	118.05	113.95
38	EN	502	GDP	C5-C6-N1	2.32	118.05	113.95
38	GJ	502	GDP	C5-C6-N1	2.32	118.05	113.95
38	TN	502	GDP	C5-C6-N1	2.32	118.05	113.95
38	HH	502	GDP	C5-C6-N1	2.32	118.05	113.95
38	JL	502	GDP	C8-N7-C5	2.32	107.41	102.99
36	BK	501	GTP	O6-C6-C5	-2.32	119.84	124.37
38	FJ	502	GDP	C5-C6-N1	2.32	118.05	113.95
38	FB	502	GDP	C8-N7-C5	2.32	107.41	102.99
38	MF	502	GDP	C8-N7-C5	2.32	107.41	102.99
38	ID	502	GDP	C5-C6-N1	2.32	118.05	113.95
38	JH	502	GDP	C8-N7-C5	2.32	107.41	102.99
38	HN	502	GDP	C5-C6-N1	2.32	118.04	113.95
38	MB	502	GDP	C8-N7-C5	2.32	107.40	102.99
38	PF	502	GDP	C8-N7-C5	2.32	107.40	102.99
38	TD	502	GDP	C5-C6-N1	2.32	118.04	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	AJ	502	GDP	C8-N7-C5	2.32	107.40	102.99
38	MN	502	GDP	C8-N7-C5	2.32	107.40	102.99
38	UJ	502	GDP	C5-C6-N1	2.32	118.04	113.95
38	KD	502	GDP	C8-N7-C5	2.31	107.39	102.99
38	UH	502	GDP	C8-N7-C5	2.31	107.39	102.99
38	GL	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	RJ	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	IN	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	SF	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	QH	502	GDP	C8-N7-C5	2.31	107.39	102.99
36	VE	501	GTP	O6-C6-C5	-2.31	119.86	124.37
38	OD	502	GDP	C8-N7-C5	2.31	107.39	102.99
38	WF	502	GDP	C5-C6-N1	2.31	118.03	113.95
36	LE	501	GTP	O6-C6-C5	-2.31	119.86	124.37
38	NH	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	TJ	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	IF	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	CB	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	GH	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	GN	502	GDP	C5-C6-N1	2.31	118.03	113.95
38	UF	502	GDP	C8-N7-C5	2.31	107.38	102.99
38	EJ	502	GDP	C8-N7-C5	2.30	107.38	102.99
38	JJ	502	GDP	C8-N7-C5	2.30	107.38	102.99
38	OF	502	GDP	C8-N7-C5	2.30	107.38	102.99
38	SD	502	GDP	C8-N7-C5	2.30	107.38	102.99
38	LL	502	GDP	C8-N7-C5	2.30	107.38	102.99
38	JF	502	GDP	C5-C6-N1	2.30	118.02	113.95
36	MM	501	GTP	C3'-C2'-C1'	2.30	104.44	100.98
38	EN	502	GDP	C8-N7-C5	2.30	107.37	102.99
38	QF	502	GDP	C8-N7-C5	2.30	107.37	102.99
38	GB	502	GDP	C8-N7-C5	2.30	107.37	102.99
38	GF	502	GDP	C8-N7-C5	2.30	107.37	102.99
36	UI	501	GTP	O6-C6-C5	-2.30	119.88	124.37
38	JL	502	GDP	C5-C6-N1	2.30	118.01	113.95
38	DD	502	GDP	C5-C6-N1	2.30	118.01	113.95
36	LM	501	GTP	C3'-C2'-C1'	2.30	104.44	100.98
36	NI	501	GTP	O6-C6-C5	-2.30	119.89	124.37
36	RG	501	GTP	O6-C6-C5	-2.30	119.89	124.37
38	BD	502	GDP	C8-N7-C5	2.30	107.36	102.99
38	FJ	502	GDP	C8-N7-C5	2.30	107.36	102.99
38	RF	502	GDP	C8-N7-C5	2.30	107.36	102.99
38	TP	502	GDP	C8-N7-C5	2.30	107.36	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	AH	502	GDP	C8-N7-C5	2.29	107.36	102.99
38	MD	502	GDP	C8-N7-C5	2.29	107.36	102.99
38	GD	502	GDP	C5-C6-N1	2.29	118.00	113.95
38	QD	502	GDP	C5-C6-N1	2.29	118.00	113.95
38	BH	502	GDP	C8-N7-C5	2.29	107.36	102.99
38	ML	502	GDP	C8-N7-C5	2.29	107.36	102.99
36	FE	501	GTP	O6-C6-C5	-2.29	119.90	124.37
38	WL	502	GDP	C5-C6-N1	2.29	118.00	113.95
38	RJ	502	GDP	C8-N7-C5	2.29	107.36	102.99
38	RH	502	GDP	C8-N7-C5	2.29	107.35	102.99
38	AD	502	GDP	C8-N7-C5	2.29	107.35	102.99
36	KE	501	GTP	O6-C6-C5	-2.29	119.90	124.37
38	KL	502	GDP	C8-N7-C5	2.29	107.35	102.99
38	UD	502	GDP	C8-N7-C5	2.29	107.35	102.99
38	DH	502	GDP	C5-C6-N1	2.29	117.99	113.95
38	NN	502	GDP	C8-N7-C5	2.29	107.35	102.99
38	QL	502	GDP	C8-N7-C5	2.29	107.35	102.99
38	UD	502	GDP	C5-C6-N1	2.29	117.99	113.95
38	EF	502	GDP	C8-N7-C5	2.28	107.34	102.99
38	TH	502	GDP	C5-C6-N1	2.28	117.98	113.95
36	HI	501	GTP	O6-C6-C5	-2.28	119.91	124.37
38	KF	502	GDP	C8-N7-C5	2.28	107.34	102.99
38	IB	502	GDP	C5-C6-N1	2.28	117.98	113.95
36	HO	501	GTP	O6-C6-C5	-2.28	119.92	124.37
38	RL	502	GDP	C8-N7-C5	2.28	107.33	102.99
36	WE	501	GTP	C3'-C2'-C1'	2.28	104.41	100.98
38	WH	502	GDP	C5-C6-N1	2.28	117.97	113.95
38	NJ	502	GDP	C8-N7-C5	2.28	107.33	102.99
38	SF	502	GDP	C8-N7-C5	2.28	107.33	102.99
38	BB	502	GDP	C8-N7-C5	2.27	107.32	102.99
38	FF	502	GDP	C5-C6-N1	2.27	117.97	113.95
38	EB	502	GDP	C8-N7-C5	2.27	107.32	102.99
36	UG	501	GTP	O6-C6-C5	-2.27	119.93	124.37
38	GB	502	GDP	C5-C6-N1	2.27	117.96	113.95
38	HB	502	GDP	C5-C6-N1	2.27	117.96	113.95
38	EL	502	GDP	C5-C6-N1	2.27	117.96	113.95
38	JB	502	GDP	C8-N7-C5	2.27	107.31	102.99
38	HL	502	GDP	C5-C6-N1	2.27	117.96	113.95
38	BJ	502	GDP	C8-N7-C5	2.27	107.31	102.99
38	TF	502	GDP	C5-C6-N1	2.27	117.96	113.95
38	FF	502	GDP	C8-N7-C5	2.27	107.31	102.99
36	HM	501	GTP	O6-C6-C5	-2.27	119.95	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	SJ	502	GDP	O6-C6-C5	-2.27	119.95	124.37
38	EH	502	GDP	C8-N7-C5	2.27	107.31	102.99
38	RD	502	GDP	C8-N7-C5	2.26	107.30	102.99
38	FH	502	GDP	C8-N7-C5	2.26	107.30	102.99
38	JN	502	GDP	C8-N7-C5	2.26	107.30	102.99
38	TL	502	GDP	C5-C6-N1	2.26	117.94	113.95
38	BL	502	GDP	C8-N7-C5	2.26	107.29	102.99
38	ED	502	GDP	C8-N7-C5	2.26	107.29	102.99
36	UM	501	GTP	O6-C6-C5	-2.25	119.97	124.37
36	AI	501	GTP	PB-O3B-PG	-2.25	125.10	132.83
36	CM	501	GTP	O6-C6-C5	-2.25	119.98	124.37
36	QG	501	GTP	O6-C6-C5	-2.25	119.98	124.37
38	WD	502	GDP	C5-C6-N1	2.25	117.92	113.95
38	DL	502	GDP	C5-C6-N1	2.25	117.92	113.95
36	UO	501	GTP	O6-C6-C5	-2.25	119.98	124.37
38	LL	502	GDP	C3'-C2'-C1'	2.24	104.36	100.98
38	QN	502	GDP	C5-C6-N1	2.24	117.92	113.95
36	OC	501	GTP	O6-C6-C5	-2.24	119.99	124.37
38	UP	502	GDP	C5-C6-N1	2.24	117.91	113.95
36	EI	501	GTP	O6-C6-C5	-2.24	119.99	124.37
36	RI	501	GTP	O6-C6-C5	-2.24	119.99	124.37
36	FC	501	GTP	O6-C6-C5	-2.24	119.99	124.37
38	RN	502	GDP	C8-N7-C5	2.24	107.26	102.99
36	NM	501	GTP	O6-C6-C5	-2.24	120.00	124.37
36	NK	501	GTP	O6-C6-C5	-2.24	120.00	124.37
36	KK	501	GTP	O6-C6-C5	-2.24	120.00	124.37
38	GF	502	GDP	C5-C6-N1	2.24	117.90	113.95
36	HK	501	GTP	O6-C6-C5	-2.24	120.00	124.37
38	RH	502	GDP	C2'-C3'-C4'	2.23	106.98	102.64
36	AE	501	GTP	O6-C6-C5	-2.23	120.01	124.37
36	VO	501	GTP	O6-C6-C5	-2.23	120.01	124.37
36	MG	501	GTP	O6-C6-C5	-2.23	120.02	124.37
36	VK	501	GTP	O6-C6-C5	-2.23	120.02	124.37
36	VI	501	GTP	O6-C6-C5	-2.22	120.03	124.37
36	ME	501	GTP	O6-C6-C5	-2.22	120.03	124.37
36	GG	501	GTP	O6-C6-C5	-2.22	120.03	124.37
36	PG	501	GTP	O6-C6-C5	-2.22	120.03	124.37
36	QK	501	GTP	O6-C6-C5	-2.22	120.03	124.37
38	FN	502	GDP	C8-N7-C5	2.22	107.22	102.99
36	HC	501	GTP	O6-C6-C5	-2.22	120.04	124.37
38	JD	502	GDP	C5-C6-N1	2.22	117.87	113.95
36	MM	501	GTP	O6-C6-C5	-2.21	120.05	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	EK	501	GTP	O6-C6-C5	-2.21	120.05	124.37
36	LK	501	GTP	O6-C6-C5	-2.21	120.05	124.37
36	KG	501	GTP	O6-C6-C5	-2.21	120.06	124.37
36	OM	501	GTP	O6-C6-C5	-2.21	120.06	124.37
36	MI	501	GTP	O6-C6-C5	-2.21	120.06	124.37
38	FD	502	GDP	C8-N7-C5	2.20	107.19	102.99
38	SJ	502	GDP	C8-N7-C5	2.20	107.18	102.99
36	KM	501	GTP	O6-C6-C5	-2.20	120.07	124.37
36	HG	501	GTP	O6-C6-C5	-2.20	120.07	124.37
36	LM	501	GTP	O6-C6-C5	-2.20	120.07	124.37
36	SE	501	GTP	O6-C6-C5	-2.20	120.08	124.37
36	AA	501	GTP	O6-C6-C5	-2.20	120.08	124.37
36	TO	501	GTP	O6-C6-C5	-2.20	120.08	124.37
36	UM	501	GTP	PA-O3A-PB	-2.19	125.30	132.83
36	OG	501	GTP	O6-C6-C5	-2.19	120.09	124.37
36	HE	501	GTP	O6-C6-C5	-2.19	120.09	124.37
36	SG	501	GTP	O6-C6-C5	-2.18	120.11	124.37
38	SH	502	GDP	C8-N7-C5	2.18	107.15	102.99
36	TK	501	GTP	O6-C6-C5	-2.18	120.12	124.37
36	SM	501	GTP	O6-C6-C5	-2.18	120.12	124.37
38	SL	502	GDP	C8-N7-C5	2.18	107.13	102.99
38	JD	502	GDP	C8-N7-C5	2.17	107.13	102.99
36	LG	501	GTP	O6-C6-C5	-2.17	120.13	124.37
36	RC	501	GTP	O6-C6-C5	-2.17	120.13	124.37
36	AC	501	GTP	O6-C6-C5	-2.17	120.13	124.37
36	QM	501	GTP	O6-C6-C5	-2.17	120.14	124.37
36	UK	501	GTP	O6-C6-C5	-2.16	120.15	124.37
36	OO	501	GTP	O6-C6-C5	-2.16	120.15	124.37
36	EE	501	GTP	O6-C6-C5	-2.16	120.16	124.37
38	FL	502	GDP	C8-N7-C5	2.16	107.10	102.99
36	MK	501	GTP	O6-C6-C5	-2.16	120.16	124.37
36	JM	501	GTP	O6-C6-C5	-2.15	120.17	124.37
36	AK	501	GTP	O6-C6-C5	-2.15	120.18	124.37
36	OE	501	GTP	O6-C6-C5	-2.15	120.18	124.37
36	AM	501	GTP	O6-C6-C5	-2.15	120.18	124.37
36	DA	501	GTP	PA-O3A-PB	-2.14	125.47	132.83
36	KO	501	GTP	O6-C6-C5	-2.14	120.19	124.37
36	SK	501	GTP	O6-C6-C5	-2.14	120.19	124.37
36	QE	501	GTP	O6-C6-C5	-2.14	120.19	124.37
36	GI	501	GTP	O6-C6-C5	-2.14	120.20	124.37
36	SO	501	GTP	O6-C6-C5	-2.14	120.20	124.37
36	VM	501	GTP	O6-C6-C5	-2.14	120.20	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	PE	501	GTP	O6-C6-C5	-2.13	120.20	124.37
36	JE	501	GTP	O6-C6-C5	-2.13	120.21	124.37
36	JI	501	GTP	O6-C6-C5	-2.13	120.21	124.37
36	PO	501	GTP	O6-C6-C5	-2.13	120.21	124.37
36	IO	501	GTP	O6-C6-C5	-2.13	120.22	124.37
38	SN	502	GDP	C8-N7-C5	2.13	107.04	102.99
36	PI	501	GTP	O6-C6-C5	-2.12	120.22	124.37
36	FK	501	GTP	C3'-C2'-C1'	2.12	104.17	100.98
36	MC	501	GTP	O6-C6-C5	-2.12	120.23	124.37
36	GE	501	GTP	O6-C6-C5	-2.12	120.23	124.37
36	EC	501	GTP	O6-C6-C5	-2.12	120.23	124.37
36	QO	501	GTP	O6-C6-C5	-2.12	120.23	124.37
36	PK	501	GTP	O6-C6-C5	-2.12	120.23	124.37
36	JK	501	GTP	O6-C6-C5	-2.12	120.24	124.37
36	CK	501	GTP	O6-C6-C5	-2.12	120.24	124.37
36	CC	501	GTP	O6-C6-C5	-2.11	120.25	124.37
36	FK	501	GTP	O6-C6-C5	-2.11	120.25	124.37
36	OK	501	GTP	O6-C6-C5	-2.11	120.26	124.37
36	SI	501	GTP	O6-C6-C5	-2.11	120.26	124.37
36	FI	501	GTP	C3'-C2'-C1'	2.11	104.15	100.98
36	FM	501	GTP	O6-C6-C5	-2.10	120.26	124.37
36	EM	501	GTP	O6-C6-C5	-2.10	120.27	124.37
36	TI	501	GTP	O6-C6-C5	-2.10	120.28	124.37
36	RM	501	GTP	O6-C6-C5	-2.10	120.28	124.37
36	QI	501	GTP	O6-C6-C5	-2.09	120.28	124.37
36	CG	501	GTP	O6-C6-C5	-2.09	120.28	124.37
36	PM	501	GTP	O6-C6-C5	-2.09	120.29	124.37
36	LC	501	GTP	O6-C6-C5	-2.09	120.29	124.37
36	FI	501	GTP	O6-C6-C5	-2.09	120.29	124.37
36	QC	501	GTP	O6-C6-C5	-2.09	120.29	124.37
36	RO	501	GTP	O6-C6-C5	-2.09	120.29	124.37
38	SH	502	GDP	O6-C6-C5	-2.08	120.30	124.37
36	KC	501	GTP	O6-C6-C5	-2.08	120.30	124.37
36	VG	501	GTP	O6-C6-C5	-2.08	120.30	124.37
36	IC	501	GTP	O6-C6-C5	-2.08	120.31	124.37
36	FG	501	GTP	O6-C6-C5	-2.08	120.31	124.37
38	SD	502	GDP	O6-C6-C5	-2.08	120.32	124.37
36	LI	501	GTP	O6-C6-C5	-2.08	120.32	124.37
36	IE	501	GTP	O6-C6-C5	-2.07	120.33	124.37
36	II	501	GTP	O6-C6-C5	-2.07	120.33	124.37
38	FD	502	GDP	O6-C6-C5	-2.07	120.33	124.37
36	VM	501	GTP	PA-O3A-PB	-2.07	125.72	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	GK	501	GTP	O6-C6-C5	-2.07	120.34	124.37
36	JG	501	GTP	O6-C6-C5	-2.06	120.34	124.37
36	TG	501	GTP	O6-C6-C5	-2.06	120.35	124.37
36	EG	501	GTP	O6-C6-C5	-2.06	120.35	124.37
38	EF	502	GDP	O6-C6-C5	-2.05	120.37	124.37
36	CE	501	GTP	O6-C6-C5	-2.05	120.38	124.37
36	GC	501	GTP	O6-C6-C5	-2.04	120.39	124.37
38	SL	502	GDP	O6-C6-C5	-2.03	120.40	124.37
38	FL	502	GDP	C3'-C2'-C1'	2.03	104.04	100.98
38	FN	502	GDP	O6-C6-C5	-2.03	120.42	124.37
36	SK	501	GTP	PA-O3A-PB	-2.02	125.88	132.83
38	RD	502	GDP	O6-C6-C5	-2.02	120.42	124.37
38	FH	502	GDP	O2B-PB-O3A	2.02	111.41	104.64
38	RF	502	GDP	C2'-C3'-C4'	2.02	106.56	102.64
36	IK	501	GTP	O6-C6-C5	-2.01	120.44	124.37
36	TM	501	GTP	O6-C6-C5	-2.01	120.46	124.37
38	EL	502	GDP	C3'-C2'-C1'	2.00	103.99	100.98
36	KI	501	GTP	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (1035) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	AE	501	GTP	PB-O3A-PA-O5'
36	AG	501	GTP	C5'-O5'-PA-O1A
36	AK	501	GTP	C5'-O5'-PA-O3A
36	AK	501	GTP	C5'-O5'-PA-O1A
36	AM	501	GTP	PB-O3A-PA-O5'
36	AM	501	GTP	C5'-O5'-PA-O1A
36	BA	501	GTP	PB-O3A-PA-O5'
36	BC	501	GTP	C3'-C4'-C5'-O5'
36	BE	501	GTP	PB-O3A-PA-O5'
36	BE	501	GTP	O4'-C4'-C5'-O5'
36	BE	501	GTP	C3'-C4'-C5'-O5'
36	BG	501	GTP	PB-O3A-PA-O5'
36	BI	501	GTP	O4'-C4'-C5'-O5'
36	BI	501	GTP	C3'-C4'-C5'-O5'
36	BK	501	GTP	PB-O3A-PA-O5'
36	BM	501	GTP	PB-O3A-PA-O5'
36	CA	501	GTP	PB-O3A-PA-O5'
36	CA	501	GTP	C3'-C4'-C5'-O5'
36	CC	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	CC	501	GTP	C5'-O5'-PA-O2A
36	CC	501	GTP	C3'-C4'-C5'-O5'
36	CE	501	GTP	C5'-O5'-PA-O3A
36	CE	501	GTP	C5'-O5'-PA-O1A
36	CG	501	GTP	C5'-O5'-PA-O1A
36	CG	501	GTP	C5'-O5'-PA-O2A
36	CG	501	GTP	O4'-C4'-C5'-O5'
36	CG	501	GTP	C3'-C4'-C5'-O5'
36	CI	501	GTP	C5'-O5'-PA-O1A
36	CK	501	GTP	PB-O3B-PG-O2G
36	CK	501	GTP	PB-O3B-PG-O3G
36	CK	501	GTP	PB-O3A-PA-O5'
36	CK	501	GTP	C5'-O5'-PA-O3A
36	CK	501	GTP	C5'-O5'-PA-O1A
36	CK	501	GTP	C5'-O5'-PA-O2A
36	CK	501	GTP	C3'-C4'-C5'-O5'
36	CM	501	GTP	O4'-C4'-C5'-O5'
36	CM	501	GTP	C3'-C4'-C5'-O5'
36	DA	501	GTP	C5'-O5'-PA-O1A
36	DC	501	GTP	C5'-O5'-PA-O1A
36	DC	501	GTP	C5'-O5'-PA-O2A
36	DE	501	GTP	C5'-O5'-PA-O3A
36	DE	501	GTP	C5'-O5'-PA-O2A
36	DG	501	GTP	C5'-O5'-PA-O1A
36	DG	501	GTP	C5'-O5'-PA-O2A
36	DI	501	GTP	C5'-O5'-PA-O3A
36	DK	501	GTP	C5'-O5'-PA-O3A
36	DM	501	GTP	C5'-O5'-PA-O3A
36	EC	501	GTP	C5'-O5'-PA-O1A
36	EC	501	GTP	C5'-O5'-PA-O2A
36	EE	501	GTP	C5'-O5'-PA-O3A
36	EE	501	GTP	C5'-O5'-PA-O2A
36	EG	501	GTP	C5'-O5'-PA-O3A
36	EI	501	GTP	C5'-O5'-PA-O1A
36	EI	501	GTP	C5'-O5'-PA-O2A
36	EK	501	GTP	C5'-O5'-PA-O3A
36	EK	501	GTP	C5'-O5'-PA-O2A
36	EM	501	GTP	C5'-O5'-PA-O3A
36	EM	501	GTP	C5'-O5'-PA-O2A
36	FC	501	GTP	C5'-O5'-PA-O3A
36	FC	501	GTP	C5'-O5'-PA-O2A
36	FE	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	FE	501	GTP	C5'-O5'-PA-O2A
36	FG	501	GTP	C5'-O5'-PA-O3A
36	FI	501	GTP	C5'-O5'-PA-O3A
36	FK	501	GTP	PB-O3A-PA-O5'
36	FK	501	GTP	C5'-O5'-PA-O3A
36	FM	501	GTP	C5'-O5'-PA-O3A
36	GC	501	GTP	C3'-C4'-C5'-O5'
36	GE	501	GTP	PB-O3A-PA-O5'
36	GE	501	GTP	C5'-O5'-PA-O1A
36	GG	501	GTP	C5'-O5'-PA-O1A
36	GI	501	GTP	PB-O3A-PA-O5'
36	GK	501	GTP	PB-O3A-PA-O5'
36	GK	501	GTP	C5'-O5'-PA-O1A
36	GM	501	GTP	PB-O3A-PA-O5'
36	HC	501	GTP	C3'-C4'-C5'-O5'
36	HE	501	GTP	C3'-C4'-C5'-O5'
36	HG	501	GTP	O4'-C4'-C5'-O5'
36	HG	501	GTP	C3'-C4'-C5'-O5'
36	HI	501	GTP	C5'-O5'-PA-O1A
36	HK	501	GTP	O4'-C4'-C5'-O5'
36	HK	501	GTP	C3'-C4'-C5'-O5'
36	HM	501	GTP	O4'-C4'-C5'-O5'
36	HM	501	GTP	C3'-C4'-C5'-O5'
36	HO	501	GTP	PB-O3A-PA-O5'
36	HO	501	GTP	C5'-O5'-PA-O1A
36	HO	501	GTP	C5'-O5'-PA-O2A
36	HO	501	GTP	C3'-C4'-C5'-O5'
36	IC	501	GTP	O4'-C4'-C5'-O5'
36	IC	501	GTP	C3'-C4'-C5'-O5'
36	IE	501	GTP	O4'-C4'-C5'-O5'
36	IE	501	GTP	C3'-C4'-C5'-O5'
36	IG	501	GTP	C5'-O5'-PA-O1A
36	IG	501	GTP	C5'-O5'-PA-O2A
36	II	501	GTP	C5'-O5'-PA-O1A
36	IK	501	GTP	PB-O3A-PA-O5'
36	IK	501	GTP	C5'-O5'-PA-O1A
36	IM	501	GTP	C5'-O5'-PA-O1A
36	IM	501	GTP	C5'-O5'-PA-O2A
36	IO	501	GTP	C5'-O5'-PA-O3A
36	IO	501	GTP	C5'-O5'-PA-O1A
36	IO	501	GTP	C5'-O5'-PA-O2A
36	JC	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	JC	501	GTP	C5'-O5'-PA-O2A
36	JE	501	GTP	C5'-O5'-PA-O3A
36	JE	501	GTP	C5'-O5'-PA-O1A
36	JK	501	GTP	C5'-O5'-PA-O3A
36	JK	501	GTP	C5'-O5'-PA-O2A
36	JM	501	GTP	C5'-O5'-PA-O1A
36	JM	501	GTP	C5'-O5'-PA-O2A
36	KC	501	GTP	C5'-O5'-PA-O3A
36	KC	501	GTP	C5'-O5'-PA-O2A
36	KE	501	GTP	C5'-O5'-PA-O3A
36	KE	501	GTP	C5'-O5'-PA-O1A
36	KE	501	GTP	C5'-O5'-PA-O2A
36	KG	501	GTP	C5'-O5'-PA-O3A
36	KG	501	GTP	C5'-O5'-PA-O1A
36	KG	501	GTP	C5'-O5'-PA-O2A
36	KI	501	GTP	C5'-O5'-PA-O1A
36	KI	501	GTP	C5'-O5'-PA-O2A
36	KK	501	GTP	C5'-O5'-PA-O1A
36	KK	501	GTP	C5'-O5'-PA-O2A
36	KM	501	GTP	C5'-O5'-PA-O1A
36	KM	501	GTP	C5'-O5'-PA-O2A
36	KO	501	GTP	C5'-O5'-PA-O1A
36	KO	501	GTP	C5'-O5'-PA-O2A
36	LC	501	GTP	C5'-O5'-PA-O1A
36	LC	501	GTP	C5'-O5'-PA-O2A
36	LE	501	GTP	C5'-O5'-PA-O3A
36	LE	501	GTP	C5'-O5'-PA-O2A
36	LG	501	GTP	C5'-O5'-PA-O1A
36	LG	501	GTP	C5'-O5'-PA-O2A
36	LI	501	GTP	C5'-O5'-PA-O3A
36	LI	501	GTP	C5'-O5'-PA-O1A
36	LI	501	GTP	C5'-O5'-PA-O2A
36	LK	501	GTP	C5'-O5'-PA-O3A
36	LK	501	GTP	C5'-O5'-PA-O1A
36	LK	501	GTP	C5'-O5'-PA-O2A
36	MC	501	GTP	C5'-O5'-PA-O3A
36	MC	501	GTP	C5'-O5'-PA-O2A
36	MG	501	GTP	C5'-O5'-PA-O3A
36	MG	501	GTP	C5'-O5'-PA-O2A
36	MI	501	GTP	C5'-O5'-PA-O3A
36	MI	501	GTP	C5'-O5'-PA-O2A
36	MK	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	MM	501	GTP	C5'-O5'-PA-O3A
36	MM	501	GTP	C5'-O5'-PA-O2A
36	NE	501	GTP	PB-O3A-PA-O5'
36	NE	501	GTP	C3'-C4'-C5'-O5'
36	NG	501	GTP	PB-O3B-PG-O3G
36	NI	501	GTP	C5'-O5'-PA-O1A
36	NK	501	GTP	PB-O3A-PA-O5'
36	NM	501	GTP	PB-O3A-PA-O5'
36	OC	501	GTP	C5'-O5'-PA-O1A
36	OC	501	GTP	C3'-C4'-C5'-O5'
36	OE	501	GTP	PB-O3A-PA-O5'
36	OE	501	GTP	O4'-C4'-C5'-O5'
36	OE	501	GTP	C3'-C4'-C5'-O5'
36	OG	501	GTP	PB-O3A-PA-O5'
36	OI	501	GTP	C5'-O5'-PA-O3A
36	OI	501	GTP	C5'-O5'-PA-O2A
36	OK	501	GTP	O4'-C4'-C5'-O5'
36	OK	501	GTP	C3'-C4'-C5'-O5'
36	OM	501	GTP	C5'-O5'-PA-O3A
36	OM	501	GTP	C5'-O5'-PA-O2A
36	OM	501	GTP	C3'-C4'-C5'-O5'
36	OO	501	GTP	C5'-O5'-PA-O1A
36	OO	501	GTP	C5'-O5'-PA-O2A
36	PC	501	GTP	C5'-O5'-PA-O3A
36	PC	501	GTP	C5'-O5'-PA-O2A
36	PC	501	GTP	C3'-C4'-C5'-O5'
36	PE	501	GTP	PB-O3A-PA-O5'
36	PE	501	GTP	O4'-C4'-C5'-O5'
36	PE	501	GTP	C3'-C4'-C5'-O5'
36	PG	501	GTP	C5'-O5'-PA-O3A
36	PG	501	GTP	C5'-O5'-PA-O1A
36	PG	501	GTP	C5'-O5'-PA-O2A
36	PI	501	GTP	C5'-O5'-PA-O3A
36	PI	501	GTP	C5'-O5'-PA-O2A
36	PM	501	GTP	C5'-O5'-PA-O3A
36	PM	501	GTP	C5'-O5'-PA-O1A
36	PM	501	GTP	C5'-O5'-PA-O2A
36	PO	501	GTP	PB-O3A-PA-O5'
36	PO	501	GTP	O4'-C4'-C5'-O5'
36	PO	501	GTP	C3'-C4'-C5'-O5'
36	QC	501	GTP	C3'-C4'-C5'-O5'
36	QE	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	QE	501	GTP	C3’-C4’-C5’-O5’
36	QG	501	GTP	C5’-O5’-PA-O1A
36	QG	501	GTP	C5’-O5’-PA-O2A
36	QI	501	GTP	C5’-O5’-PA-O3A
36	QI	501	GTP	C5’-O5’-PA-O1A
36	QI	501	GTP	C5’-O5’-PA-O2A
36	QK	501	GTP	C5’-O5’-PA-O3A
36	QK	501	GTP	O4’-C4’-C5’-O5’
36	QK	501	GTP	C3’-C4’-C5’-O5’
36	QM	501	GTP	PB-O3A-PA-O5’
36	QM	501	GTP	C5’-O5’-PA-O3A
36	QM	501	GTP	C5’-O5’-PA-O2A
36	QM	501	GTP	C3’-C4’-C5’-O5’
36	QO	501	GTP	C5’-O5’-PA-O1A
36	QO	501	GTP	C5’-O5’-PA-O2A
36	RC	501	GTP	C5’-O5’-PA-O3A
36	RC	501	GTP	C5’-O5’-PA-O2A
36	RE	501	GTP	C5’-O5’-PA-O3A
36	RE	501	GTP	C5’-O5’-PA-O2A
36	RG	501	GTP	C5’-O5’-PA-O3A
36	RG	501	GTP	C5’-O5’-PA-O2A
36	RM	501	GTP	C5’-O5’-PA-O1A
36	RM	501	GTP	C5’-O5’-PA-O2A
36	RO	501	GTP	C5’-O5’-PA-O3A
36	RO	501	GTP	C5’-O5’-PA-O2A
36	SE	501	GTP	C5’-O5’-PA-O3A
36	SG	501	GTP	C5’-O5’-PA-O3A
36	SG	501	GTP	C5’-O5’-PA-O1A
36	SG	501	GTP	C5’-O5’-PA-O2A
36	SI	501	GTP	C5’-O5’-PA-O3A
36	SK	501	GTP	C5’-O5’-PA-O3A
36	SM	501	GTP	C5’-O5’-PA-O3A
36	SO	501	GTP	C5’-O5’-PA-O1A
36	TE	501	GTP	C5’-O5’-PA-O1A
36	TG	501	GTP	C5’-O5’-PA-O3A
36	TG	501	GTP	C5’-O5’-PA-O2A
36	TK	501	GTP	PB-O3A-PA-O5’
36	UE	501	GTP	PB-O3A-PA-O5’
36	UI	501	GTP	C3’-C4’-C5’-O5’
36	UK	501	GTP	C5’-O5’-PA-O1A
36	UM	501	GTP	C5’-O5’-PA-O3A
36	UM	501	GTP	C5’-O5’-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	UM	501	GTP	C5'-O5'-PA-O2A
36	UM	501	GTP	C3'-C4'-C5'-O5'
36	UO	501	GTP	PB-O3A-PA-O5'
36	VE	501	GTP	PB-O3A-PA-O5'
36	VG	501	GTP	C5'-O5'-PA-O1A
36	VG	501	GTP	C5'-O5'-PA-O2A
36	VG	501	GTP	O4'-C4'-C5'-O5'
36	VG	501	GTP	C3'-C4'-C5'-O5'
36	VI	501	GTP	C5'-O5'-PA-O1A
36	VI	501	GTP	C5'-O5'-PA-O2A
36	VI	501	GTP	O4'-C4'-C5'-O5'
36	VI	501	GTP	C3'-C4'-C5'-O5'
36	VK	501	GTP	O4'-C4'-C5'-O5'
36	VK	501	GTP	C3'-C4'-C5'-O5'
36	VM	501	GTP	C5'-O5'-PA-O3A
36	VM	501	GTP	C5'-O5'-PA-O2A
36	VM	501	GTP	C3'-C4'-C5'-O5'
36	VO	501	GTP	O4'-C4'-C5'-O5'
36	VO	501	GTP	C3'-C4'-C5'-O5'
36	WE	501	GTP	O4'-C4'-C5'-O5'
36	WE	501	GTP	C3'-C4'-C5'-O5'
36	WG	501	GTP	C5'-O5'-PA-O1A
36	WG	501	GTP	O4'-C4'-C5'-O5'
36	WG	501	GTP	C3'-C4'-C5'-O5'
36	WI	501	GTP	C5'-O5'-PA-O3A
36	WK	501	GTP	C5'-O5'-PA-O1A
36	WK	501	GTP	C5'-O5'-PA-O2A
36	WM	501	GTP	C5'-O5'-PA-O3A
36	WM	501	GTP	C5'-O5'-PA-O2A
36	WM	501	GTP	O4'-C4'-C5'-O5'
36	WM	501	GTP	C3'-C4'-C5'-O5'
36	WO	501	GTP	O4'-C4'-C5'-O5'
38	AB	502	GDP	C5'-O5'-PA-O1A
38	AJ	502	GDP	C5'-O5'-PA-O1A
38	BB	502	GDP	C5'-O5'-PA-O1A
38	BD	502	GDP	C5'-O5'-PA-O1A
38	BF	502	GDP	C5'-O5'-PA-O3A
38	BF	502	GDP	C5'-O5'-PA-O1A
38	BJ	502	GDP	PA-O3A-PB-O2B
38	BJ	502	GDP	C5'-O5'-PA-O1A
38	BL	502	GDP	C5'-O5'-PA-O1A
38	CB	502	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	CF	502	GDP	C5'-O5'-PA-O1A
38	DH	502	GDP	C5'-O5'-PA-O1A
38	FB	502	GDP	C5'-O5'-PA-O1A
38	FD	502	GDP	C5'-O5'-PA-O1A
38	FD	502	GDP	C3'-C4'-C5'-O5'
38	GB	502	GDP	C5'-O5'-PA-O1A
38	GJ	502	GDP	C5'-O5'-PA-O1A
38	HL	502	GDP	C5'-O5'-PA-O1A
38	IB	502	GDP	C5'-O5'-PA-O1A
38	ID	502	GDP	C5'-O5'-PA-O1A
38	IF	502	GDP	C5'-O5'-PA-O3A
38	IF	502	GDP	C5'-O5'-PA-O1A
38	IH	502	GDP	C5'-O5'-PA-O1A
38	IJ	502	GDP	C5'-O5'-PA-O1A
38	IL	502	GDP	C5'-O5'-PA-O1A
38	IN	502	GDP	C5'-O5'-PA-O1A
38	JF	502	GDP	C5'-O5'-PA-O1A
38	KD	502	GDP	C5'-O5'-PA-O1A
38	KF	502	GDP	C5'-O5'-PA-O3A
38	KF	502	GDP	C5'-O5'-PA-O1A
38	KJ	502	GDP	C5'-O5'-PA-O1A
38	KL	502	GDP	C5'-O5'-PA-O1A
38	KN	502	GDP	C5'-O5'-PA-O1A
38	LD	502	GDP	C5'-O5'-PA-O1A
38	LH	502	GDP	C5'-O5'-PA-O1A
38	LH	502	GDP	C3'-C4'-C5'-O5'
38	LJ	502	GDP	C5'-O5'-PA-O1A
38	LL	502	GDP	C5'-O5'-PA-O1A
38	LN	502	GDP	C5'-O5'-PA-O3A
38	LN	502	GDP	C5'-O5'-PA-O1A
38	MH	502	GDP	C5'-O5'-PA-O1A
38	ML	502	GDP	C5'-O5'-PA-O3A
38	ML	502	GDP	C5'-O5'-PA-O1A
38	OB	502	GDP	C5'-O5'-PA-O3A
38	OB	502	GDP	C5'-O5'-PA-O1A
38	OD	502	GDP	C5'-O5'-PA-O3A
38	OD	502	GDP	C5'-O5'-PA-O1A
38	OF	502	GDP	C5'-O5'-PA-O1A
38	OF	502	GDP	O4'-C4'-C5'-O5'
38	OF	502	GDP	C3'-C4'-C5'-O5'
38	OH	502	GDP	C5'-O5'-PA-O1A
38	OJ	502	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	OL	502	GDP	C5'-O5'-PA-O1A
38	ON	502	GDP	C5'-O5'-PA-O1A
38	PD	502	GDP	C5'-O5'-PA-O1A
38	PD	502	GDP	O4'-C4'-C5'-O5'
38	PD	502	GDP	C3'-C4'-C5'-O5'
38	PH	502	GDP	C5'-O5'-PA-O1A
38	PJ	502	GDP	C5'-O5'-PA-O1A
38	PL	502	GDP	C5'-O5'-PA-O1A
38	PN	502	GDP	C5'-O5'-PA-O3A
38	QD	502	GDP	C5'-O5'-PA-O1A
38	QH	502	GDP	C5'-O5'-PA-O1A
38	QJ	502	GDP	C5'-O5'-PA-O1A
38	QN	502	GDP	C5'-O5'-PA-O1A
38	SH	502	GDP	C5'-O5'-PA-O1A
38	SN	502	GDP	C5'-O5'-PA-O1A
38	TF	502	GDP	C5'-O5'-PA-O1A
38	TJ	502	GDP	C5'-O5'-PA-O1A
38	TL	502	GDP	C5'-O5'-PA-O3A
38	TN	502	GDP	C5'-O5'-PA-O1A
38	UD	502	GDP	C5'-O5'-PA-O1A
38	UF	502	GDP	C5'-O5'-PA-O1A
38	UJ	502	GDP	C5'-O5'-PA-O1A
38	UP	502	GDP	C5'-O5'-PA-O1A
38	VJ	502	GDP	C5'-O5'-PA-O1A
38	VL	502	GDP	C5'-O5'-PA-O1A
38	VN	502	GDP	C5'-O5'-PA-O1A
38	VP	502	GDP	C5'-O5'-PA-O1A
38	WD	502	GDP	C5'-O5'-PA-O1A
38	WF	502	GDP	C5'-O5'-PA-O3A
38	WF	502	GDP	C5'-O5'-PA-O1A
38	WH	502	GDP	C5'-O5'-PA-O1A
38	WJ	502	GDP	C5'-O5'-PA-O3A
38	WJ	502	GDP	C5'-O5'-PA-O1A
38	WL	502	GDP	C5'-O5'-PA-O1A
38	WN	502	GDP	C5'-O5'-PA-O3A
38	WN	502	GDP	C5'-O5'-PA-O1A
38	WP	502	GDP	C5'-O5'-PA-O1A
36	AC	501	GTP	C3'-C4'-C5'-O5'
36	AE	501	GTP	C3'-C4'-C5'-O5'
36	BC	501	GTP	O4'-C4'-C5'-O5'
36	BM	501	GTP	O4'-C4'-C5'-O5'
36	BM	501	GTP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	CA	501	GTP	O4'-C4'-C5'-O5'
36	CC	501	GTP	O4'-C4'-C5'-O5'
36	CK	501	GTP	O4'-C4'-C5'-O5'
36	GC	501	GTP	O4'-C4'-C5'-O5'
36	GI	501	GTP	C3'-C4'-C5'-O5'
36	HC	501	GTP	O4'-C4'-C5'-O5'
36	HE	501	GTP	O4'-C4'-C5'-O5'
36	HO	501	GTP	O4'-C4'-C5'-O5'
36	IK	501	GTP	C3'-C4'-C5'-O5'
36	NE	501	GTP	O4'-C4'-C5'-O5'
36	OC	501	GTP	O4'-C4'-C5'-O5'
36	OG	501	GTP	C3'-C4'-C5'-O5'
36	OM	501	GTP	O4'-C4'-C5'-O5'
36	OO	501	GTP	C3'-C4'-C5'-O5'
36	PC	501	GTP	O4'-C4'-C5'-O5'
36	PM	501	GTP	C3'-C4'-C5'-O5'
36	QC	501	GTP	O4'-C4'-C5'-O5'
36	QE	501	GTP	O4'-C4'-C5'-O5'
36	QM	501	GTP	O4'-C4'-C5'-O5'
36	UI	501	GTP	O4'-C4'-C5'-O5'
36	UM	501	GTP	O4'-C4'-C5'-O5'
36	VE	501	GTP	O4'-C4'-C5'-O5'
36	VE	501	GTP	C3'-C4'-C5'-O5'
36	VM	501	GTP	O4'-C4'-C5'-O5'
36	WO	501	GTP	C3'-C4'-C5'-O5'
38	FD	502	GDP	O4'-C4'-C5'-O5'
38	LH	502	GDP	O4'-C4'-C5'-O5'
38	ML	502	GDP	C3'-C4'-C5'-O5'
38	QD	502	GDP	C3'-C4'-C5'-O5'
38	TL	502	GDP	O4'-C4'-C5'-O5'
38	TL	502	GDP	C3'-C4'-C5'-O5'
38	TN	502	GDP	C3'-C4'-C5'-O5'
36	DI	501	GTP	C4'-C5'-O5'-PA
36	WI	501	GTP	C4'-C5'-O5'-PA
36	AC	501	GTP	O4'-C4'-C5'-O5'
36	AE	501	GTP	O4'-C4'-C5'-O5'
36	BA	501	GTP	O4'-C4'-C5'-O5'
36	BA	501	GTP	C3'-C4'-C5'-O5'
36	CE	501	GTP	O4'-C4'-C5'-O5'
36	CE	501	GTP	C3'-C4'-C5'-O5'
36	GI	501	GTP	O4'-C4'-C5'-O5'
36	IK	501	GTP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	OG	501	GTP	O4'-C4'-C5'-O5'
36	OO	501	GTP	O4'-C4'-C5'-O5'
36	PK	501	GTP	O4'-C4'-C5'-O5'
36	PK	501	GTP	C3'-C4'-C5'-O5'
36	PM	501	GTP	O4'-C4'-C5'-O5'
38	FH	502	GDP	O4'-C4'-C5'-O5'
38	FH	502	GDP	C3'-C4'-C5'-O5'
38	ML	502	GDP	O4'-C4'-C5'-O5'
38	QD	502	GDP	O4'-C4'-C5'-O5'
38	TN	502	GDP	O4'-C4'-C5'-O5'
36	FI	501	GTP	C4'-C5'-O5'-PA
36	NG	501	GTP	O4'-C4'-C5'-O5'
36	NG	501	GTP	C3'-C4'-C5'-O5'
38	OB	502	GDP	C3'-C4'-C5'-O5'
36	AA	501	GTP	C3'-C4'-C5'-O5'
36	BG	501	GTP	C3'-C4'-C5'-O5'
36	CI	501	GTP	C3'-C4'-C5'-O5'
36	DG	501	GTP	C3'-C4'-C5'-O5'
36	IO	501	GTP	C3'-C4'-C5'-O5'
36	NC	501	GTP	C3'-C4'-C5'-O5'
36	NK	501	GTP	C3'-C4'-C5'-O5'
38	LD	502	GDP	C3'-C4'-C5'-O5'
38	QN	502	GDP	C3'-C4'-C5'-O5'
38	SN	502	GDP	C3'-C4'-C5'-O5'
38	TD	502	GDP	C3'-C4'-C5'-O5'
36	AA	501	GTP	O4'-C4'-C5'-O5'
36	BG	501	GTP	O4'-C4'-C5'-O5'
36	BK	501	GTP	C3'-C4'-C5'-O5'
36	DG	501	GTP	O4'-C4'-C5'-O5'
36	HI	501	GTP	C3'-C4'-C5'-O5'
36	IM	501	GTP	C3'-C4'-C5'-O5'
36	IO	501	GTP	O4'-C4'-C5'-O5'
36	LE	501	GTP	C3'-C4'-C5'-O5'
36	NK	501	GTP	O4'-C4'-C5'-O5'
36	NM	501	GTP	C3'-C4'-C5'-O5'
36	QO	501	GTP	C3'-C4'-C5'-O5'
36	RK	501	GTP	C3'-C4'-C5'-O5'
36	UO	501	GTP	C3'-C4'-C5'-O5'
38	ED	502	GDP	C3'-C4'-C5'-O5'
38	GJ	502	GDP	C3'-C4'-C5'-O5'
38	LD	502	GDP	O4'-C4'-C5'-O5'
38	OB	502	GDP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	PH	502	GDP	C3'-C4'-C5'-O5'
38	SN	502	GDP	O4'-C4'-C5'-O5'
38	TD	502	GDP	O4'-C4'-C5'-O5'
38	WD	502	GDP	C3'-C4'-C5'-O5'
36	DK	501	GTP	C4'-C5'-O5'-PA
36	OI	501	GTP	C4'-C5'-O5'-PA
36	LC	501	GTP	C3'-C4'-C5'-O5'
36	LM	501	GTP	C3'-C4'-C5'-O5'
36	NC	501	GTP	O4'-C4'-C5'-O5'
36	QI	501	GTP	C3'-C4'-C5'-O5'
38	GD	502	GDP	C3'-C4'-C5'-O5'
38	ON	502	GDP	C3'-C4'-C5'-O5'
38	TJ	502	GDP	C3'-C4'-C5'-O5'
38	BF	502	GDP	PA-O3A-PB-O1B
38	BH	502	GDP	PA-O3A-PB-O1B
38	BJ	502	GDP	PA-O3A-PB-O1B
36	SK	501	GTP	C4'-C5'-O5'-PA
36	DA	501	GTP	PB-O3A-PA-O1A
36	DG	501	GTP	PB-O3A-PA-O1A
36	FE	501	GTP	PA-O3A-PB-O1B
36	FI	501	GTP	PB-O3A-PA-O1A
36	HI	501	GTP	PB-O3A-PA-O1A
36	QE	501	GTP	PA-O3A-PB-O1B
36	QK	501	GTP	PA-O3A-PB-O1B
36	QK	501	GTP	PB-O3A-PA-O1A
36	TE	501	GTP	PA-O3A-PB-O1B
36	WG	501	GTP	PB-O3A-PA-O1A
36	AI	501	GTP	C3'-C4'-C5'-O5'
38	KB	502	GDP	C3'-C4'-C5'-O5'
38	QL	502	GDP	C3'-C4'-C5'-O5'
36	FM	501	GTP	C4'-C5'-O5'-PA
36	CI	501	GTP	O4'-C4'-C5'-O5'
36	HI	501	GTP	O4'-C4'-C5'-O5'
36	LE	501	GTP	O4'-C4'-C5'-O5'
38	ED	502	GDP	O4'-C4'-C5'-O5'
38	QN	502	GDP	O4'-C4'-C5'-O5'
36	CI	501	GTP	C4'-C5'-O5'-PA
36	CK	501	GTP	C4'-C5'-O5'-PA
36	DC	501	GTP	C4'-C5'-O5'-PA
36	HI	501	GTP	C4'-C5'-O5'-PA
36	HO	501	GTP	C4'-C5'-O5'-PA
36	II	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	IM	501	GTP	C4'-C5'-O5'-PA
36	JG	501	GTP	C4'-C5'-O5'-PA
36	JK	501	GTP	C4'-C5'-O5'-PA
36	LI	501	GTP	C4'-C5'-O5'-PA
36	LK	501	GTP	C4'-C5'-O5'-PA
36	MC	501	GTP	C4'-C5'-O5'-PA
36	OC	501	GTP	C4'-C5'-O5'-PA
36	PI	501	GTP	C4'-C5'-O5'-PA
36	QE	501	GTP	C4'-C5'-O5'-PA
36	QK	501	GTP	C4'-C5'-O5'-PA
36	SM	501	GTP	C4'-C5'-O5'-PA
36	TE	501	GTP	C4'-C5'-O5'-PA
36	WE	501	GTP	C4'-C5'-O5'-PA
36	WK	501	GTP	C4'-C5'-O5'-PA
36	WO	501	GTP	C4'-C5'-O5'-PA
36	AA	501	GTP	PB-O3A-PA-O5'
36	AC	501	GTP	PB-O3A-PA-O5'
36	AG	501	GTP	PB-O3A-PA-O5'
36	AI	501	GTP	PB-O3A-PA-O5'
36	AK	501	GTP	PB-O3A-PA-O5'
36	BC	501	GTP	PB-O3A-PA-O5'
36	BI	501	GTP	PB-O3A-PA-O5'
36	CC	501	GTP	PB-O3A-PA-O5'
36	GC	501	GTP	PB-O3A-PA-O5'
36	GG	501	GTP	PB-O3A-PA-O5'
36	HC	501	GTP	PB-O3A-PA-O5'
36	HE	501	GTP	PB-O3A-PA-O5'
36	HG	501	GTP	PB-O3A-PA-O5'
36	HK	501	GTP	PB-O3A-PA-O5'
36	HM	501	GTP	PB-O3A-PA-O5'
36	IC	501	GTP	PB-O3A-PA-O5'
36	IE	501	GTP	PB-O3A-PA-O5'
36	KE	501	GTP	PB-O3A-PA-O5'
36	LE	501	GTP	PB-O3A-PA-O5'
36	LM	501	GTP	PB-O3A-PA-O5'
36	ME	501	GTP	PB-O3A-PA-O5'
36	MM	501	GTP	PB-O3A-PA-O5'
36	NC	501	GTP	PB-O3A-PA-O5'
36	NG	501	GTP	PB-O3A-PA-O5'
36	NI	501	GTP	PB-O3A-PA-O5'
36	OK	501	GTP	PB-O3A-PA-O5'
36	OM	501	GTP	PB-O3A-PA-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	PC	501	GTP	PB-O3A-PA-O5’
36	PK	501	GTP	PB-O3A-PA-O5’
36	QE	501	GTP	PB-O3A-PA-O5’
36	QK	501	GTP	PB-O3A-PA-O5’
36	SO	501	GTP	PB-O3A-PA-O5’
36	TE	501	GTP	PB-O3A-PA-O5’
36	TI	501	GTP	PB-O3A-PA-O5’
36	TM	501	GTP	PB-O3A-PA-O5’
36	TO	501	GTP	PB-O3A-PA-O5’
36	UG	501	GTP	PB-O3A-PA-O5’
36	UI	501	GTP	PB-O3A-PA-O5’
36	UK	501	GTP	PB-O3A-PA-O5’
36	UM	501	GTP	PB-O3A-PA-O5’
36	VG	501	GTP	PB-O3A-PA-O5’
36	VK	501	GTP	PB-O3A-PA-O5’
36	VM	501	GTP	PB-O3A-PA-O5’
36	VO	501	GTP	PB-O3A-PA-O5’
36	WE	501	GTP	PB-O3A-PA-O5’
36	WM	501	GTP	PB-O3A-PA-O5’
36	QO	501	GTP	O4’-C4’-C5’-O5’
36	UO	501	GTP	O4’-C4’-C5’-O5’
38	GJ	502	GDP	O4’-C4’-C5’-O5’
36	DM	501	GTP	C4’-C5’-O5’-PA
36	EG	501	GTP	C4’-C5’-O5’-PA
36	KE	501	GTP	C4’-C5’-O5’-PA
36	KG	501	GTP	C4’-C5’-O5’-PA
36	KK	501	GTP	C4’-C5’-O5’-PA
36	LG	501	GTP	C4’-C5’-O5’-PA
36	OO	501	GTP	C4’-C5’-O5’-PA
36	RK	501	GTP	C4’-C5’-O5’-PA
36	SI	501	GTP	C4’-C5’-O5’-PA
36	UM	501	GTP	C4’-C5’-O5’-PA
36	VK	501	GTP	C4’-C5’-O5’-PA
36	WG	501	GTP	C4’-C5’-O5’-PA
38	BH	502	GDP	PA-O3A-PB-O2B
36	CI	501	GTP	C5’-O5’-PA-O3A
36	DA	501	GTP	C5’-O5’-PA-O3A
36	EI	501	GTP	C5’-O5’-PA-O3A
36	HI	501	GTP	C5’-O5’-PA-O3A
36	II	501	GTP	C5’-O5’-PA-O3A
36	OC	501	GTP	C5’-O5’-PA-O3A
36	QG	501	GTP	C5’-O5’-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	RI	501	GTP	C5'-O5'-PA-O3A
36	SO	501	GTP	C5'-O5'-PA-O3A
36	WG	501	GTP	C5'-O5'-PA-O3A
38	BJ	502	GDP	C5'-O5'-PA-O3A
38	LH	502	GDP	C5'-O5'-PA-O3A
38	LJ	502	GDP	C5'-O5'-PA-O3A
38	QD	502	GDP	C5'-O5'-PA-O3A
38	UJ	502	GDP	C5'-O5'-PA-O3A
36	BK	501	GTP	O4'-C4'-C5'-O5'
36	KK	501	GTP	C3'-C4'-C5'-O5'
36	LM	501	GTP	O4'-C4'-C5'-O5'
36	NM	501	GTP	O4'-C4'-C5'-O5'
36	PG	501	GTP	C3'-C4'-C5'-O5'
36	TK	501	GTP	C3'-C4'-C5'-O5'
38	OL	502	GDP	C3'-C4'-C5'-O5'
38	PH	502	GDP	O4'-C4'-C5'-O5'
38	TH	502	GDP	C3'-C4'-C5'-O5'
36	CC	501	GTP	PA-O3A-PB-O2B
36	CI	501	GTP	PB-O3A-PA-O2A
36	EE	501	GTP	PB-O3A-PA-O2A
36	EG	501	GTP	PB-O3A-PA-O2A
36	EI	501	GTP	PB-O3A-PA-O2A
36	FK	501	GTP	PA-O3A-PB-O1B
36	IM	501	GTP	PB-O3A-PA-O2A
36	KG	501	GTP	PA-O3A-PB-O2B
36	KK	501	GTP	PA-O3A-PB-O2B
36	KO	501	GTP	PA-O3A-PB-O2B
36	LC	501	GTP	PA-O3A-PB-O2B
36	MI	501	GTP	PA-O3A-PB-O2B
36	MK	501	GTP	PA-O3A-PB-O2B
36	OM	501	GTP	PA-O3A-PB-O2B
36	OO	501	GTP	PA-O3A-PB-O2B
36	QG	501	GTP	PB-O3A-PA-O2A
36	QO	501	GTP	PA-O3A-PB-O2B
36	SM	501	GTP	PA-O3A-PB-O2B
36	TG	501	GTP	PA-O3A-PB-O2B
36	UM	501	GTP	PB-O3A-PA-O1A
36	VM	501	GTP	PA-O3A-PB-O2B
36	WM	501	GTP	PA-O3A-PB-O2B
36	CC	501	GTP	C4'-C5'-O5'-PA
36	CG	501	GTP	C4'-C5'-O5'-PA
36	CM	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	DA	501	GTP	C4'-C5'-O5'-PA
36	EC	501	GTP	C4'-C5'-O5'-PA
36	EE	501	GTP	C4'-C5'-O5'-PA
36	EI	501	GTP	C4'-C5'-O5'-PA
36	FC	501	GTP	C4'-C5'-O5'-PA
36	FE	501	GTP	C4'-C5'-O5'-PA
36	FG	501	GTP	C4'-C5'-O5'-PA
36	HG	501	GTP	C4'-C5'-O5'-PA
36	IG	501	GTP	C4'-C5'-O5'-PA
36	IO	501	GTP	C4'-C5'-O5'-PA
36	JC	501	GTP	C4'-C5'-O5'-PA
36	KC	501	GTP	C4'-C5'-O5'-PA
36	KI	501	GTP	C4'-C5'-O5'-PA
36	KM	501	GTP	C4'-C5'-O5'-PA
36	KO	501	GTP	C4'-C5'-O5'-PA
36	LC	501	GTP	C4'-C5'-O5'-PA
36	LE	501	GTP	C4'-C5'-O5'-PA
36	MG	501	GTP	C4'-C5'-O5'-PA
36	MI	501	GTP	C4'-C5'-O5'-PA
36	MK	501	GTP	C4'-C5'-O5'-PA
36	MM	501	GTP	C4'-C5'-O5'-PA
36	OK	501	GTP	C4'-C5'-O5'-PA
36	OM	501	GTP	C4'-C5'-O5'-PA
36	PC	501	GTP	C4'-C5'-O5'-PA
36	PM	501	GTP	C4'-C5'-O5'-PA
36	QG	501	GTP	C4'-C5'-O5'-PA
36	QI	501	GTP	C4'-C5'-O5'-PA
36	QM	501	GTP	C4'-C5'-O5'-PA
36	QO	501	GTP	C4'-C5'-O5'-PA
36	RC	501	GTP	C4'-C5'-O5'-PA
36	RG	501	GTP	C4'-C5'-O5'-PA
36	RO	501	GTP	C4'-C5'-O5'-PA
36	SE	501	GTP	C4'-C5'-O5'-PA
36	SG	501	GTP	C4'-C5'-O5'-PA
36	TG	501	GTP	C4'-C5'-O5'-PA
36	UK	501	GTP	C4'-C5'-O5'-PA
36	VI	501	GTP	C4'-C5'-O5'-PA
36	VM	501	GTP	C4'-C5'-O5'-PA
36	WM	501	GTP	C4'-C5'-O5'-PA
36	CI	501	GTP	C5'-O5'-PA-O2A
36	DA	501	GTP	C5'-O5'-PA-O2A
36	DE	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	DI	501	GTP	C5'-O5'-PA-O2A
36	DK	501	GTP	C5'-O5'-PA-O2A
36	DM	501	GTP	C5'-O5'-PA-O2A
36	EG	501	GTP	C5'-O5'-PA-O2A
36	EK	501	GTP	C5'-O5'-PA-O1A
36	FG	501	GTP	C5'-O5'-PA-O2A
36	FI	501	GTP	C5'-O5'-PA-O2A
36	FK	501	GTP	C5'-O5'-PA-O1A
36	FM	501	GTP	C5'-O5'-PA-O2A
36	HI	501	GTP	C5'-O5'-PA-O2A
36	II	501	GTP	C5'-O5'-PA-O2A
36	MK	501	GTP	C5'-O5'-PA-O2A
36	OC	501	GTP	C5'-O5'-PA-O2A
36	QE	501	GTP	C5'-O5'-PA-O2A
36	QK	501	GTP	C5'-O5'-PA-O2A
36	SE	501	GTP	C5'-O5'-PA-O2A
36	SI	501	GTP	C5'-O5'-PA-O2A
36	SK	501	GTP	C5'-O5'-PA-O2A
36	SM	501	GTP	C5'-O5'-PA-O2A
36	WG	501	GTP	C5'-O5'-PA-O2A
38	HN	502	GDP	C5'-O5'-PA-O1A
38	KB	502	GDP	C5'-O5'-PA-O1A
38	PN	502	GDP	C5'-O5'-PA-O1A
38	QF	502	GDP	C5'-O5'-PA-O1A
38	TL	502	GDP	C5'-O5'-PA-O1A
36	GE	501	GTP	C3'-C4'-C5'-O5'
36	GM	501	GTP	C3'-C4'-C5'-O5'
36	KO	501	GTP	C3'-C4'-C5'-O5'
36	ME	501	GTP	C3'-C4'-C5'-O5'
36	UG	501	GTP	C3'-C4'-C5'-O5'
38	FL	502	GDP	C3'-C4'-C5'-O5'
38	GB	502	GDP	C3'-C4'-C5'-O5'
38	LN	502	GDP	C3'-C4'-C5'-O5'
38	MJ	502	GDP	C3'-C4'-C5'-O5'
38	QH	502	GDP	C3'-C4'-C5'-O5'
38	SH	502	GDP	C3'-C4'-C5'-O5'
36	BK	501	GTP	C4'-C5'-O5'-PA
36	CA	501	GTP	C4'-C5'-O5'-PA
36	GE	501	GTP	C4'-C5'-O5'-PA
36	GK	501	GTP	C4'-C5'-O5'-PA
36	HE	501	GTP	C4'-C5'-O5'-PA
36	JI	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	PG	501	GTP	C4'-C5'-O5'-PA
36	RI	501	GTP	C4'-C5'-O5'-PA
36	TK	501	GTP	C4'-C5'-O5'-PA
36	VE	501	GTP	C4'-C5'-O5'-PA
36	VG	501	GTP	C4'-C5'-O5'-PA
36	IM	501	GTP	O4'-C4'-C5'-O5'
36	LC	501	GTP	O4'-C4'-C5'-O5'
36	QI	501	GTP	O4'-C4'-C5'-O5'
36	RC	501	GTP	C3'-C4'-C5'-O5'
36	UE	501	GTP	C3'-C4'-C5'-O5'
38	GD	502	GDP	O4'-C4'-C5'-O5'
38	JN	502	GDP	C3'-C4'-C5'-O5'
38	ON	502	GDP	O4'-C4'-C5'-O5'
38	PF	502	GDP	C3'-C4'-C5'-O5'
38	TJ	502	GDP	O4'-C4'-C5'-O5'
38	WD	502	GDP	O4'-C4'-C5'-O5'
38	VN	502	GDP	PA-O3A-PB-O1B
36	AK	501	GTP	C4'-C5'-O5'-PA
36	BG	501	GTP	C4'-C5'-O5'-PA
36	EK	501	GTP	C4'-C5'-O5'-PA
36	EM	501	GTP	C4'-C5'-O5'-PA
36	HK	501	GTP	C4'-C5'-O5'-PA
36	IC	501	GTP	C4'-C5'-O5'-PA
36	IE	501	GTP	C4'-C5'-O5'-PA
36	NI	501	GTP	C4'-C5'-O5'-PA
36	NK	501	GTP	C4'-C5'-O5'-PA
36	PO	501	GTP	C4'-C5'-O5'-PA
36	UE	501	GTP	C4'-C5'-O5'-PA
36	UO	501	GTP	C4'-C5'-O5'-PA
36	VO	501	GTP	C4'-C5'-O5'-PA
36	GK	501	GTP	C3'-C4'-C5'-O5'
36	RK	501	GTP	O4'-C4'-C5'-O5'
36	TK	501	GTP	O4'-C4'-C5'-O5'
38	KB	502	GDP	O4'-C4'-C5'-O5'
38	LL	502	GDP	C3'-C4'-C5'-O5'
38	QL	502	GDP	O4'-C4'-C5'-O5'
36	CK	501	GTP	PA-O3A-PB-O2B
36	EC	501	GTP	PB-O3A-PA-O2A
36	FC	501	GTP	PA-O3A-PB-O1B
36	FG	501	GTP	PA-O3A-PB-O2B
36	FI	501	GTP	PA-O3A-PB-O1B
36	FM	501	GTP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	GE	501	GTP	PA-O3A-PB-O1B
36	HO	501	GTP	PA-O3A-PB-O2B
36	IG	501	GTP	PB-O3A-PA-O2A
36	JC	501	GTP	PA-O3A-PB-O2B
36	JM	501	GTP	PB-O3A-PA-O2A
36	KC	501	GTP	PA-O3A-PB-O2B
36	KE	501	GTP	PA-O3A-PB-O2B
36	KI	501	GTP	PA-O3A-PB-O2B
36	KM	501	GTP	PA-O3A-PB-O2B
36	LE	501	GTP	PA-O3A-PB-O1B
36	LG	501	GTP	PA-O3A-PB-O2B
36	LI	501	GTP	PA-O3A-PB-O2B
36	LK	501	GTP	PA-O3A-PB-O2B
36	MC	501	GTP	PA-O3A-PB-O2B
36	MG	501	GTP	PA-O3A-PB-O2B
36	MM	501	GTP	PA-O3A-PB-O2B
36	PC	501	GTP	PA-O3A-PB-O2B
36	PG	501	GTP	PA-O3A-PB-O2B
36	QM	501	GTP	PA-O3A-PB-O2B
36	RC	501	GTP	PA-O3A-PB-O2B
36	RM	501	GTP	PB-O3A-PA-O2A
36	SE	501	GTP	PA-O3A-PB-O2B
36	SG	501	GTP	PA-O3A-PB-O2B
36	SI	501	GTP	PA-O3A-PB-O1B
36	SK	501	GTP	PA-O3A-PB-O2B
36	WK	501	GTP	PB-O3A-PA-O2A
36	AG	501	GTP	C4'-C5'-O5'-PA
36	BA	501	GTP	C4'-C5'-O5'-PA
36	BE	501	GTP	C4'-C5'-O5'-PA
36	FK	501	GTP	C4'-C5'-O5'-PA
36	GC	501	GTP	C4'-C5'-O5'-PA
36	GG	501	GTP	C4'-C5'-O5'-PA
36	HM	501	GTP	C4'-C5'-O5'-PA
36	LM	501	GTP	C4'-C5'-O5'-PA
36	NG	501	GTP	C4'-C5'-O5'-PA
36	NM	501	GTP	C4'-C5'-O5'-PA
36	OE	501	GTP	C4'-C5'-O5'-PA
36	TO	501	GTP	C4'-C5'-O5'-PA
36	UG	501	GTP	C4'-C5'-O5'-PA
36	UI	501	GTP	C4'-C5'-O5'-PA
36	JI	501	GTP	C3'-C4'-C5'-O5'
38	JD	502	GDP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	OJ	502	GDP	C3'-C4'-C5'-O5'
36	AA	501	GTP	C4'-C5'-O5'-PA
36	AC	501	GTP	C4'-C5'-O5'-PA
36	BM	501	GTP	C4'-C5'-O5'-PA
36	GI	501	GTP	C4'-C5'-O5'-PA
36	HC	501	GTP	C4'-C5'-O5'-PA
36	IK	501	GTP	C4'-C5'-O5'-PA
36	NC	501	GTP	C4'-C5'-O5'-PA
36	PK	501	GTP	C4'-C5'-O5'-PA
36	TI	501	GTP	C4'-C5'-O5'-PA
36	AG	501	GTP	C3'-C4'-C5'-O5'
36	TM	501	GTP	C3'-C4'-C5'-O5'
38	AJ	502	GDP	C3'-C4'-C5'-O5'
36	AM	501	GTP	C4'-C5'-O5'-PA
36	GM	501	GTP	C4'-C5'-O5'-PA
36	NE	501	GTP	C4'-C5'-O5'-PA
36	PE	501	GTP	C4'-C5'-O5'-PA
36	AI	501	GTP	O4'-C4'-C5'-O5'
38	LB	502	GDP	C3'-C4'-C5'-O5'
38	WN	502	GDP	C3'-C4'-C5'-O5'
36	EM	501	GTP	PB-O3A-PA-O2A
36	HO	501	GTP	PA-O3A-PB-O1B
36	QE	501	GTP	PB-O3A-PA-O1A
36	QK	501	GTP	PA-O3A-PB-O2B
36	QM	501	GTP	PA-O3A-PB-O1B
36	RO	501	GTP	PA-O3A-PB-O2B
36	RO	501	GTP	PB-O3A-PA-O1A
36	SE	501	GTP	PA-O3A-PB-O1B
36	SK	501	GTP	PB-O3A-PA-O1A
36	VG	501	GTP	PA-O3A-PB-O2B
36	GM	501	GTP	O4'-C4'-C5'-O5'
36	IG	501	GTP	C3'-C4'-C5'-O5'
36	KK	501	GTP	O4'-C4'-C5'-O5'
36	KO	501	GTP	O4'-C4'-C5'-O5'
36	PG	501	GTP	O4'-C4'-C5'-O5'
38	FF	502	GDP	C3'-C4'-C5'-O5'
38	FL	502	GDP	O4'-C4'-C5'-O5'
38	GB	502	GDP	O4'-C4'-C5'-O5'
38	KN	502	GDP	C3'-C4'-C5'-O5'
38	MJ	502	GDP	O4'-C4'-C5'-O5'
38	OL	502	GDP	O4'-C4'-C5'-O5'
38	SD	502	GDP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	TH	502	GDP	O4'-C4'-C5'-O5'
36	QC	501	GTP	PB-O3A-PA-O5'
36	BC	501	GTP	C4'-C5'-O5'-PA
36	BI	501	GTP	C4'-C5'-O5'-PA
36	ME	501	GTP	C4'-C5'-O5'-PA
36	OG	501	GTP	C4'-C5'-O5'-PA
36	DA	501	GTP	C3'-C4'-C5'-O5'
36	GE	501	GTP	O4'-C4'-C5'-O5'
36	ME	501	GTP	O4'-C4'-C5'-O5'
36	UE	501	GTP	O4'-C4'-C5'-O5'
36	UG	501	GTP	O4'-C4'-C5'-O5'
38	CD	502	GDP	C3'-C4'-C5'-O5'
38	KJ	502	GDP	C3'-C4'-C5'-O5'
38	MD	502	GDP	C3'-C4'-C5'-O5'
38	QH	502	GDP	O4'-C4'-C5'-O5'
38	SH	502	GDP	O4'-C4'-C5'-O5'
38	BL	502	GDP	PA-O3A-PB-O1B
36	AI	501	GTP	C4'-C5'-O5'-PA
36	RM	501	GTP	C4'-C5'-O5'-PA
36	RC	501	GTP	O4'-C4'-C5'-O5'
36	TO	501	GTP	C3'-C4'-C5'-O5'
38	CL	502	GDP	C3'-C4'-C5'-O5'
38	EH	502	GDP	C3'-C4'-C5'-O5'
38	EL	502	GDP	C3'-C4'-C5'-O5'
38	QF	502	GDP	C3'-C4'-C5'-O5'
36	AM	501	GTP	C5'-O5'-PA-O3A
36	CC	501	GTP	C5'-O5'-PA-O3A
36	CG	501	GTP	C5'-O5'-PA-O3A
36	DC	501	GTP	C5'-O5'-PA-O3A
36	DG	501	GTP	C5'-O5'-PA-O3A
36	EC	501	GTP	C5'-O5'-PA-O3A
36	GC	501	GTP	C5'-O5'-PA-O3A
36	GG	501	GTP	C5'-O5'-PA-O3A
36	HO	501	GTP	C5'-O5'-PA-O3A
36	IG	501	GTP	C5'-O5'-PA-O3A
36	IM	501	GTP	C5'-O5'-PA-O3A
36	JG	501	GTP	C5'-O5'-PA-O3A
36	JM	501	GTP	C5'-O5'-PA-O3A
36	KI	501	GTP	C5'-O5'-PA-O3A
36	KK	501	GTP	C5'-O5'-PA-O3A
36	KM	501	GTP	C5'-O5'-PA-O3A
36	KO	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	LC	501	GTP	C5'-O5'-PA-O3A
36	LG	501	GTP	C5'-O5'-PA-O3A
36	NI	501	GTP	C5'-O5'-PA-O3A
36	OO	501	GTP	C5'-O5'-PA-O3A
36	PE	501	GTP	C5'-O5'-PA-O3A
36	QO	501	GTP	C5'-O5'-PA-O3A
36	RM	501	GTP	C5'-O5'-PA-O3A
36	UI	501	GTP	C5'-O5'-PA-O3A
36	VG	501	GTP	C5'-O5'-PA-O3A
36	VI	501	GTP	C5'-O5'-PA-O3A
36	WK	501	GTP	C5'-O5'-PA-O3A
38	CB	502	GDP	C5'-O5'-PA-O3A
38	DH	502	GDP	C5'-O5'-PA-O3A
38	FD	502	GDP	C5'-O5'-PA-O3A
38	GJ	502	GDP	C5'-O5'-PA-O3A
38	ID	502	GDP	C5'-O5'-PA-O3A
38	IH	502	GDP	C5'-O5'-PA-O3A
38	IL	502	GDP	C5'-O5'-PA-O3A
38	KD	502	GDP	C5'-O5'-PA-O3A
38	KJ	502	GDP	C5'-O5'-PA-O3A
38	KN	502	GDP	C5'-O5'-PA-O3A
38	LD	502	GDP	C5'-O5'-PA-O3A
38	LL	502	GDP	C5'-O5'-PA-O3A
38	OL	502	GDP	C5'-O5'-PA-O3A
38	PD	502	GDP	C5'-O5'-PA-O3A
38	PJ	502	GDP	C5'-O5'-PA-O3A
38	PL	502	GDP	C5'-O5'-PA-O3A
38	QH	502	GDP	C5'-O5'-PA-O3A
38	QJ	502	GDP	C5'-O5'-PA-O3A
38	QN	502	GDP	C5'-O5'-PA-O3A
38	SH	502	GDP	C5'-O5'-PA-O3A
38	TN	502	GDP	C5'-O5'-PA-O3A
38	UF	502	GDP	C5'-O5'-PA-O3A
38	VJ	502	GDP	C5'-O5'-PA-O3A
38	VN	502	GDP	C5'-O5'-PA-O3A
38	WD	502	GDP	C5'-O5'-PA-O3A
38	WH	502	GDP	C5'-O5'-PA-O3A
38	WP	502	GDP	C5'-O5'-PA-O3A
36	RI	501	GTP	C3'-C4'-C5'-O5'
36	TE	501	GTP	C3'-C4'-C5'-O5'
36	WI	501	GTP	C3'-C4'-C5'-O5'
38	AF	502	GDP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	KF	502	GDP	C3'-C4'-C5'-O5'
38	LJ	502	GDP	C3'-C4'-C5'-O5'
38	LN	502	GDP	O4'-C4'-C5'-O5'
38	RJ	502	GDP	C3'-C4'-C5'-O5'
38	UJ	502	GDP	C3'-C4'-C5'-O5'
38	WP	502	GDP	C3'-C4'-C5'-O5'
36	CI	501	GTP	PB-O3A-PA-O1A
36	DA	501	GTP	PA-O3A-PB-O1B
36	DA	501	GTP	PA-O3A-PB-O2B
36	DA	501	GTP	PB-O3A-PA-O2A
36	DC	501	GTP	PB-O3A-PA-O2A
36	DG	501	GTP	PB-O3A-PA-O2A
36	EE	501	GTP	PB-O3A-PA-O1A
36	EG	501	GTP	PB-O3A-PA-O1A
36	EI	501	GTP	PB-O3A-PA-O1A
36	EK	501	GTP	PB-O3A-PA-O2A
36	EM	501	GTP	PB-O3A-PA-O1A
36	FC	501	GTP	PA-O3A-PB-O2B
36	FG	501	GTP	PA-O3A-PB-O1B
36	FI	501	GTP	PA-O3A-PB-O2B
36	FM	501	GTP	PA-O3A-PB-O2B
36	HI	501	GTP	PB-O3A-PA-O2A
36	IG	501	GTP	PB-O3A-PA-O1A
36	IM	501	GTP	PB-O3A-PA-O1A
36	JK	501	GTP	PA-O3A-PB-O1B
36	JK	501	GTP	PA-O3A-PB-O2B
36	KE	501	GTP	PA-O3A-PB-O1B
36	KG	501	GTP	PA-O3A-PB-O1B
36	KK	501	GTP	PA-O3A-PB-O1B
36	LE	501	GTP	PA-O3A-PB-O2B
36	LK	501	GTP	PA-O3A-PB-O1B
36	MC	501	GTP	PA-O3A-PB-O1B
36	MG	501	GTP	PA-O3A-PB-O1B
36	MI	501	GTP	PA-O3A-PB-O1B
36	MK	501	GTP	PA-O3A-PB-O1B
36	PM	501	GTP	PA-O3A-PB-O1B
36	PM	501	GTP	PA-O3A-PB-O2B
36	QE	501	GTP	PA-O3A-PB-O2B
36	QG	501	GTP	PB-O3A-PA-O1A
36	QO	501	GTP	PA-O3A-PB-O1B
36	RM	501	GTP	PB-O3A-PA-O1A
36	SI	501	GTP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	SK	501	GTP	PA-O3A-PB-O1B
36	SM	501	GTP	PA-O3A-PB-O1B
36	TG	501	GTP	PA-O3A-PB-O1B
38	TH	502	GDP	PB-O3A-PA-O2A
36	DG	501	GTP	C4'-C5'-O5'-PA
36	RE	501	GTP	C4'-C5'-O5'-PA
36	BA	501	GTP	C5'-O5'-PA-O1A
36	BG	501	GTP	C5'-O5'-PA-O1A
36	BK	501	GTP	C5'-O5'-PA-O1A
36	GM	501	GTP	C5'-O5'-PA-O1A
36	IC	501	GTP	C5'-O5'-PA-O1A
36	LE	501	GTP	C5'-O5'-PA-O1A
36	LM	501	GTP	C5'-O5'-PA-O1A
36	ME	501	GTP	C5'-O5'-PA-O1A
36	NC	501	GTP	C5'-O5'-PA-O1A
36	NK	501	GTP	C5'-O5'-PA-O1A
36	NM	501	GTP	C5'-O5'-PA-O1A
36	OG	501	GTP	C5'-O5'-PA-O1A
36	PC	501	GTP	C5'-O5'-PA-O1A
36	TK	501	GTP	C5'-O5'-PA-O1A
36	TM	501	GTP	C5'-O5'-PA-O1A
36	TO	501	GTP	C5'-O5'-PA-O1A
36	UG	501	GTP	C5'-O5'-PA-O1A
36	UO	501	GTP	C5'-O5'-PA-O1A
36	VK	501	GTP	C5'-O5'-PA-O1A
36	WE	501	GTP	C5'-O5'-PA-O1A
36	WM	501	GTP	C5'-O5'-PA-O1A
38	AD	502	GDP	C5'-O5'-PA-O1A
38	AF	502	GDP	C5'-O5'-PA-O1A
38	AH	502	GDP	C5'-O5'-PA-O1A
38	AL	502	GDP	C5'-O5'-PA-O1A
38	BH	502	GDP	C5'-O5'-PA-O1A
38	CD	502	GDP	C5'-O5'-PA-O1A
38	CH	502	GDP	C5'-O5'-PA-O1A
38	CJ	502	GDP	C5'-O5'-PA-O1A
38	CL	502	GDP	C5'-O5'-PA-O1A
38	DD	502	GDP	C5'-O5'-PA-O1A
38	DF	502	GDP	C5'-O5'-PA-O1A
38	DJ	502	GDP	C5'-O5'-PA-O1A
38	DL	502	GDP	C5'-O5'-PA-O1A
38	ED	502	GDP	C5'-O5'-PA-O1A
38	EH	502	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	EJ	502	GDP	C5’-O5’-PA-O1A
38	EL	502	GDP	C5’-O5’-PA-O1A
38	EN	502	GDP	C5’-O5’-PA-O1A
38	FF	502	GDP	C5’-O5’-PA-O1A
38	FH	502	GDP	C5’-O5’-PA-O1A
38	FJ	502	GDP	C5’-O5’-PA-O1A
38	FL	502	GDP	C5’-O5’-PA-O1A
38	GD	502	GDP	C5’-O5’-PA-O1A
38	GF	502	GDP	C5’-O5’-PA-O1A
38	GH	502	GDP	C5’-O5’-PA-O1A
38	GN	502	GDP	C5’-O5’-PA-O1A
38	HB	502	GDP	C5’-O5’-PA-O1A
38	HD	502	GDP	C5’-O5’-PA-O1A
38	HJ	502	GDP	C5’-O5’-PA-O1A
38	JB	502	GDP	C5’-O5’-PA-O1A
38	JD	502	GDP	C5’-O5’-PA-O1A
38	JH	502	GDP	C5’-O5’-PA-O1A
38	JJ	502	GDP	C5’-O5’-PA-O1A
38	JL	502	GDP	C5’-O5’-PA-O1A
38	JN	502	GDP	C5’-O5’-PA-O1A
38	LB	502	GDP	C5’-O5’-PA-O1A
38	LF	502	GDP	C5’-O5’-PA-O1A
38	MB	502	GDP	C5’-O5’-PA-O1A
38	MD	502	GDP	C5’-O5’-PA-O1A
38	MF	502	GDP	C5’-O5’-PA-O1A
38	MJ	502	GDP	C5’-O5’-PA-O1A
38	MN	502	GDP	C5’-O5’-PA-O1A
38	NB	502	GDP	C5’-O5’-PA-O1A
38	NF	502	GDP	C5’-O5’-PA-O1A
38	NH	502	GDP	C5’-O5’-PA-O1A
38	NJ	502	GDP	C5’-O5’-PA-O1A
38	NL	502	GDP	C5’-O5’-PA-O1A
38	NN	502	GDP	C5’-O5’-PA-O1A
38	PF	502	GDP	C5’-O5’-PA-O1A
38	QL	502	GDP	C5’-O5’-PA-O1A
38	RD	502	GDP	C5’-O5’-PA-O1A
38	RF	502	GDP	C5’-O5’-PA-O1A
38	RN	502	GDP	C5’-O5’-PA-O1A
38	SD	502	GDP	C5’-O5’-PA-O1A
38	TD	502	GDP	C5’-O5’-PA-O1A
38	TP	502	GDP	C5’-O5’-PA-O1A
38	UH	502	GDP	C5’-O5’-PA-O1A

Continued on next page...

Continued from previous page...

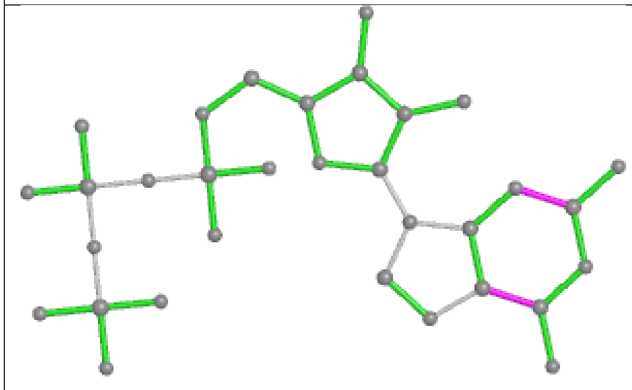
Mol	Chain	Res	Type	Atoms
38	UL	502	GDP	C5'-O5'-PA-O1A
38	UN	502	GDP	C5'-O5'-PA-O1A
38	VF	502	GDP	C5'-O5'-PA-O1A
36	GK	501	GTP	O4'-C4'-C5'-O5'
38	CF	502	GDP	C3'-C4'-C5'-O5'
38	PF	502	GDP	O4'-C4'-C5'-O5'
38	SD	502	GDP	O4'-C4'-C5'-O5'
38	PN	502	GDP	C3'-C4'-C5'-O5'

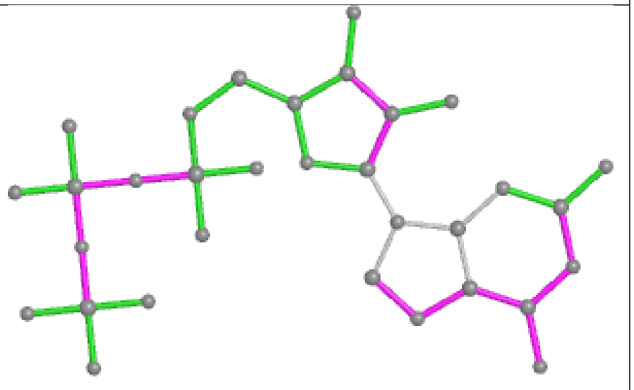
There are no ring outliers.

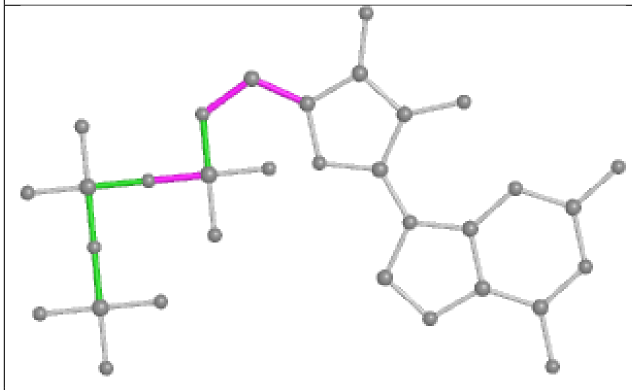
No monomer is involved in short contacts.

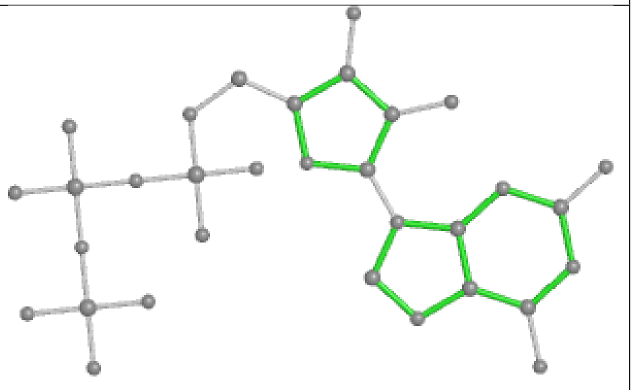
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP PO 501

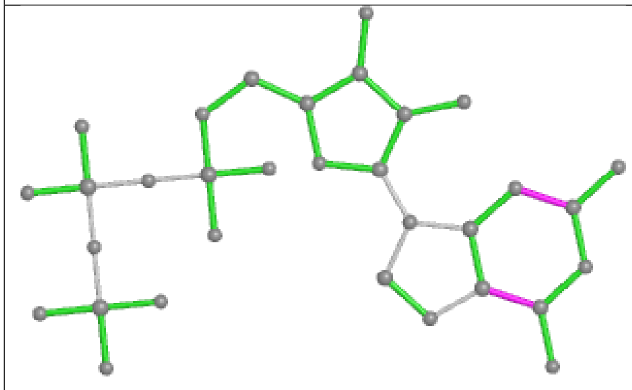

Bond lengths

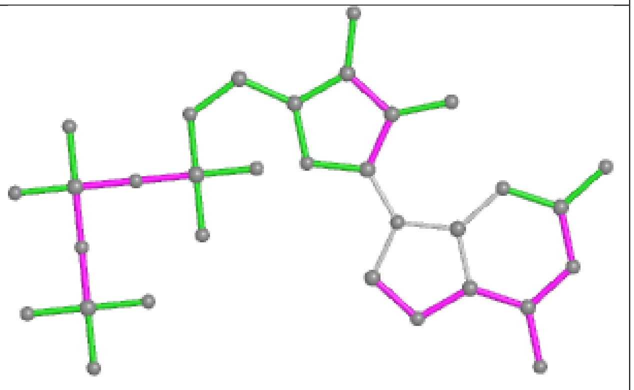

Bond angles

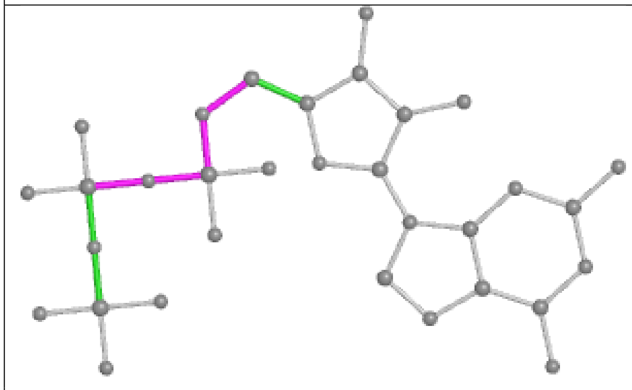

Torsions

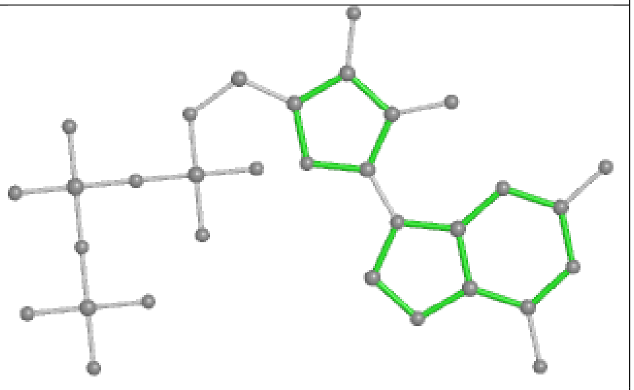

Rings

Ligand GTP KE 501

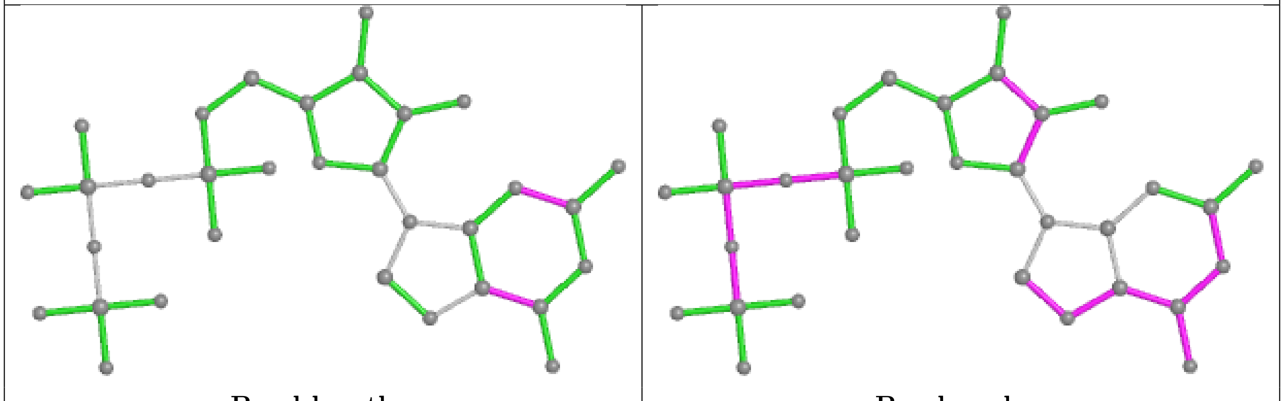

Bond lengths


Bond angles

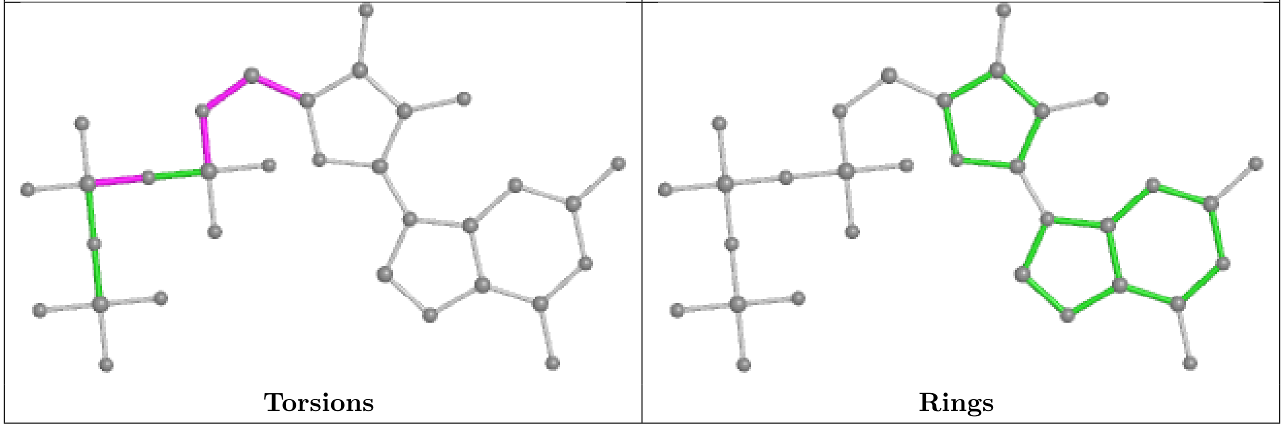

Torsions


Rings

Ligand GTP KO 501

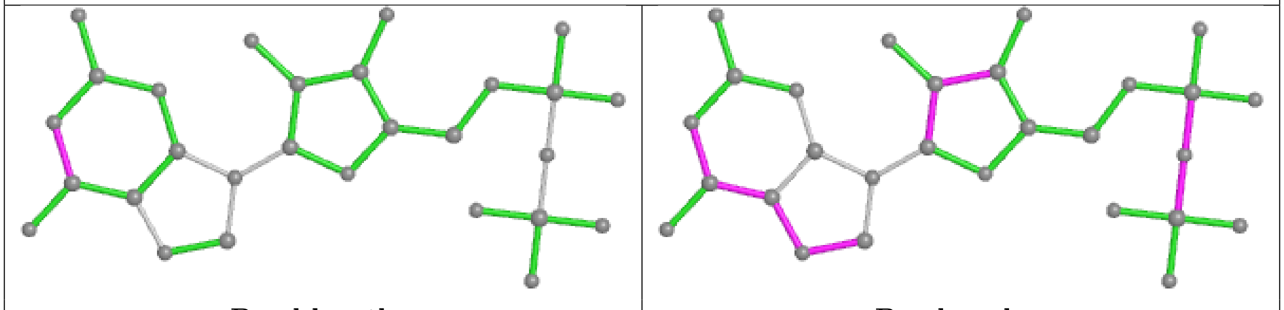


Bond lengths **Bond angles**

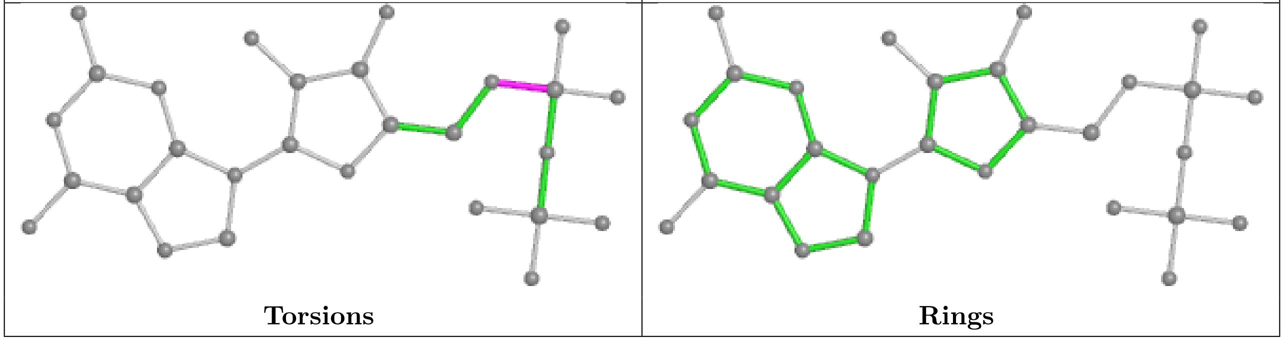


Torsions **Rings**

Ligand GDP PL 502

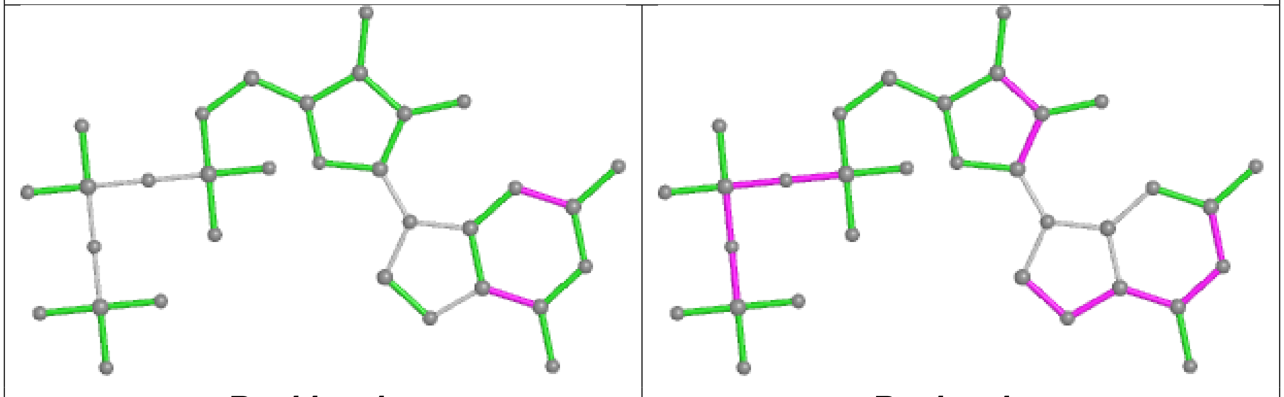


Bond lengths **Bond angles**

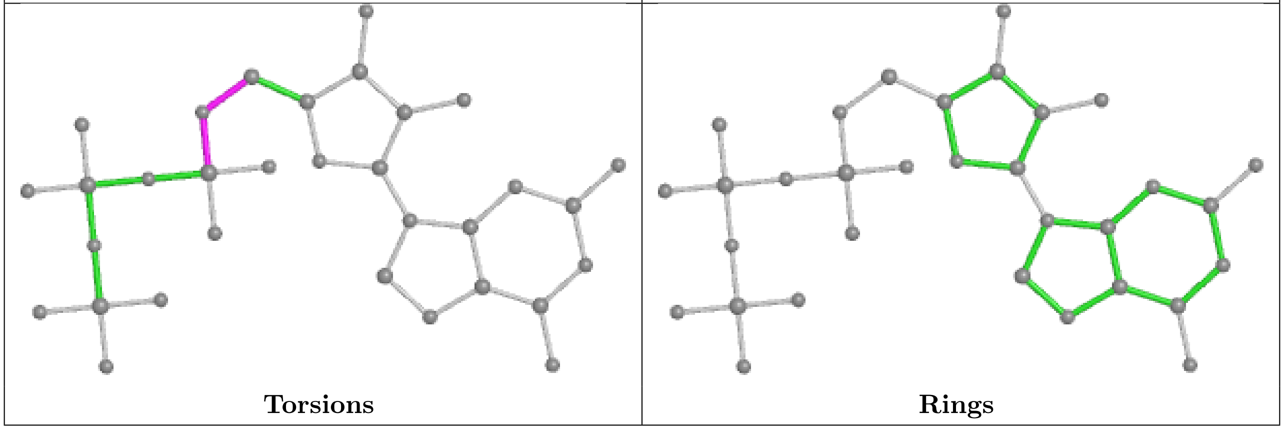


Torsions **Rings**

Ligand GTP DM 501

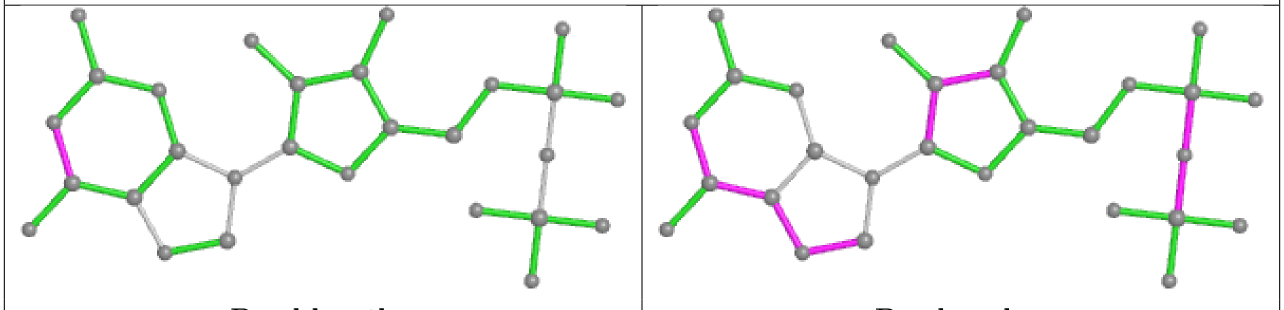


Bond lengths Bond angles

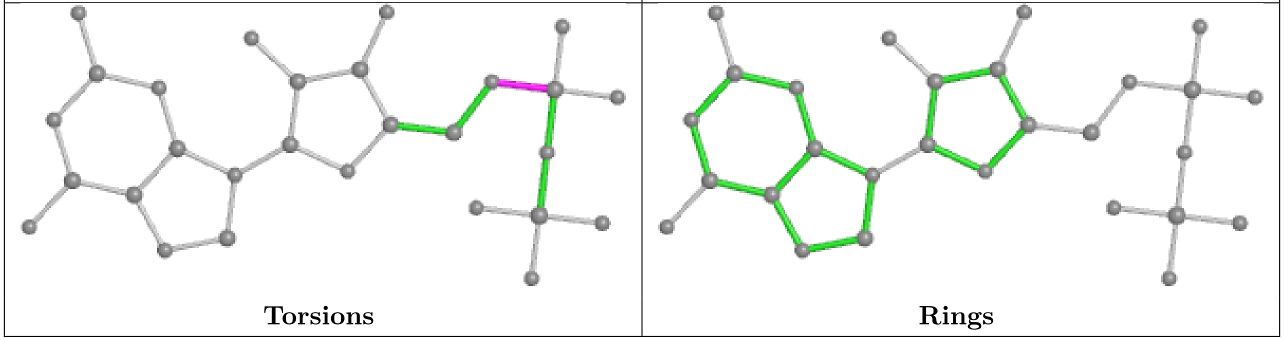


Torsions Rings

Ligand GDP AB 502

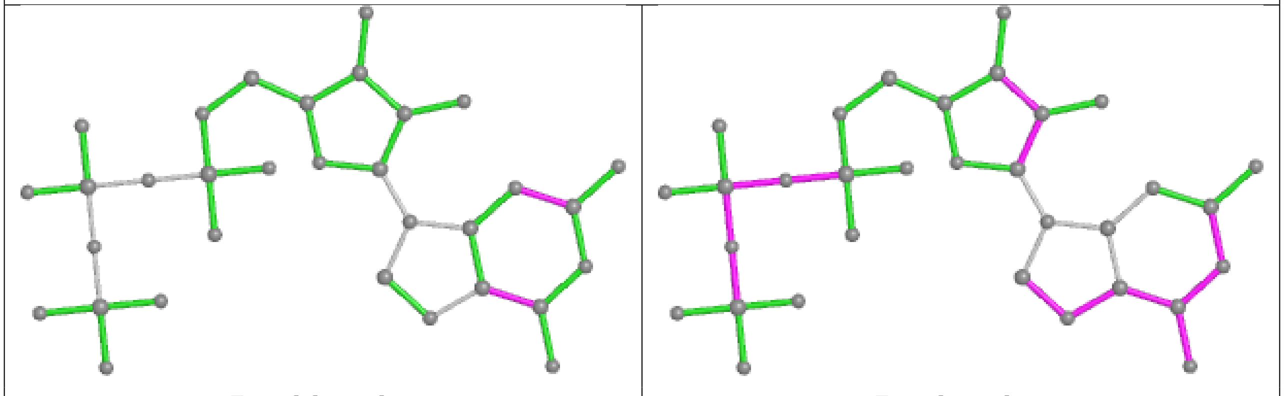


Bond lengths Bond angles



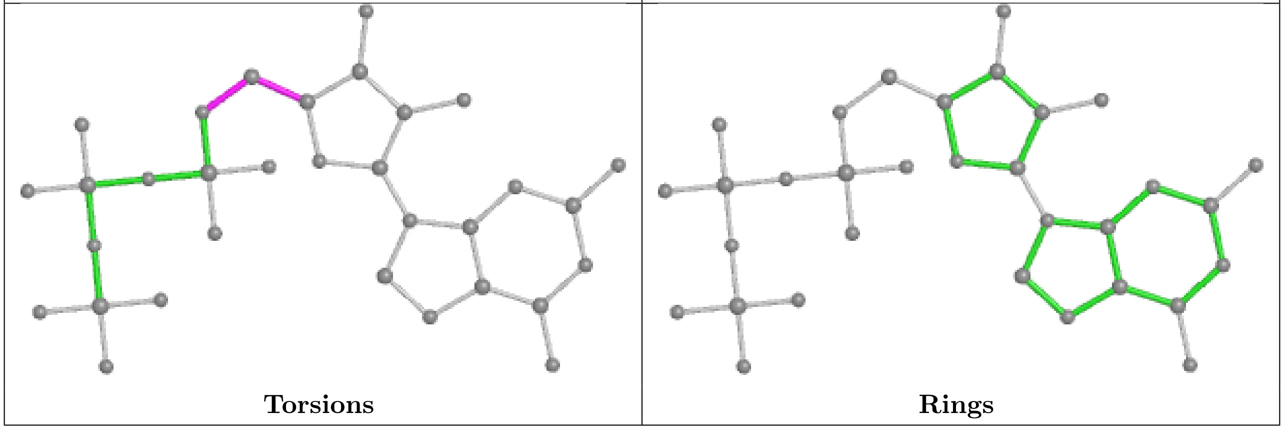
Torsions Rings

Ligand GTP RK 501



Bond lengths

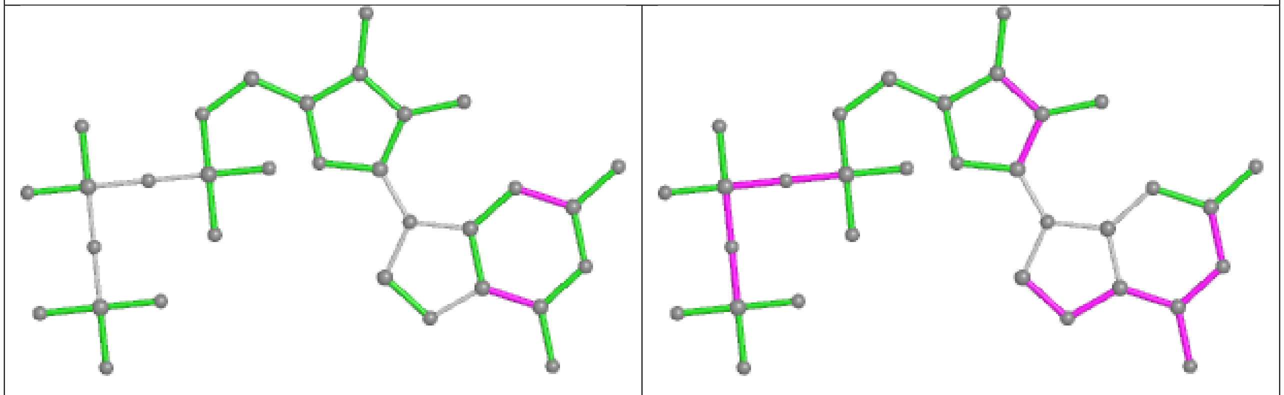
Bond angles



Torsions

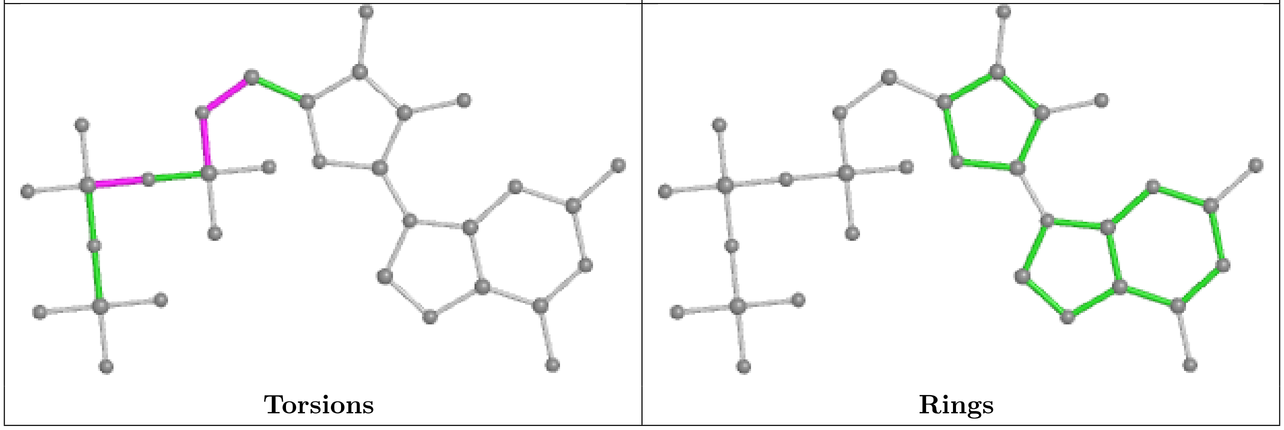
Rings

Ligand GTP TG 501



Bond lengths

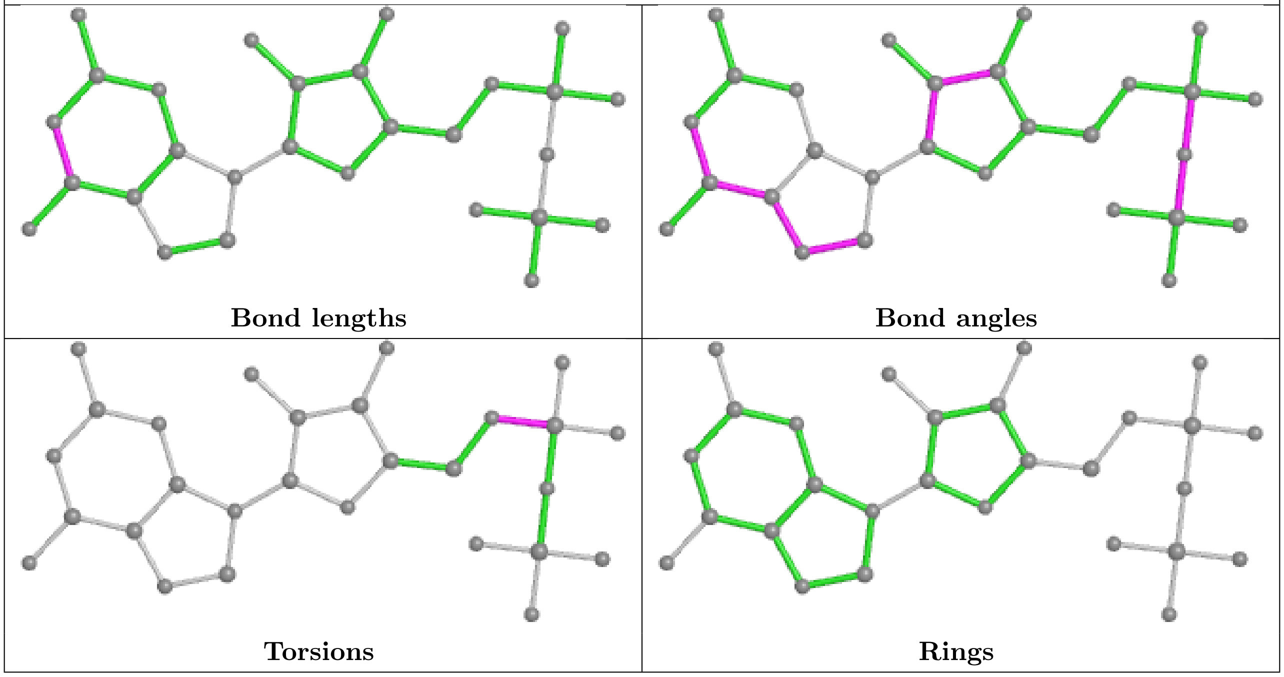
Bond angles



Torsions

Rings

Ligand GDP DH 502



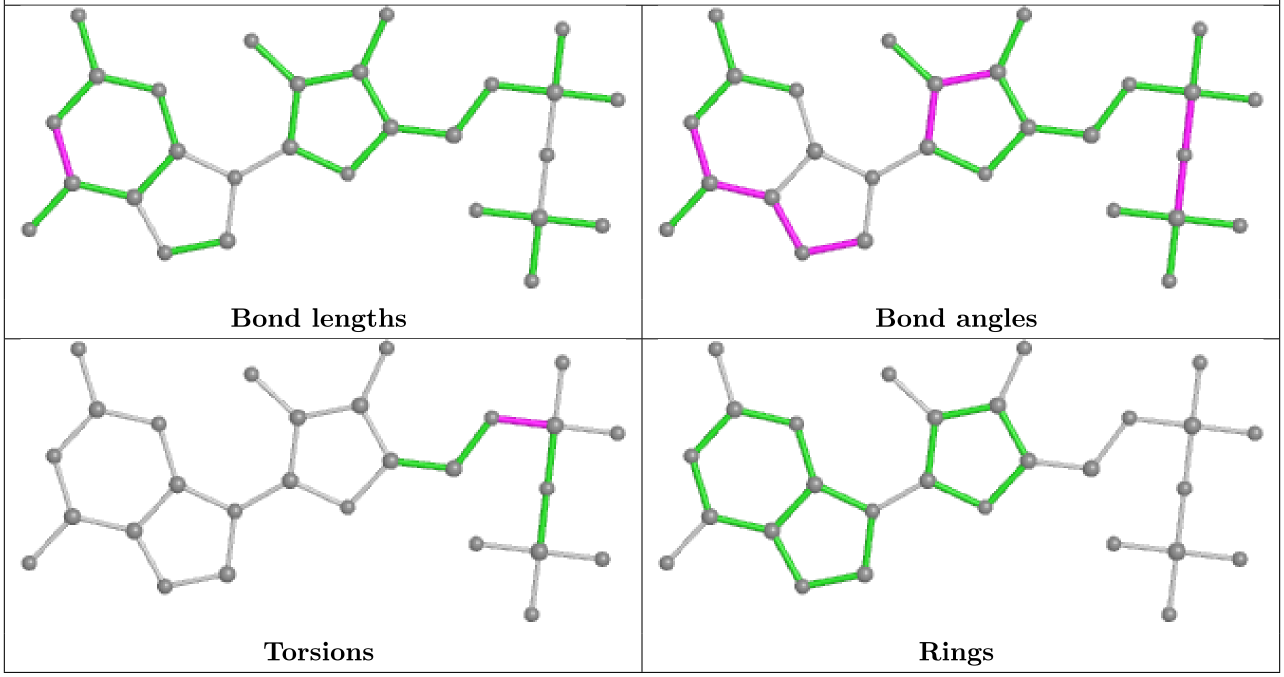
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP BD 502



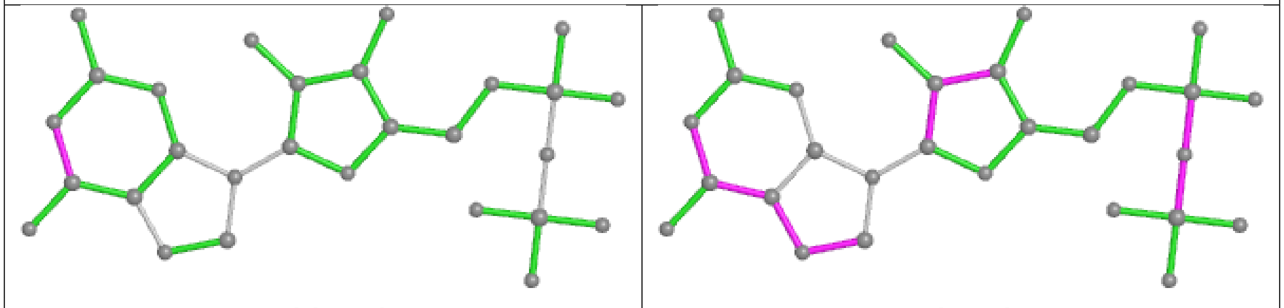
Bond lengths

Bond angles

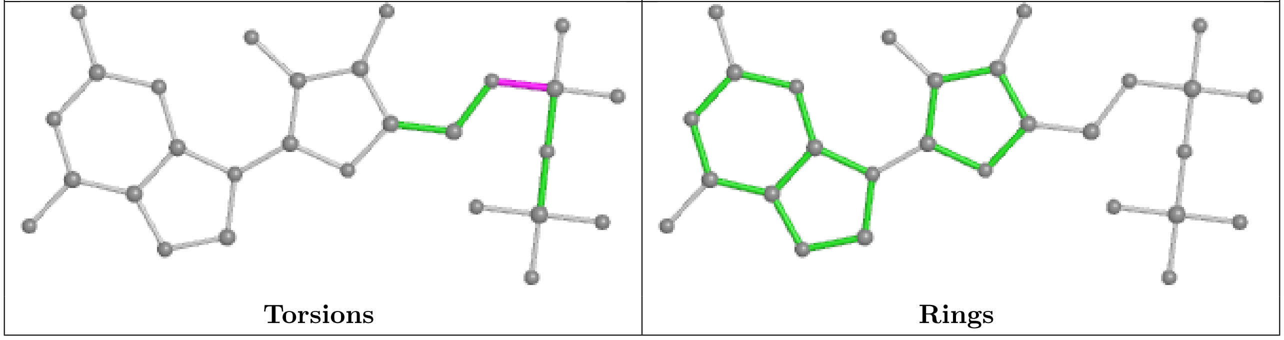
Torsions

Rings

Ligand GDP GF 502

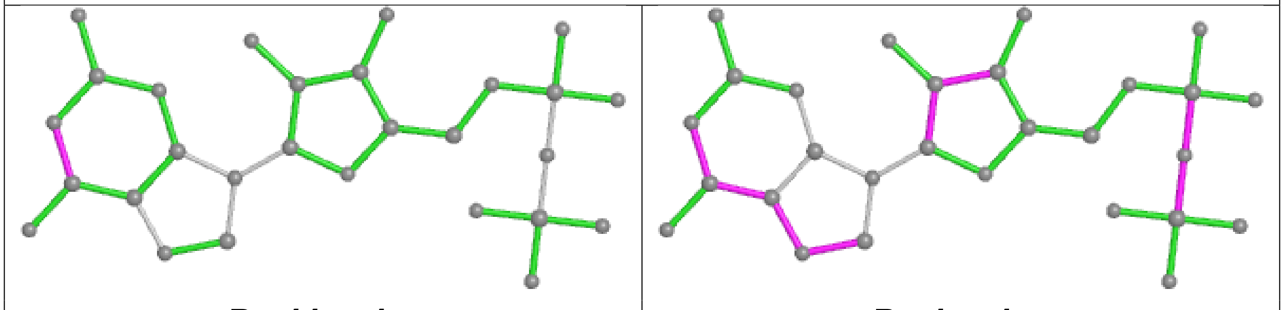


Bond lengths **Bond angles**

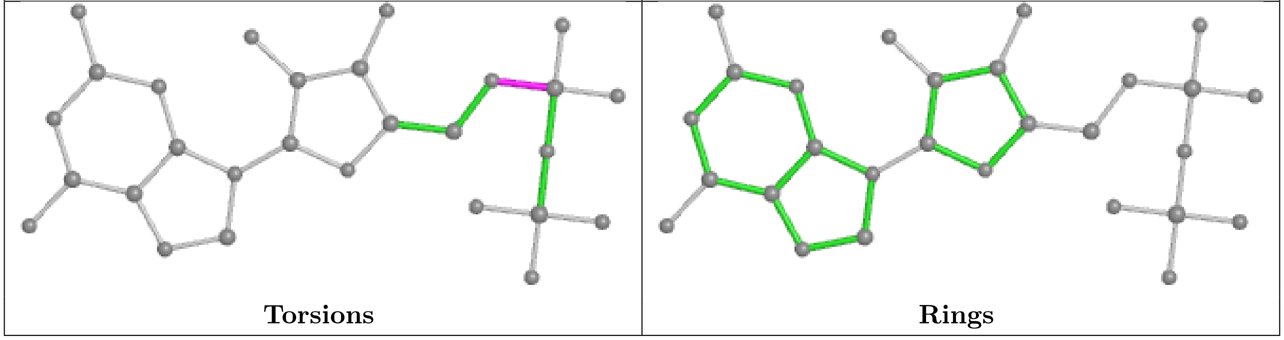


Torsions **Rings**

Ligand GDP DL 502

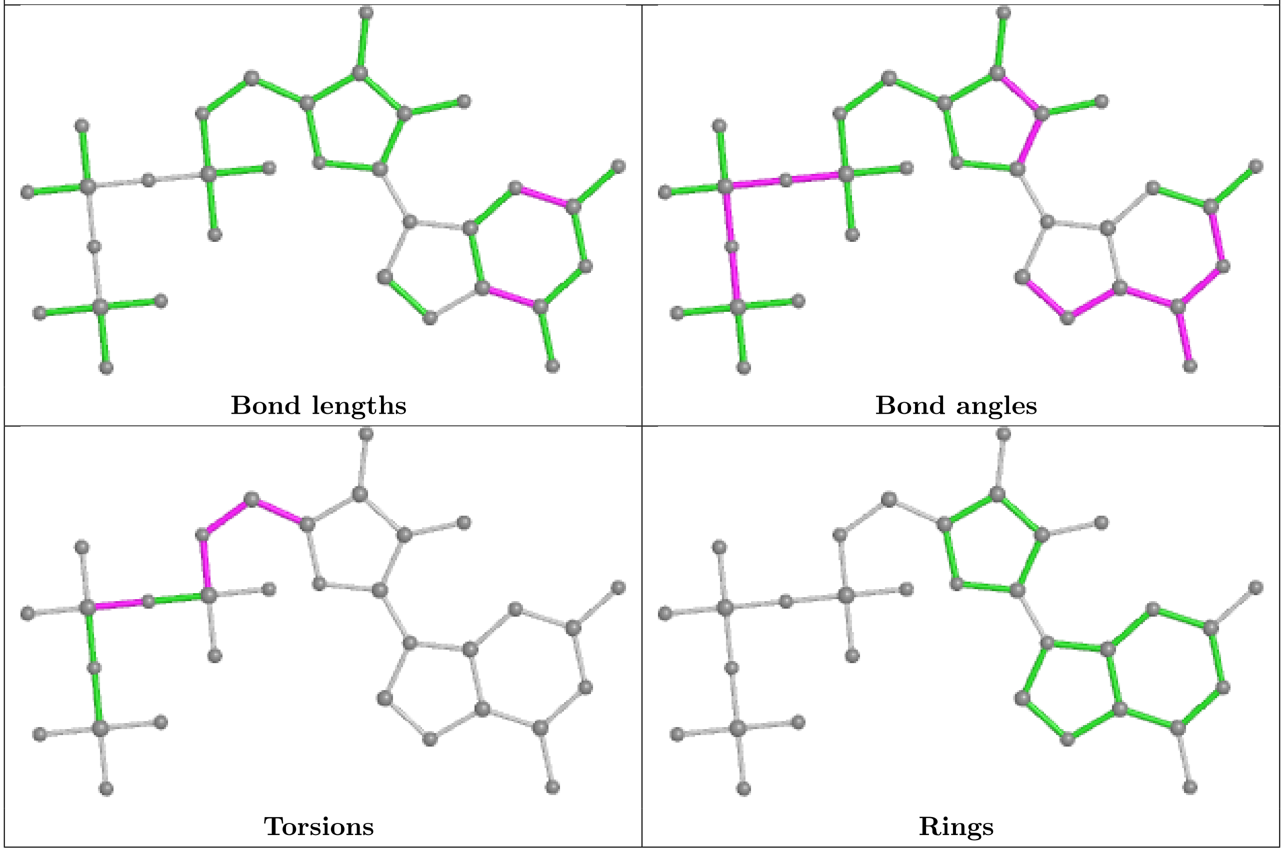


Bond lengths **Bond angles**

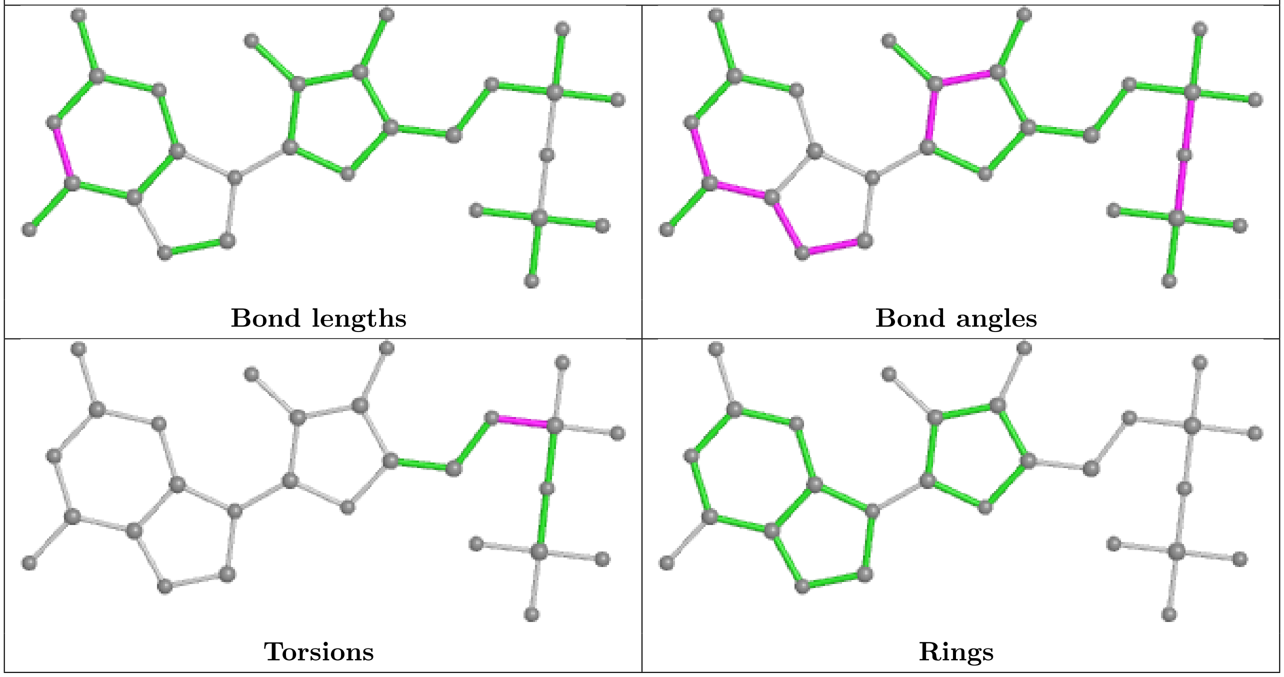


Torsions **Rings**

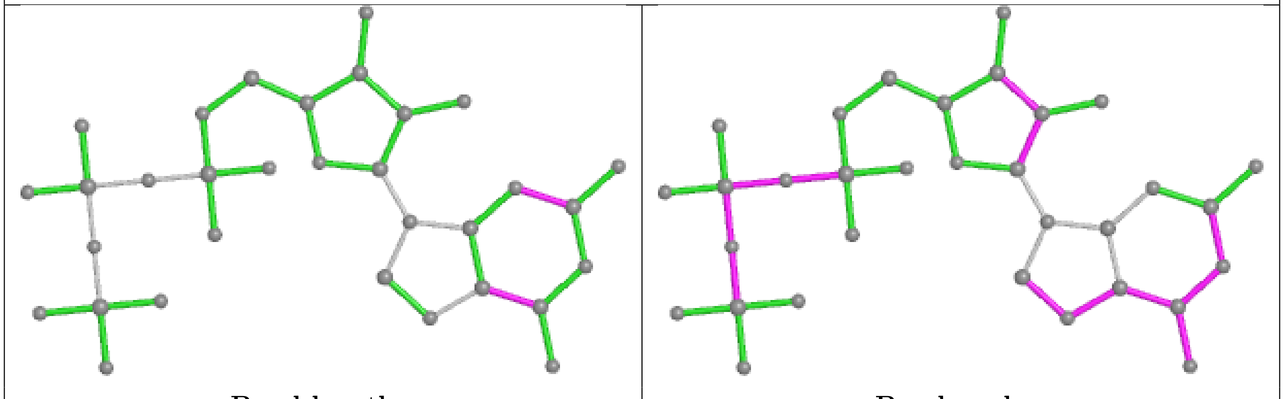
Ligand GTP QO 501



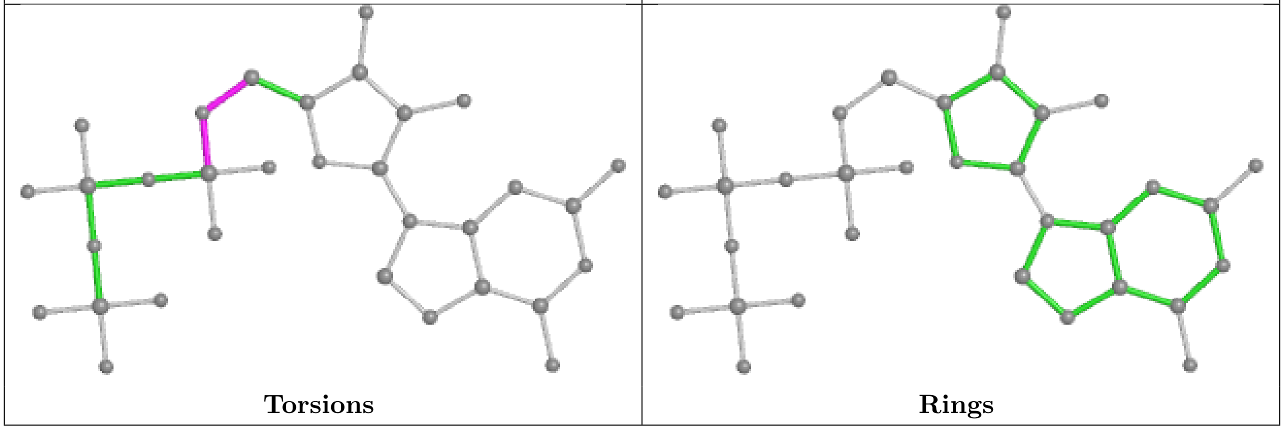
Ligand GDP WF 502



Ligand GTP II 501

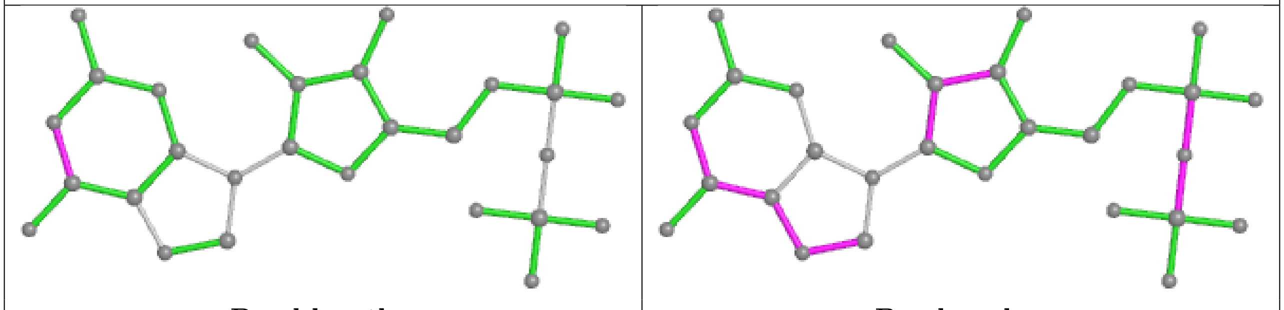

Bond lengths

Bond angles

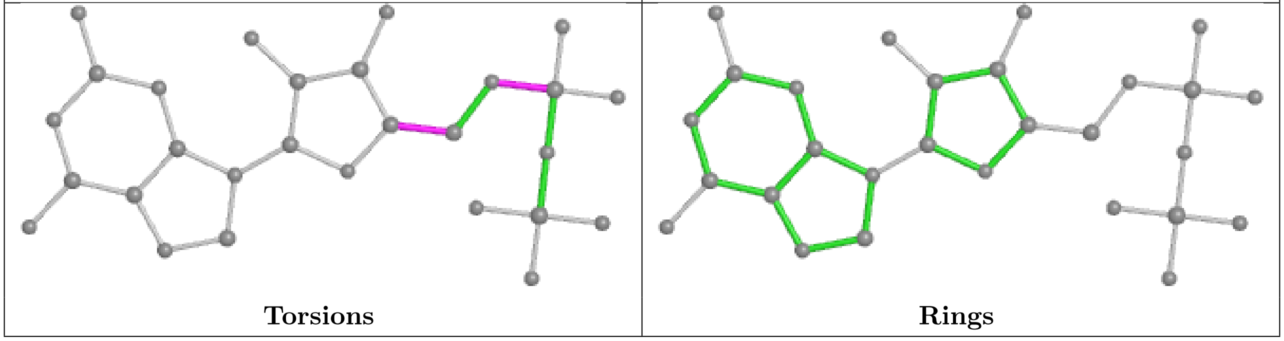

Torsions

Rings

Ligand GDP LN 502

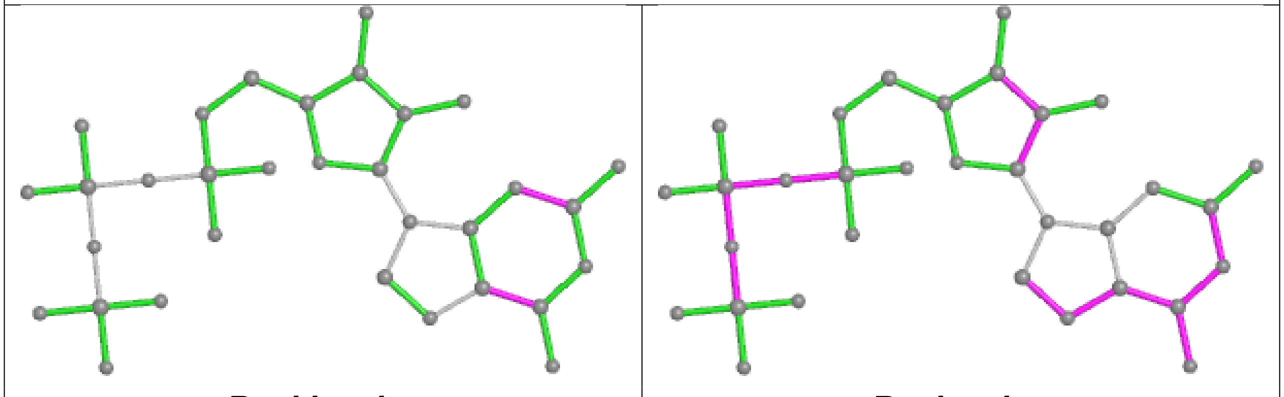

Bond lengths

Bond angles

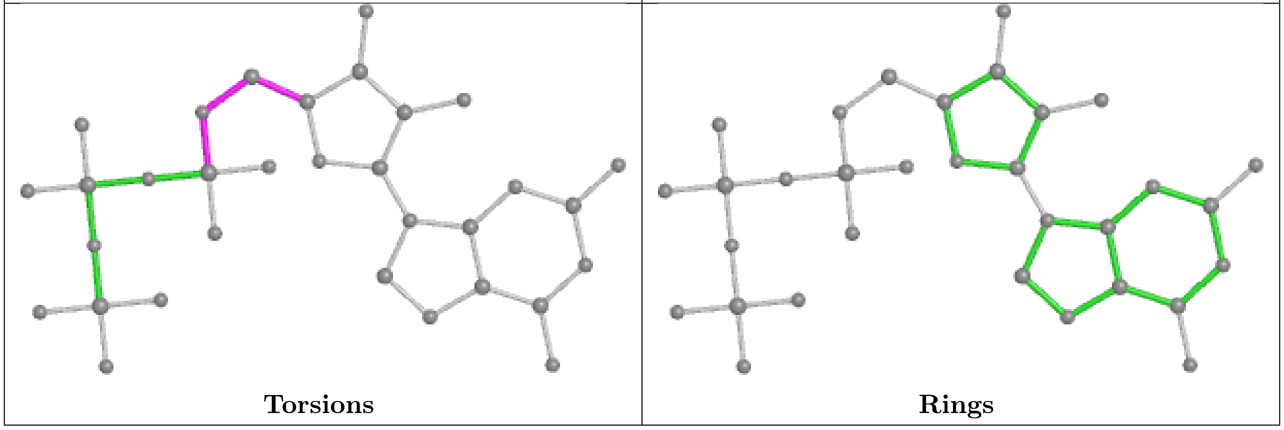

Torsions

Rings

Ligand GTP IO 501

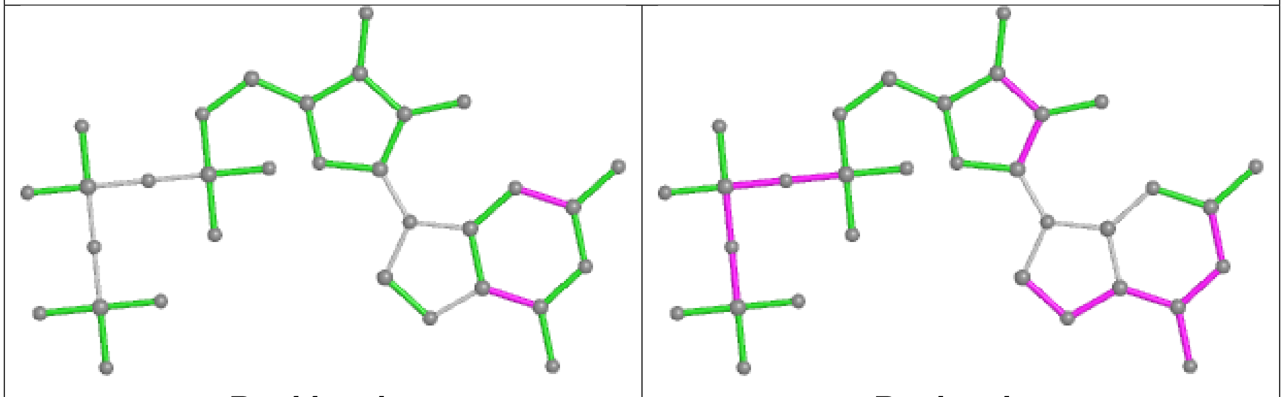


Bond lengths **Bond angles**

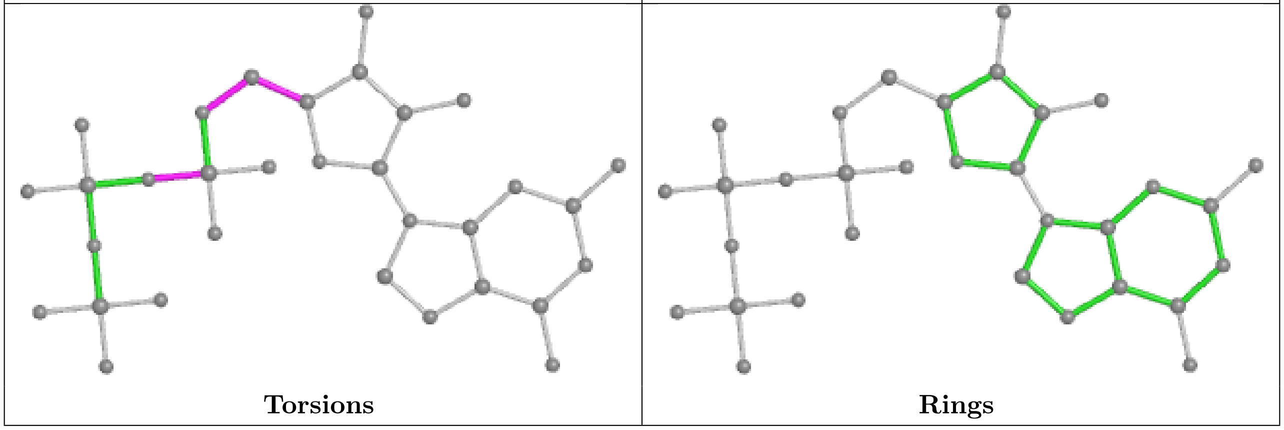


Torsions **Rings**

Ligand GTP GI 501

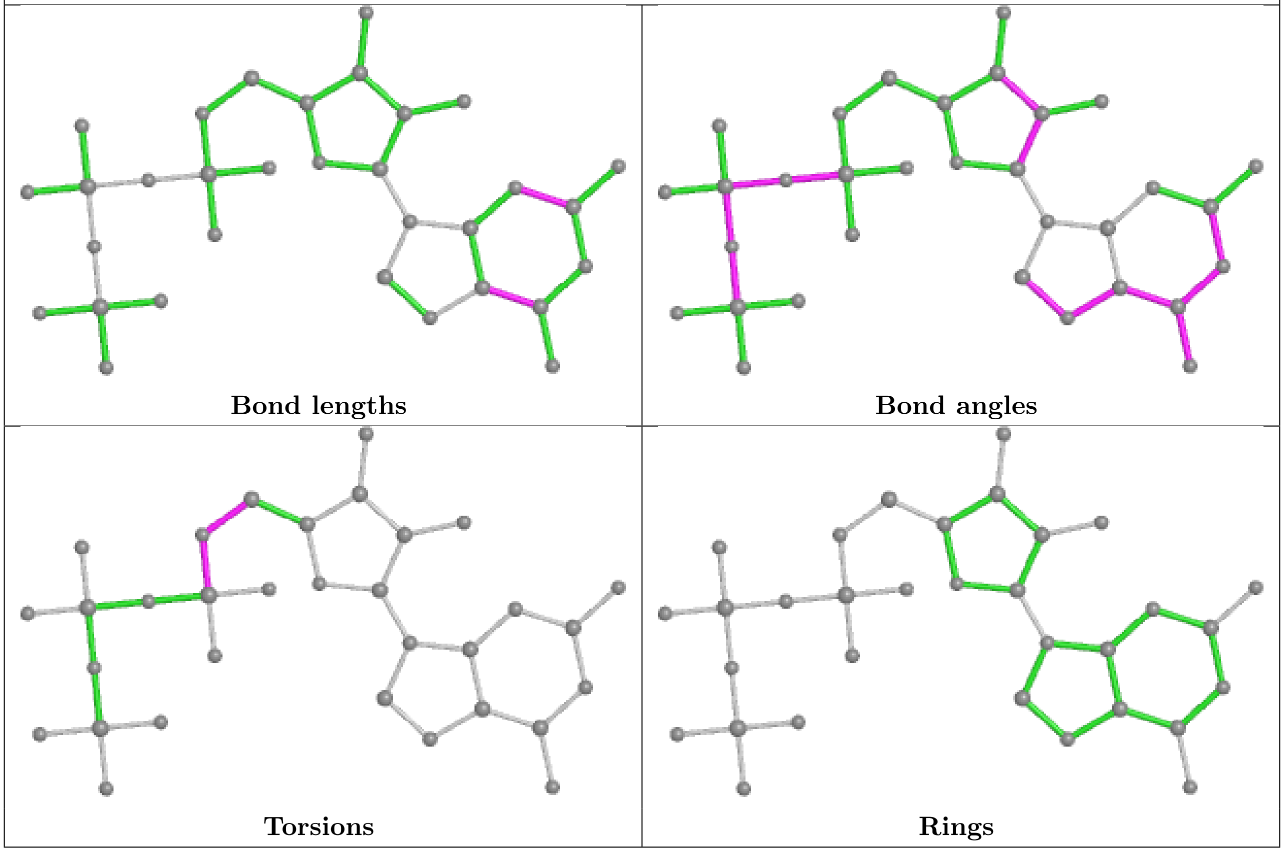


Bond lengths **Bond angles**

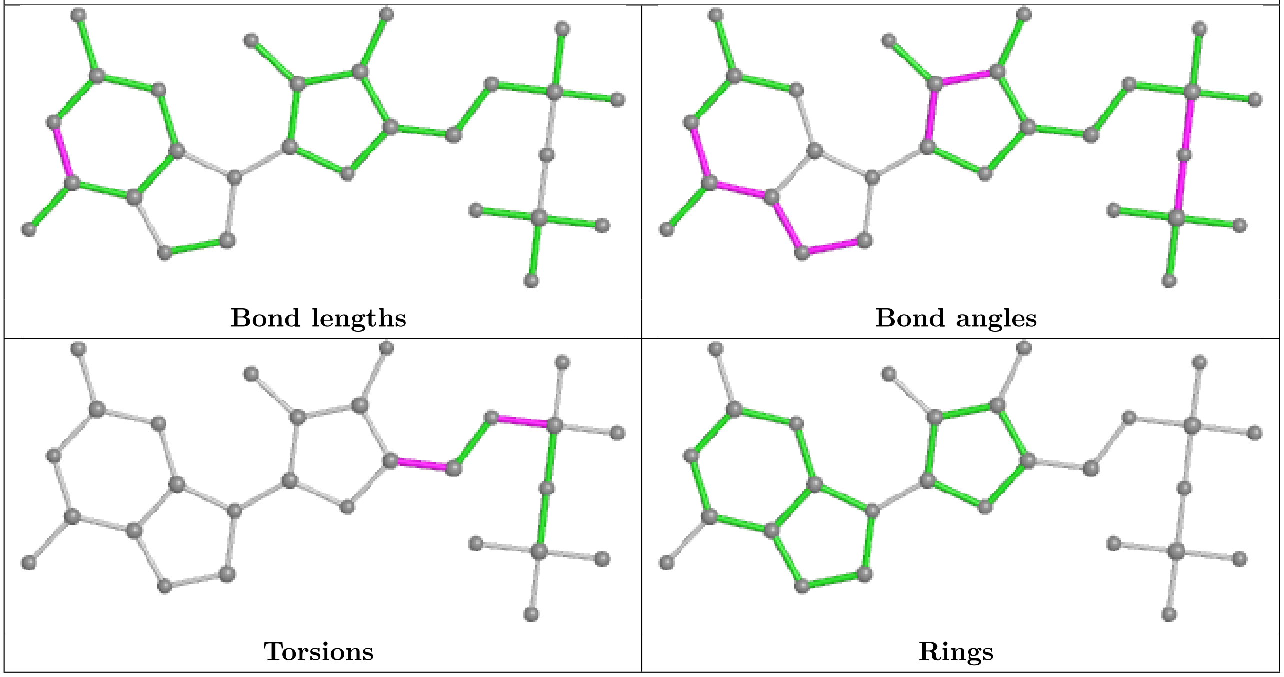


Torsions **Rings**

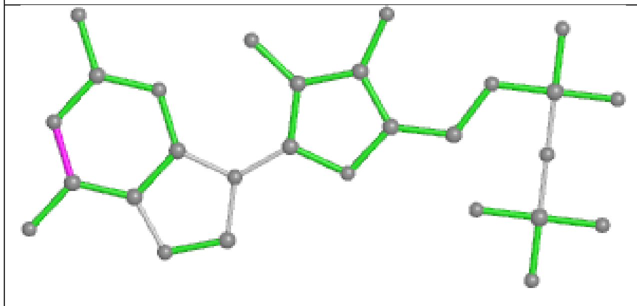
Ligand GTP RG 501



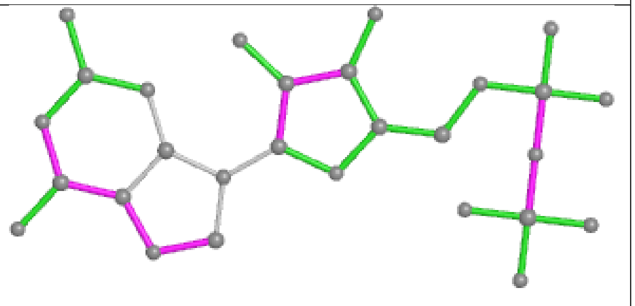
Ligand GDP MD 502



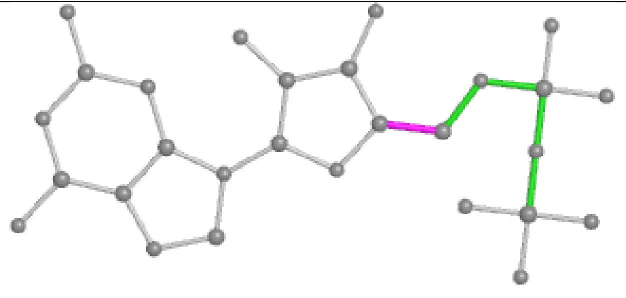
Ligand GDP RJ 502



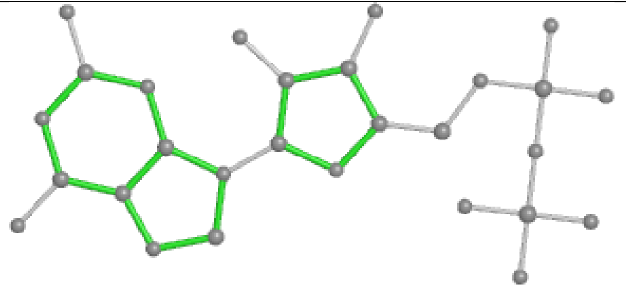
Bond lengths



Bond angles

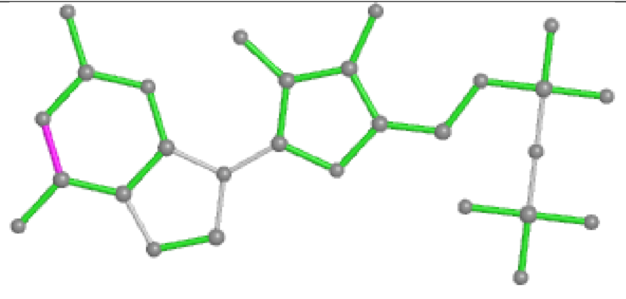


Torsions

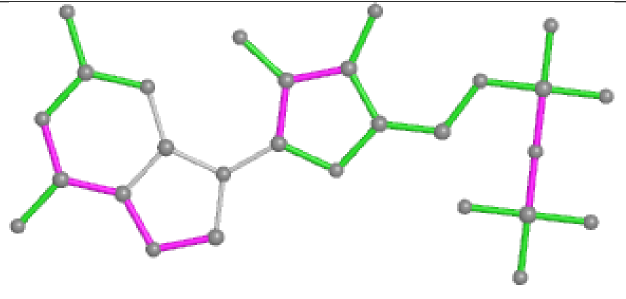


Rings

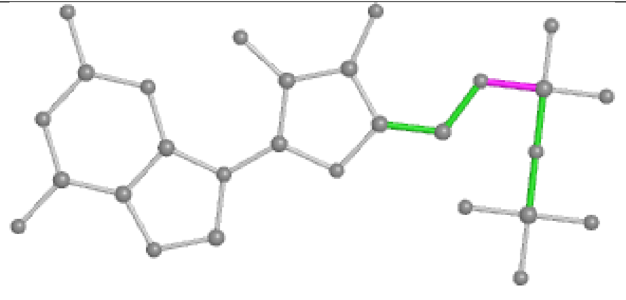
Ligand GDP WL 502



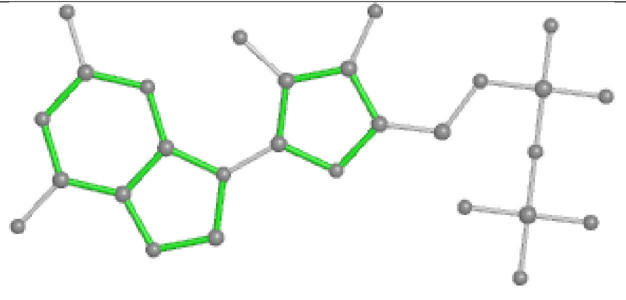
Bond lengths



Bond angles

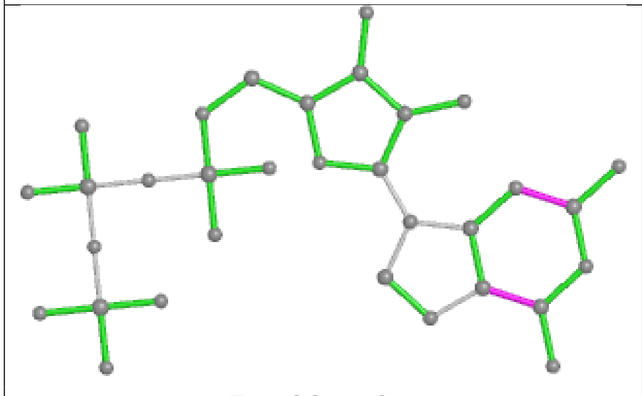


Torsions

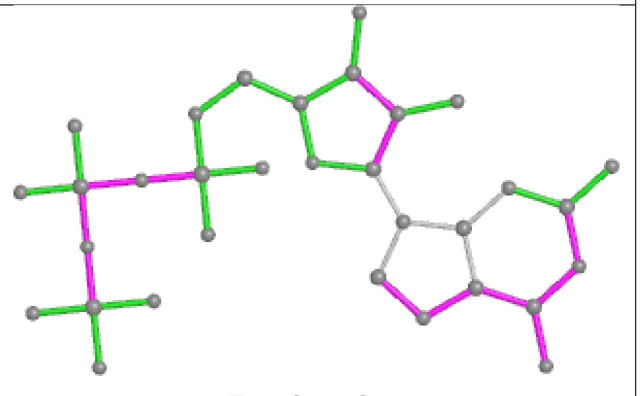


Rings

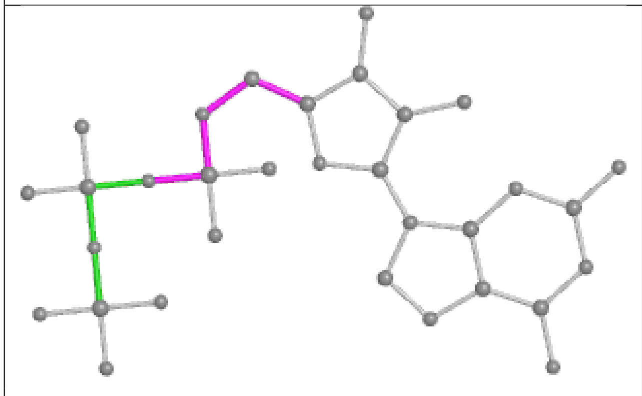
Ligand GTP AG 501



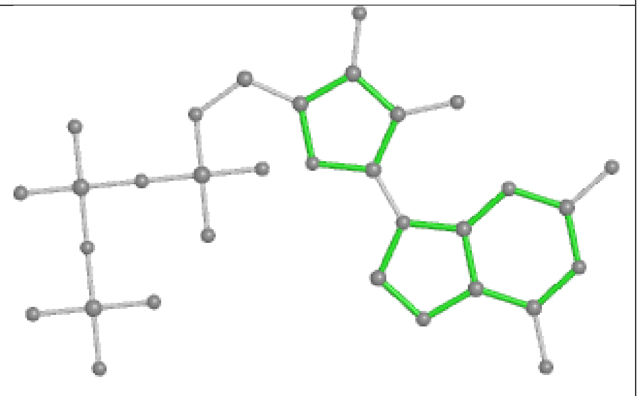
Bond lengths



Bond angles

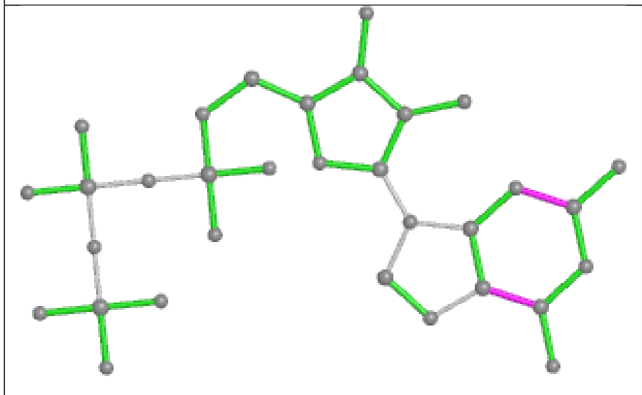


Torsions

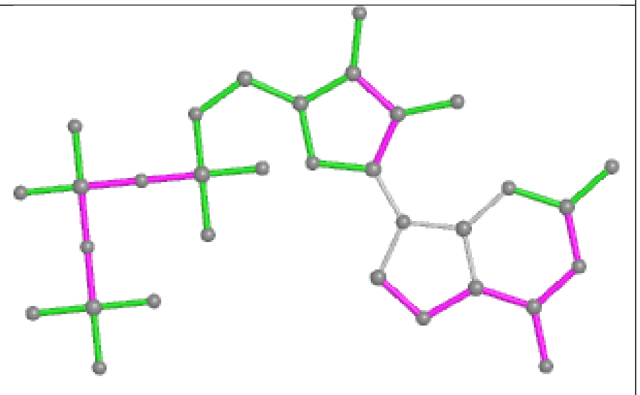


Rings

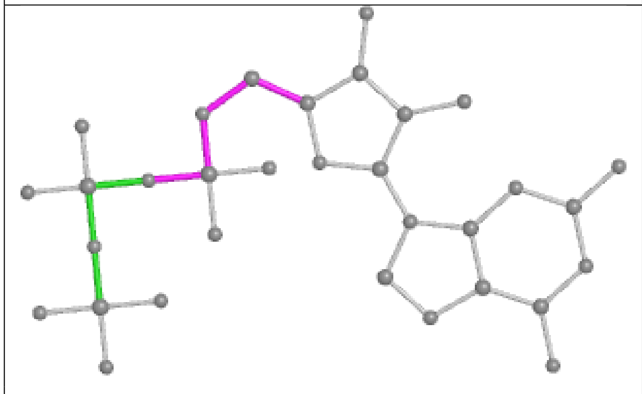
Ligand GTP TO 501



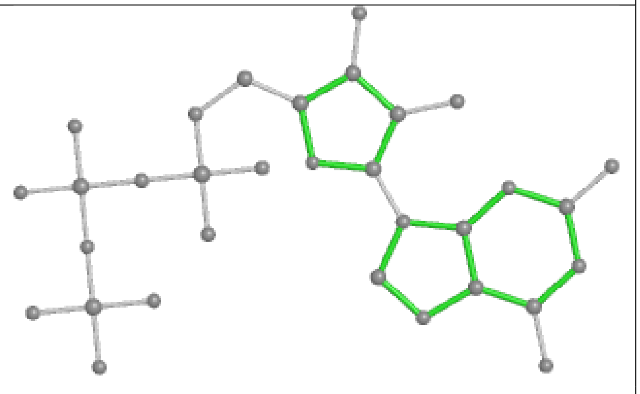
Bond lengths



Bond angles

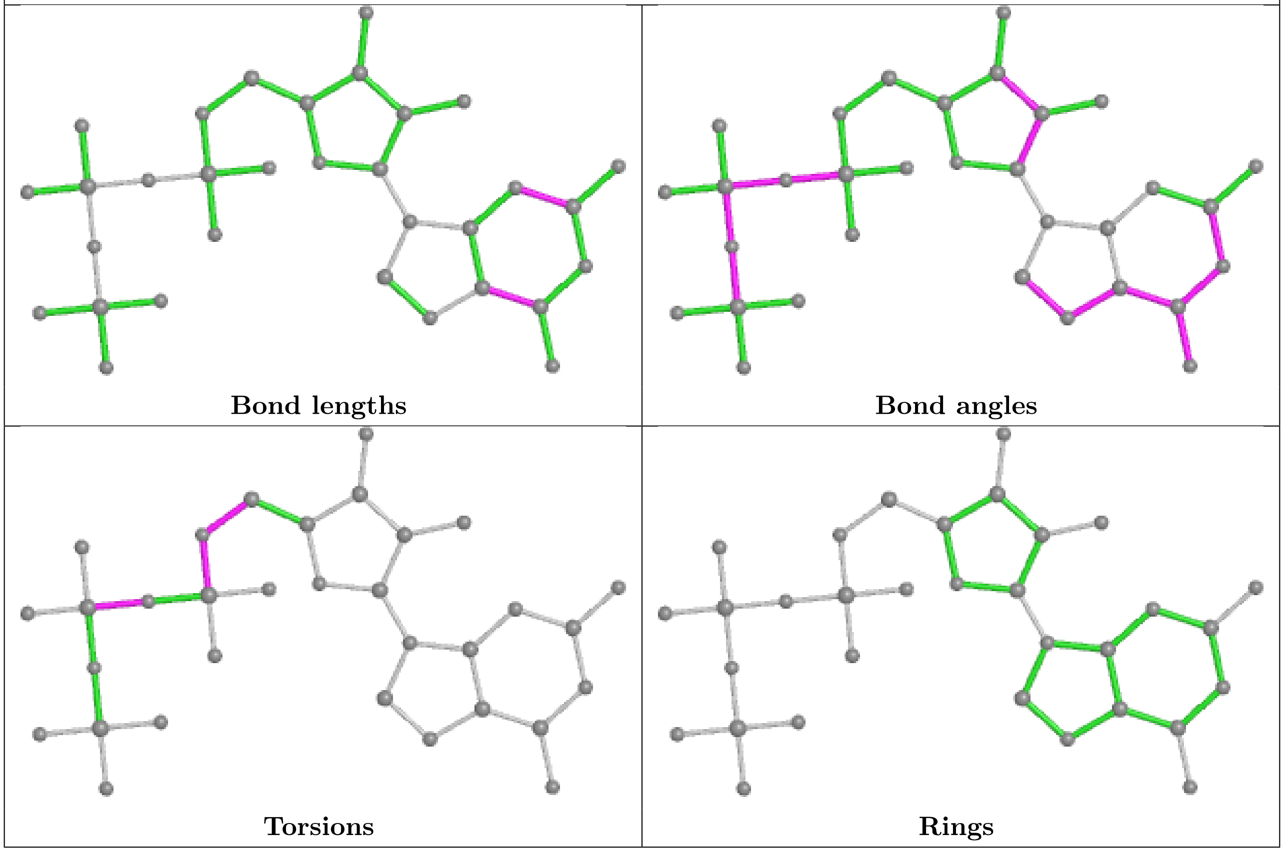


Torsions



Rings

Ligand GTP KI 501



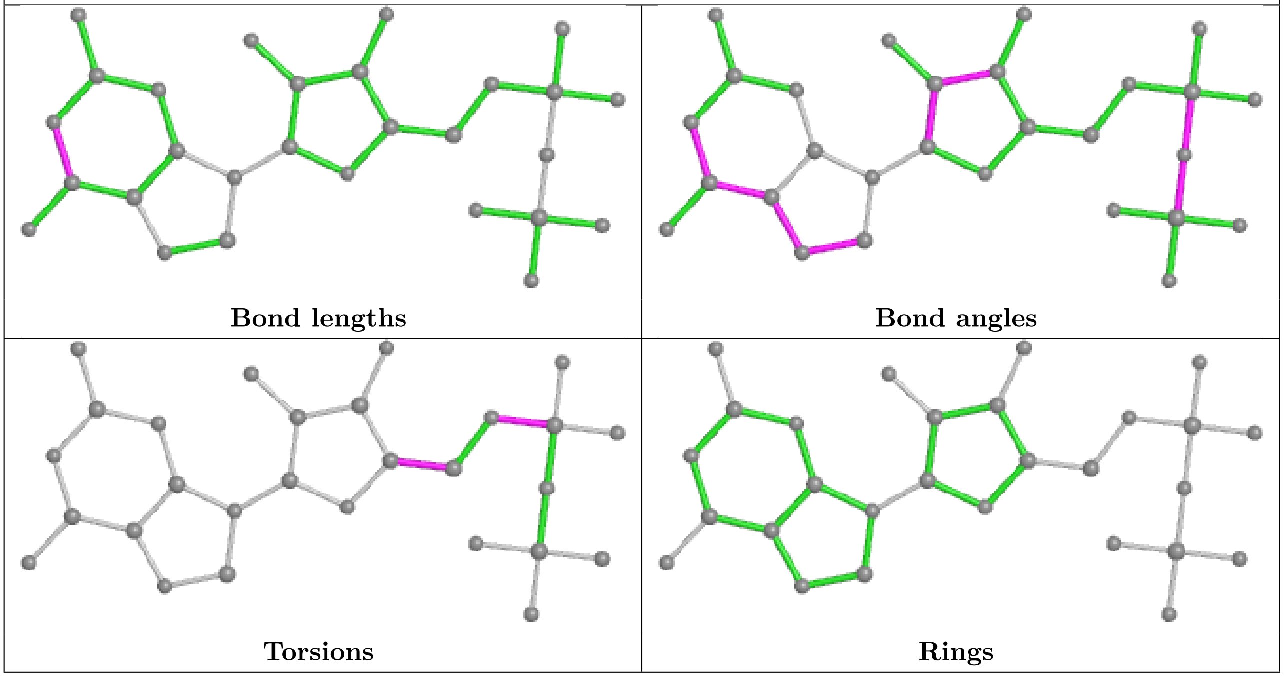
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP TJ 502



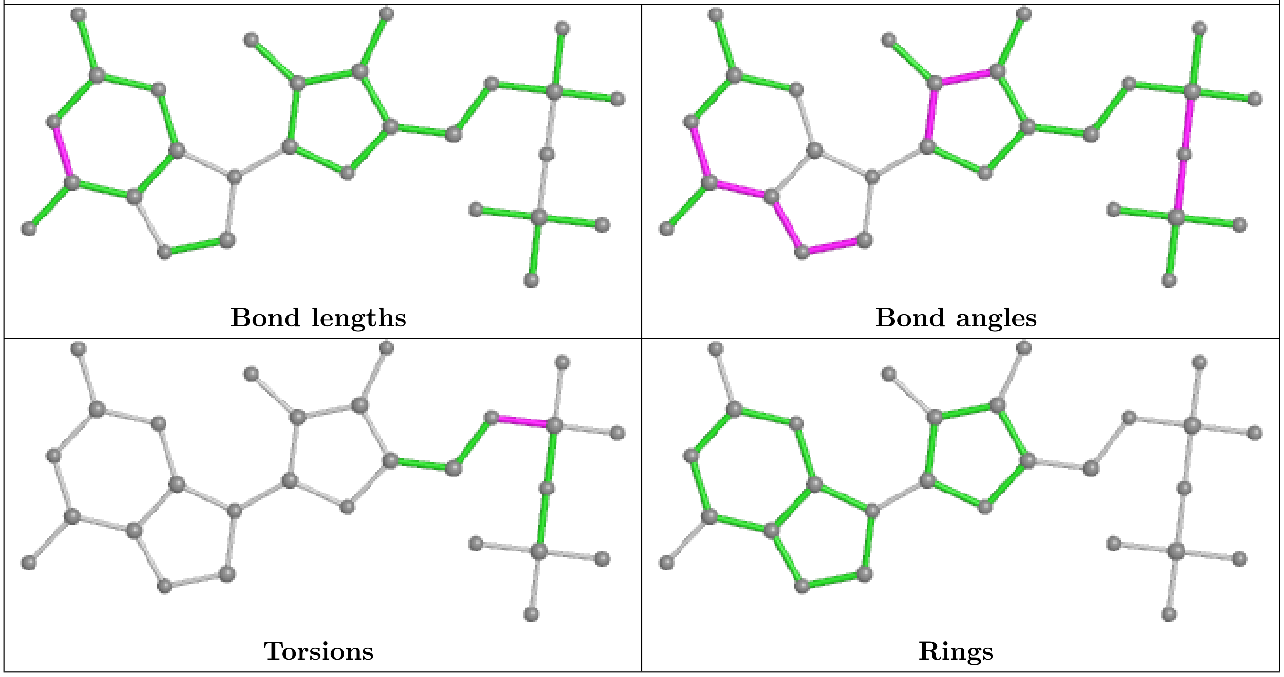
Bond lengths

Bond angles

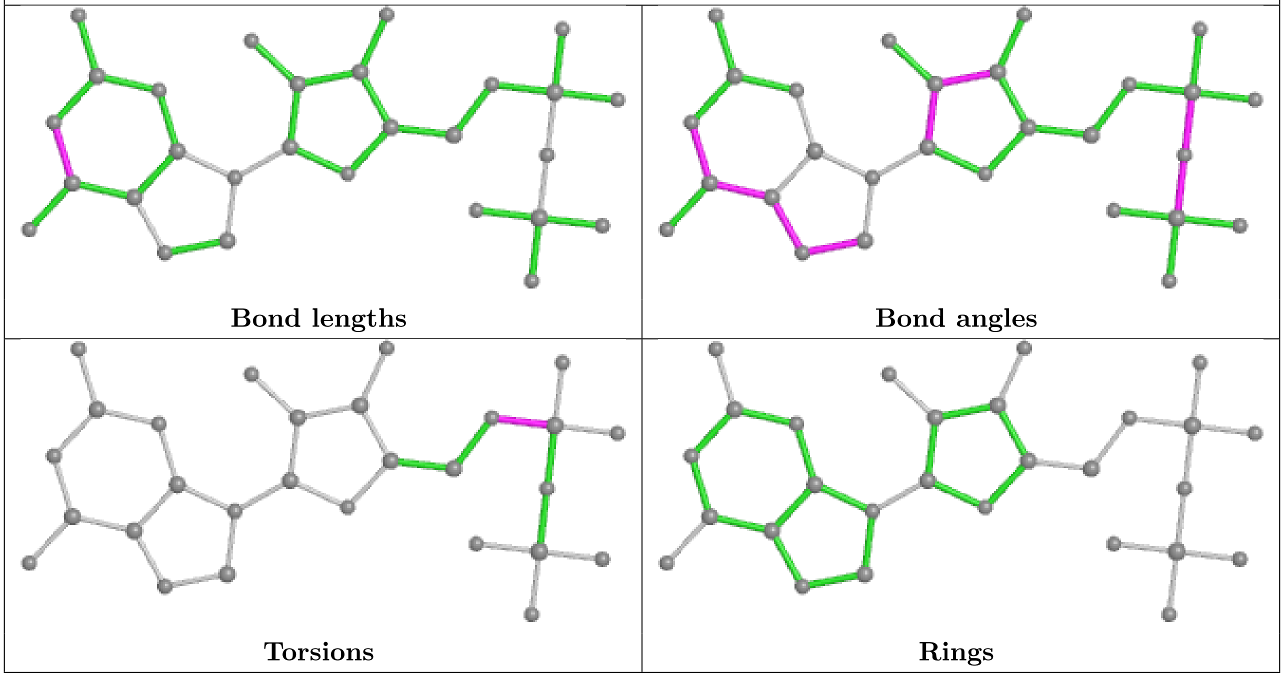
Torsions

Rings

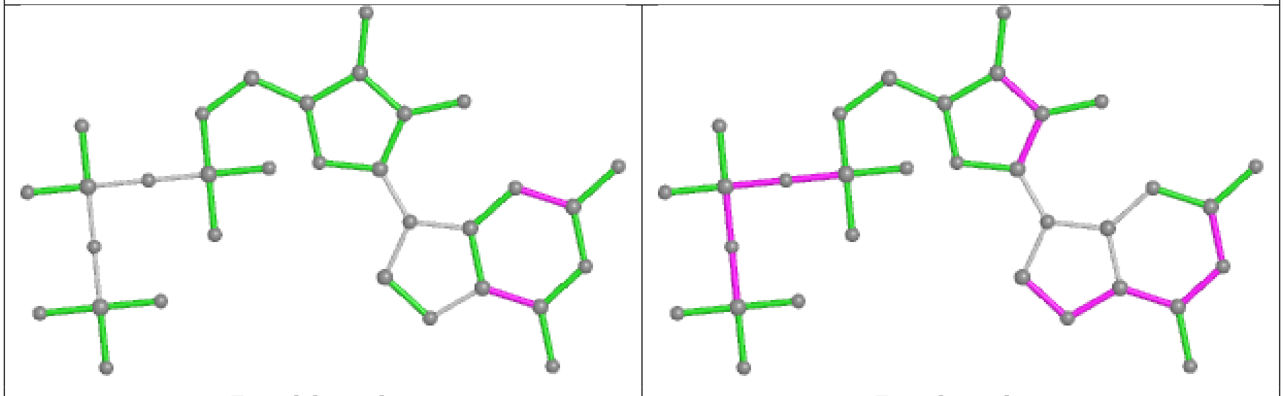
Ligand GDP WJ 502



Ligand GDP BB 502

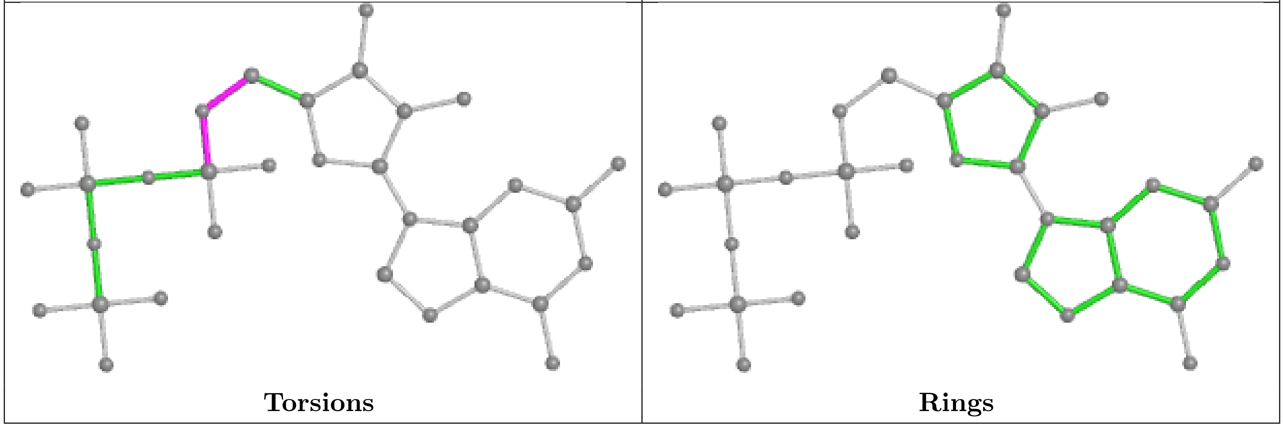


Ligand GTP OI 501



Bond lengths

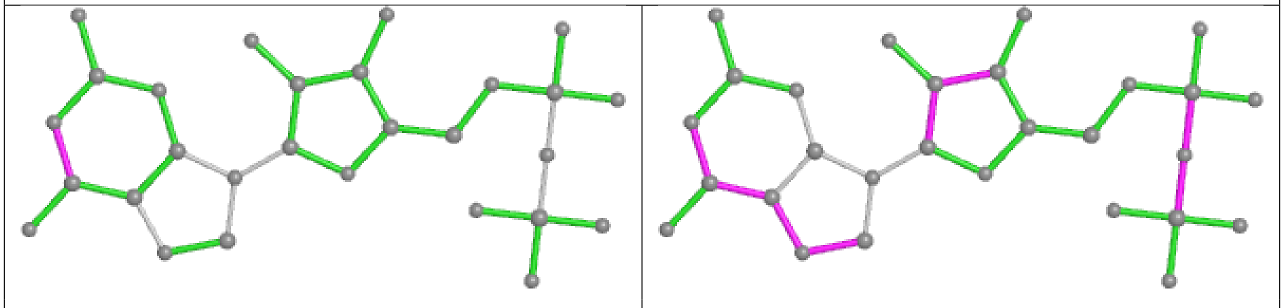
Bond angles



Torsions

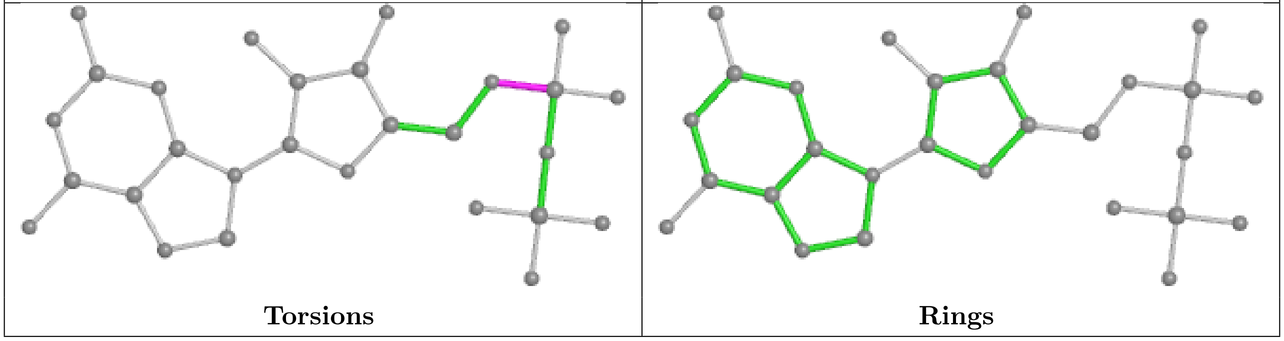
Rings

Ligand GDP TF 502



Bond lengths

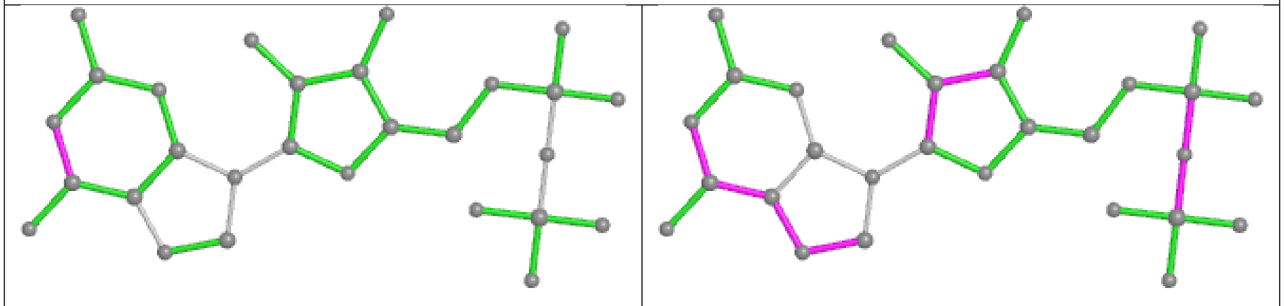
Bond angles



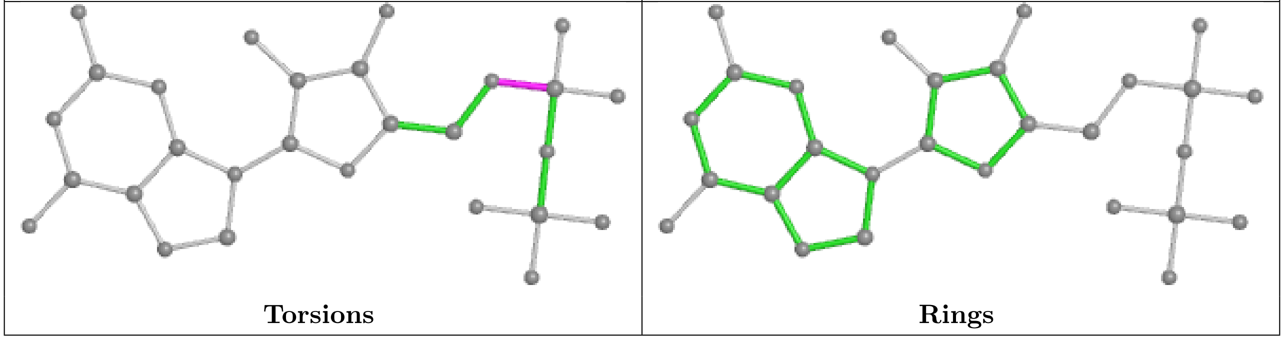
Torsions

Rings

Ligand GDP TP 502

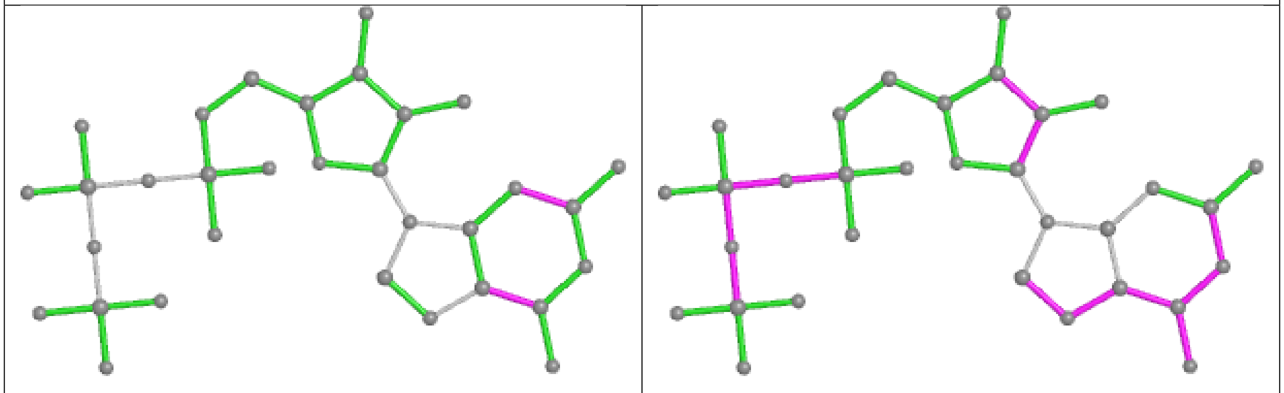


Bond lengths **Bond angles**

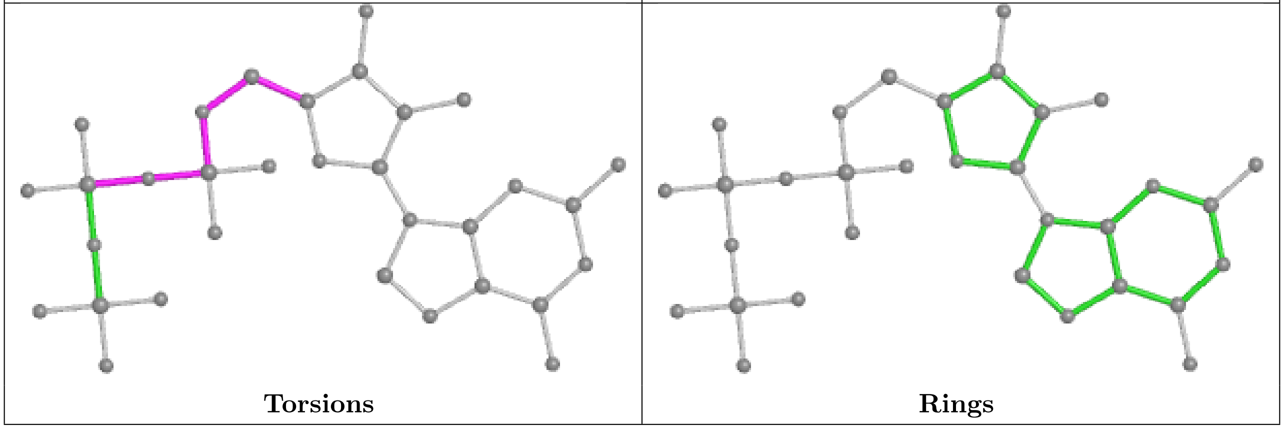


Torsions **Rings**

Ligand GTP OM 501

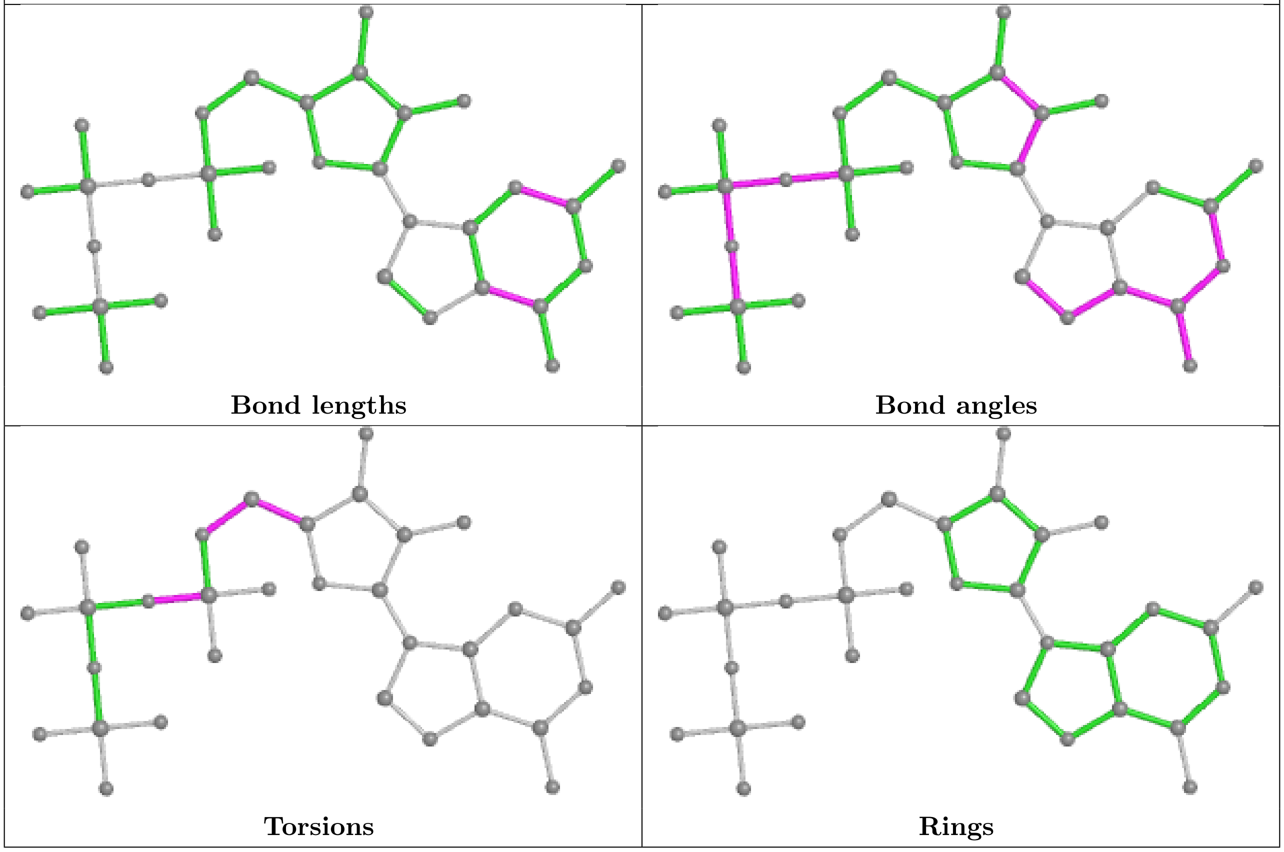


Bond lengths **Bond angles**

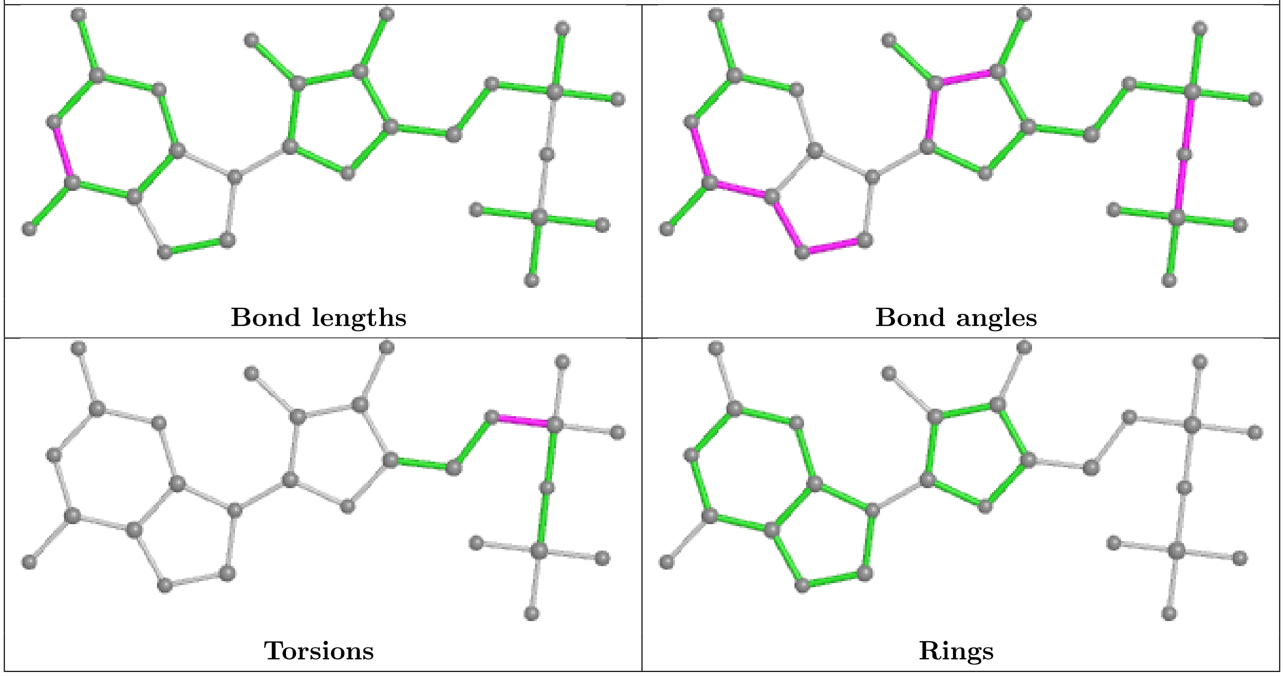


Torsions **Rings**

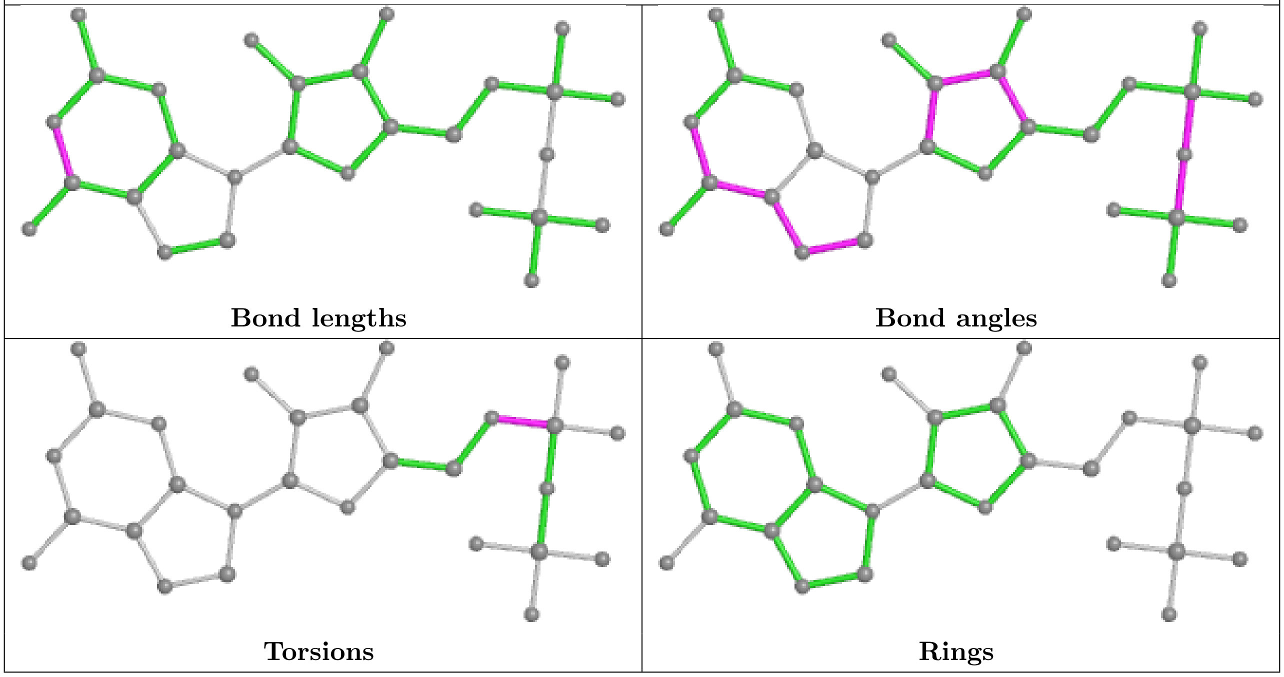
Ligand GTP HC 501



Ligand GDP IF 502



Ligand GDP RF 502



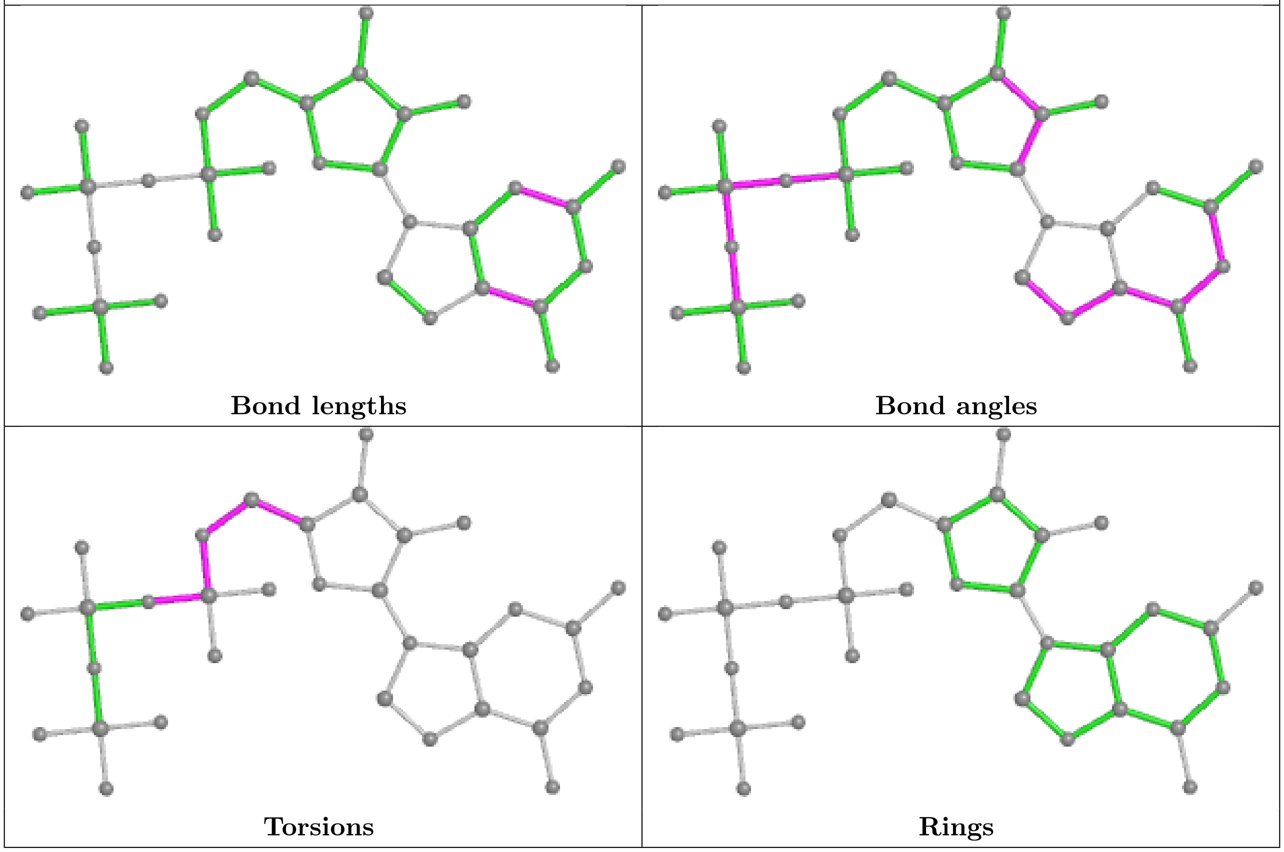
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP CI 501



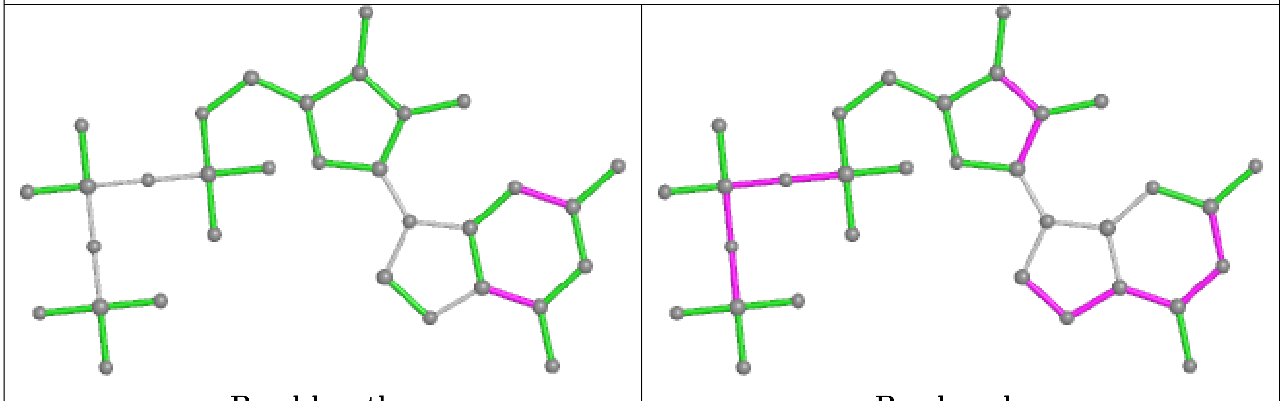
Bond lengths

Bond angles

Torsions

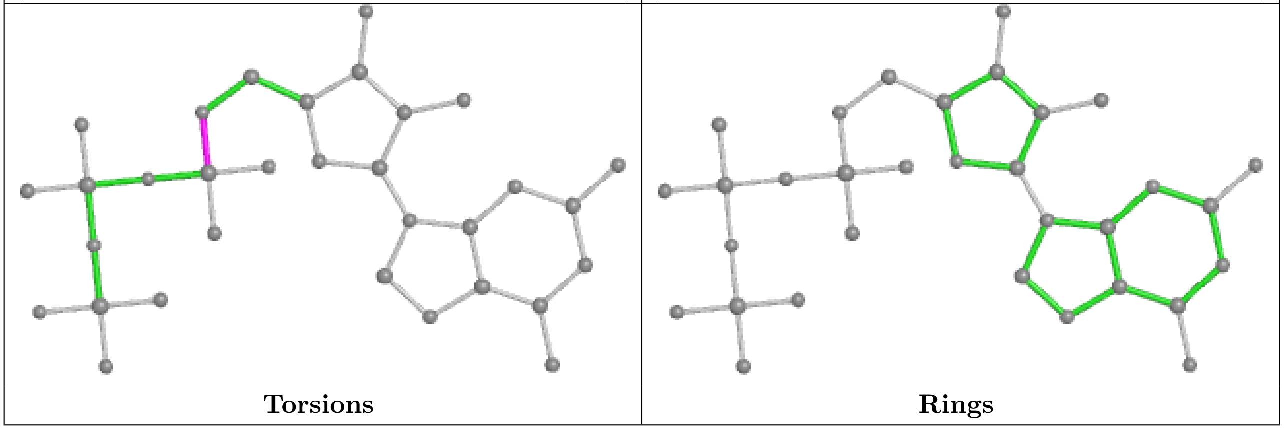
Rings

Ligand GTP DE 501



Bond lengths

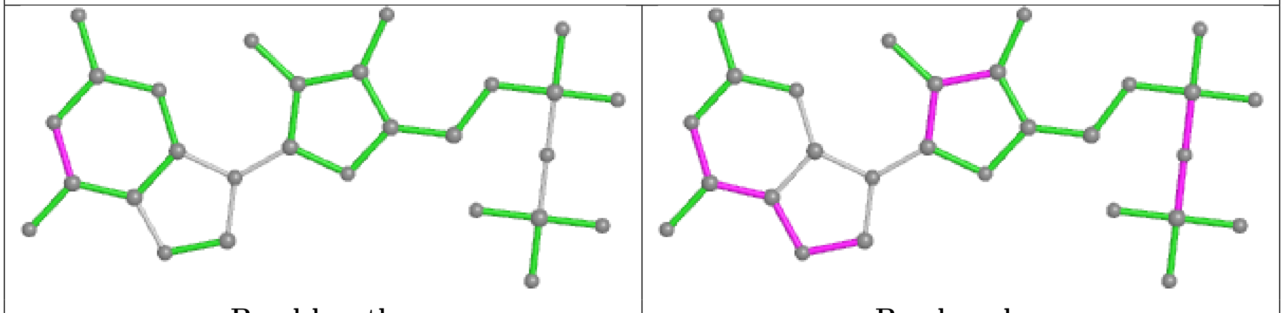
Bond angles



Torsions

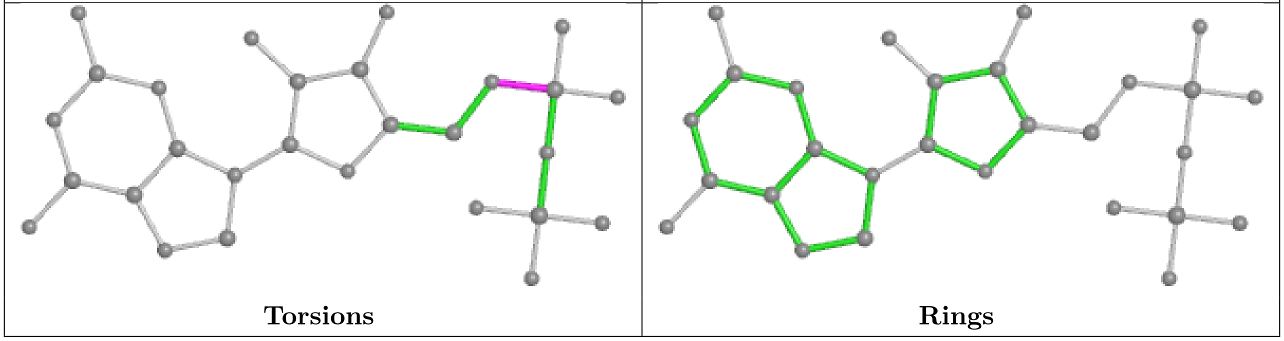
Rings

Ligand GDP JJ 502



Bond lengths

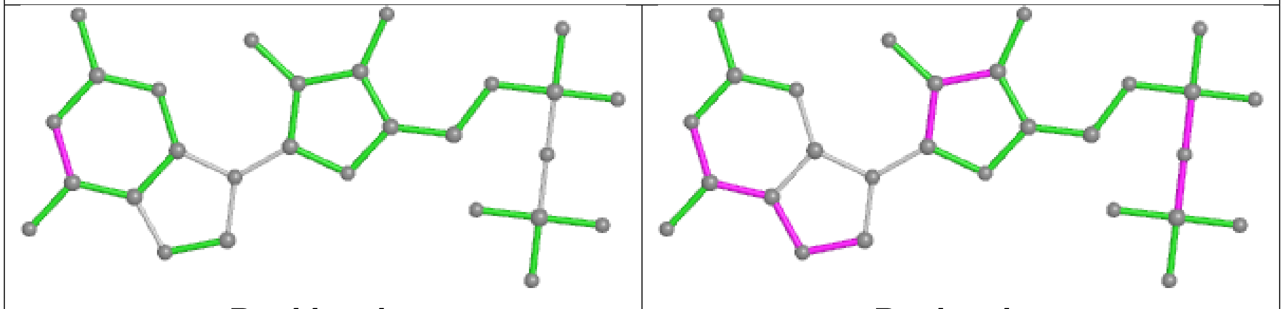
Bond angles



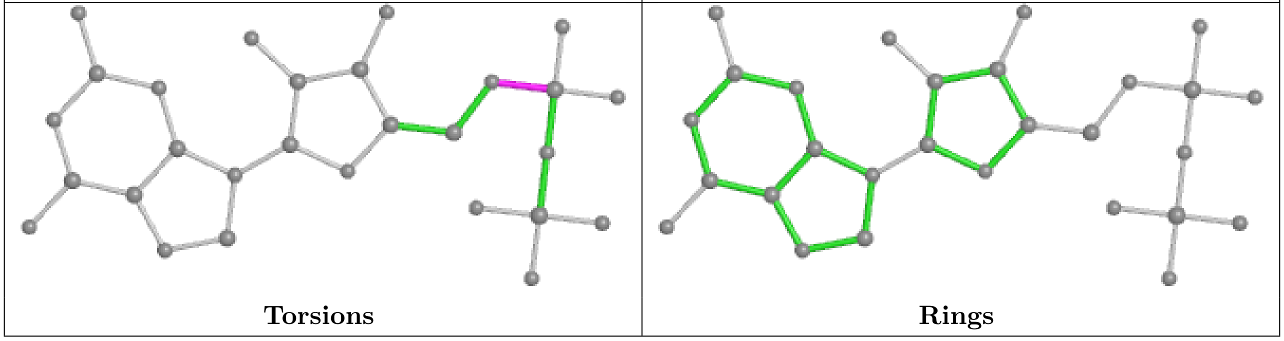
Torsions

Rings

Ligand GDP CB 502

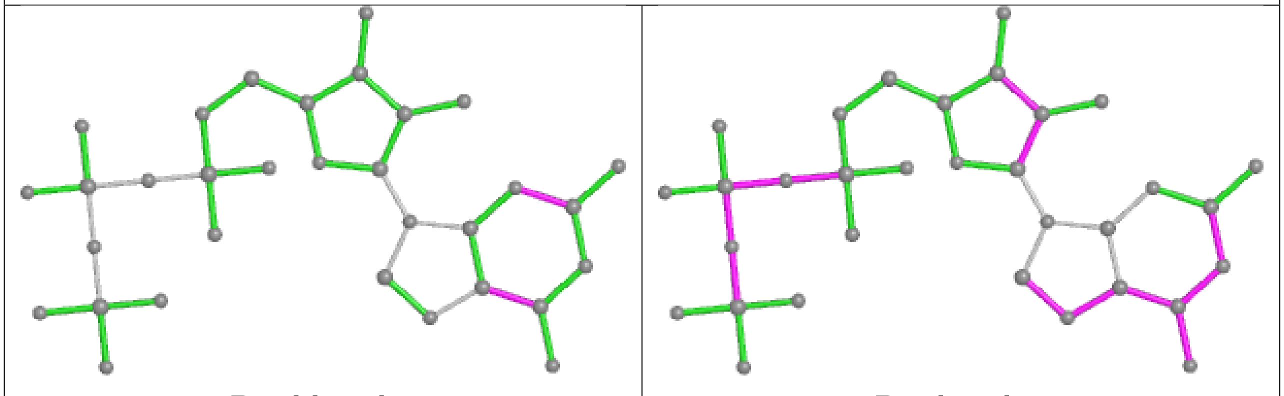


Bond lengths Bond angles

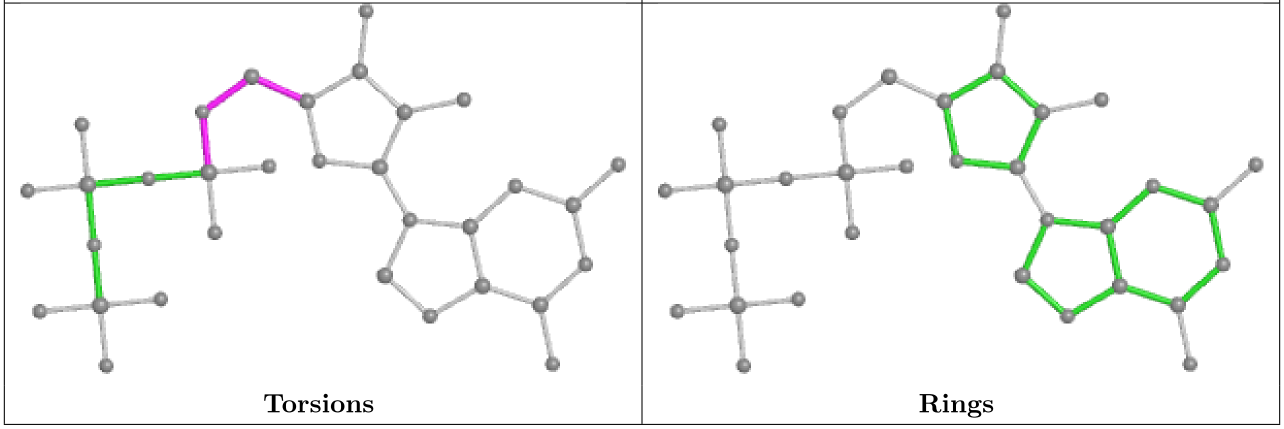


Torsions Rings

Ligand GTP OC 501

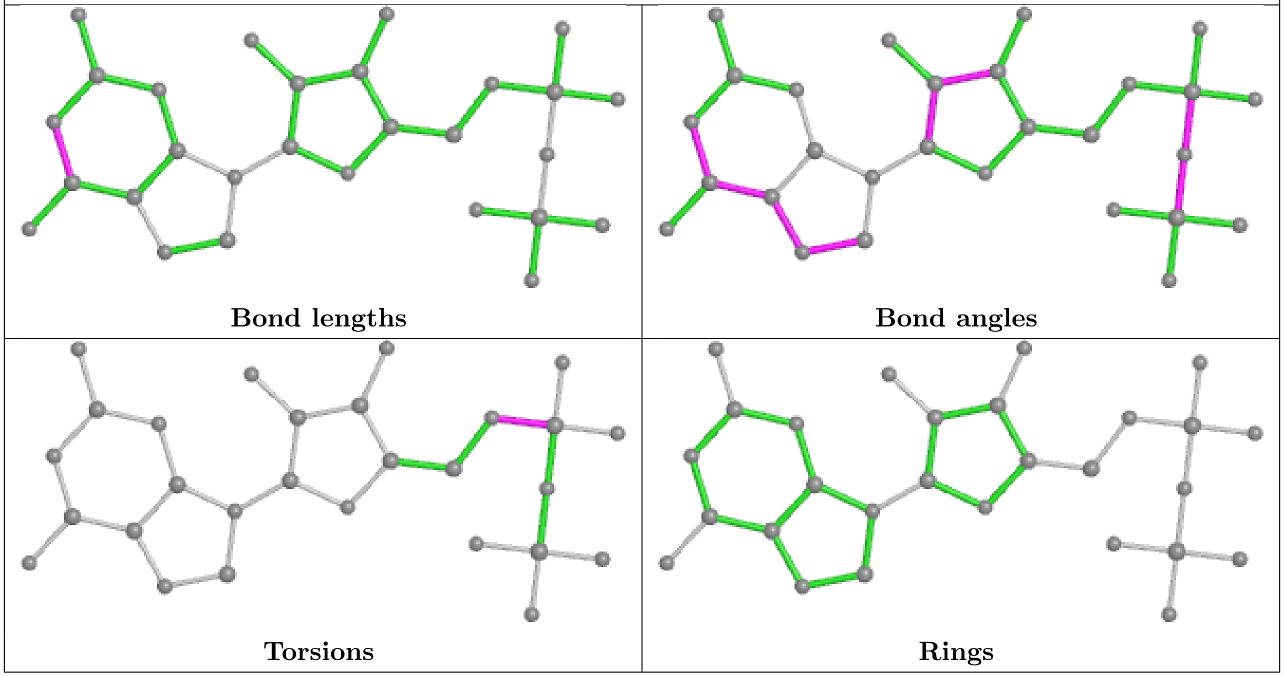


Bond lengths Bond angles



Torsions Rings

Ligand GDP DD 502



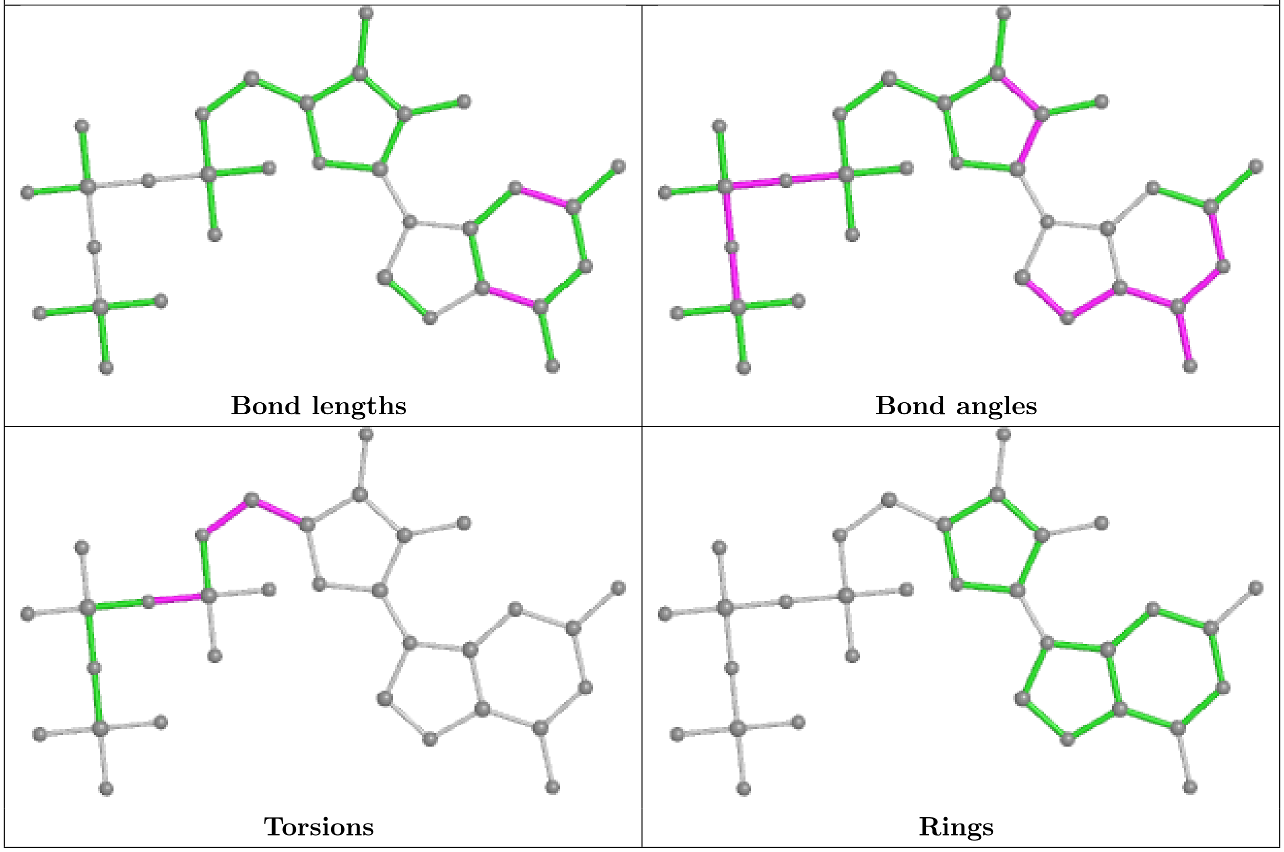
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP AA 501



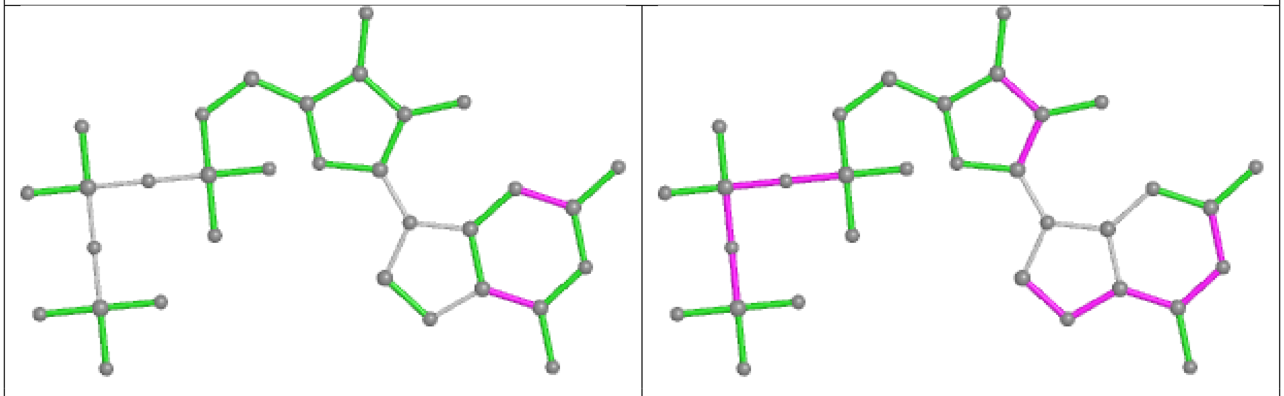
Bond lengths

Bond angles

Torsions

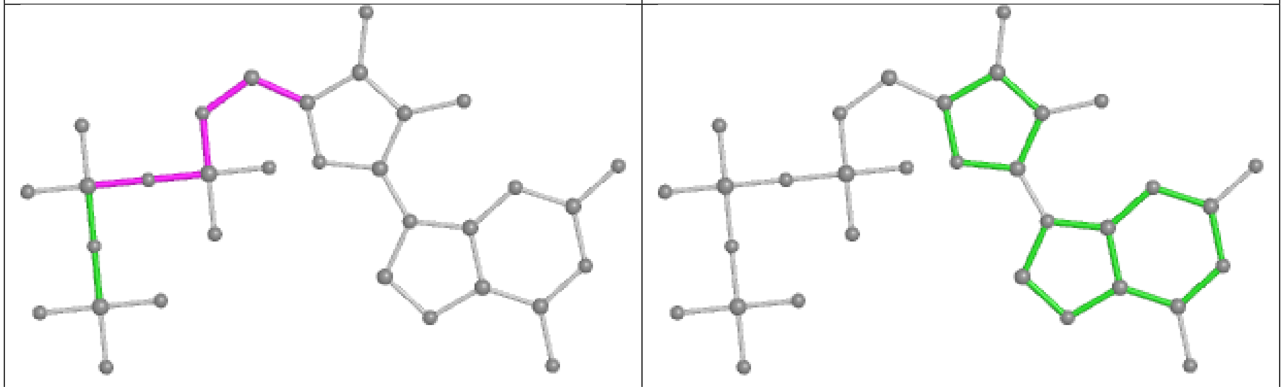
Rings

Ligand GTP PC 501



Bond lengths

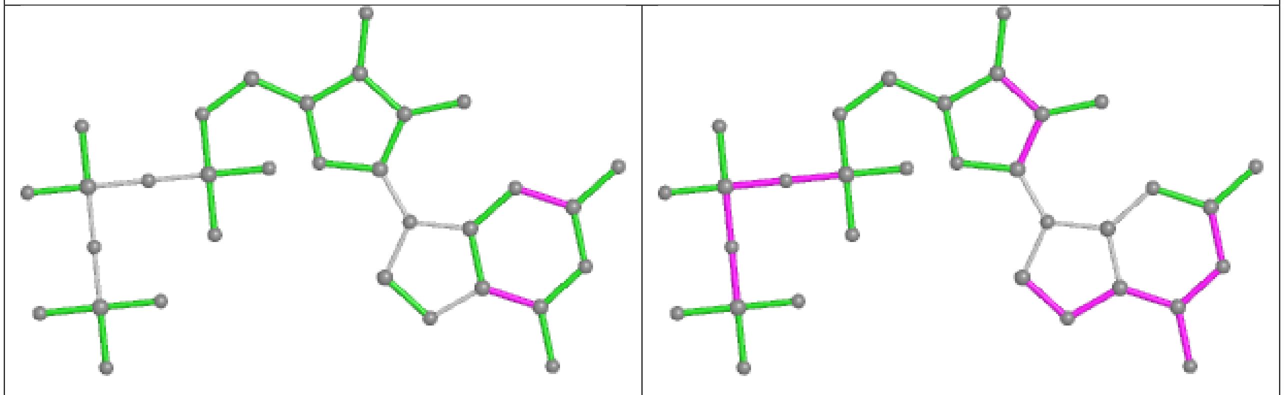
Bond angles



Torsions

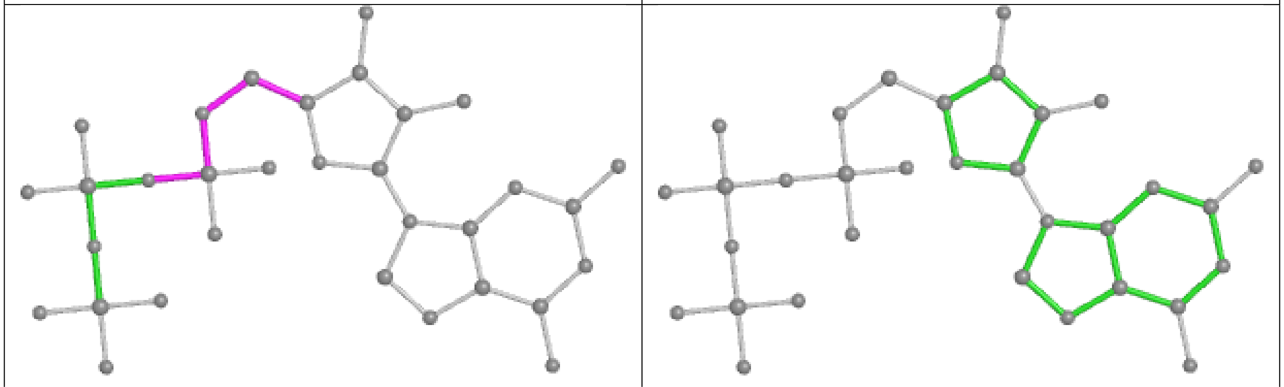
Rings

Ligand GTP HI 501



Bond lengths

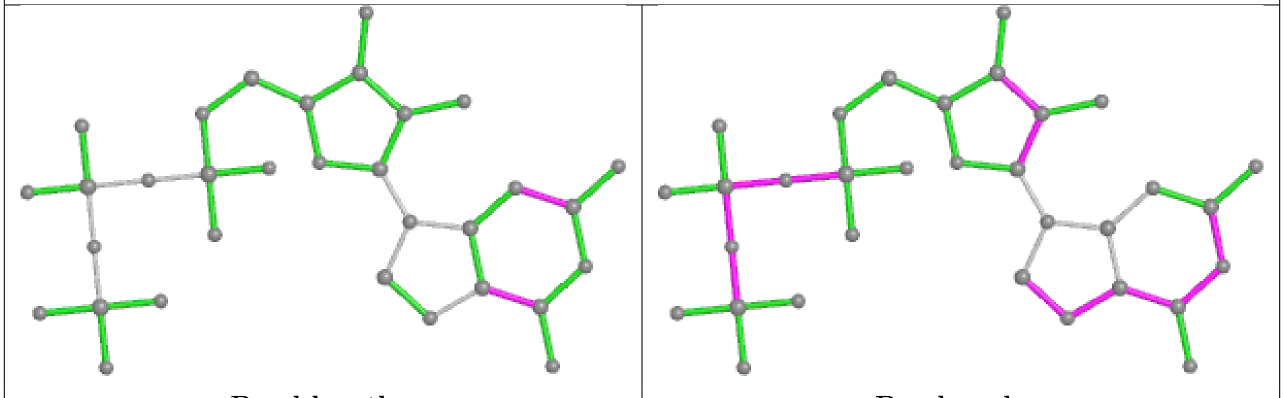
Bond angles



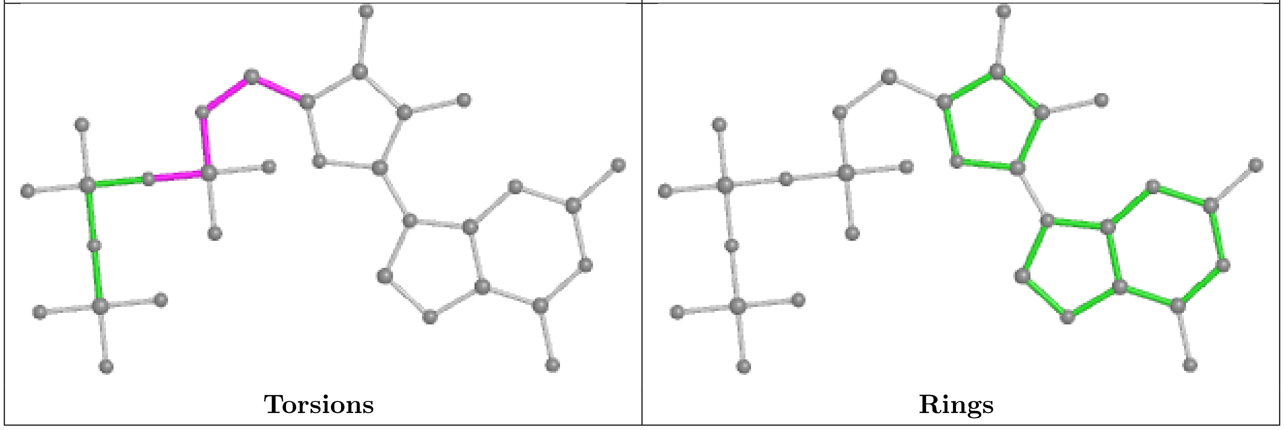
Torsions

Rings

Ligand GTP WG 501

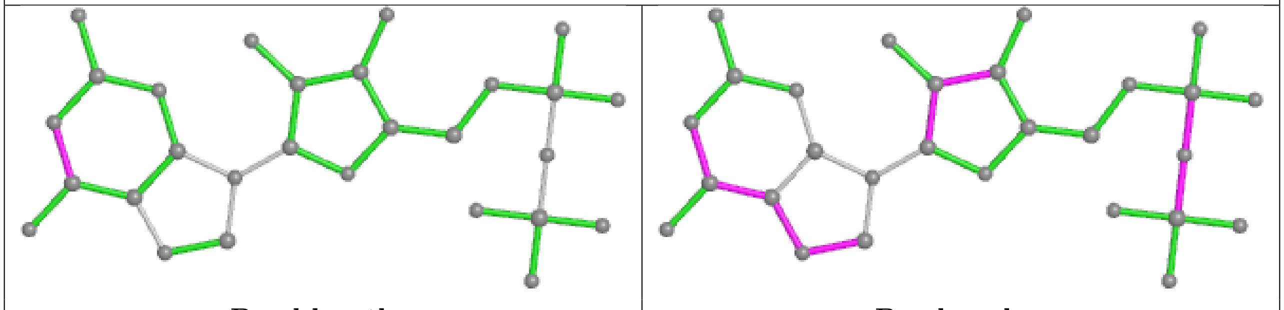


Bond lengths Bond angles

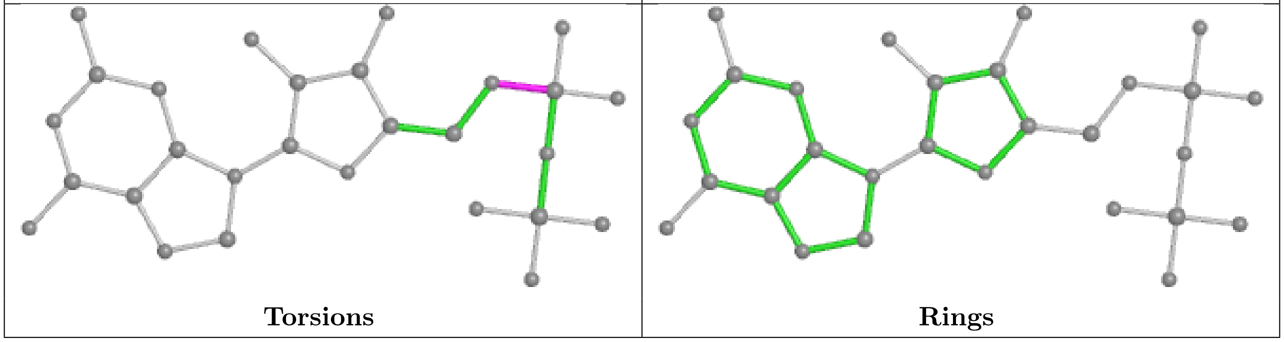


Torsions Rings

Ligand GDP HL 502

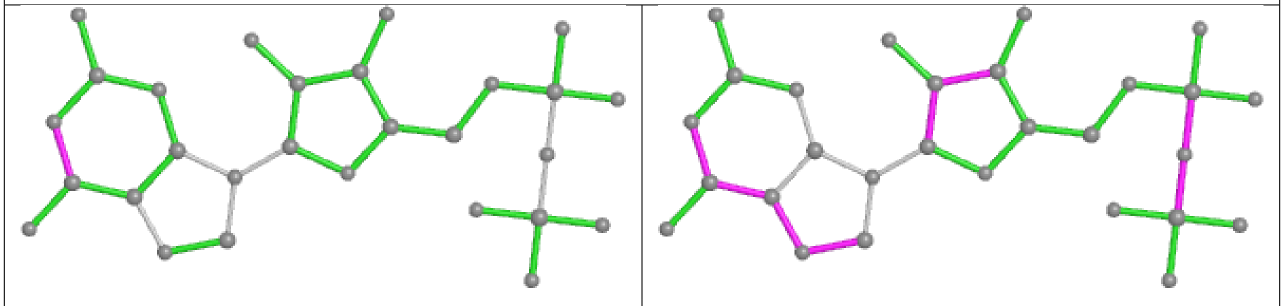


Bond lengths Bond angles

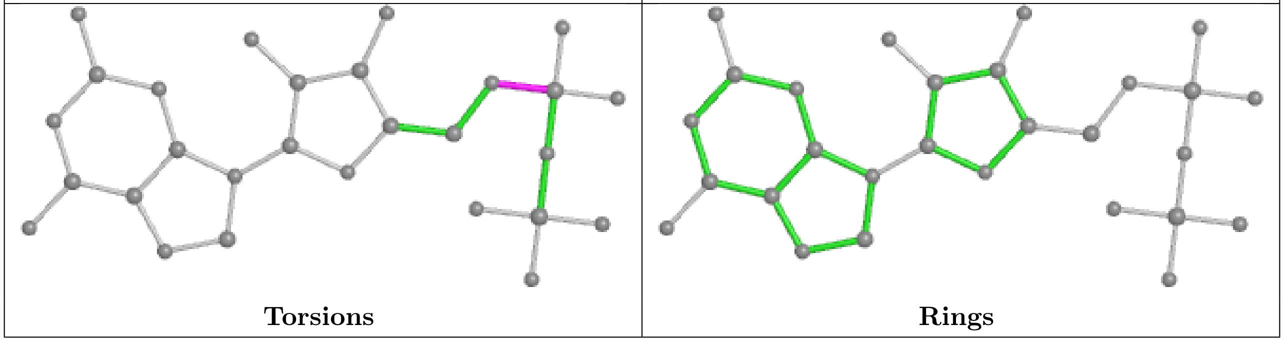


Torsions Rings

Ligand GDP PJ 502

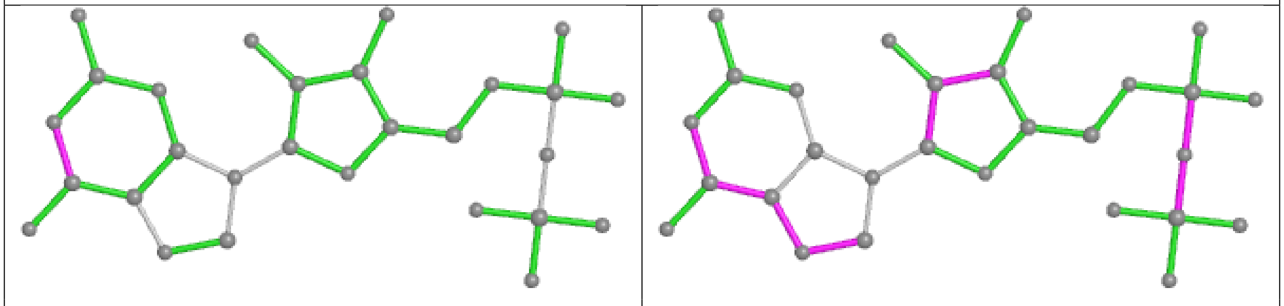


Bond lengths **Bond angles**

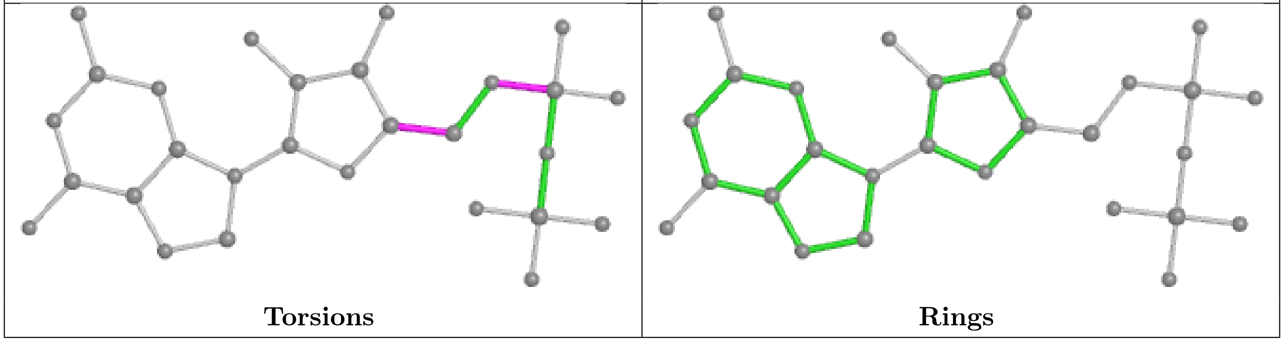


Torsions **Rings**

Ligand GDP JN 502

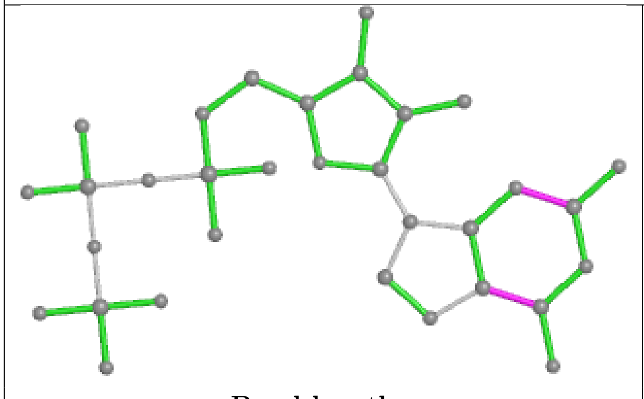


Bond lengths **Bond angles**

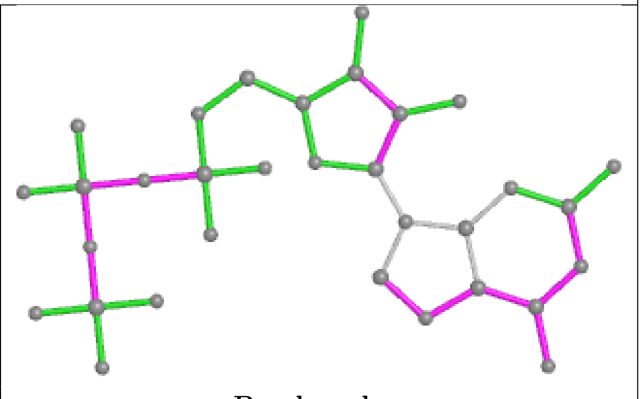


Torsions **Rings**

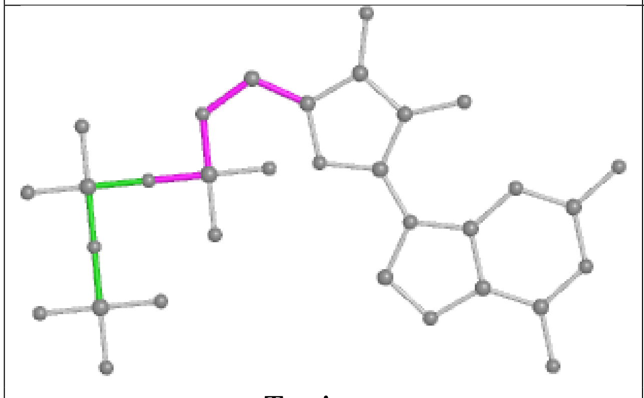
Ligand GTP PE 501



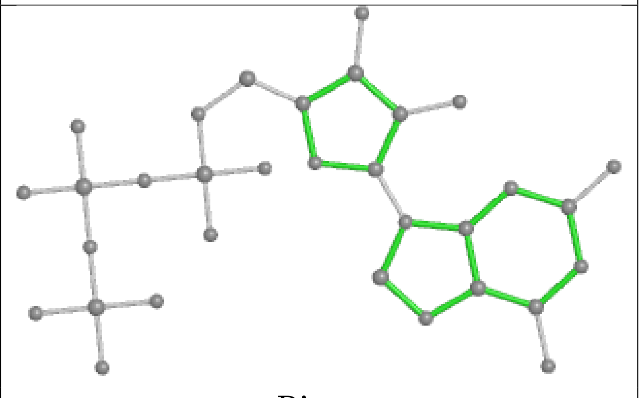
Bond lengths



Bond angles

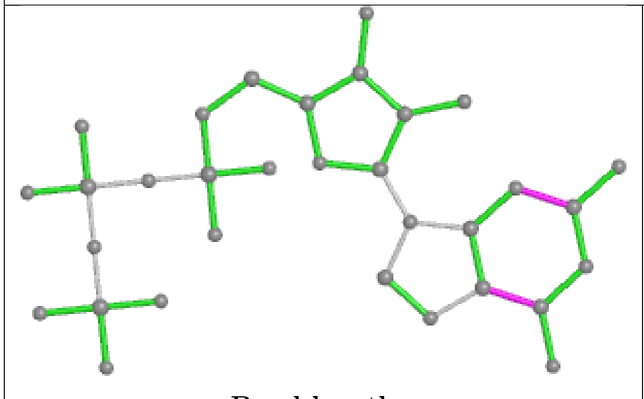


Torsions

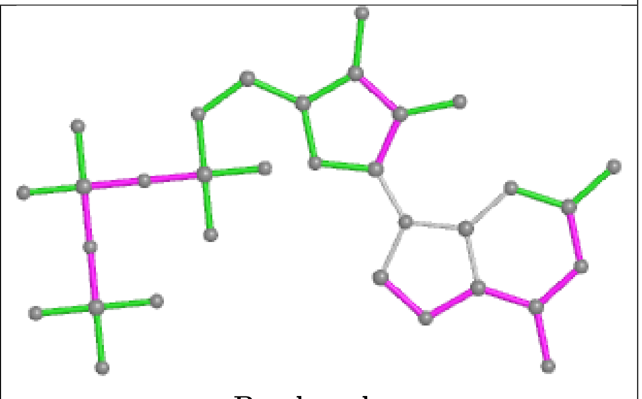


Rings

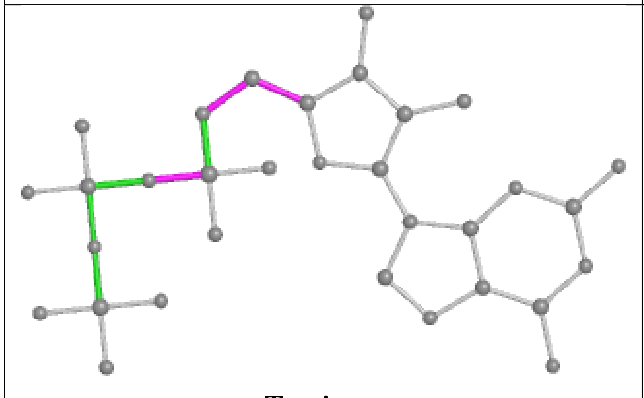
Ligand GTP HM 501



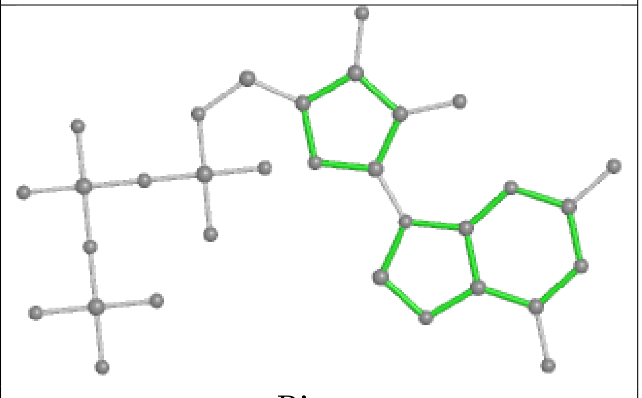
Bond lengths



Bond angles

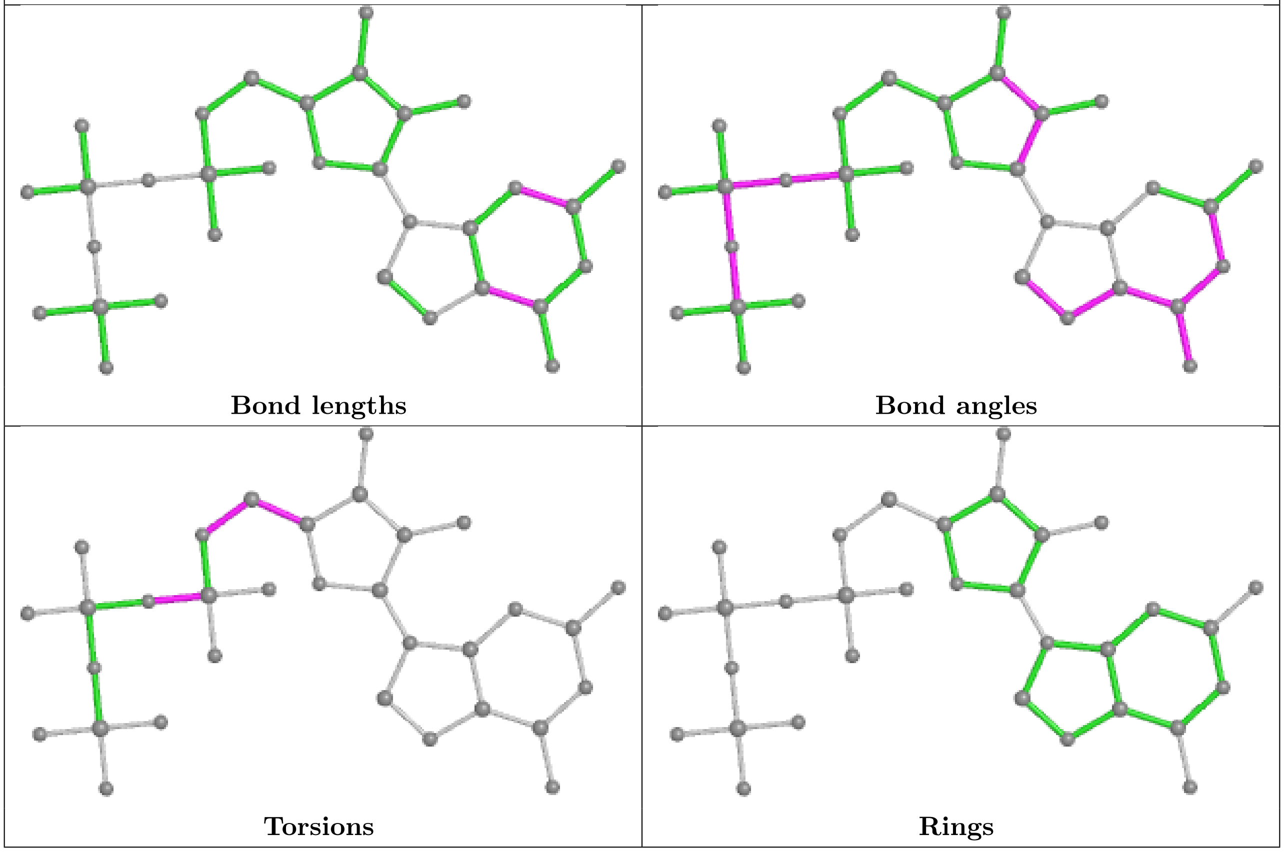


Torsions



Rings

Ligand GTP AI 501



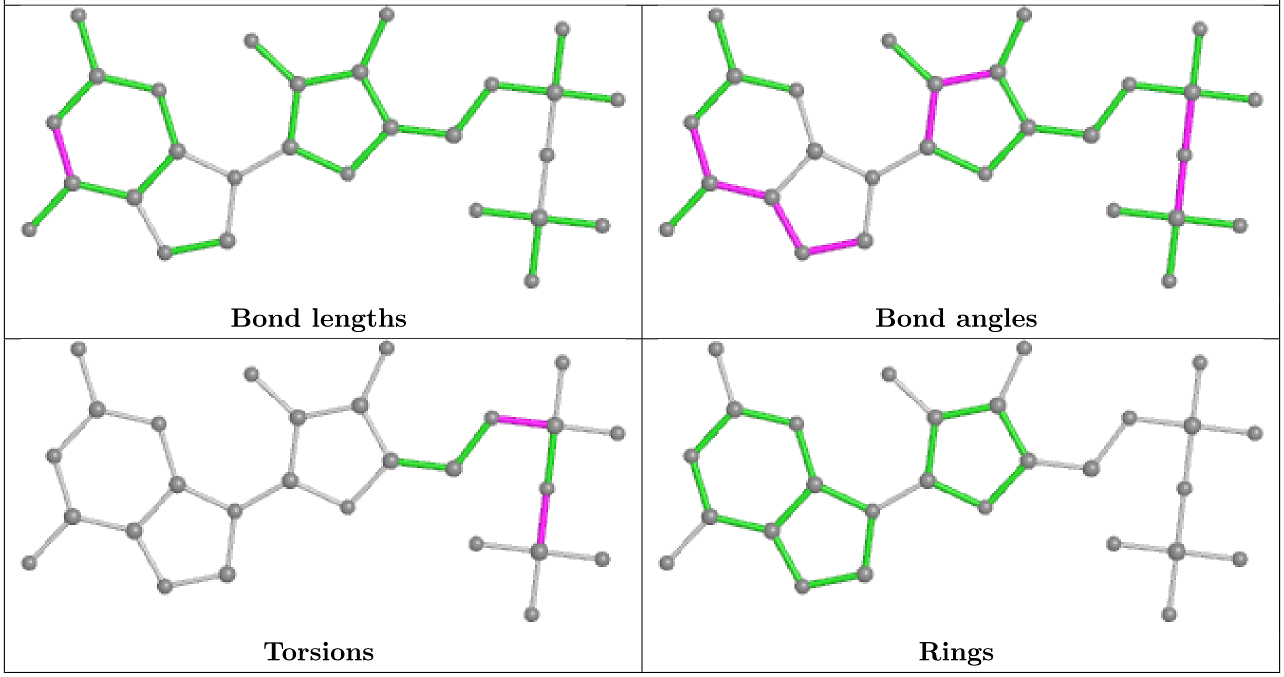
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP BJ 502



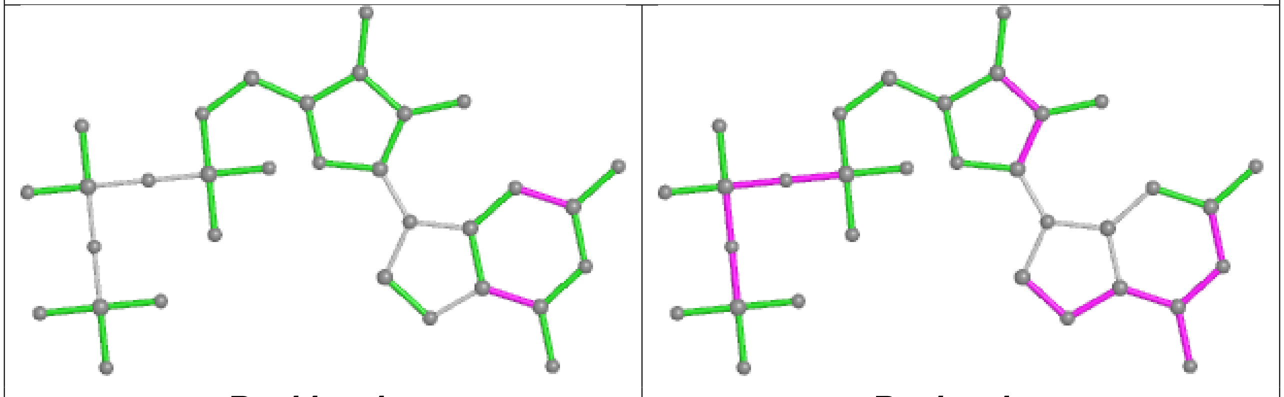
Bond lengths

Bond angles

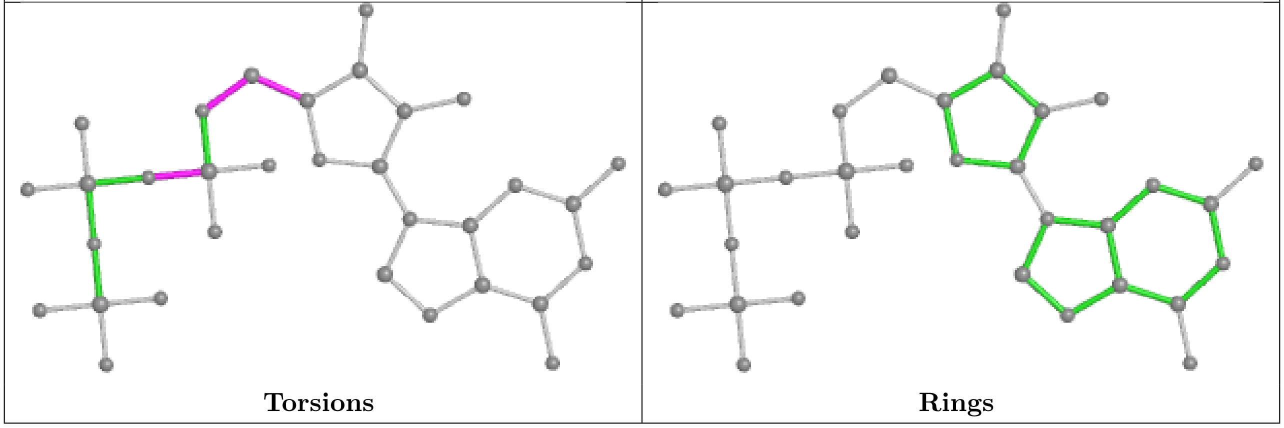
Torsions

Rings

Ligand GTP VE 501

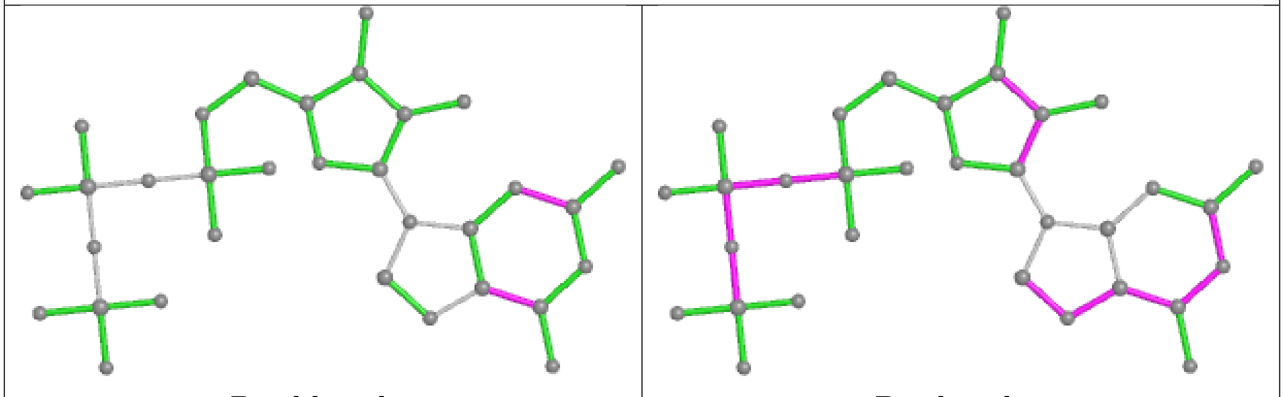


Bond lengths Bond angles

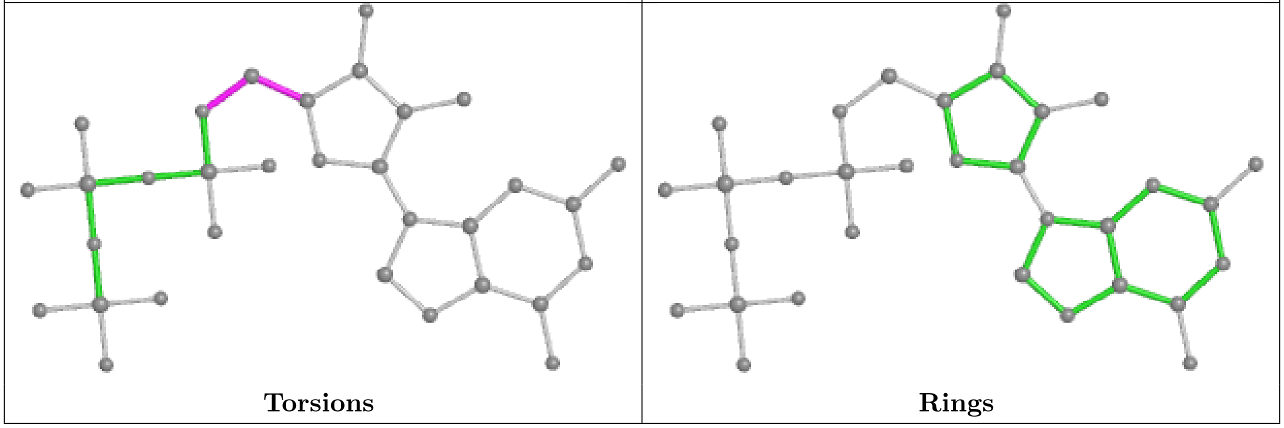


Torsions Rings

Ligand GTP WO 501

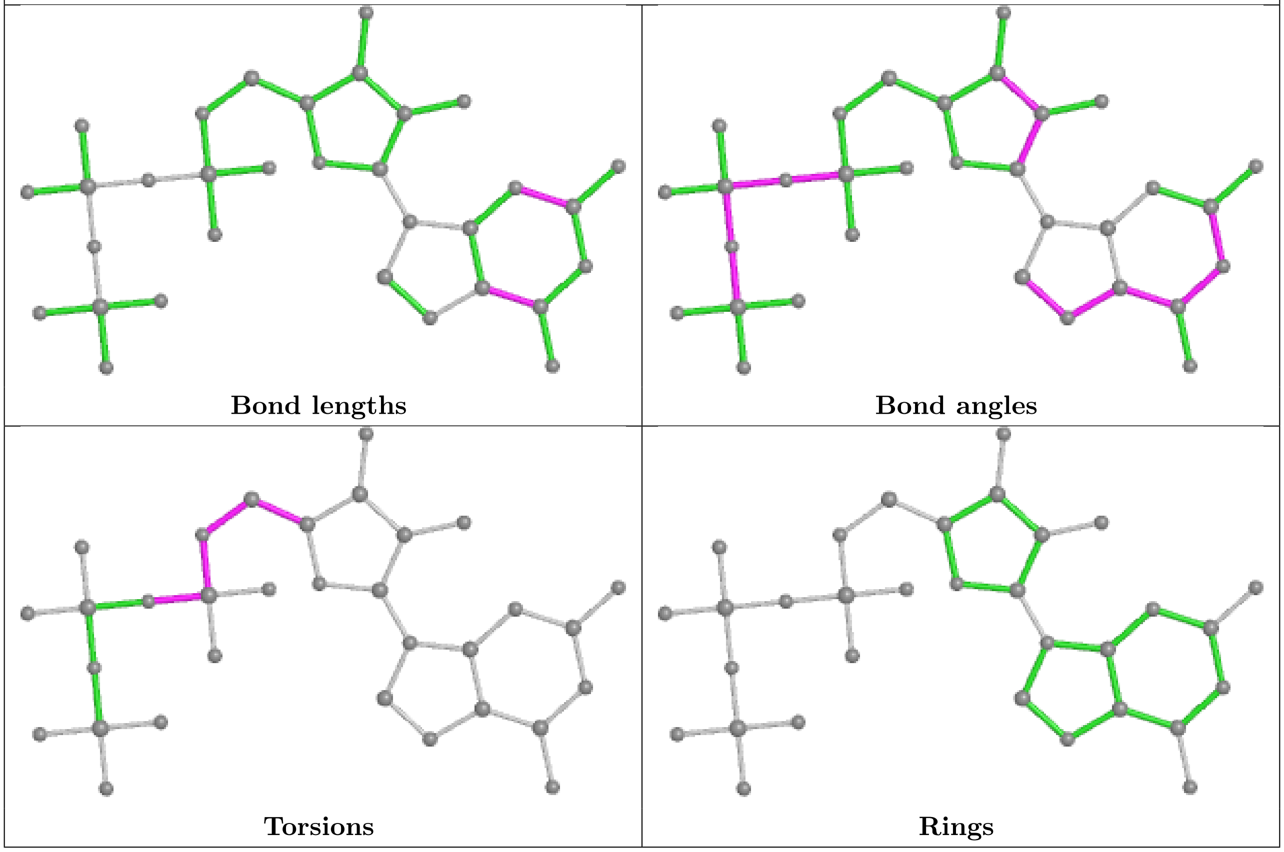


Bond lengths Bond angles



Torsions Rings

Ligand GTP GM 501



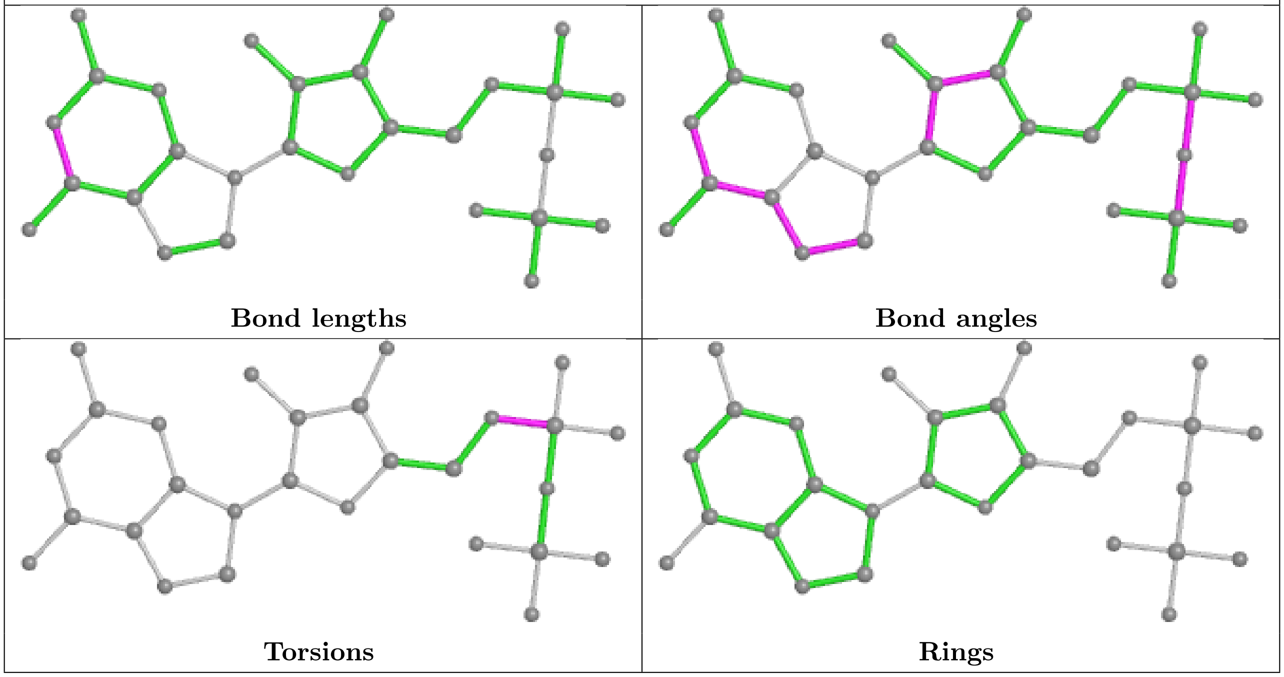
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP JL 502



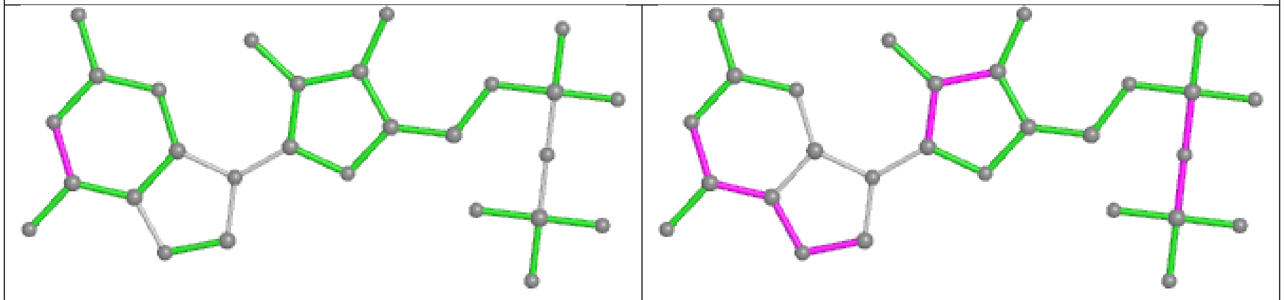
Bond lengths

Bond angles

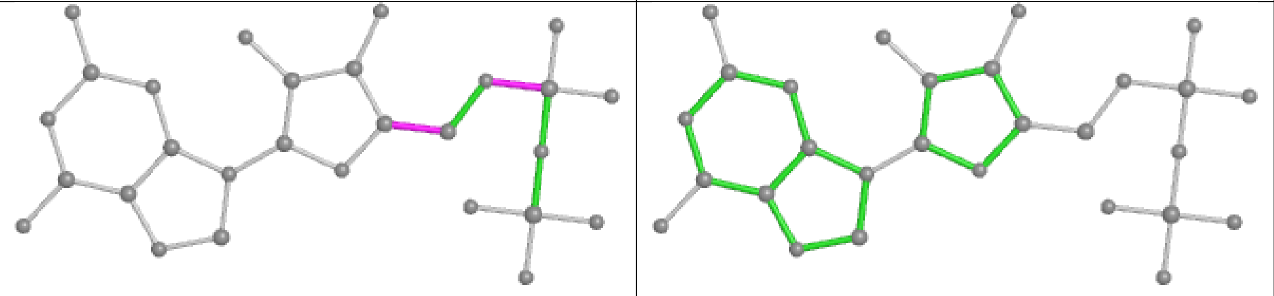
Torsions

Rings

Ligand GDP WN 502

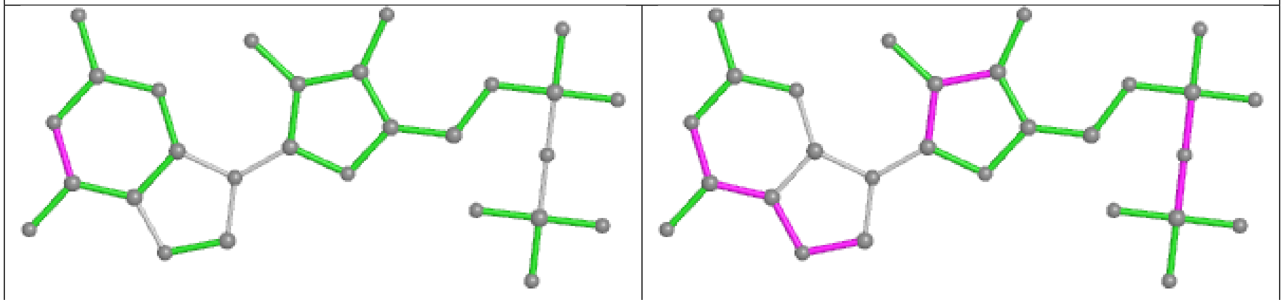


Bond lengths Bond angles

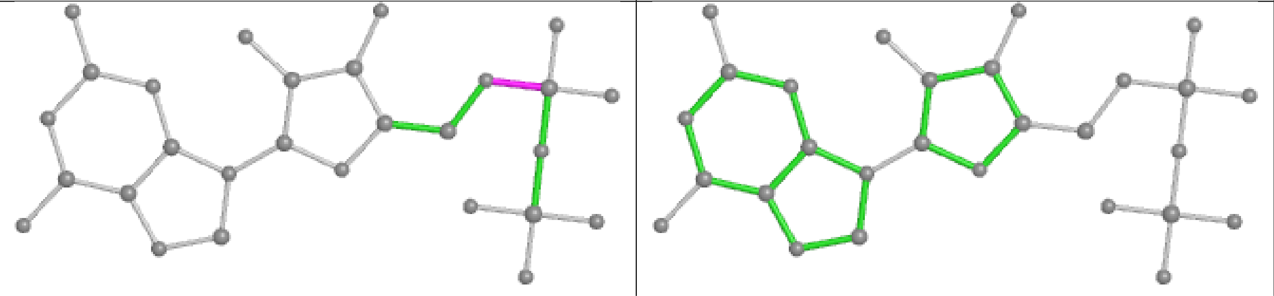


Torsions Rings

Ligand GDP IB 502

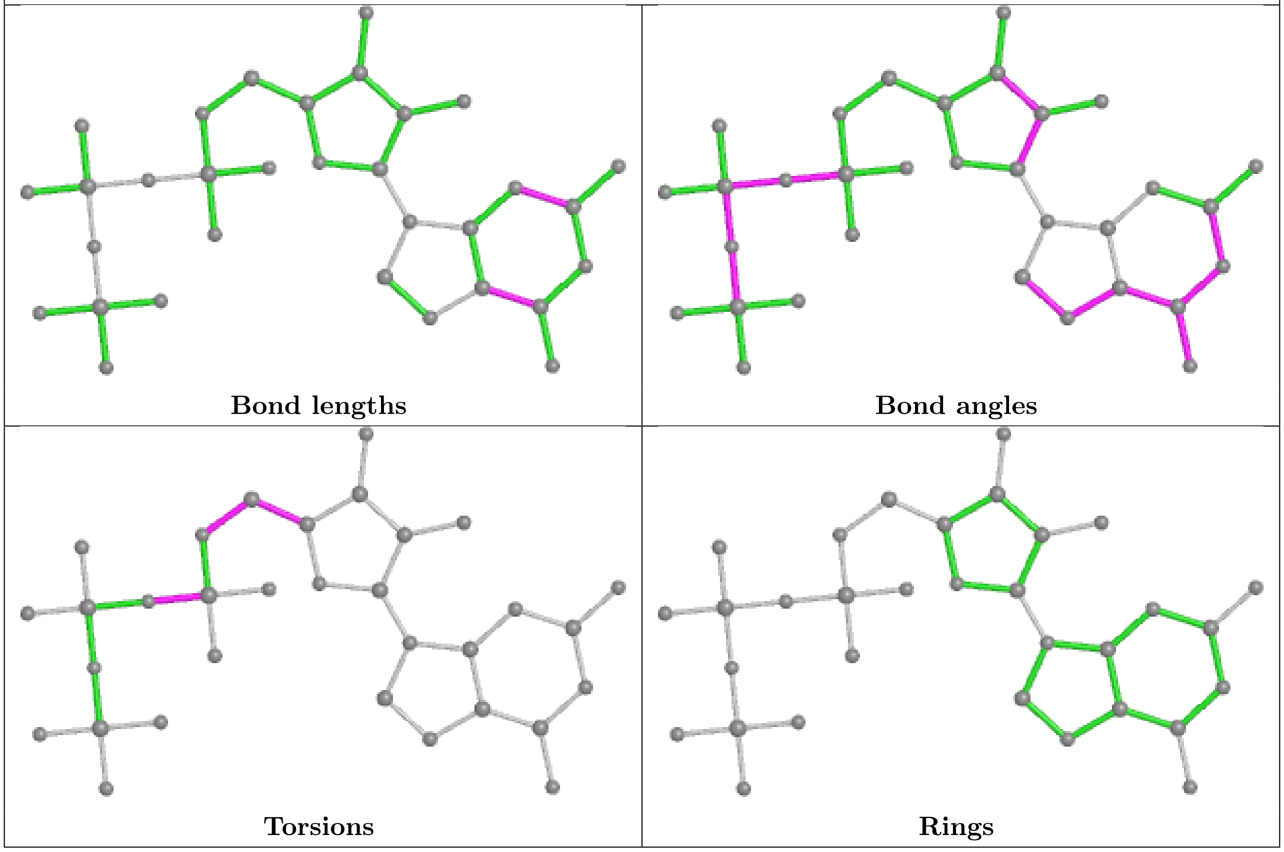


Bond lengths Bond angles



Torsions Rings

Ligand GTP PK 501

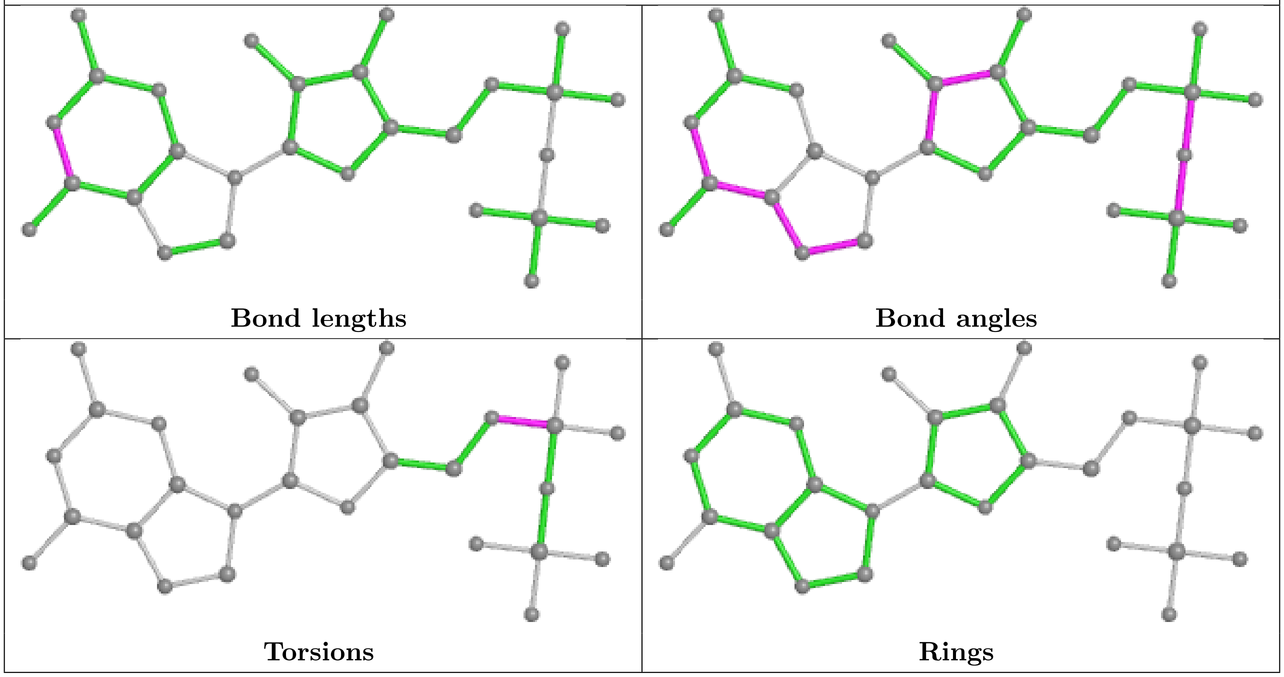

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP UN 502

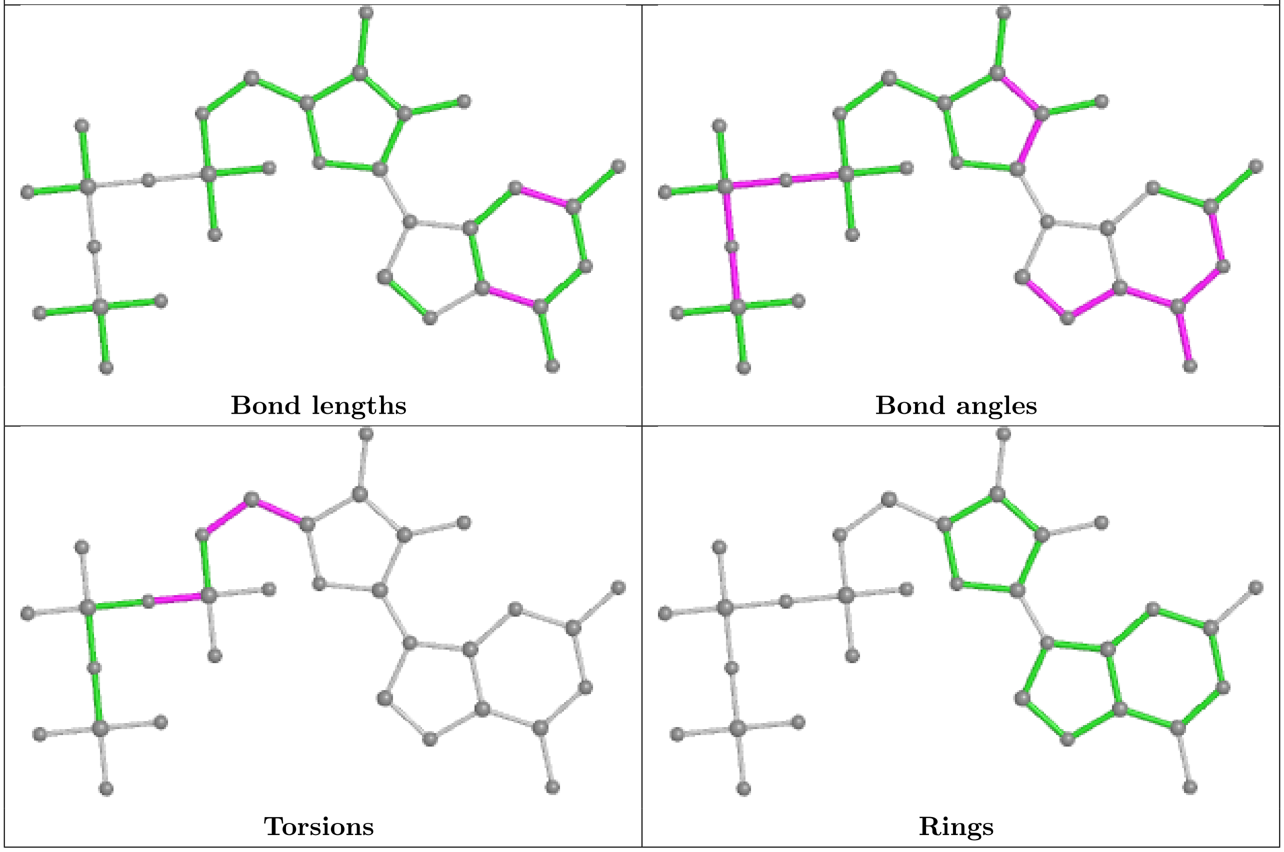

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP VO 501



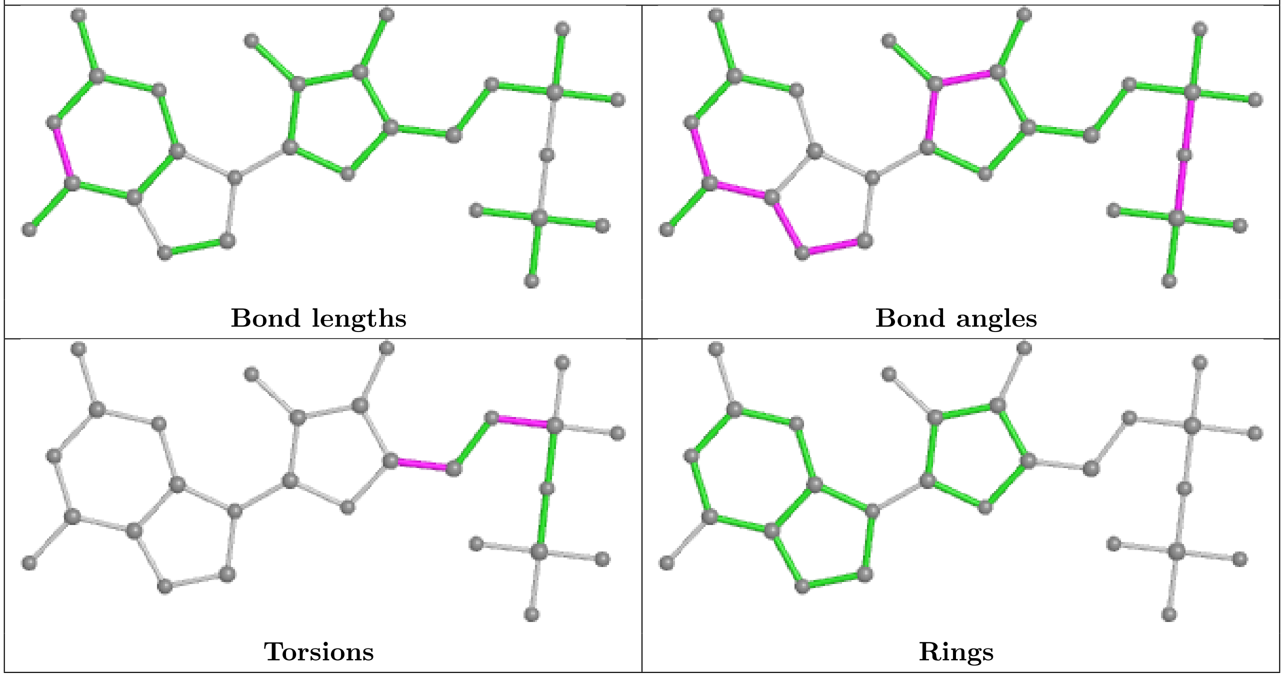
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP EH 502



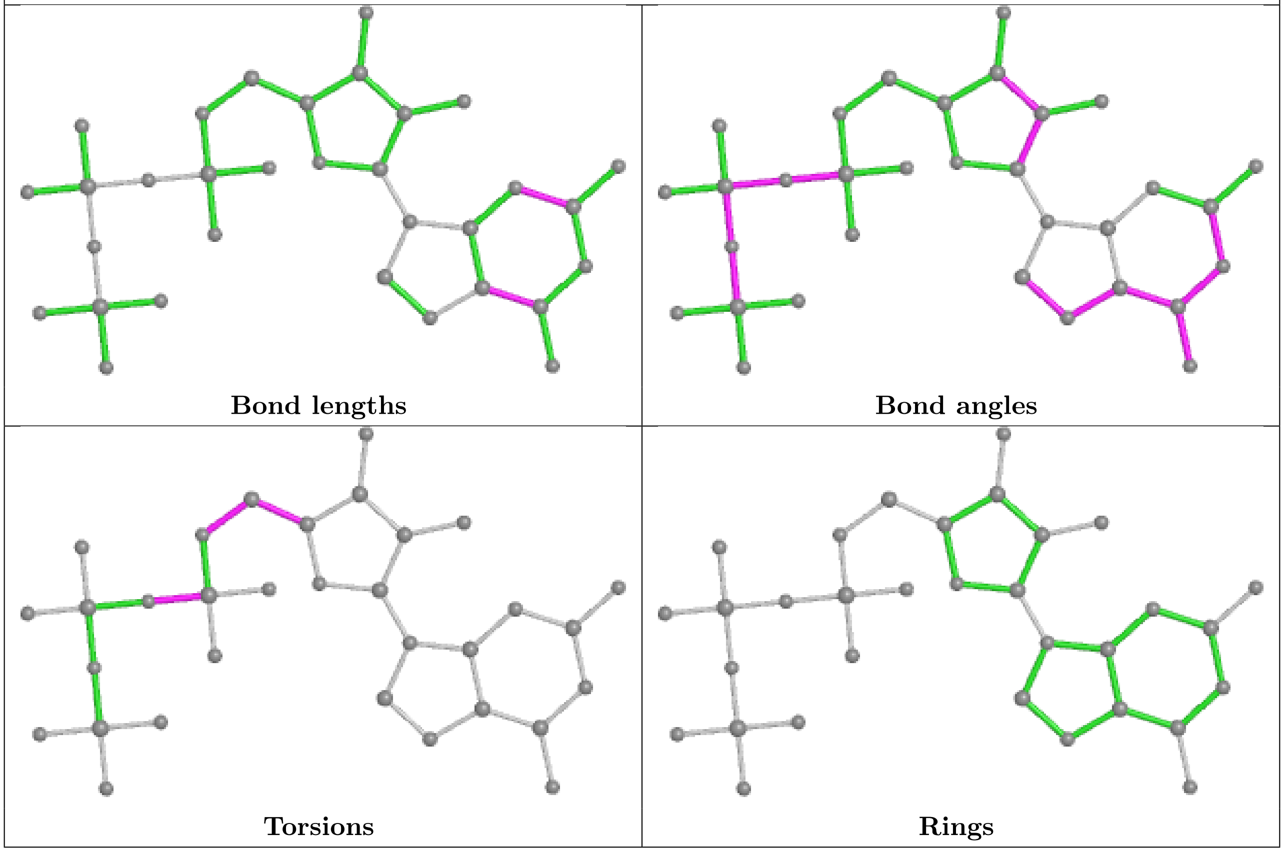
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP HG 501



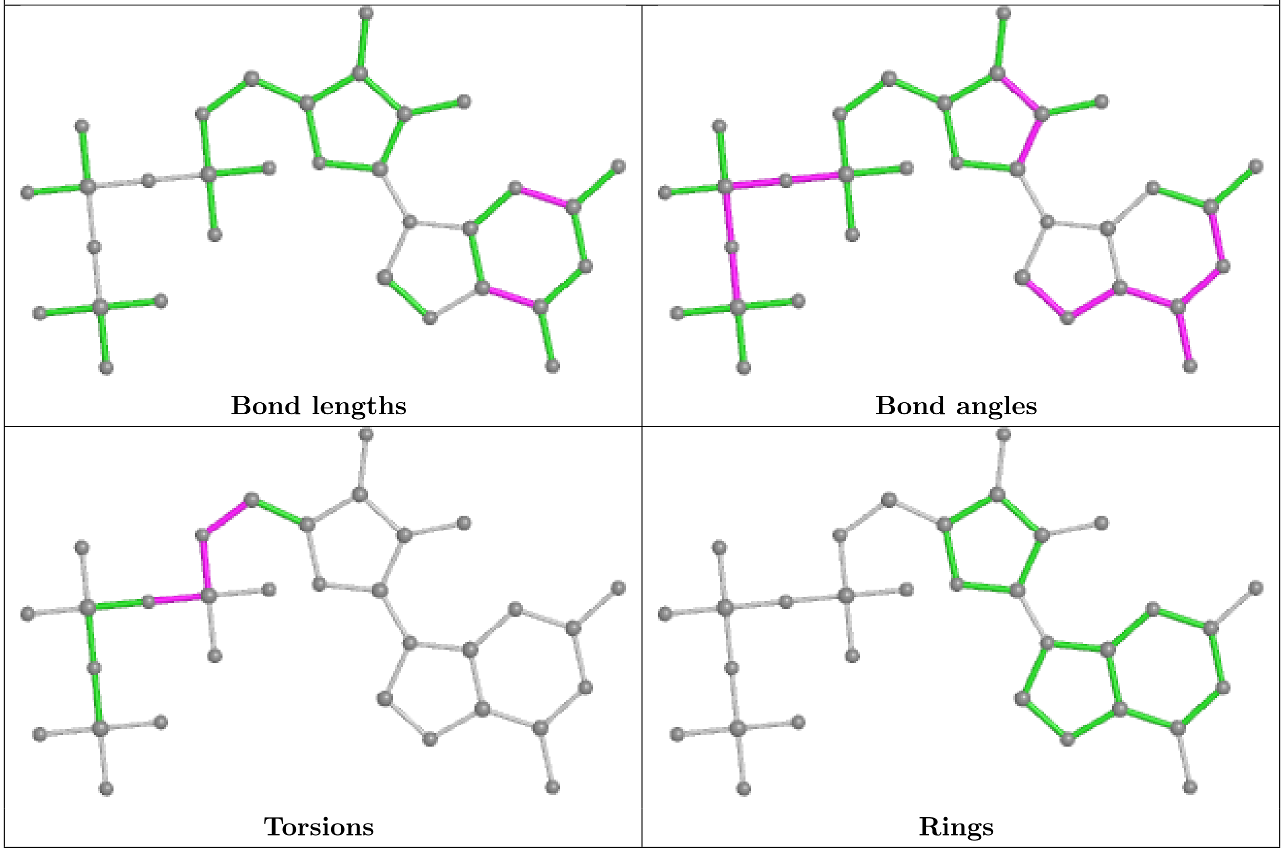
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP RM 501



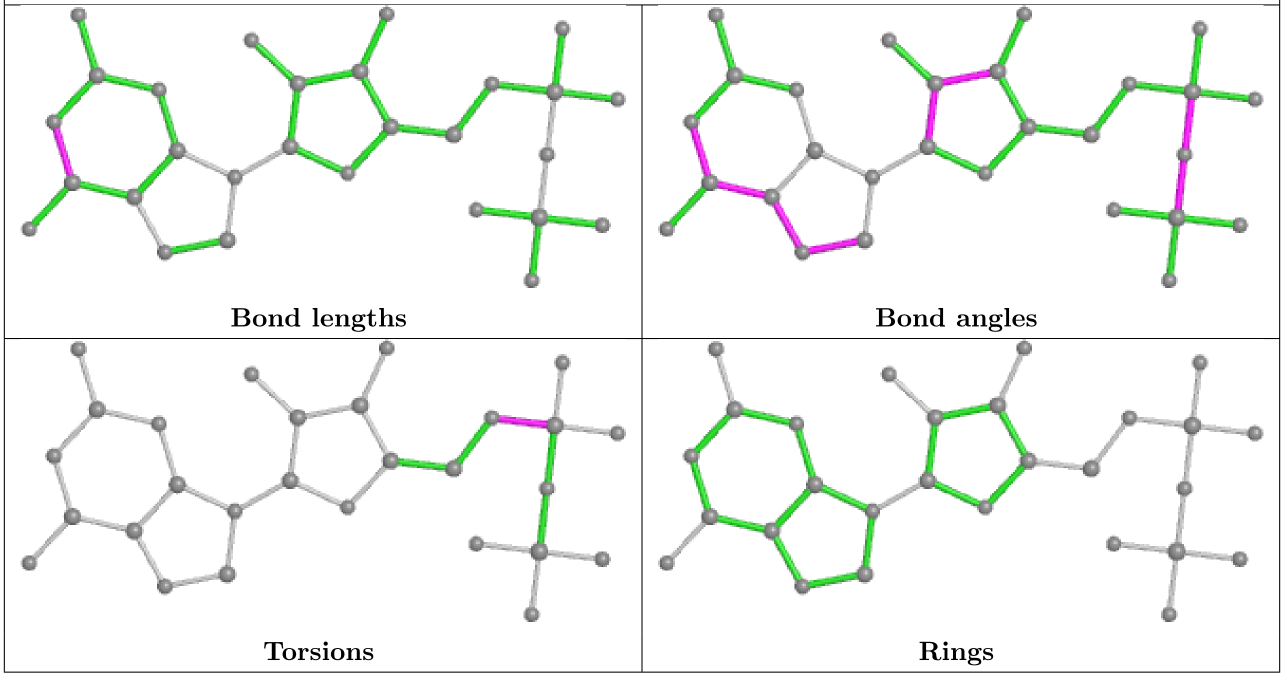
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP JF 502



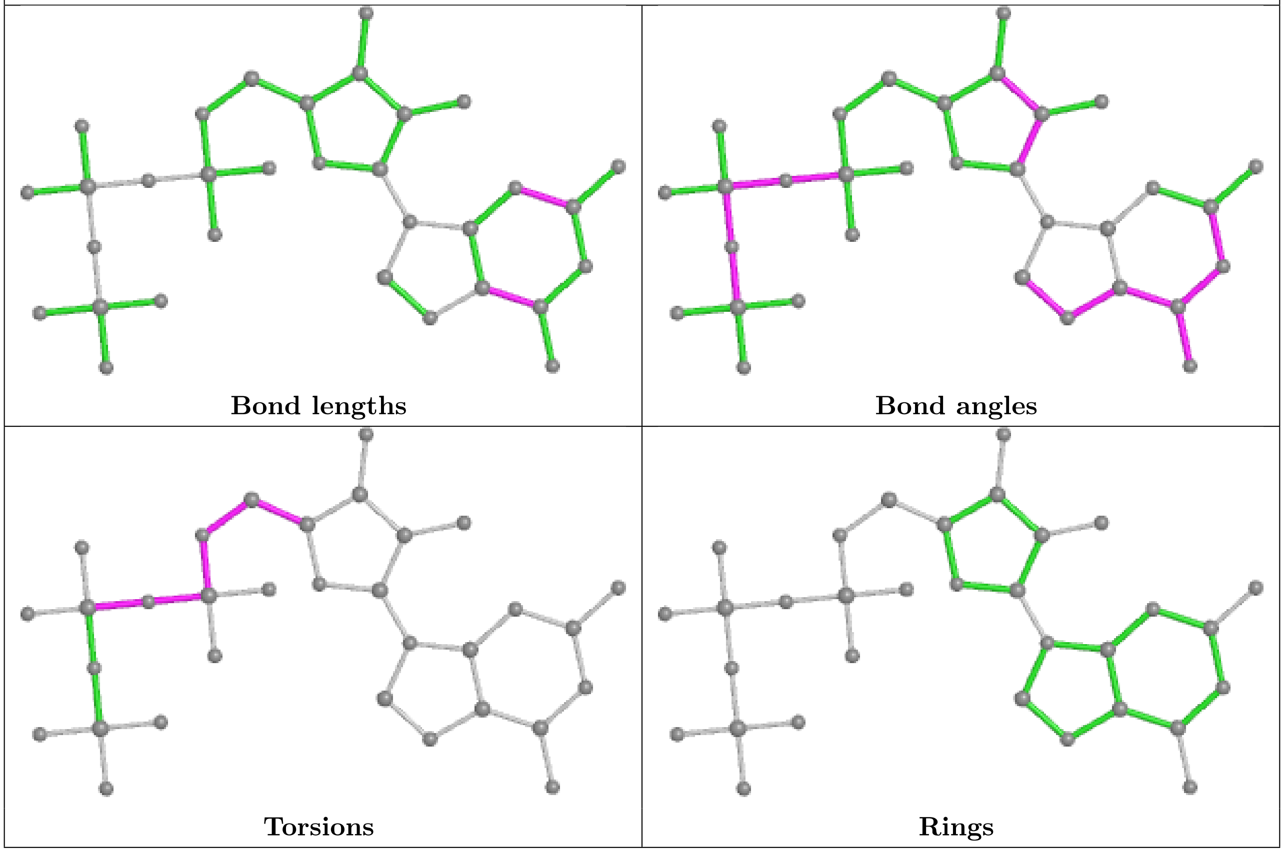
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP GE 501



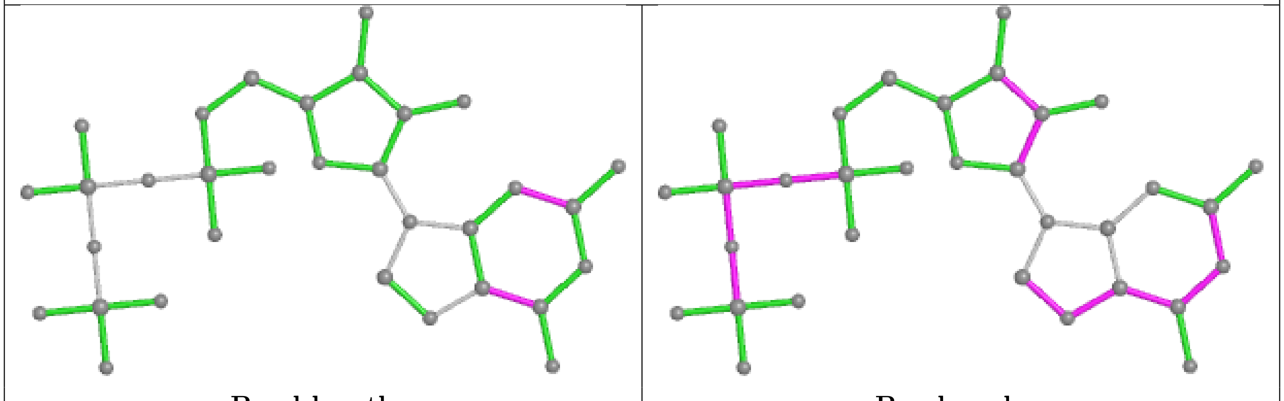
Bond lengths

Bond angles

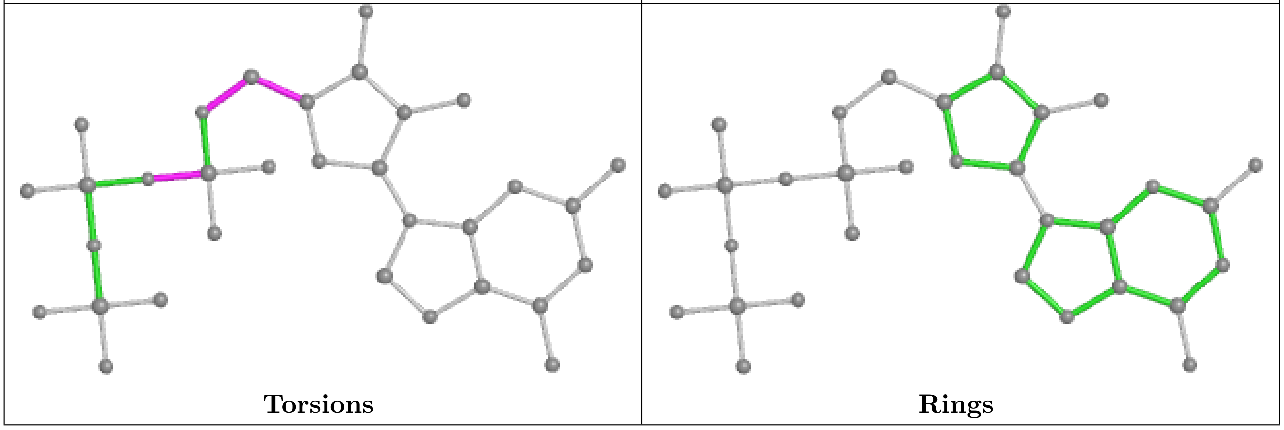
Torsions

Rings

Ligand GTP CA 501

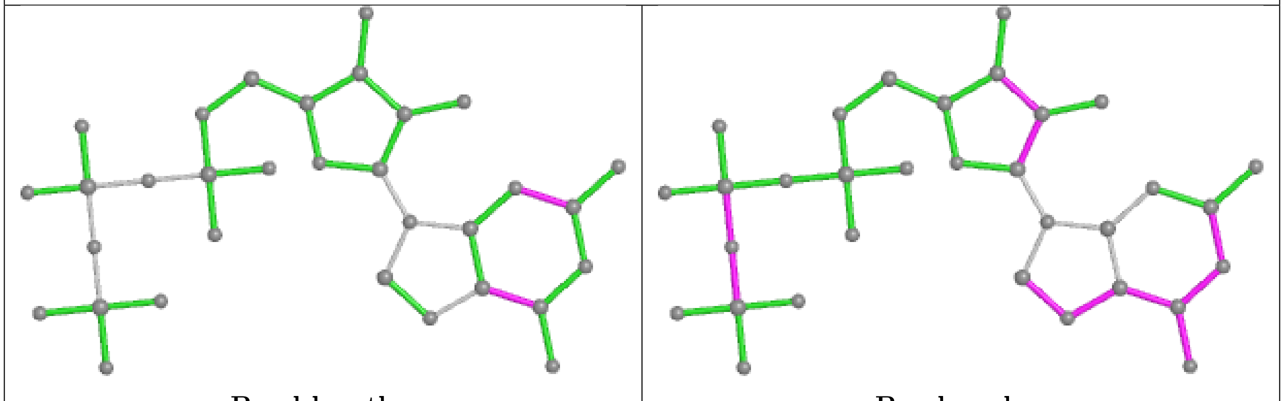


Bond lengths **Bond angles**

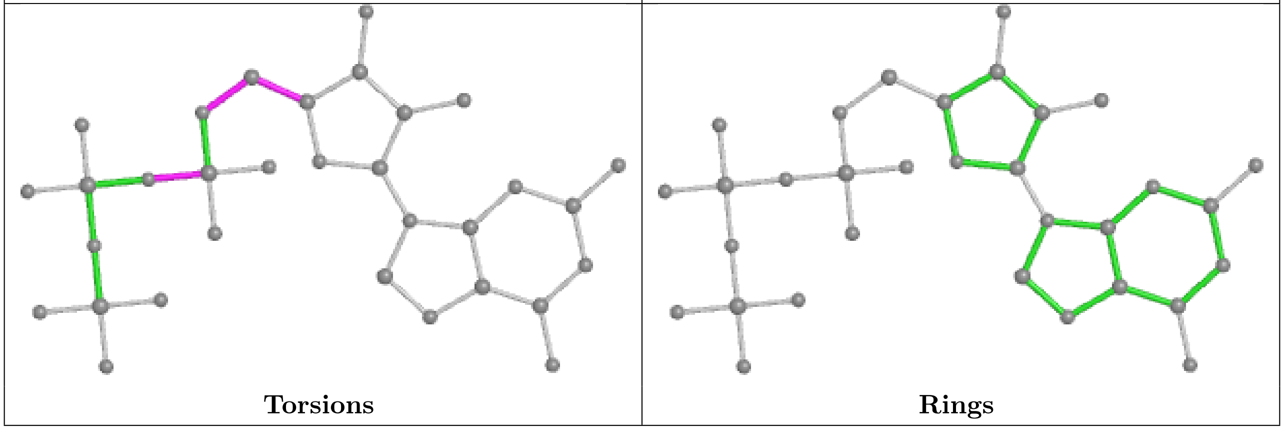


Torsions **Rings**

Ligand GTP OK 501

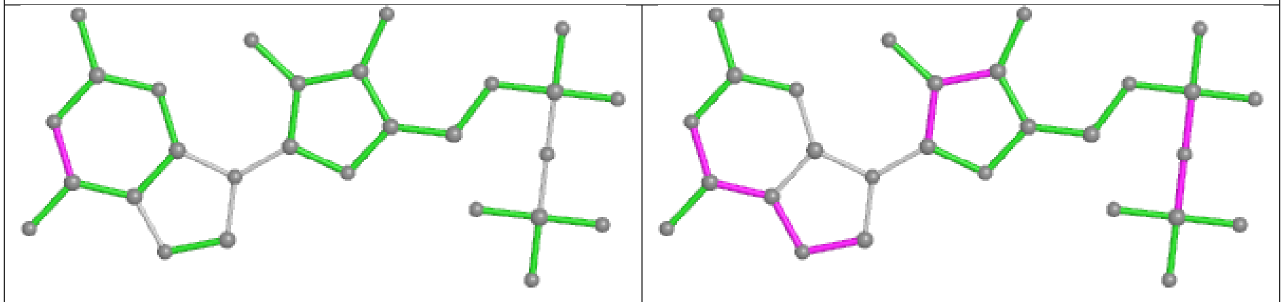


Bond lengths **Bond angles**



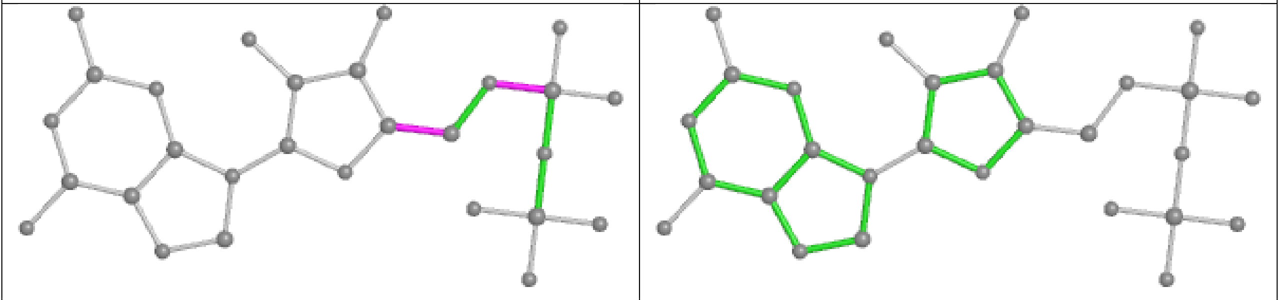
Torsions **Rings**

Ligand GDP ML 502



Bond lengths

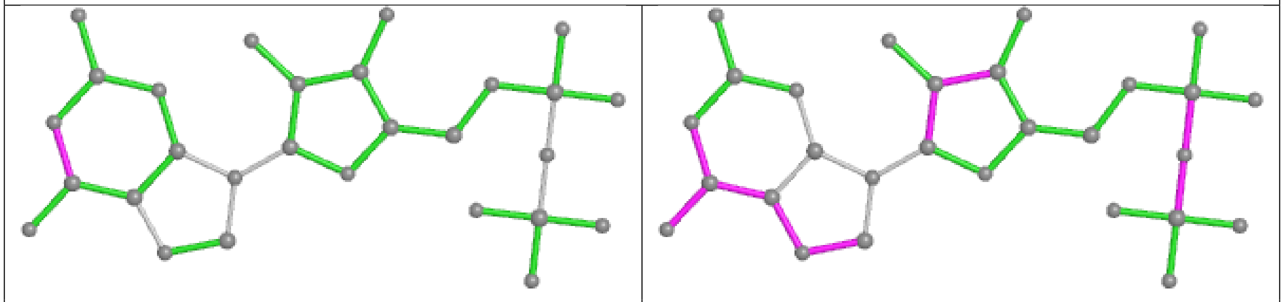
Bond angles



Torsions

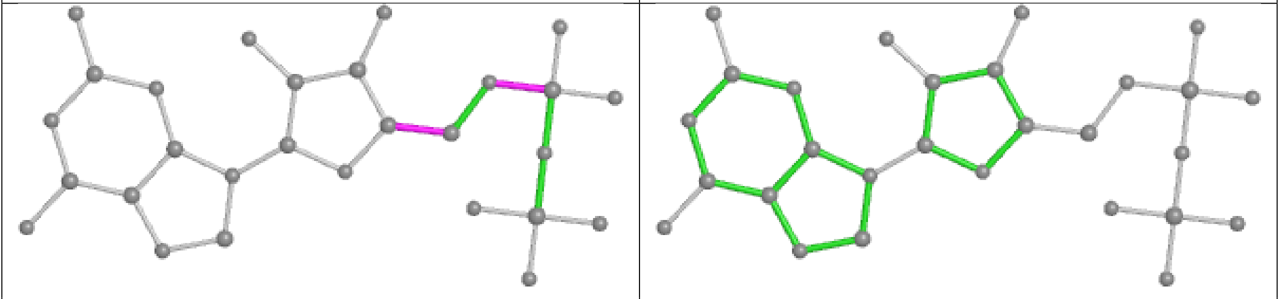
Rings

Ligand GDP SH 502



Bond lengths

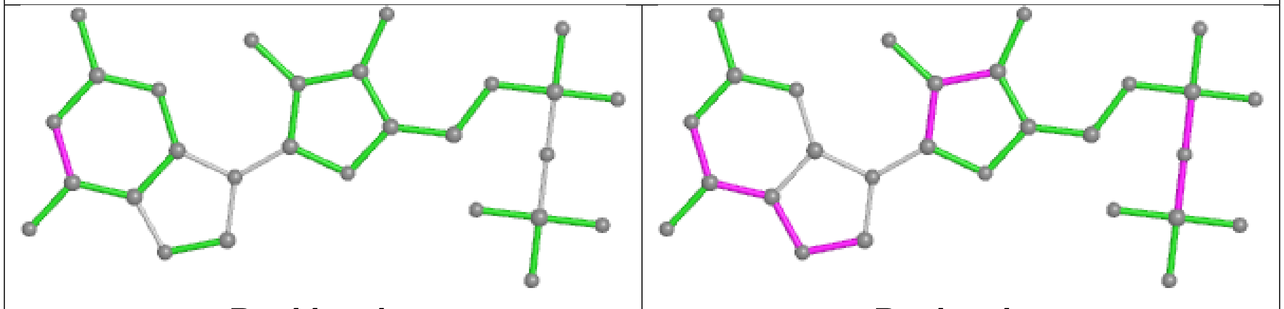
Bond angles



Torsions

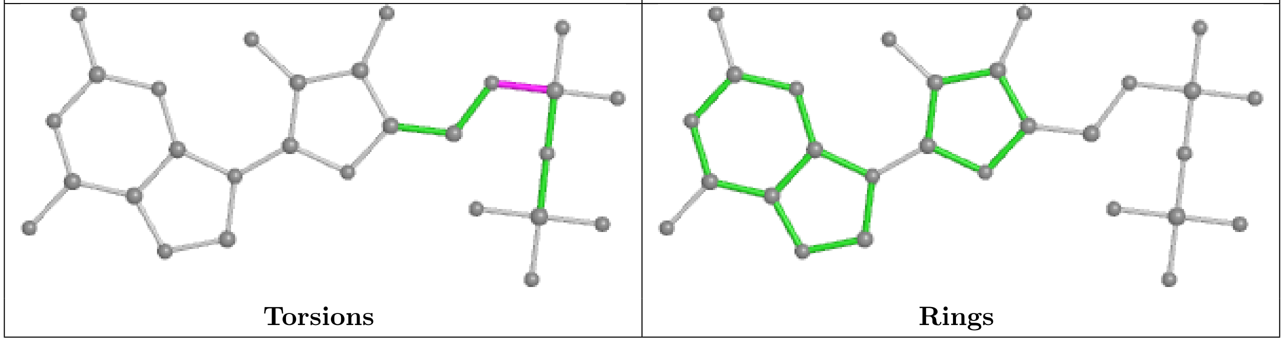
Rings

Ligand GDP UD 502



Bond lengths

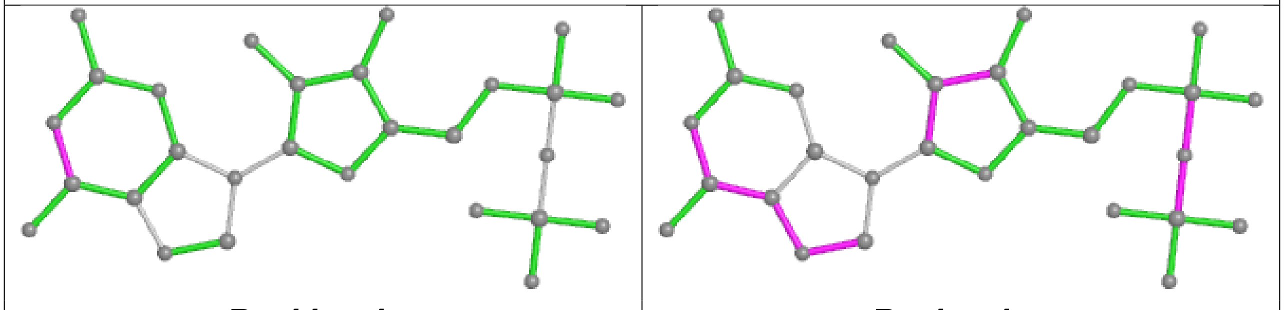
Bond angles



Torsions

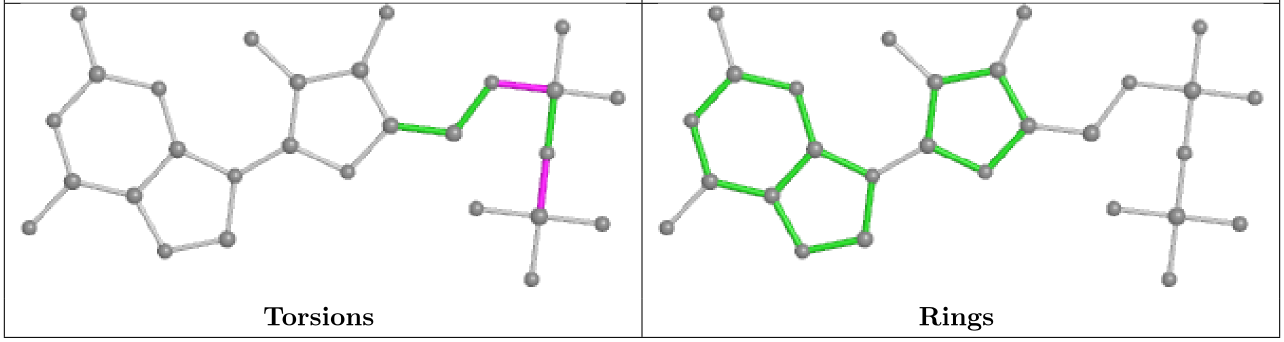
Rings

Ligand GDP VN 502



Bond lengths

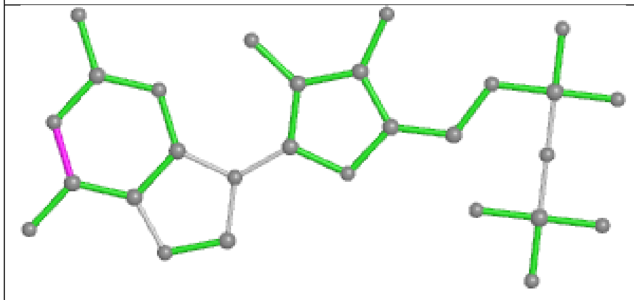
Bond angles

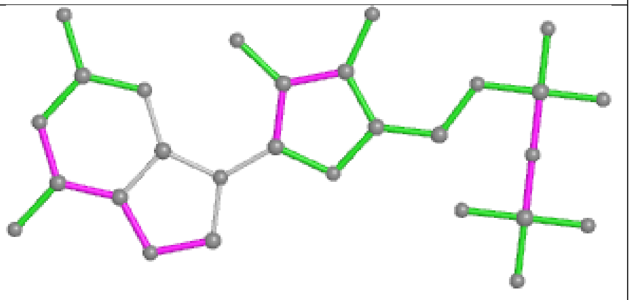


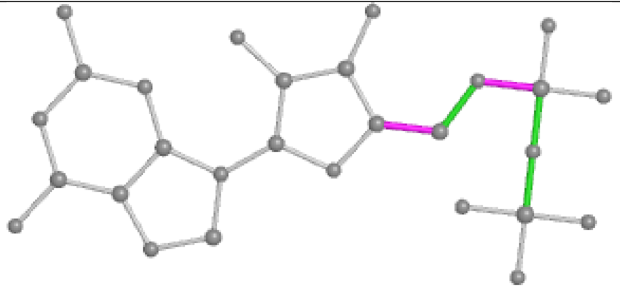
Torsions

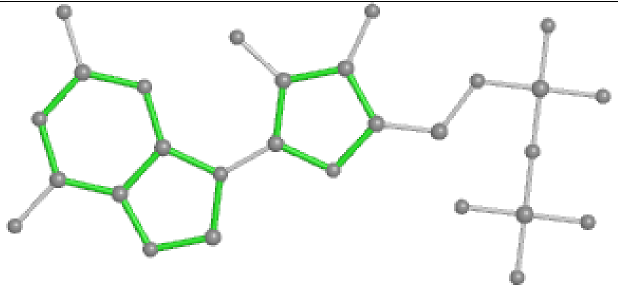
Rings

Ligand GDP KJ 502

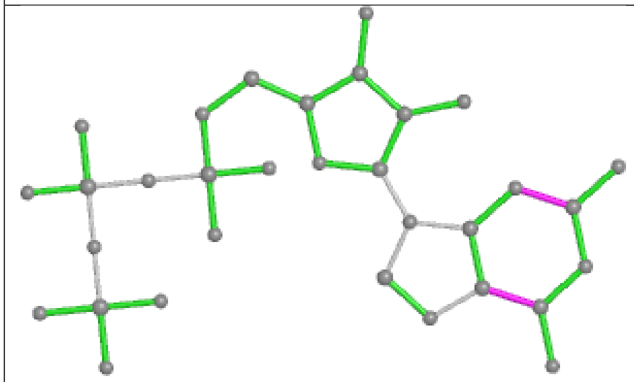

Bond lengths

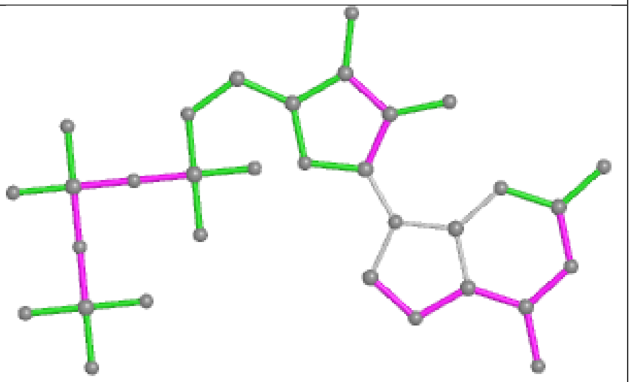

Bond angles

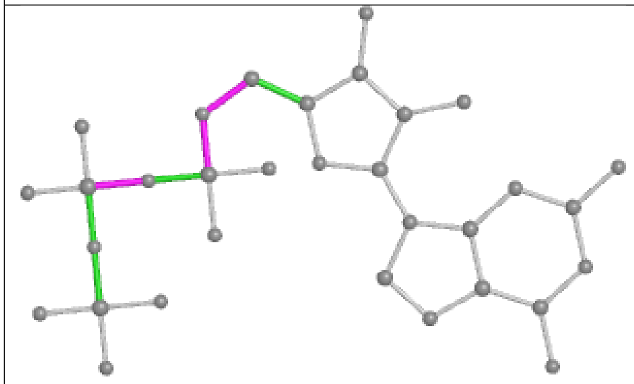

Torsions

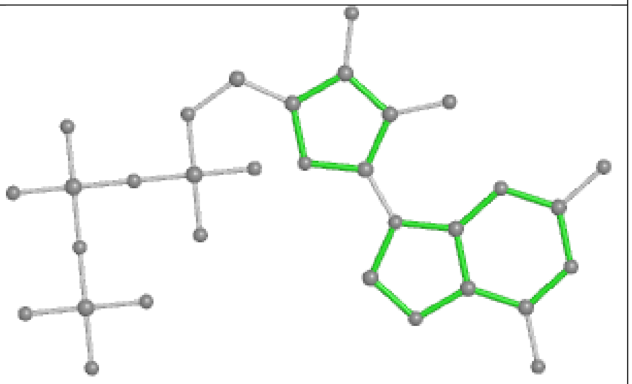

Rings

Ligand GTP SI 501

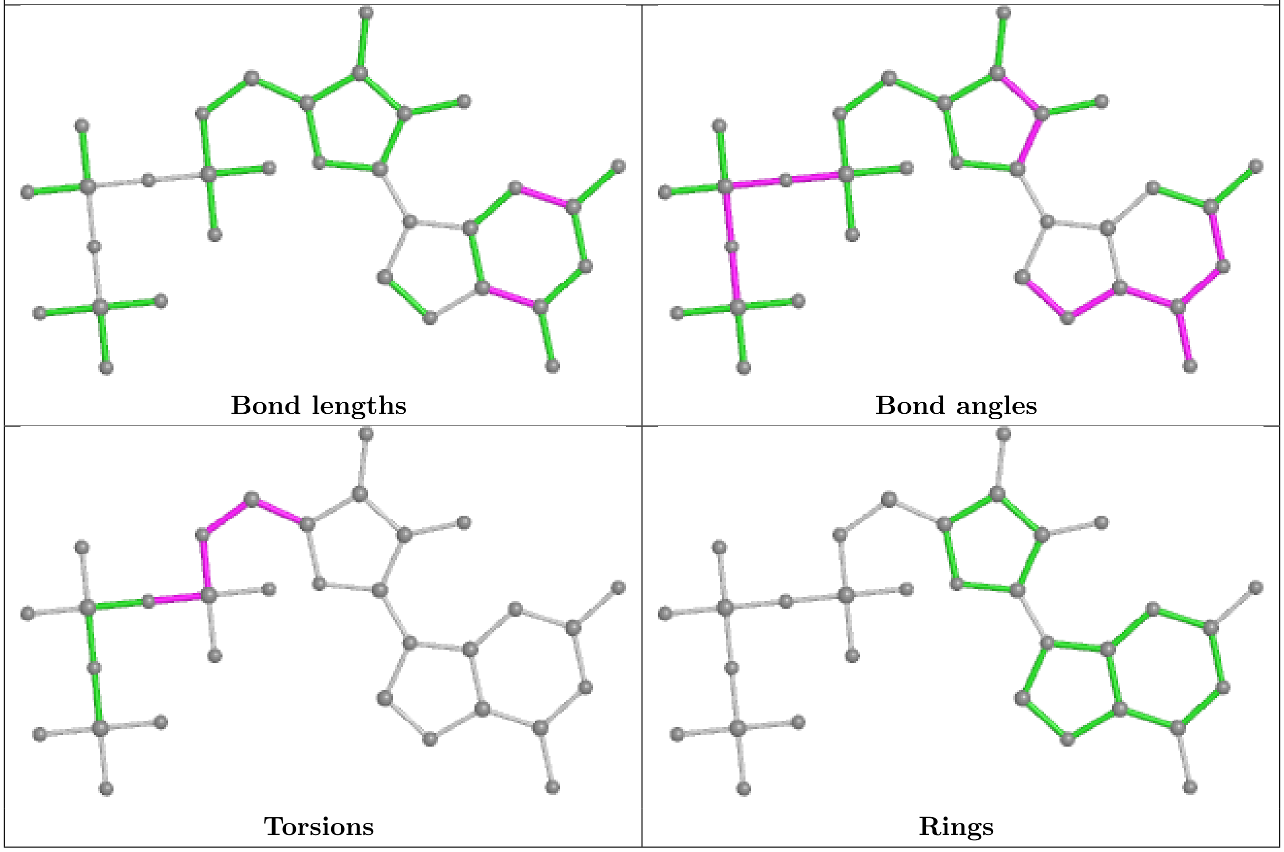

Bond lengths


Bond angles


Torsions


Rings

Ligand GTP LM 501



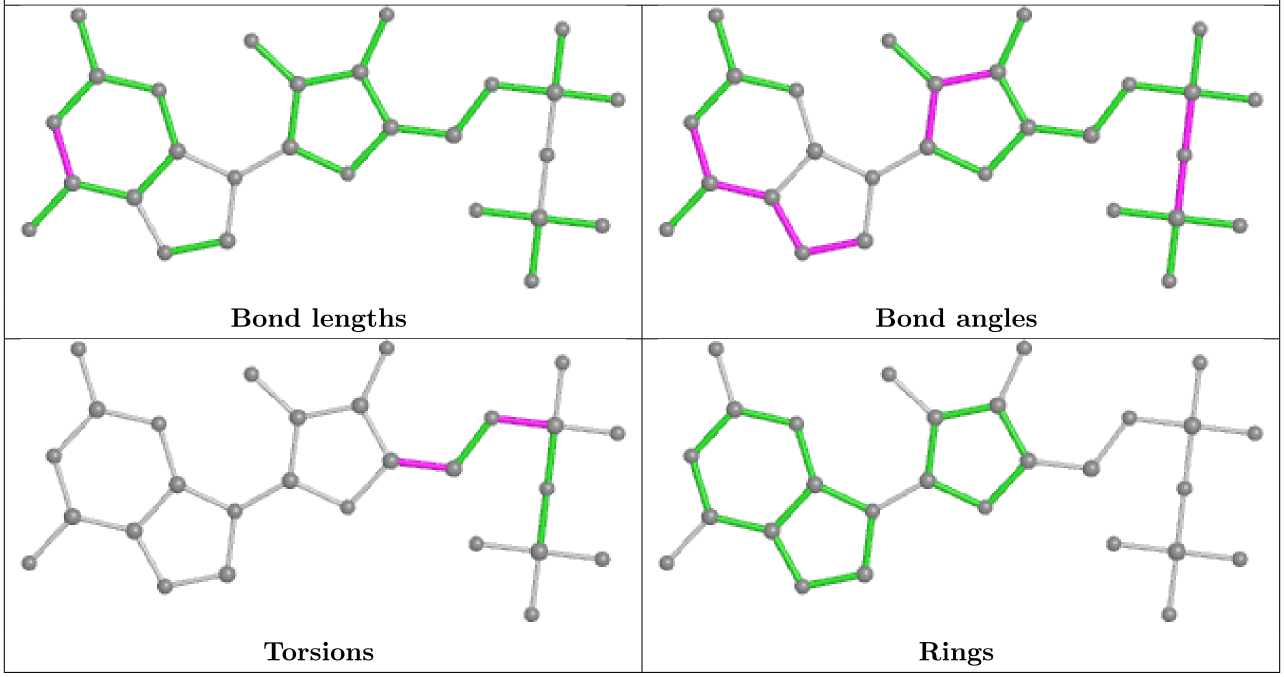
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP JD 502



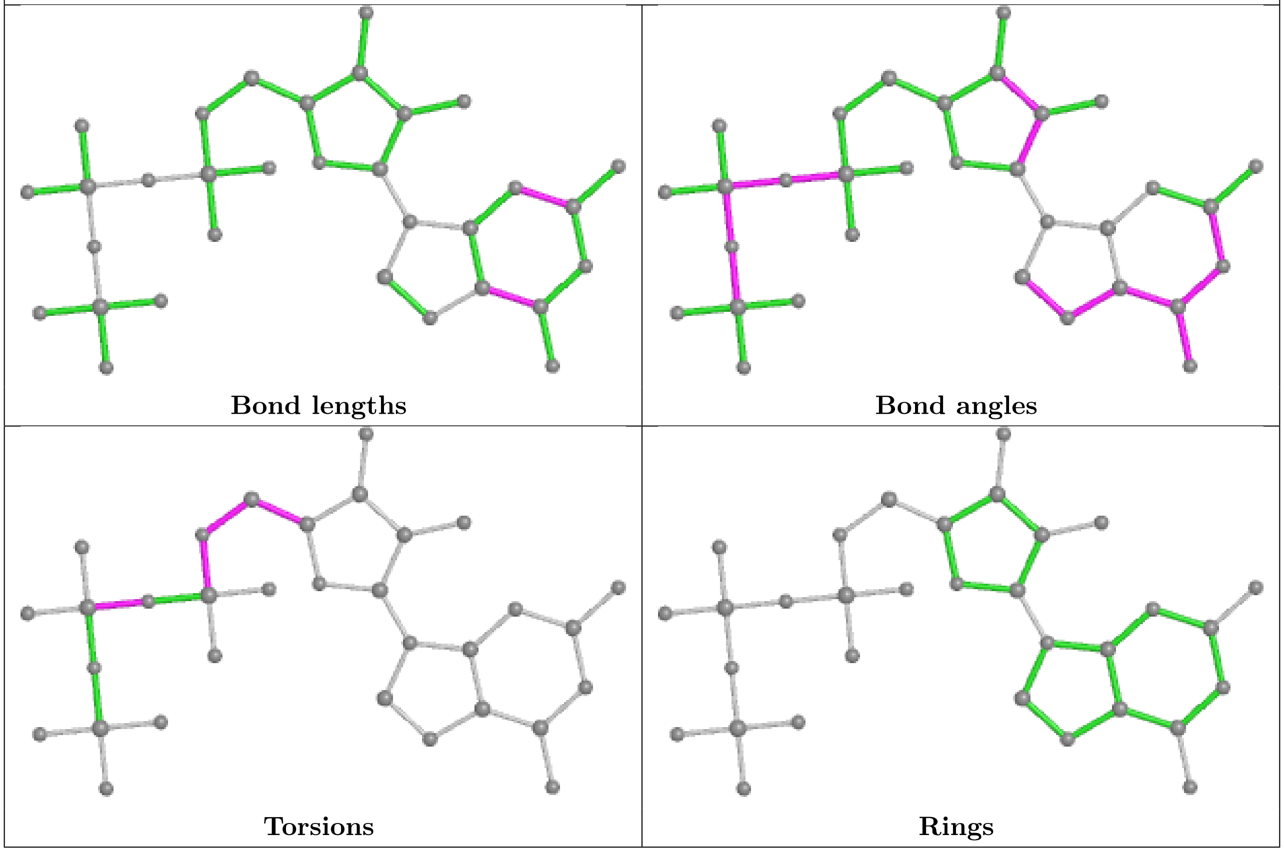
Bond lengths

Bond angles

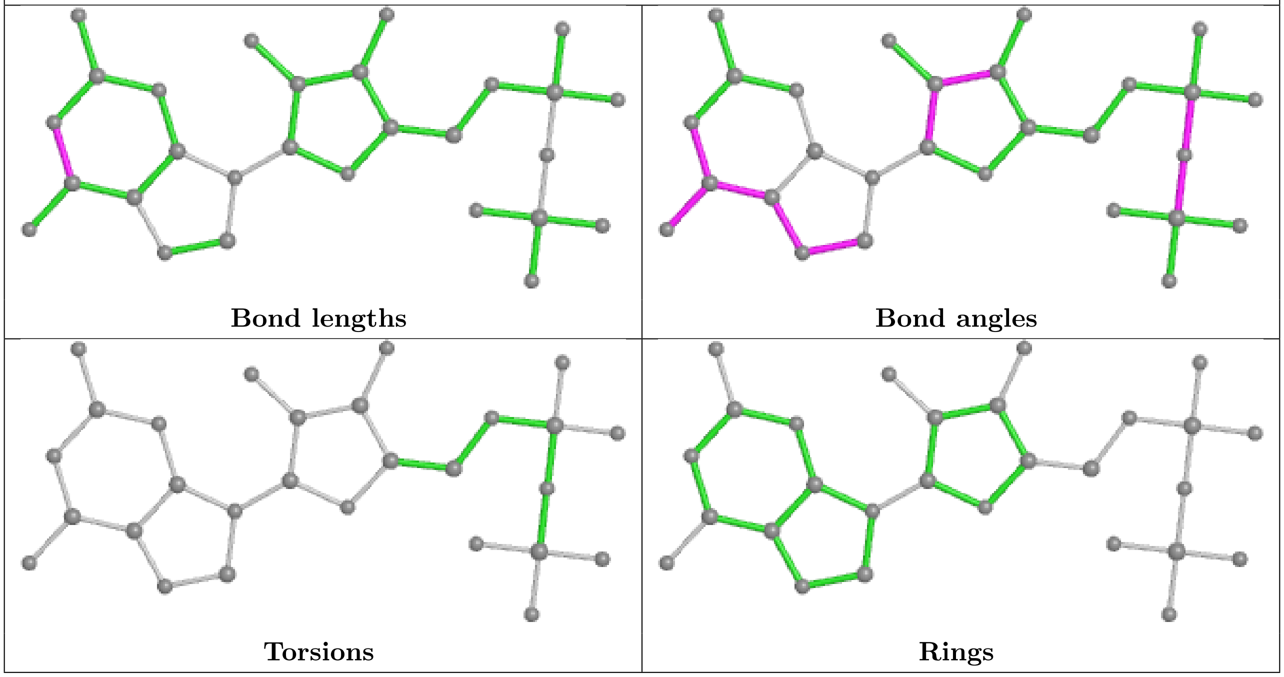
Torsions

Rings

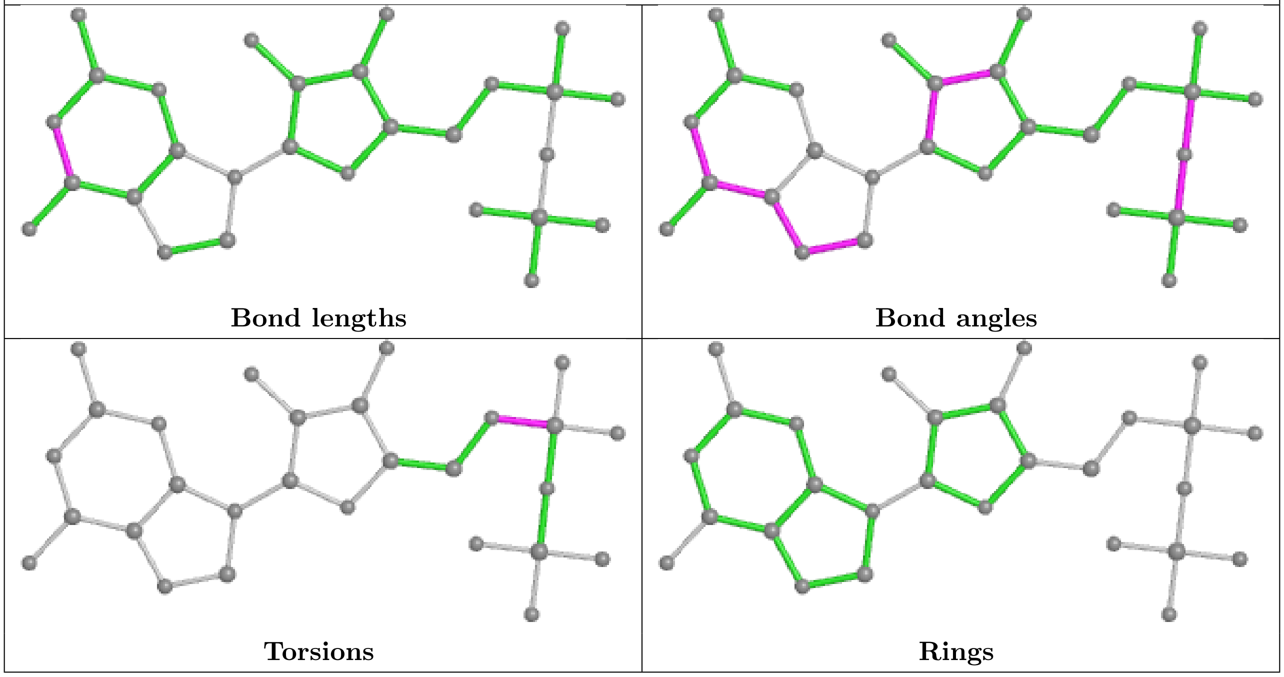
Ligand GTP KK 501



Ligand GDP FN 502



Ligand GDP NH 502



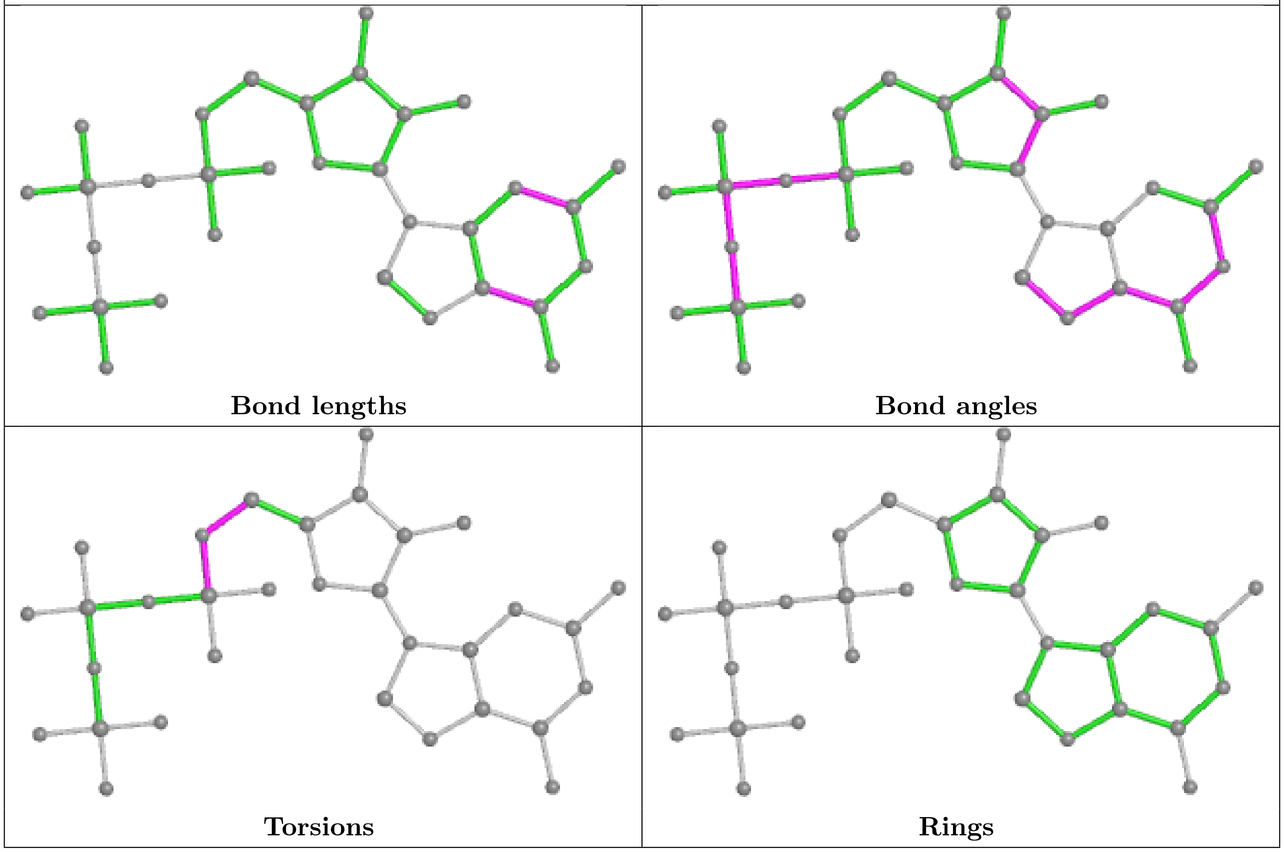
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP DK 501



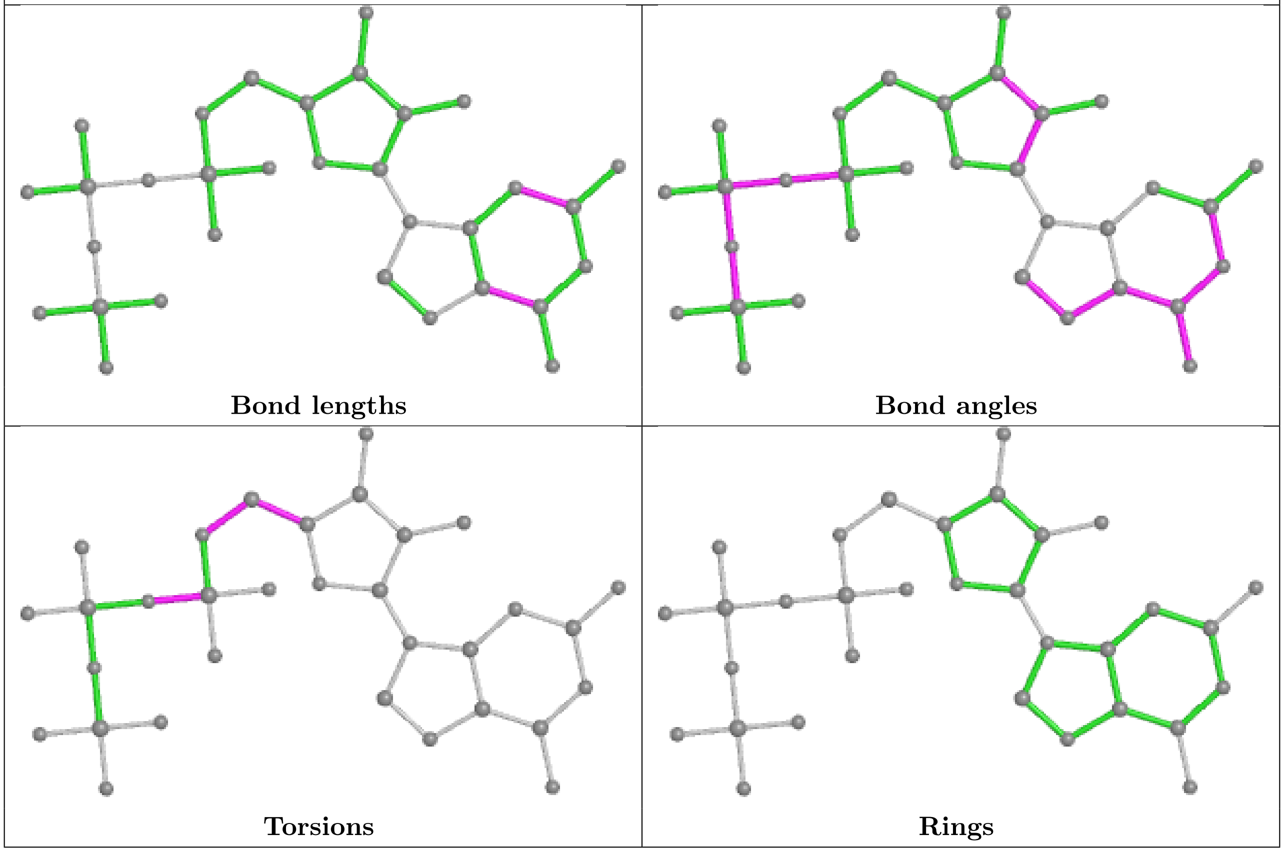
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP AC 501



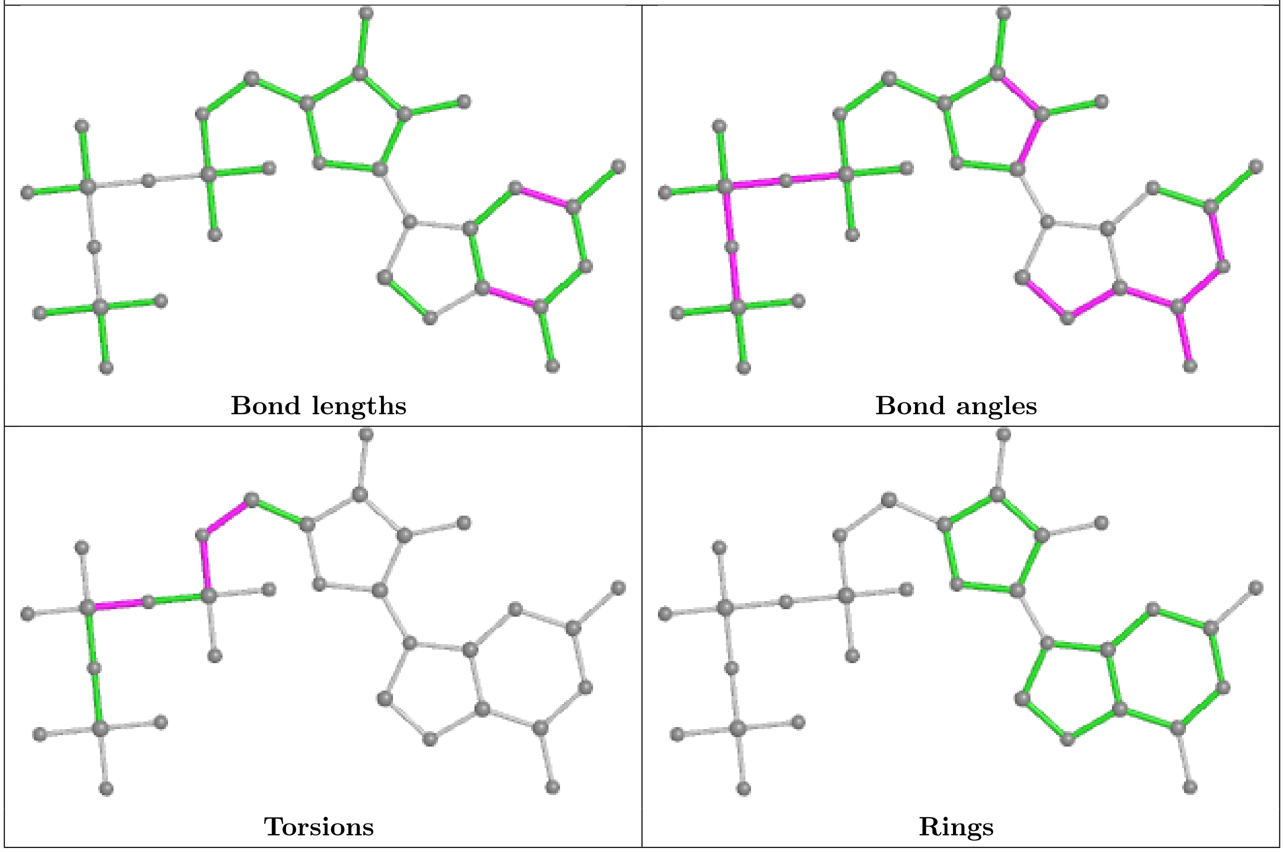
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP LI 501



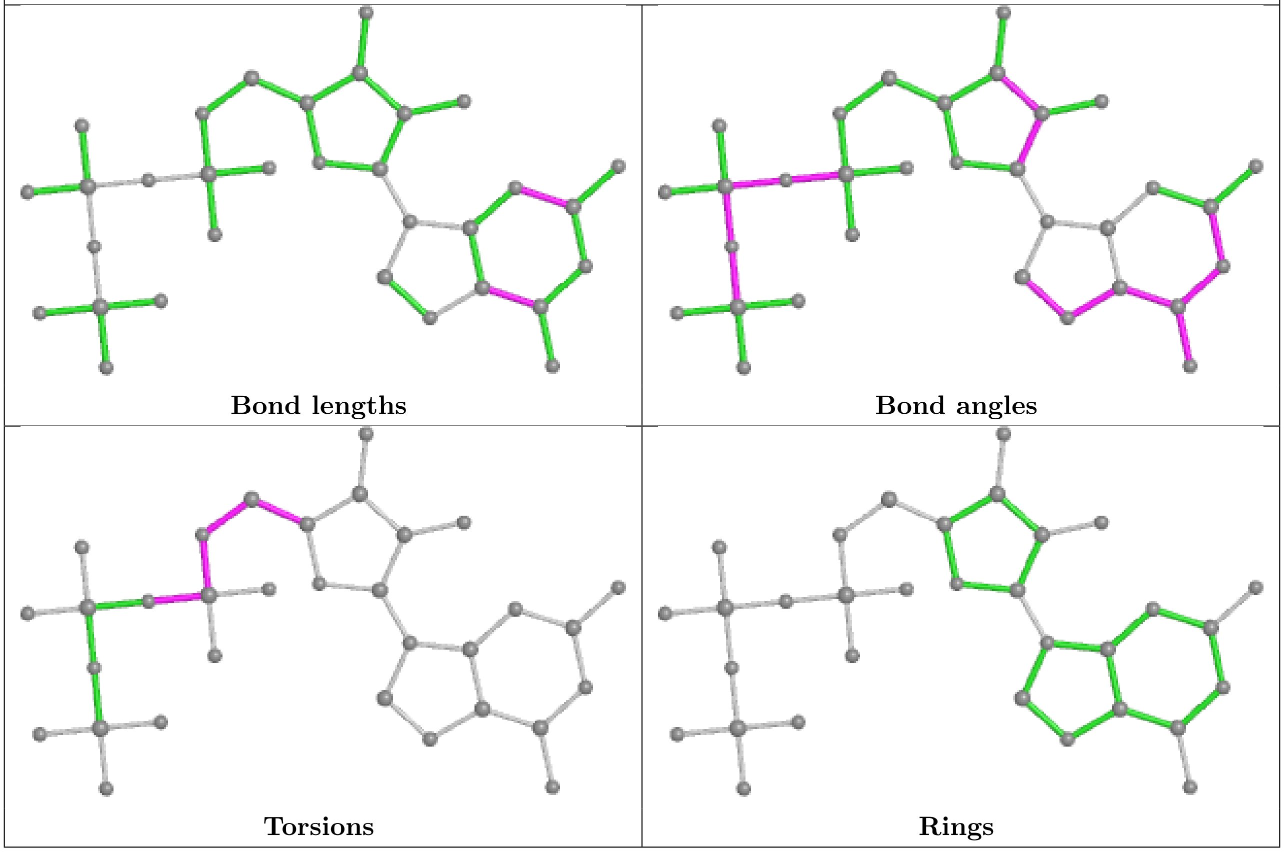
Bond lengths

Bond angles

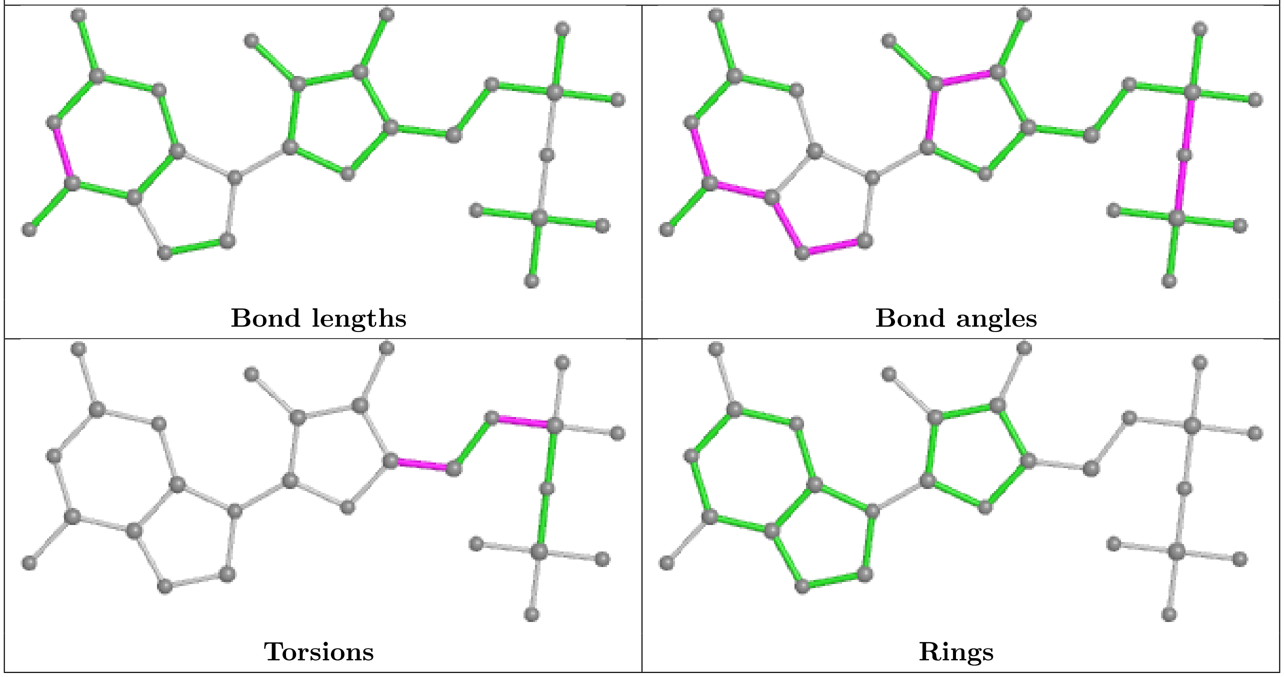
Torsions

Rings

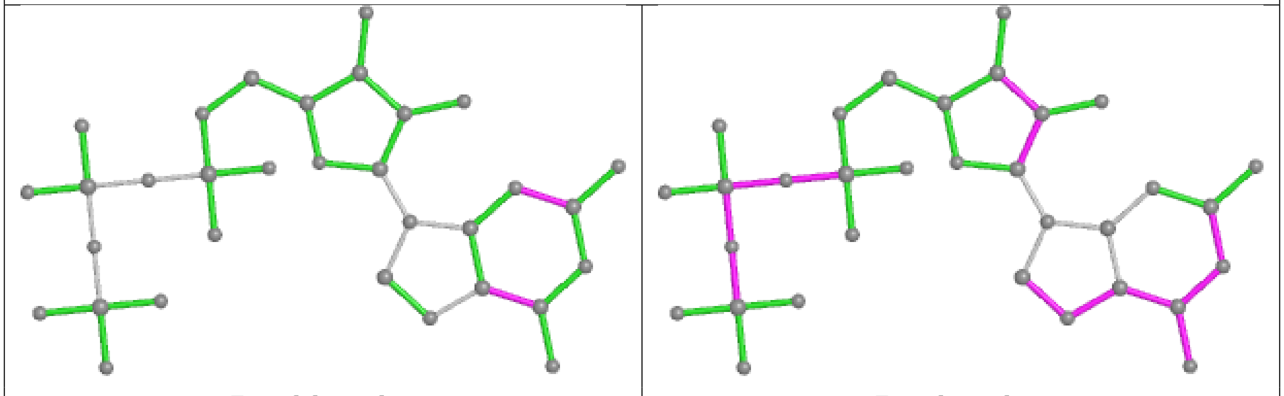
Ligand GTP NK 501



Ligand GDP KN 502

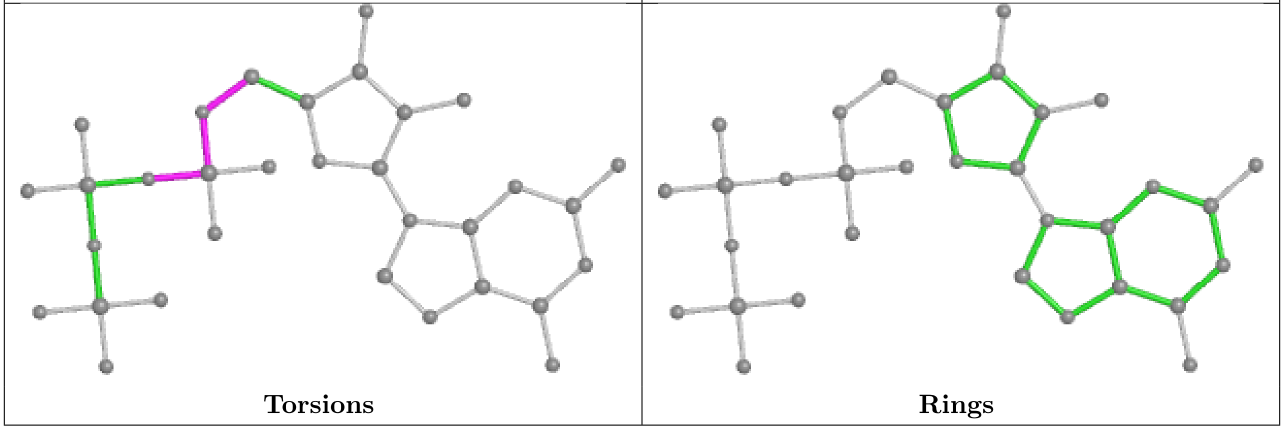


Ligand GTP NI 501



Bond lengths

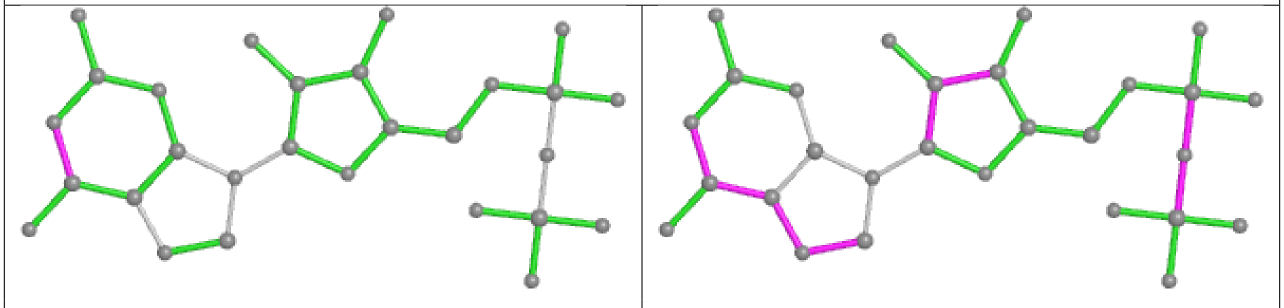
Bond angles



Torsions

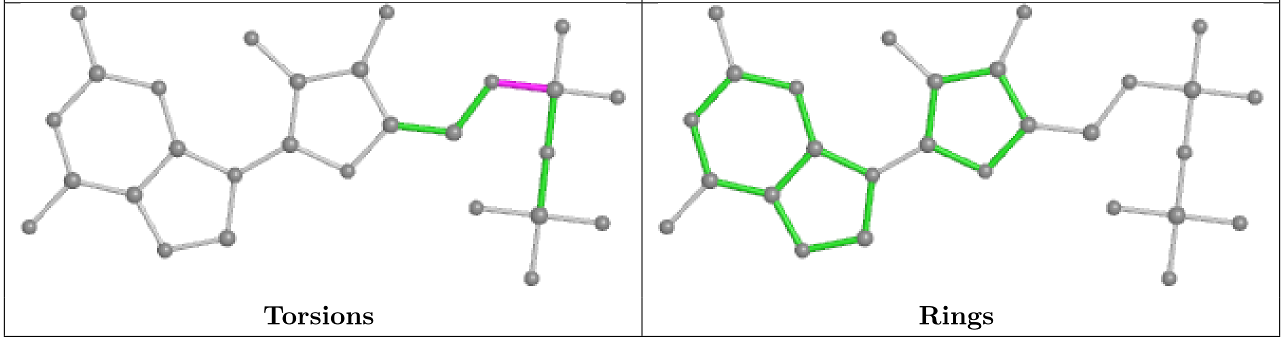
Rings

Ligand GDP LF 502



Bond lengths

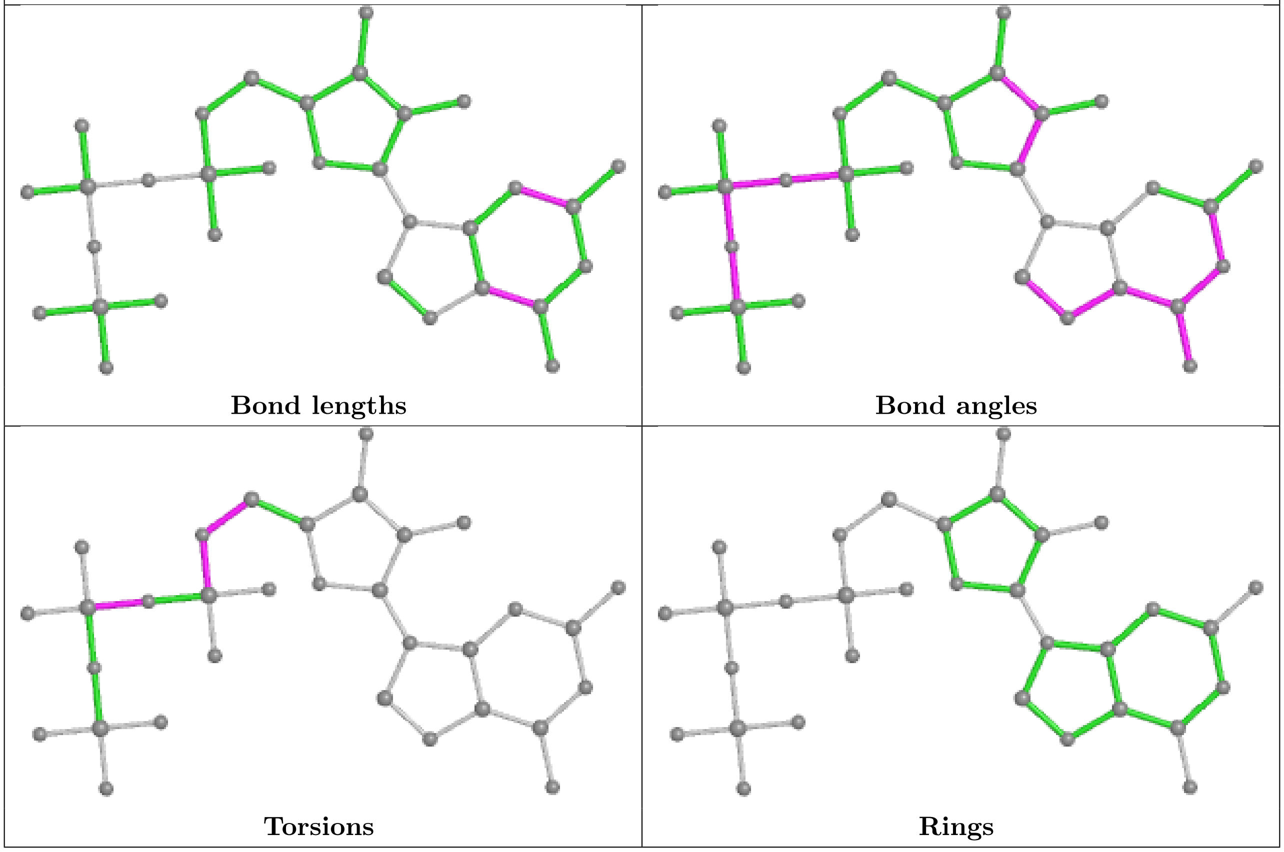
Bond angles



Torsions

Rings

Ligand GTP MI 501



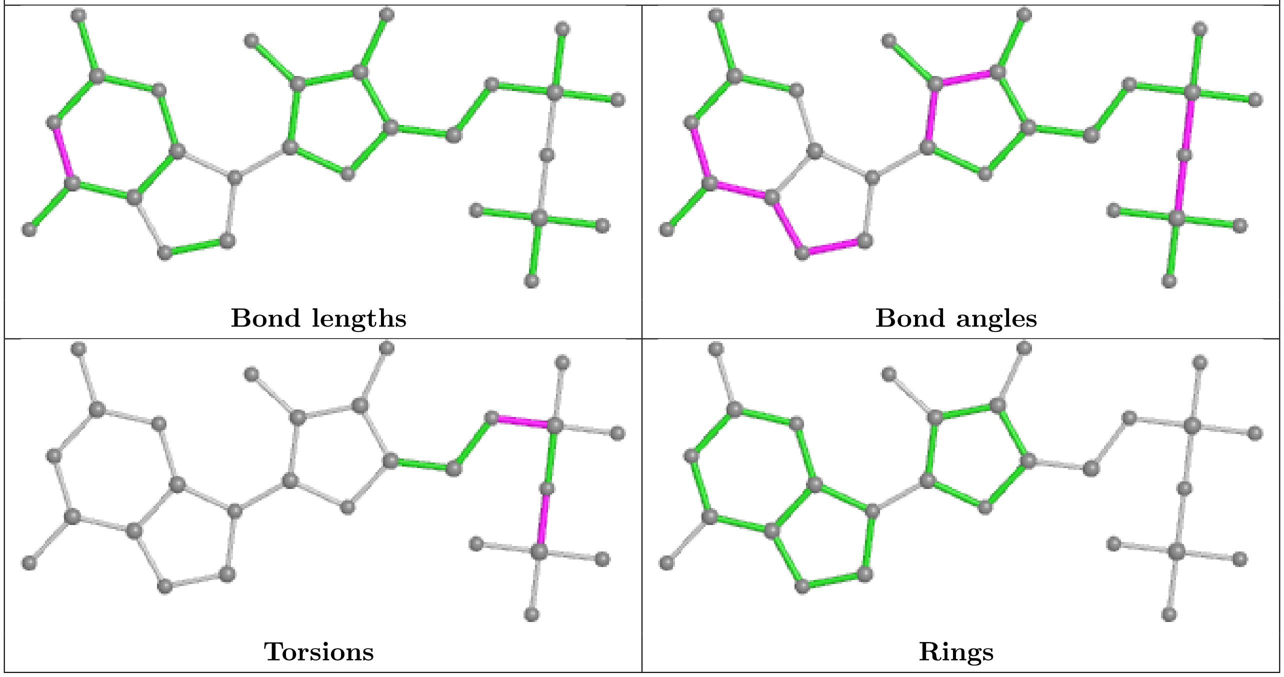
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP BF 502



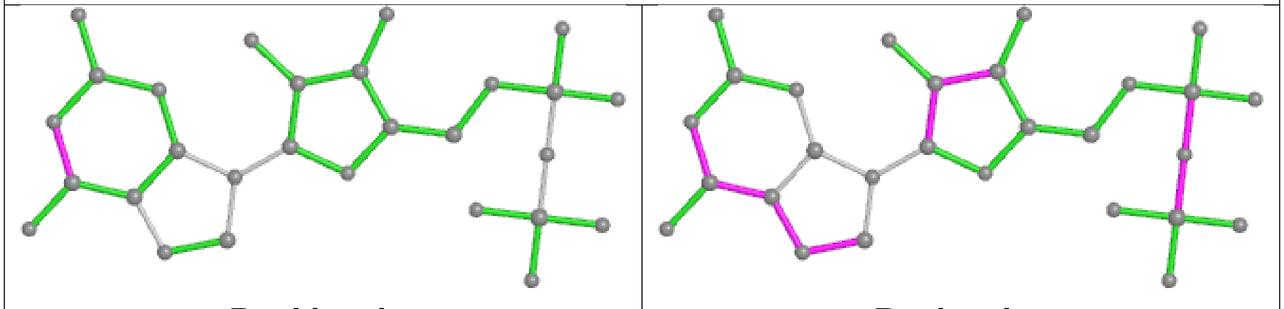
Bond lengths

Bond angles

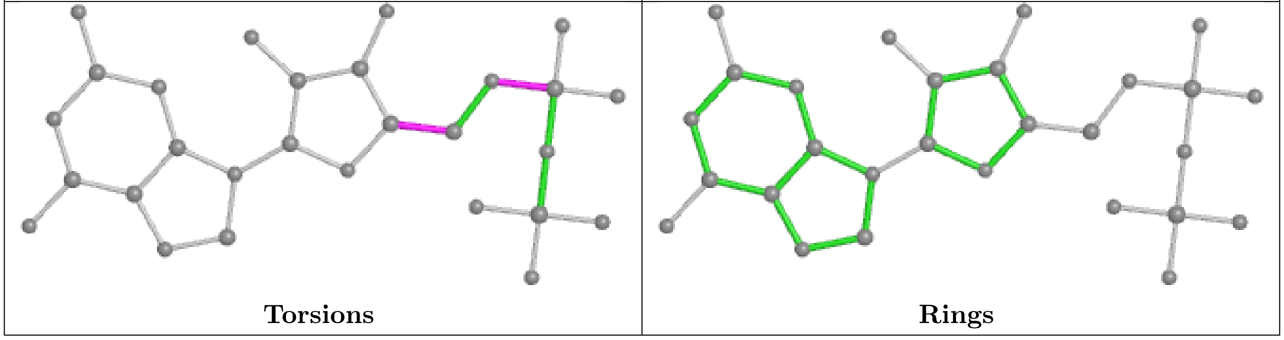
Torsions

Rings

Ligand GDP OF 502

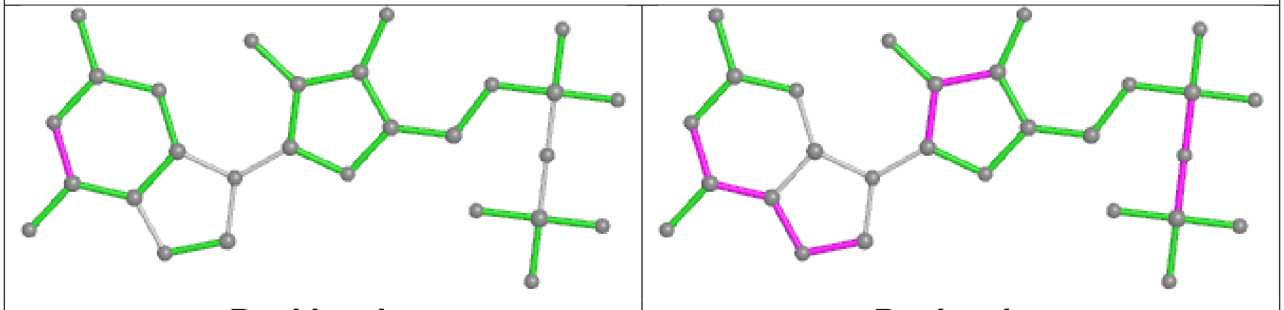


Bond lengths Bond angles

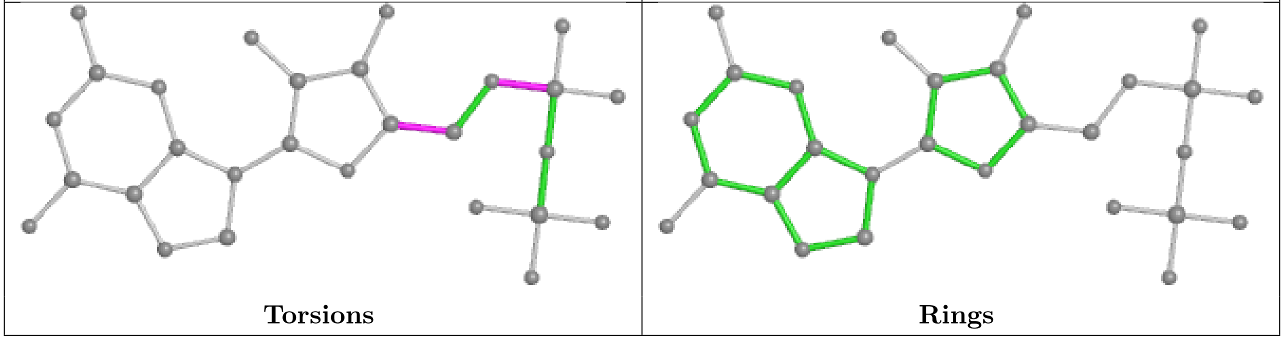


Torsions Rings

Ligand GDP PN 502

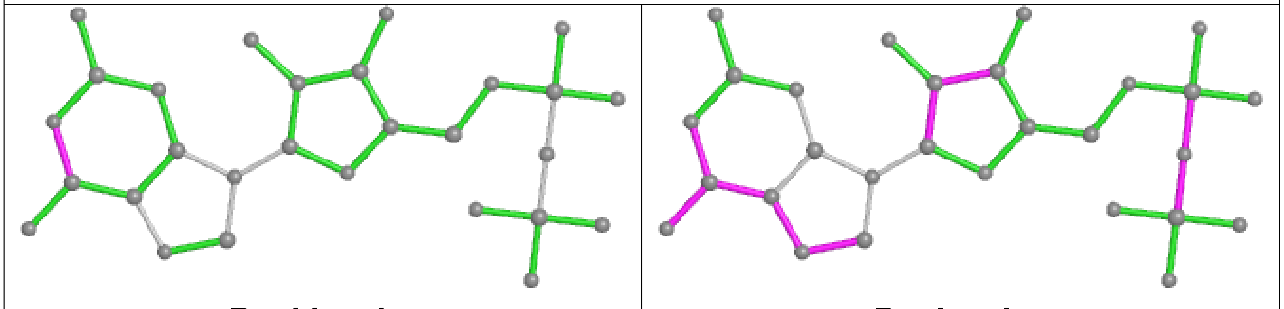


Bond lengths Bond angles

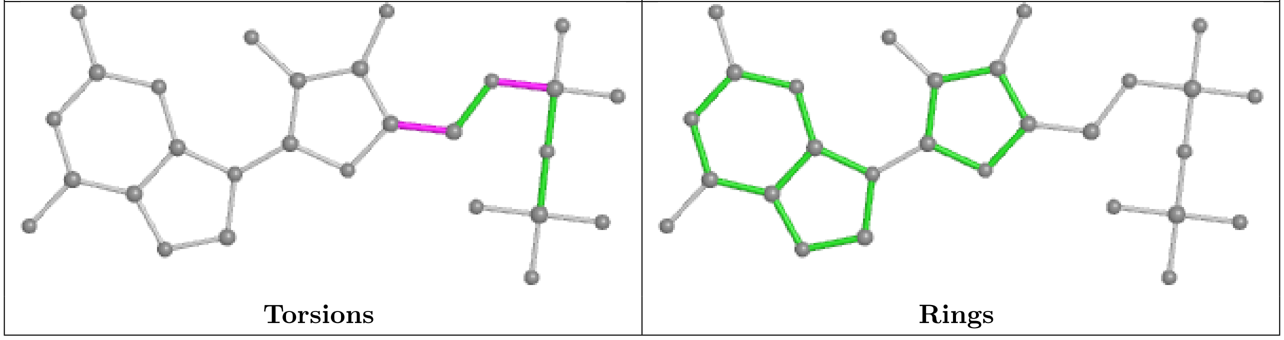


Torsions Rings

Ligand GDP SD 502

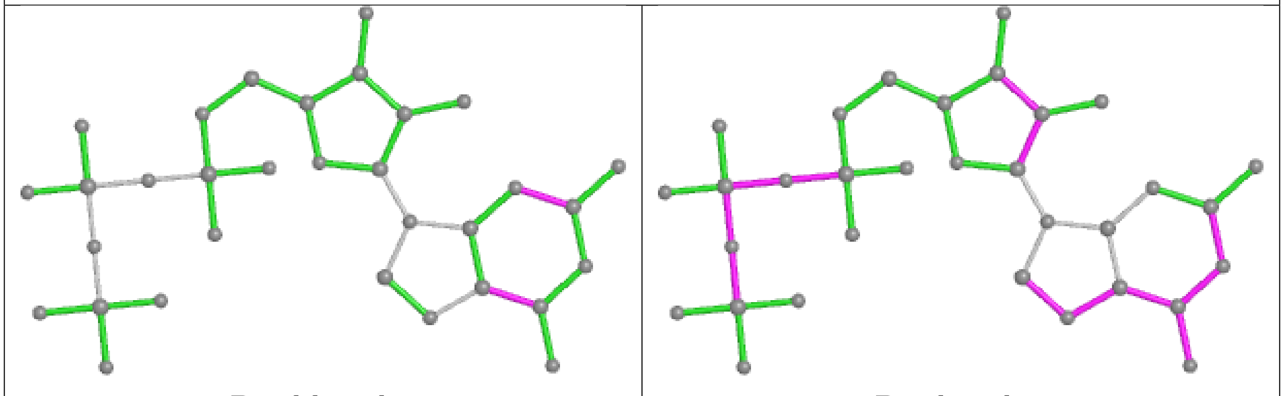


Bond lengths Bond angles

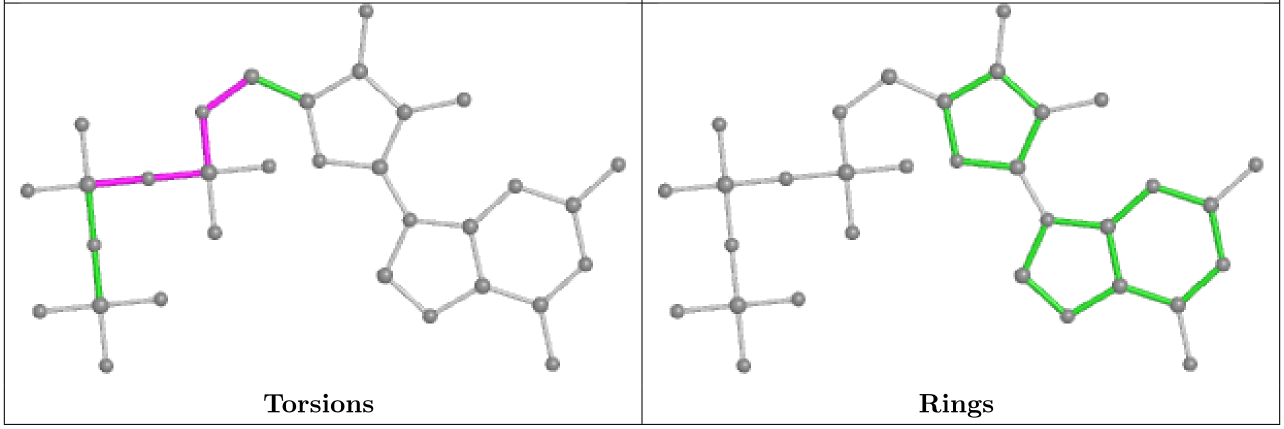


Torsions Rings

Ligand GTP SK 501

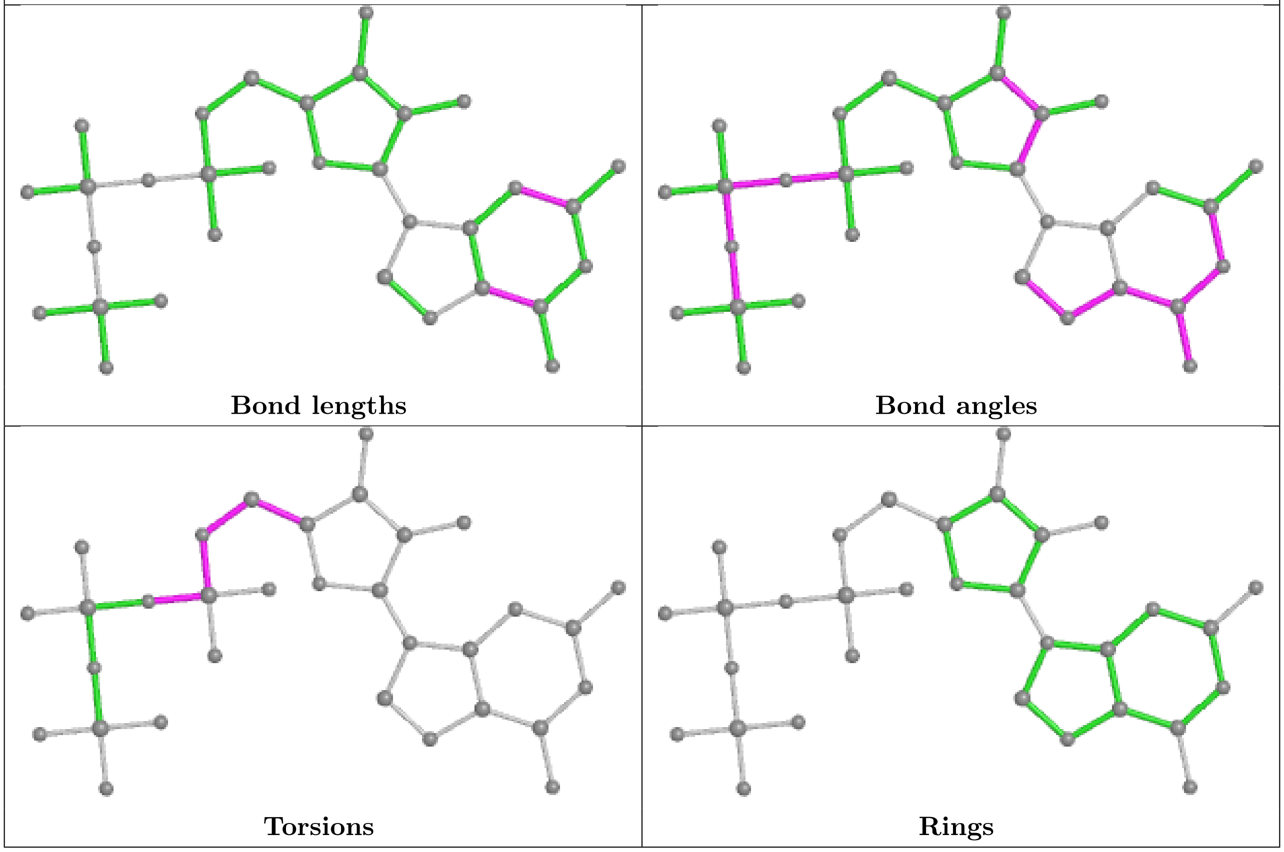


Bond lengths Bond angles



Torsions Rings

Ligand GTP VK 501



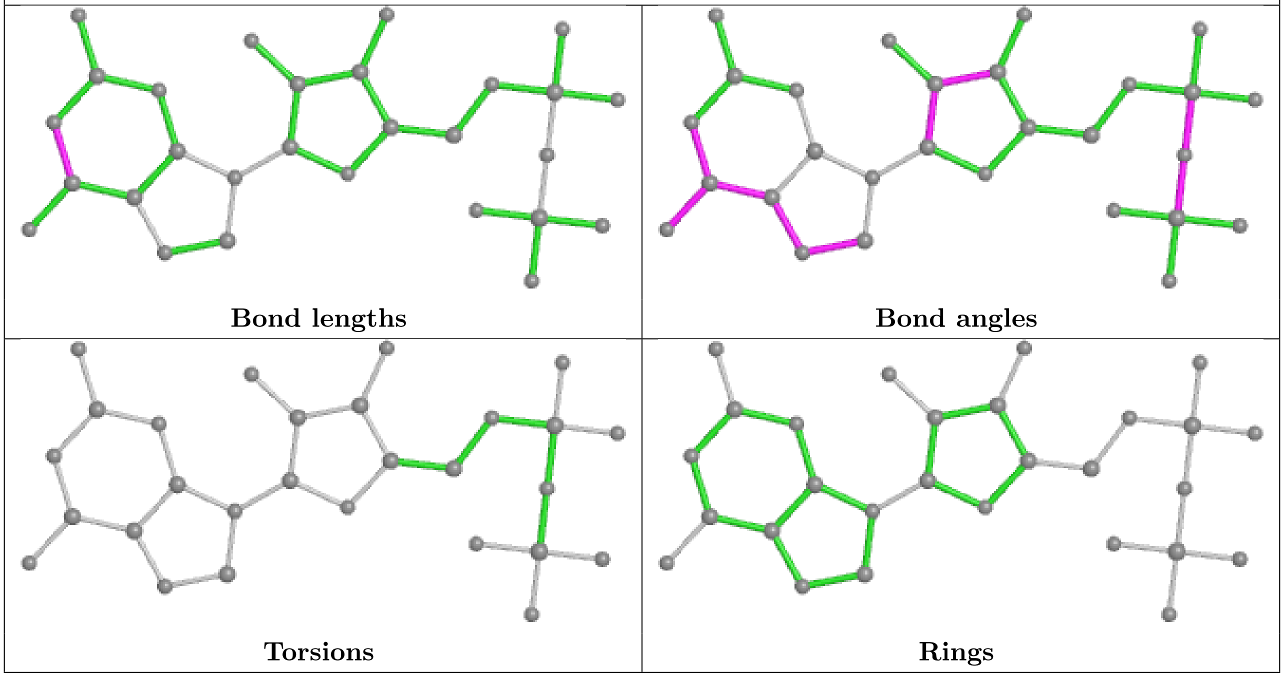
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP SL 502



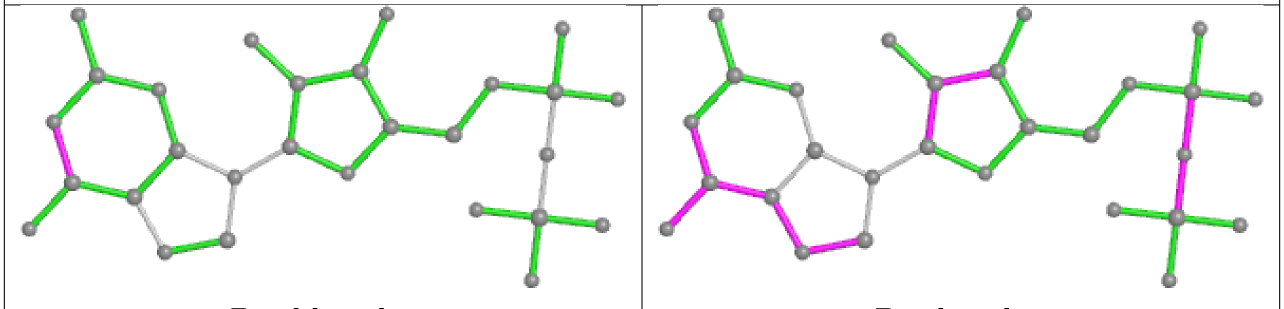
Bond lengths

Bond angles

Torsions

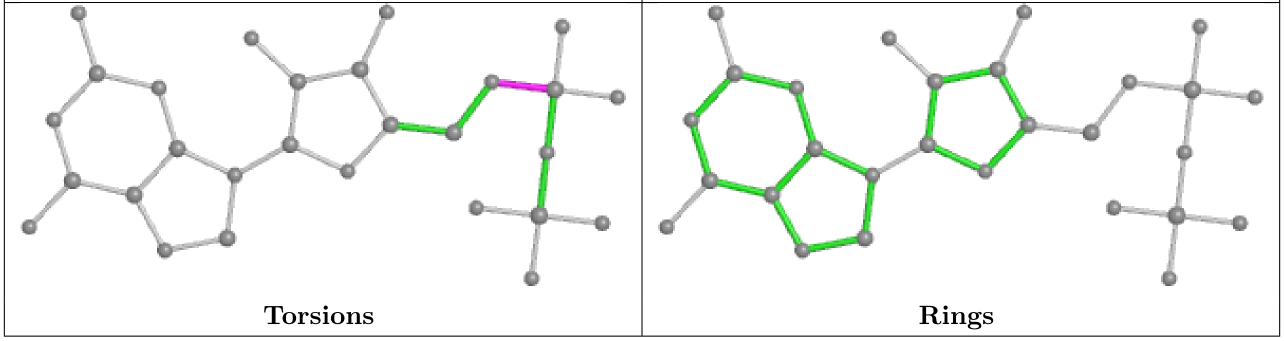
Rings

Ligand GDP RD 502



Bond lengths

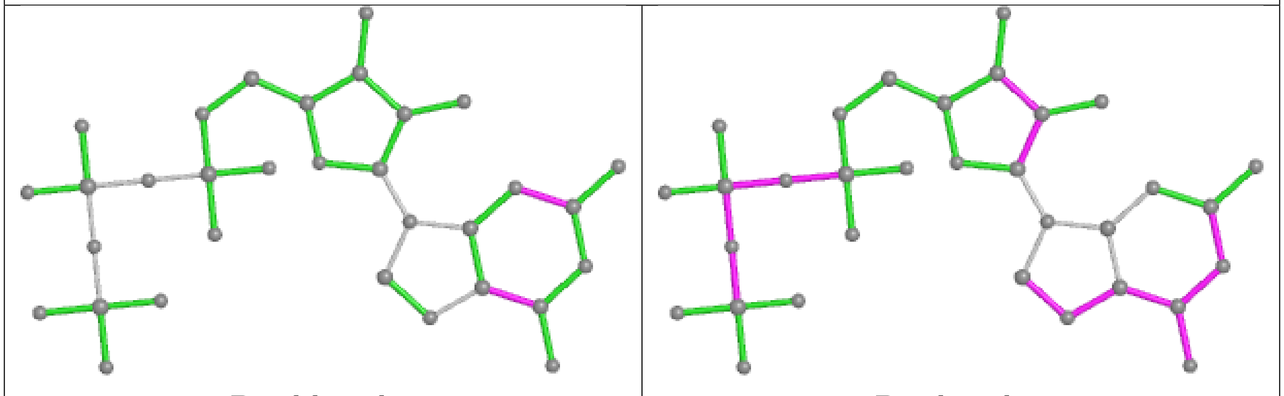
Bond angles



Torsions

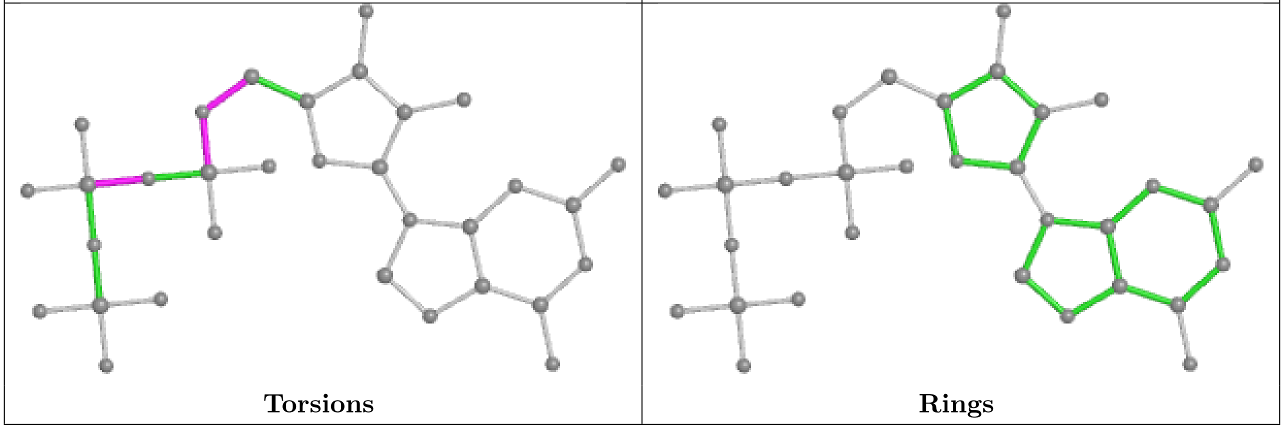
Rings

Ligand GTP MG 501



Bond lengths

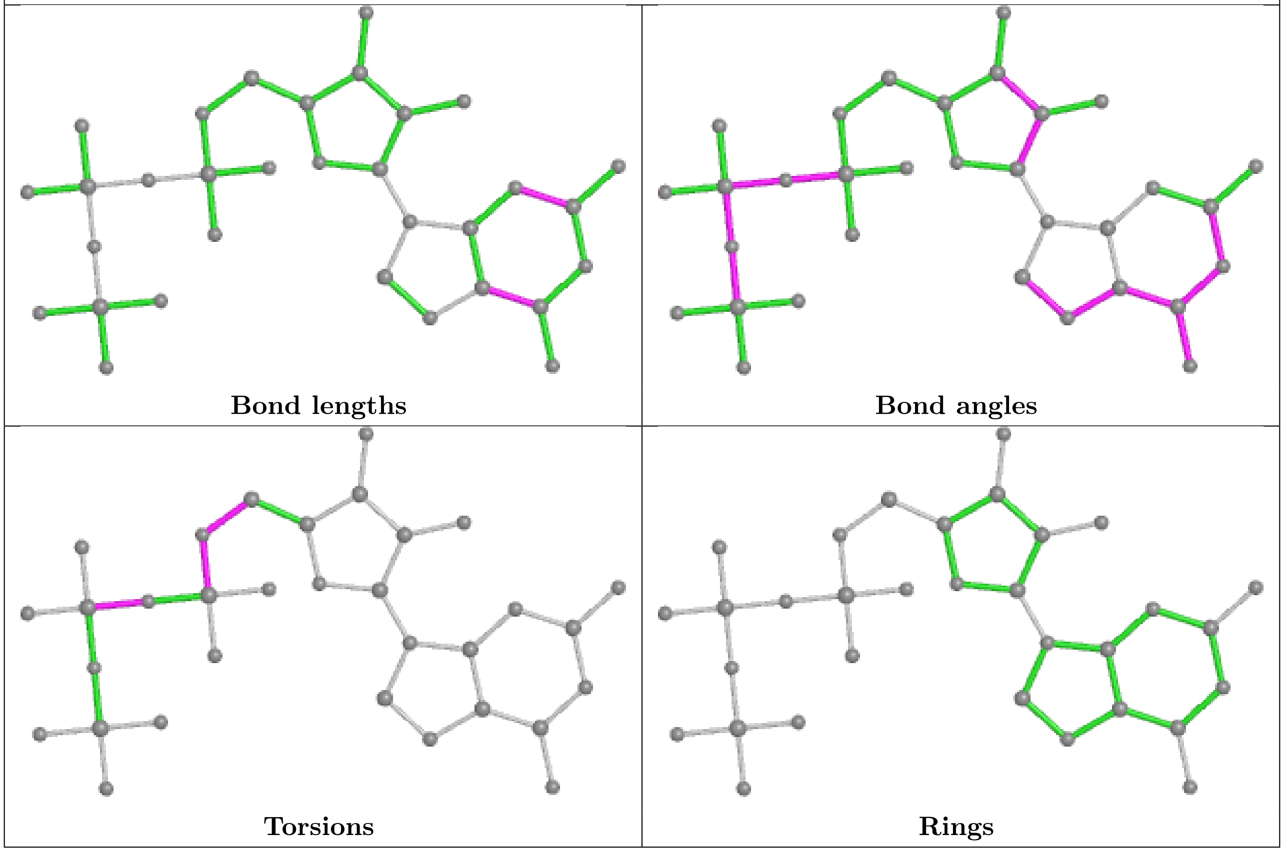
Bond angles



Torsions

Rings

Ligand GTP SG 501



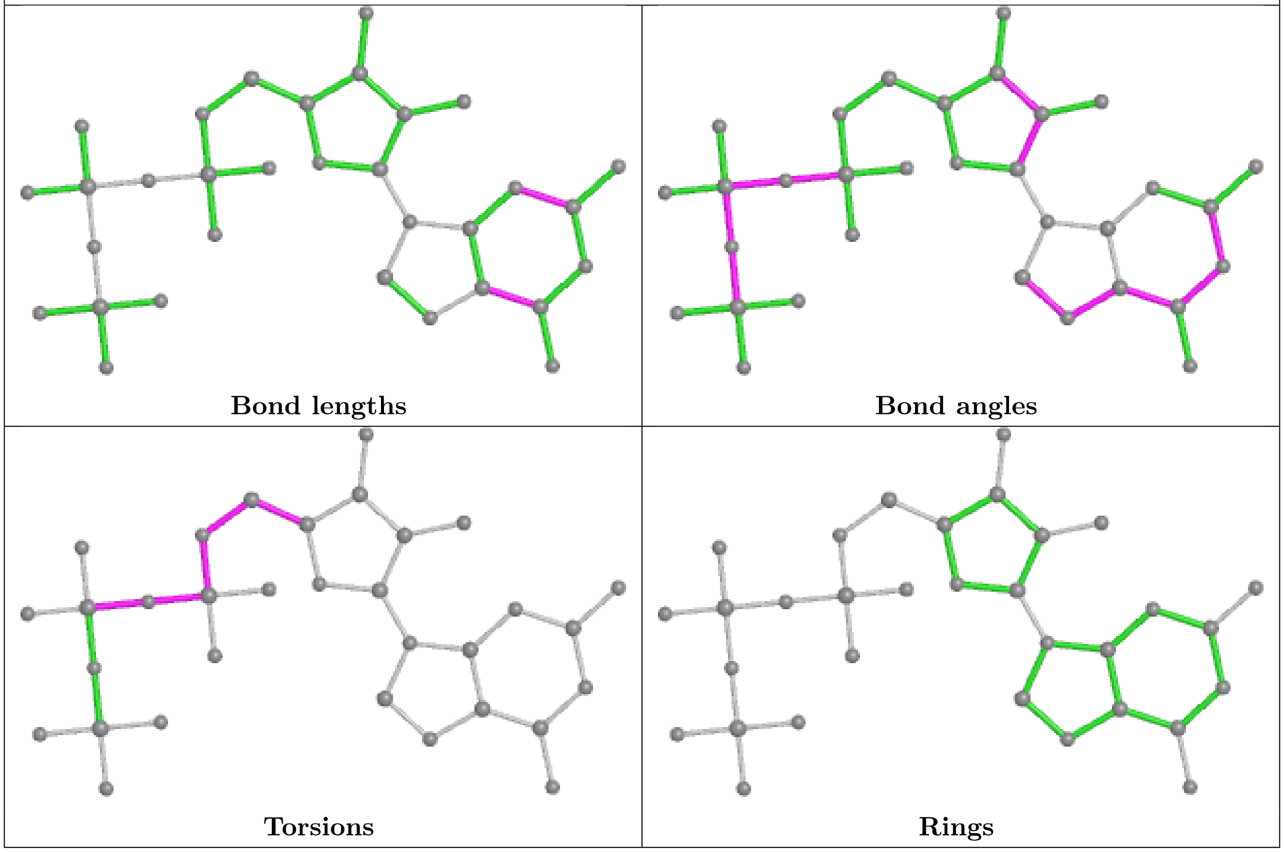
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP DA 501



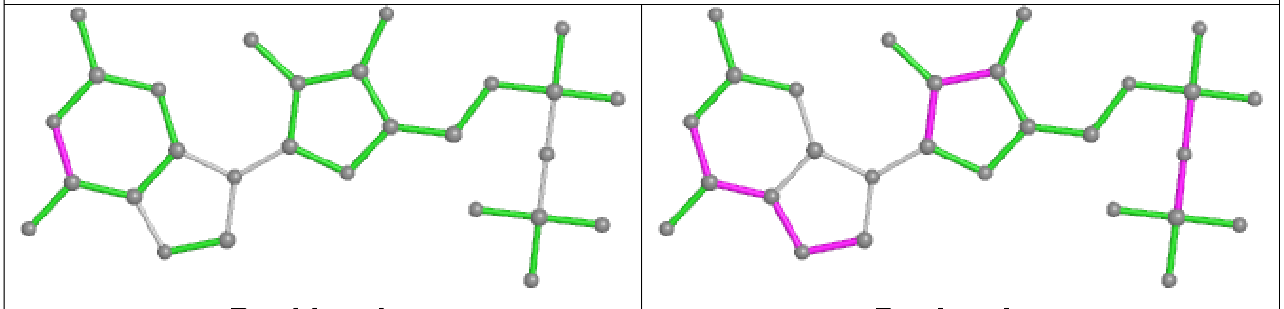
Bond lengths

Bond angles

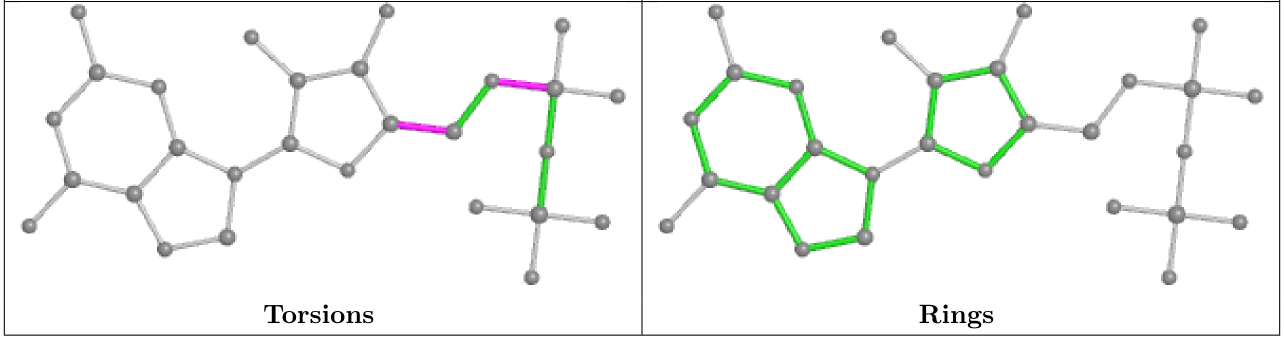
Torsions

Rings

Ligand GDP PD 502

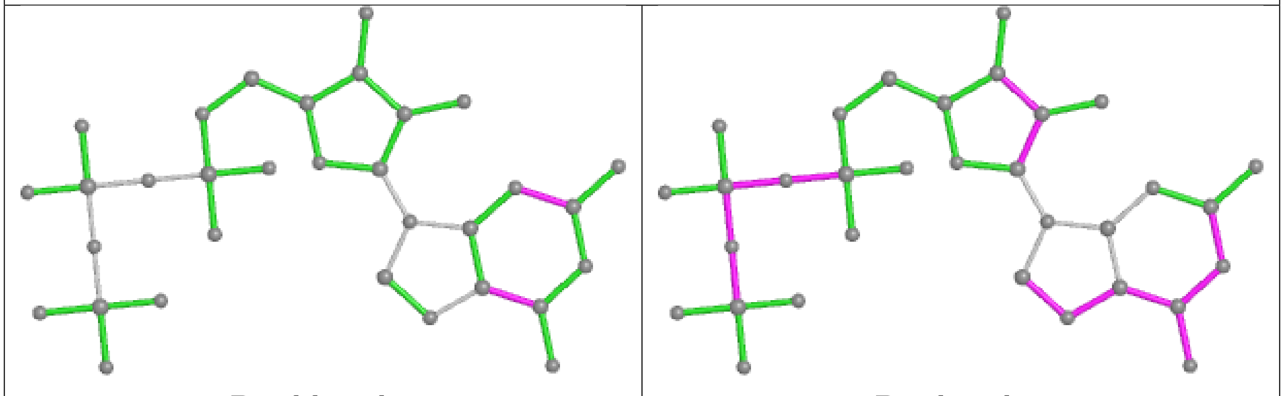


Bond lengths Bond angles

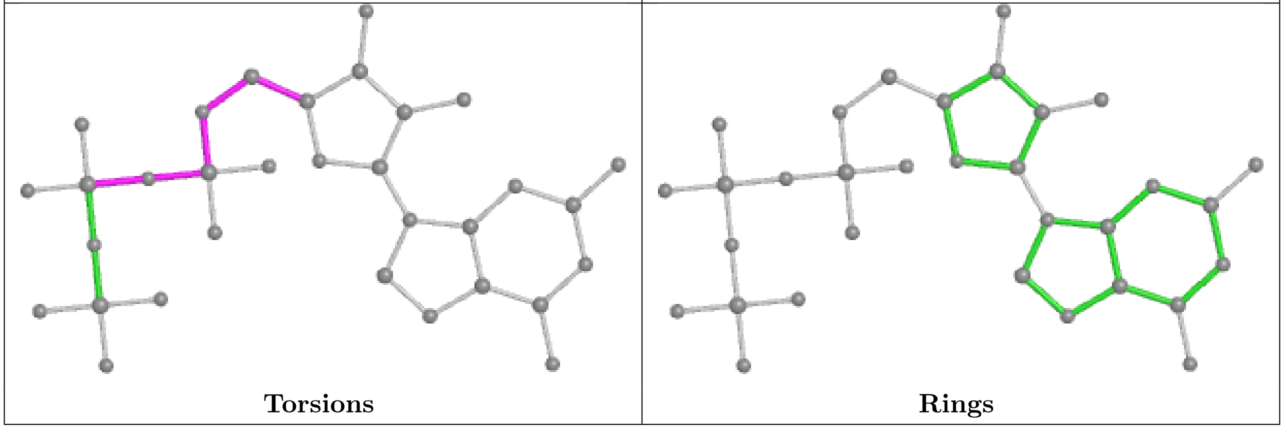


Torsions Rings

Ligand GTP VG 501

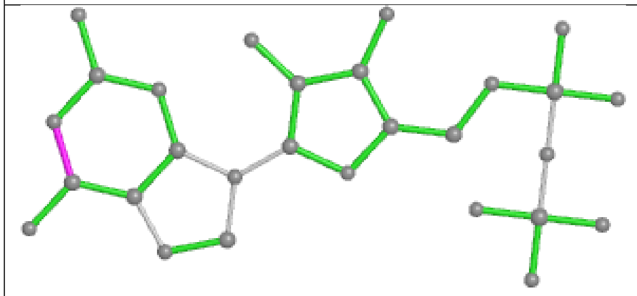


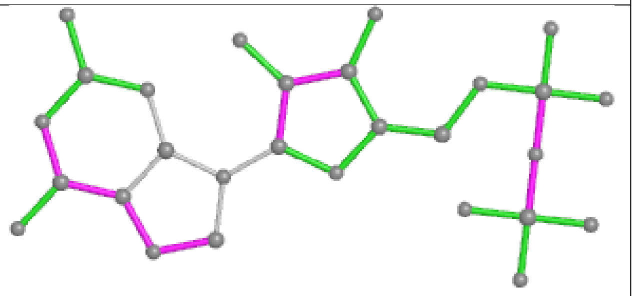
Bond lengths Bond angles

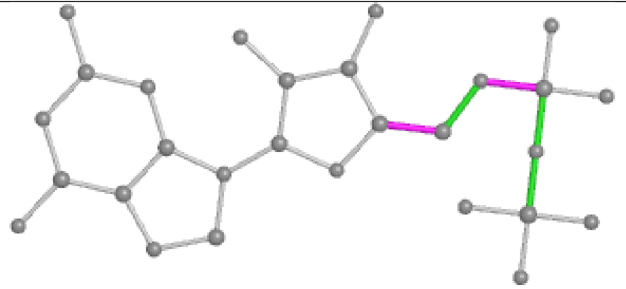


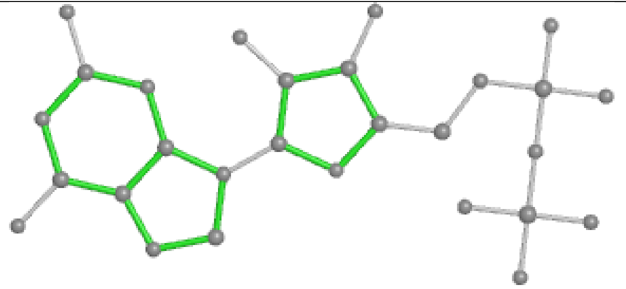
Torsions Rings

Ligand GDP QD 502

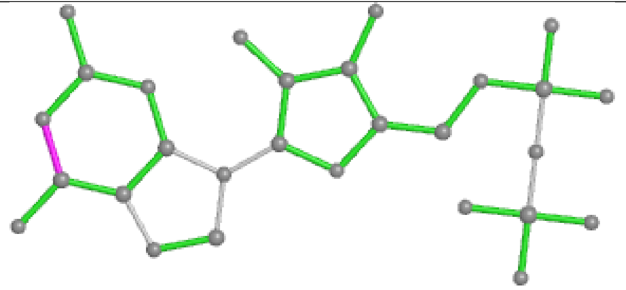

Bond lengths

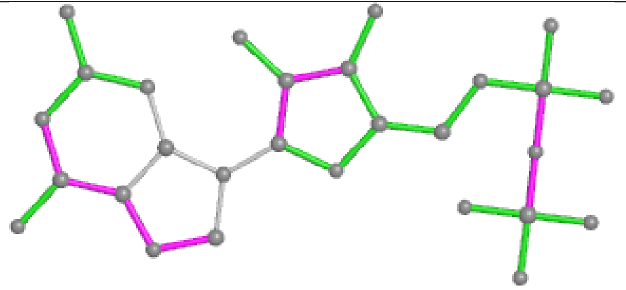

Bond angles

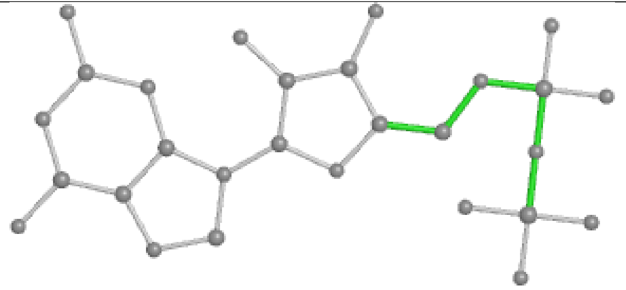

Torsions

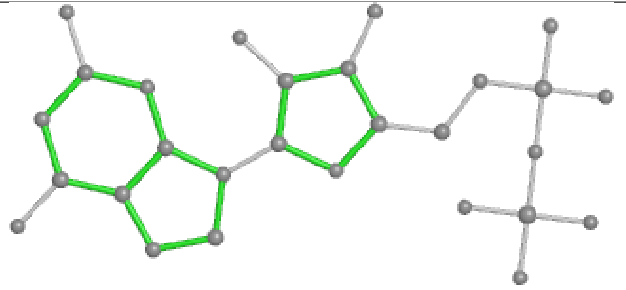

Rings

Ligand GDP SF 502

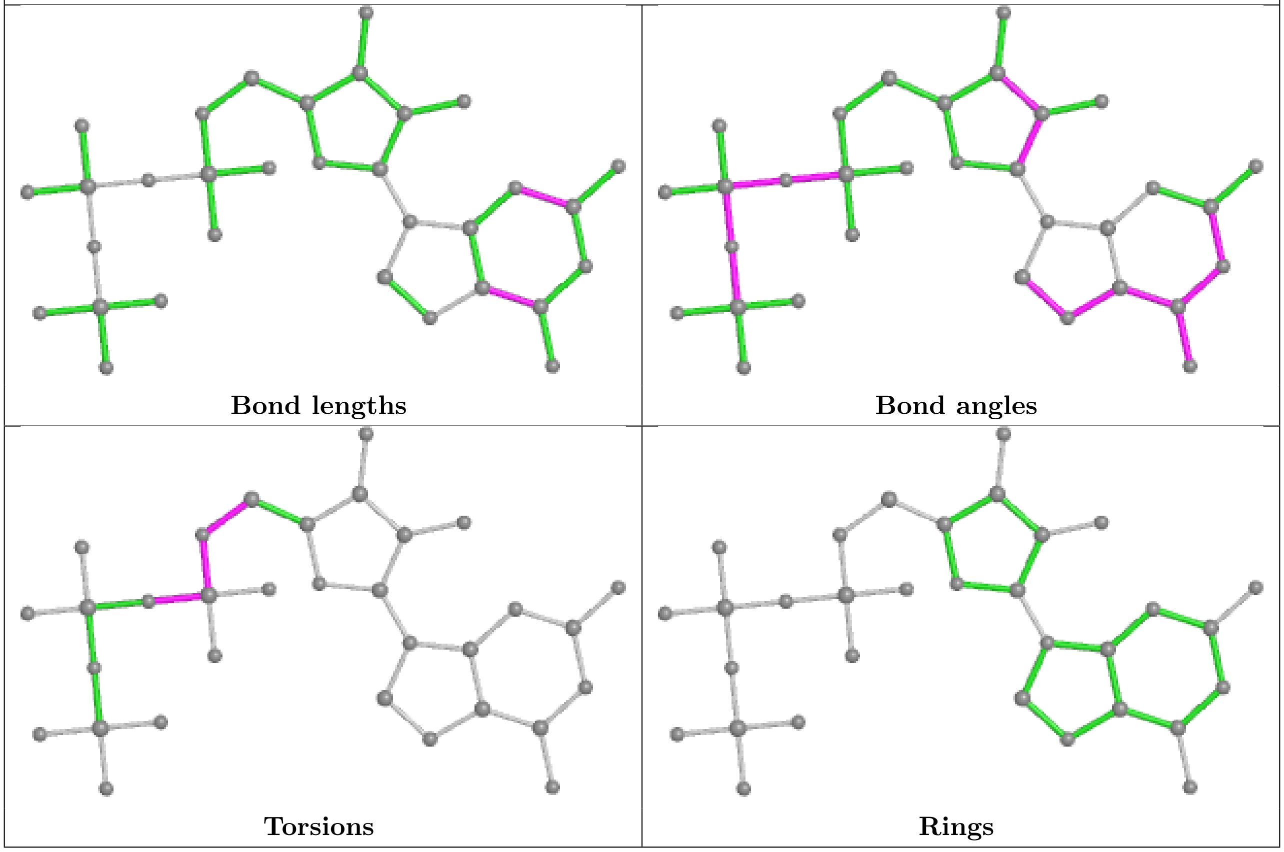

Bond lengths


Bond angles


Torsions


Rings

Ligand GTP EK 501



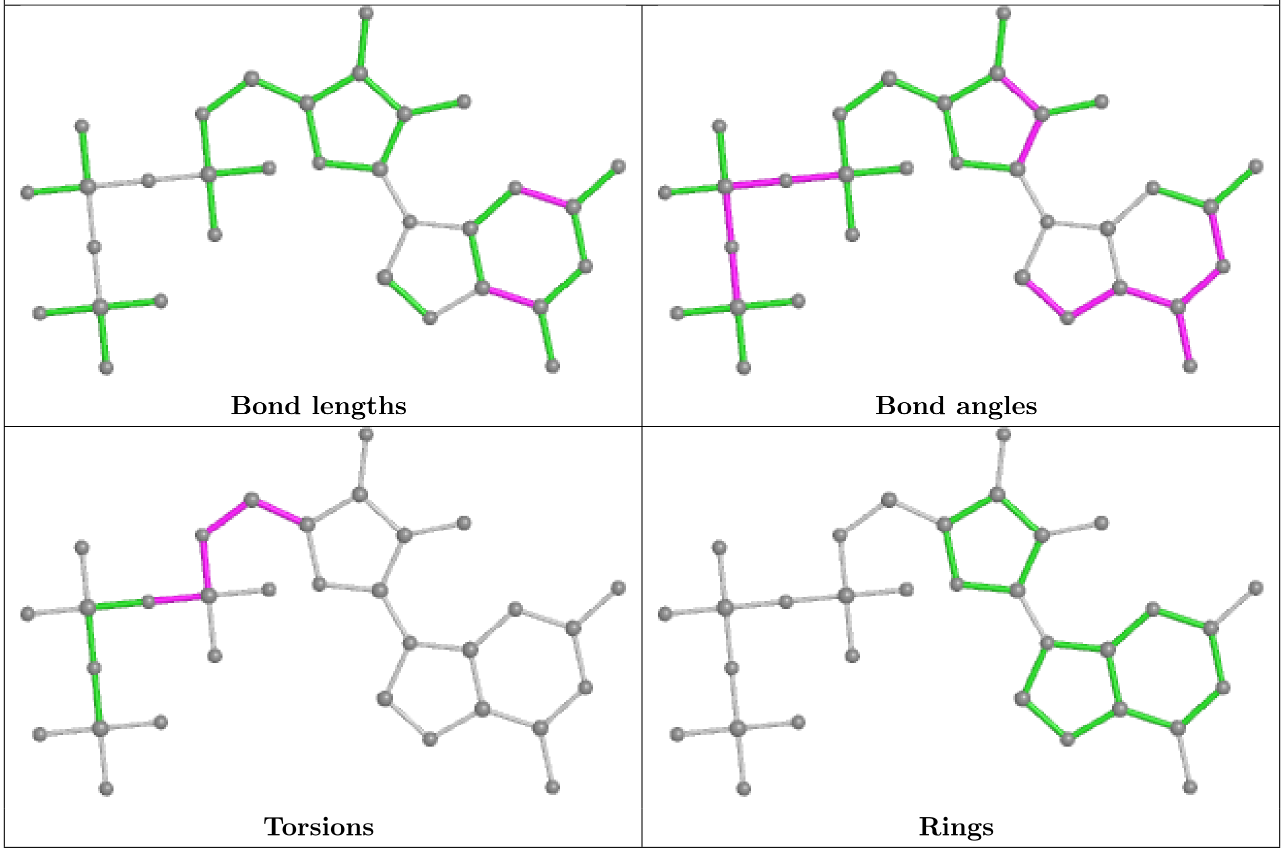
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP IC 501



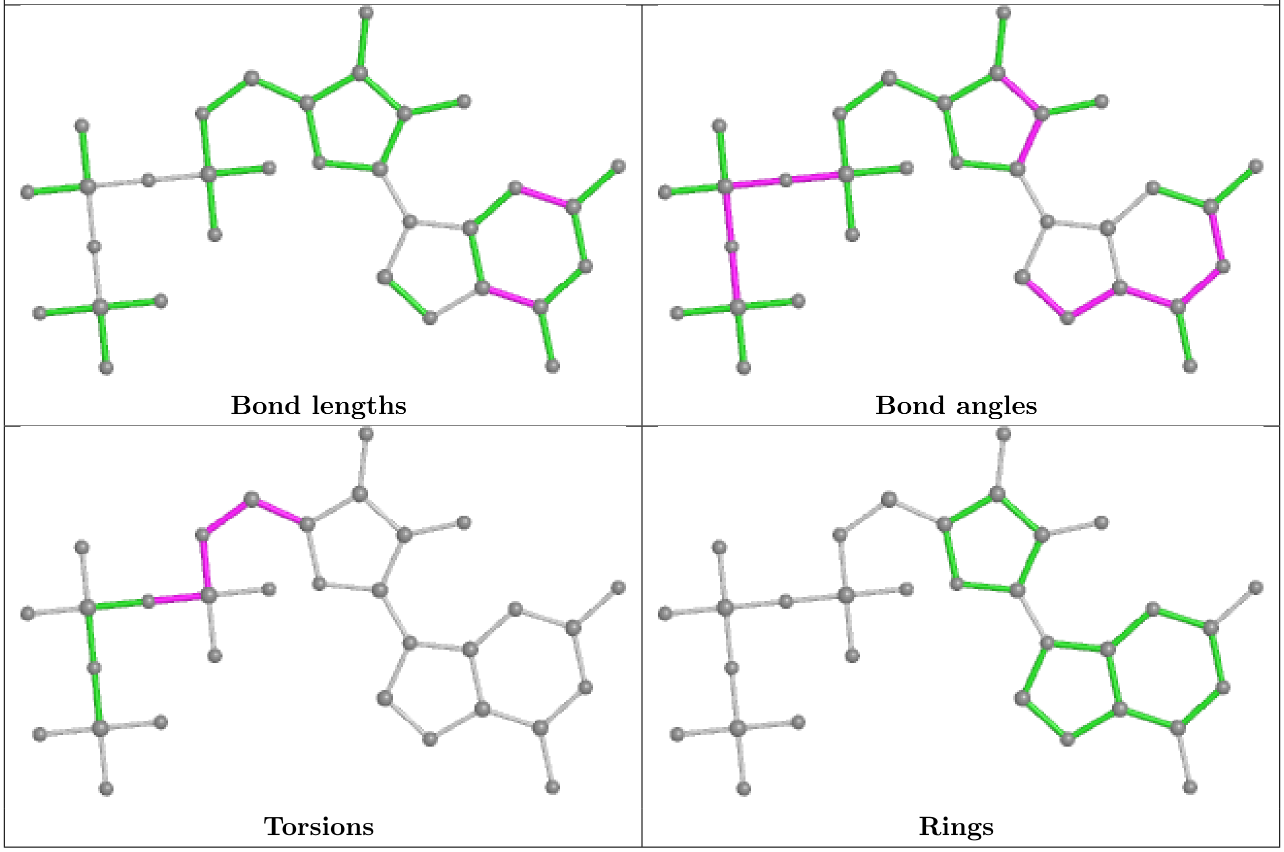
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP WE 501



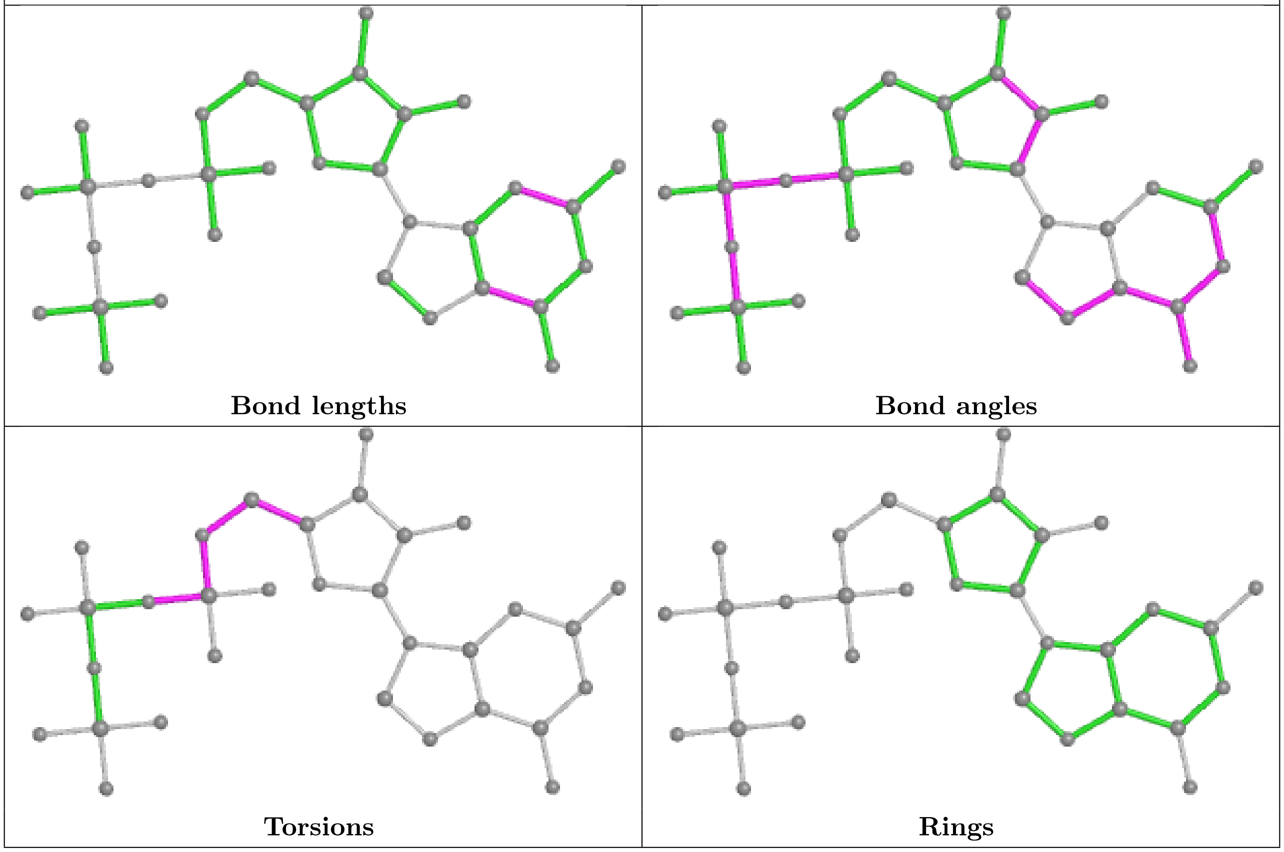
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP NC 501



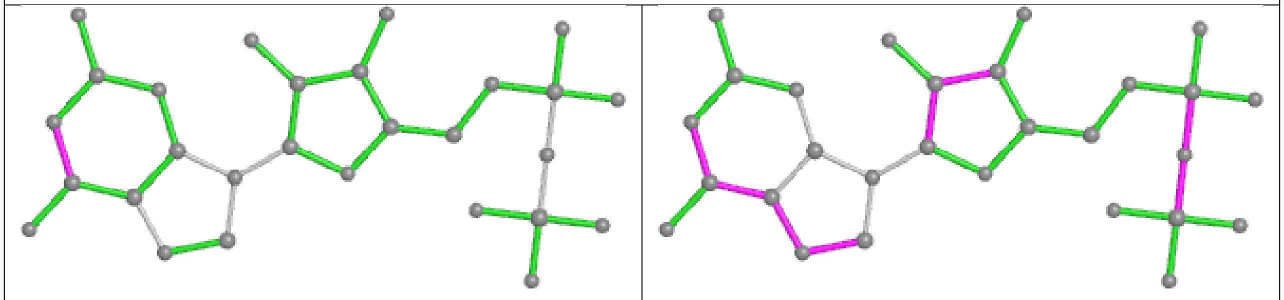
Bond lengths

Bond angles

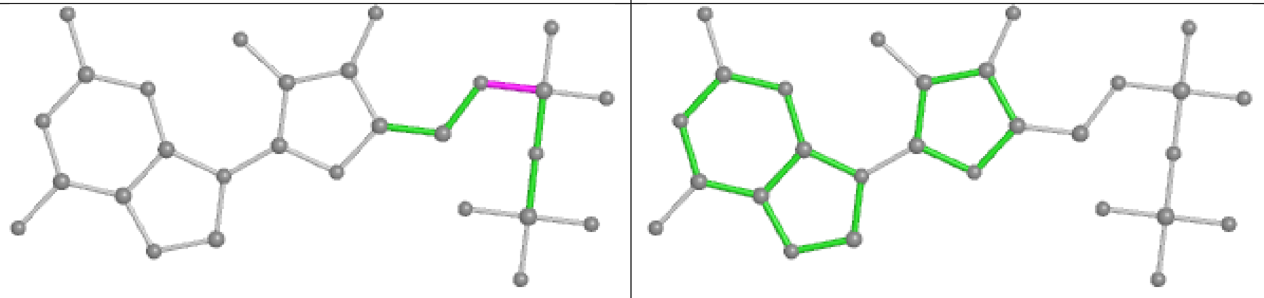
Torsions

Rings

Ligand GDP WH 502

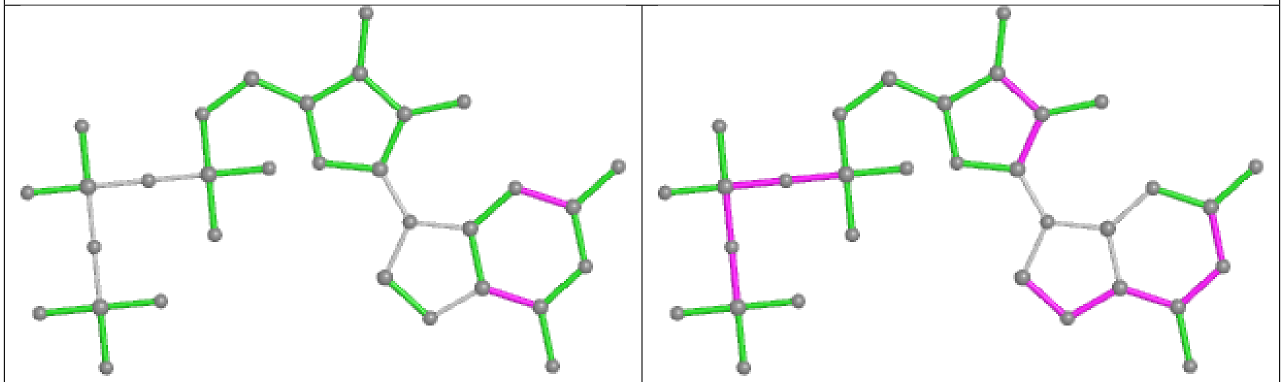


Bond lengths **Bond angles**

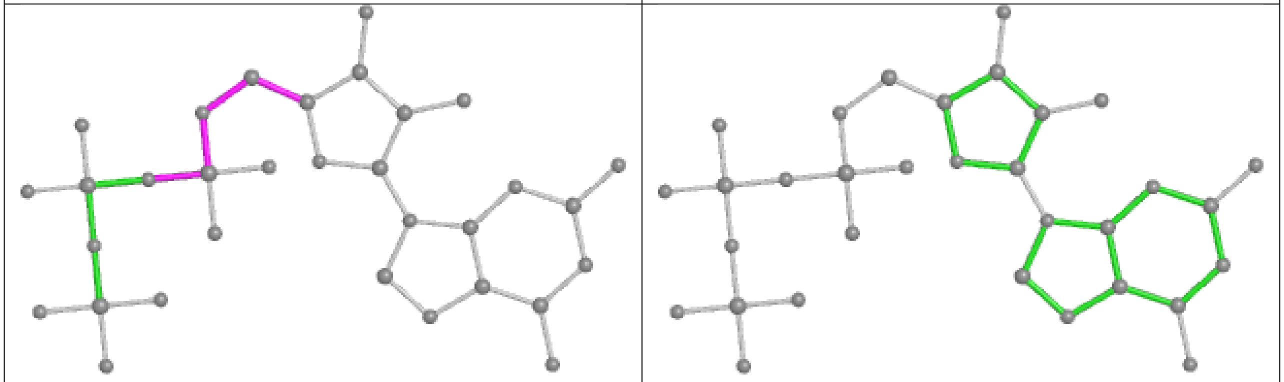


Torsions **Rings**

Ligand GTP IG 501

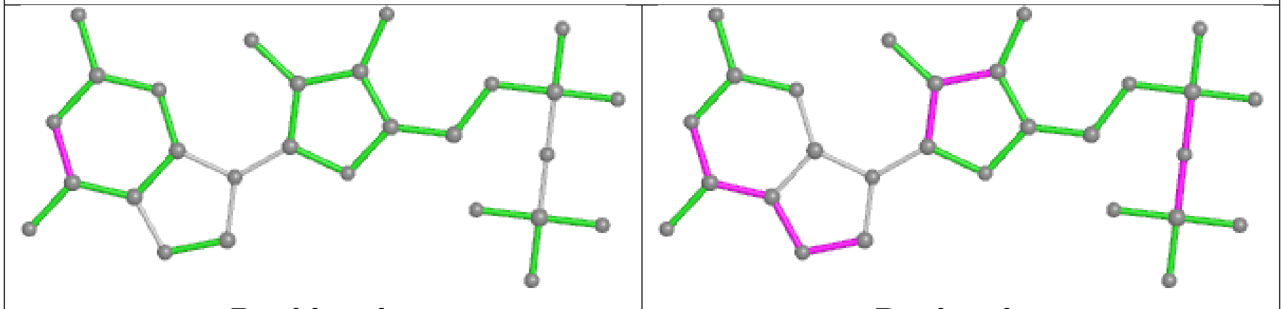


Bond lengths **Bond angles**



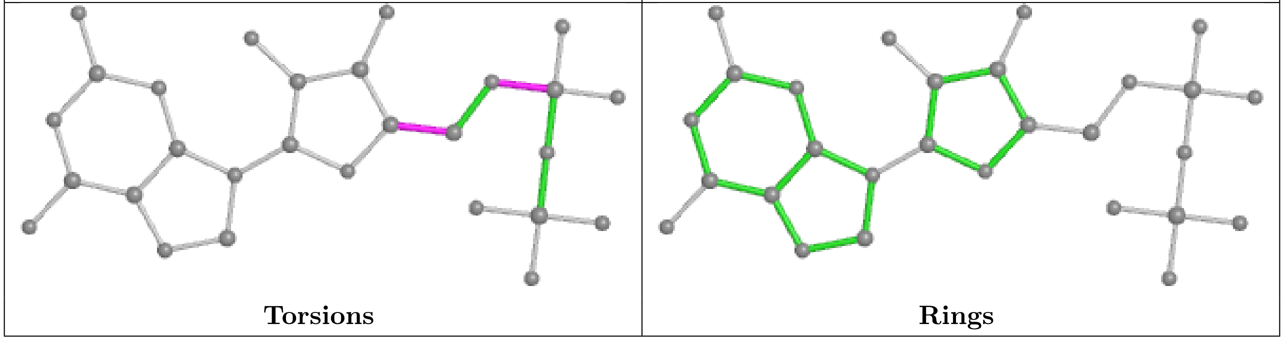
Torsions **Rings**

Ligand GDP MJ 502



Bond lengths

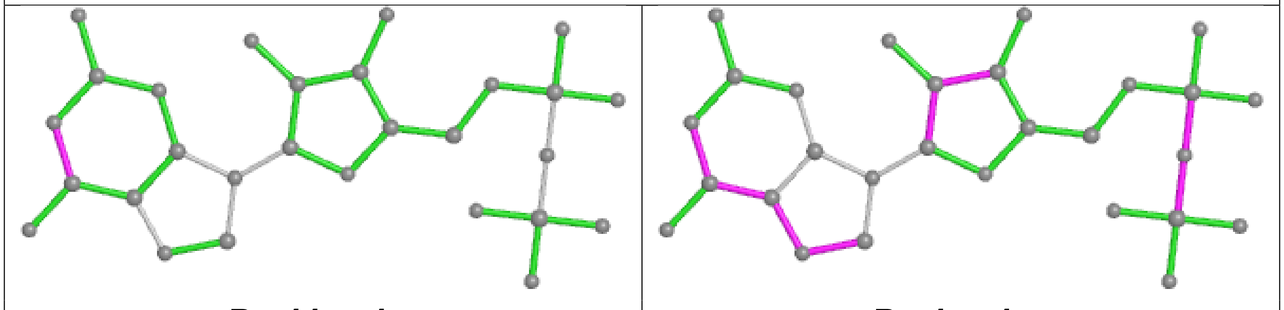
Bond angles



Torsions

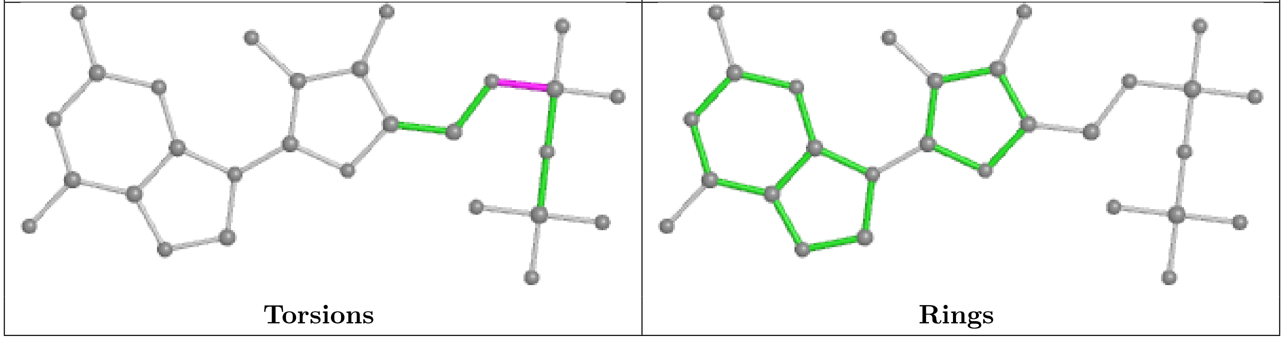
Rings

Ligand GDP KD 502



Bond lengths

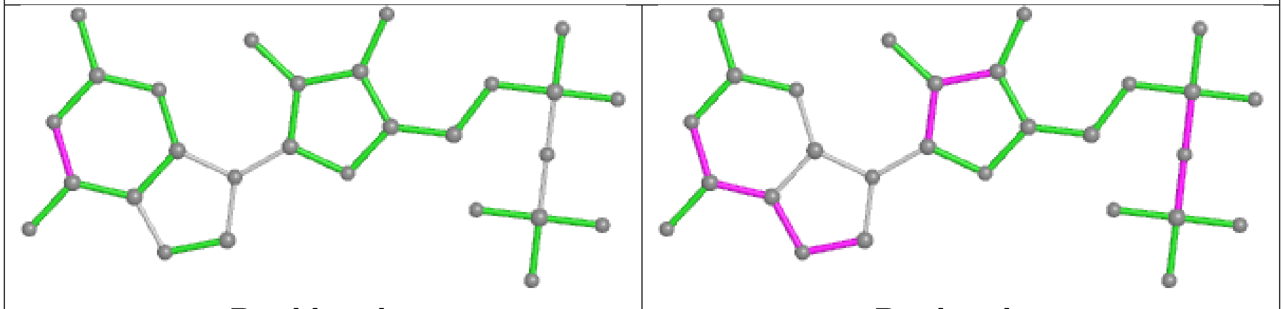
Bond angles



Torsions

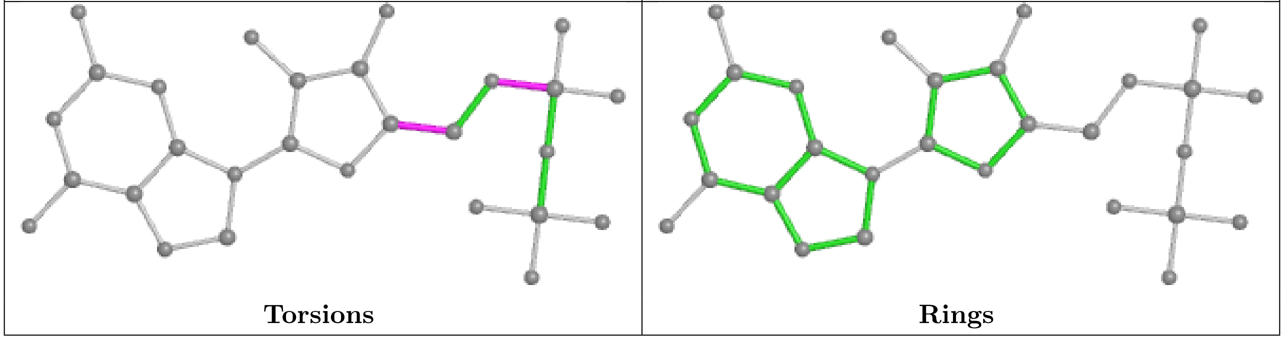
Rings

Ligand GDP TN 502



Bond lengths

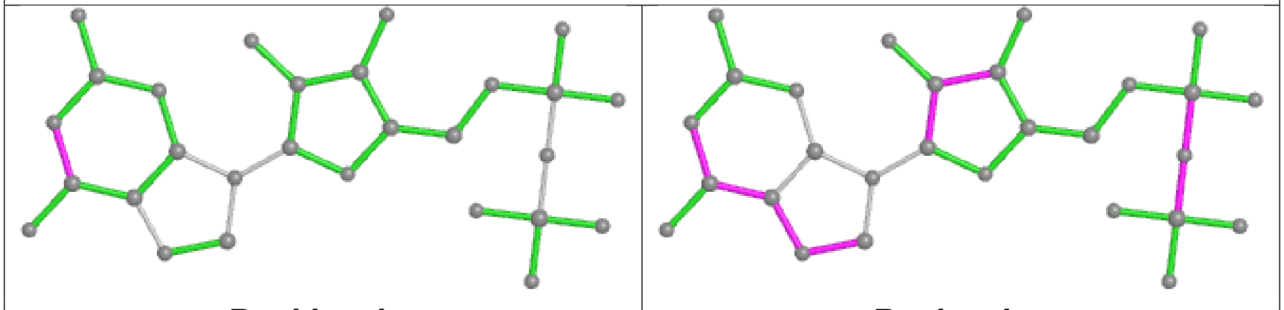
Bond angles



Torsions

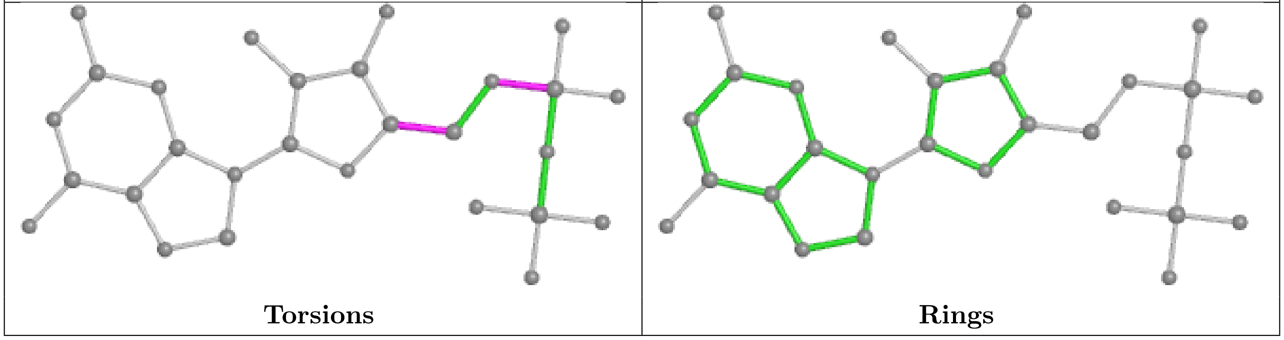
Rings

Ligand GDP QL 502



Bond lengths

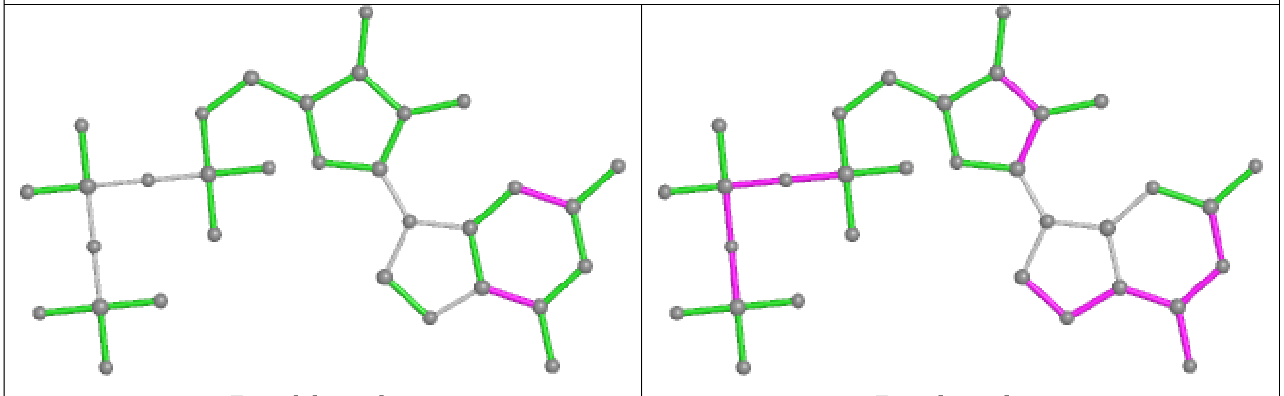
Bond angles



Torsions

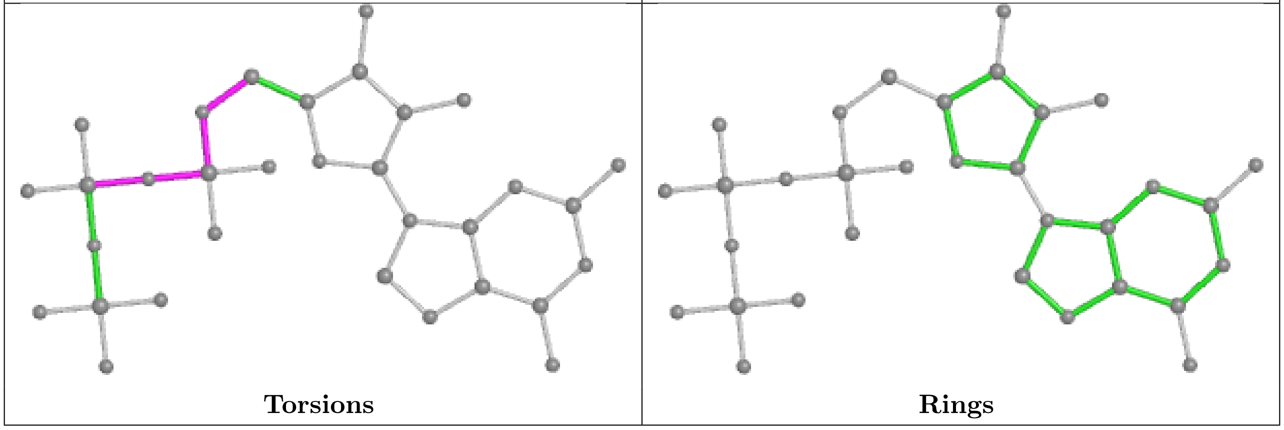
Rings

Ligand GTP MM 501



Bond lengths

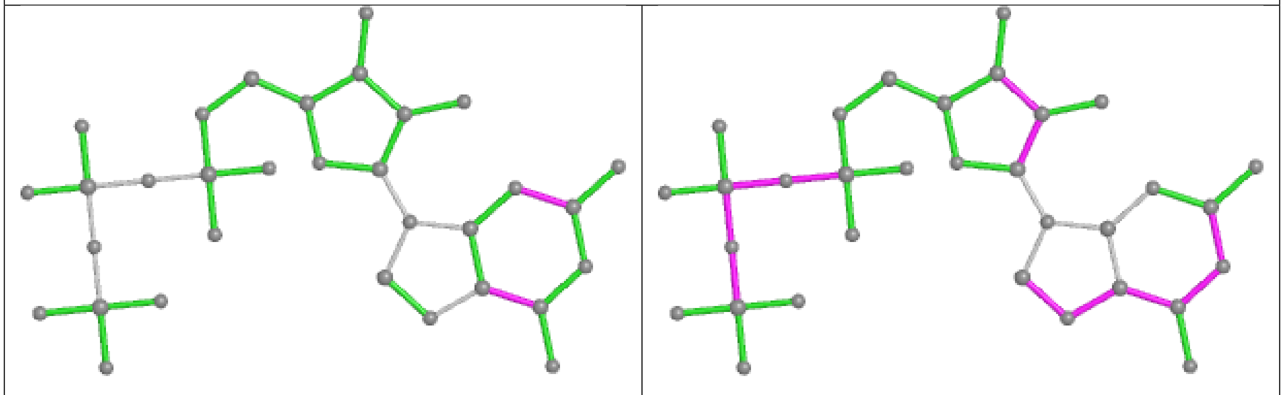
Bond angles



Torsions

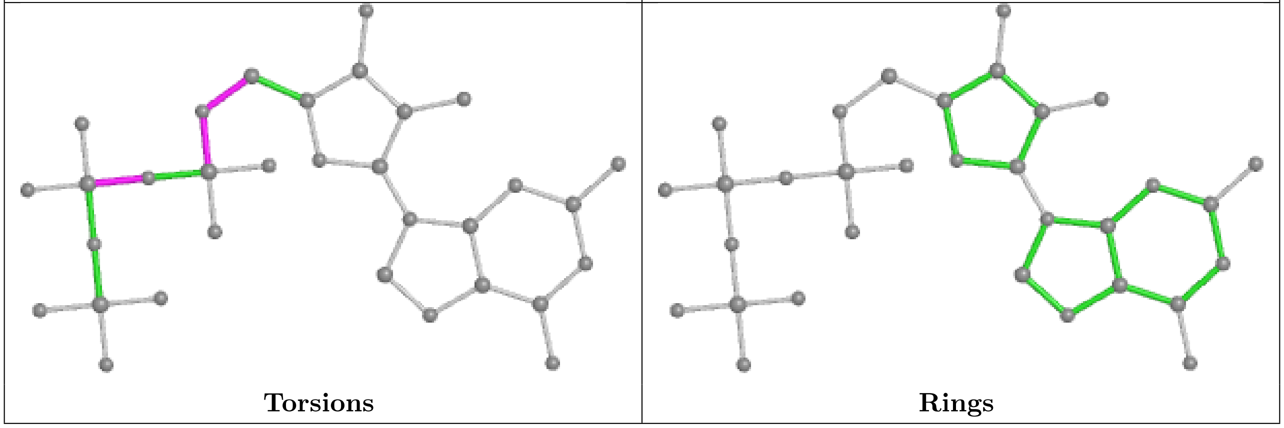
Rings

Ligand GTP JC 501



Bond lengths

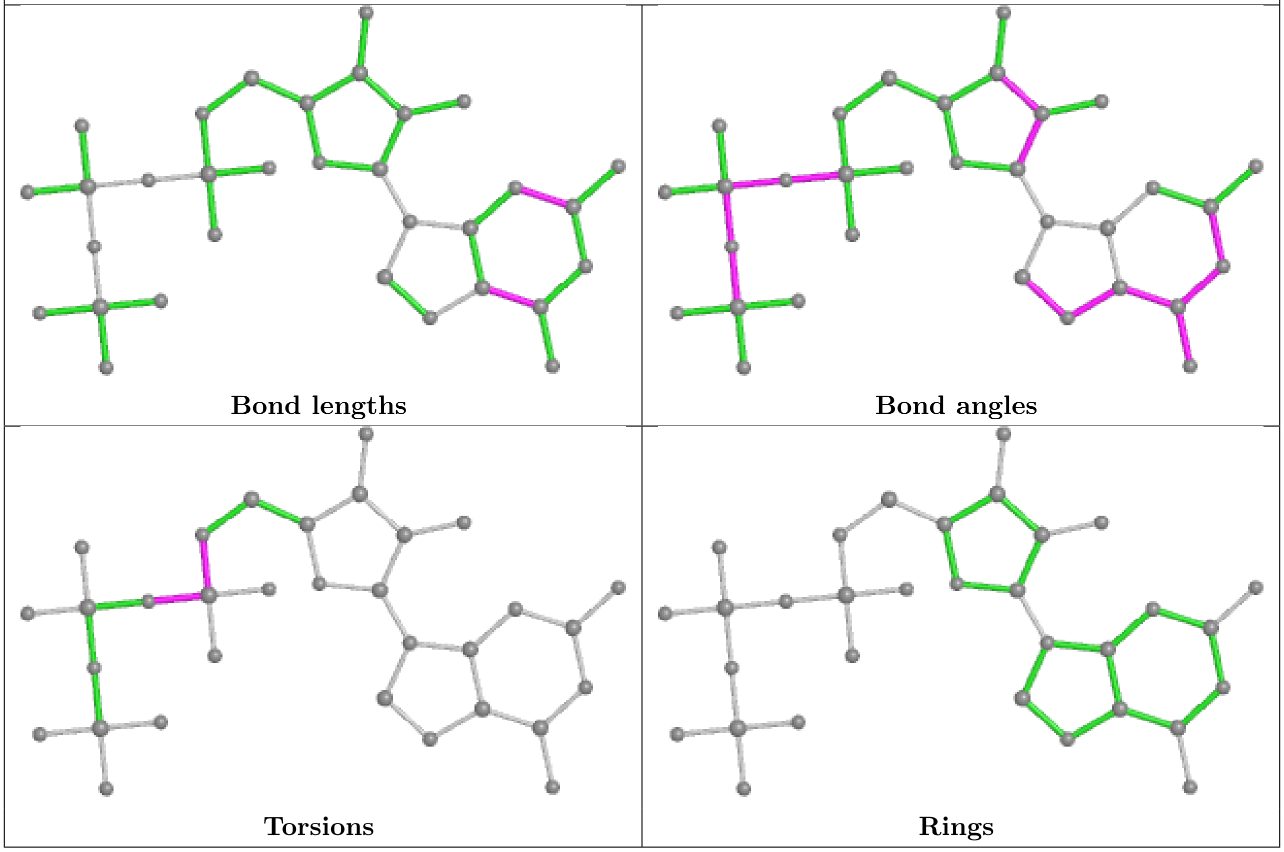
Bond angles



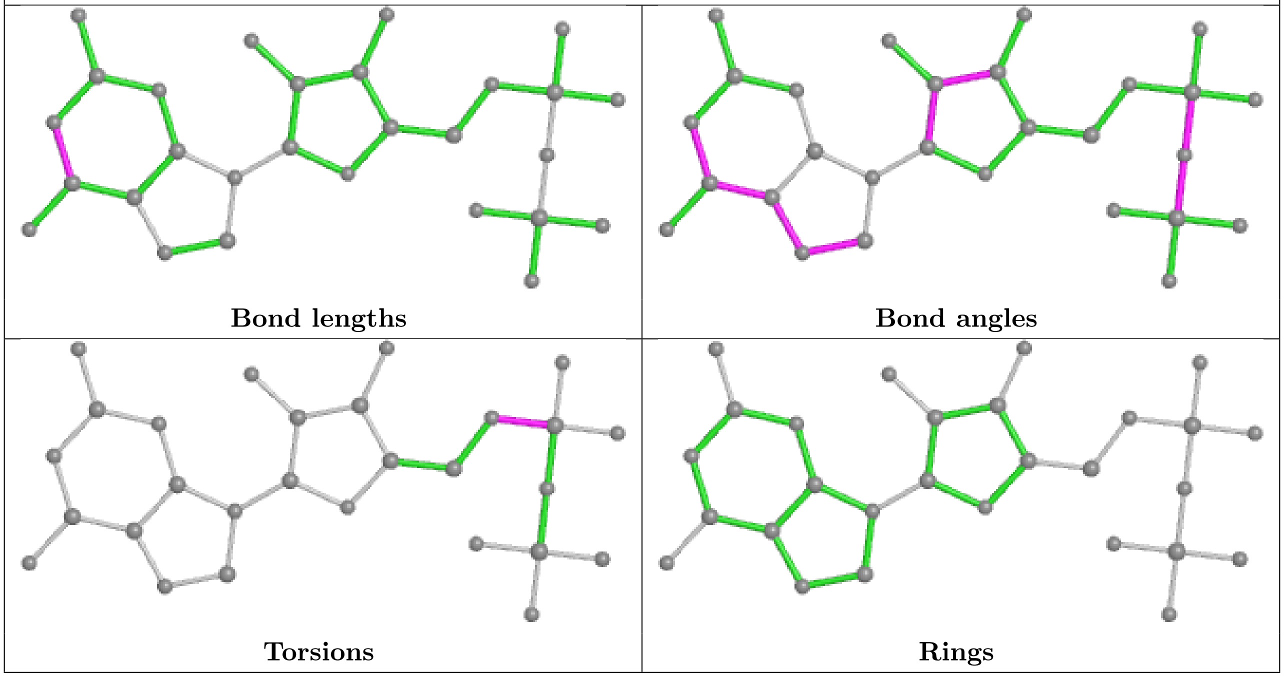
Torsions

Rings

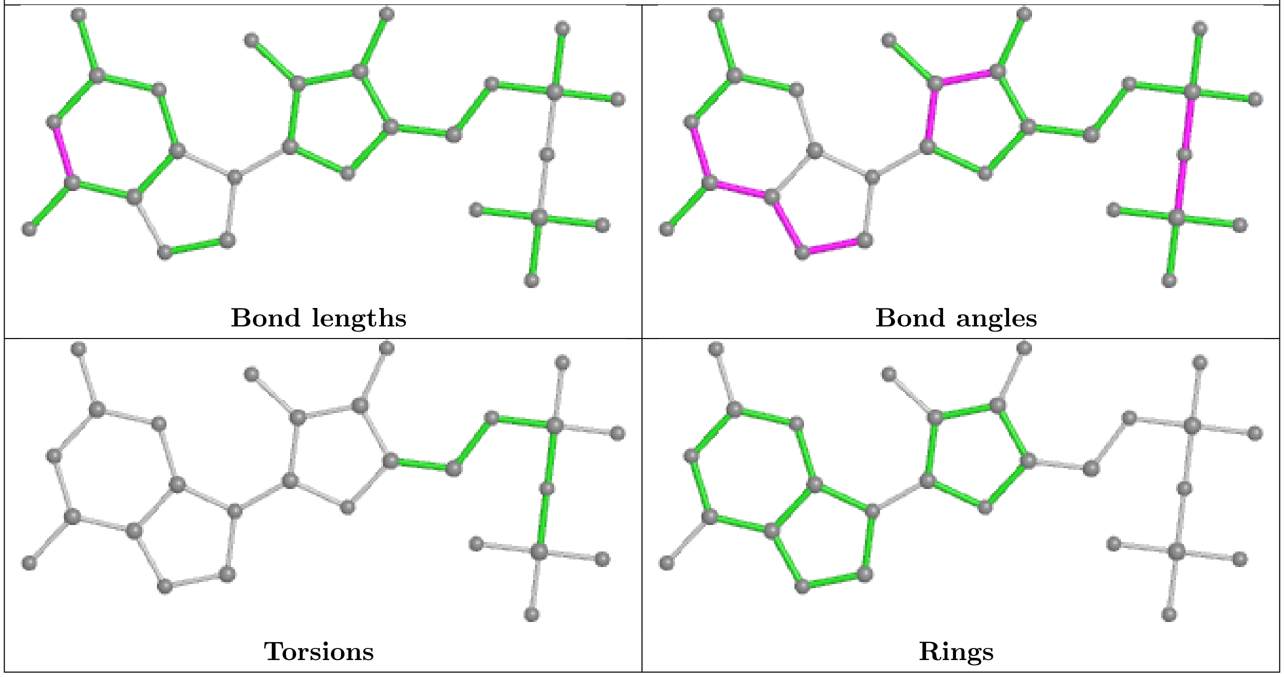
Ligand GTP SO 501


Bond lengths
Bond angles
Torsions
Rings

Ligand GDP GN 502


Bond lengths
Bond angles
Torsions
Rings

Ligand GDP VH 502



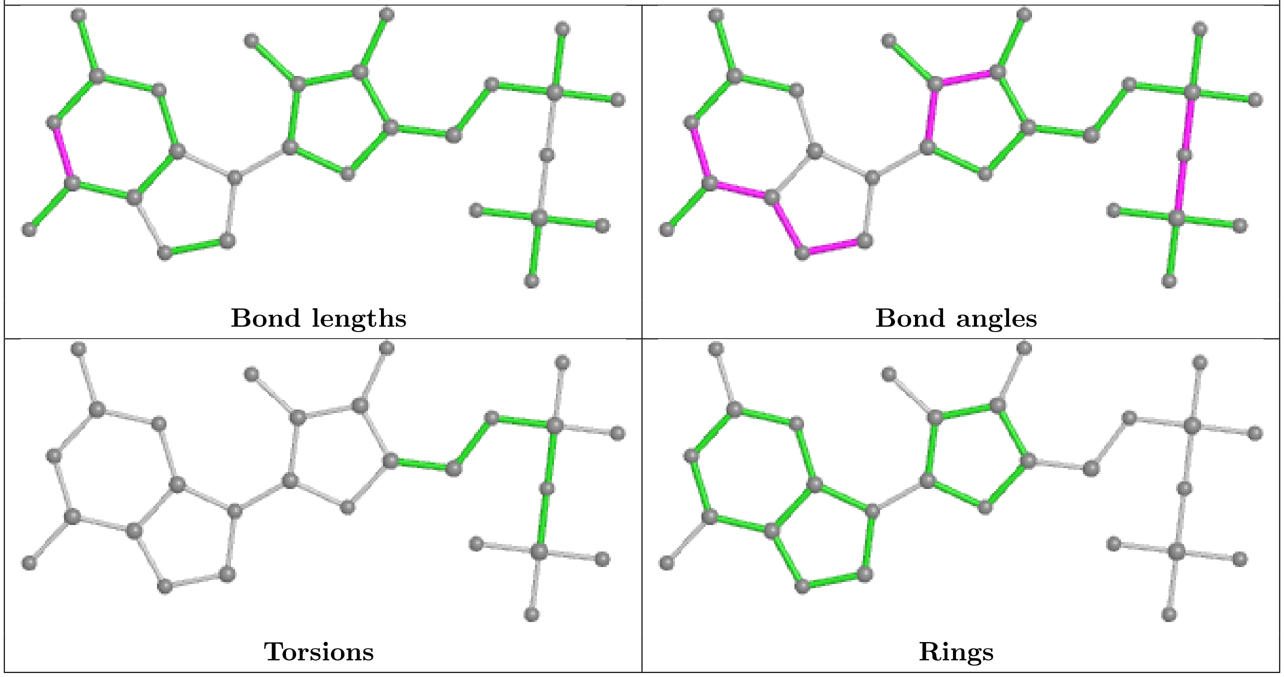
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP DB 502



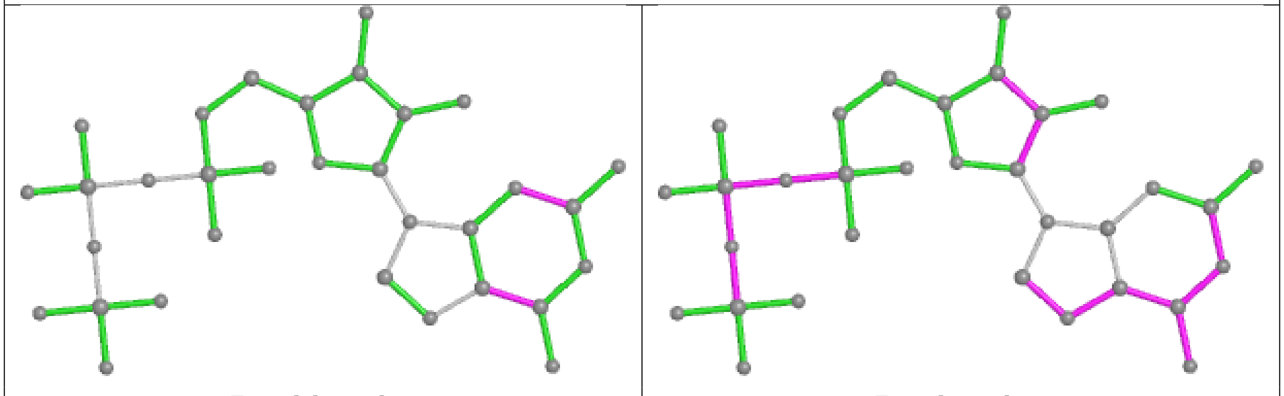
Bond lengths

Bond angles

Torsions

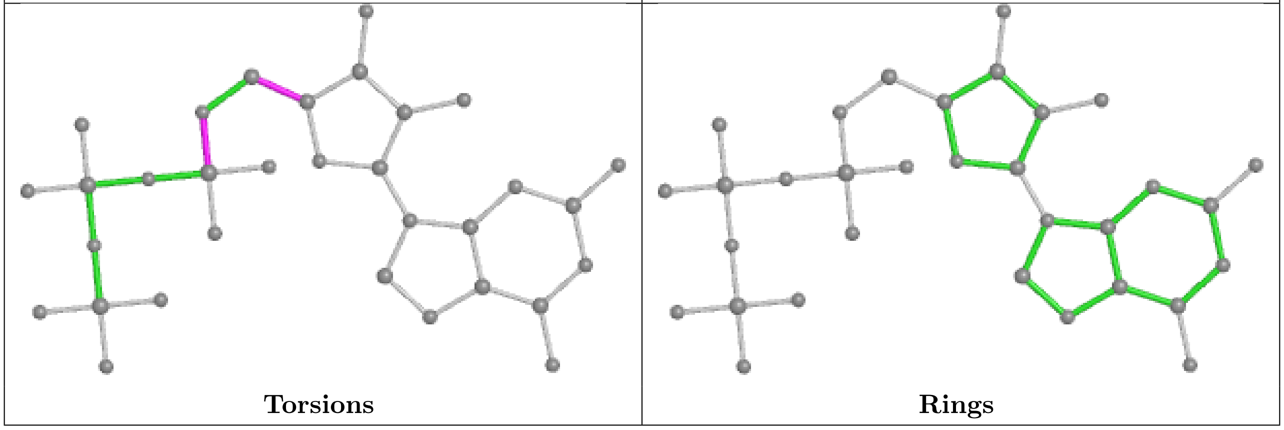
Rings

Ligand GTP CE 501



Bond lengths

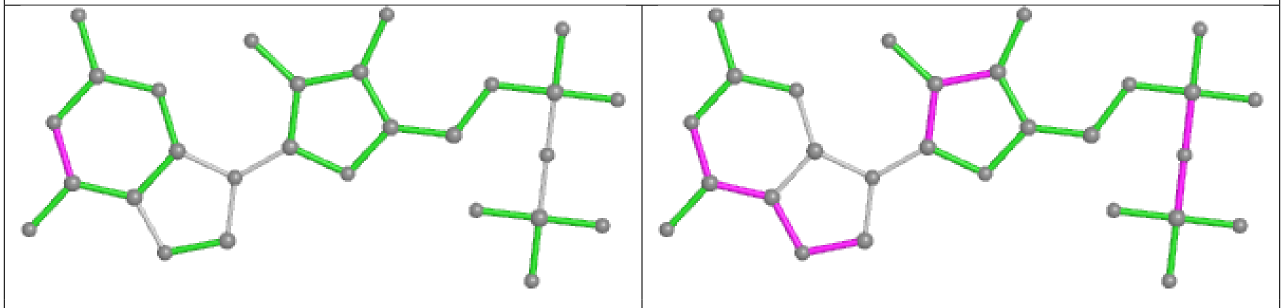
Bond angles



Torsions

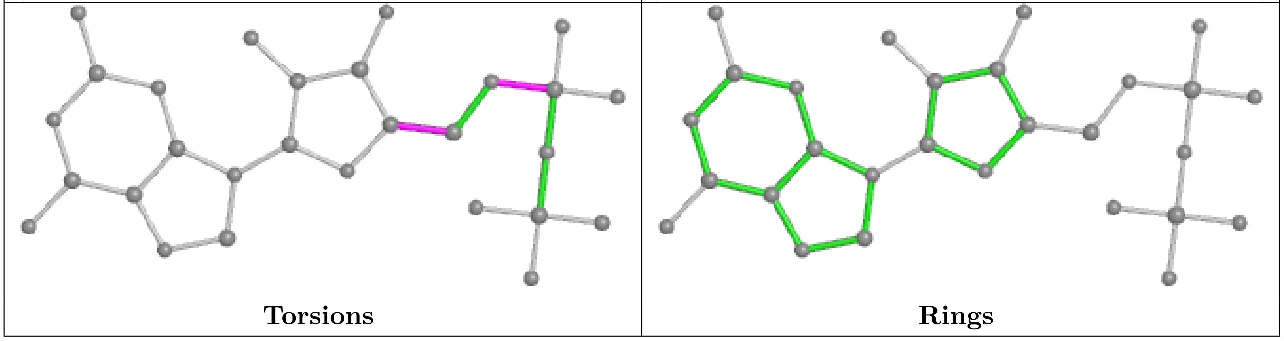
Rings

Ligand GDP LB 502



Bond lengths

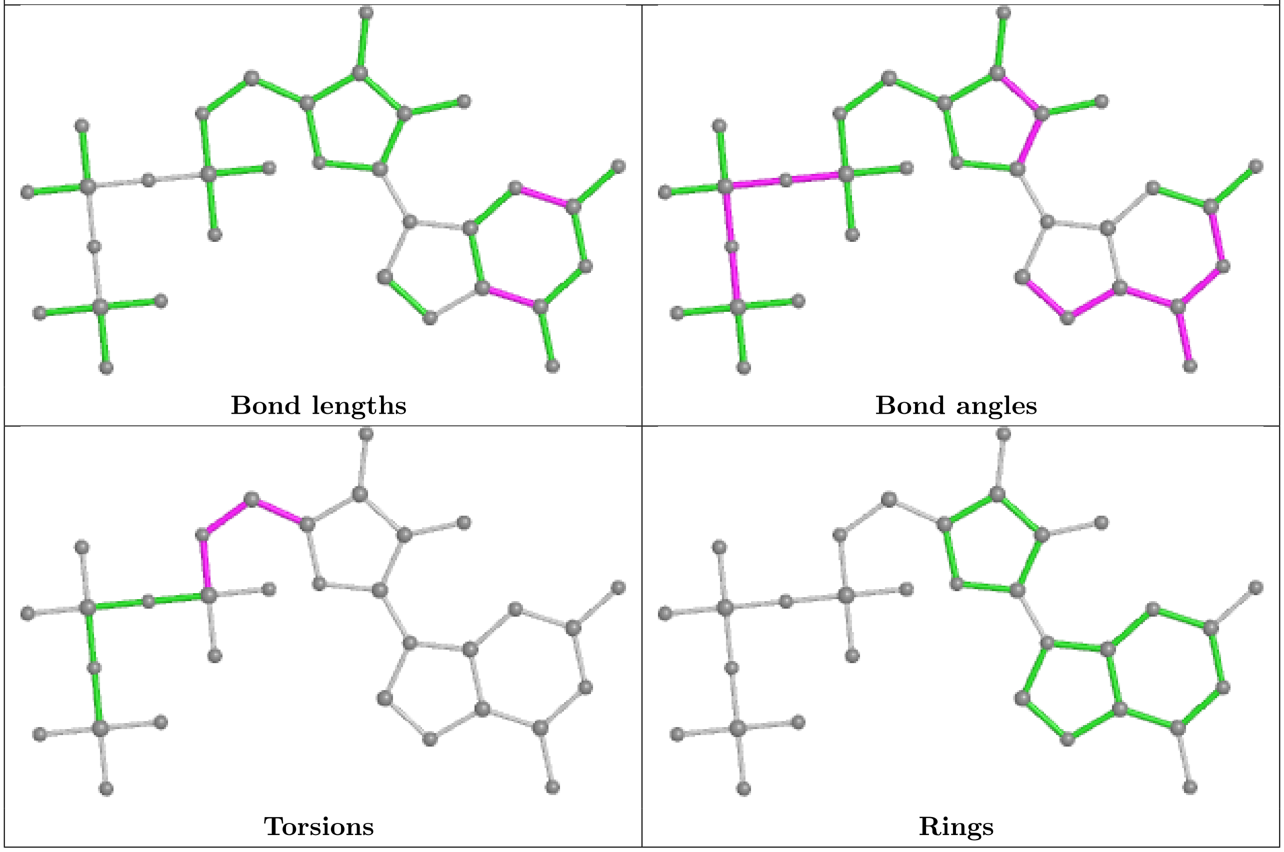
Bond angles



Torsions

Rings

Ligand GTP RI 501



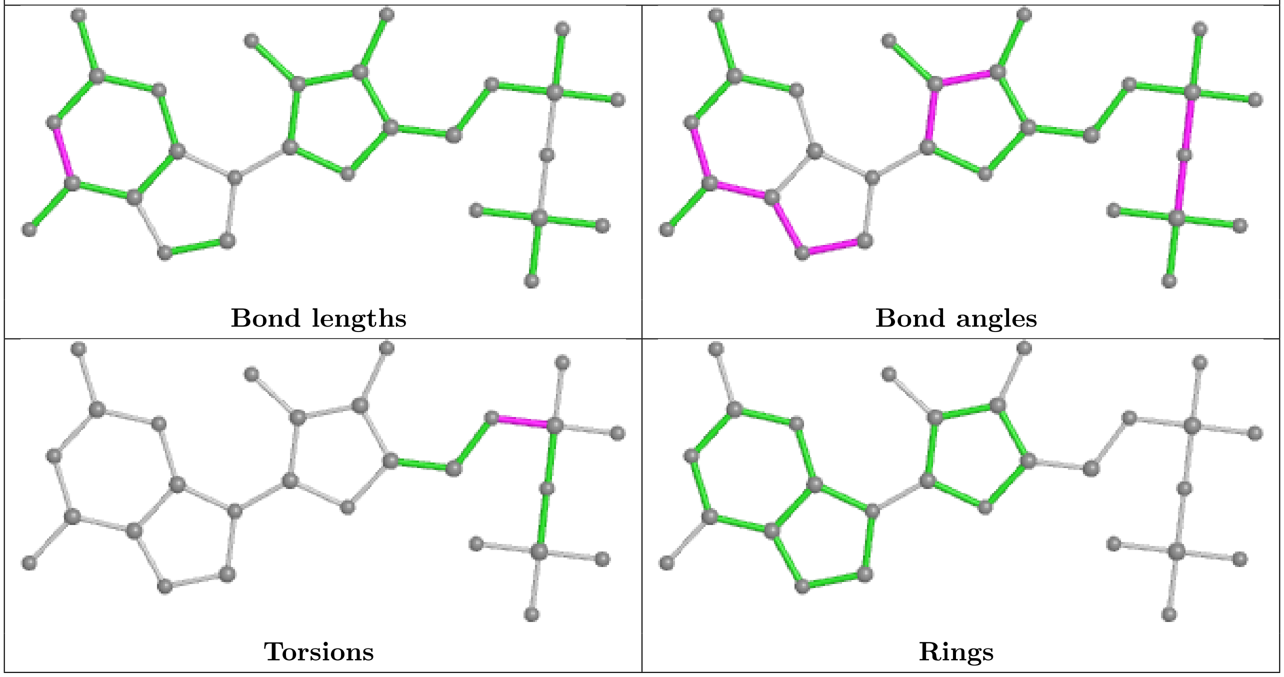
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP EN 502



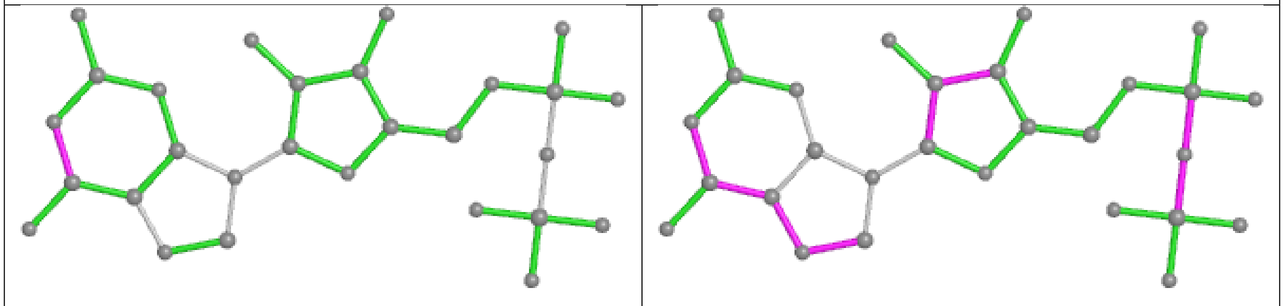
Bond lengths

Bond angles

Torsions

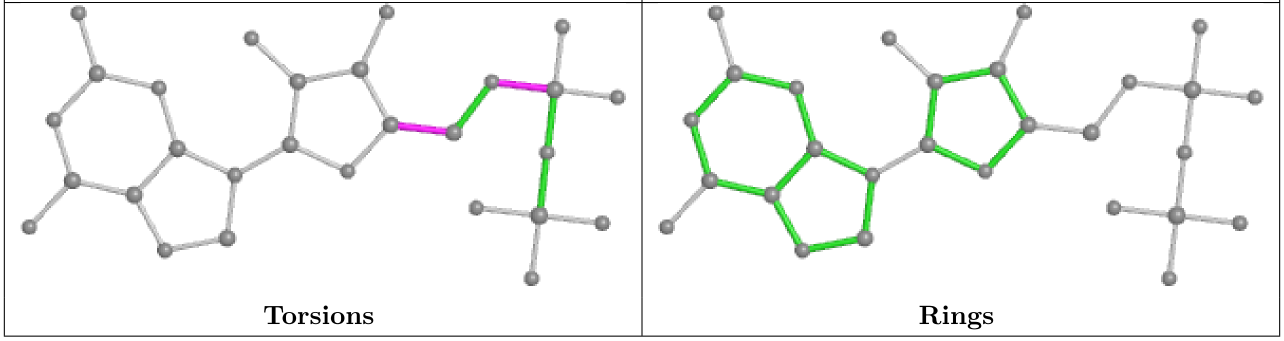
Rings

Ligand GDP AJ 502



Bond lengths

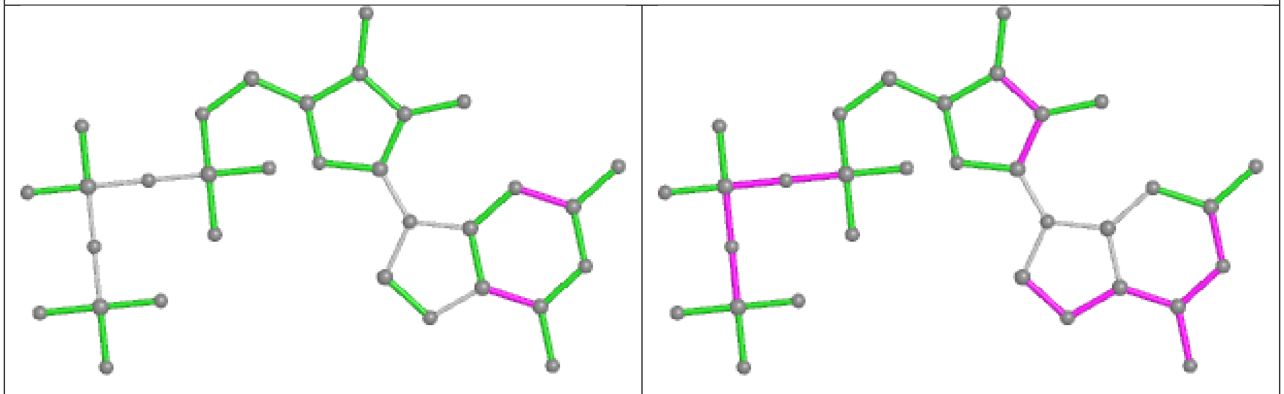
Bond angles



Torsions

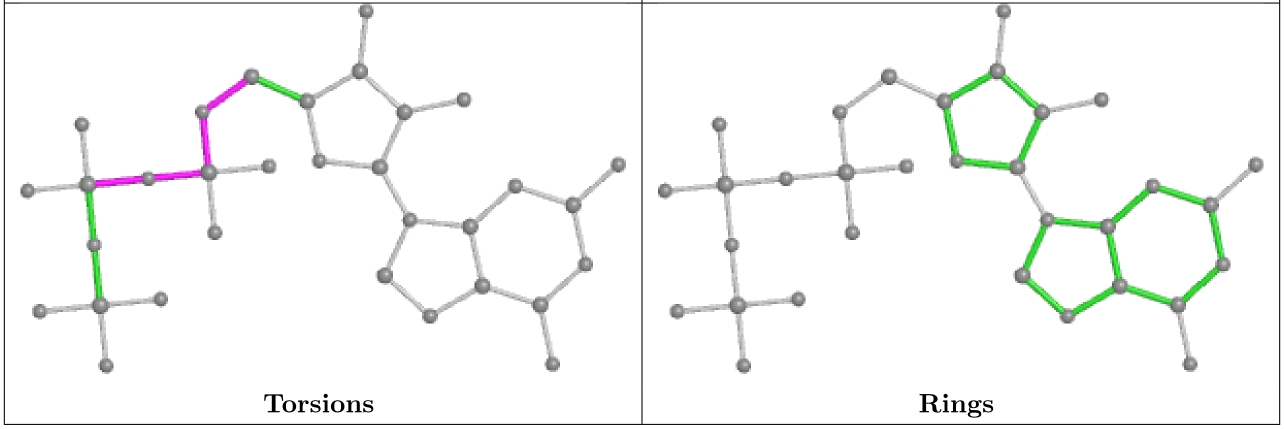
Rings

Ligand GTP RO 501



Bond lengths

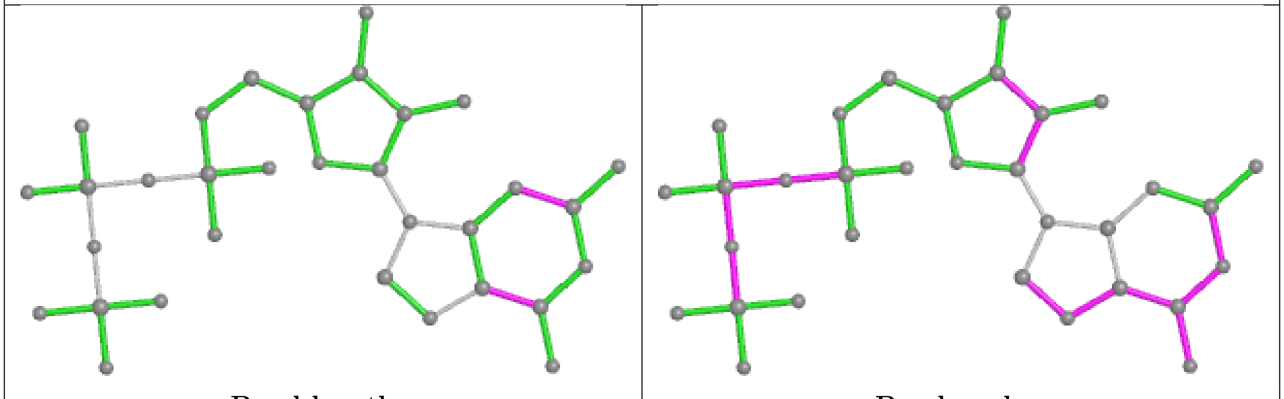
Bond angles



Torsions

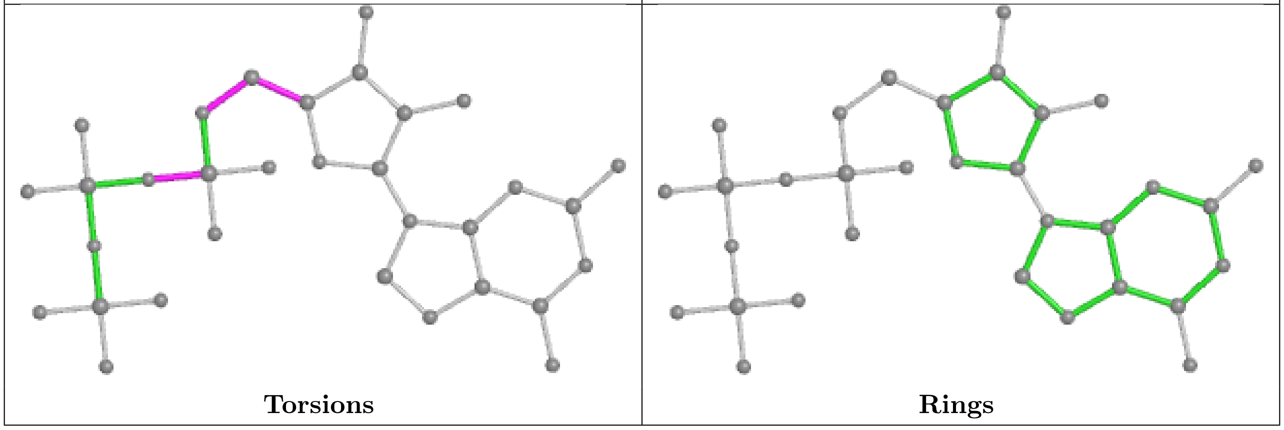
Rings

Ligand GTP IE 501



Bond lengths

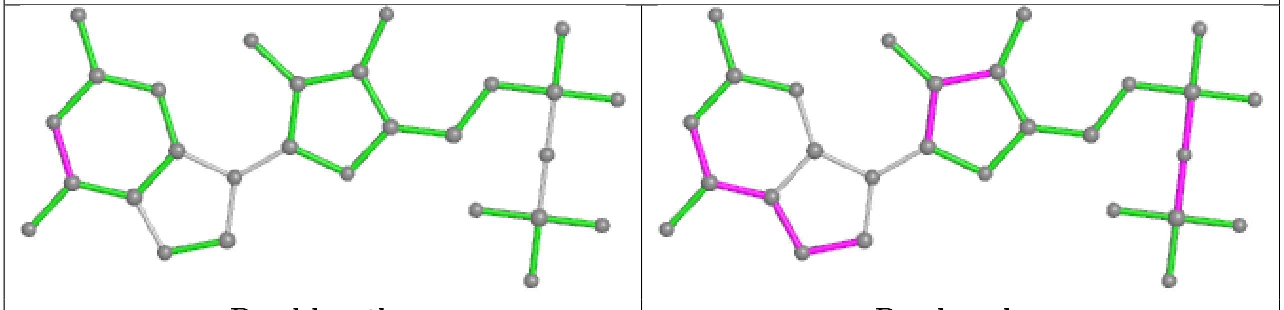
Bond angles



Torsions

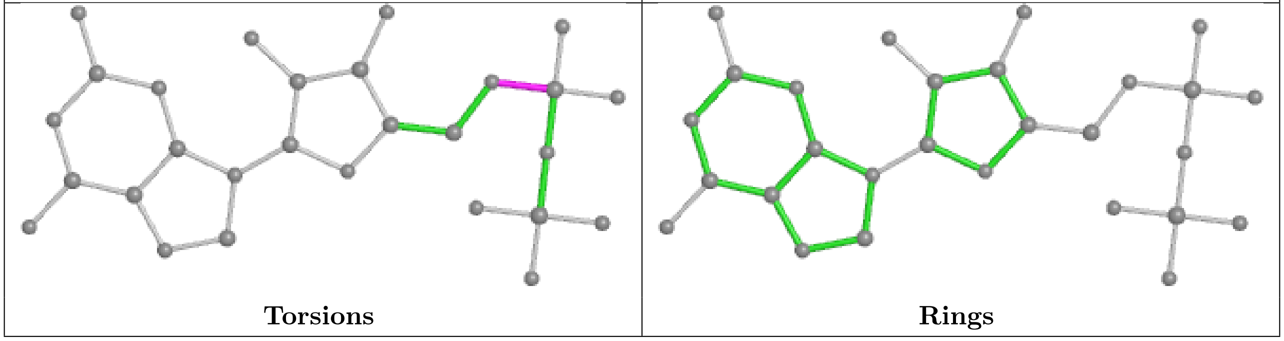
Rings

Ligand GDP NF 502



Bond lengths

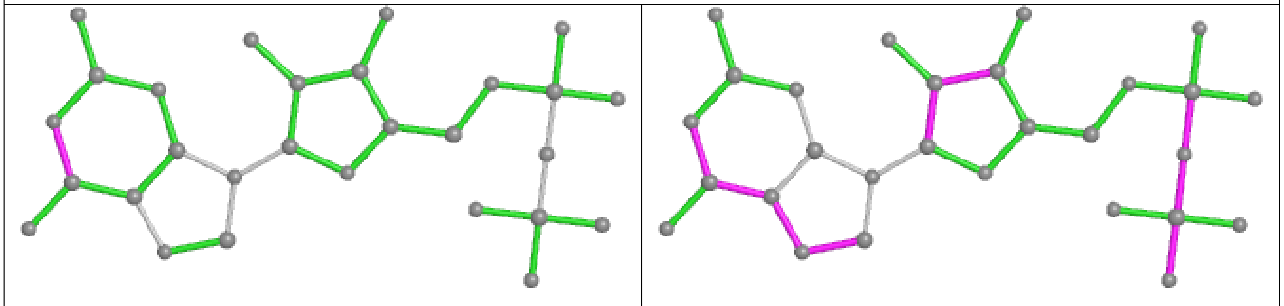
Bond angles



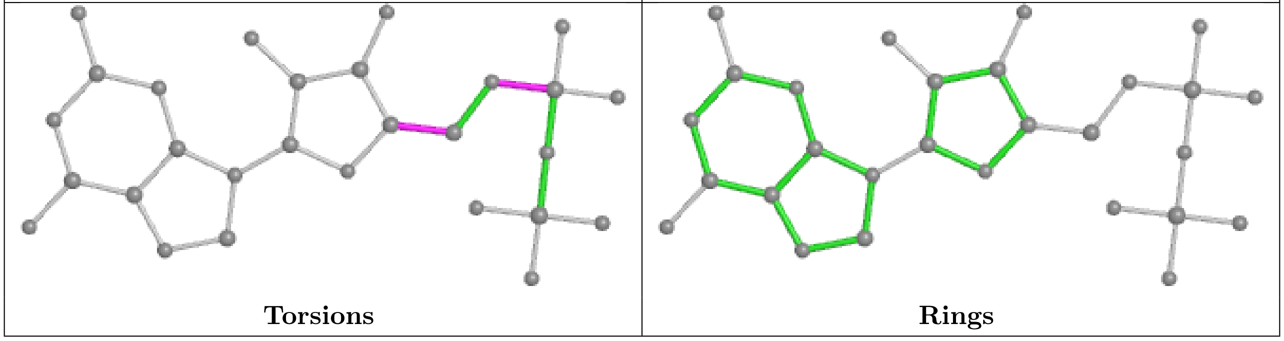
Torsions

Rings

Ligand GDP FH 502

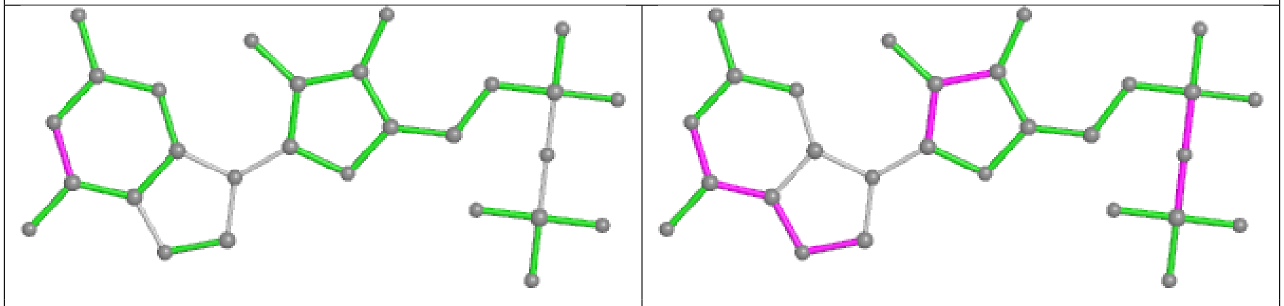


Bond lengths Bond angles

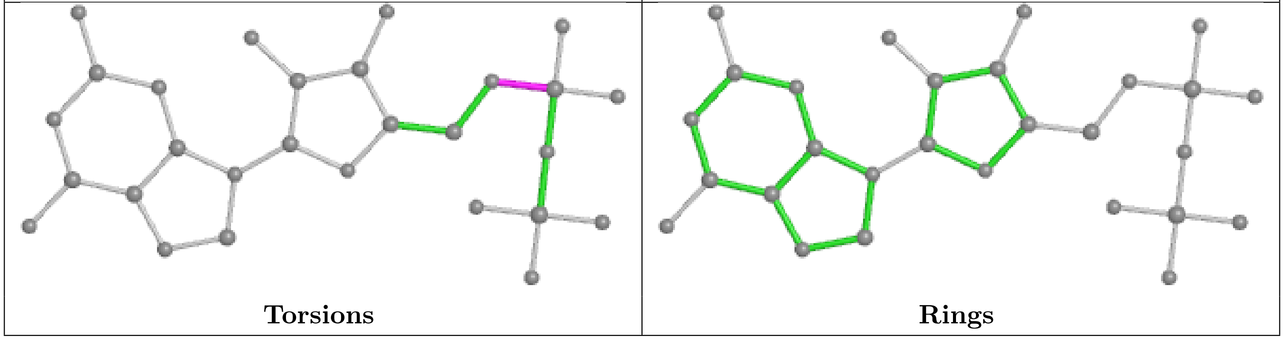


Torsions Rings

Ligand GDP IL 502

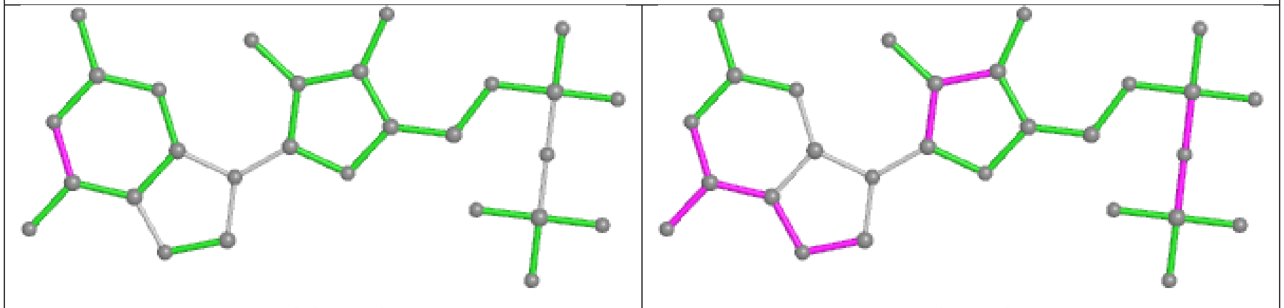


Bond lengths Bond angles



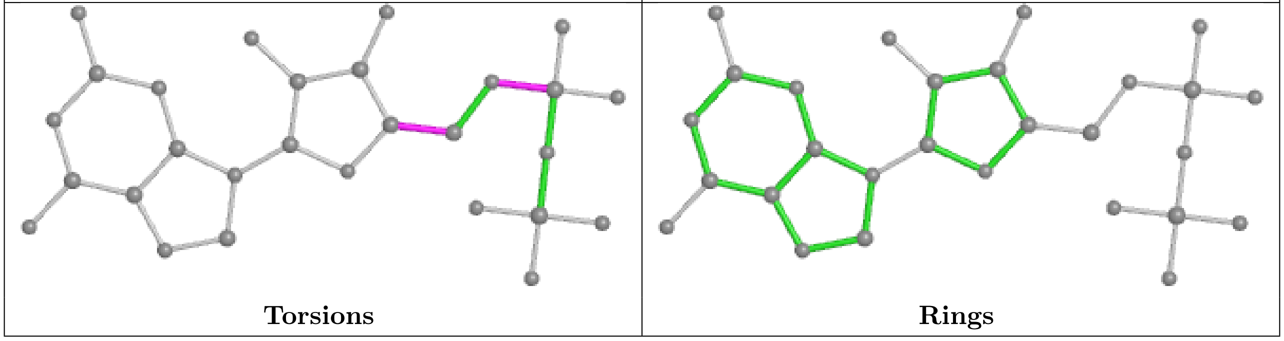
Torsions Rings

Ligand GDP SN 502



Bond lengths

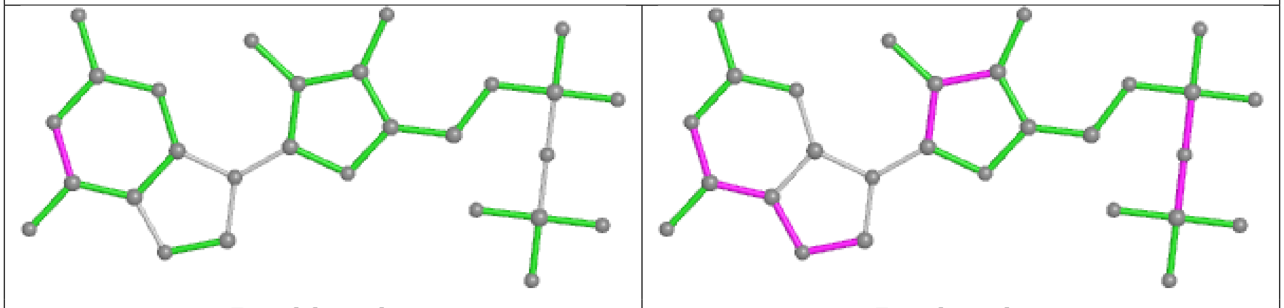
Bond angles



Torsions

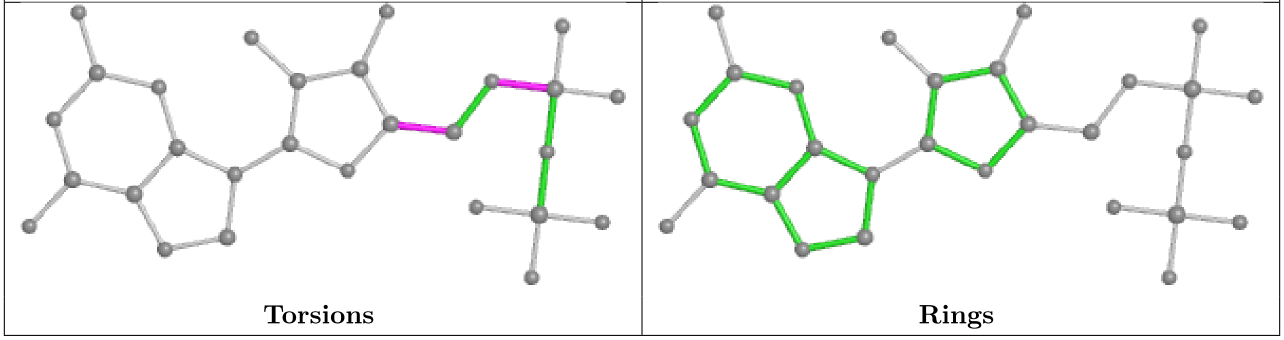
Rings

Ligand GDP GD 502



Bond lengths

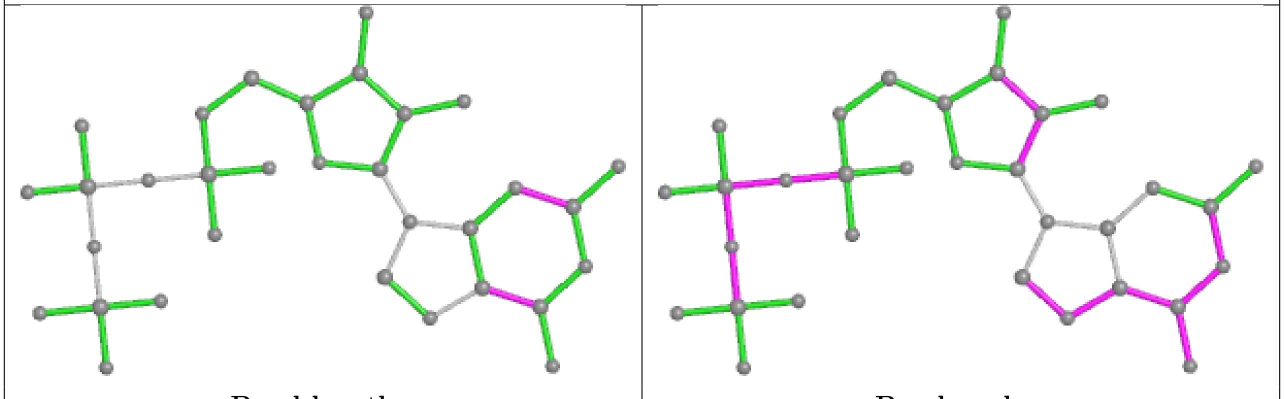
Bond angles



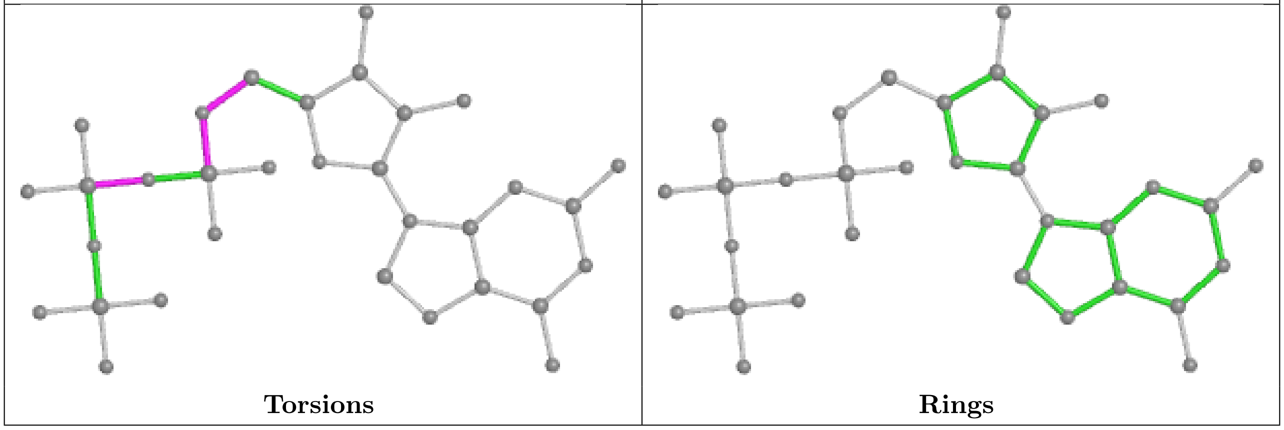
Torsions

Rings

Ligand GTP SM 501

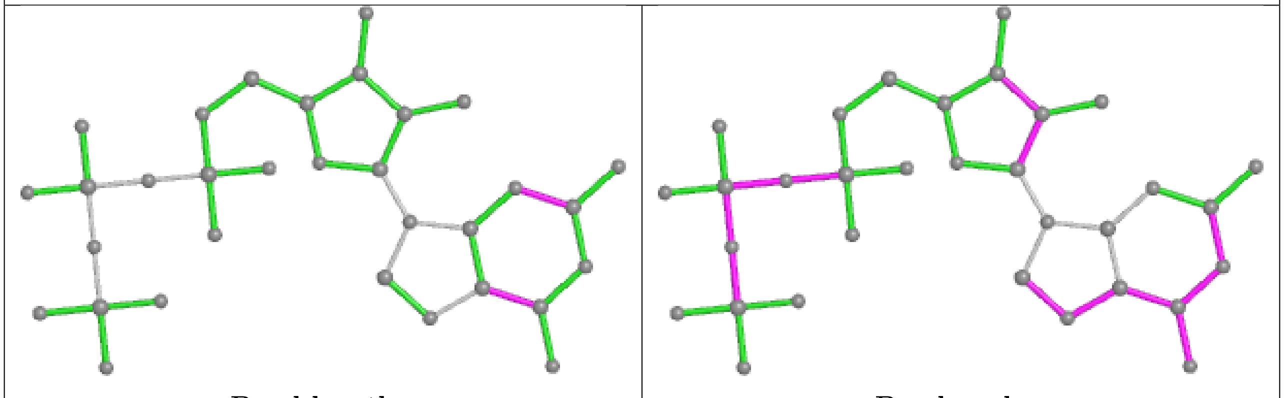


Bond lengths **Bond angles**

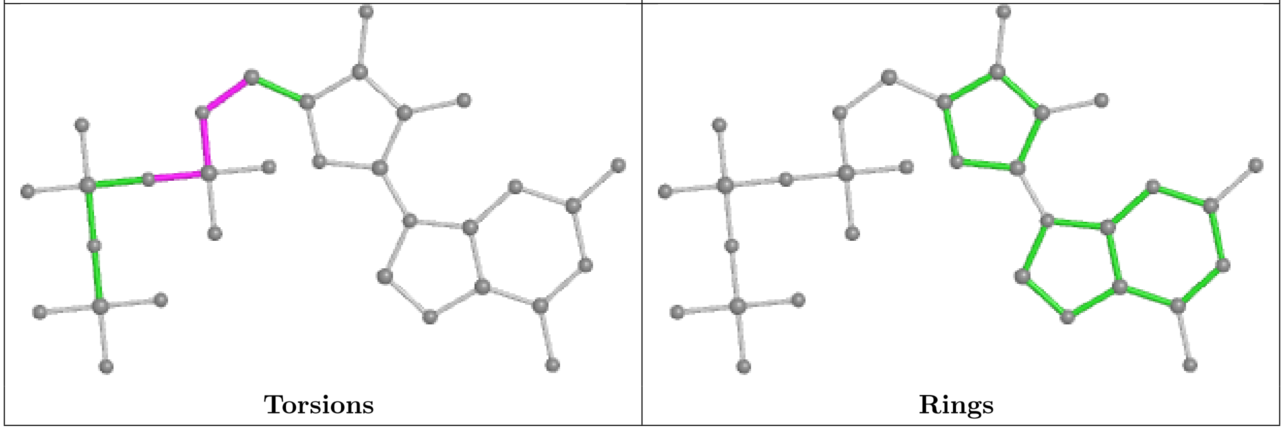


Torsions **Rings**

Ligand GTP GG 501

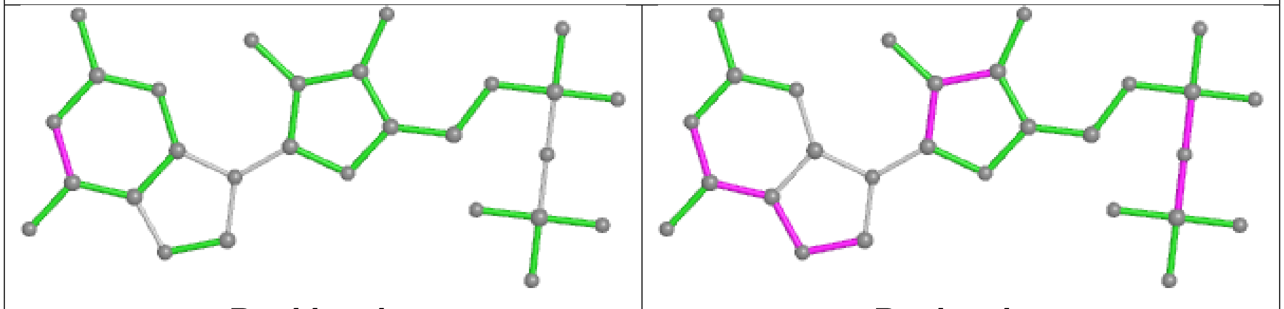


Bond lengths **Bond angles**

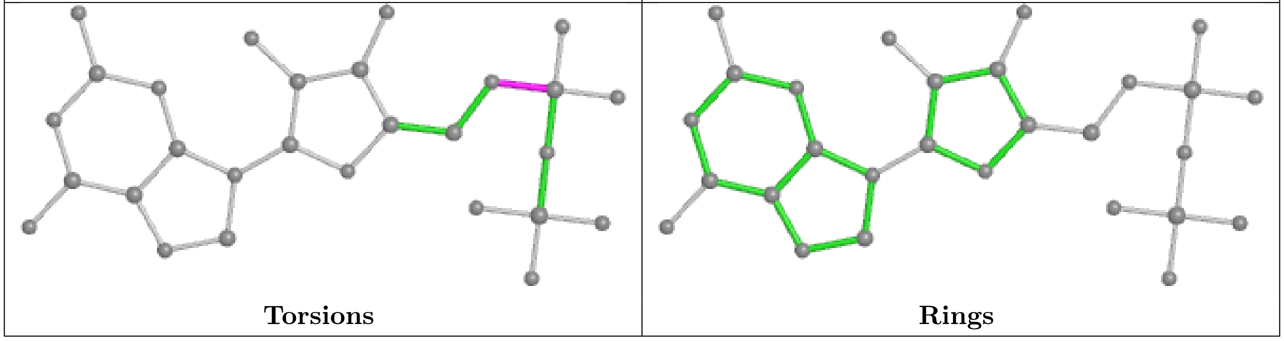


Torsions **Rings**

Ligand GDP MB 502

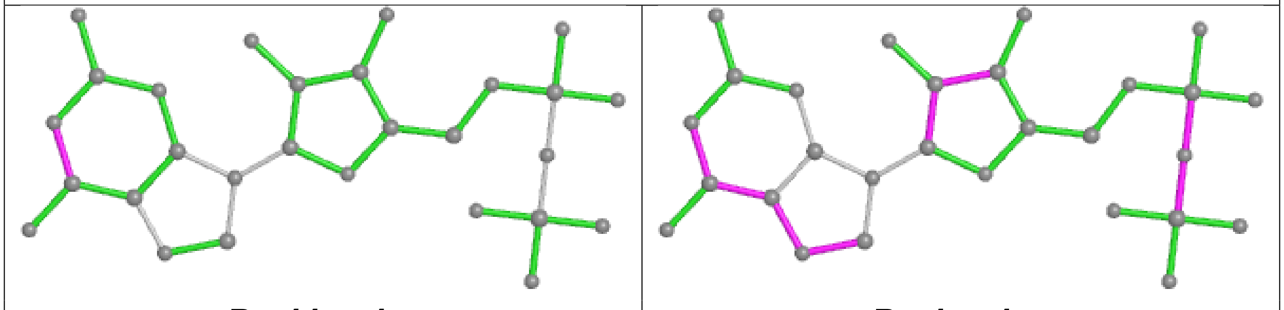


Bond lengths Bond angles

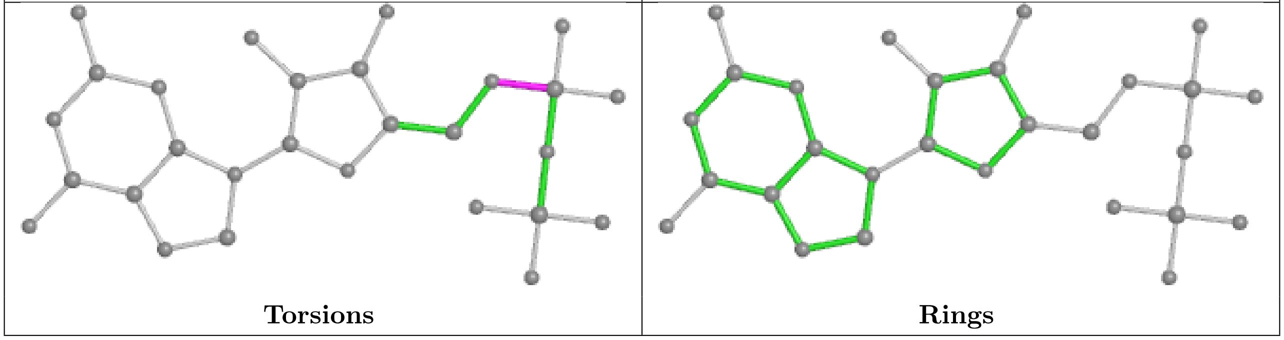


Torsions Rings

Ligand GDP OD 502

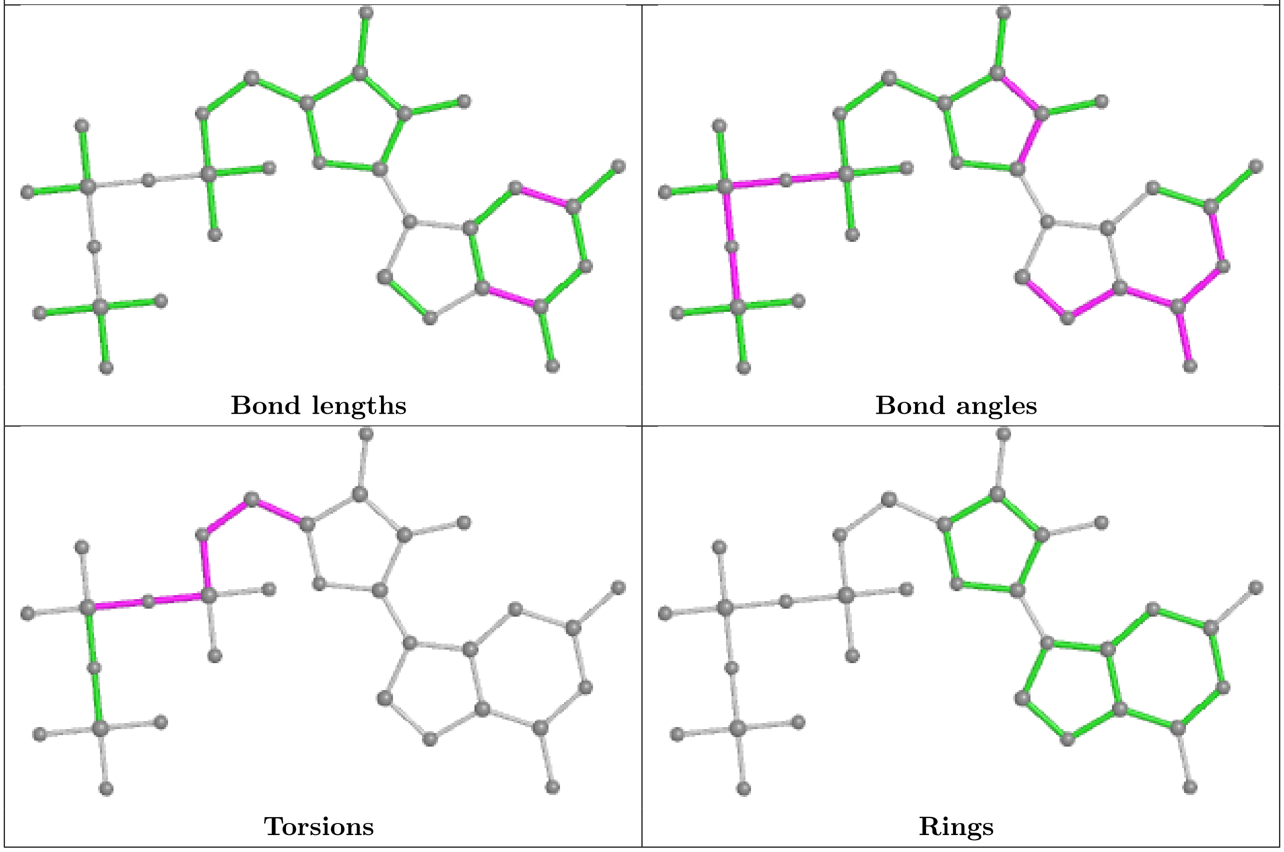


Bond lengths Bond angles



Torsions Rings

Ligand GTP LE 501



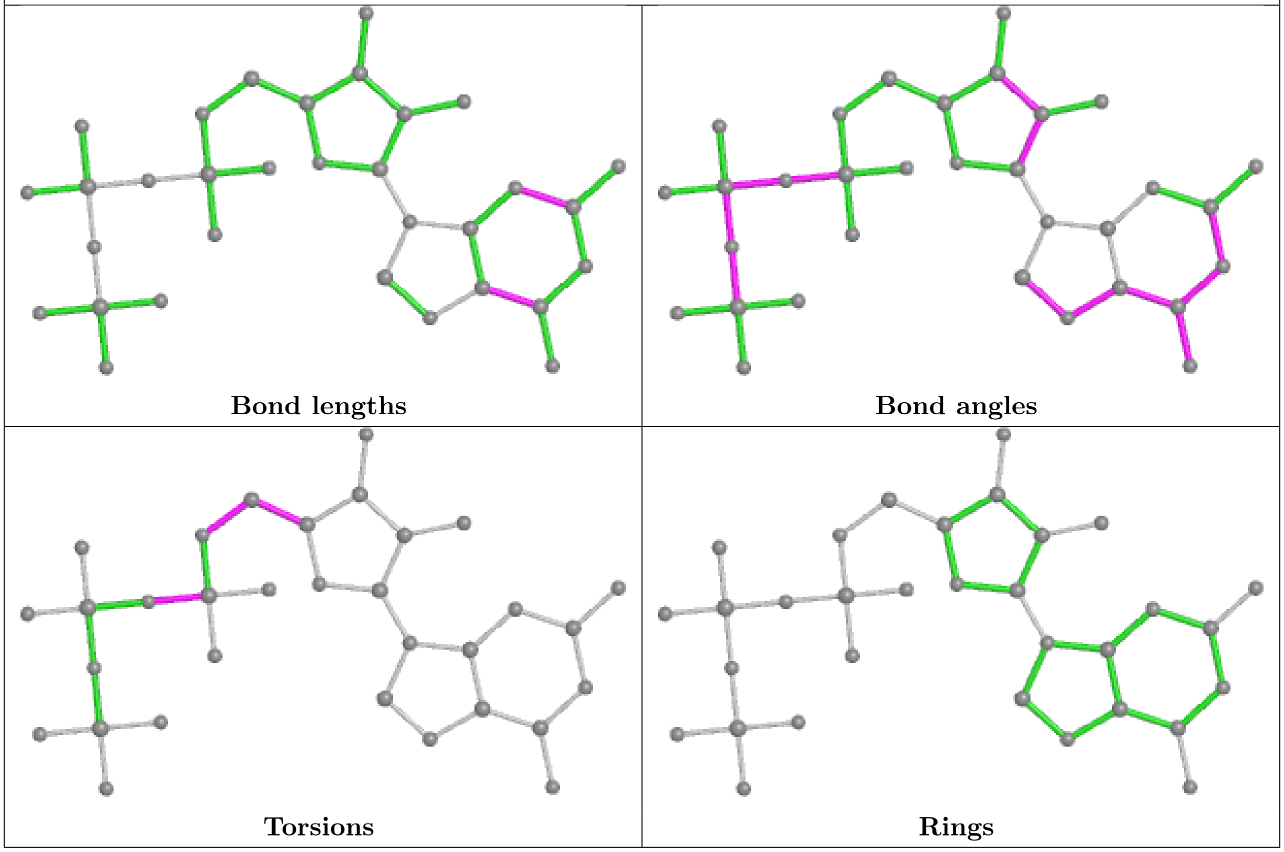
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP BI 501



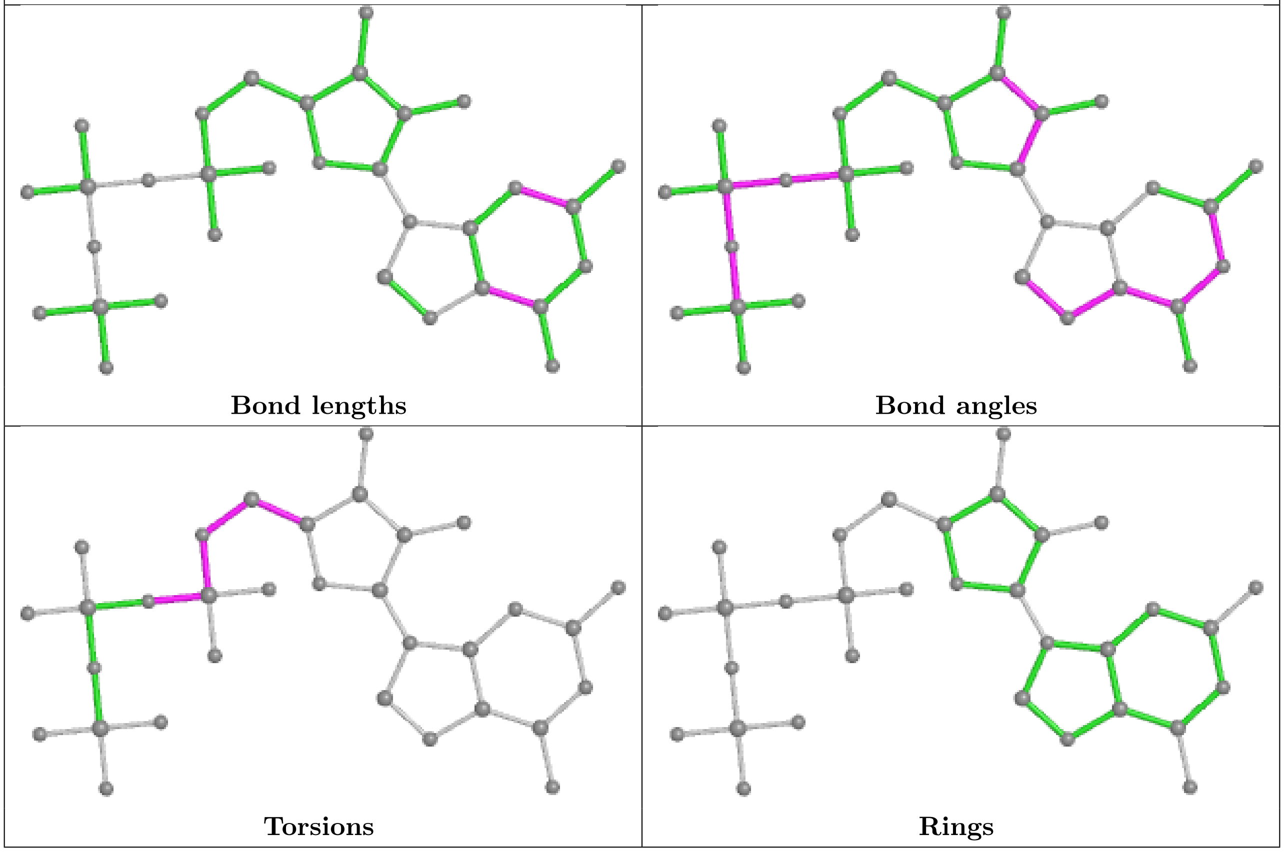
Bond lengths

Bond angles

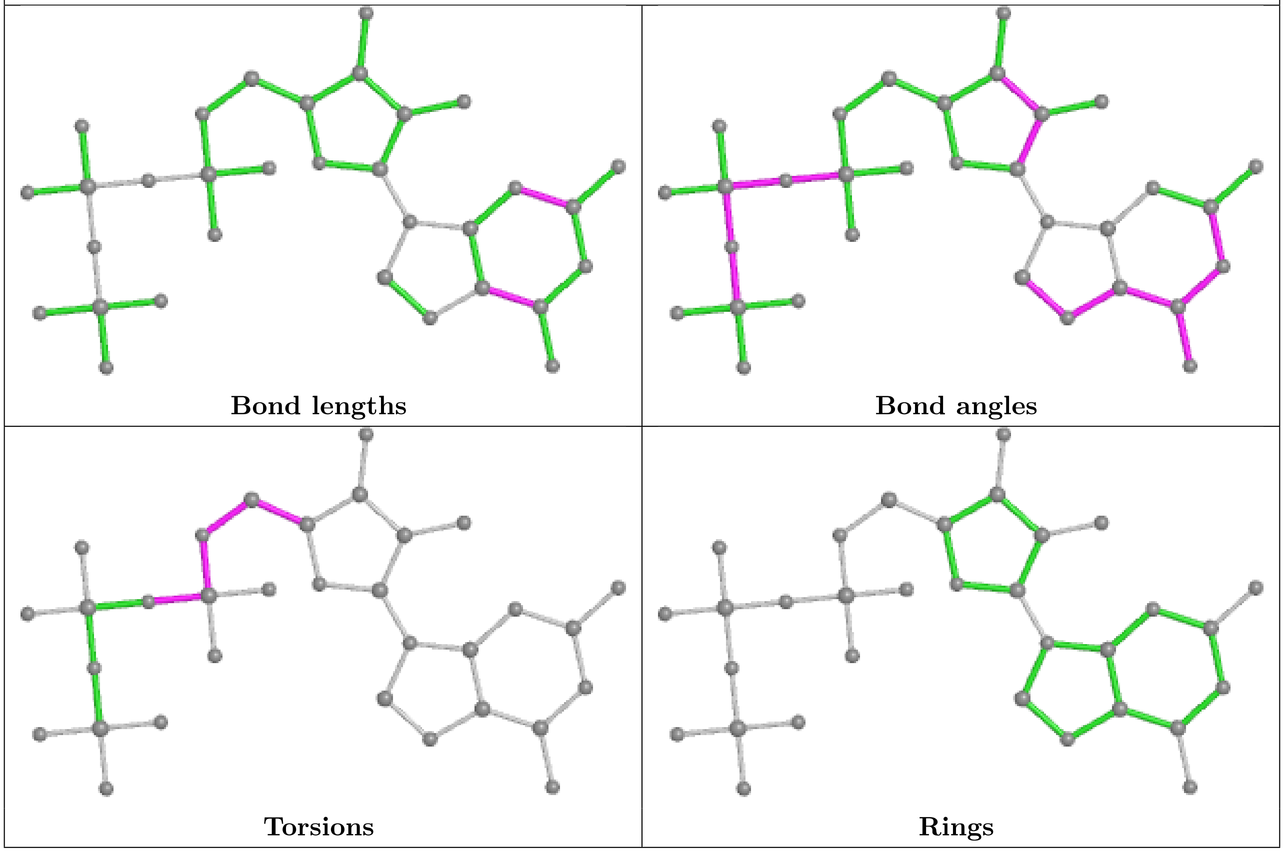
Torsions

Rings

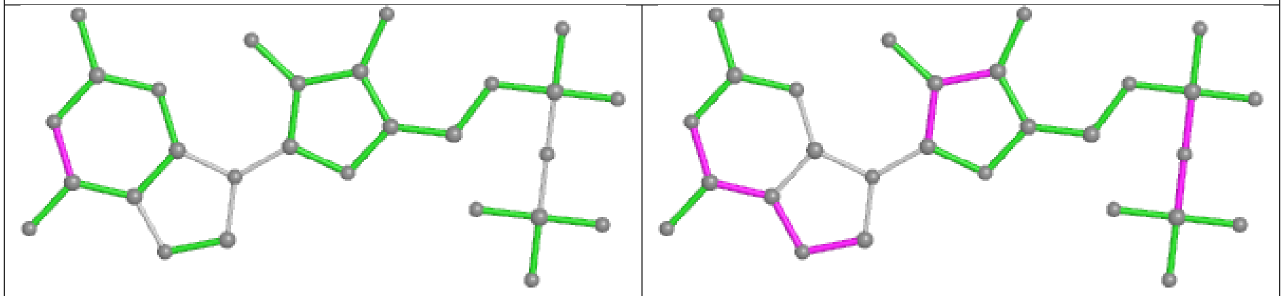
Ligand GTP DG 501


Bond lengths
Bond angles
Torsions
Rings

Ligand GTP NM 501

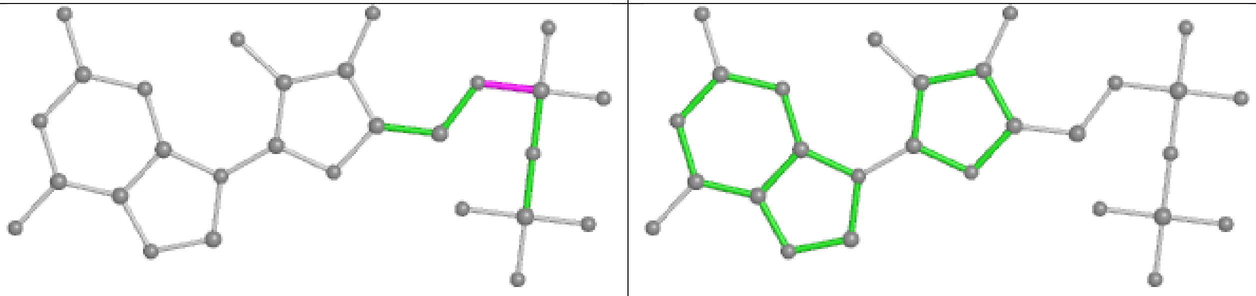

Bond lengths
Bond angles
Torsions
Rings

Ligand GDP HD 502



Bond lengths

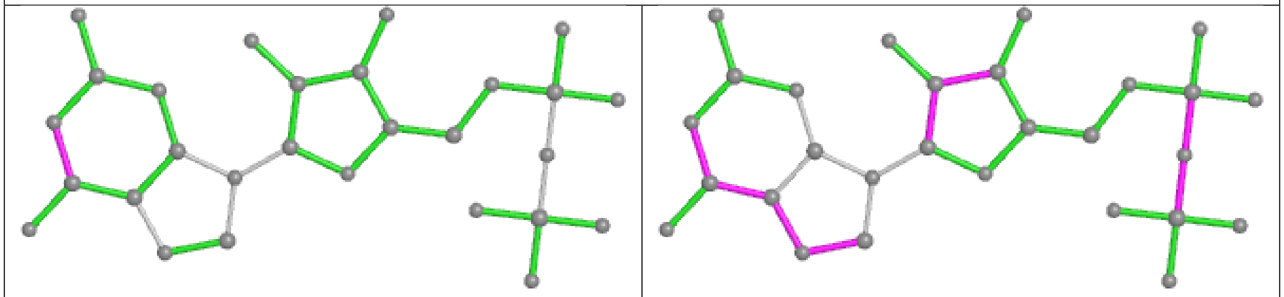
Bond angles



Torsions

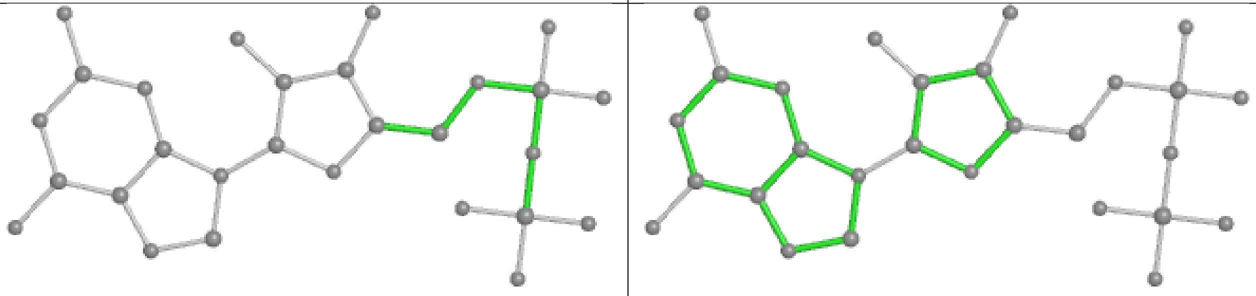
Rings

Ligand GDP KH 502



Bond lengths

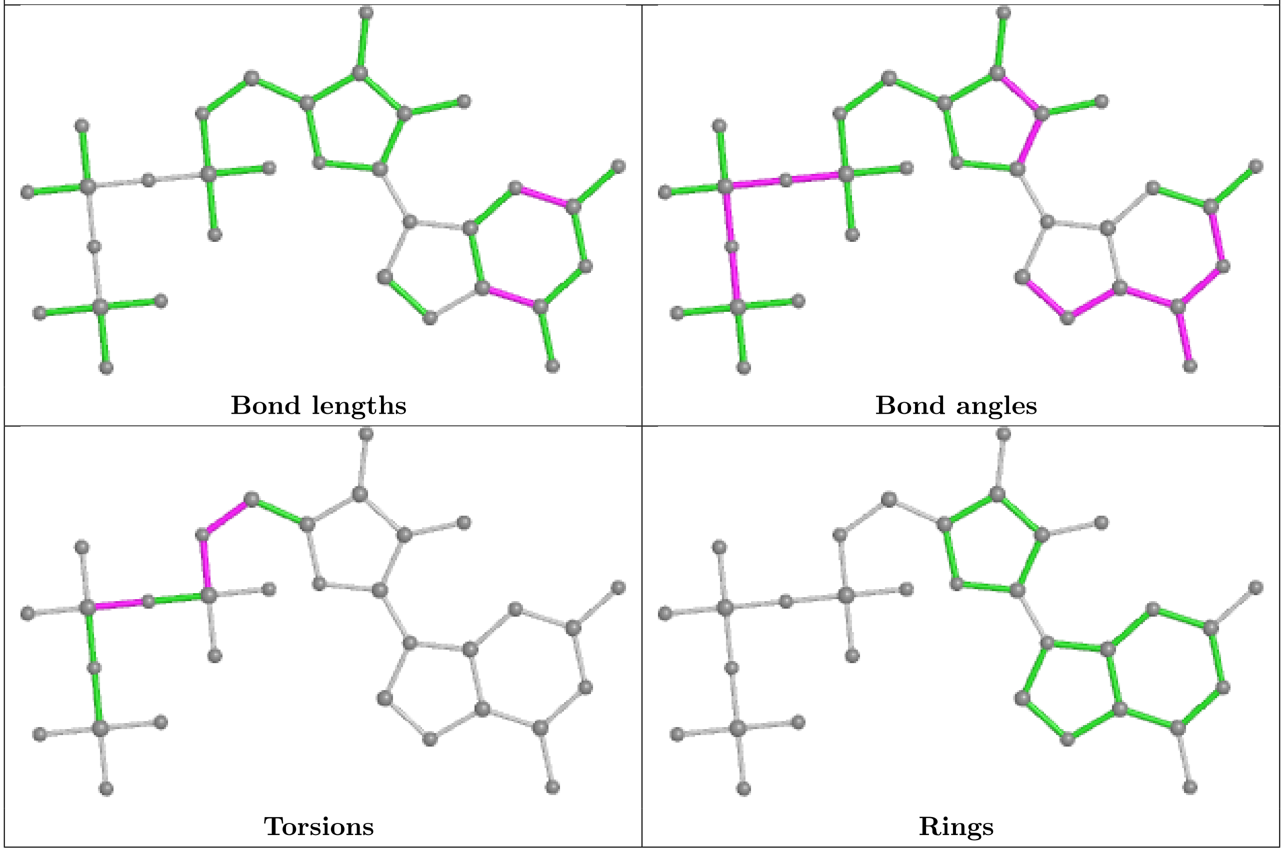
Bond angles



Torsions

Rings

Ligand GTP SE 501



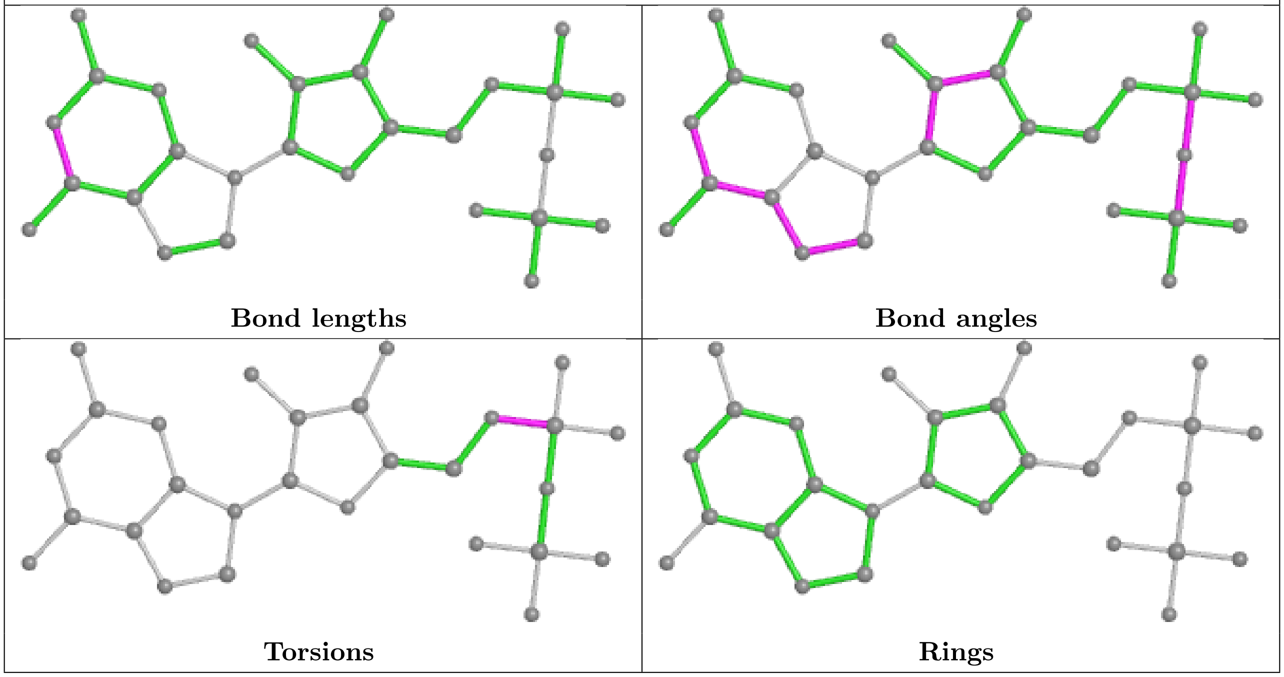
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP MF 502



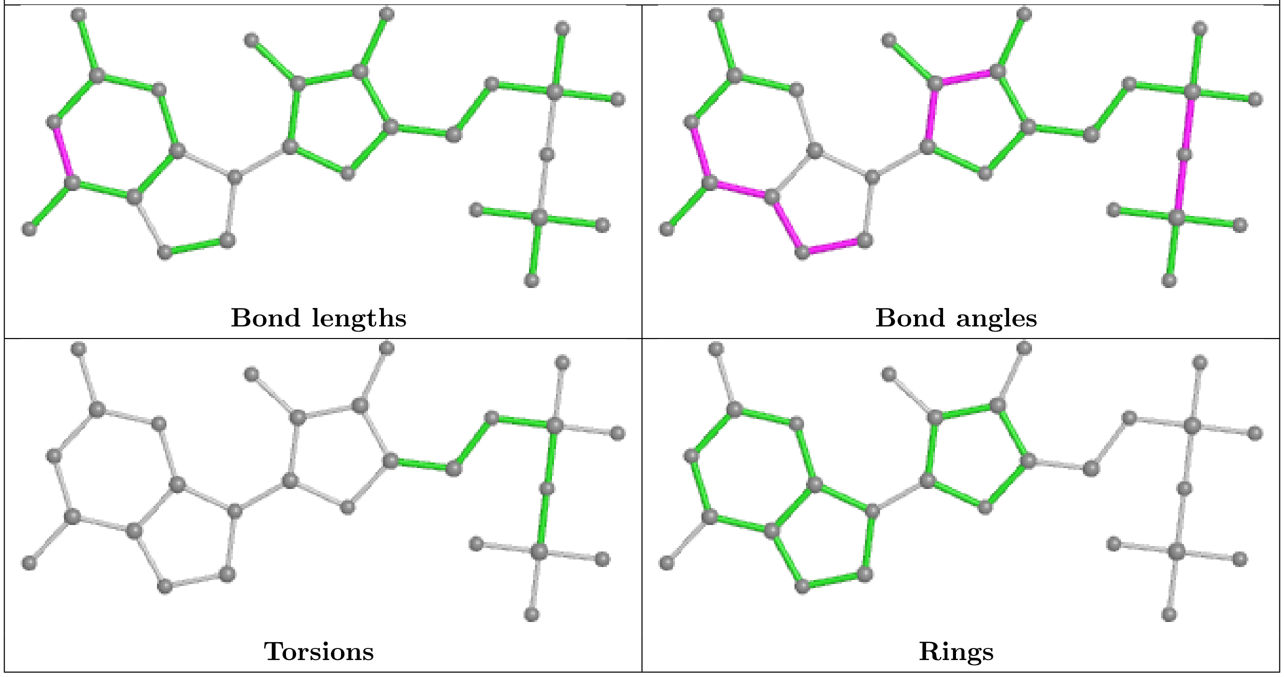
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP EB 502



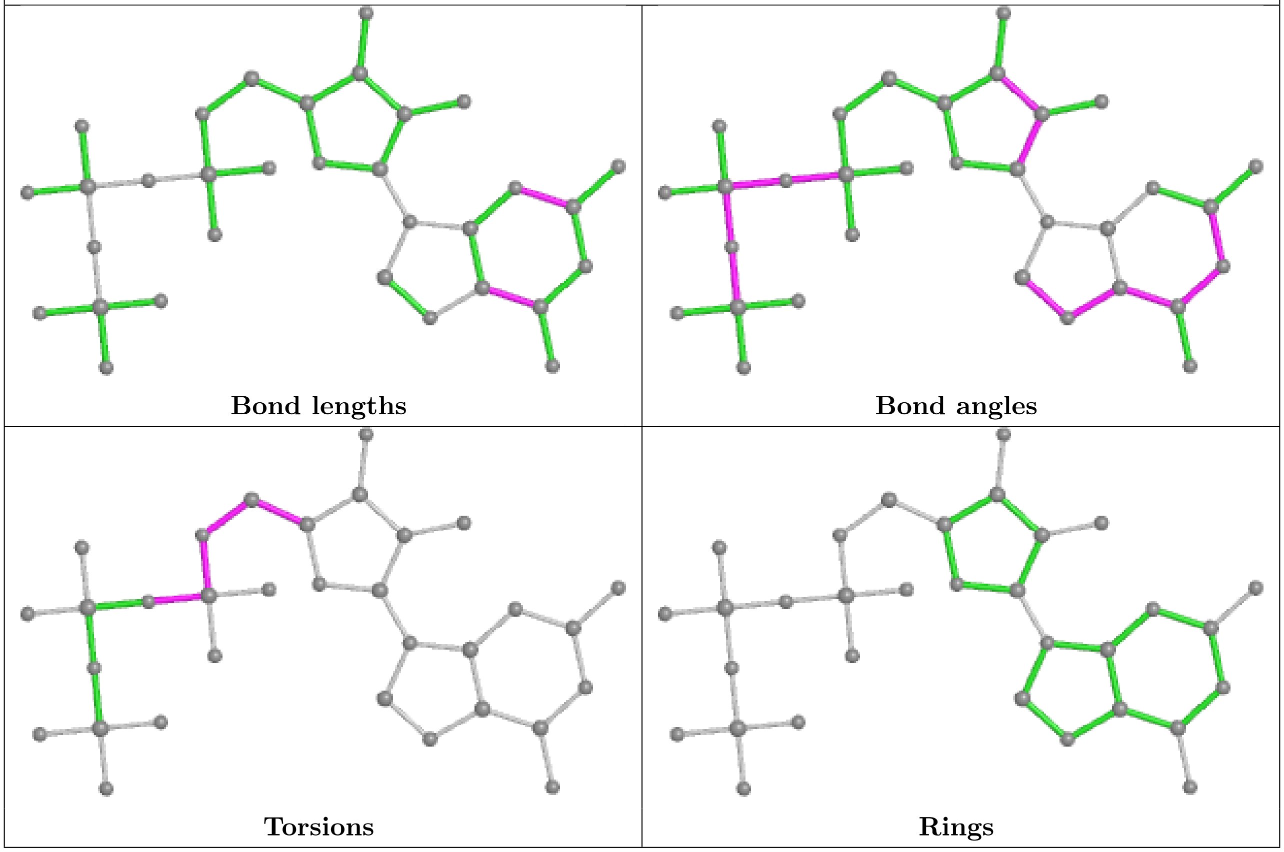
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP IM 501



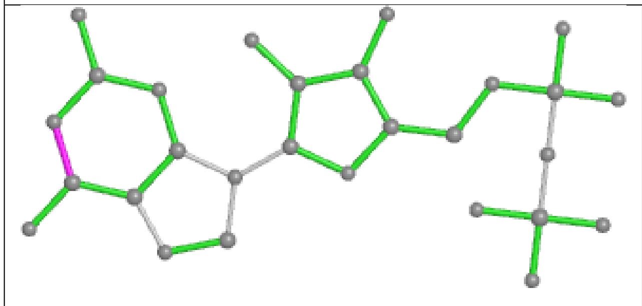
Bond lengths

Bond angles

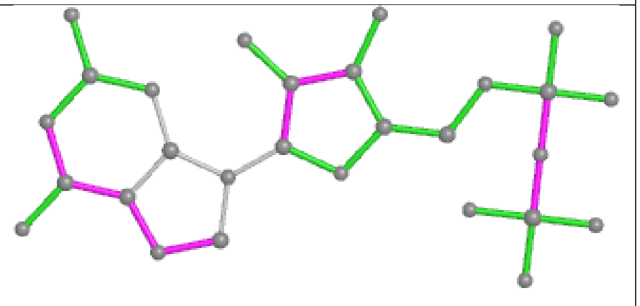
Torsions

Rings

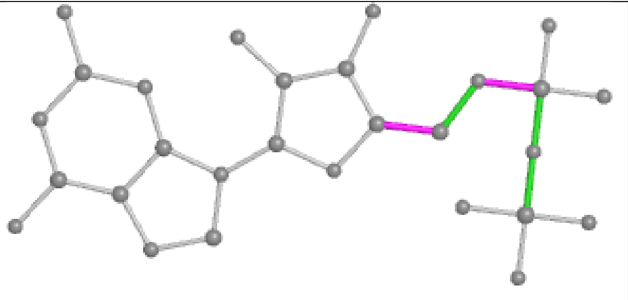
Ligand GDP FF 502



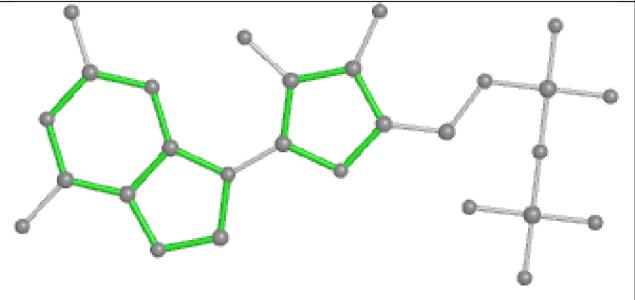
Bond lengths



Bond angles

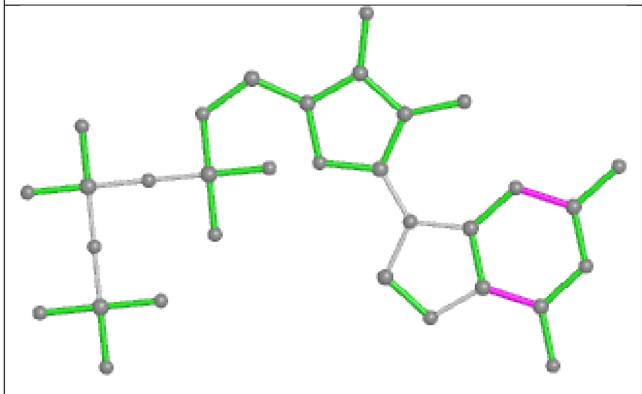


Torsions

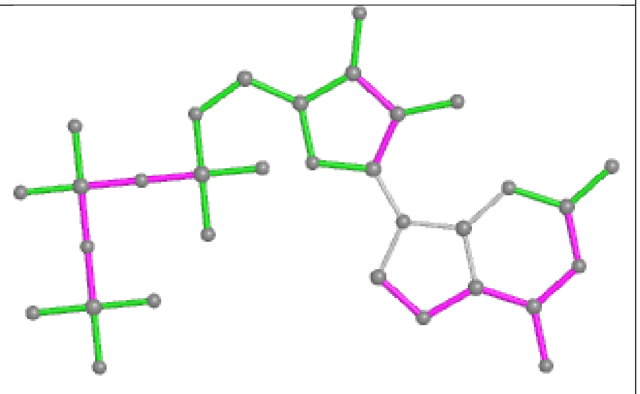


Rings

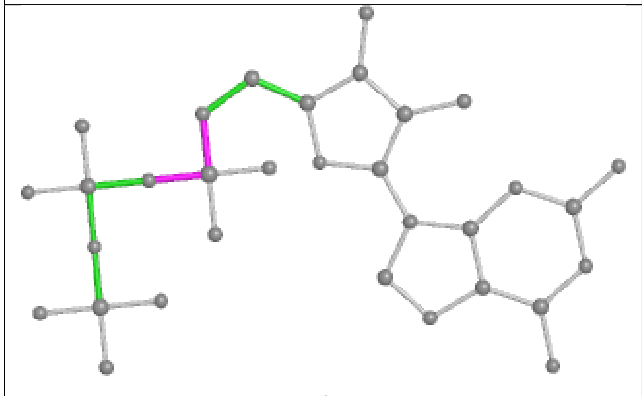
Ligand GTP JM 501



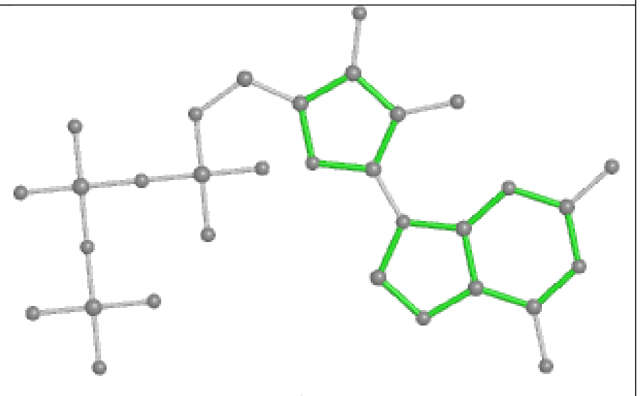
Bond lengths



Bond angles

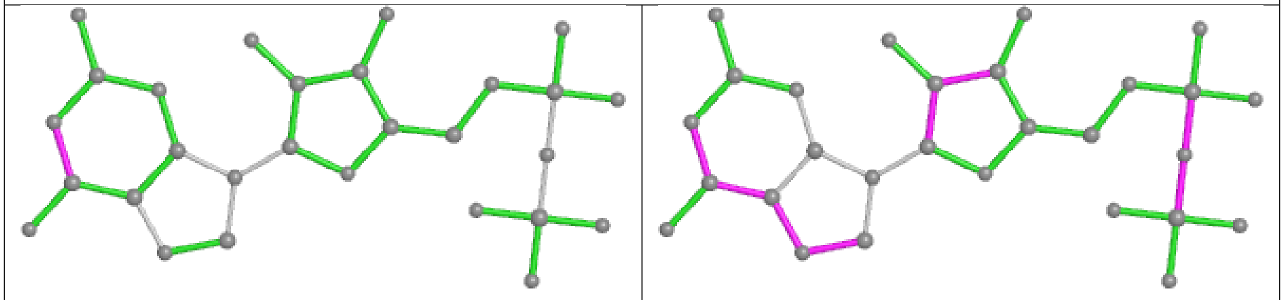


Torsions

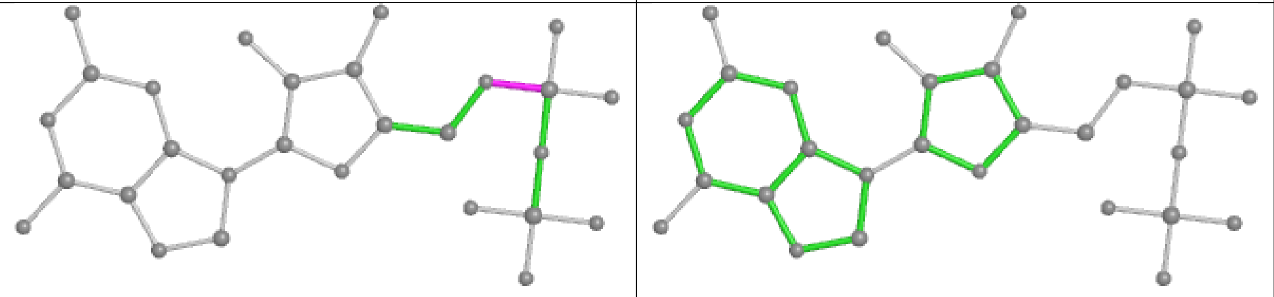


Rings

Ligand GDP IN 502

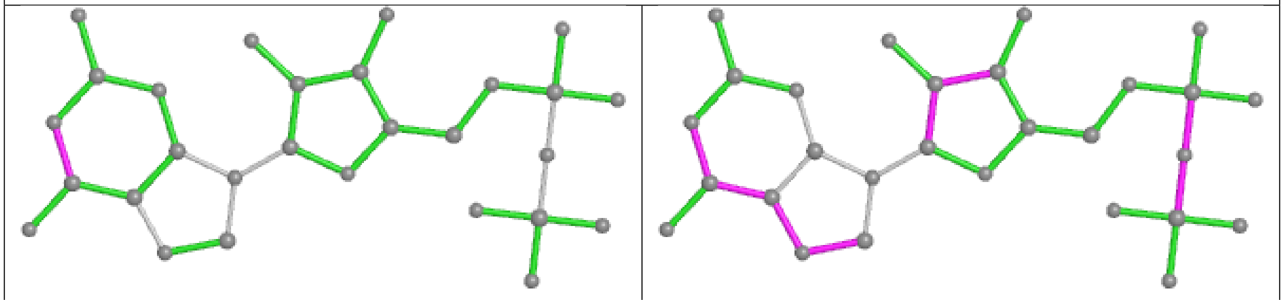

Bond lengths

Bond angles

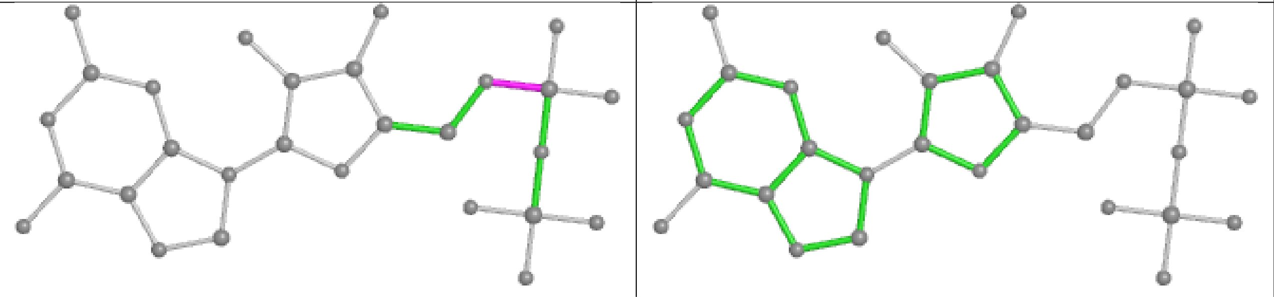

Torsions

Rings

Ligand GDP GH 502

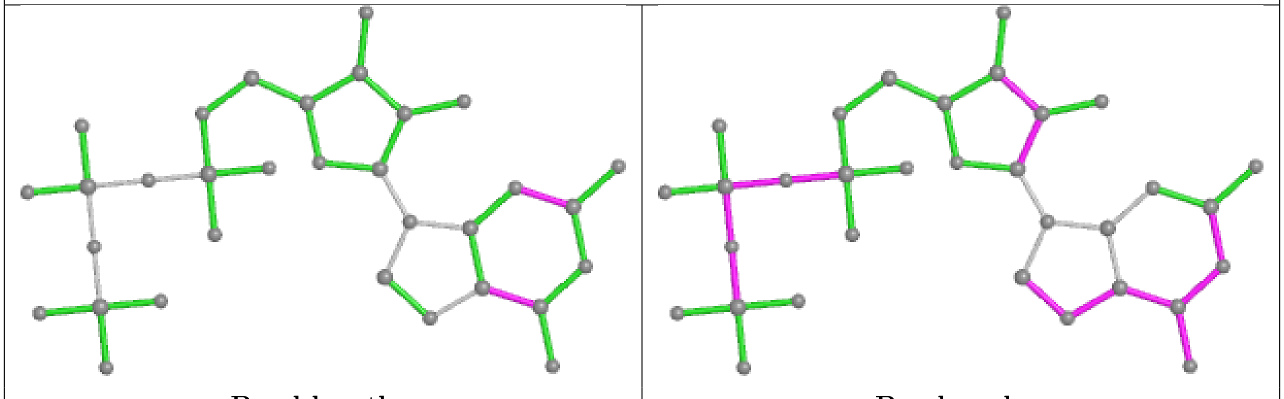

Bond lengths

Bond angles


Torsions

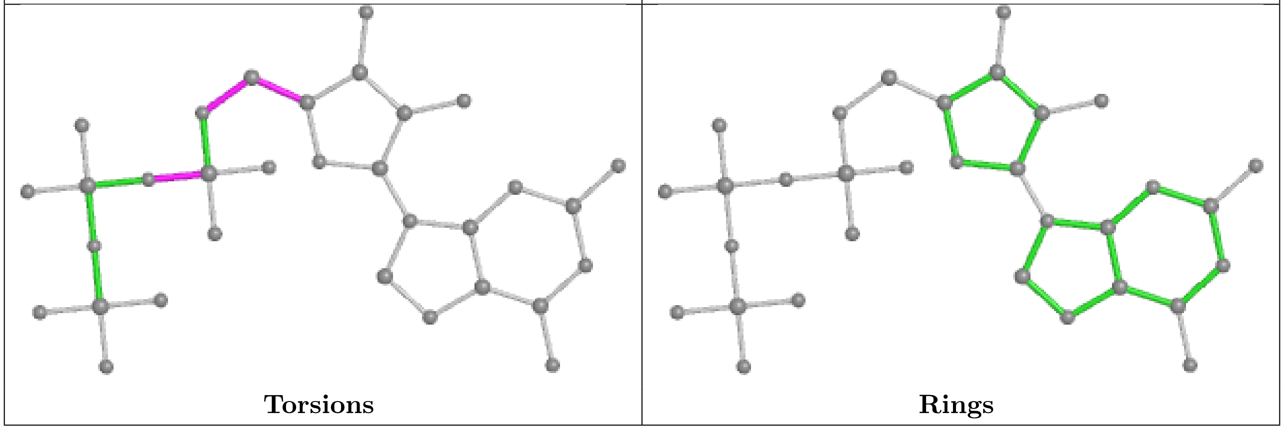
Rings

Ligand GTP BM 501



Bond lengths

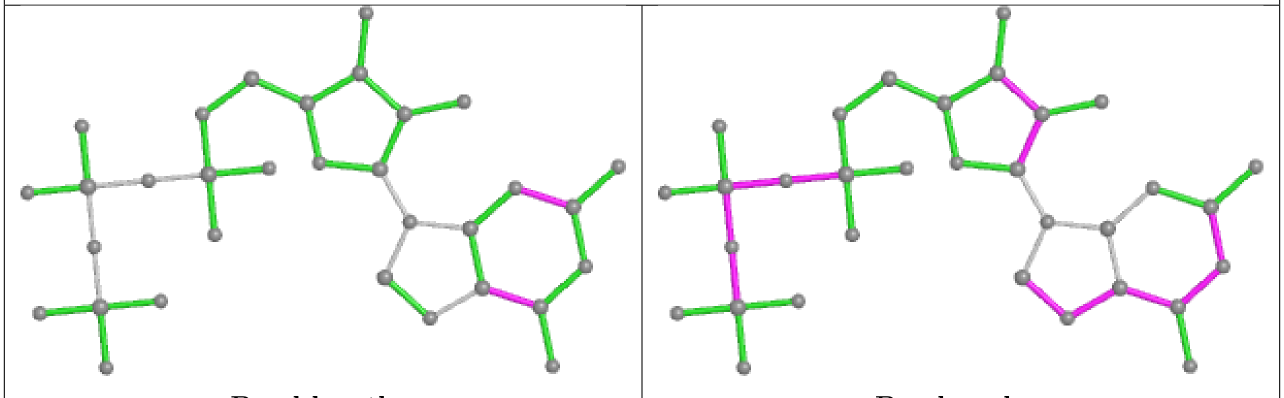
Bond angles



Torsions

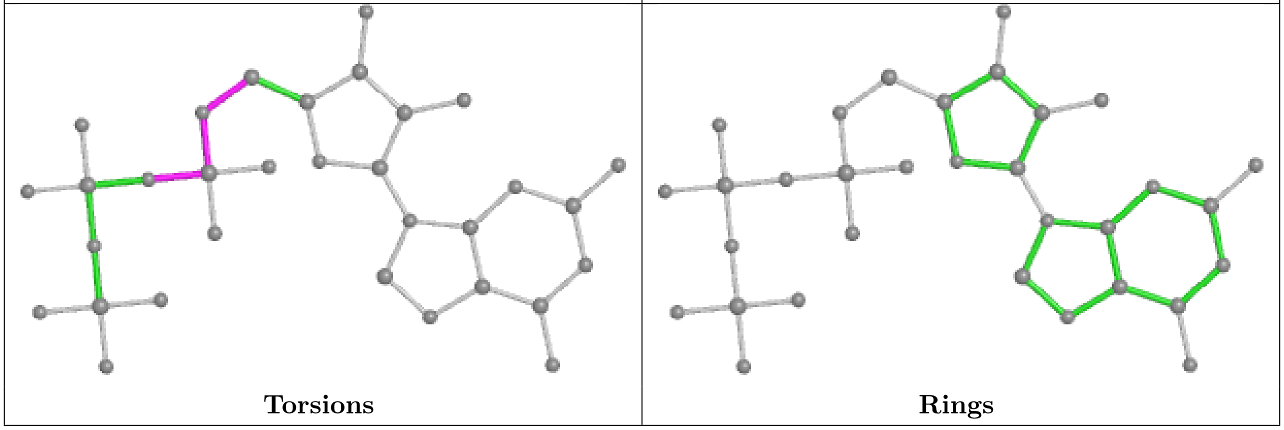
Rings

Ligand GTP DC 501



Bond lengths

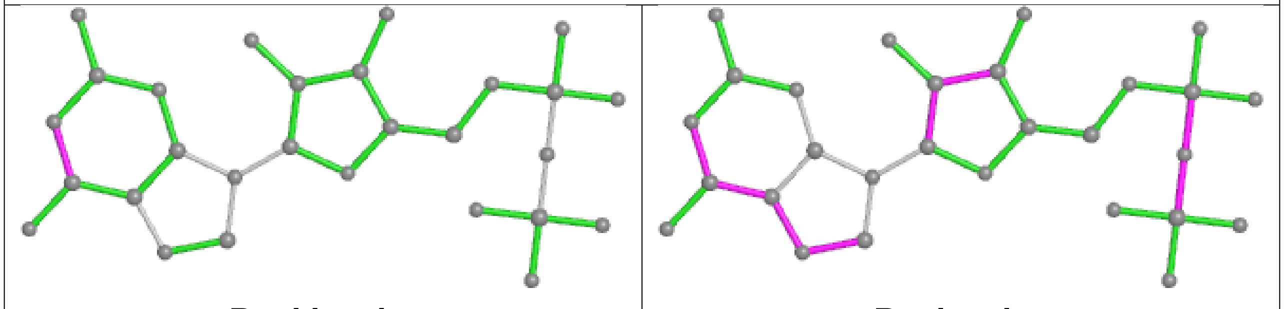
Bond angles



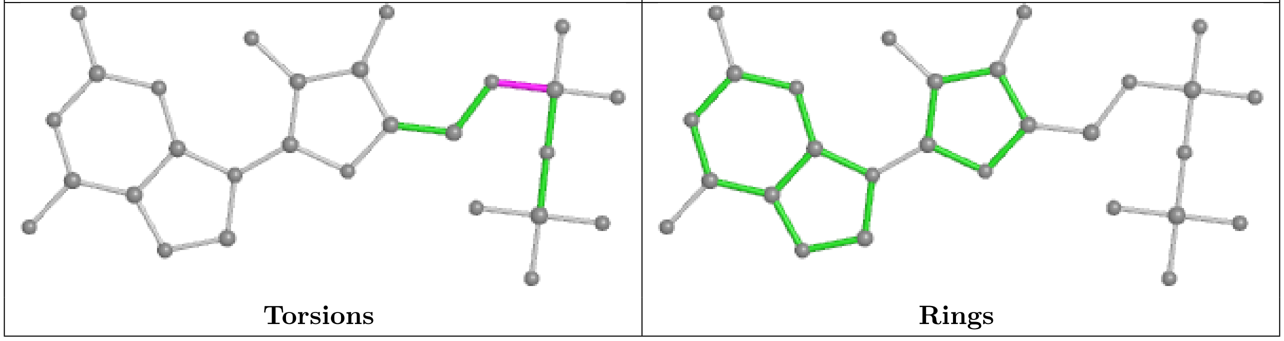
Torsions

Rings

Ligand GDP AD 502

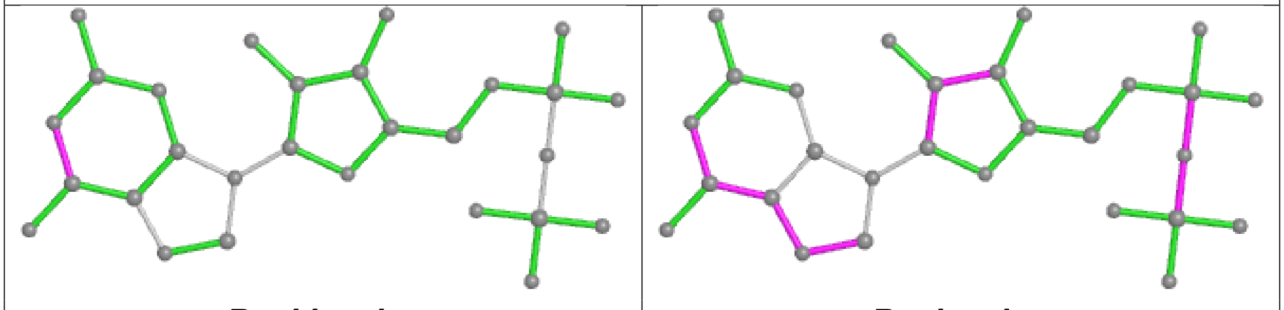


Bond lengths Bond angles

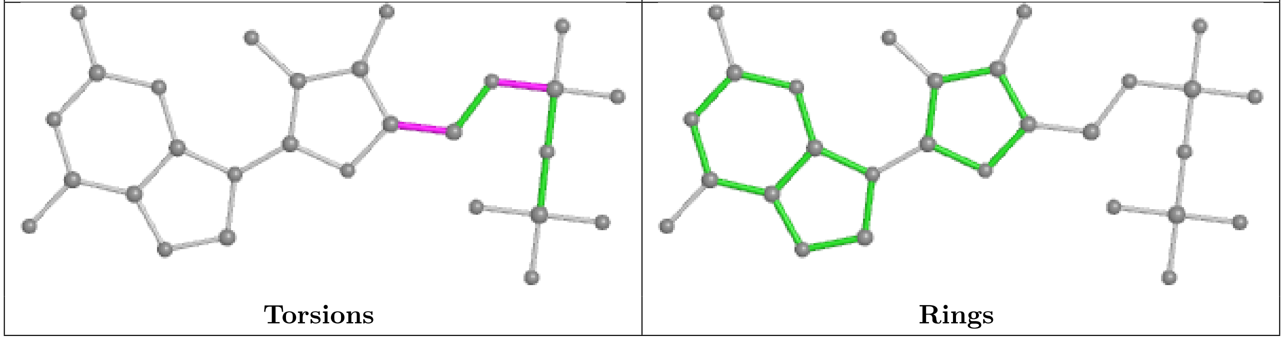


Torsions Rings

Ligand GDP AF 502

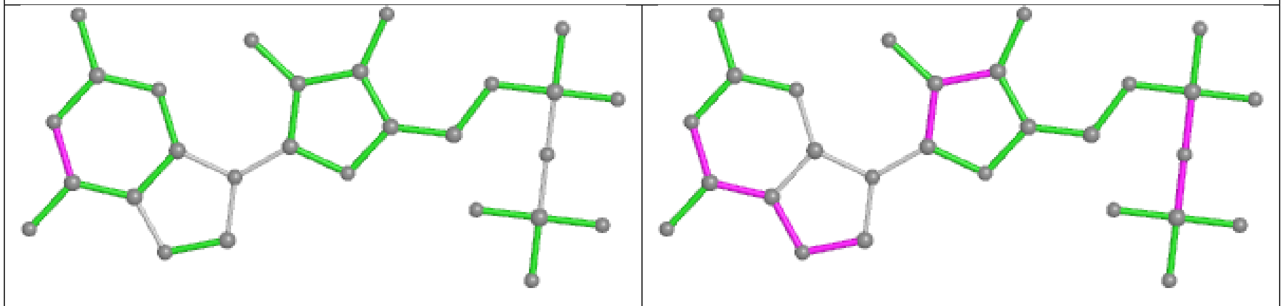


Bond lengths Bond angles

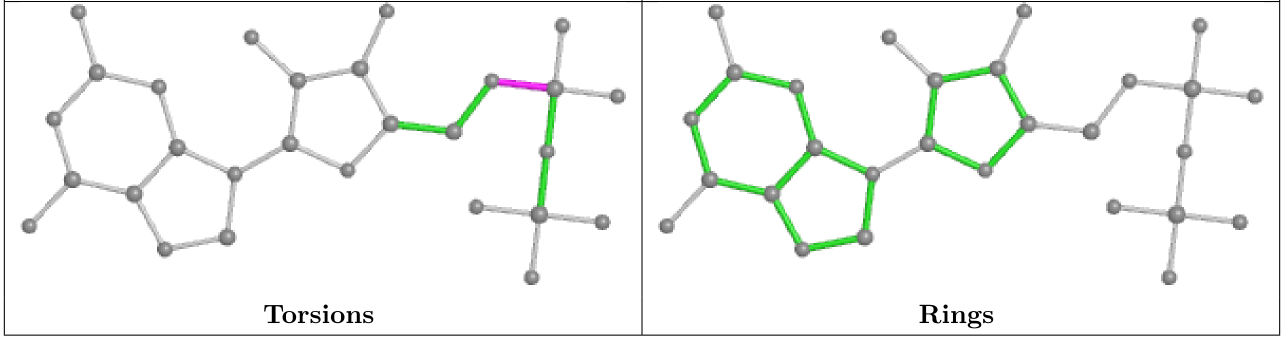


Torsions Rings

Ligand GDP MH 502

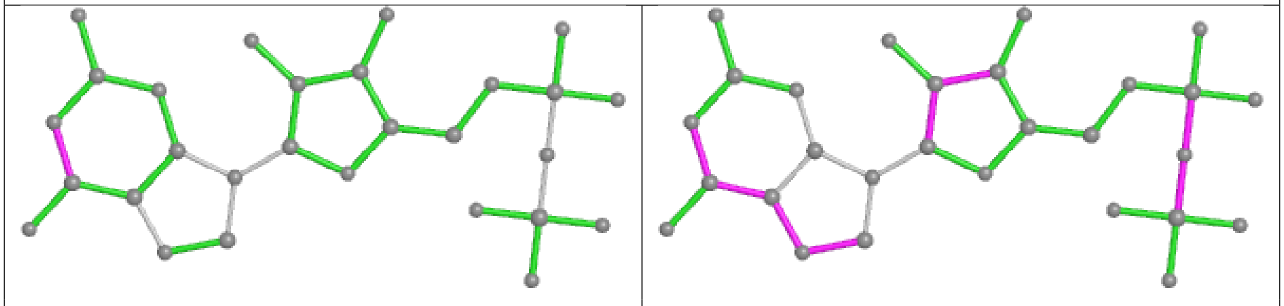


Bond lengths Bond angles

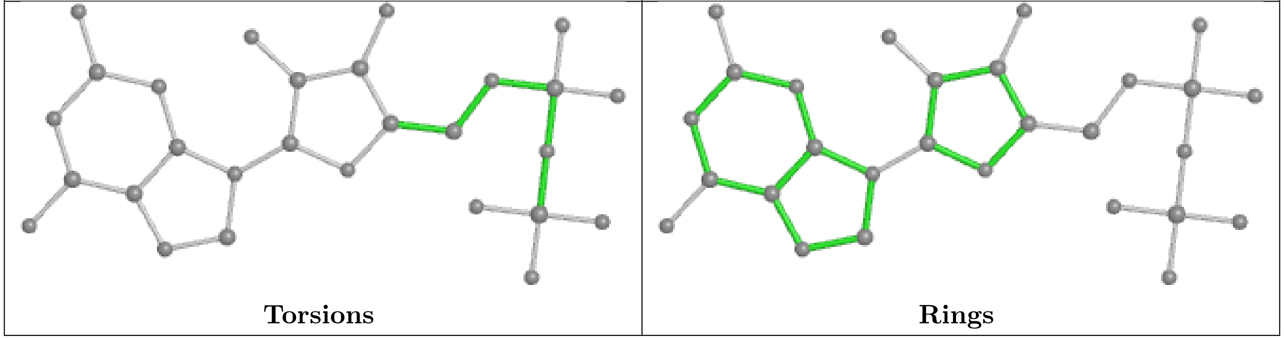


Torsions Rings

Ligand GDP ND 502

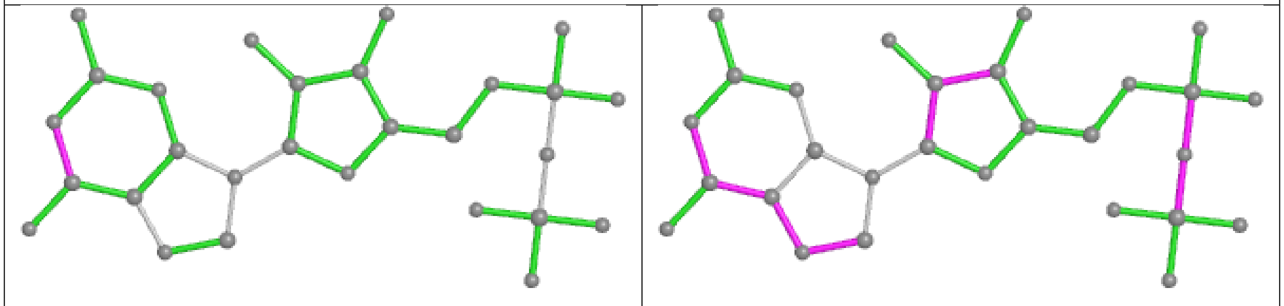


Bond lengths Bond angles

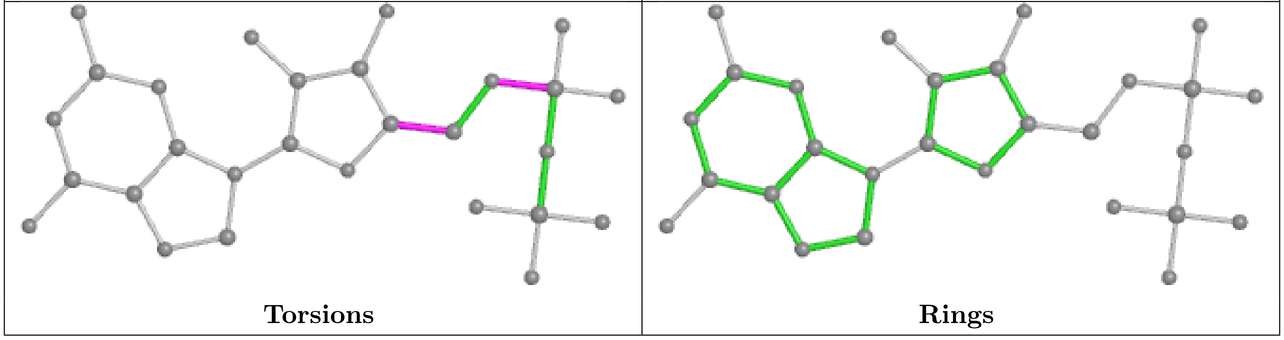


Torsions Rings

Ligand GDP QF 502

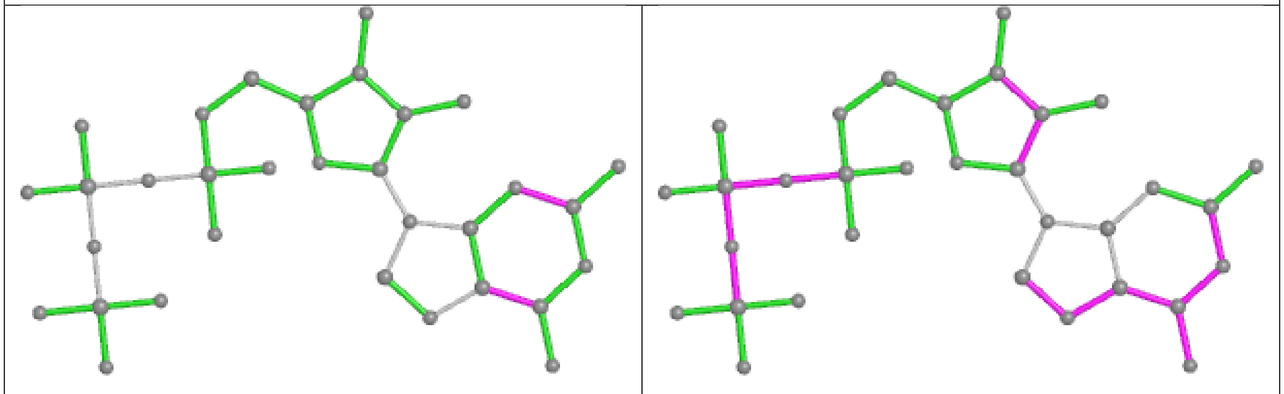


Bond lengths **Bond angles**

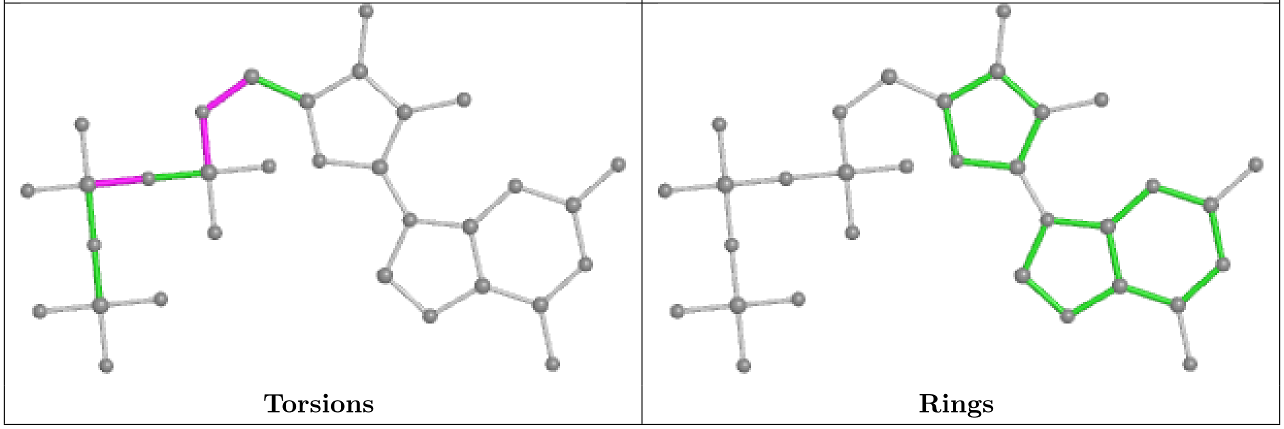


Torsions **Rings**

Ligand GTP LG 501

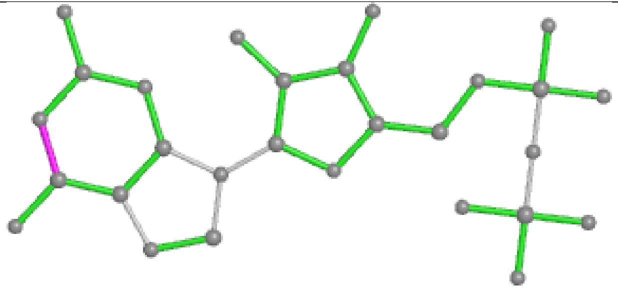


Bond lengths **Bond angles**

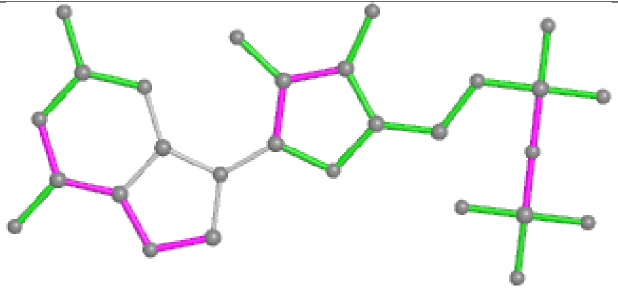


Torsions **Rings**

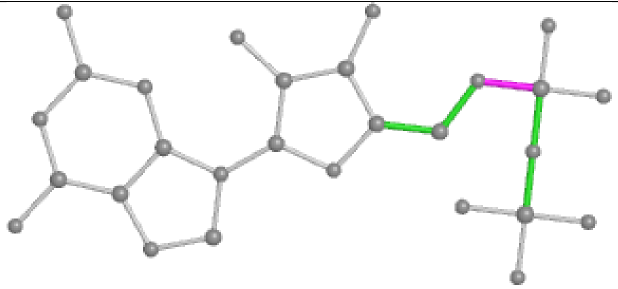
Ligand GDP KL 502



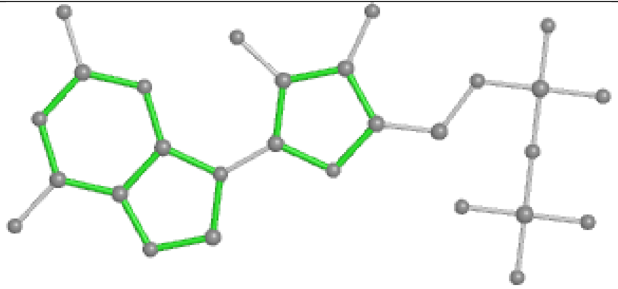
Bond lengths



Bond angles

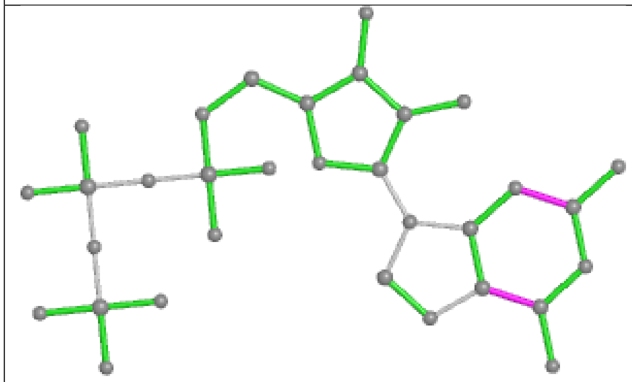


Torsions

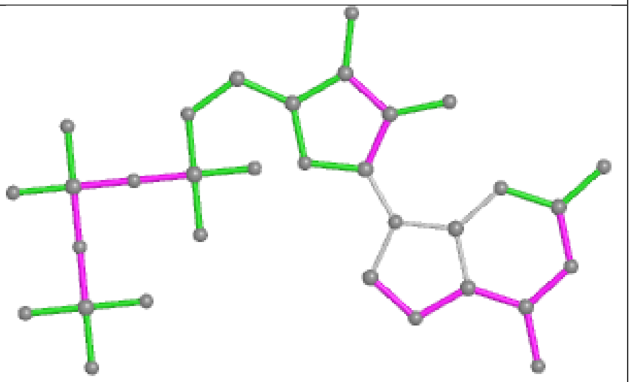


Rings

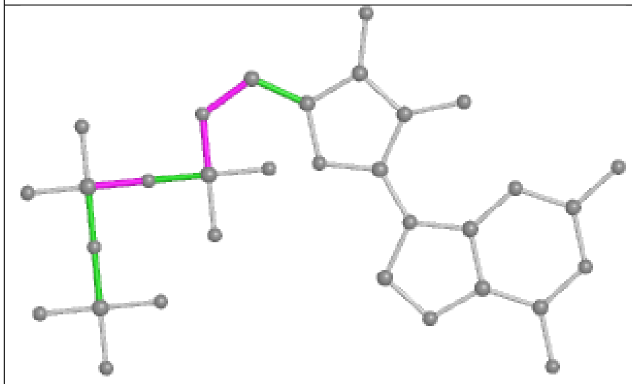
Ligand GTP MK 501



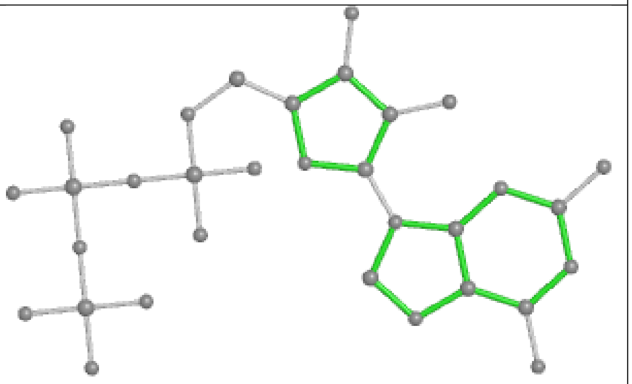
Bond lengths



Bond angles

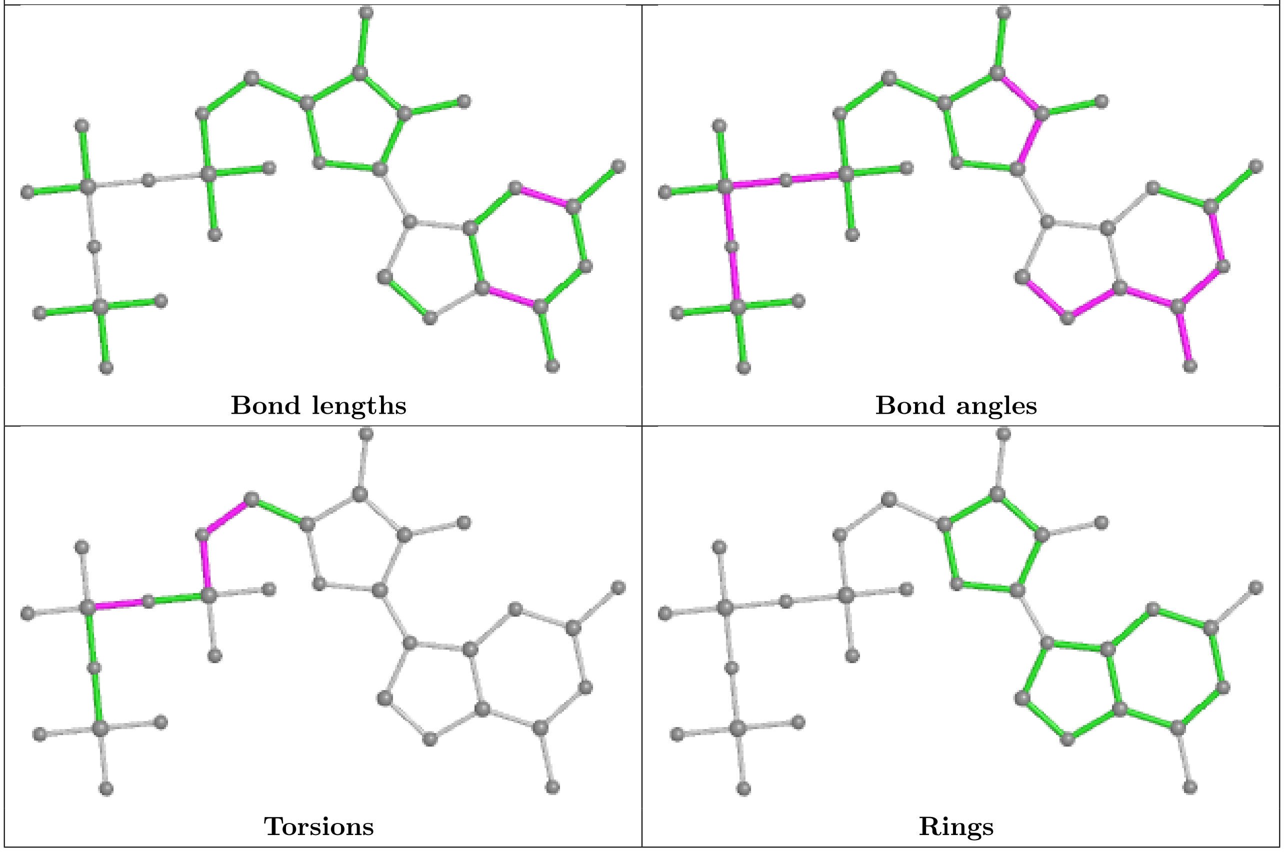


Torsions



Rings

Ligand GTP FE 501



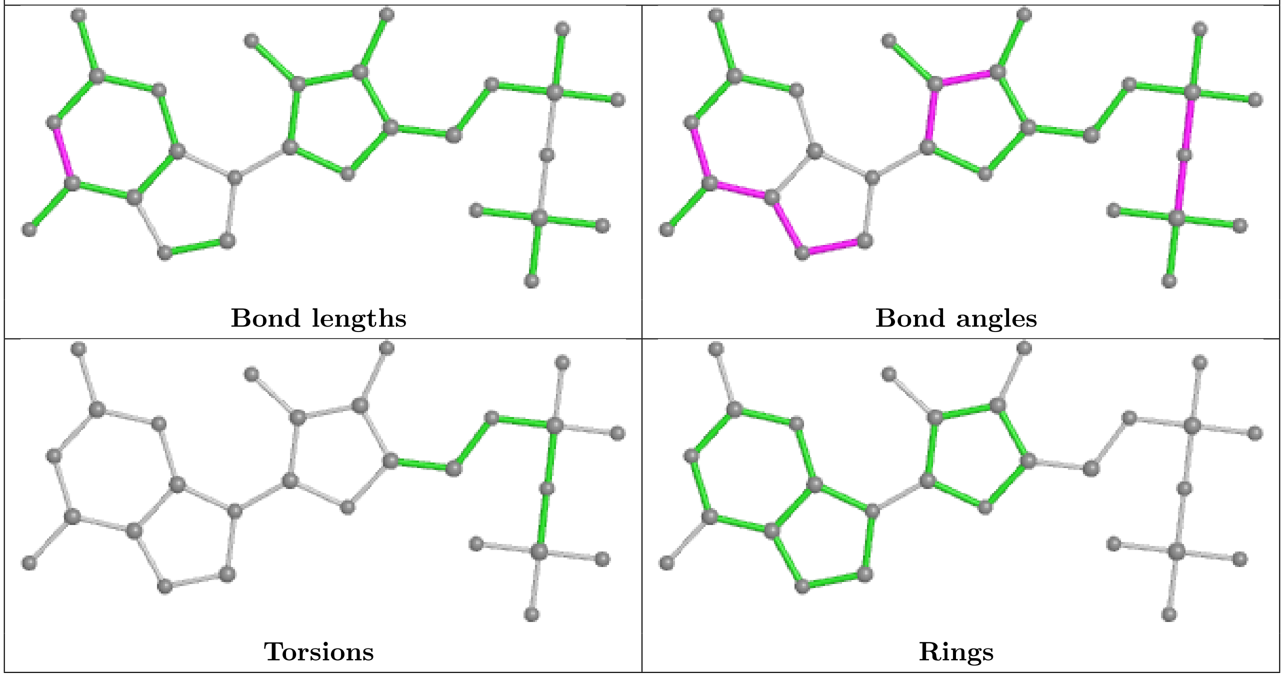
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP RL 502



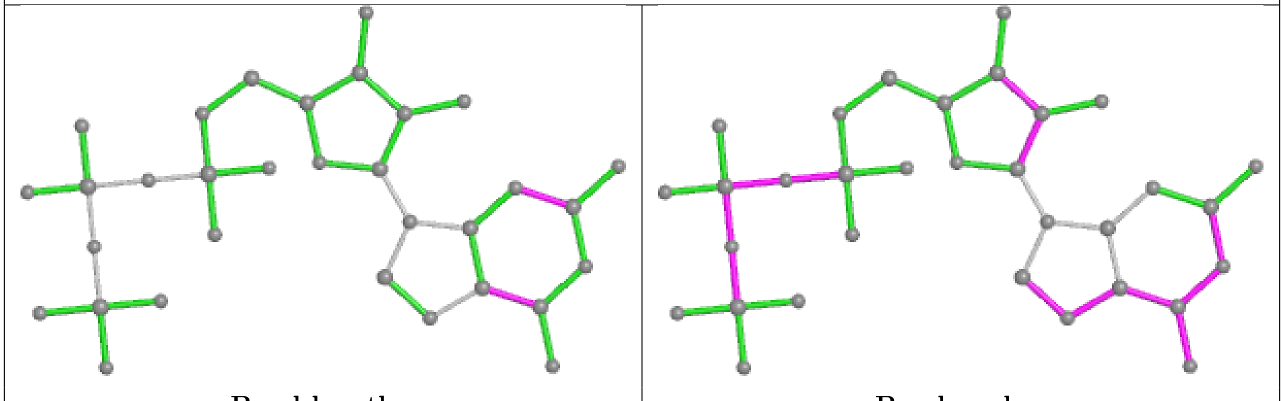
Bond lengths

Bond angles

Torsions

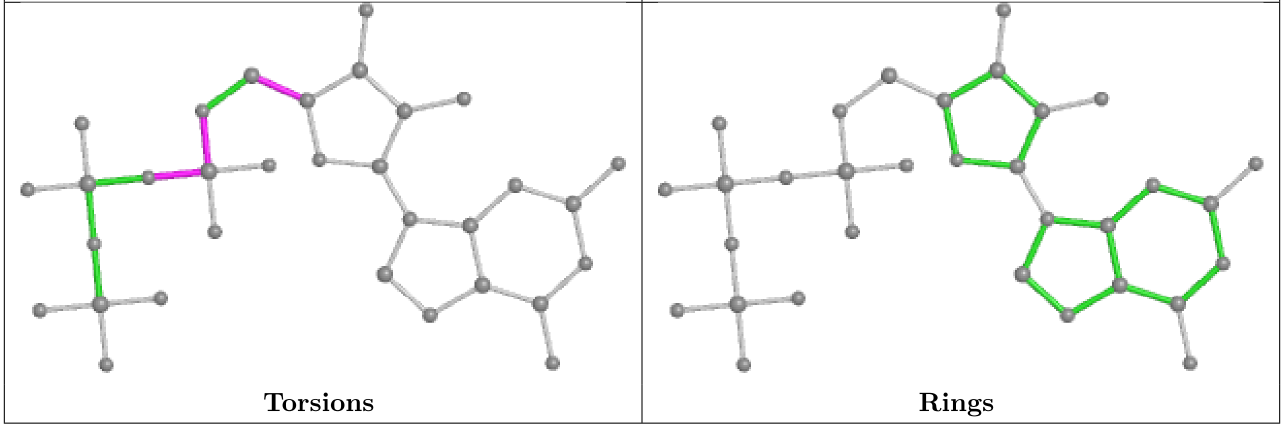
Rings

Ligand GTP TM 501



Bond lengths

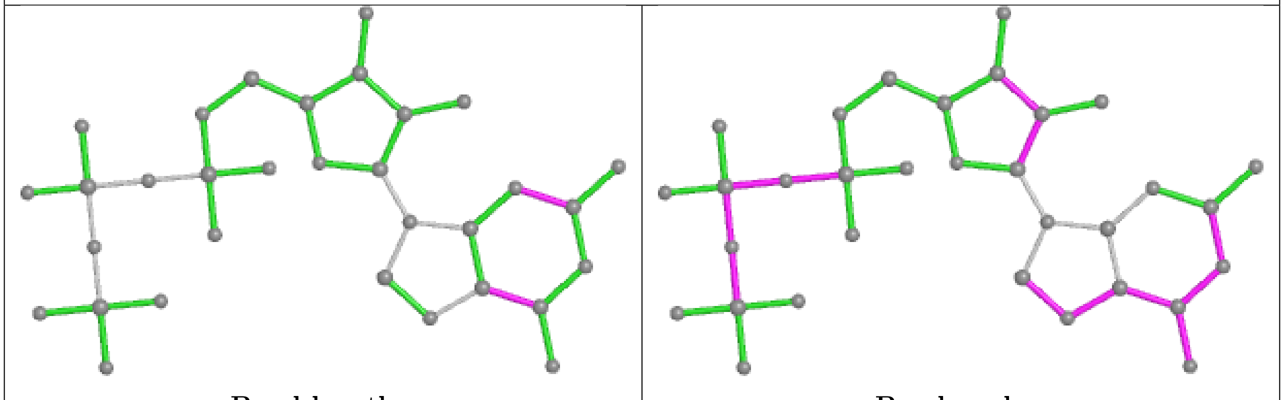
Bond angles



Torsions

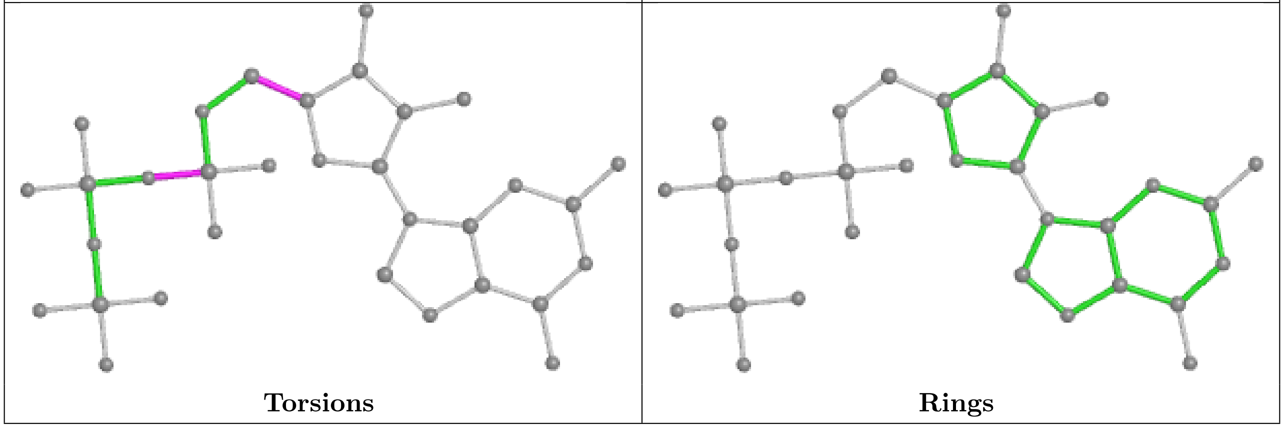
Rings

Ligand GTP QC 501



Bond lengths

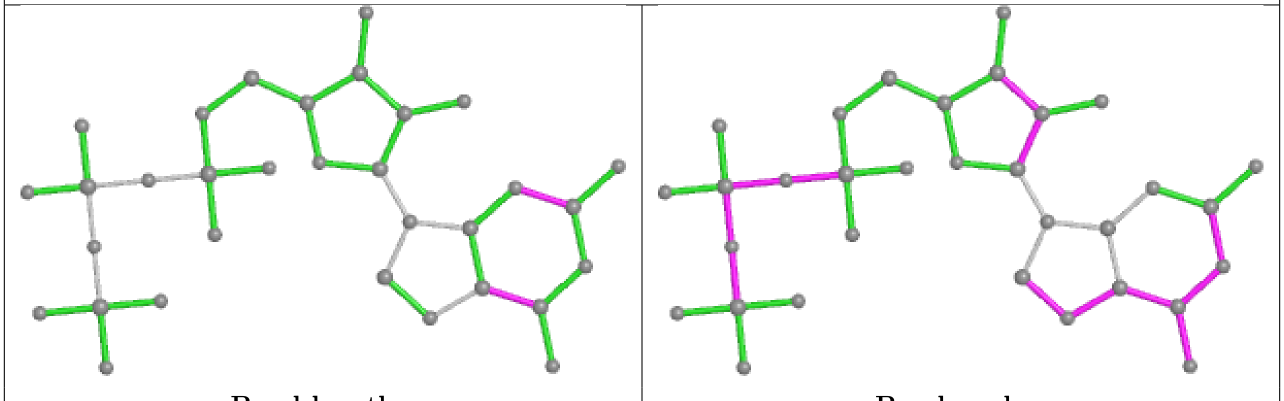
Bond angles



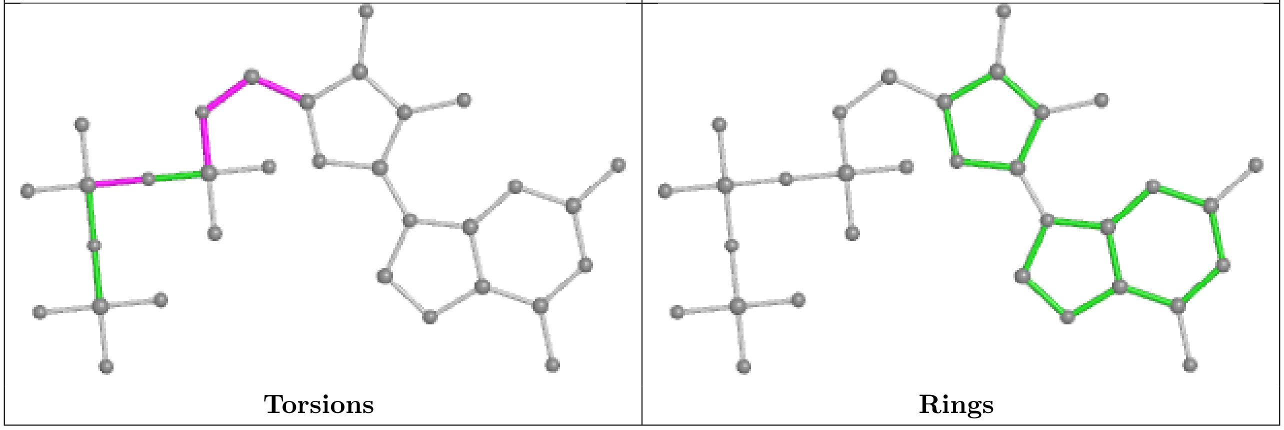
Torsions

Rings

Ligand GTP OO 501

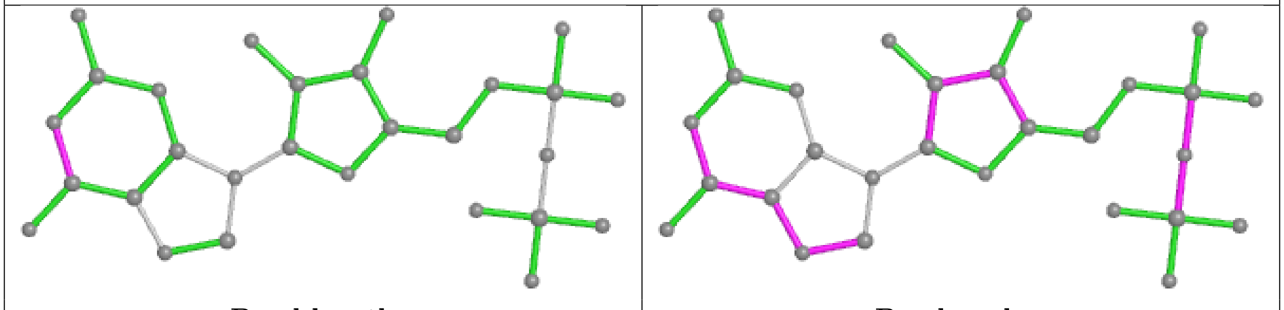


Bond lengths Bond angles

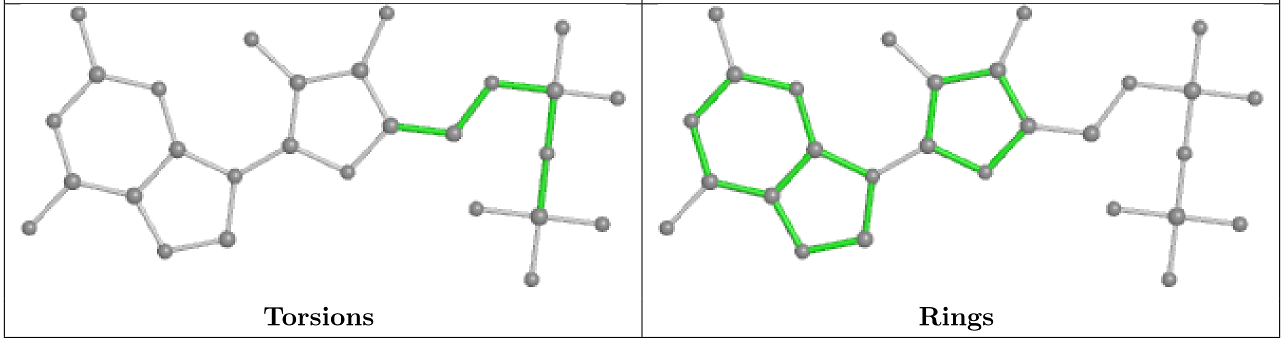


Torsions Rings

Ligand GDP RH 502

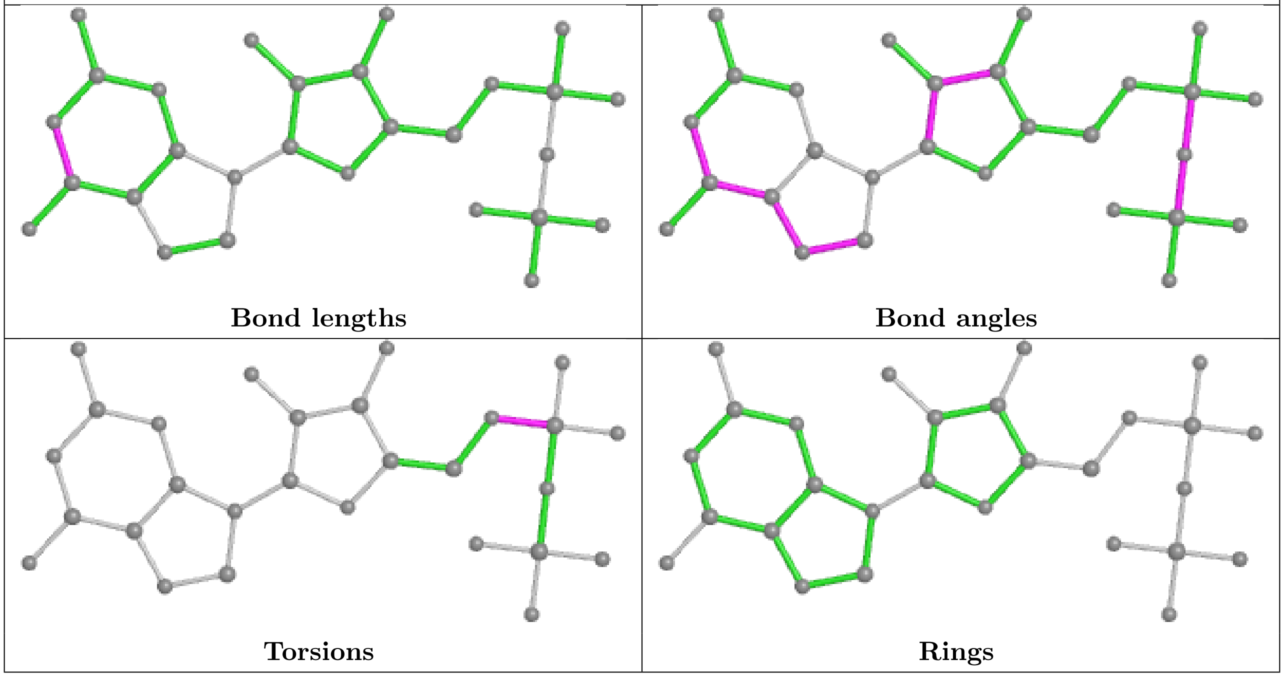


Bond lengths Bond angles



Torsions Rings

Ligand GDP VL 502



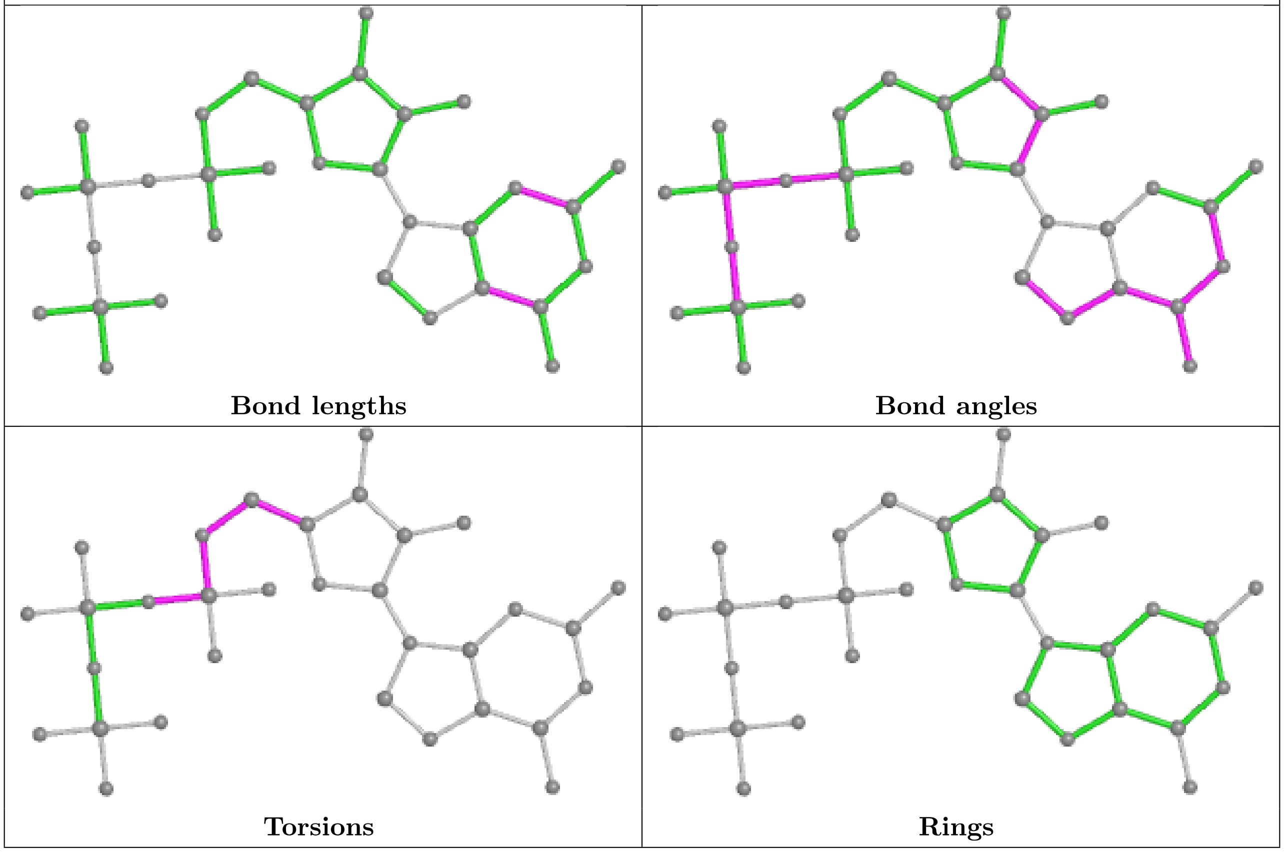
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP OG 501



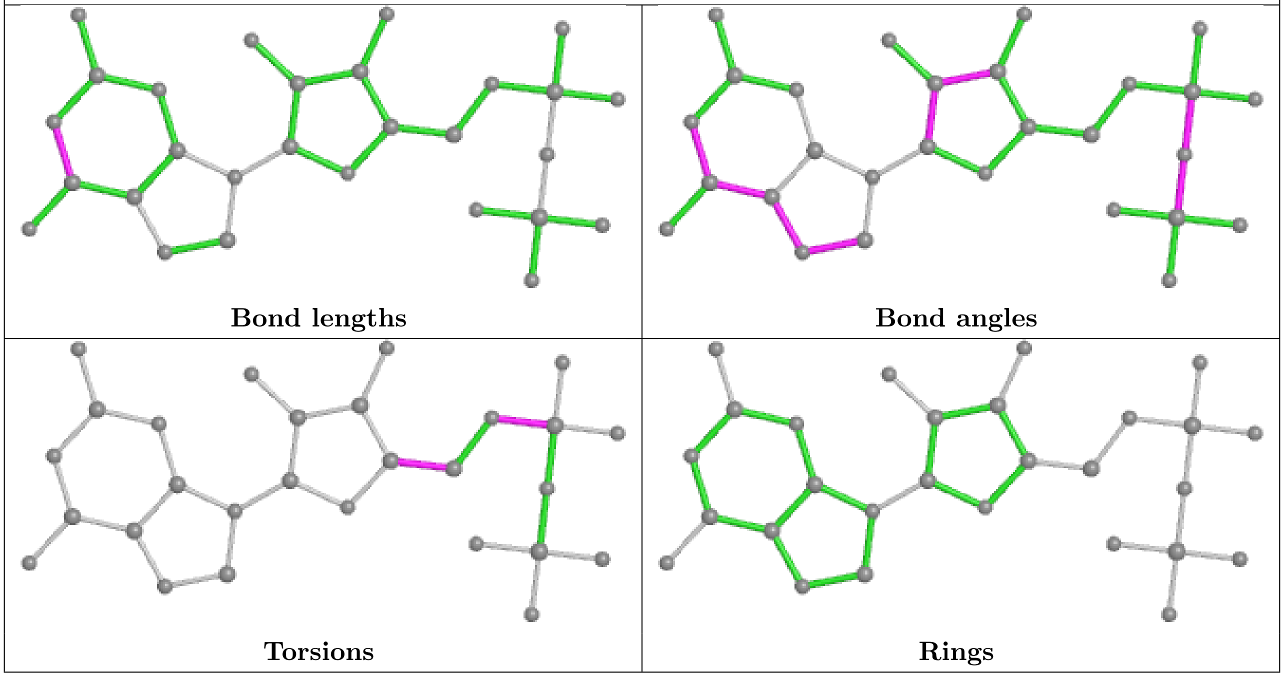
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP CF 502



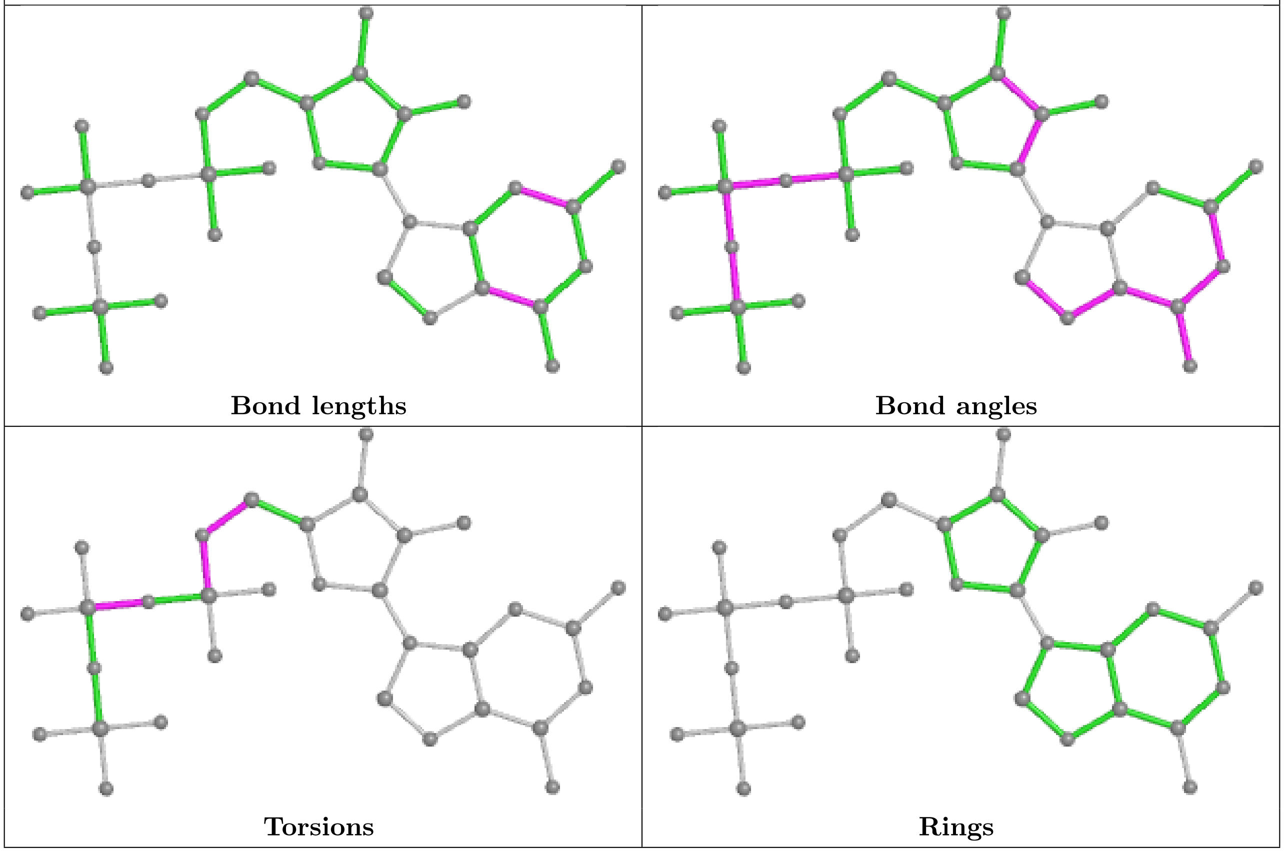
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP MC 501



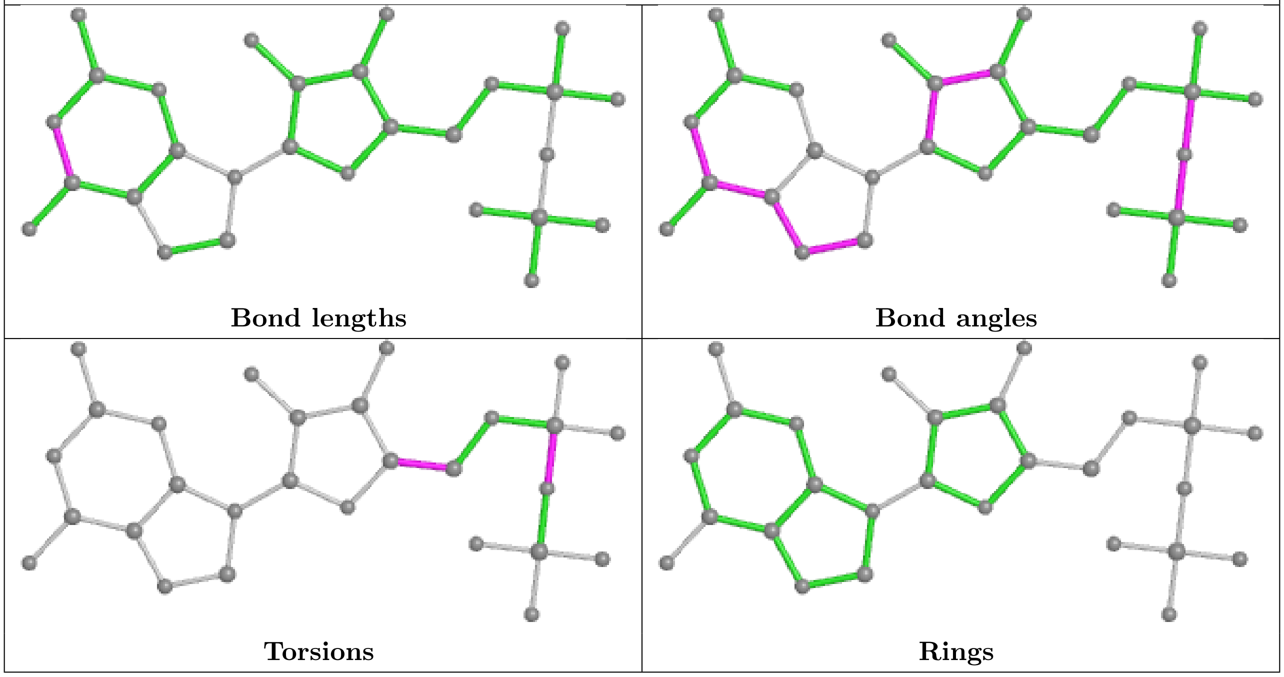
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP TH 502



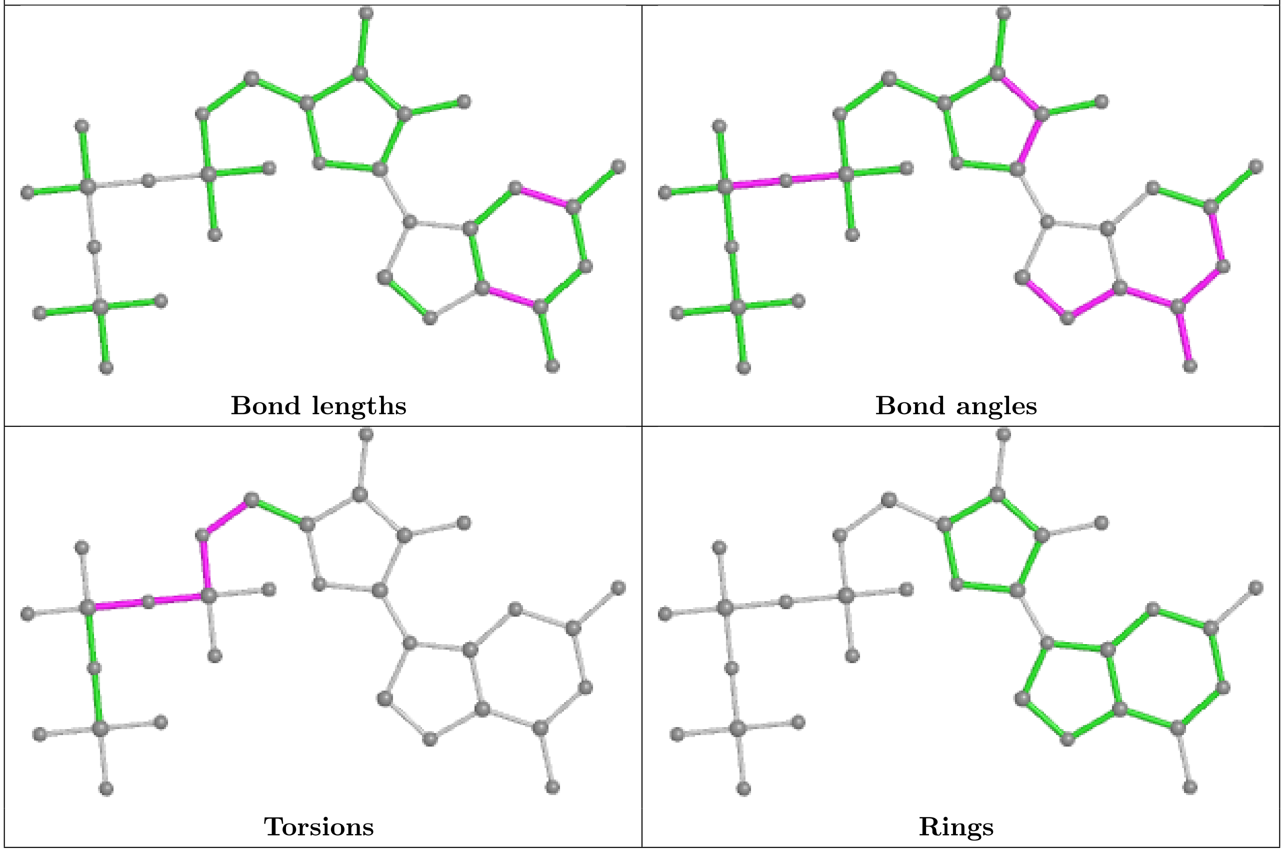
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP FK 501



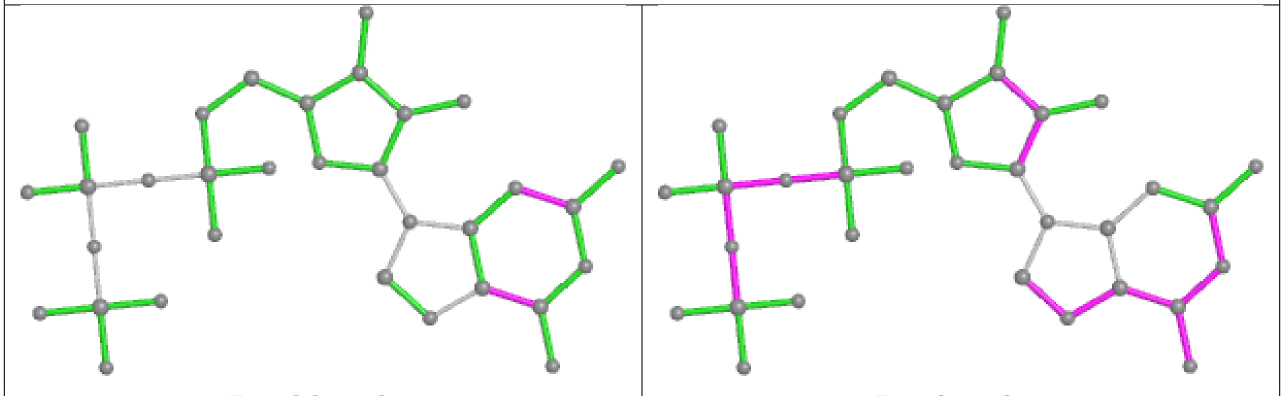
Bond lengths

Bond angles

Torsions

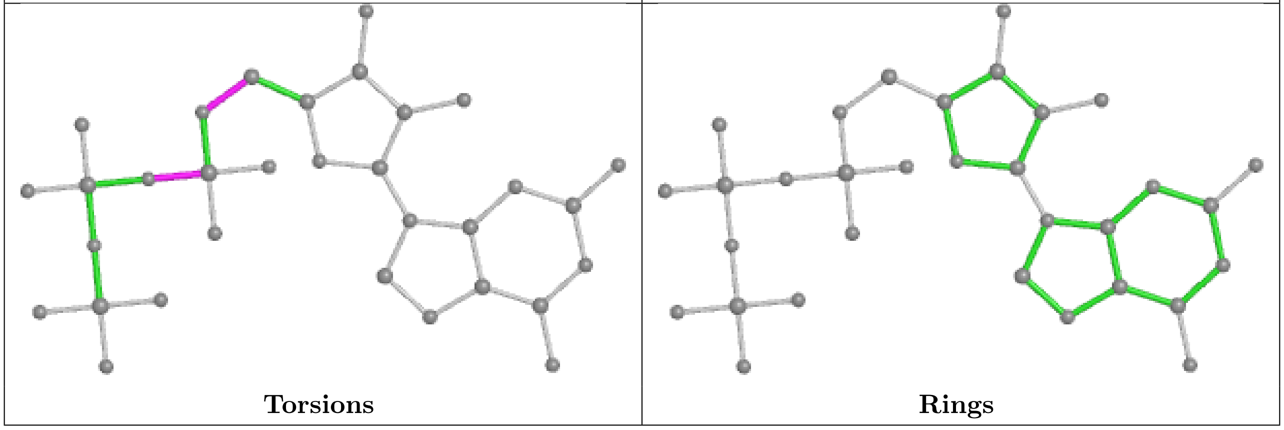
Rings

Ligand GTP TI 501



Bond lengths

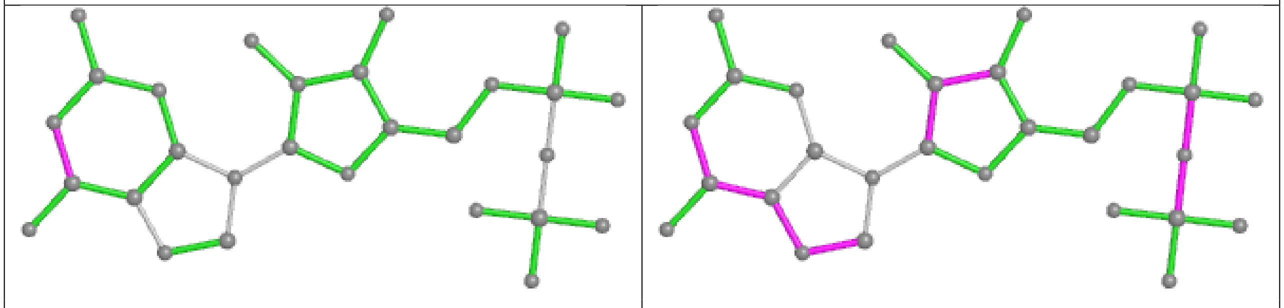
Bond angles



Torsions

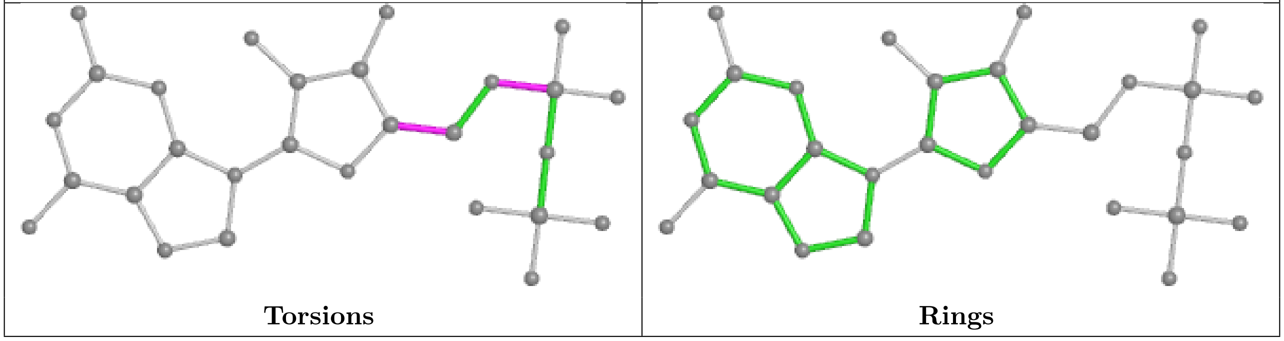
Rings

Ligand GDP GB 502



Bond lengths

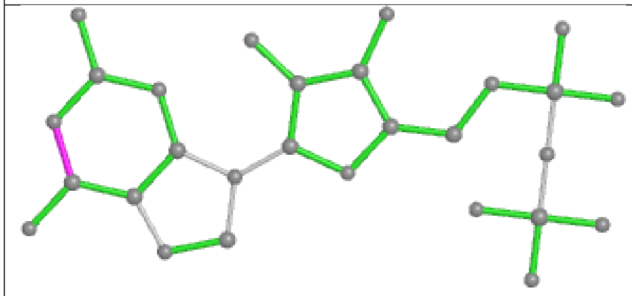
Bond angles



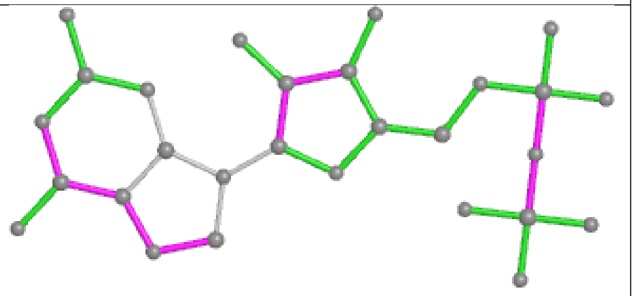
Torsions

Rings

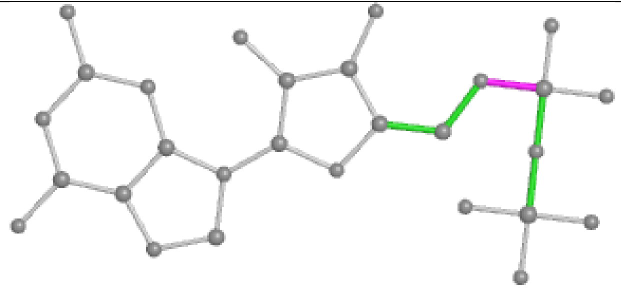
Ligand GDP VJ 502



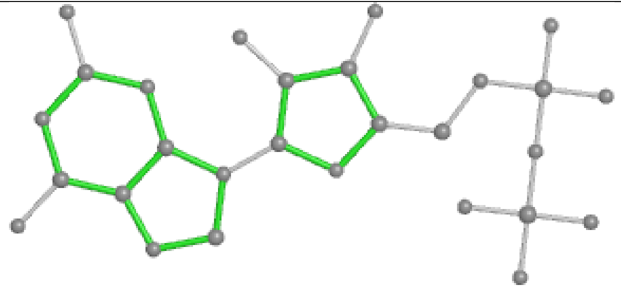
Bond lengths



Bond angles

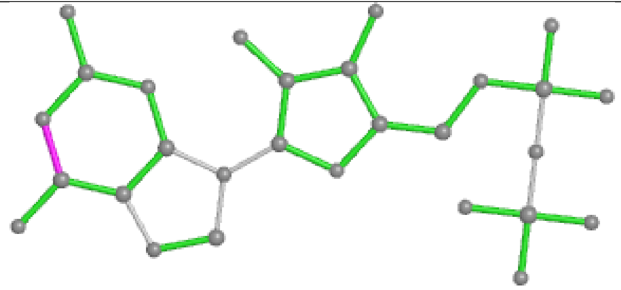


Torsions

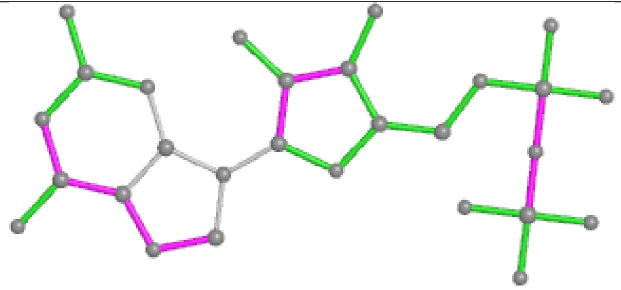


Rings

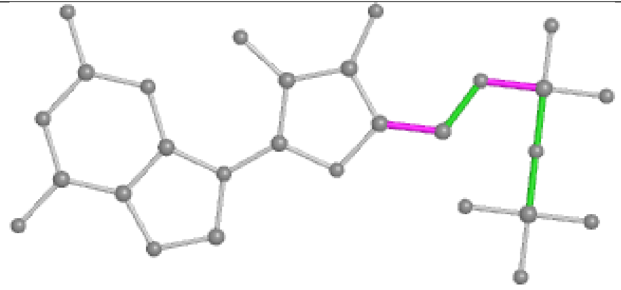
Ligand GDP TL 502



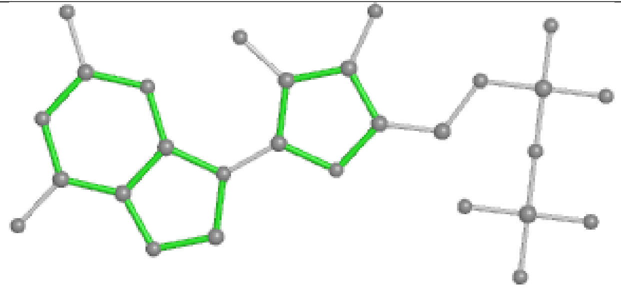
Bond lengths



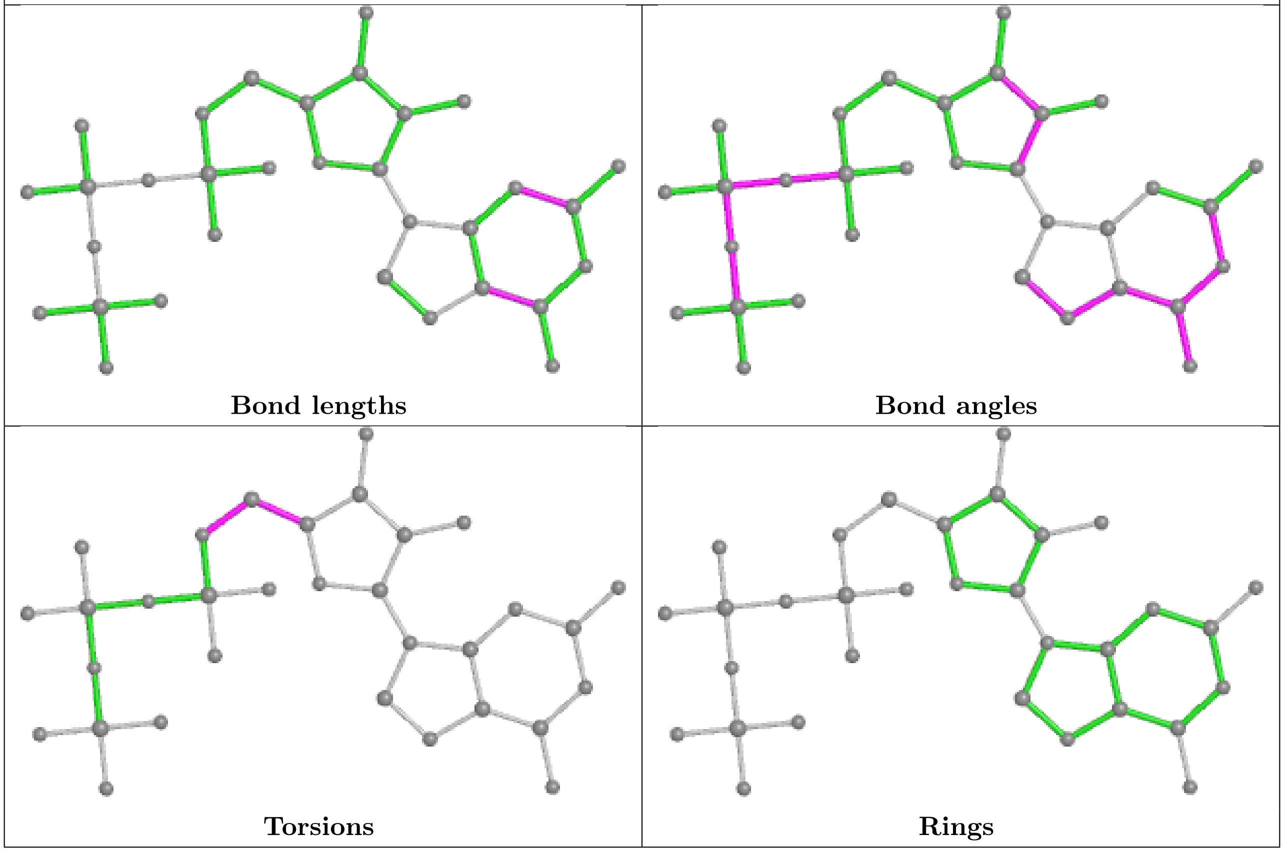
Bond angles



Torsions



Rings



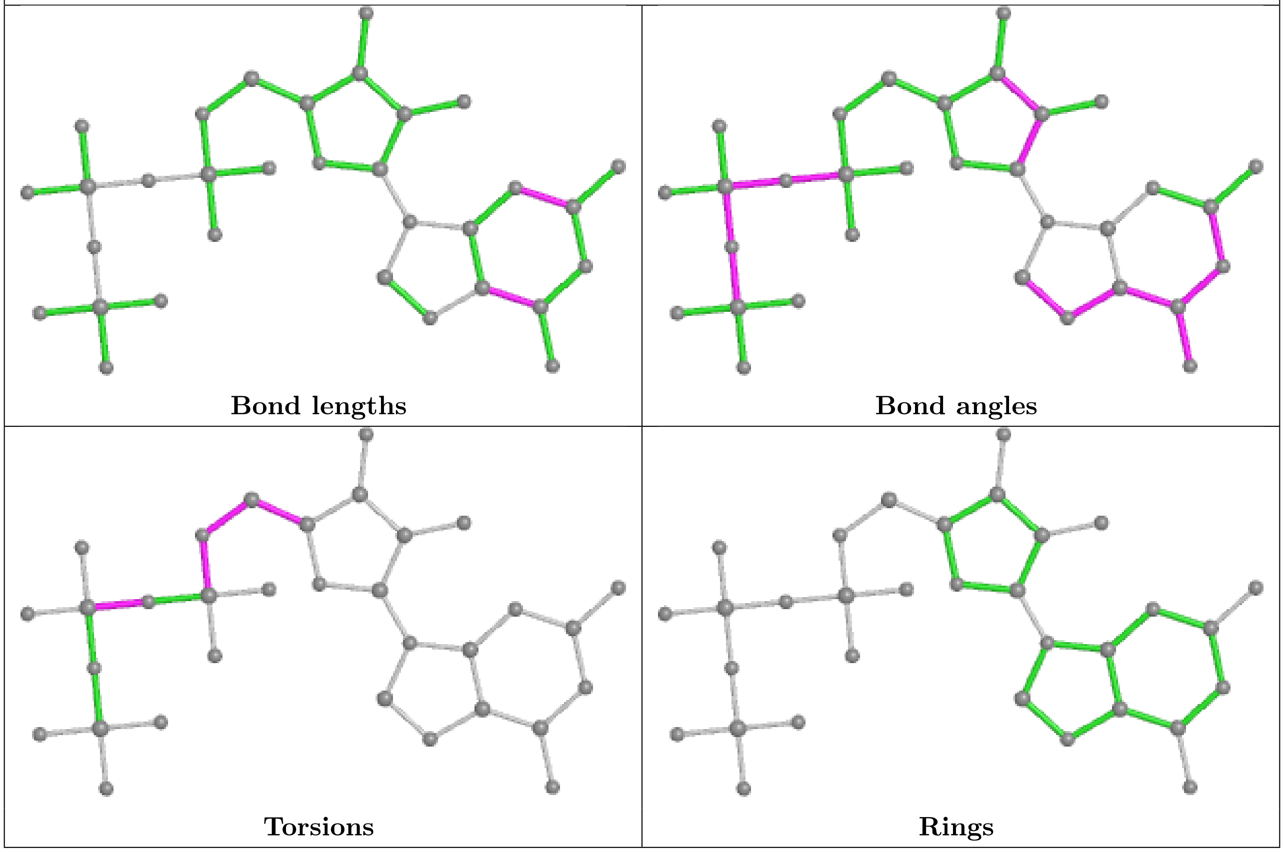
Ligand GTP CM 501

Bond lengths

Bond angles

Torsions

Rings



Ligand GTP PG 501

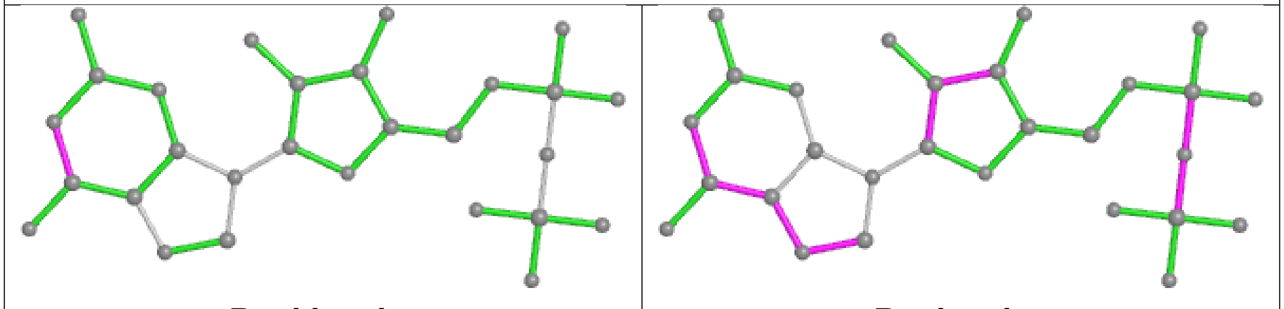
Bond lengths

Bond angles

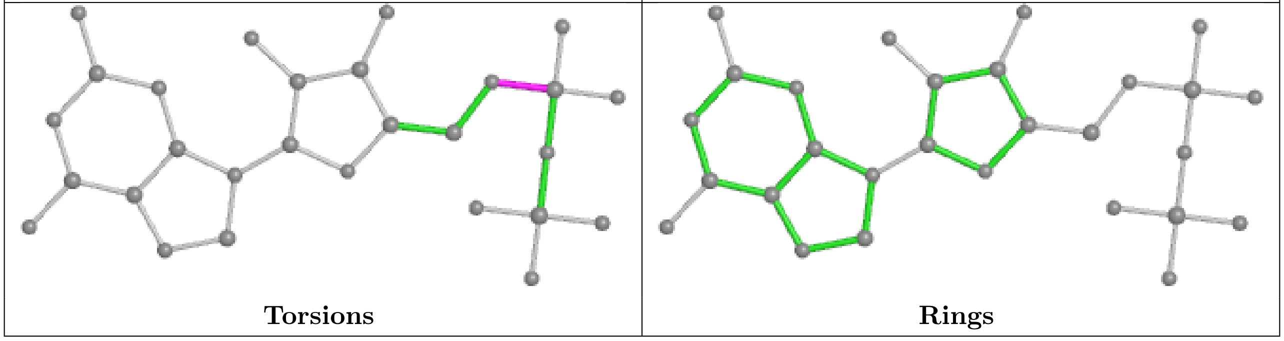
Torsions

Rings

Ligand GDP AH 502

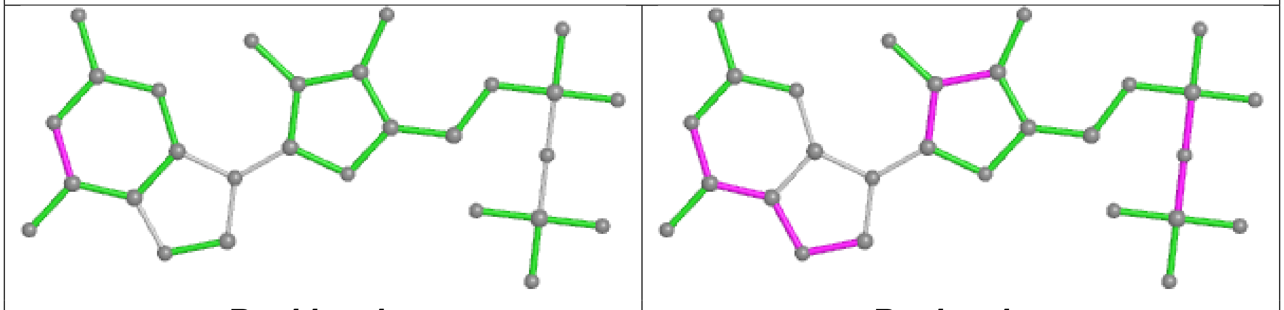


Bond lengths Bond angles

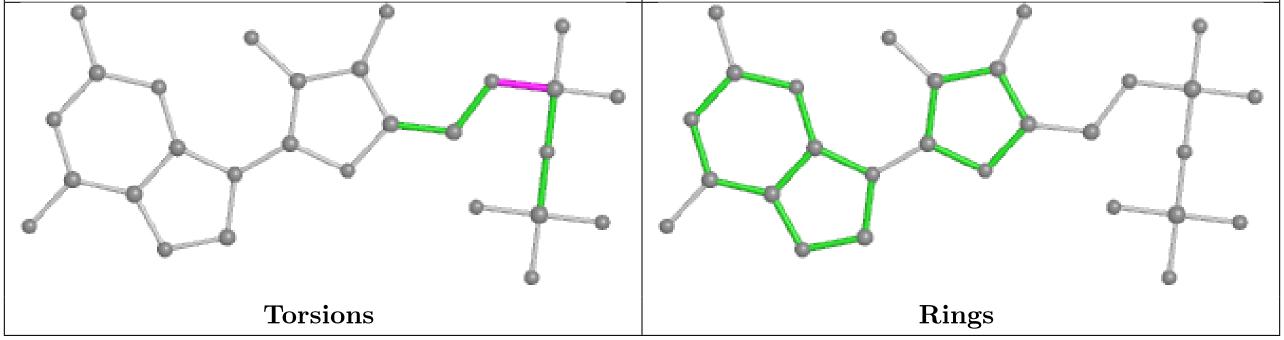


Torsions Rings

Ligand GDP UF 502

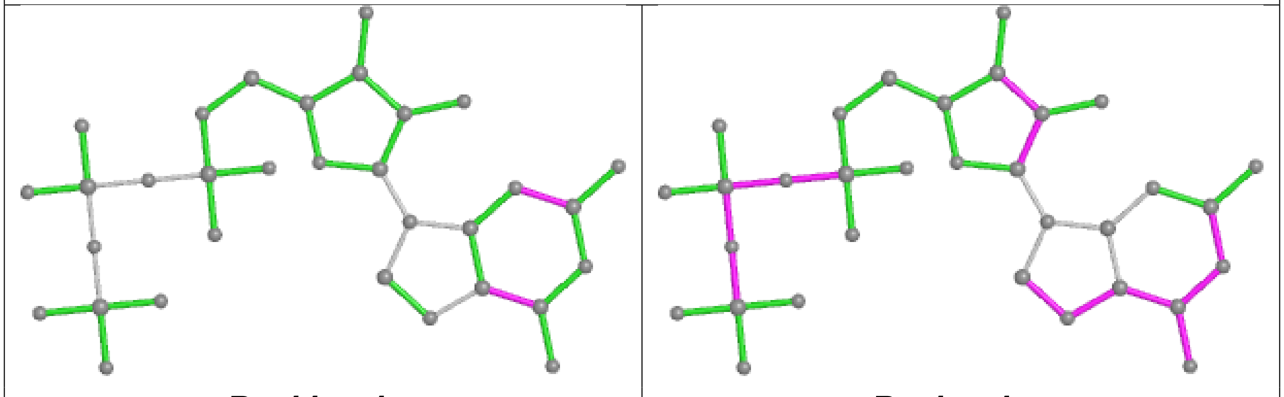


Bond lengths Bond angles

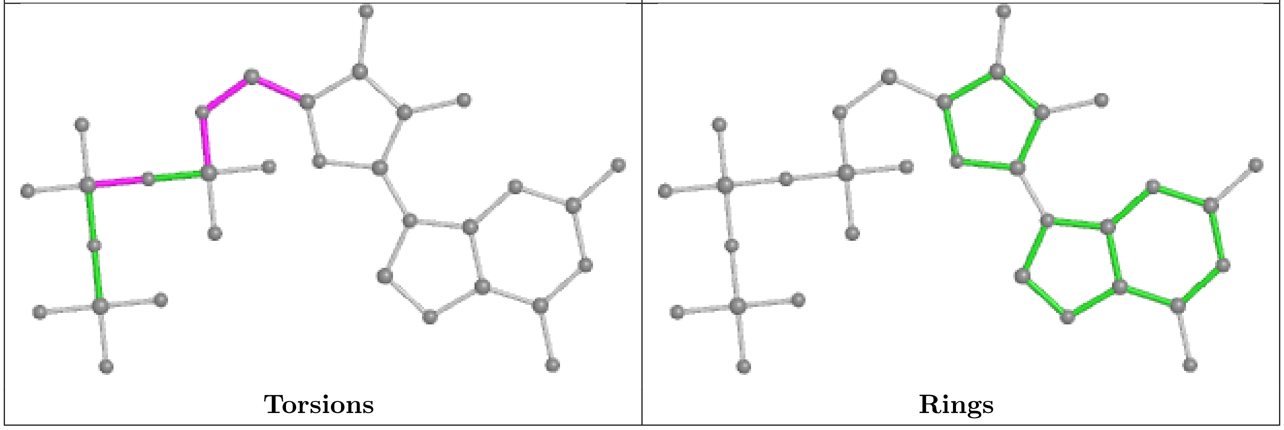


Torsions Rings

Ligand GTP RC 501

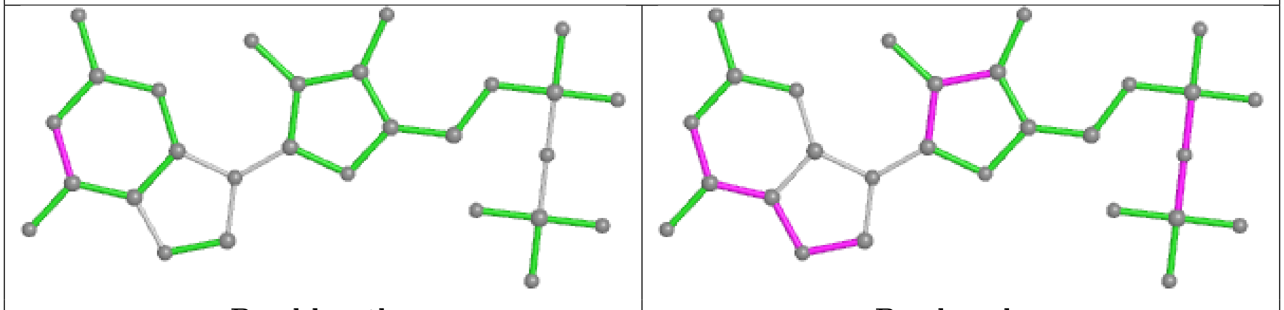


Bond lengths Bond angles

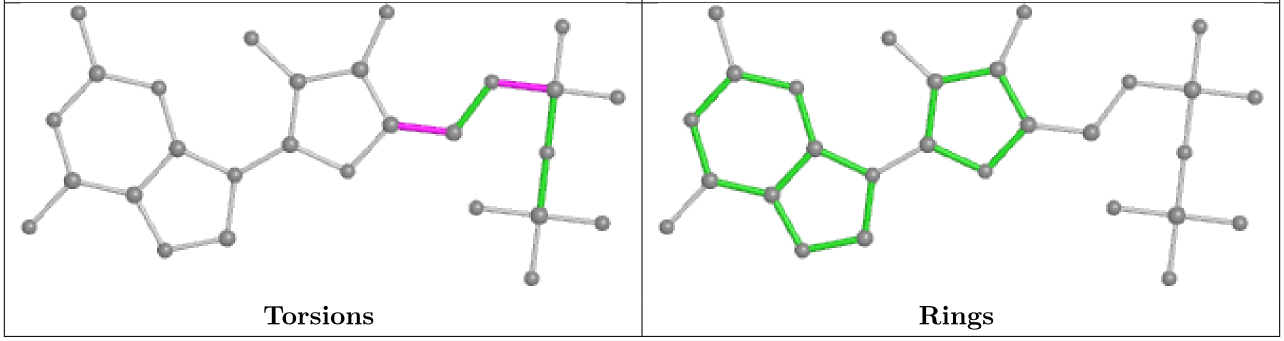


Torsions Rings

Ligand GDP LD 502

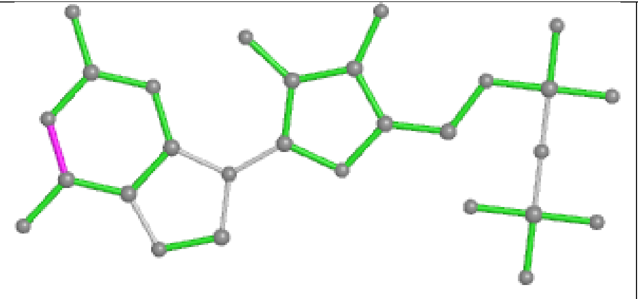


Bond lengths Bond angles

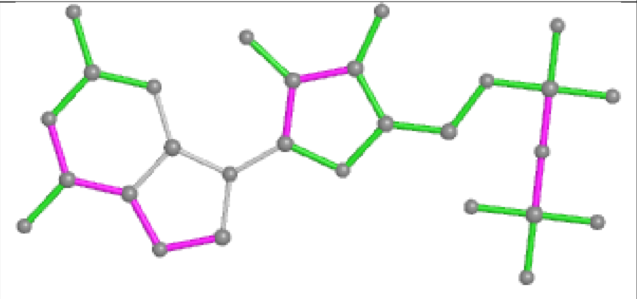


Torsions Rings

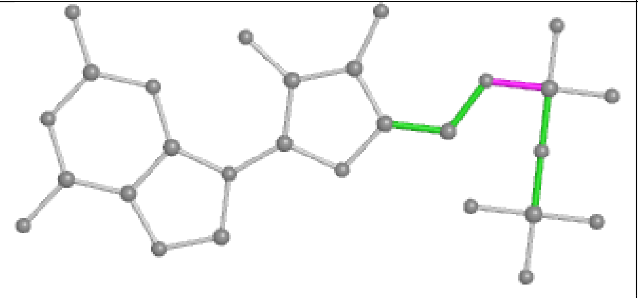
Ligand GDP AL 502



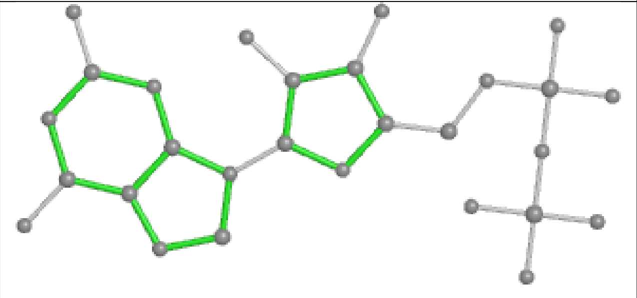
Bond lengths



Bond angles

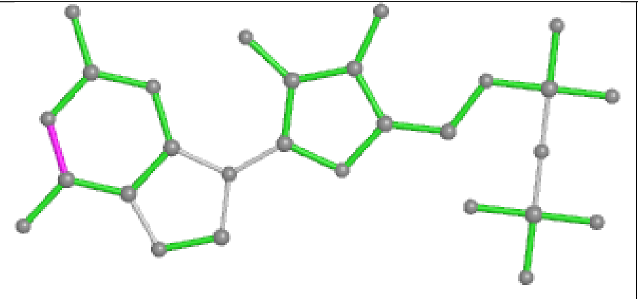


Torsions

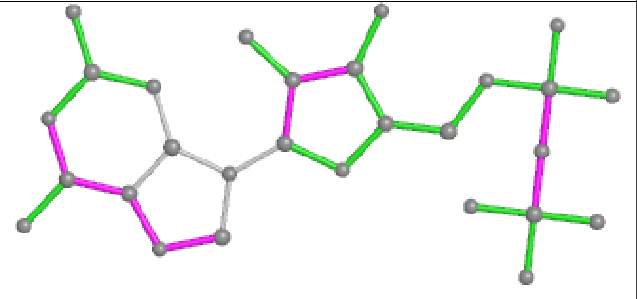


Rings

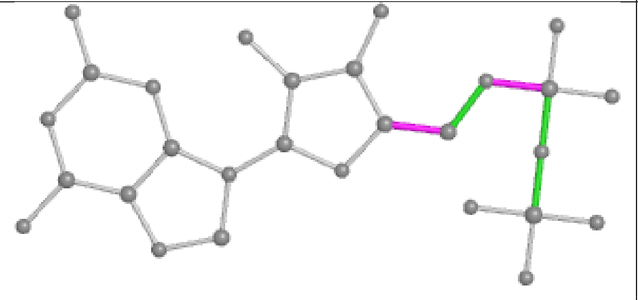
Ligand GDP CD 502



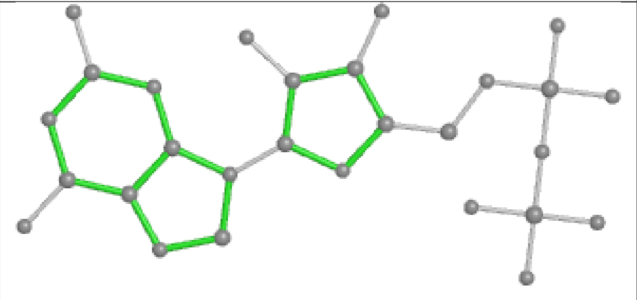
Bond lengths



Bond angles

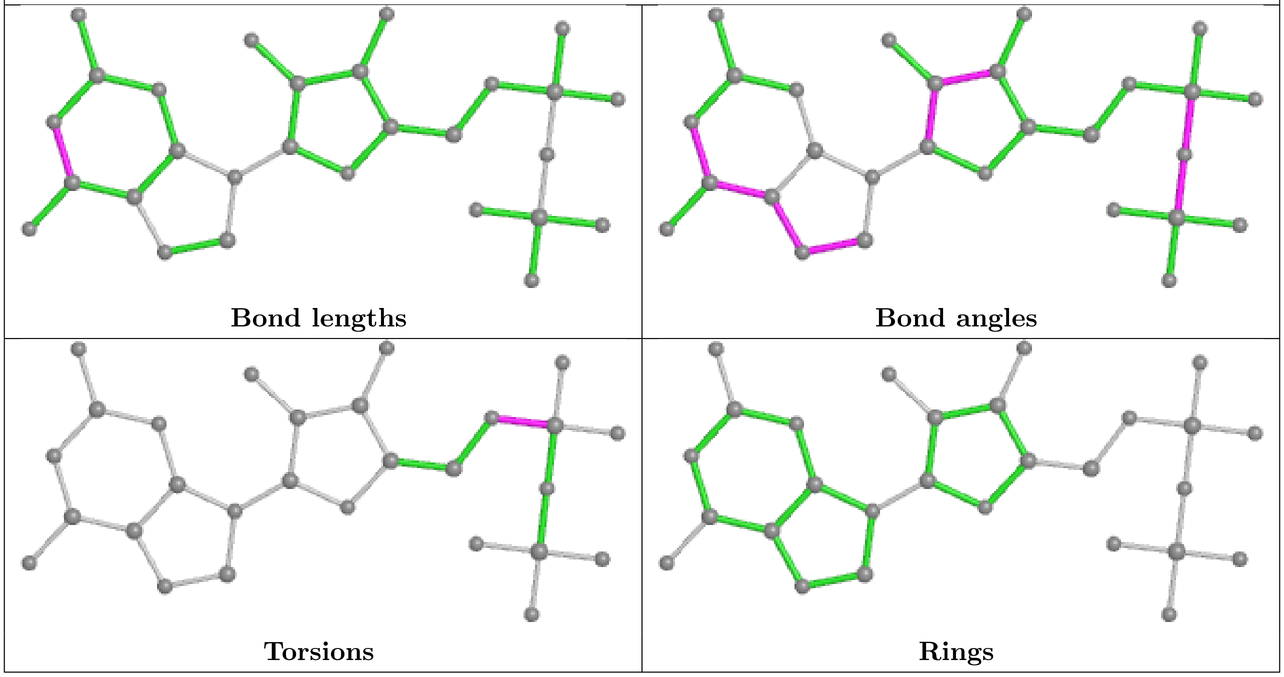


Torsions



Rings

Ligand GDP VP 502



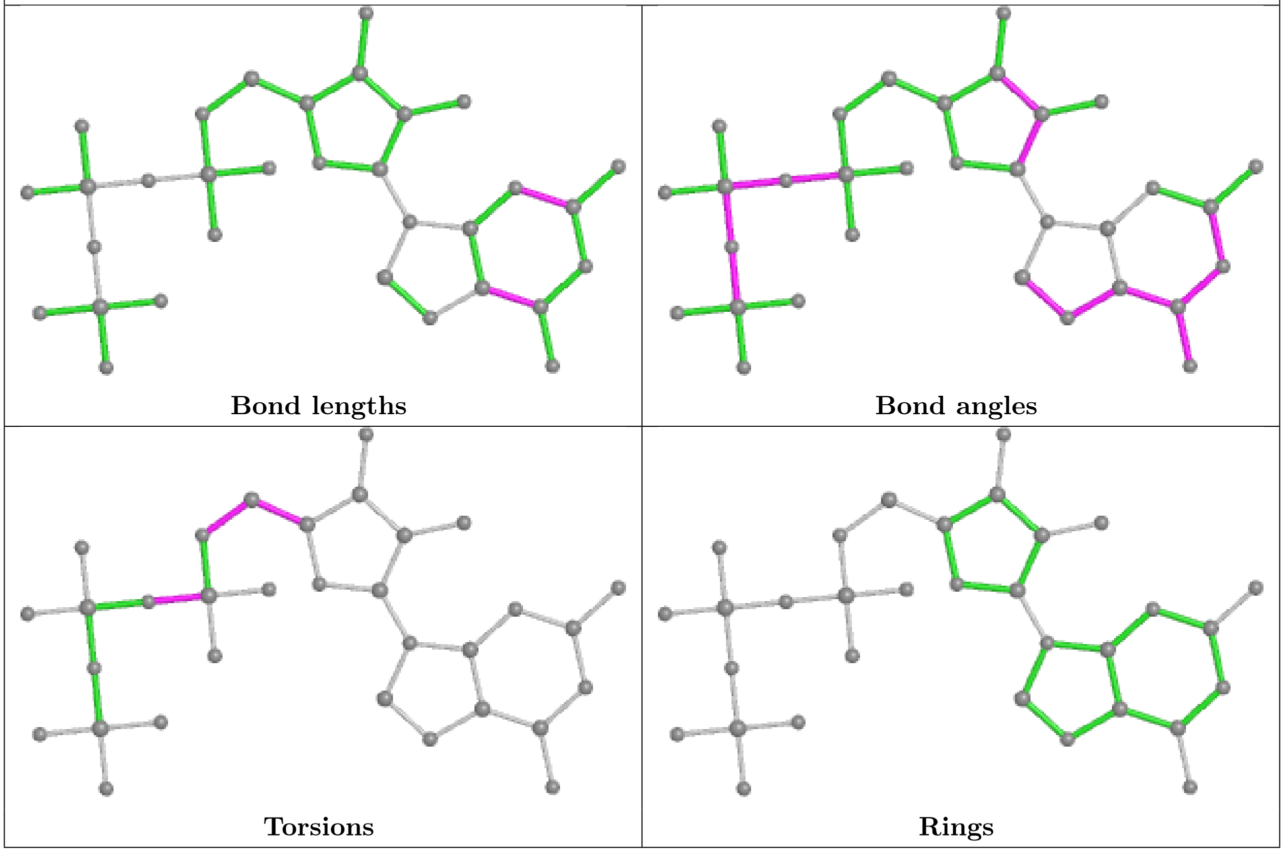
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP BC 501



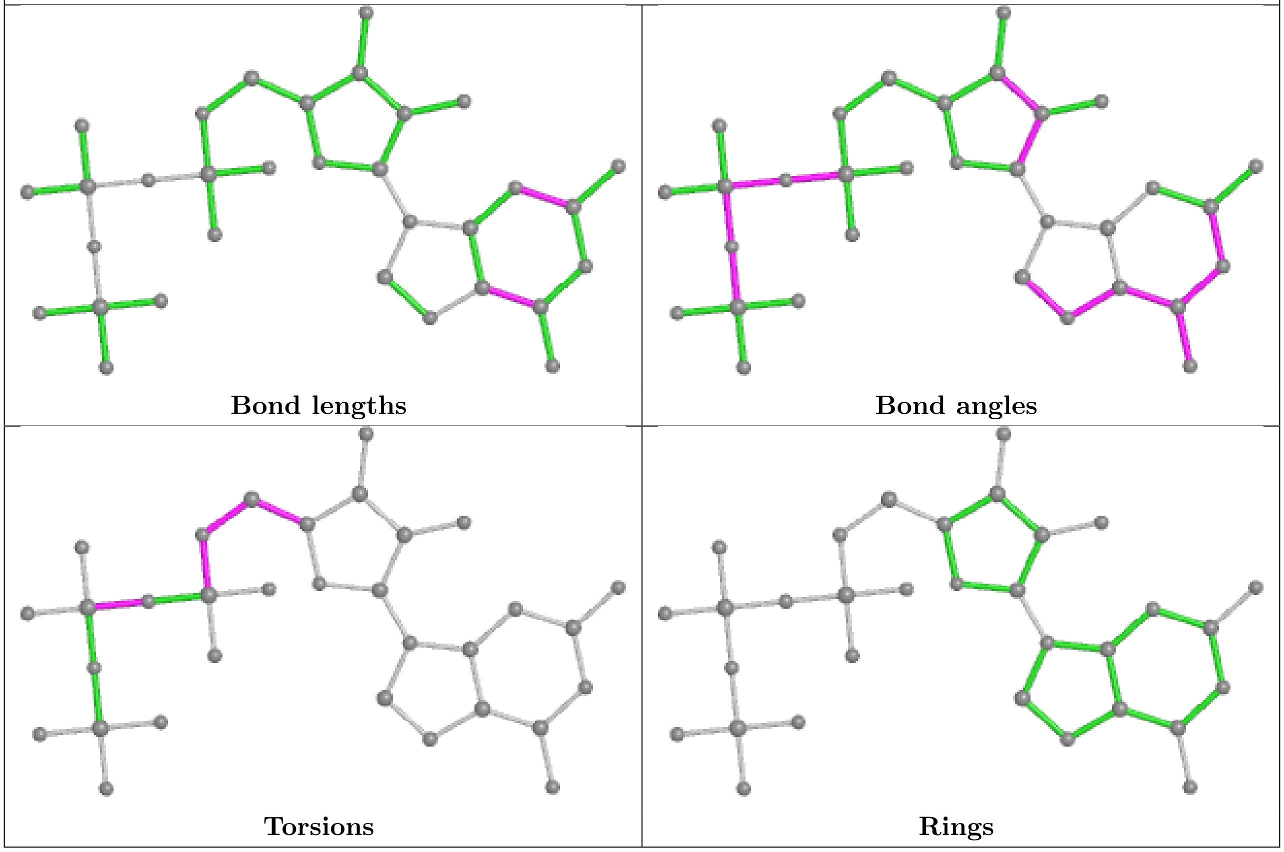
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP PM 501



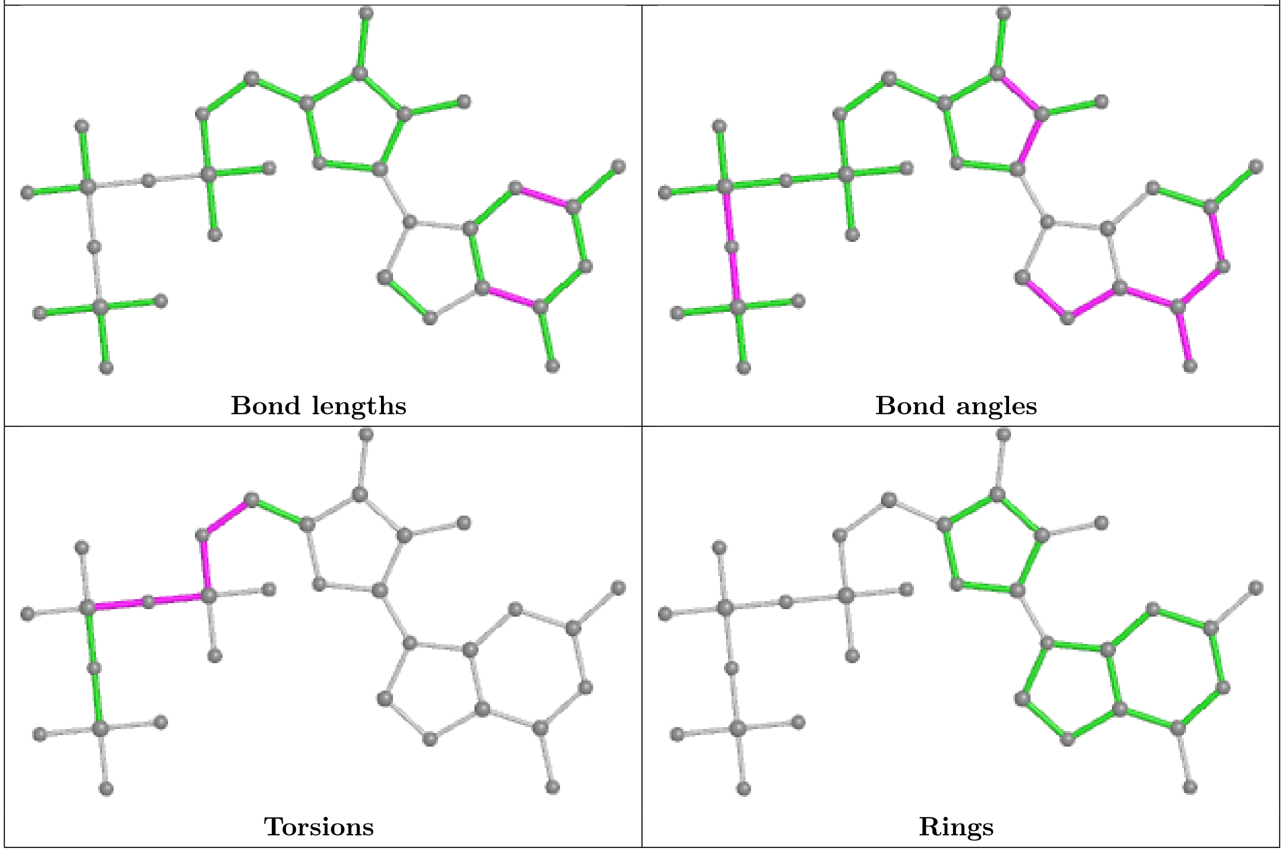
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP FI 501



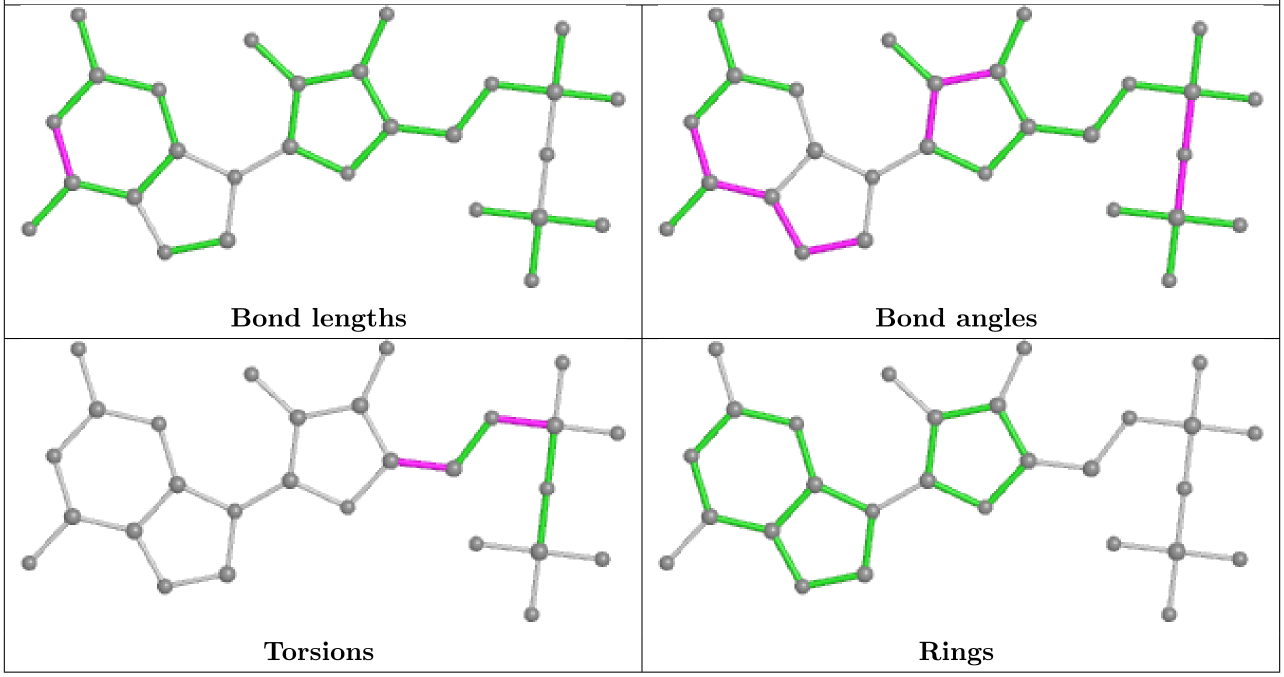
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP KB 502



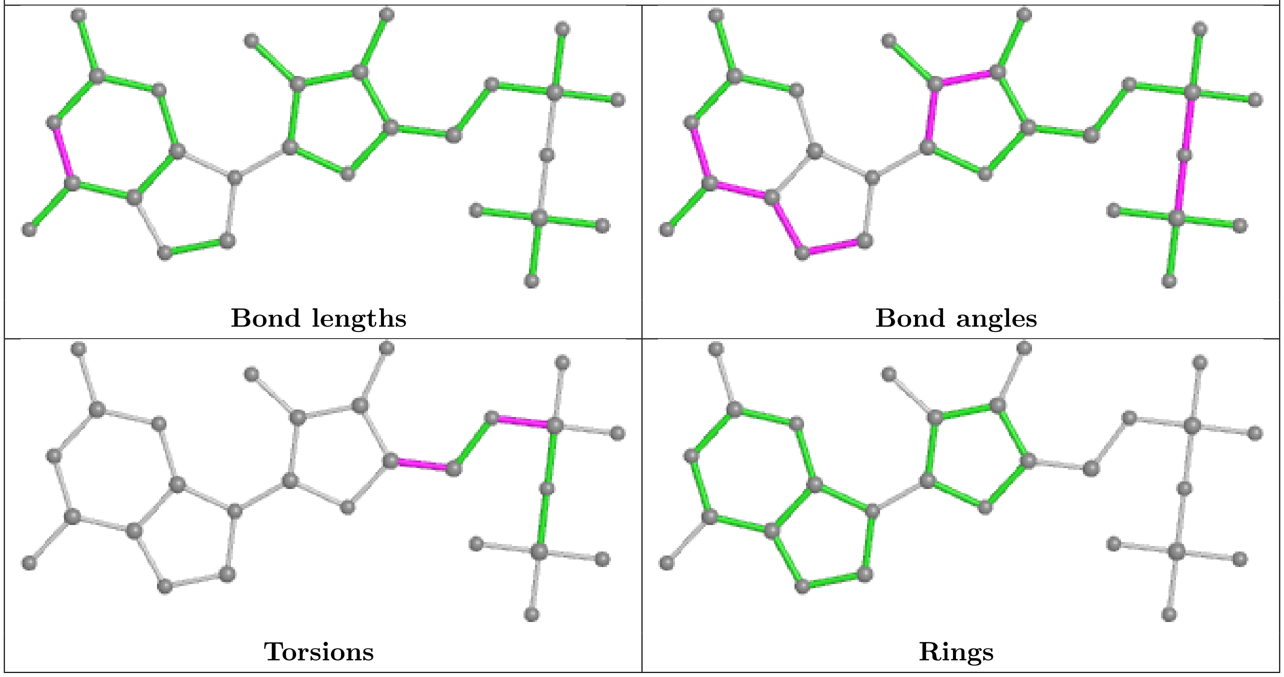
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP WP 502



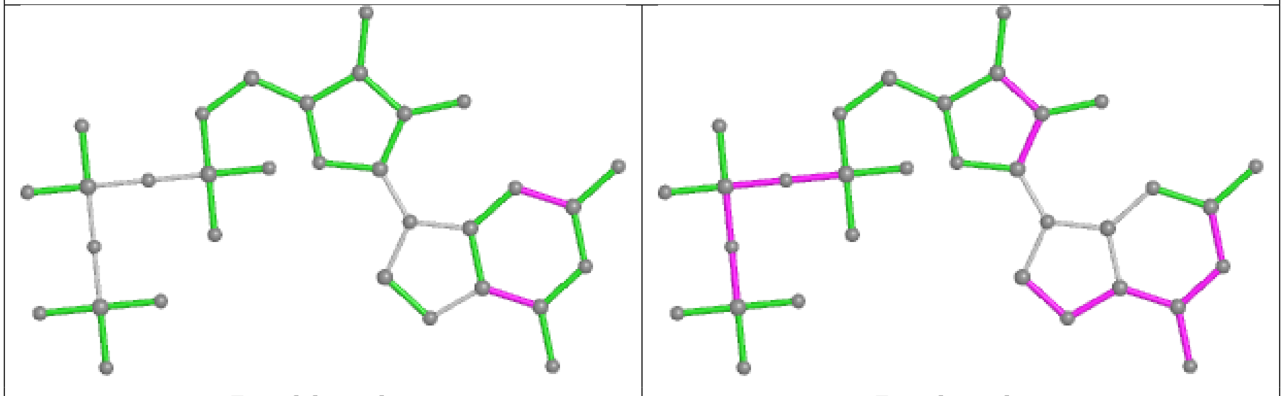
Bond lengths

Bond angles

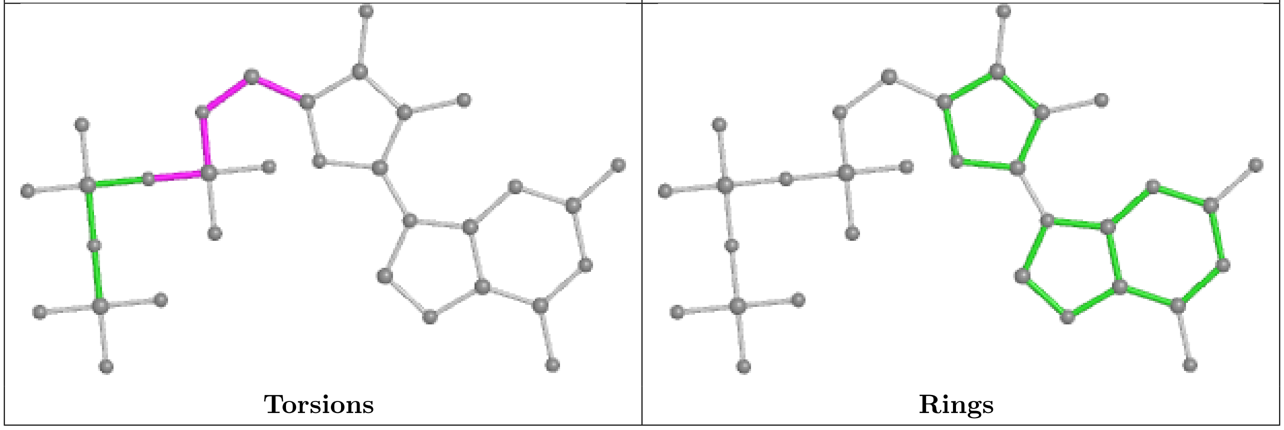
Torsions

Rings

Ligand GTP BA 501

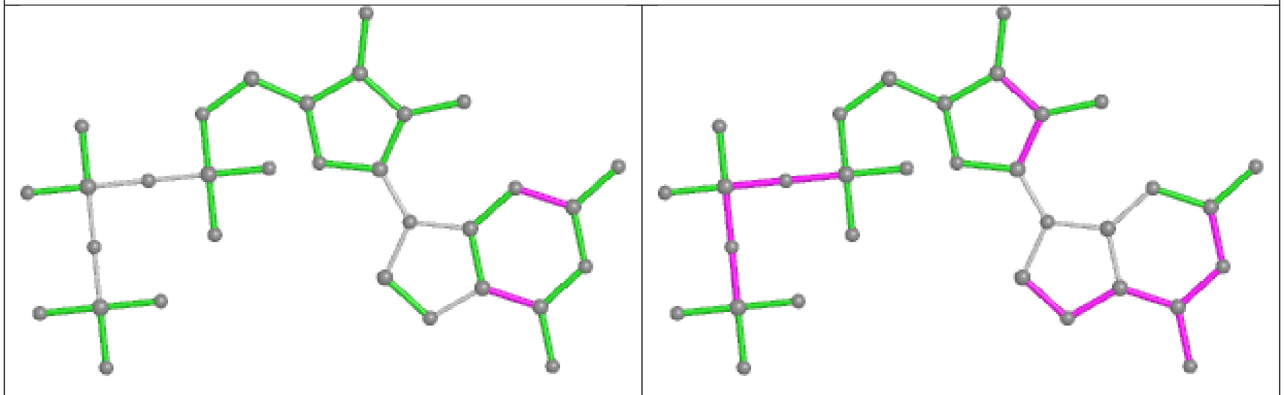


Bond lengths Bond angles

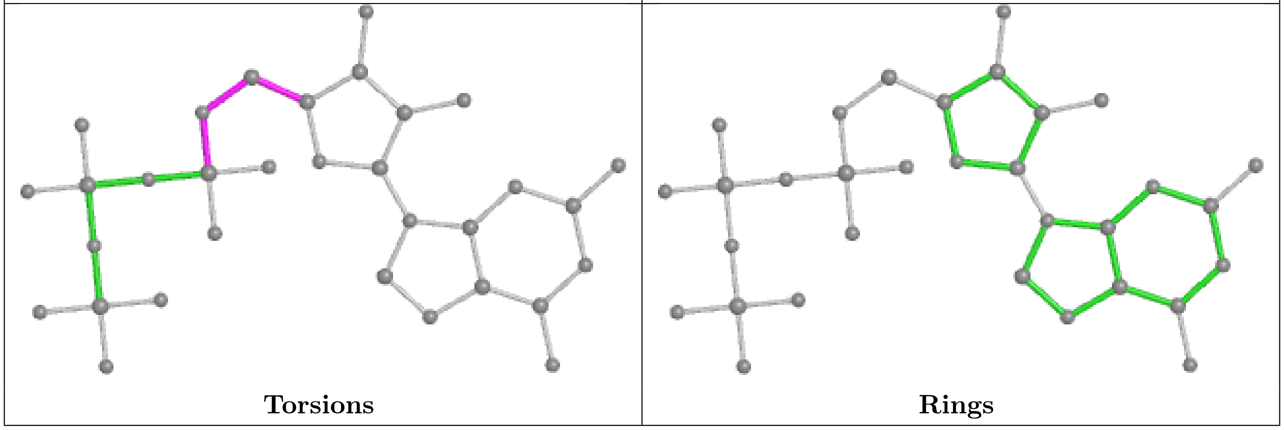


Torsions Rings

Ligand GTP QI 501

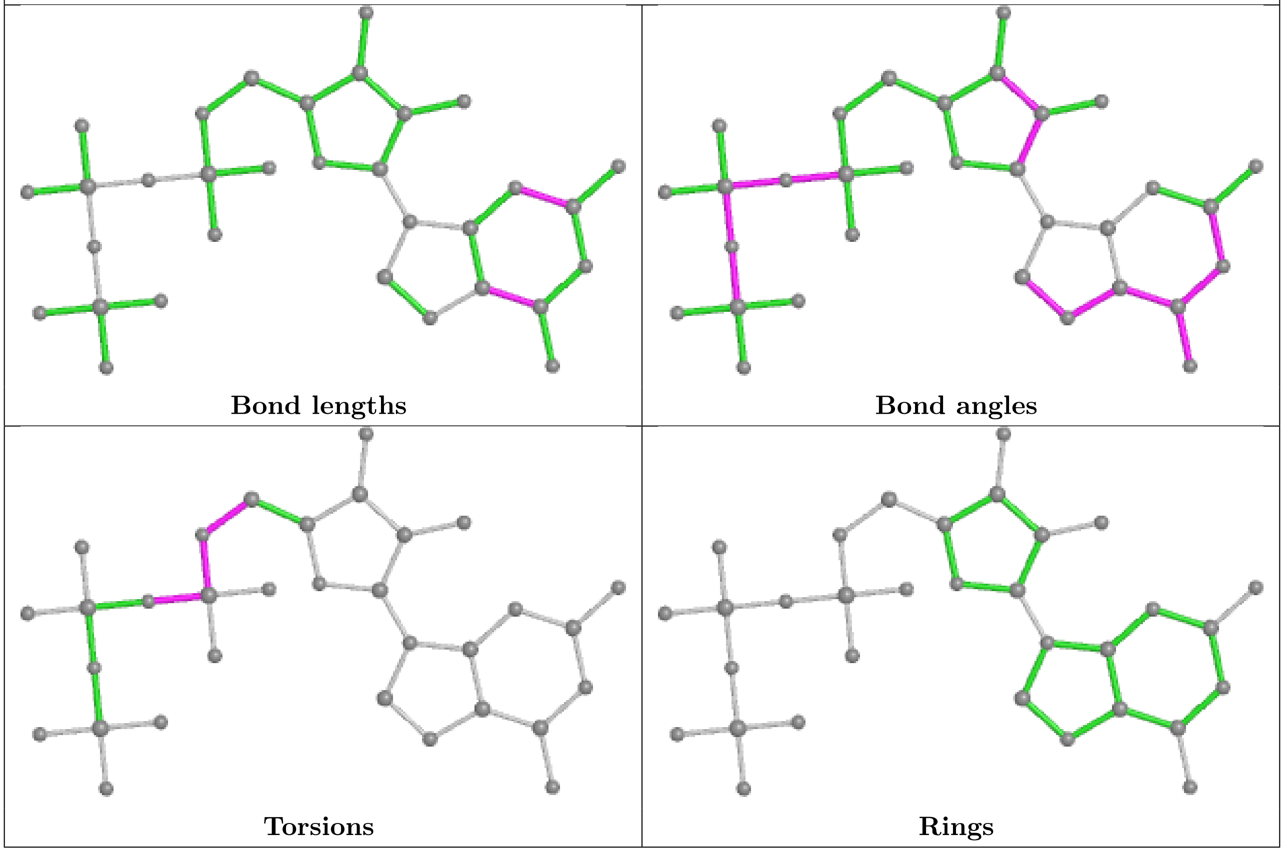


Bond lengths Bond angles



Torsions Rings

Ligand GTP AK 501



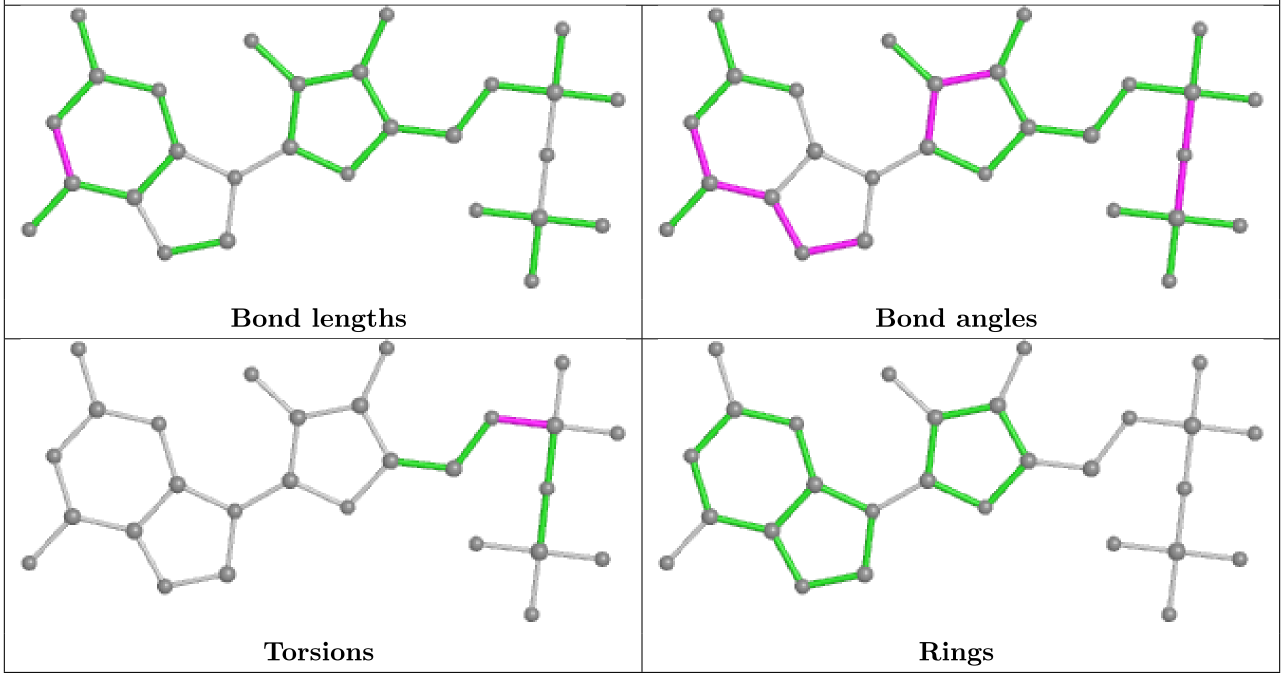
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP QJ 502



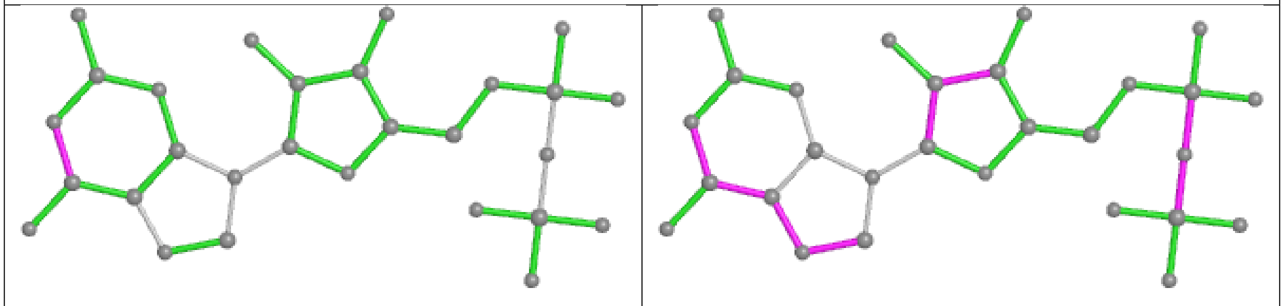
Bond lengths

Bond angles

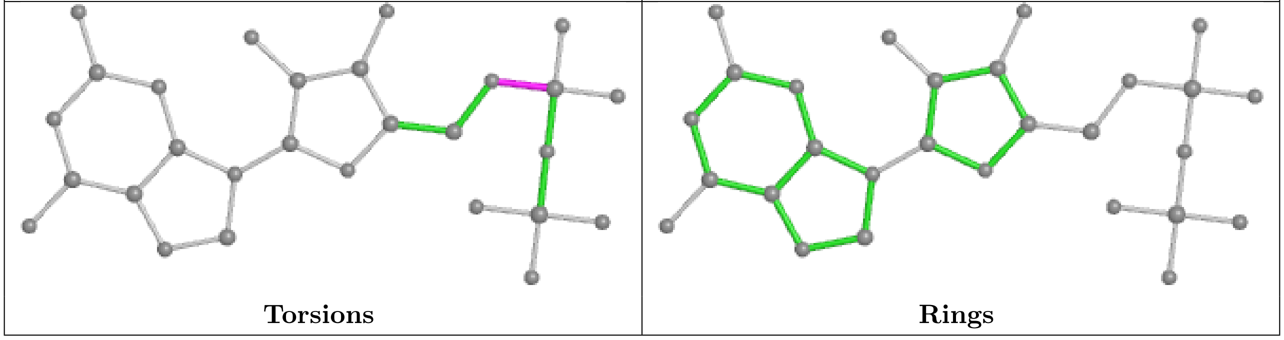
Torsions

Rings

Ligand GDP HJ 502

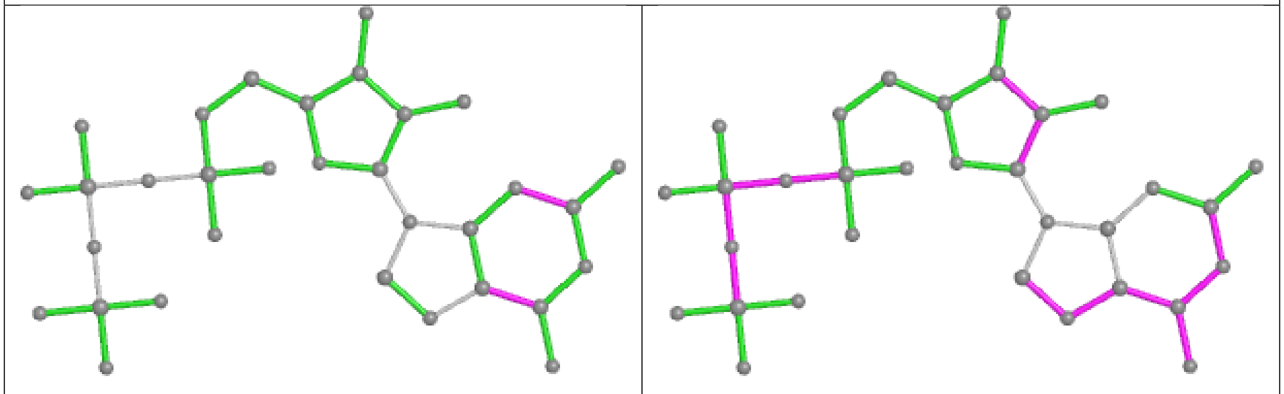


Bond lengths **Bond angles**

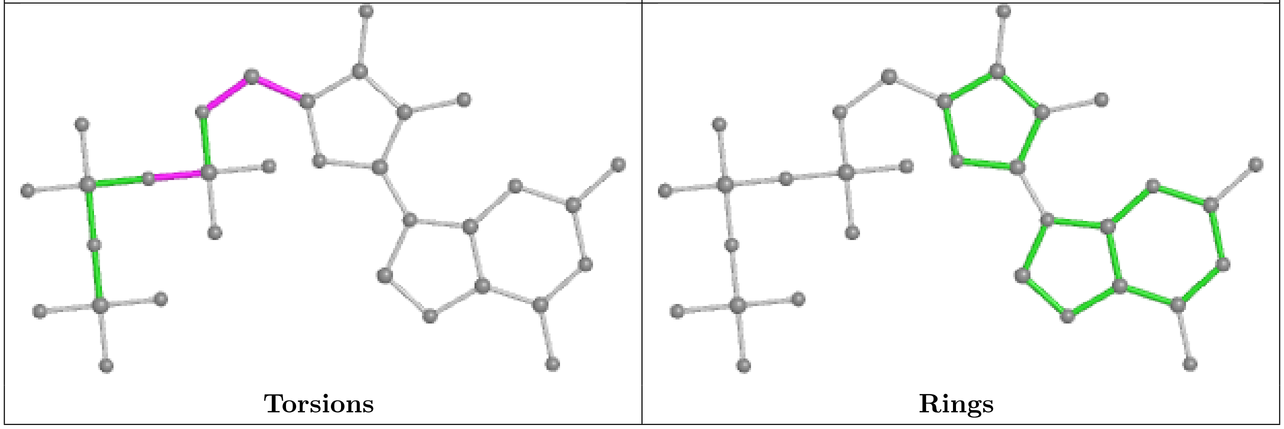


Torsions **Rings**

Ligand GTP BE 501

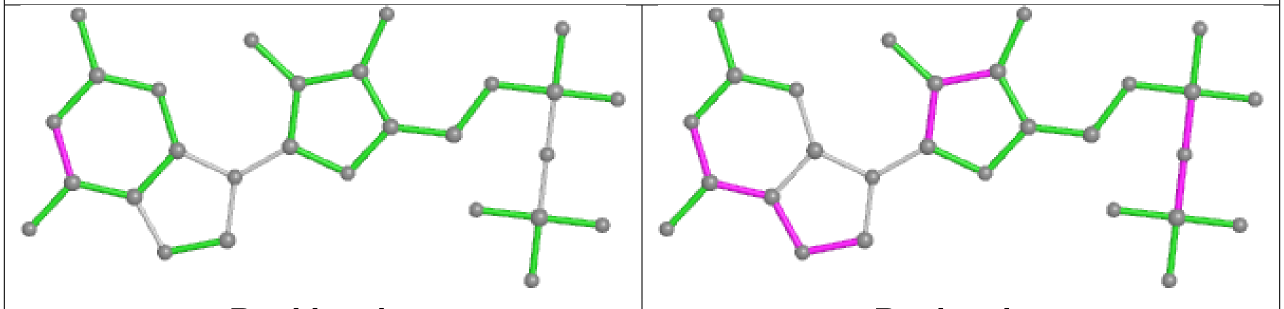


Bond lengths **Bond angles**

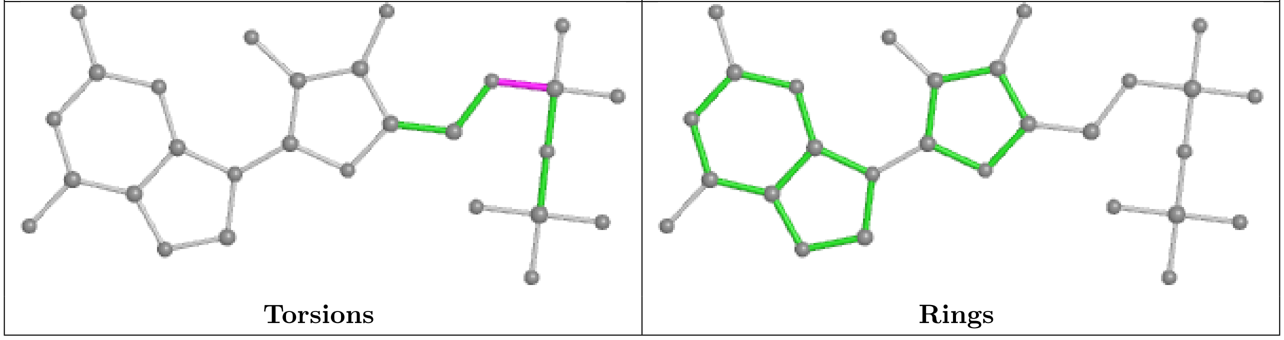


Torsions **Rings**

Ligand GDP NN 502

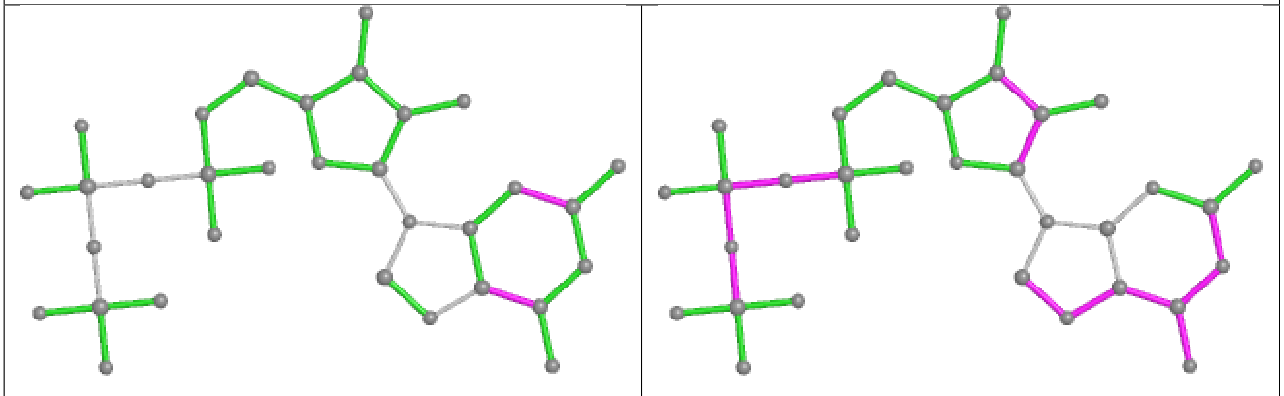


Bond lengths **Bond angles**

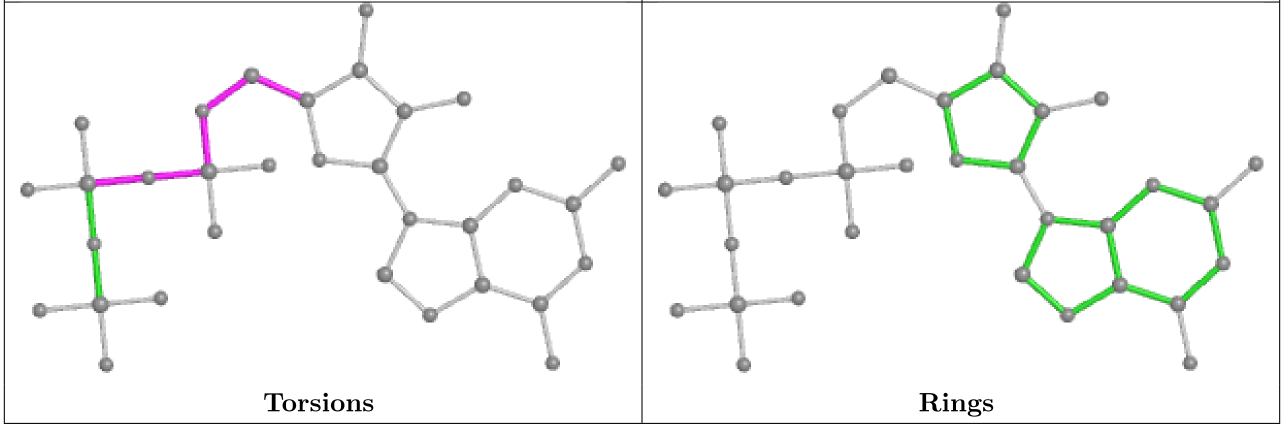


Torsions **Rings**

Ligand GTP QM 501

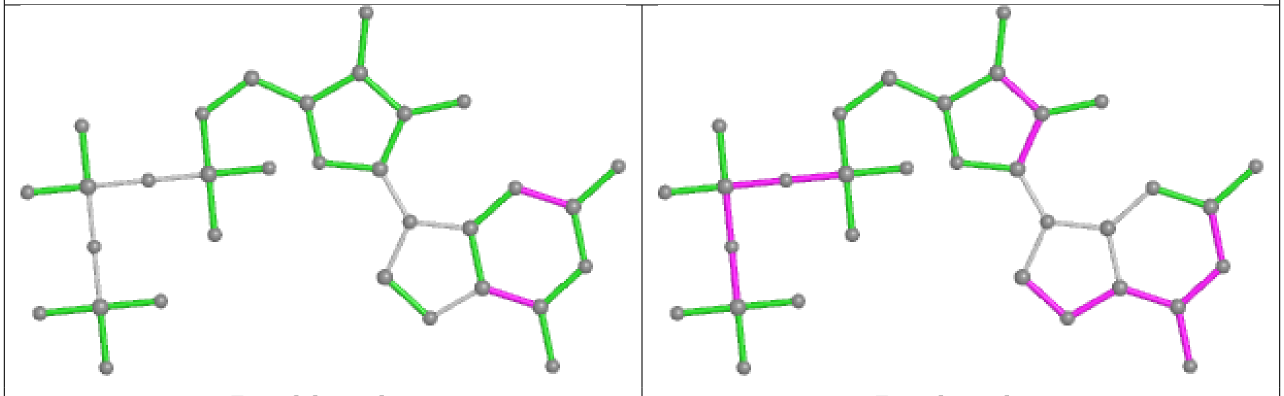


Bond lengths **Bond angles**



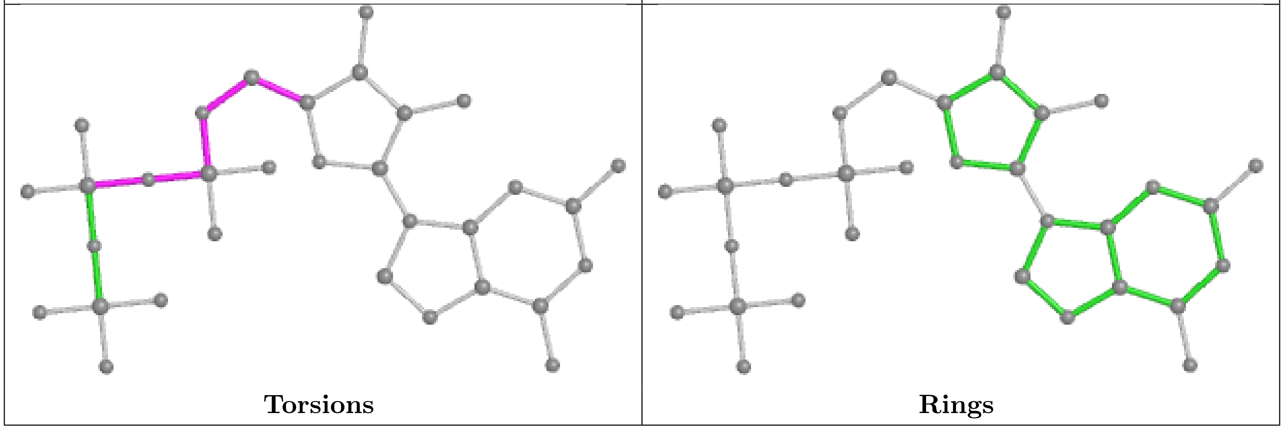
Torsions **Rings**

Ligand GTP HO 501



Bond lengths

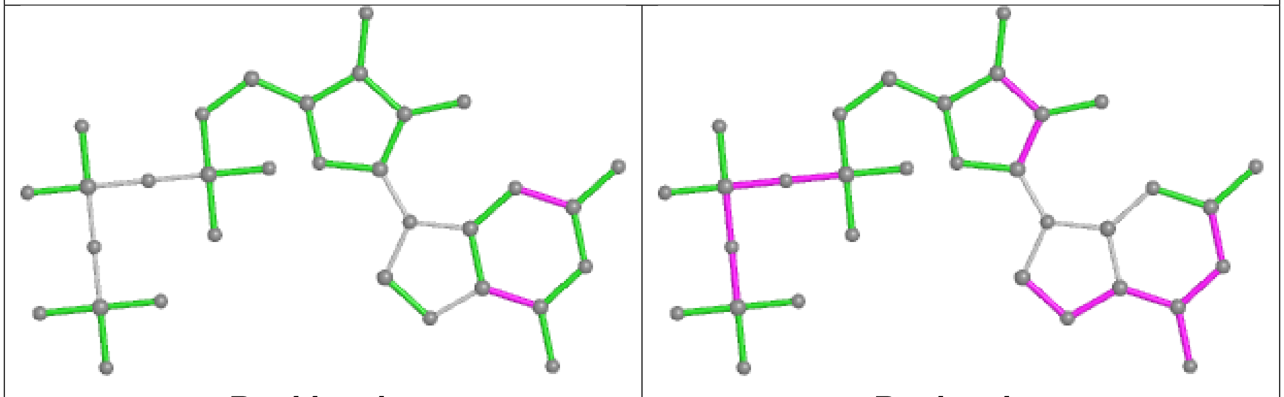
Bond angles



Torsions

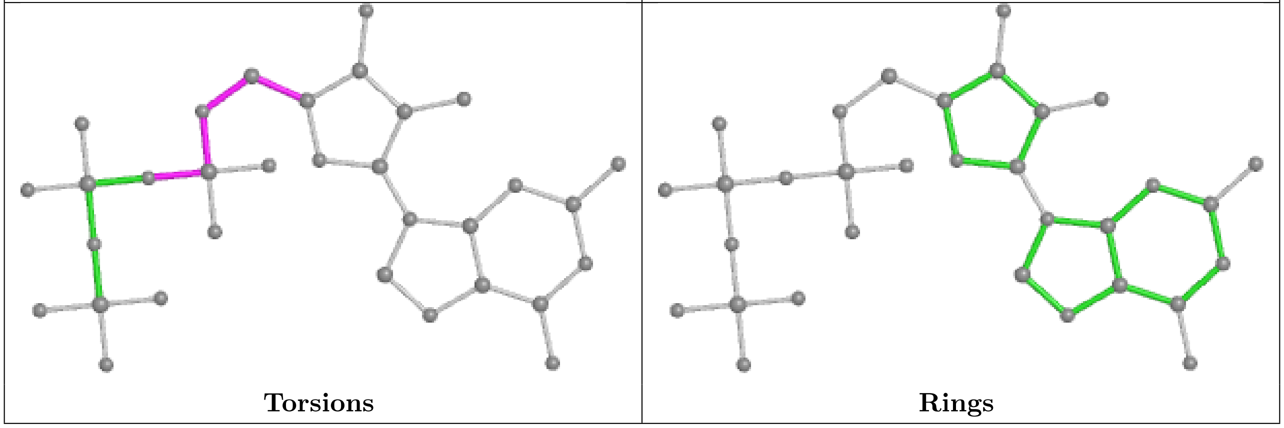
Rings

Ligand GTP TK 501



Bond lengths

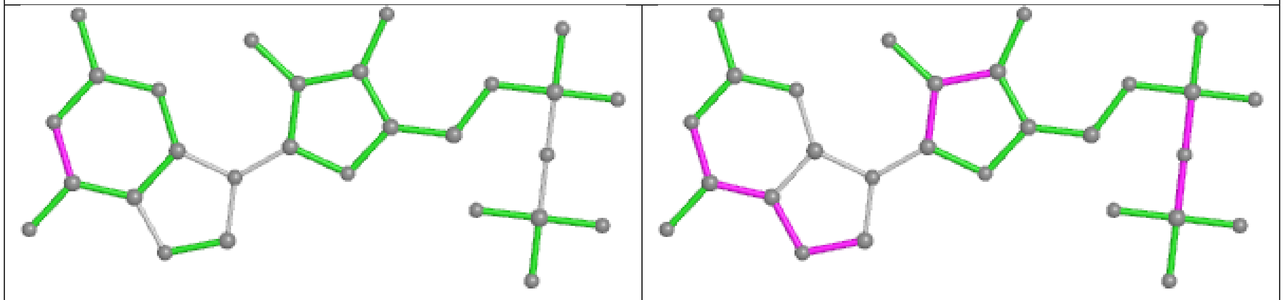
Bond angles



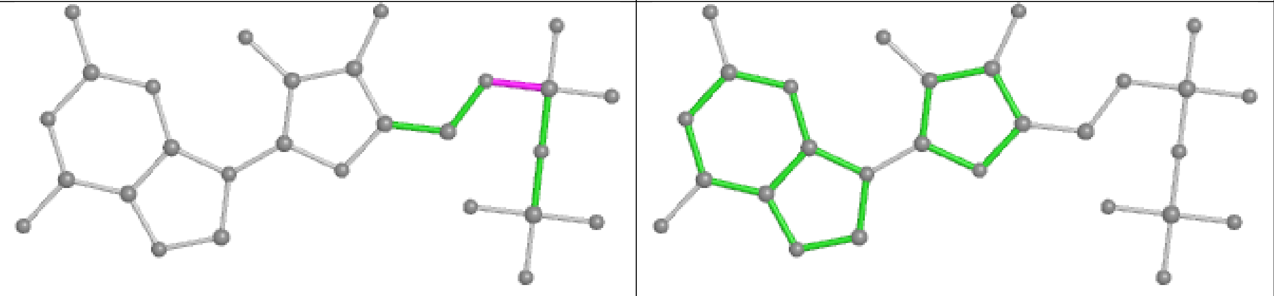
Torsions

Rings

Ligand GDP DJ 502

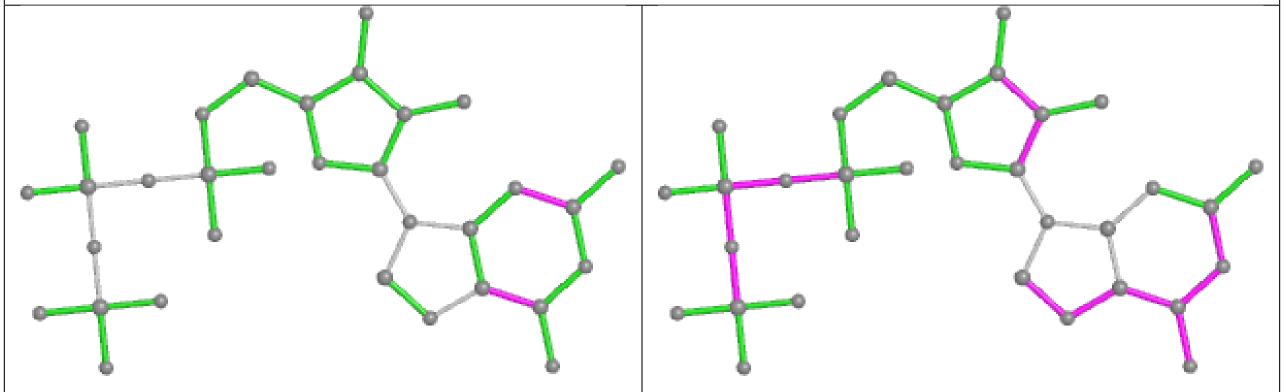


Bond lengths **Bond angles**

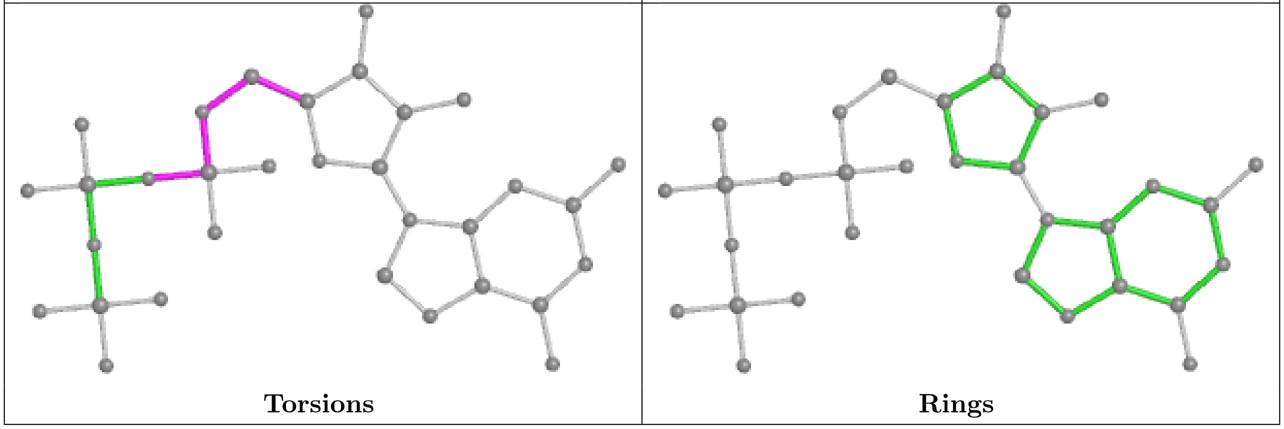


Torsions **Rings**

Ligand GTP ME 501

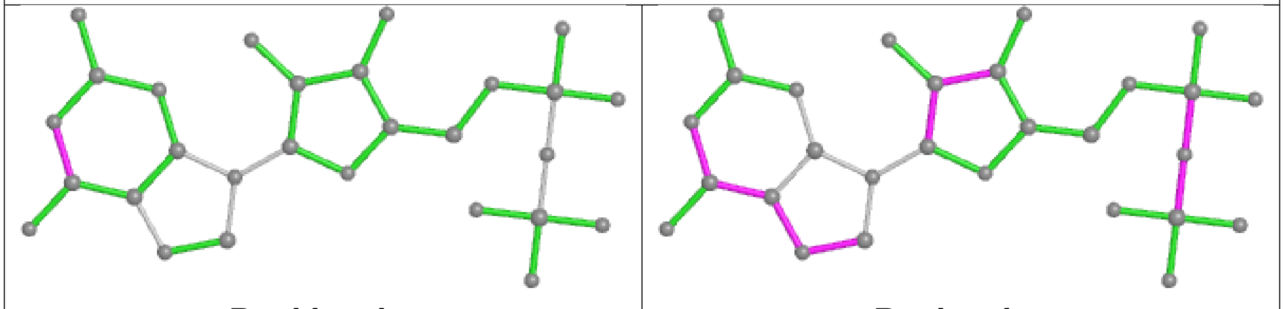


Bond lengths **Bond angles**

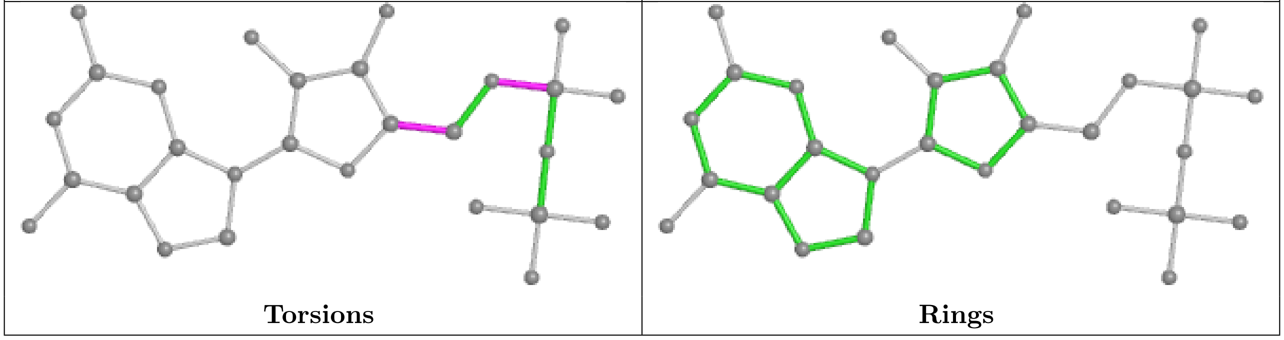


Torsions **Rings**

Ligand GDP OB 502

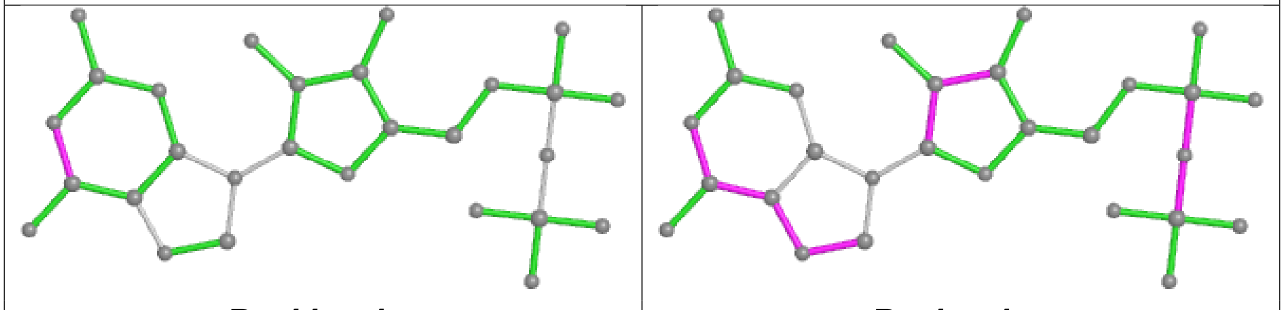


Bond lengths Bond angles

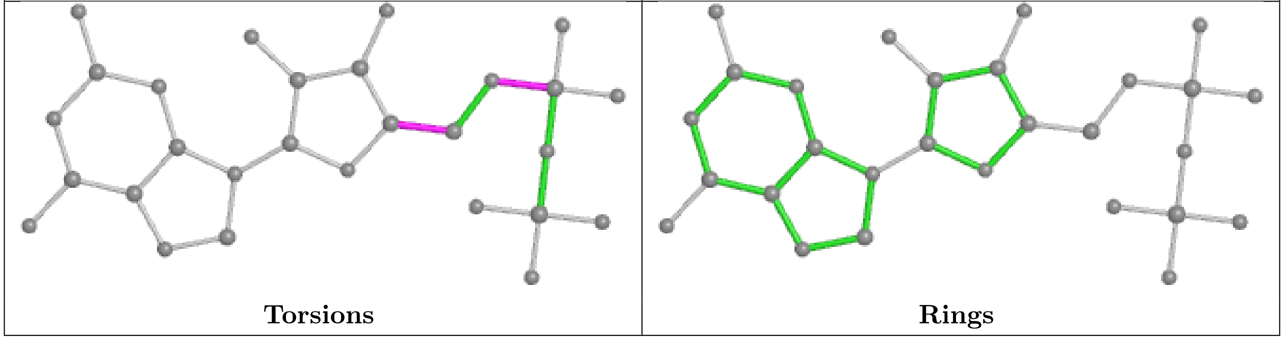


Torsions Rings

Ligand GDP QN 502

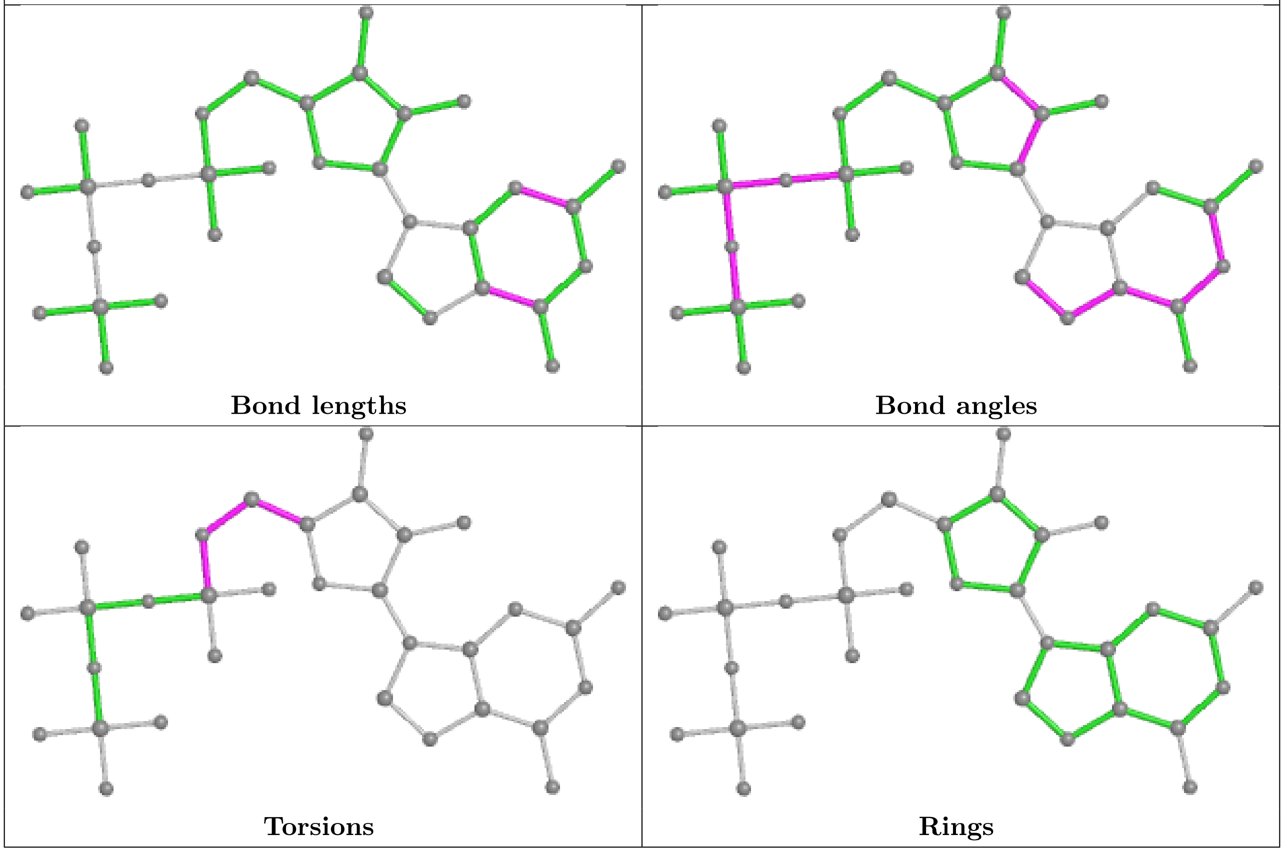


Bond lengths Bond angles

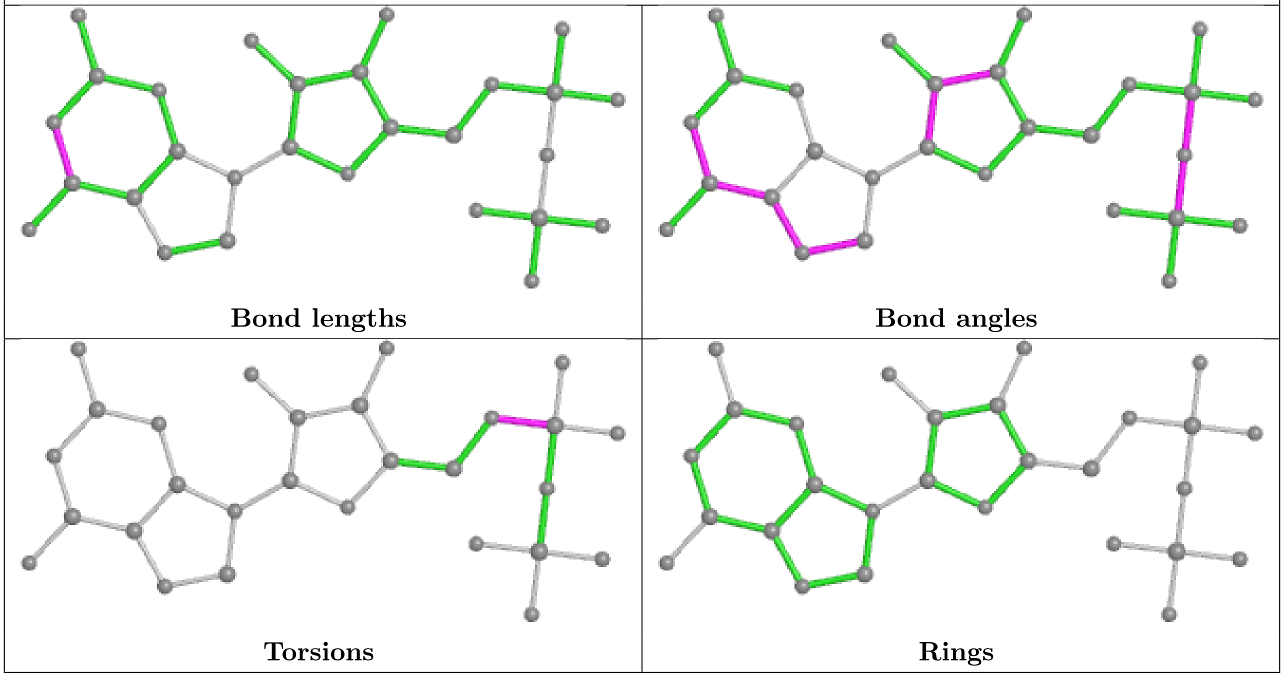


Torsions Rings

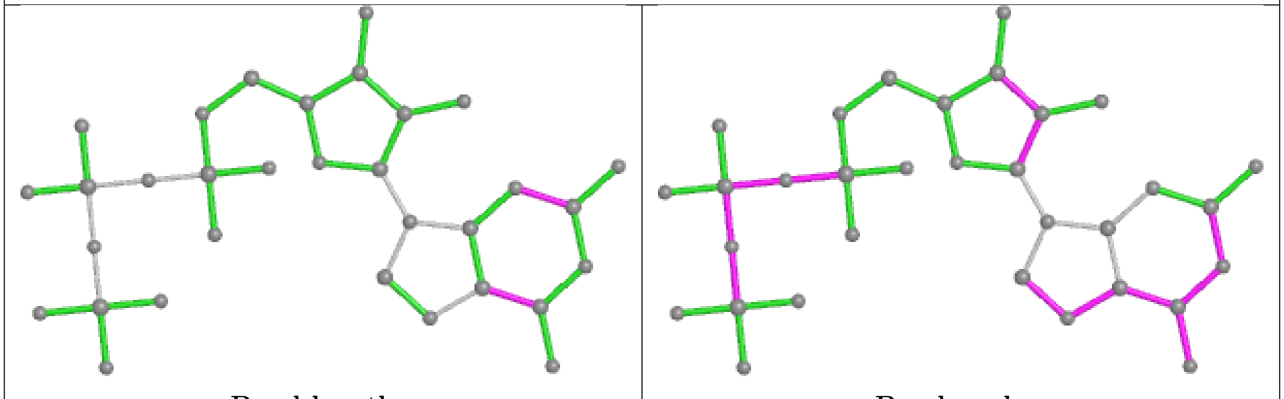
Ligand GTP WI 501



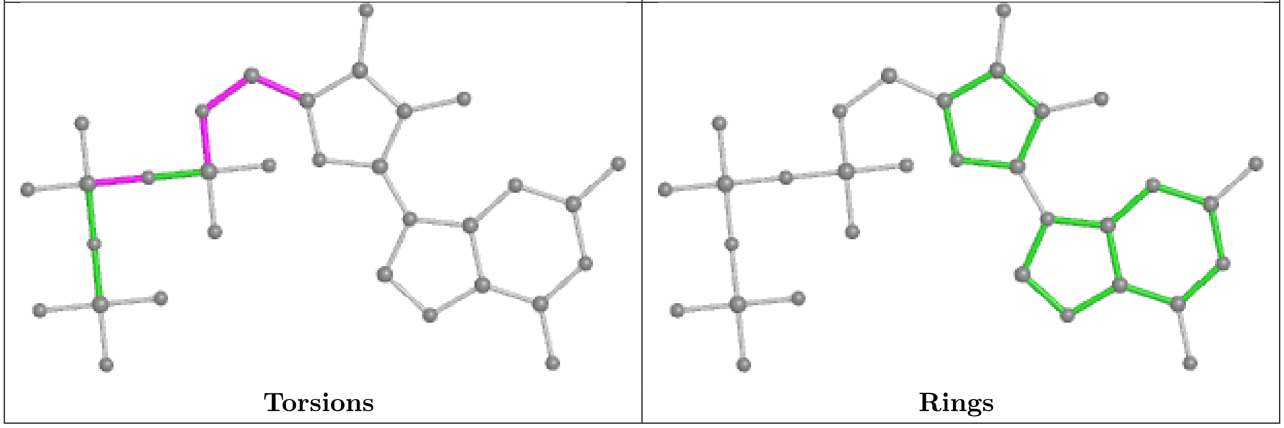
Ligand GDP NB 502



Ligand GTP LC 501

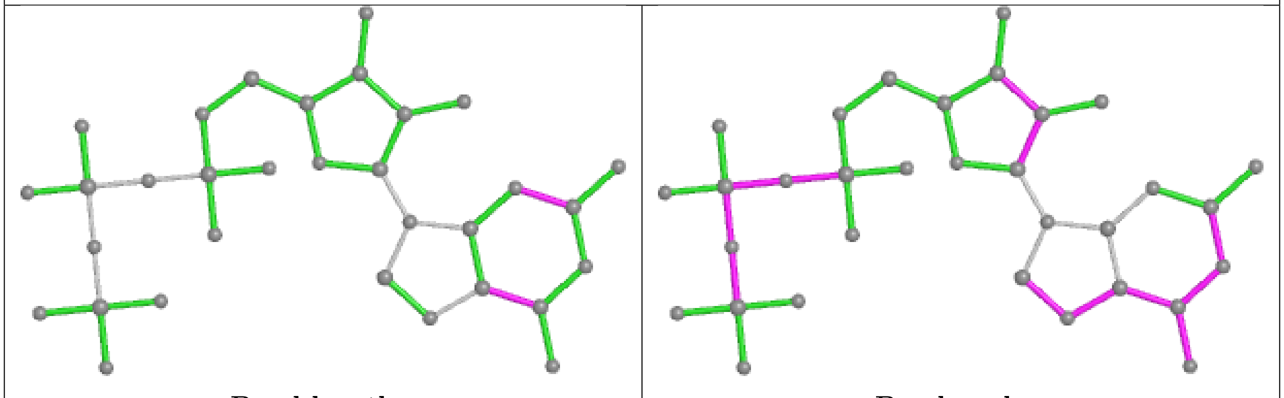


Bond lengths Bond angles

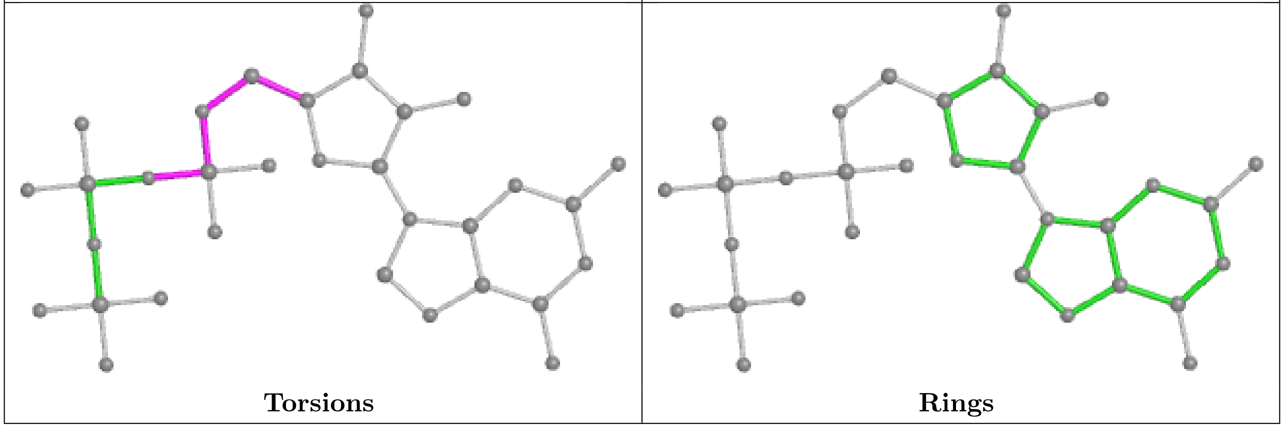


Torsions Rings

Ligand GTP GC 501

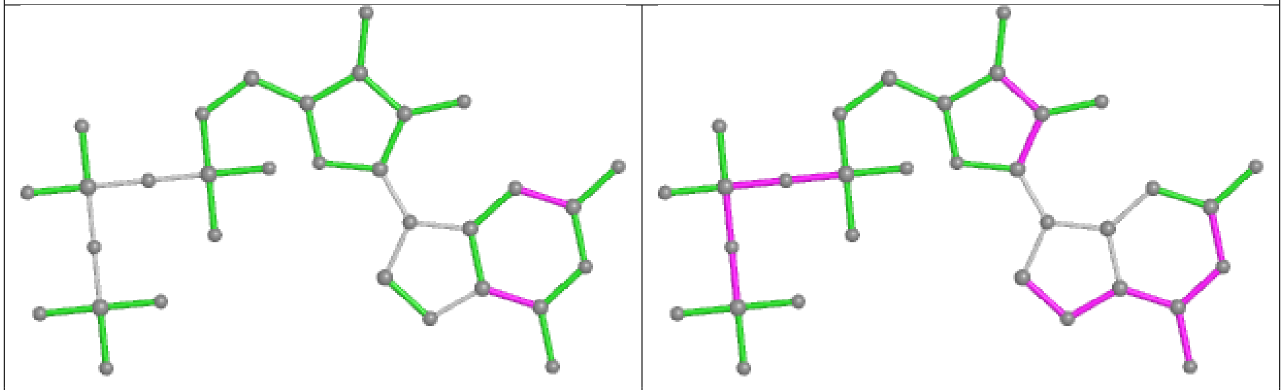


Bond lengths Bond angles

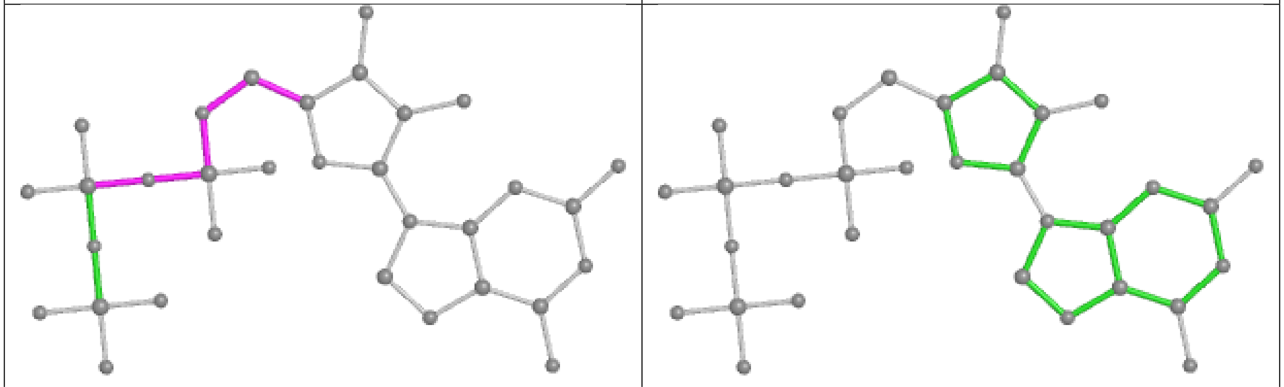


Torsions Rings

Ligand GTP QE 501

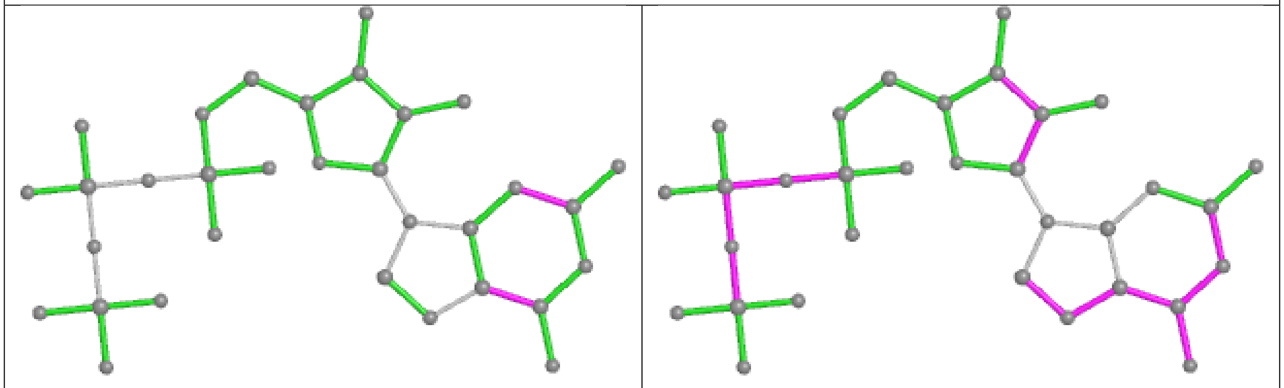


Bond lengths **Bond angles**

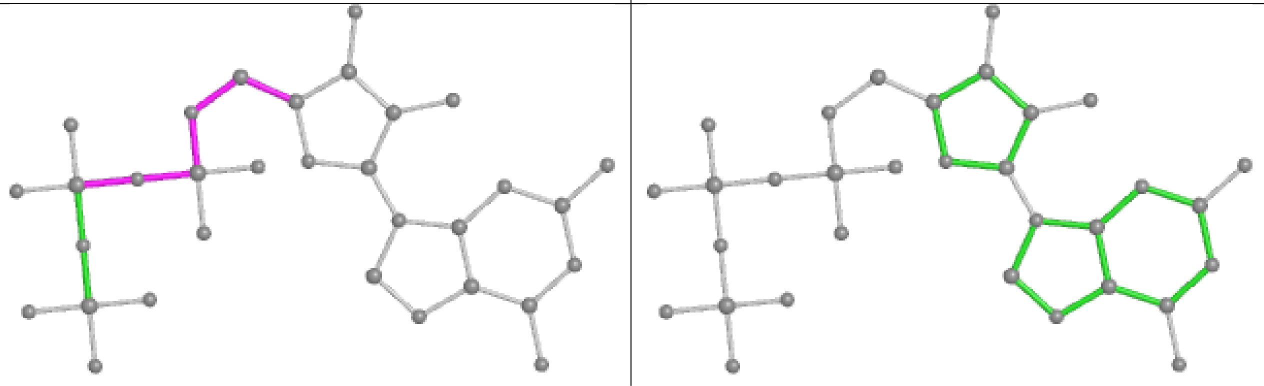


Torsions **Rings**

Ligand GTP VM 501

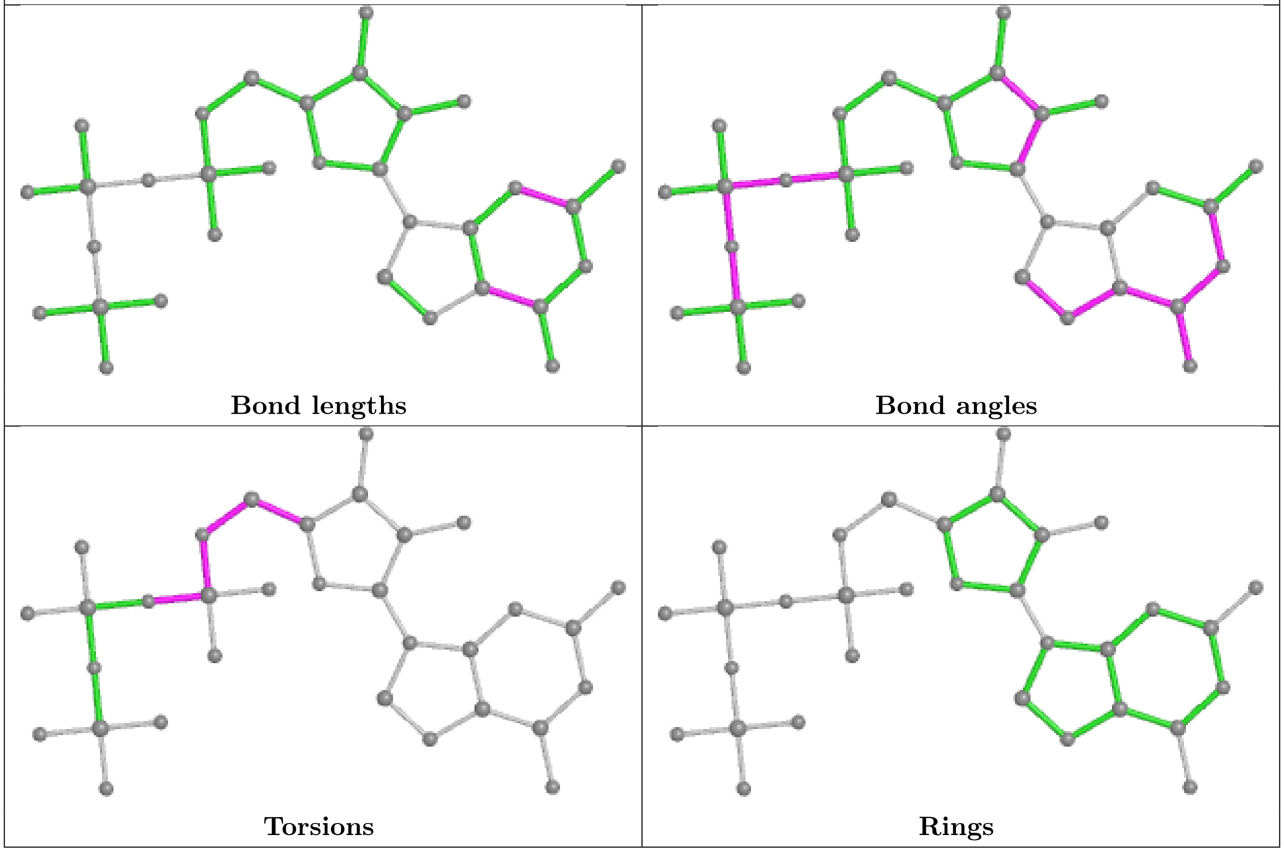


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GTP UO 501



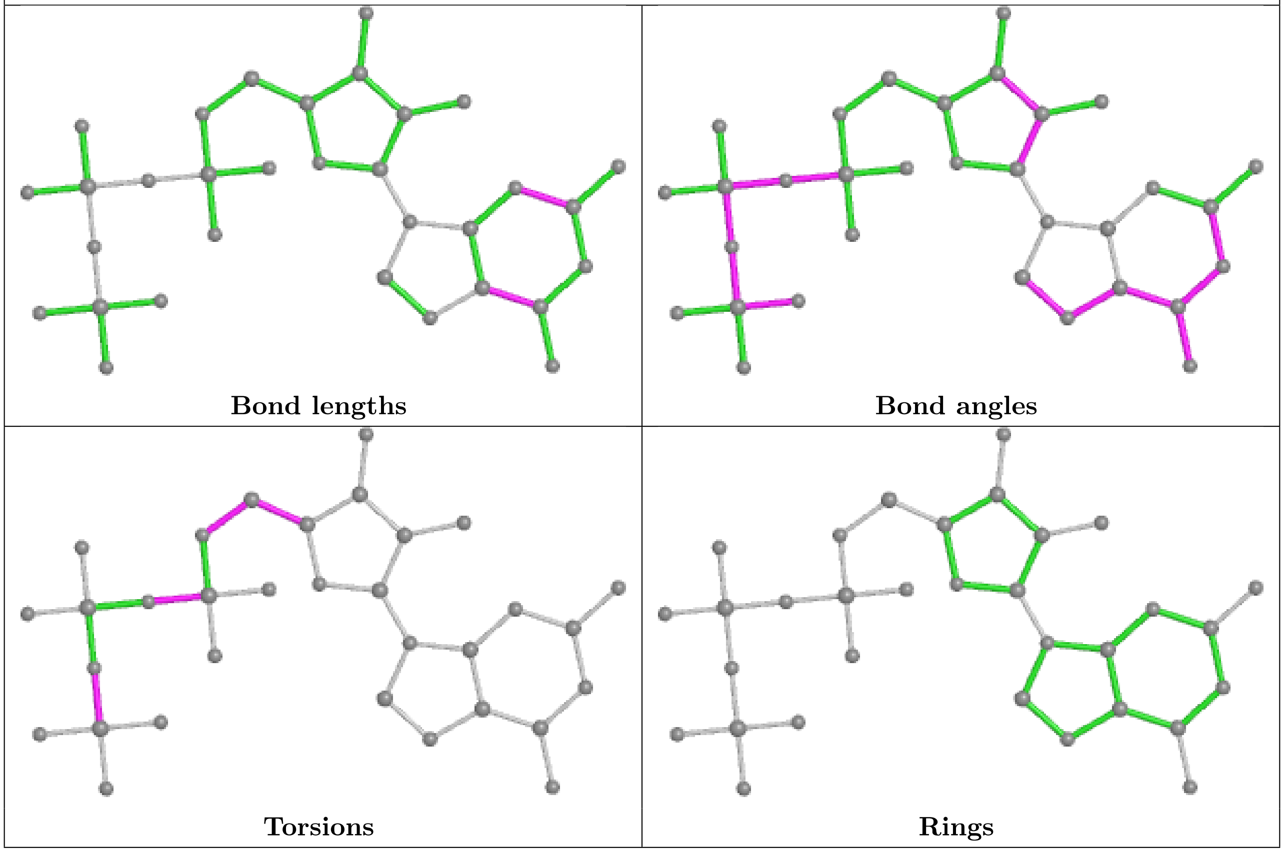
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP NG 501



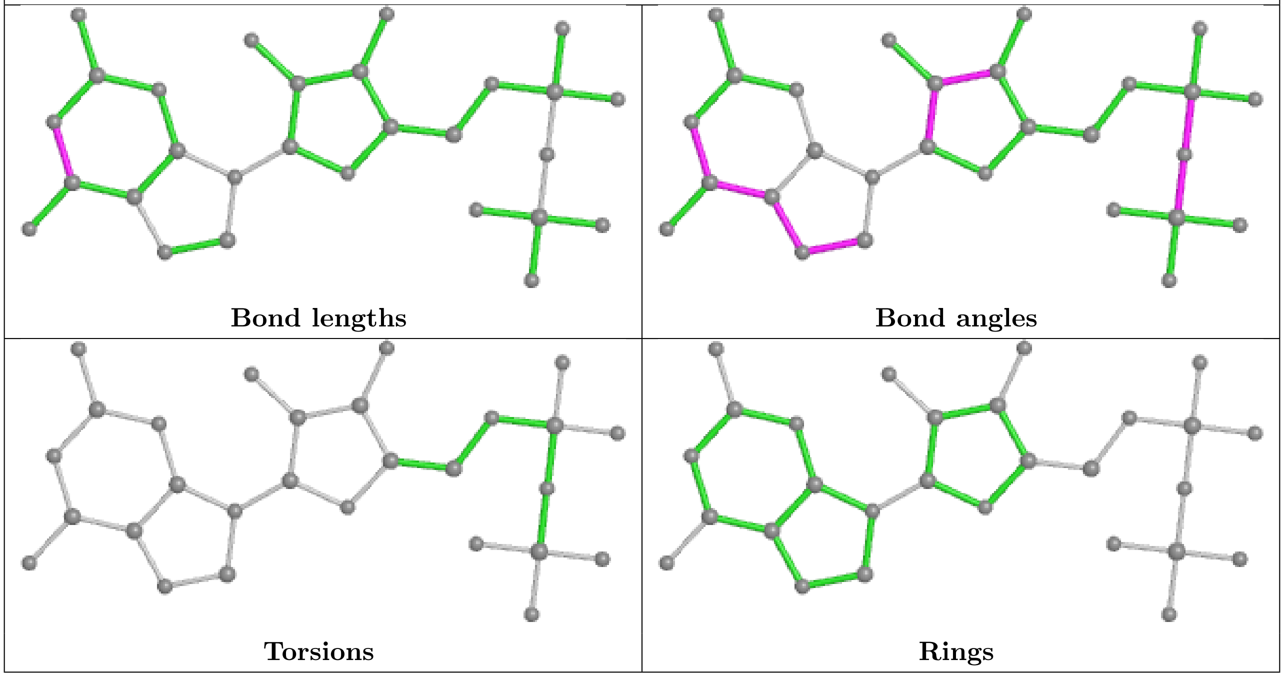
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP GL 502



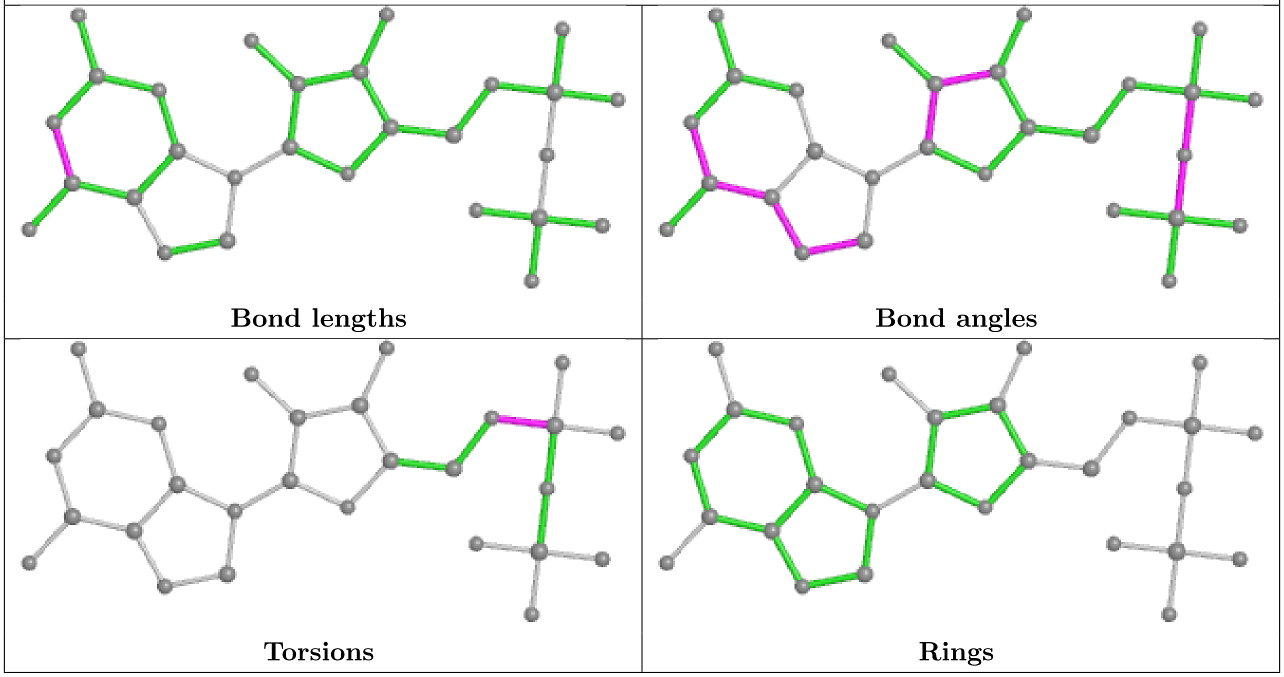
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP IJ 502



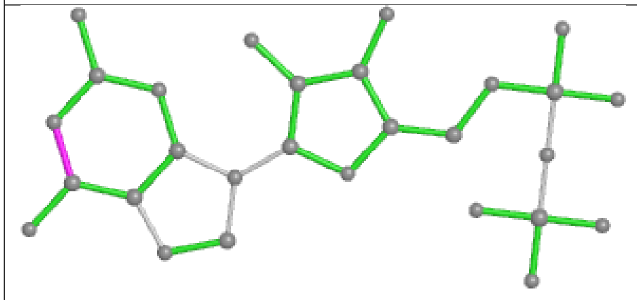
Bond lengths

Bond angles

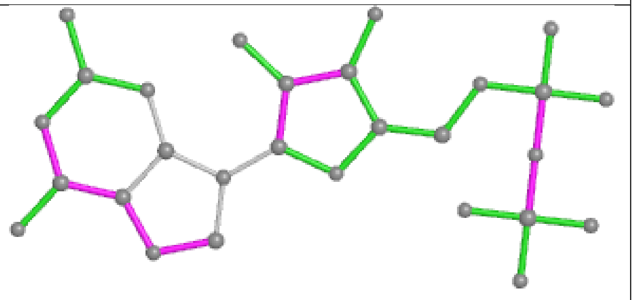
Torsions

Rings

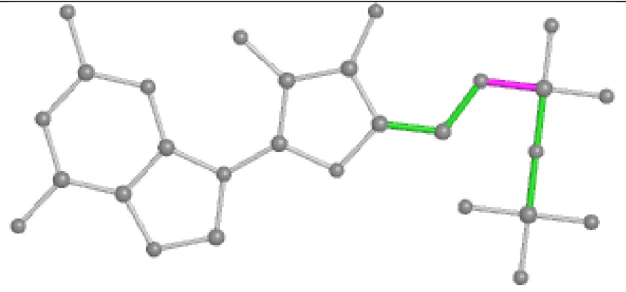
Ligand GDP EJ 502



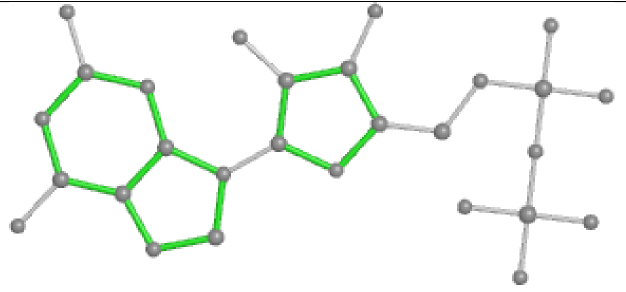
Bond lengths



Bond angles

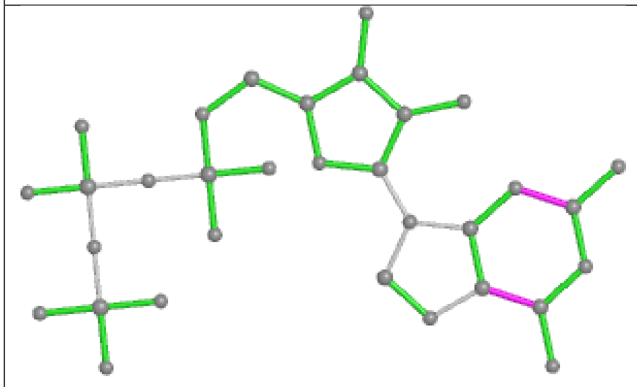


Torsions

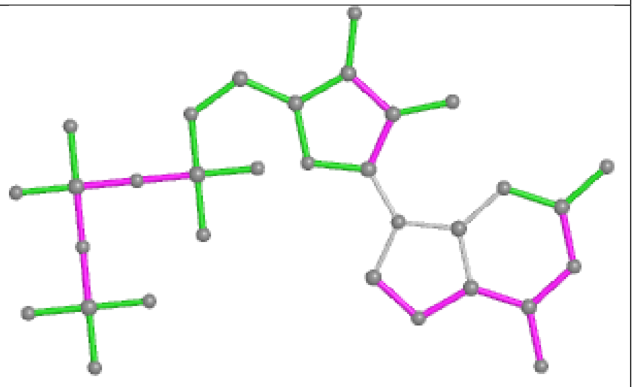


Rings

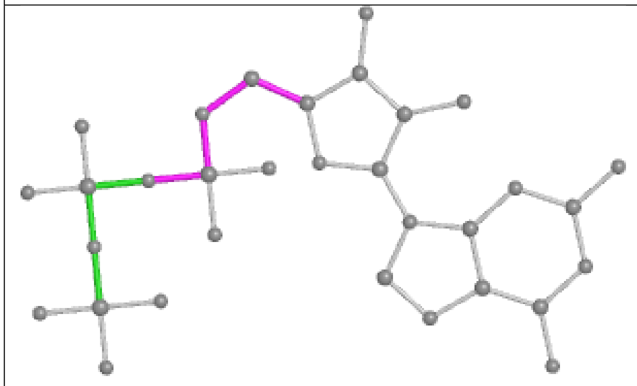
Ligand GTP BK 501



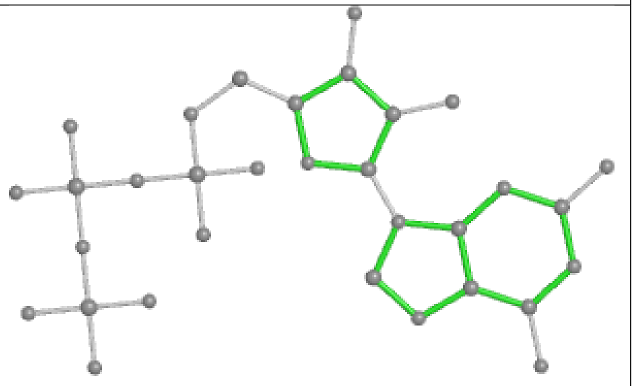
Bond lengths



Bond angles

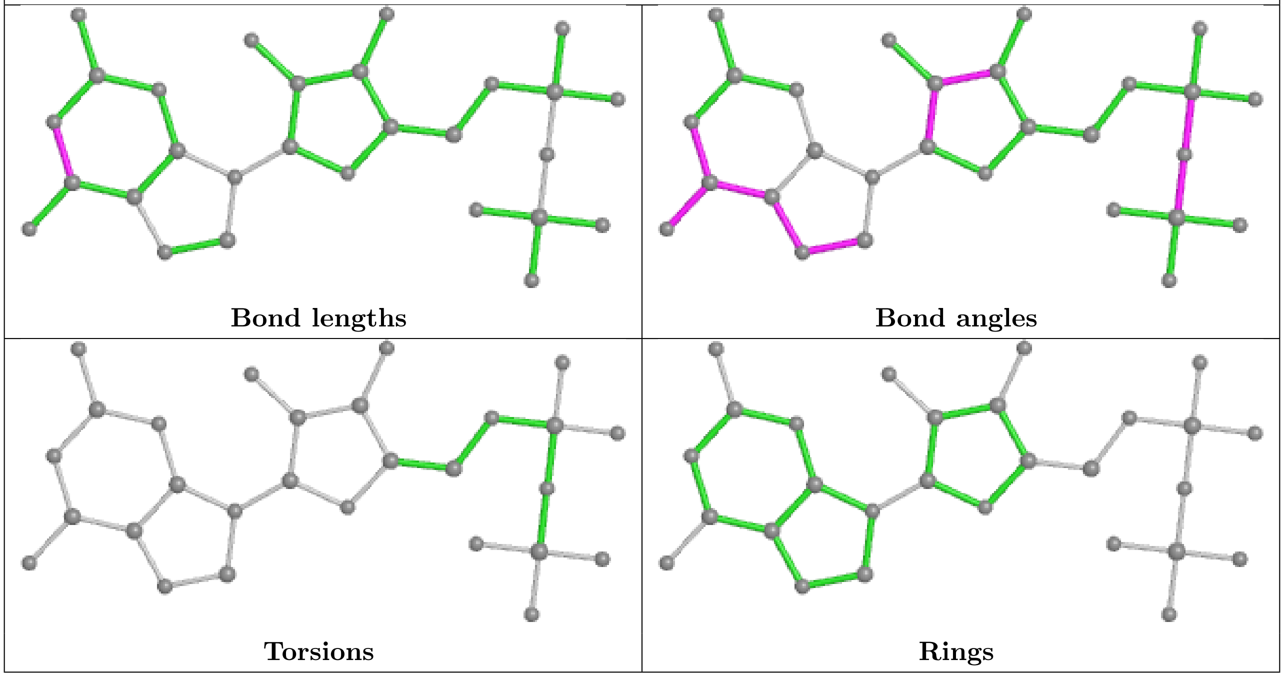


Torsions



Rings

Ligand GDP EF 502



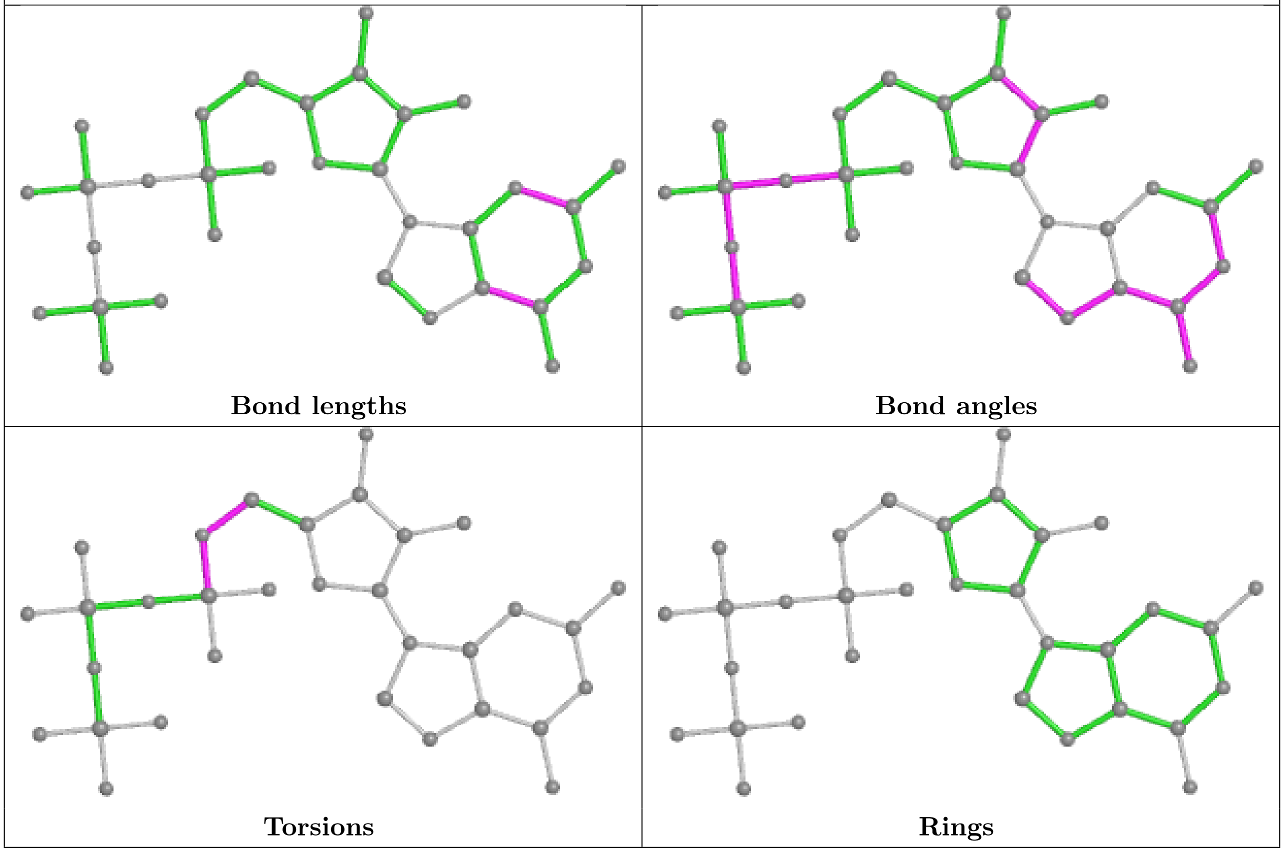
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP RE 501



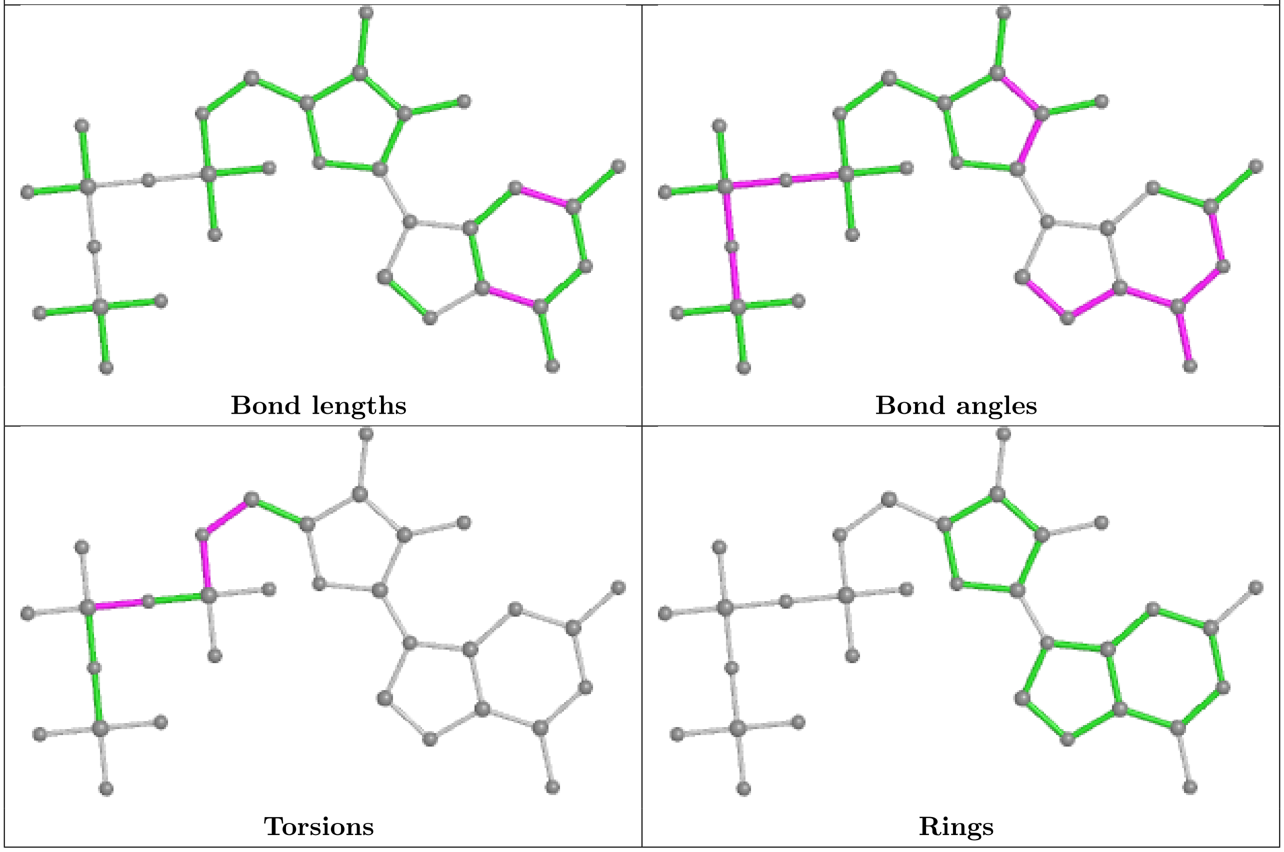
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP LK 501



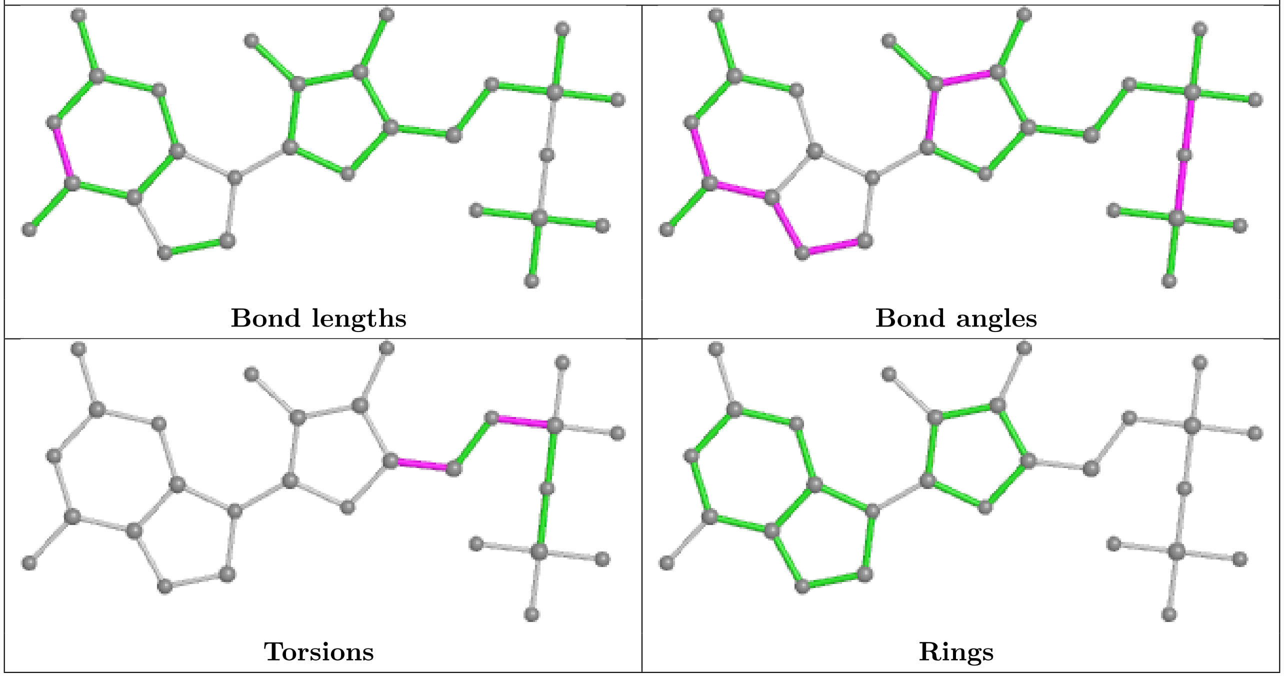
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP ON 502



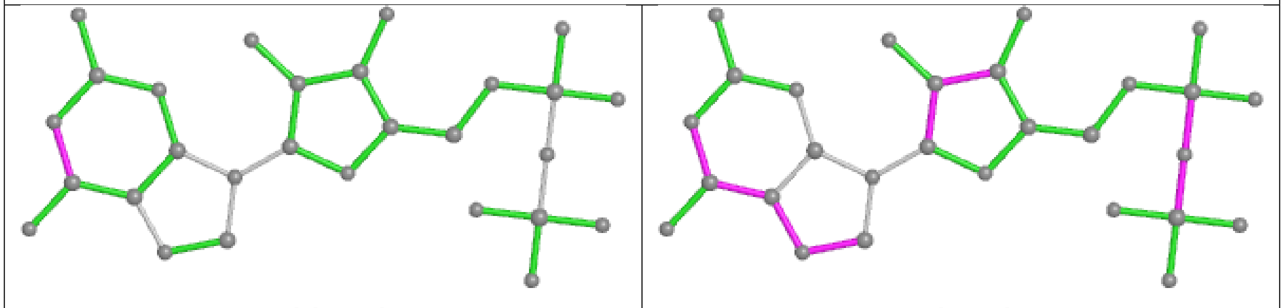
Bond lengths

Bond angles

Torsions

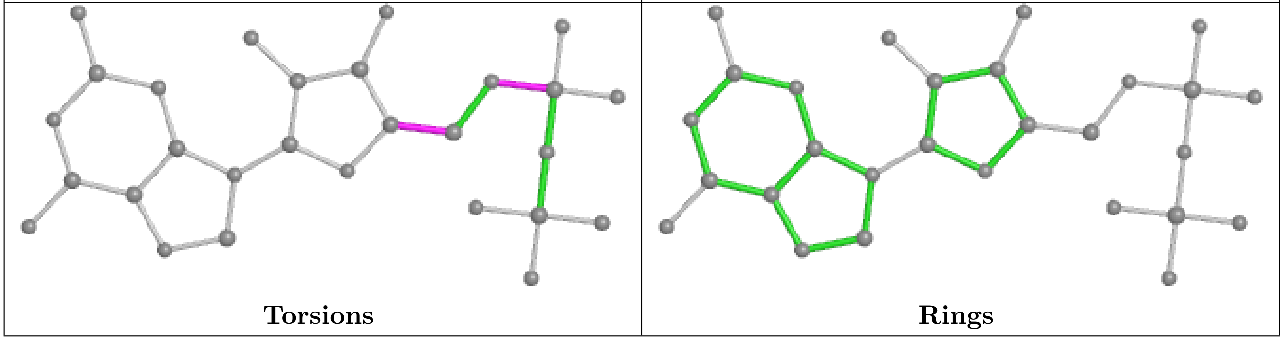
Rings

Ligand GDP UJ 502



Bond lengths

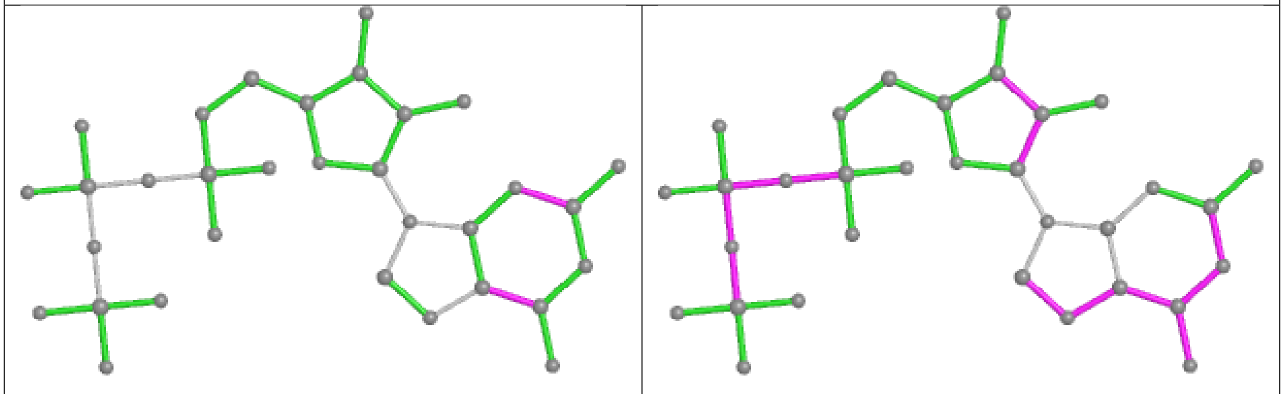
Bond angles



Torsions

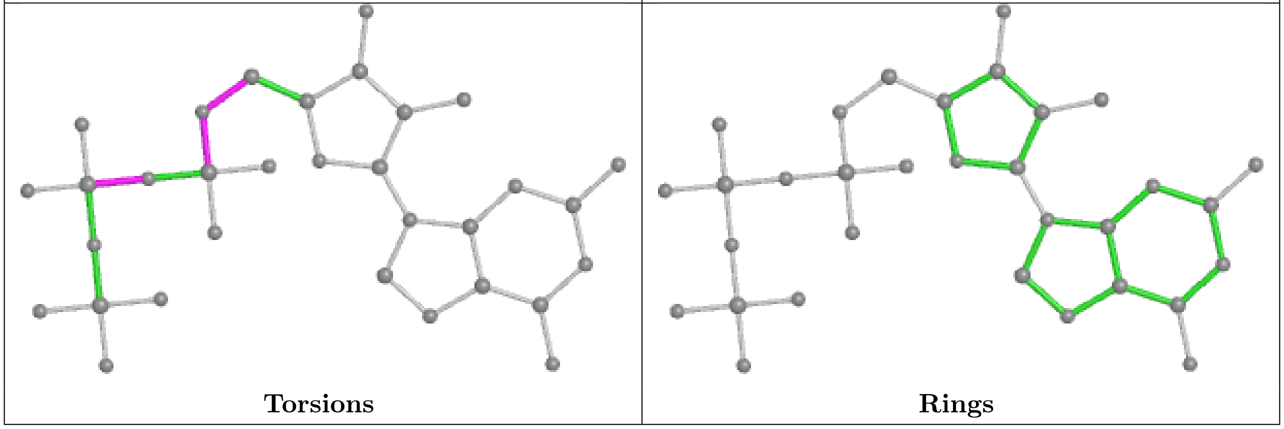
Rings

Ligand GTP KM 501



Bond lengths

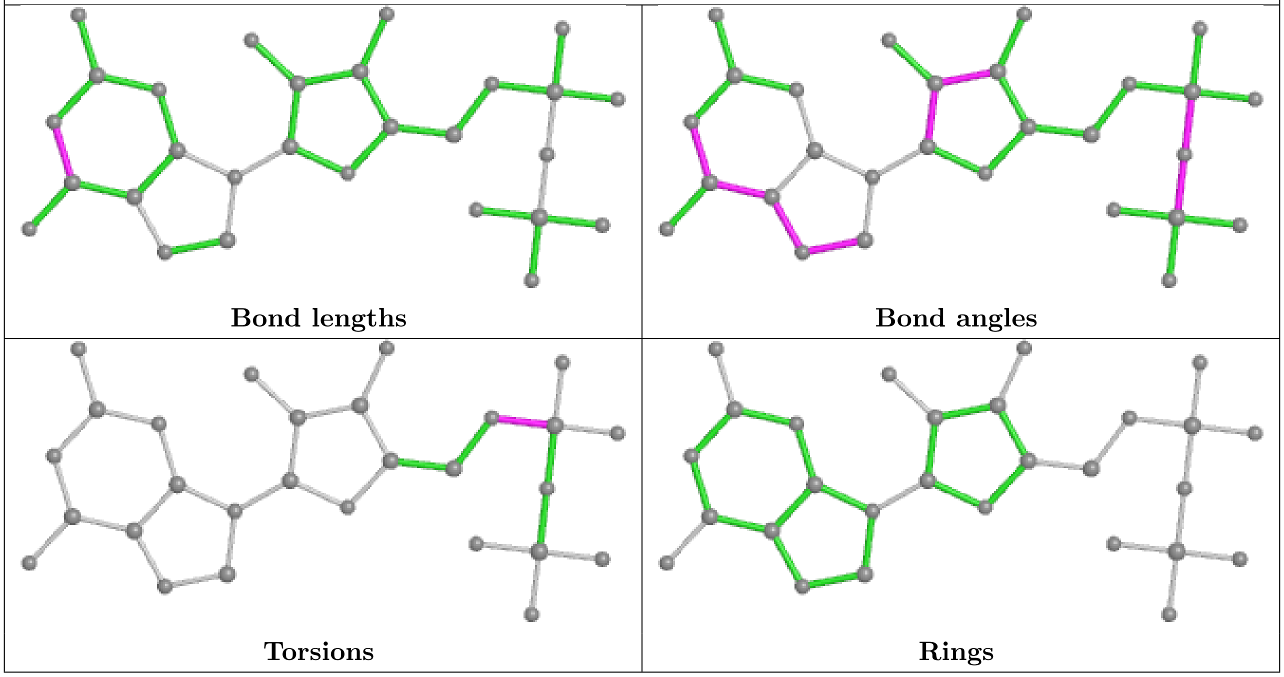
Bond angles



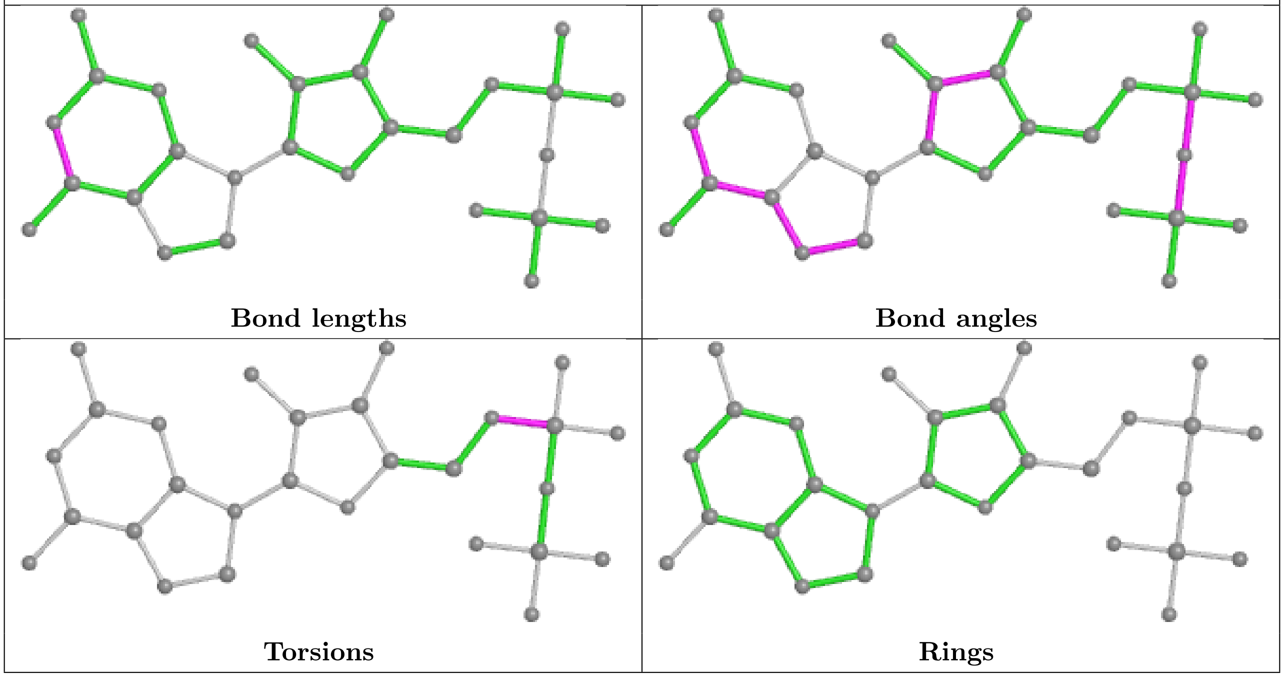
Torsions

Rings

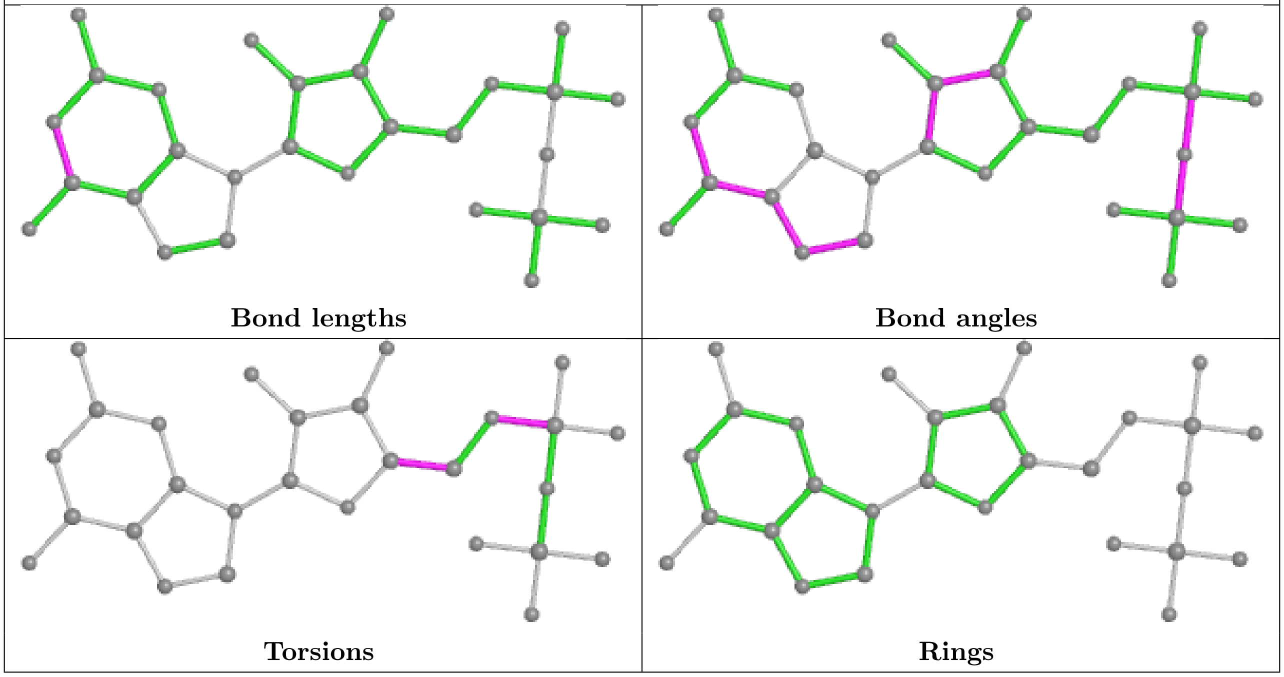
Ligand GDP JH 502



Ligand GDP IH 502



Ligand GDP CL 502



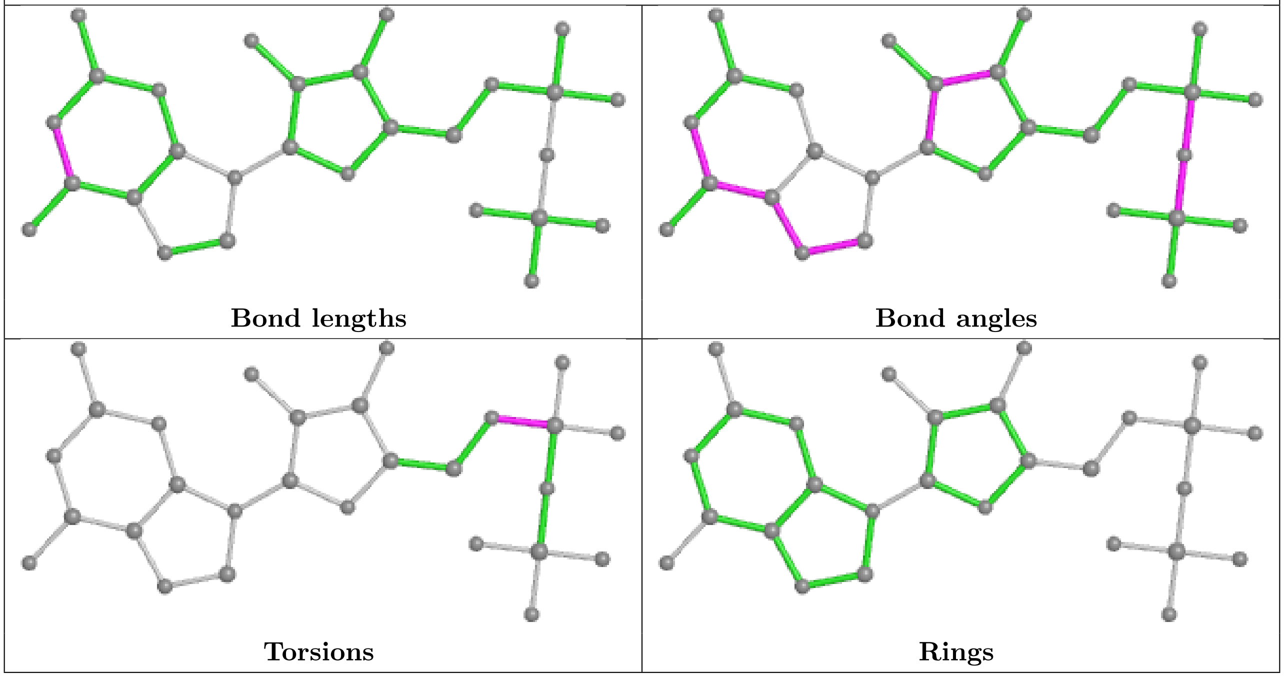
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP UH 502



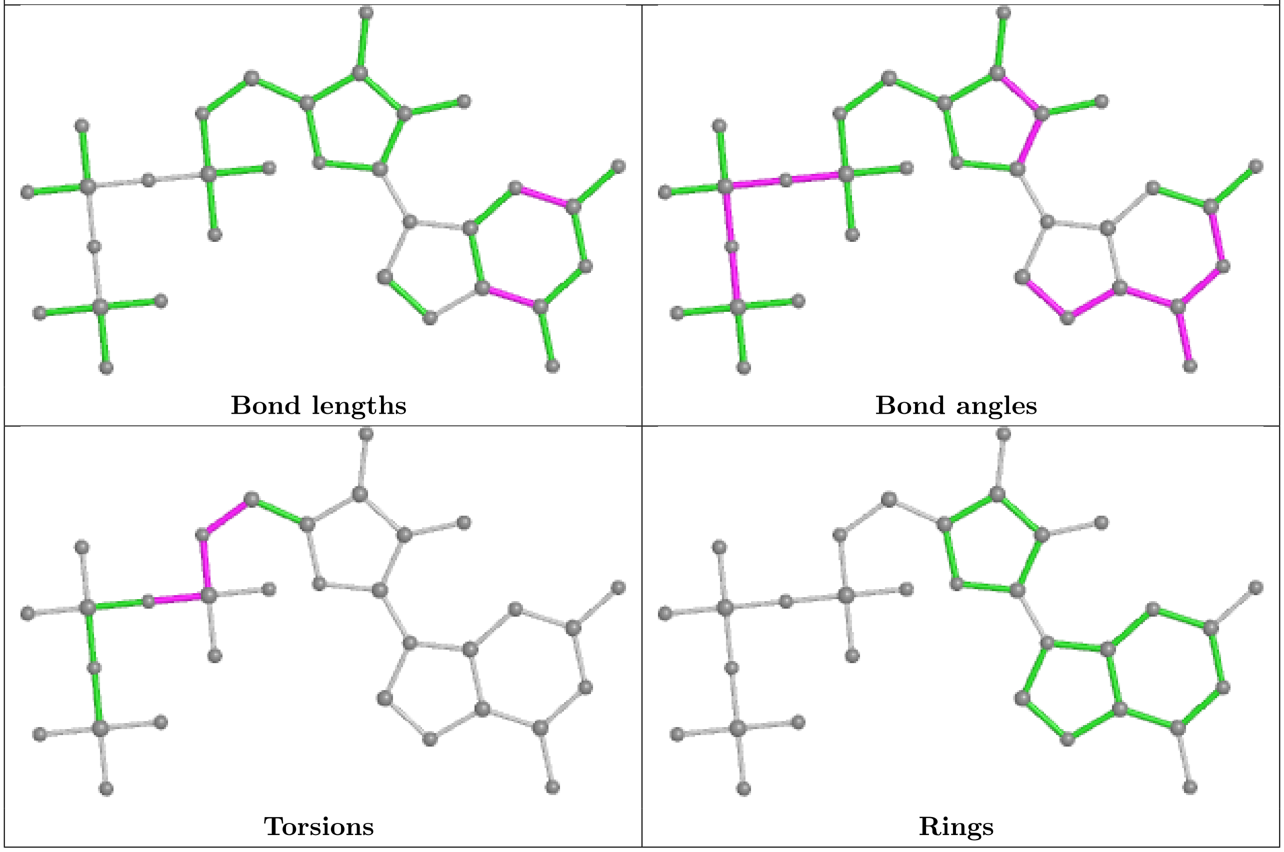
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP UK 501



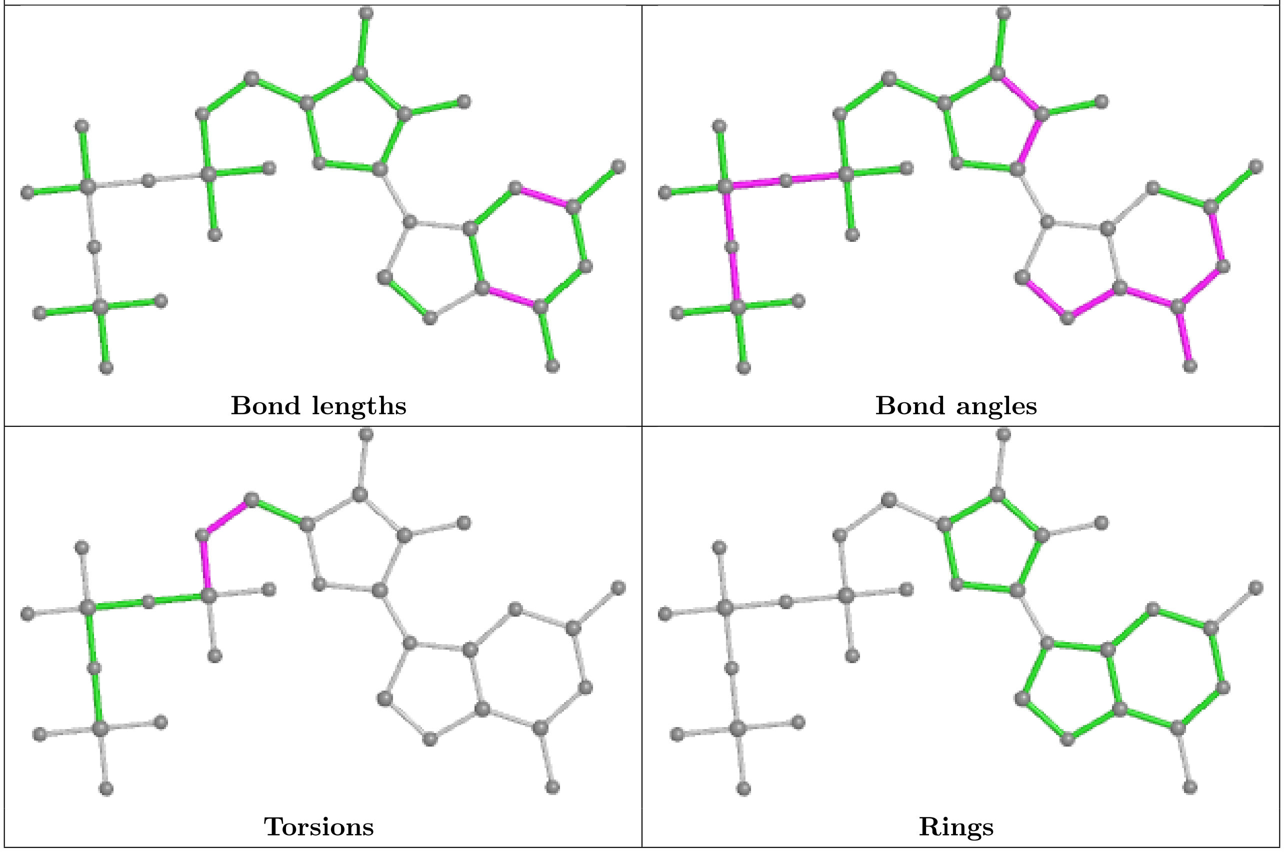
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP JG 501



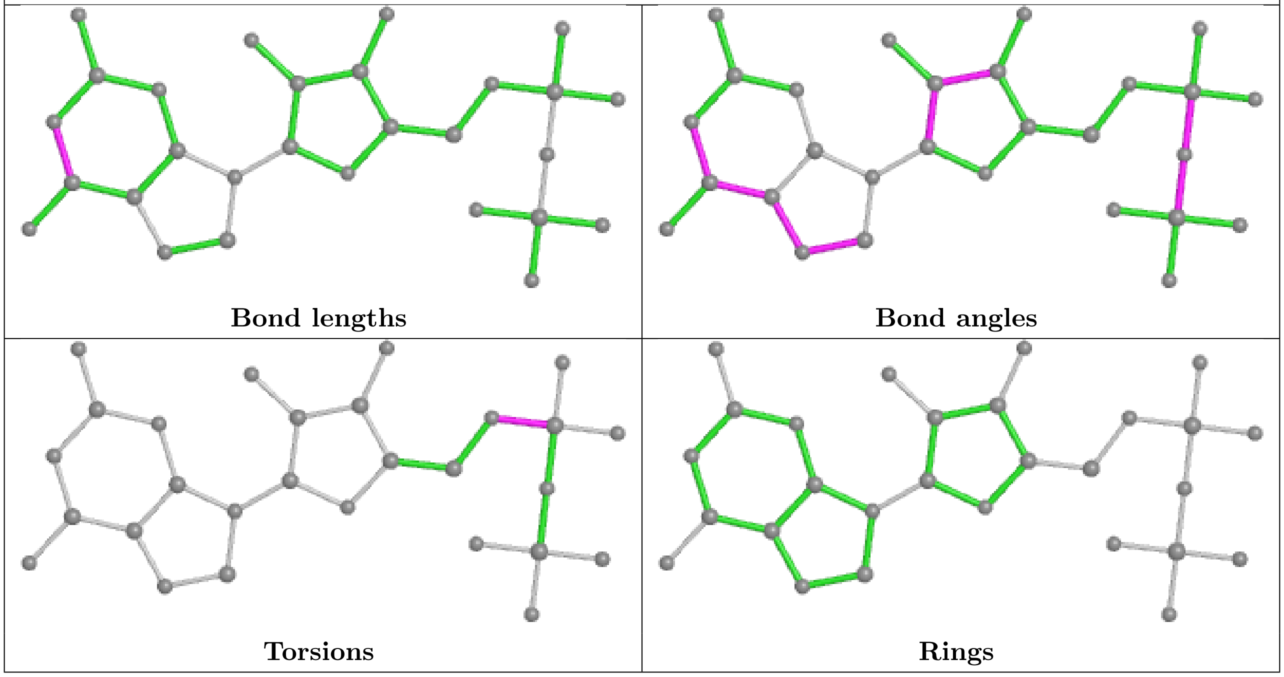
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP CH 502



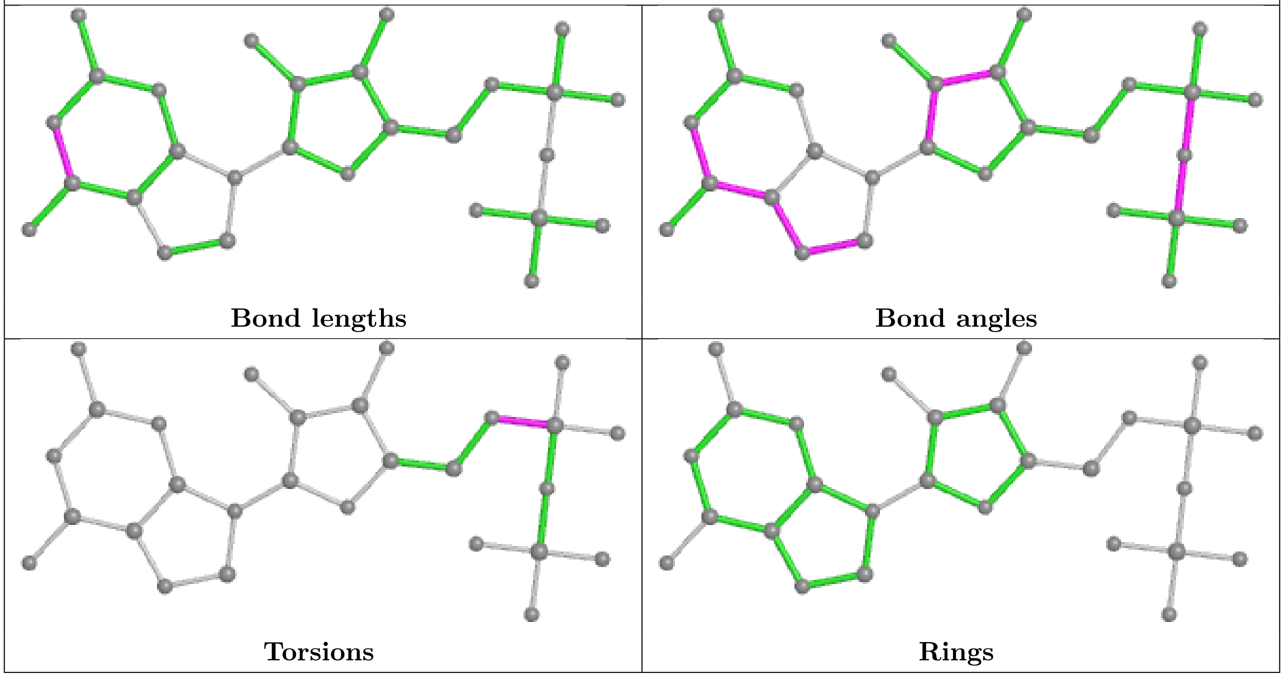
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP ID 502



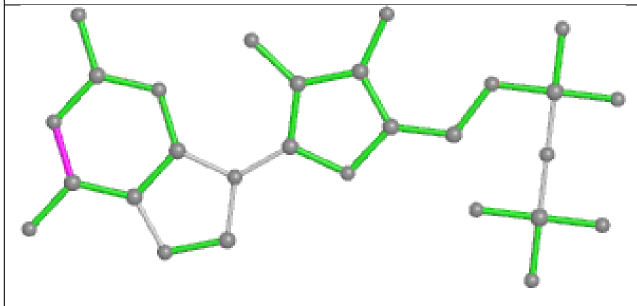
Bond lengths

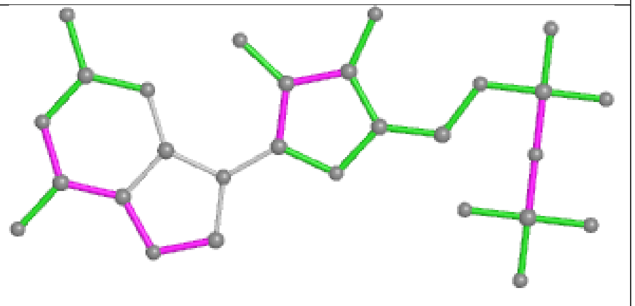
Bond angles

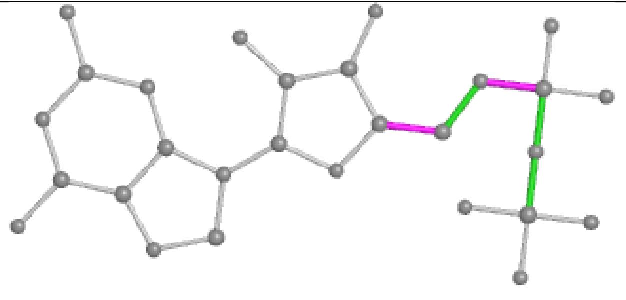
Torsions

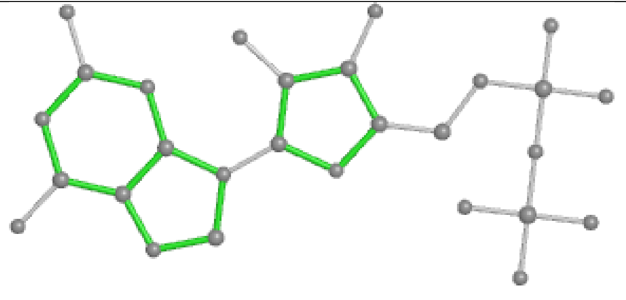
Rings

Ligand GDP LH 502

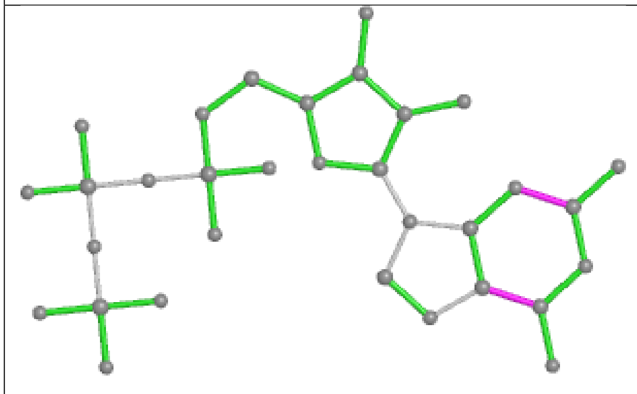

Bond lengths

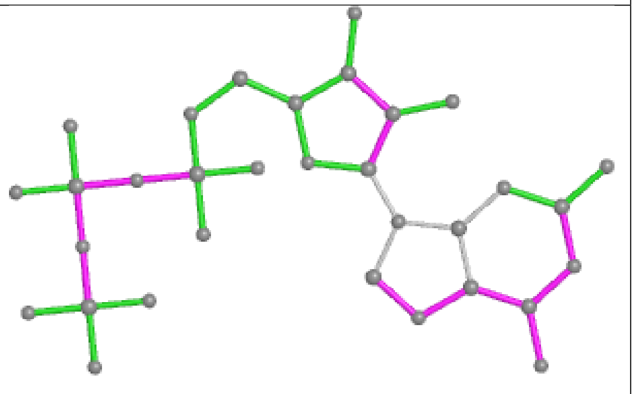

Bond angles

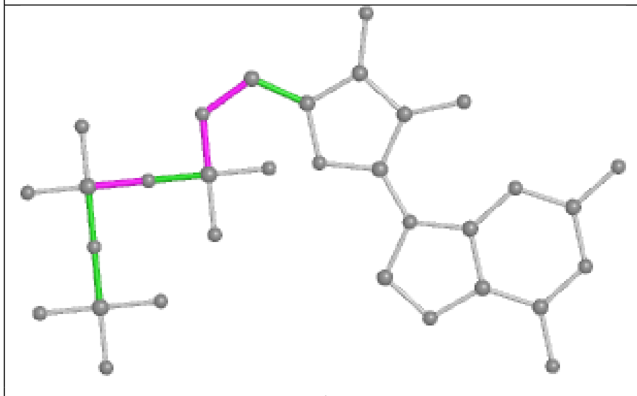

Torsions

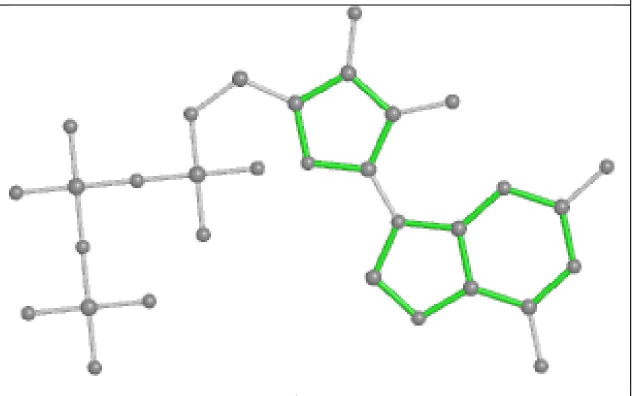

Rings

Ligand GTP KG 501

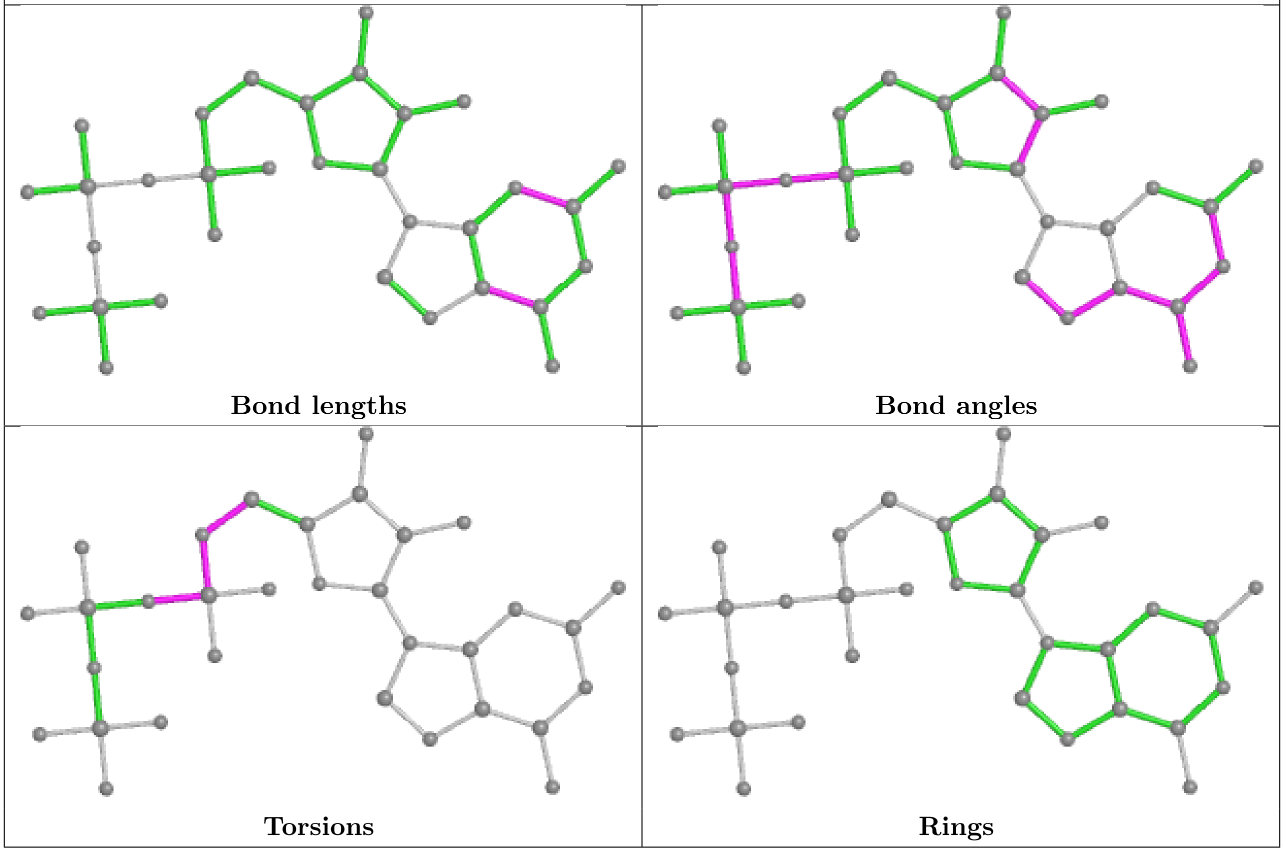

Bond lengths


Bond angles


Torsions


Rings

Ligand GTP EE 501



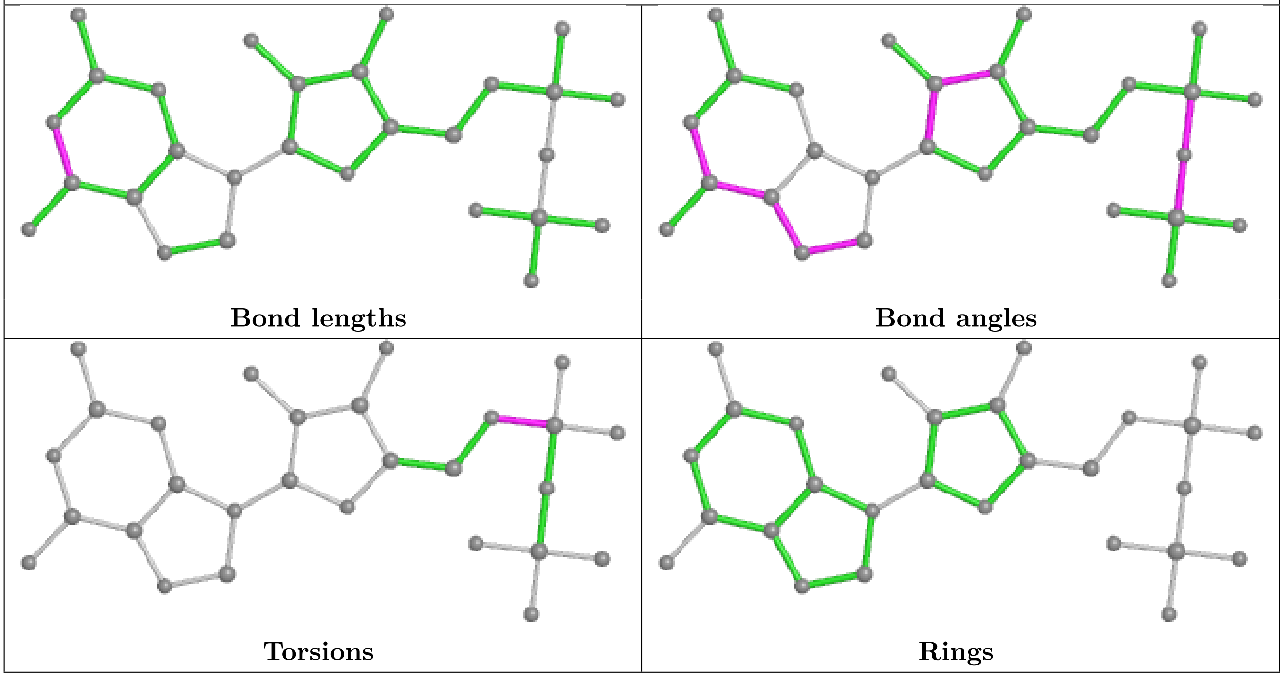
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP NJ 502



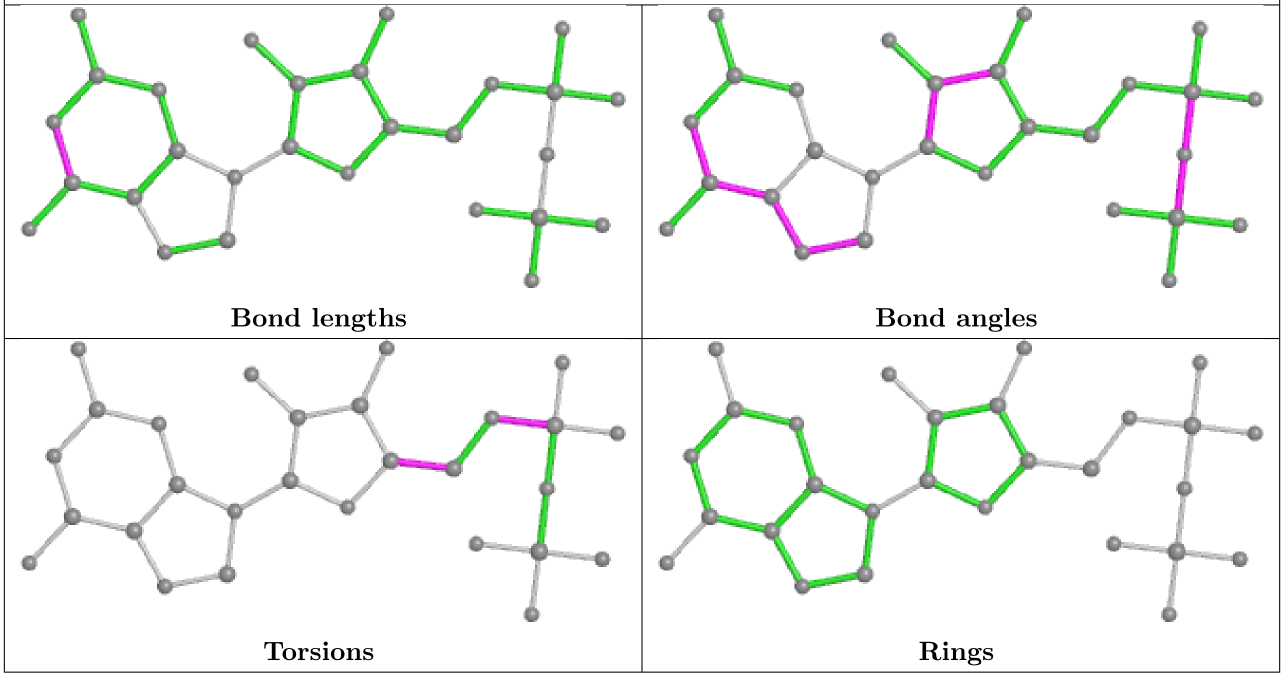
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP ED 502



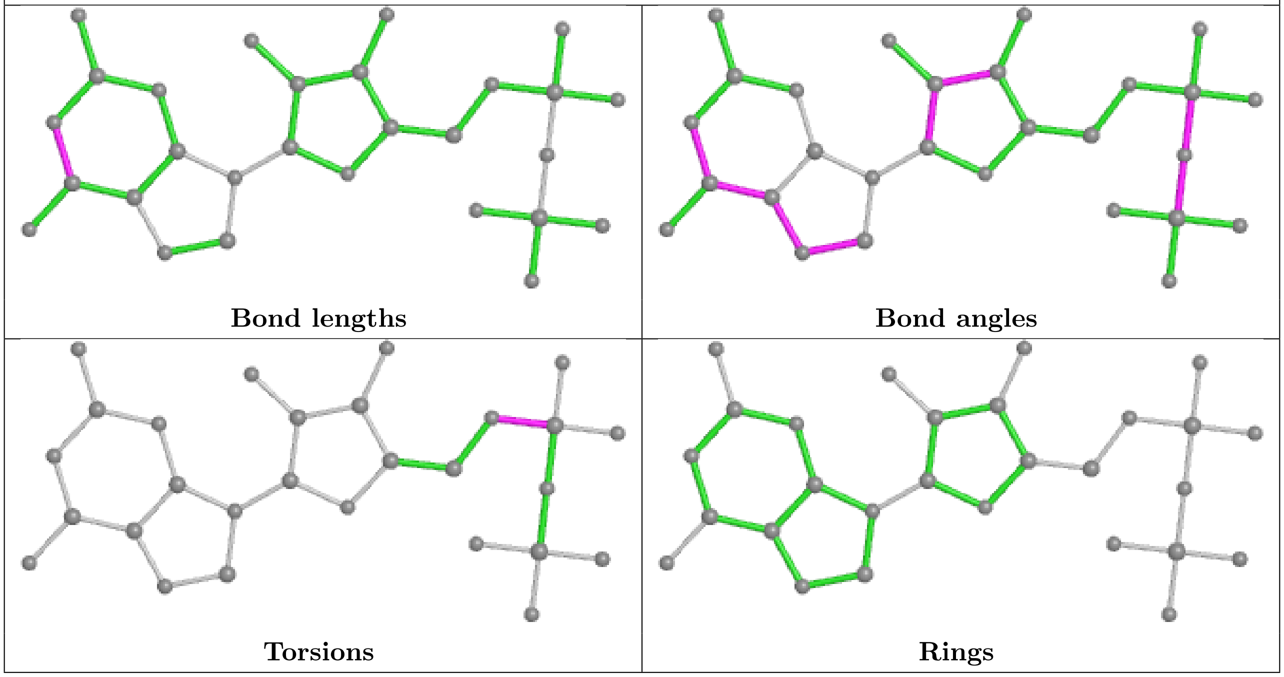
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP UL 502



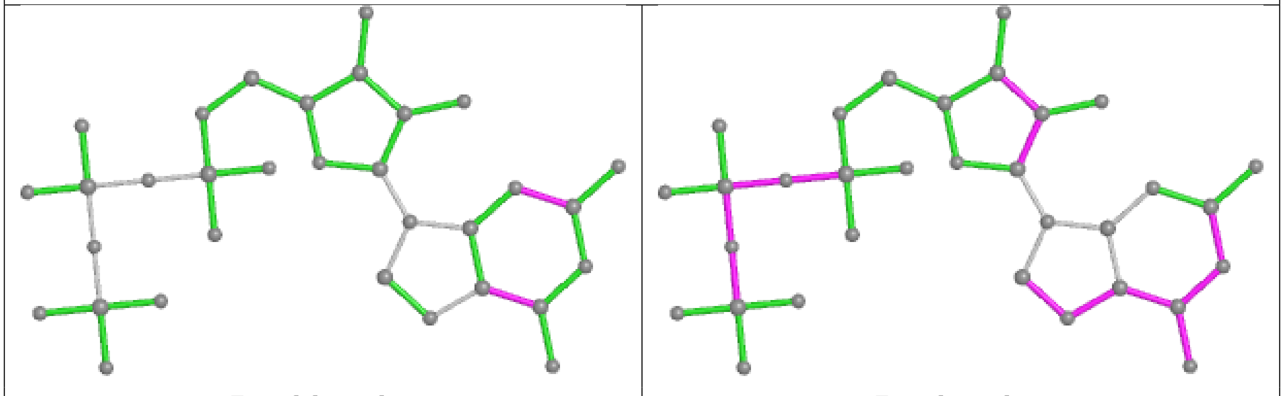
Bond lengths

Bond angles

Torsions

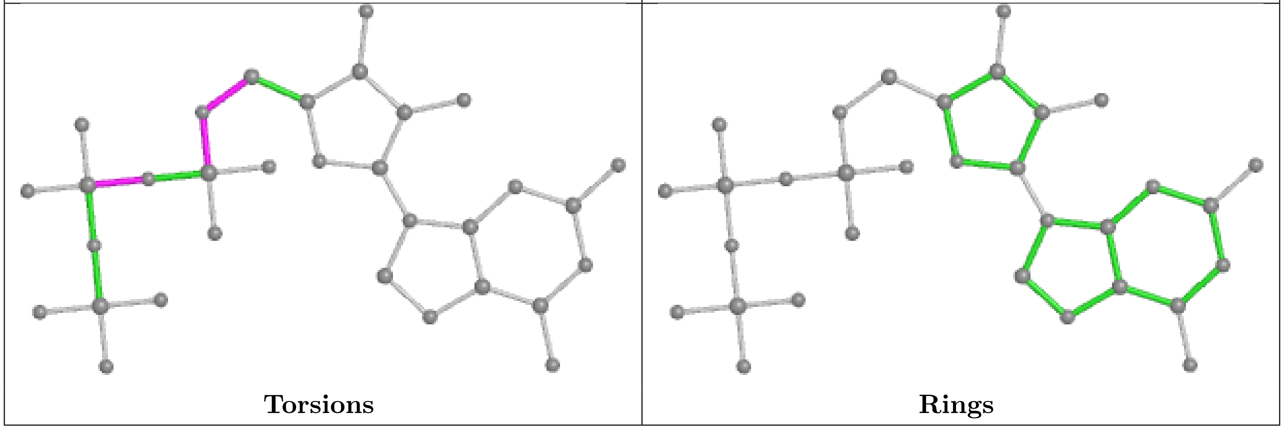
Rings

Ligand GTP JK 501



Bond lengths

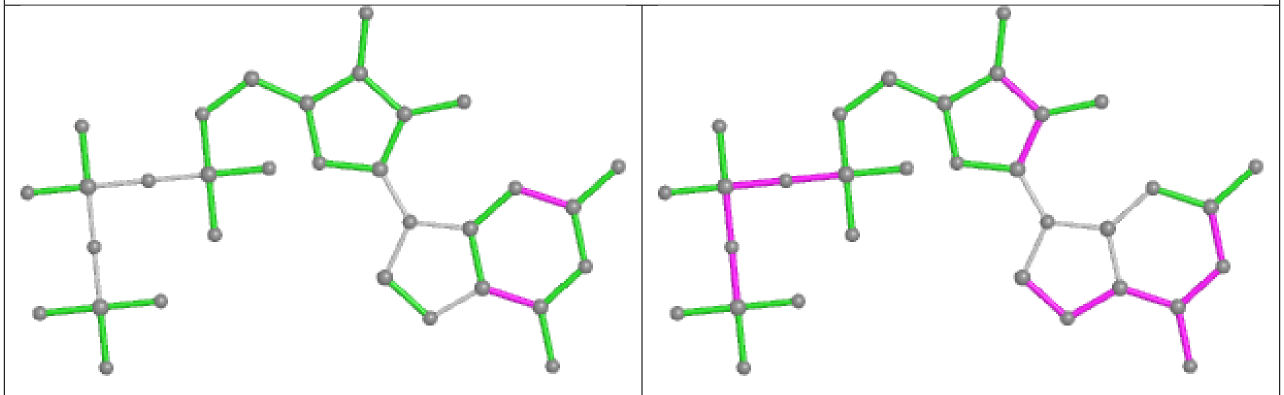
Bond angles



Torsions

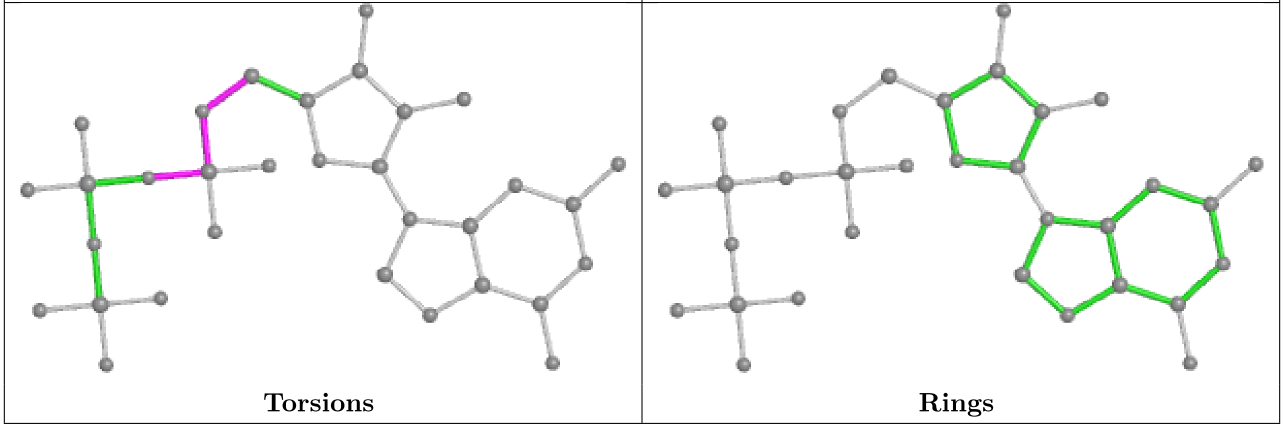
Rings

Ligand GTP EC 501



Bond lengths

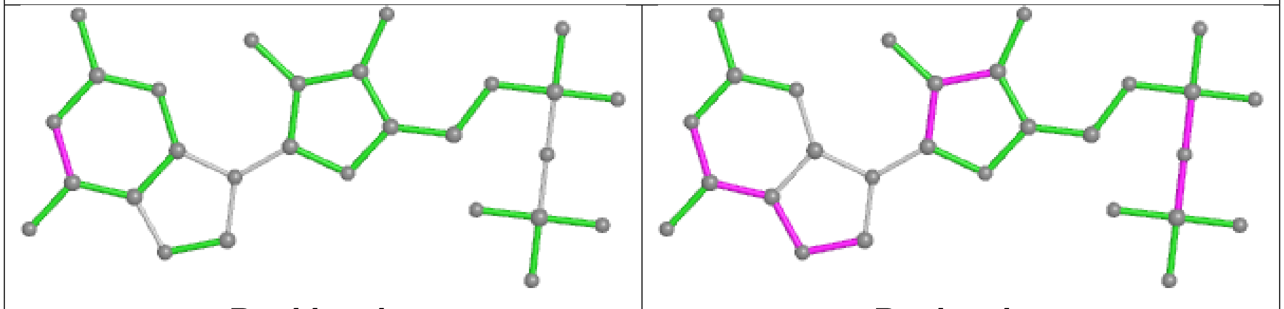
Bond angles



Torsions

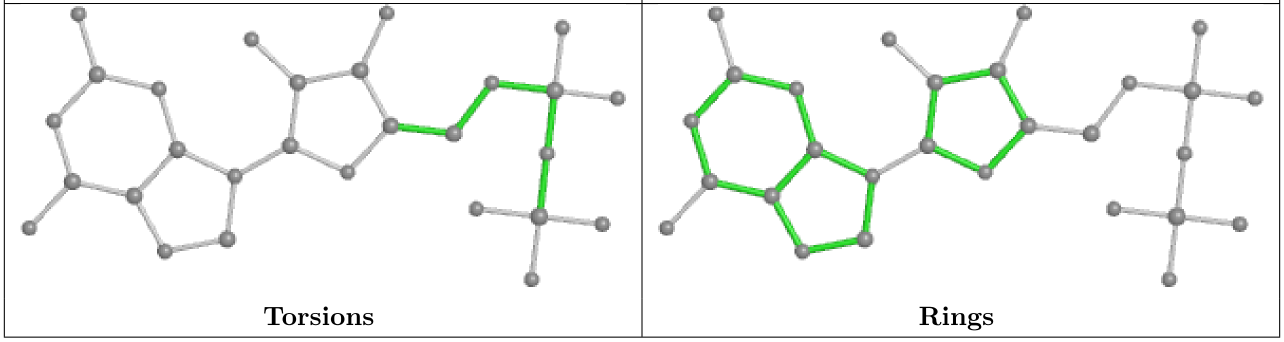
Rings

Ligand GDP VD 502



Bond lengths

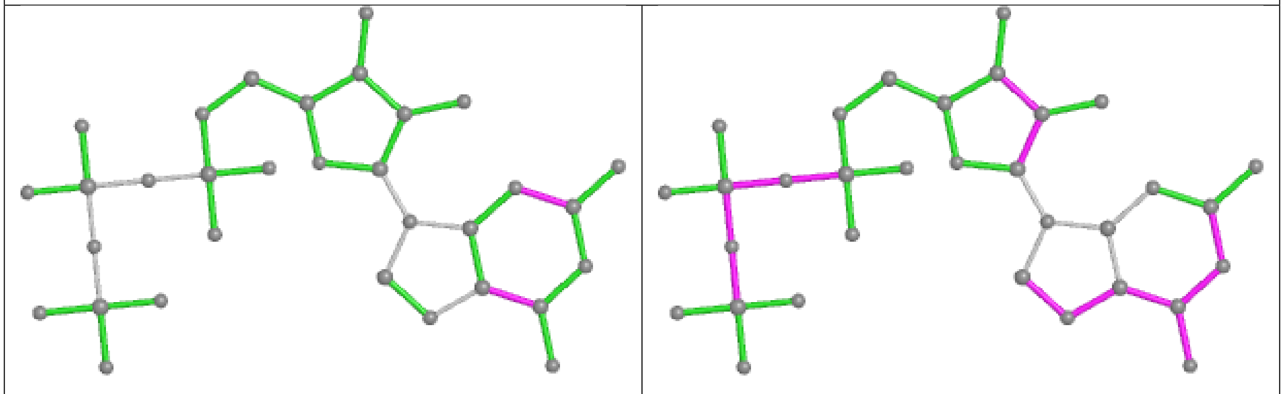
Bond angles



Torsions

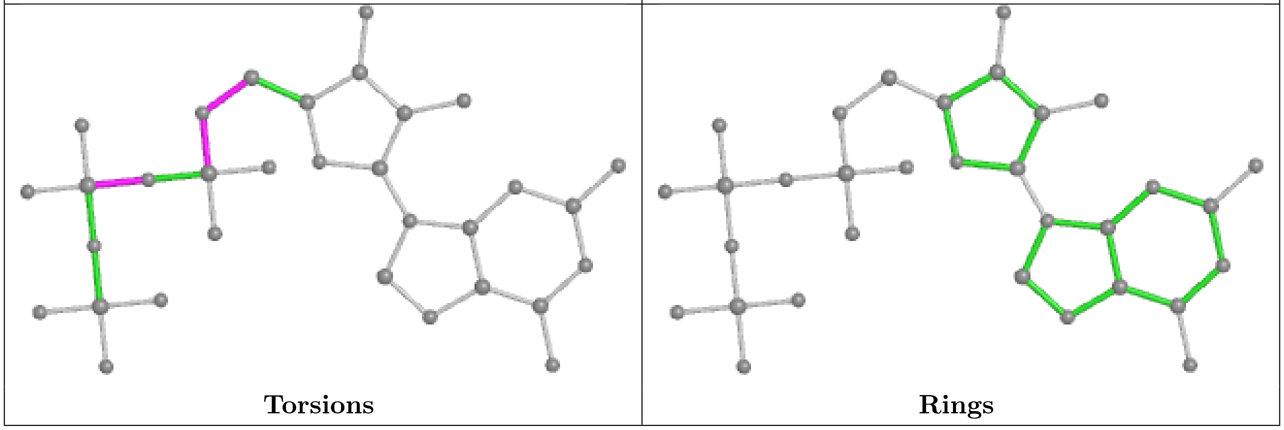
Rings

Ligand GTP FM 501



Bond lengths

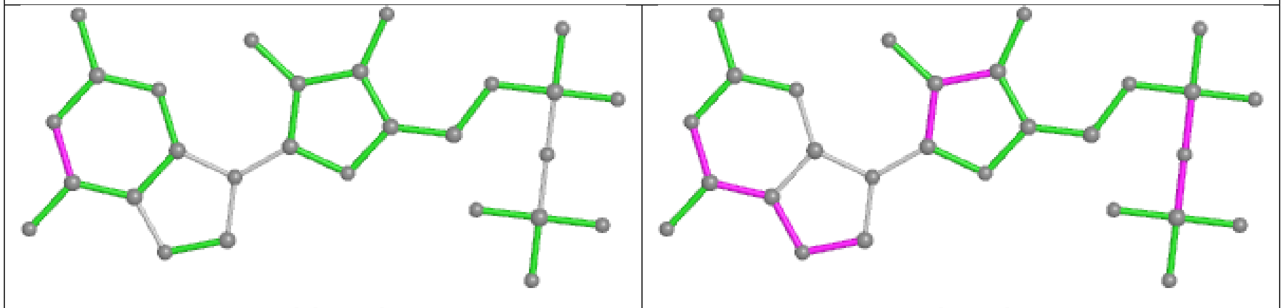
Bond angles



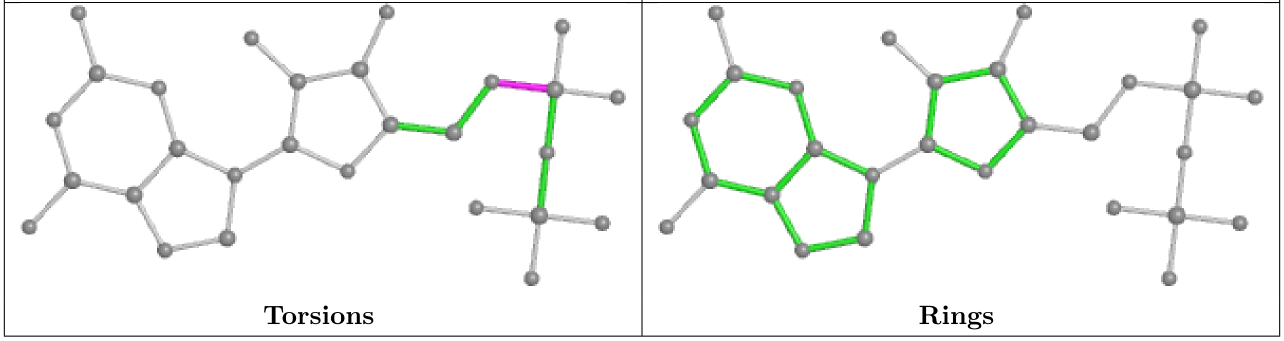
Torsions

Rings

Ligand GDP NL 502

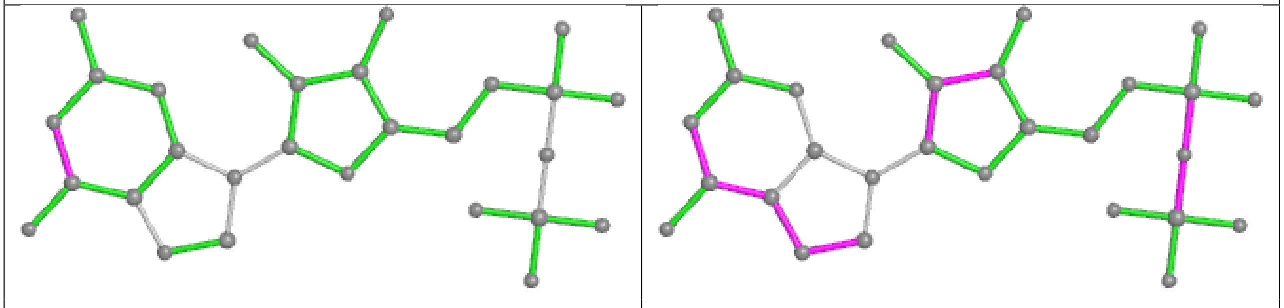


Bond lengths **Bond angles**

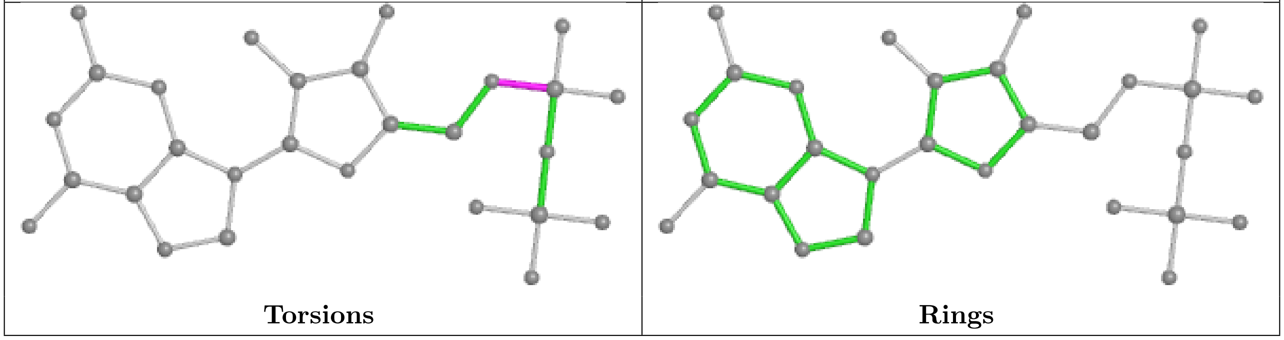


Torsions **Rings**

Ligand GDP CJ 502

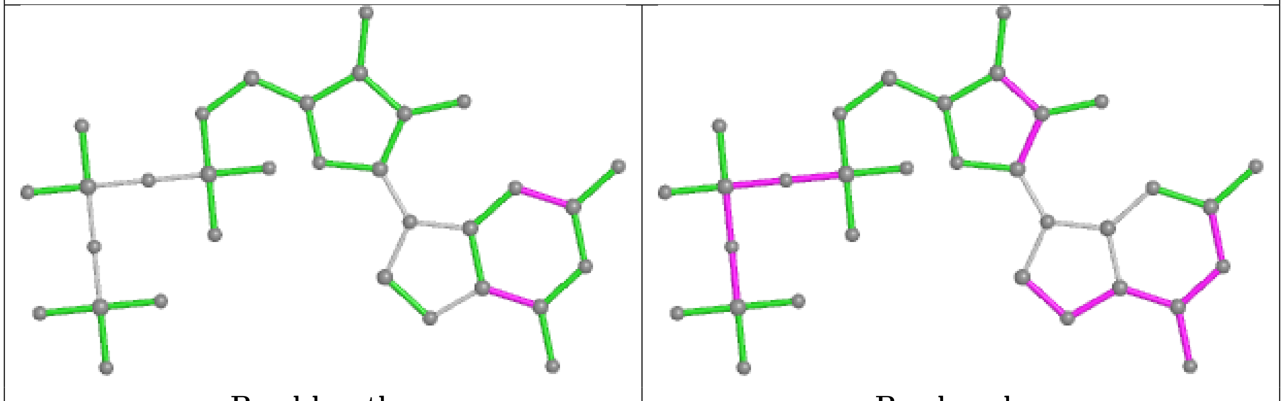


Bond lengths **Bond angles**



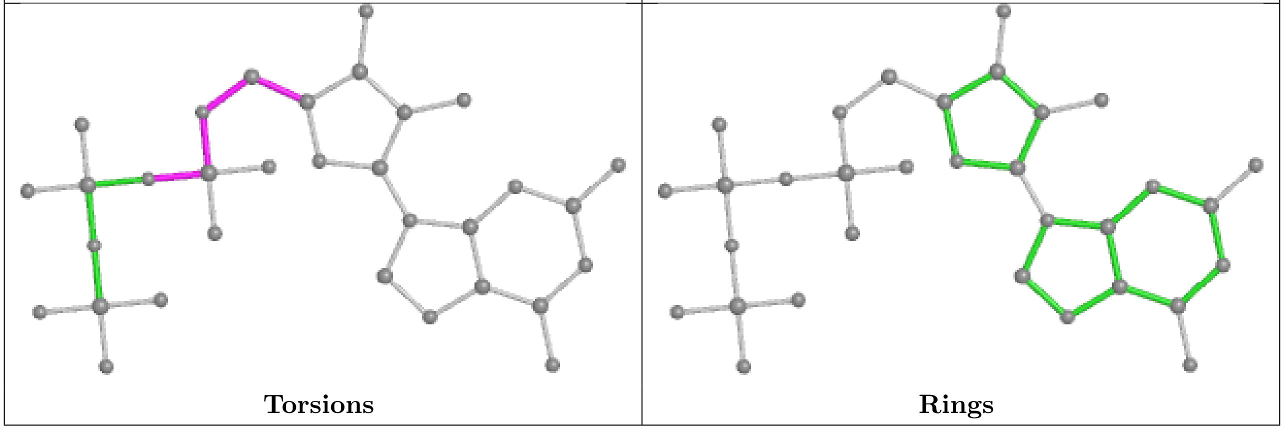
Torsions **Rings**

Ligand GTP BG 501



Bond lengths

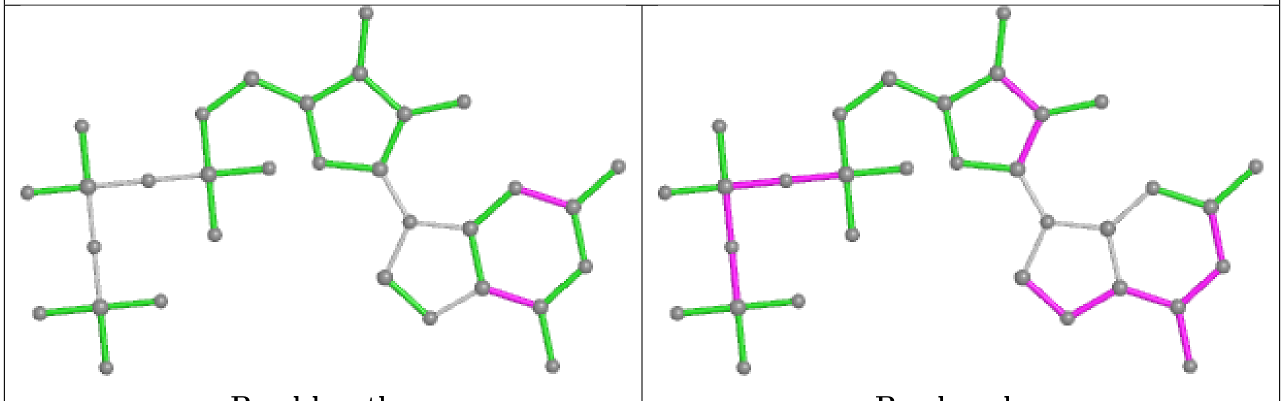
Bond angles



Torsions

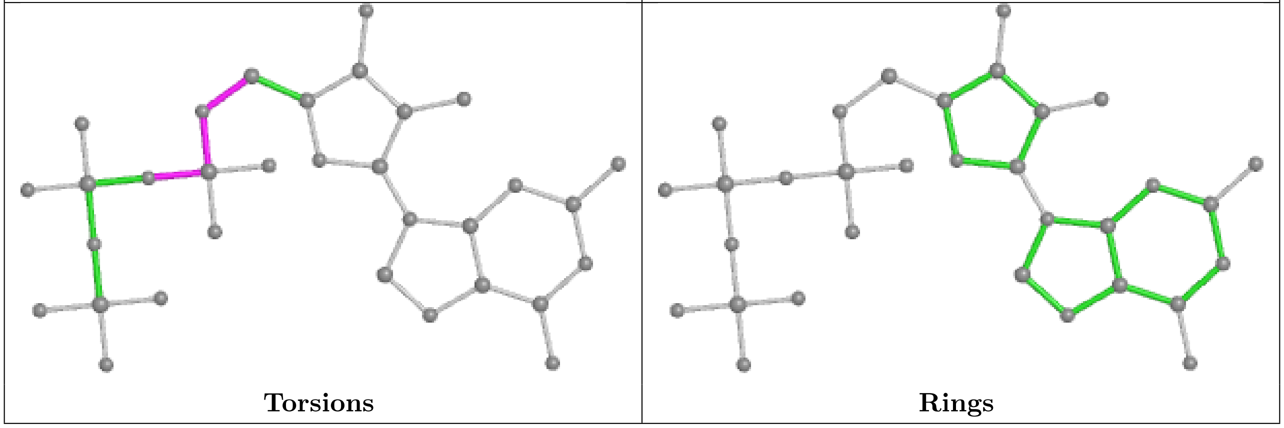
Rings

Ligand GTP EM 501



Bond lengths

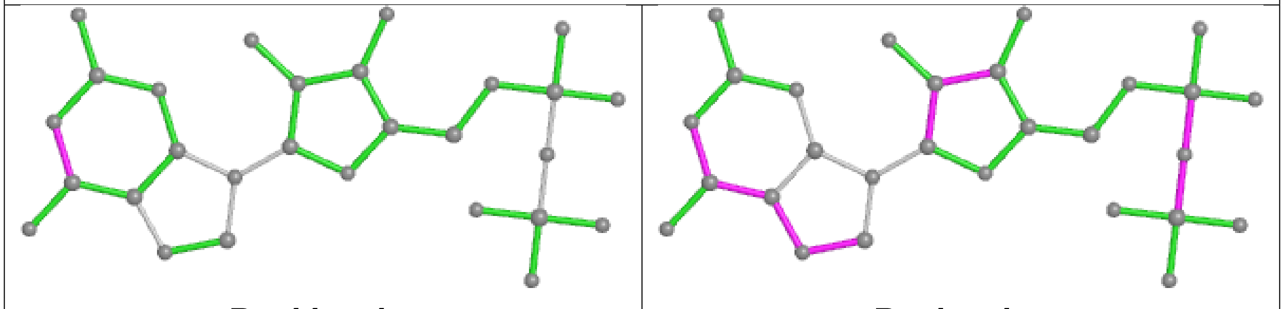
Bond angles



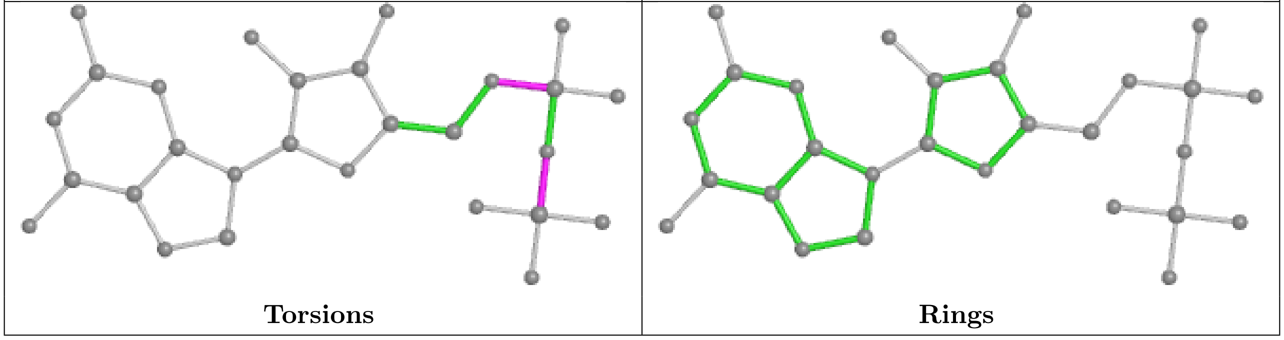
Torsions

Rings

Ligand GDP BH 502

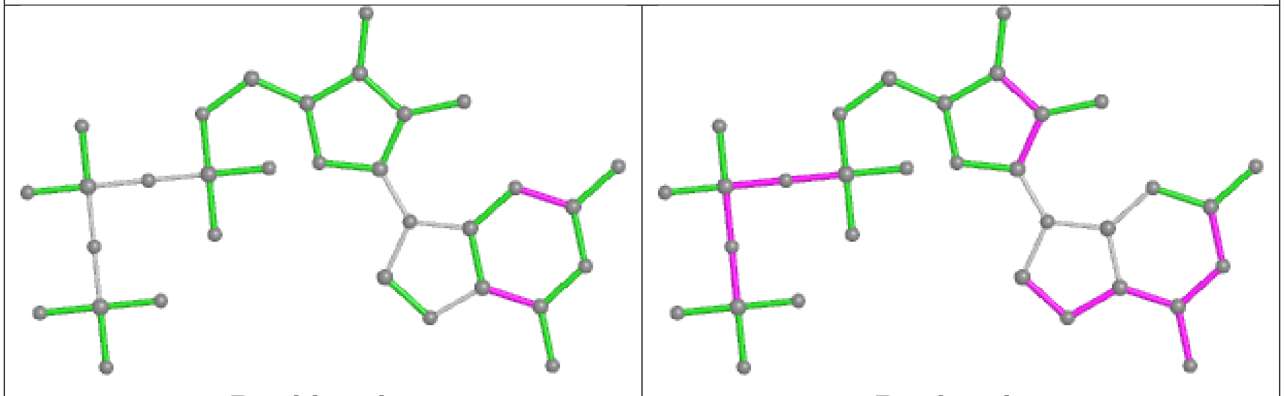


Bond lengths **Bond angles**

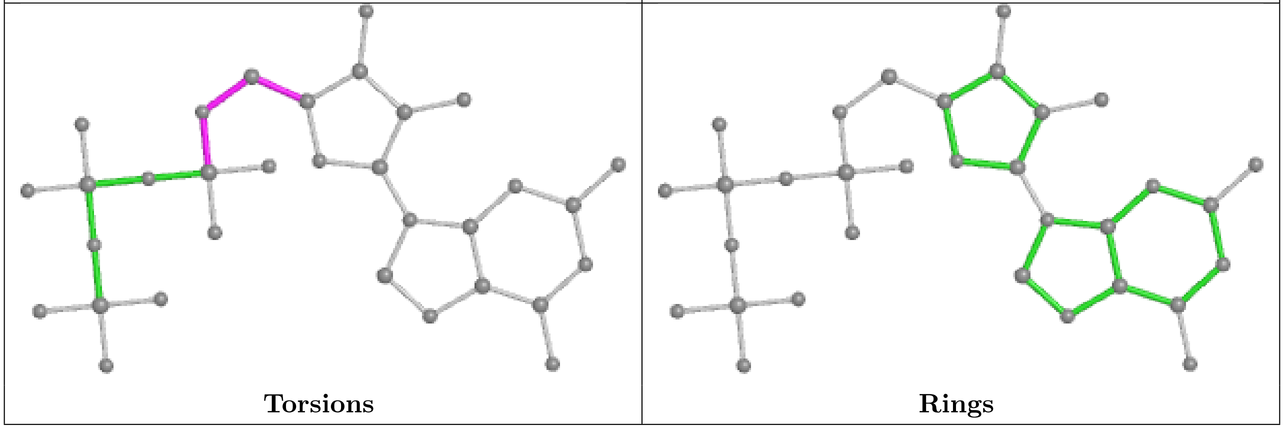


Torsions **Rings**

Ligand GTP CG 501

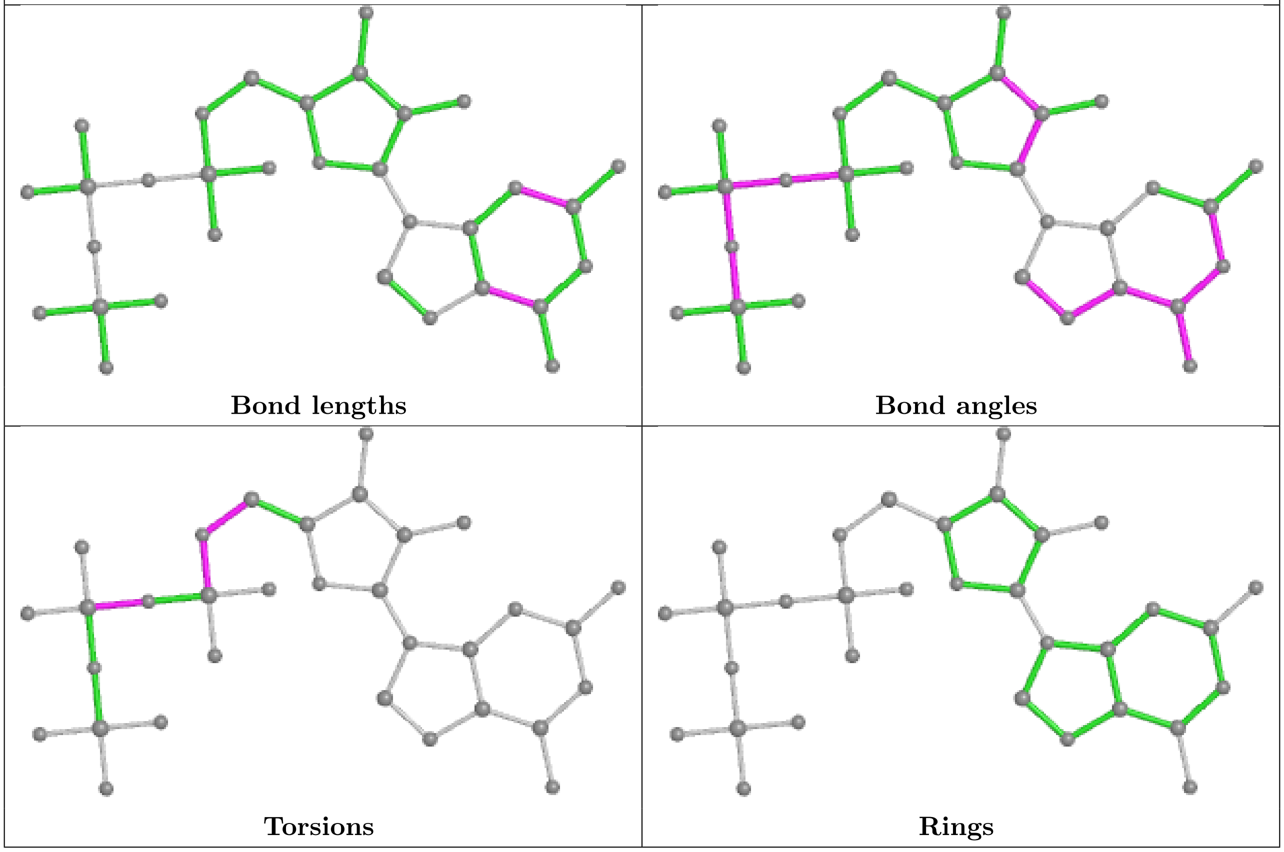


Bond lengths **Bond angles**

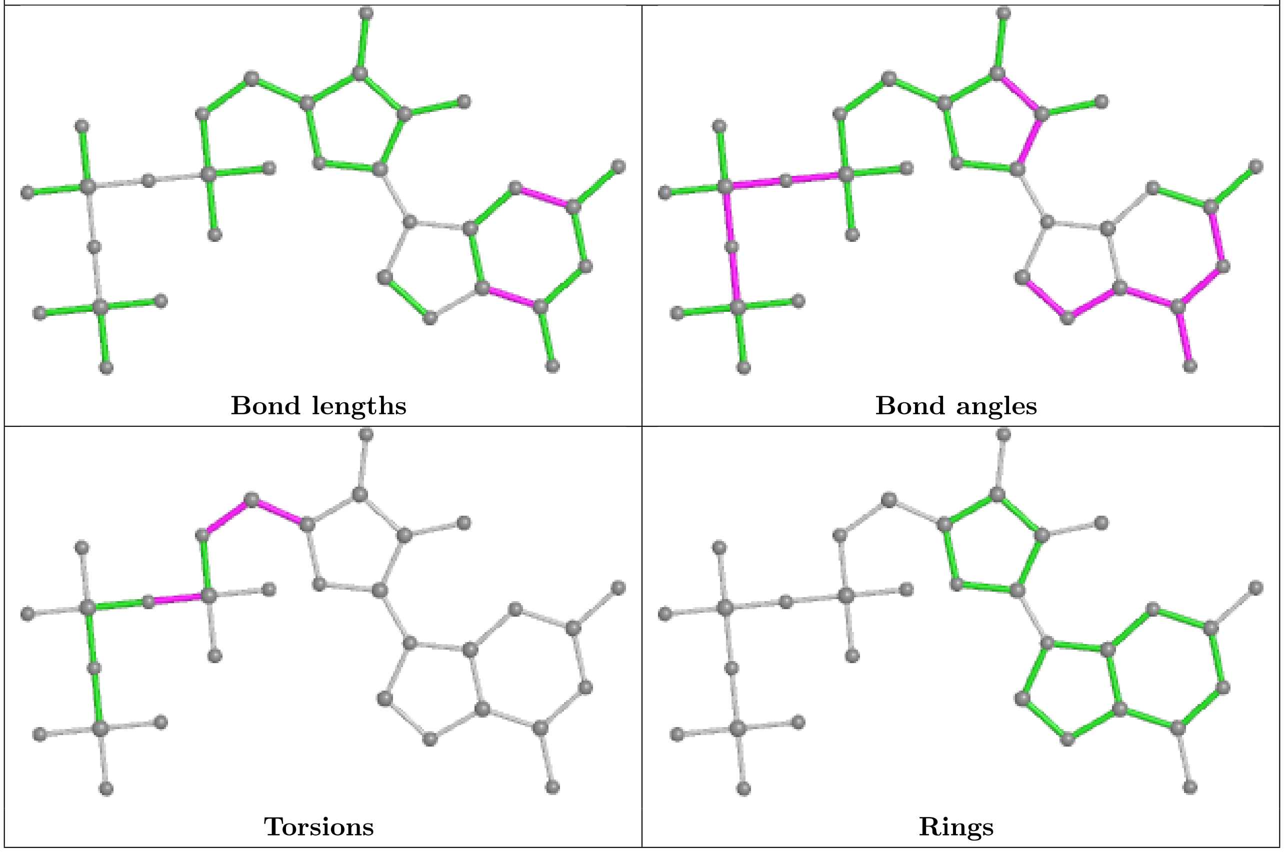


Torsions **Rings**

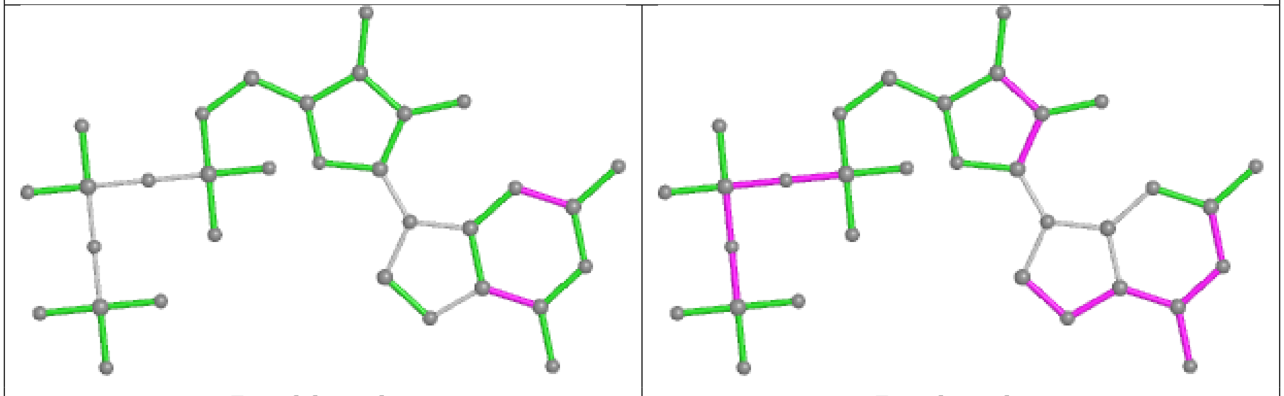
Ligand GTP KC 501



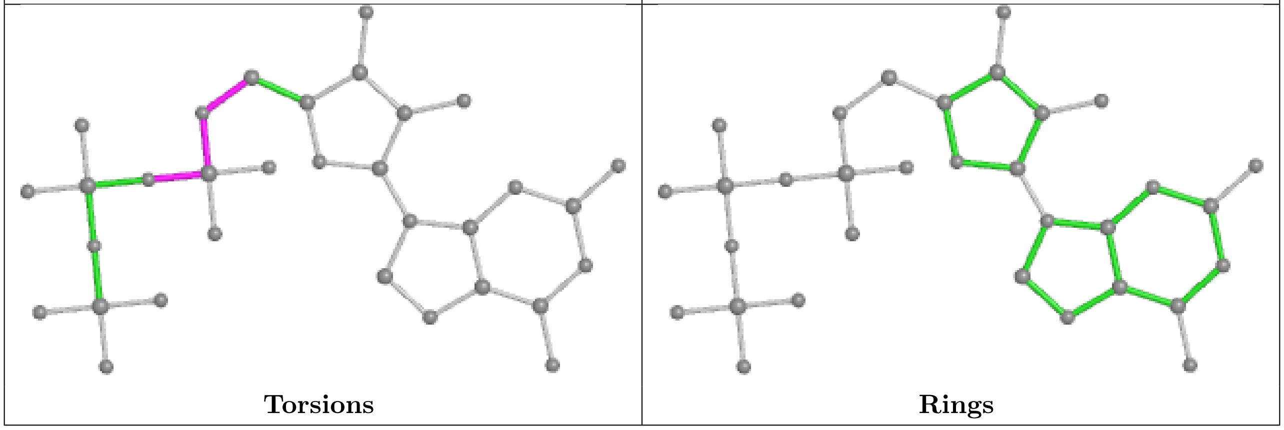
Ligand GTP NE 501



Ligand GTP AM 501

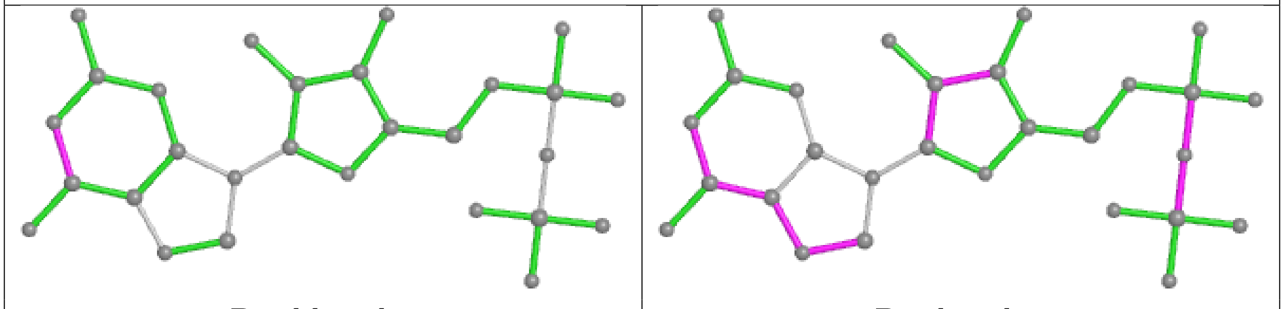


Bond lengths **Bond angles**

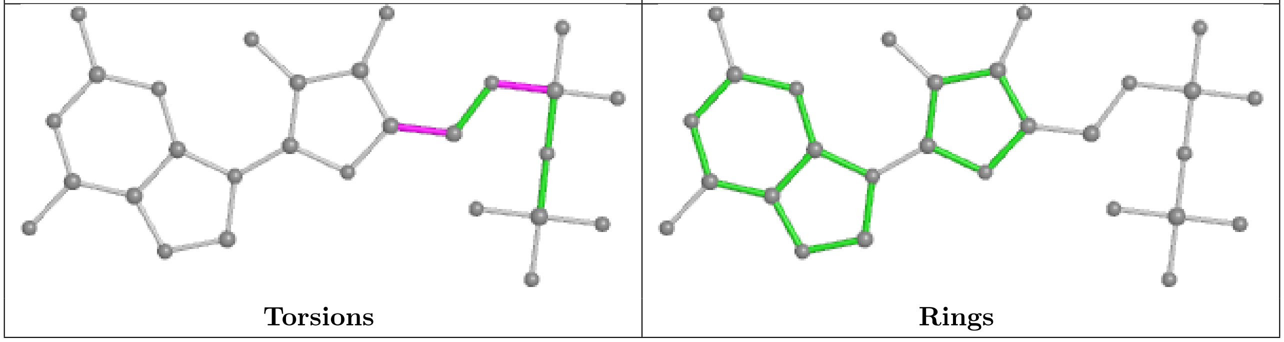


Torsions **Rings**

Ligand GDP PF 502

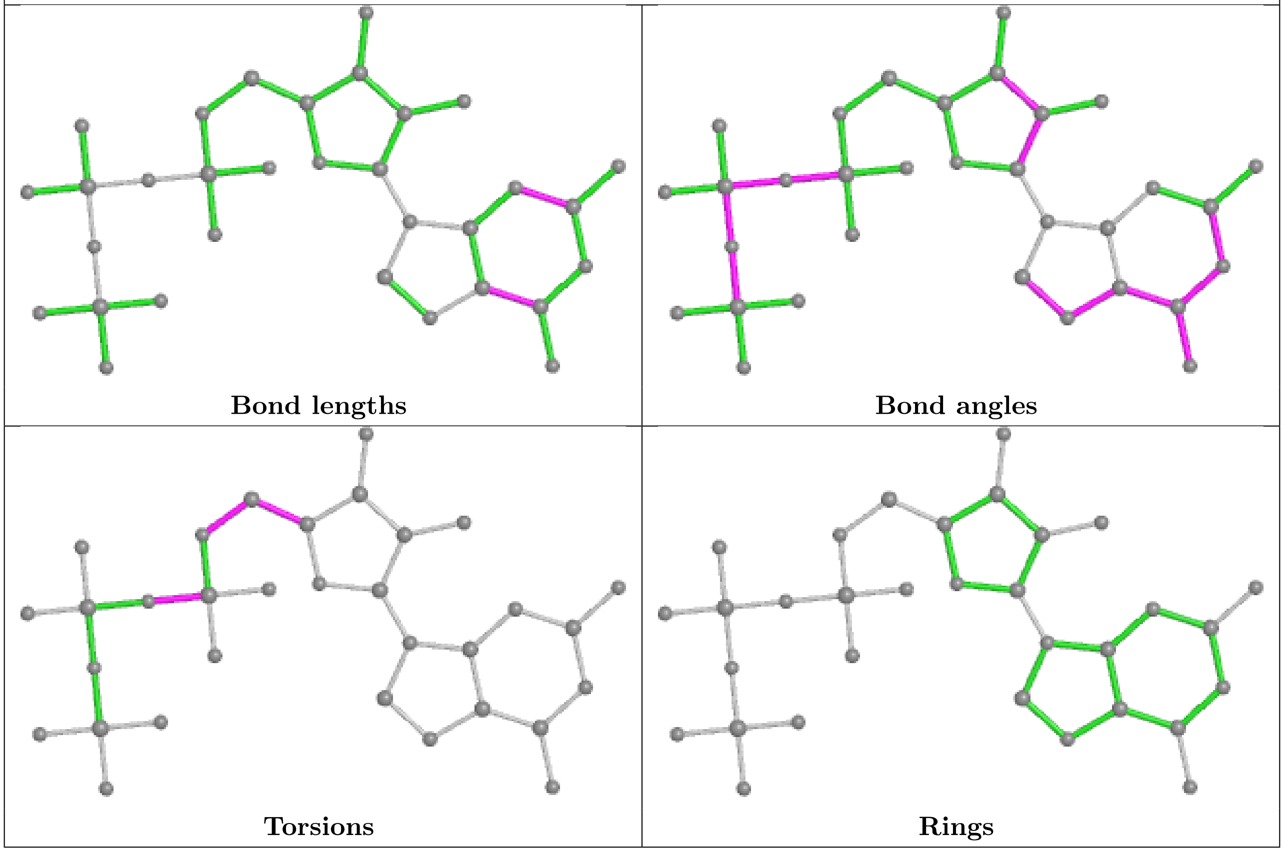


Bond lengths **Bond angles**

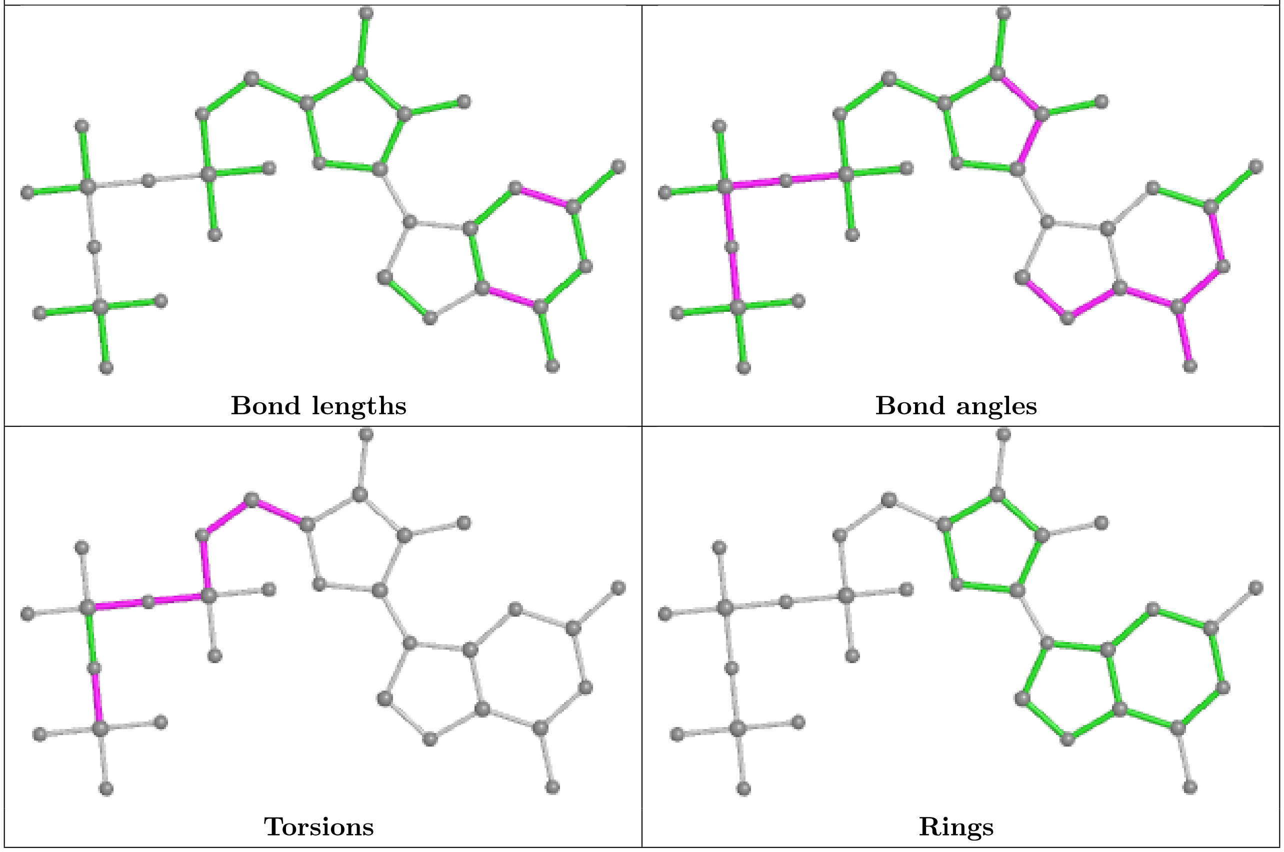


Torsions **Rings**

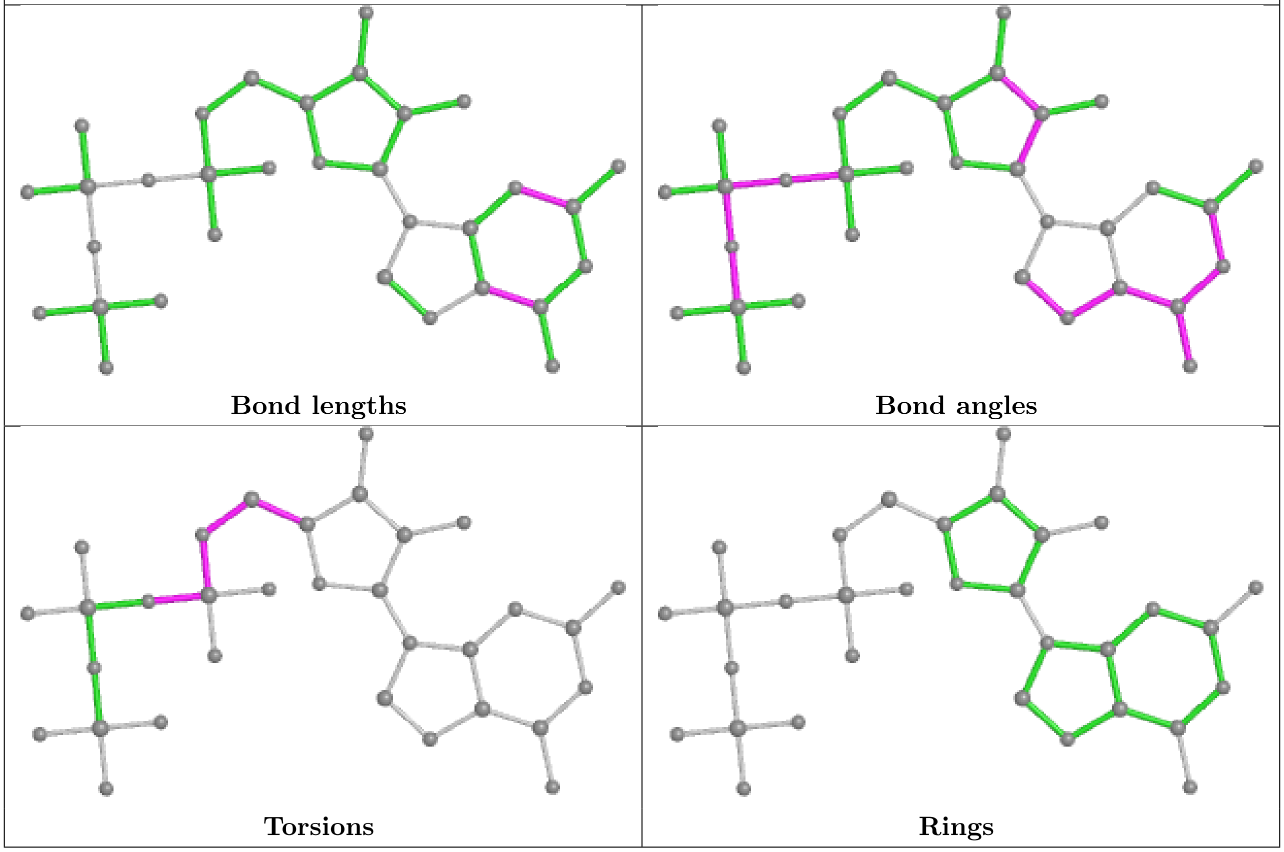
Ligand GTP UE 501



Ligand GTP CK 501



Ligand GTP GK 501



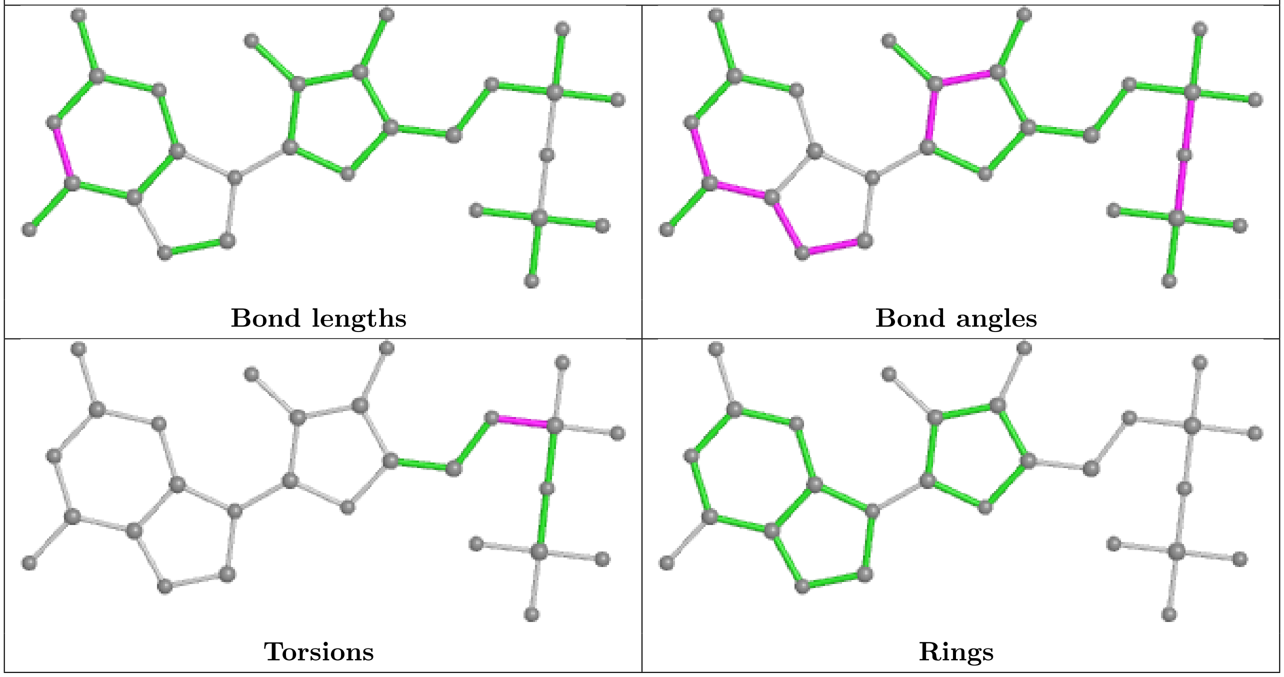
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP UP 502



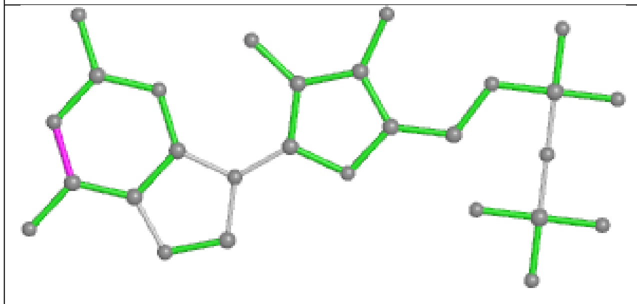
Bond lengths

Bond angles

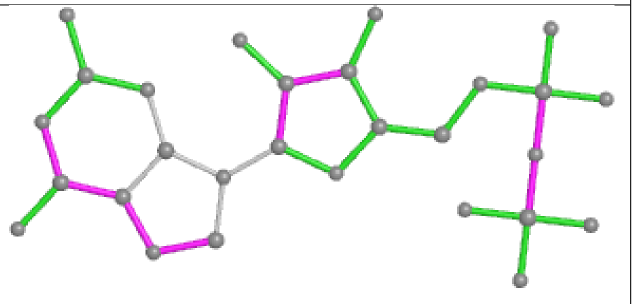
Torsions

Rings

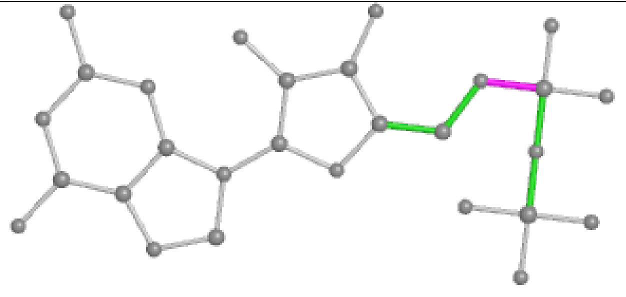
Ligand GDP HB 502



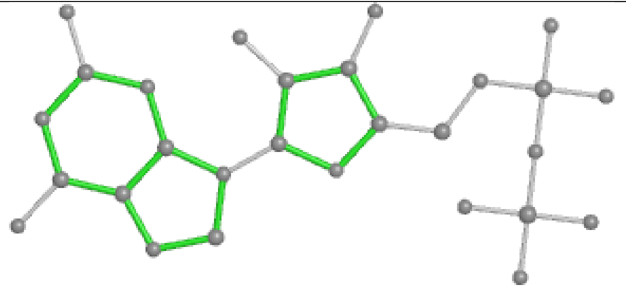
Bond lengths



Bond angles

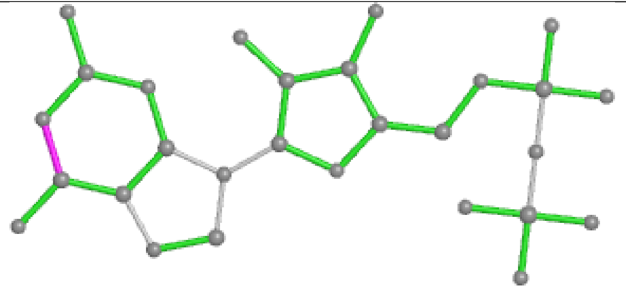


Torsions

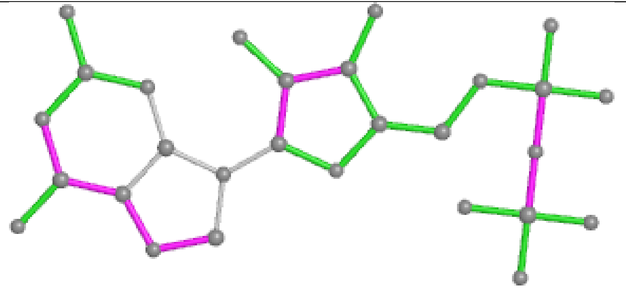


Rings

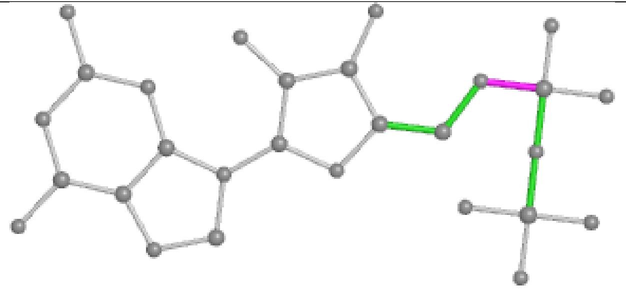
Ligand GDP OH 502



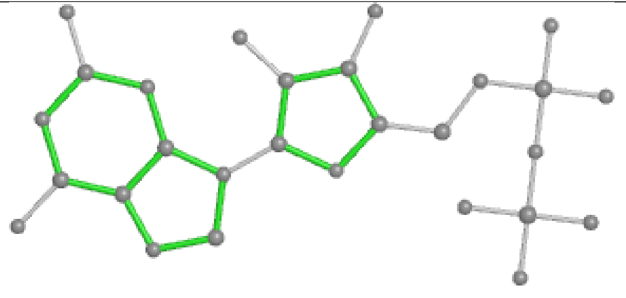
Bond lengths



Bond angles

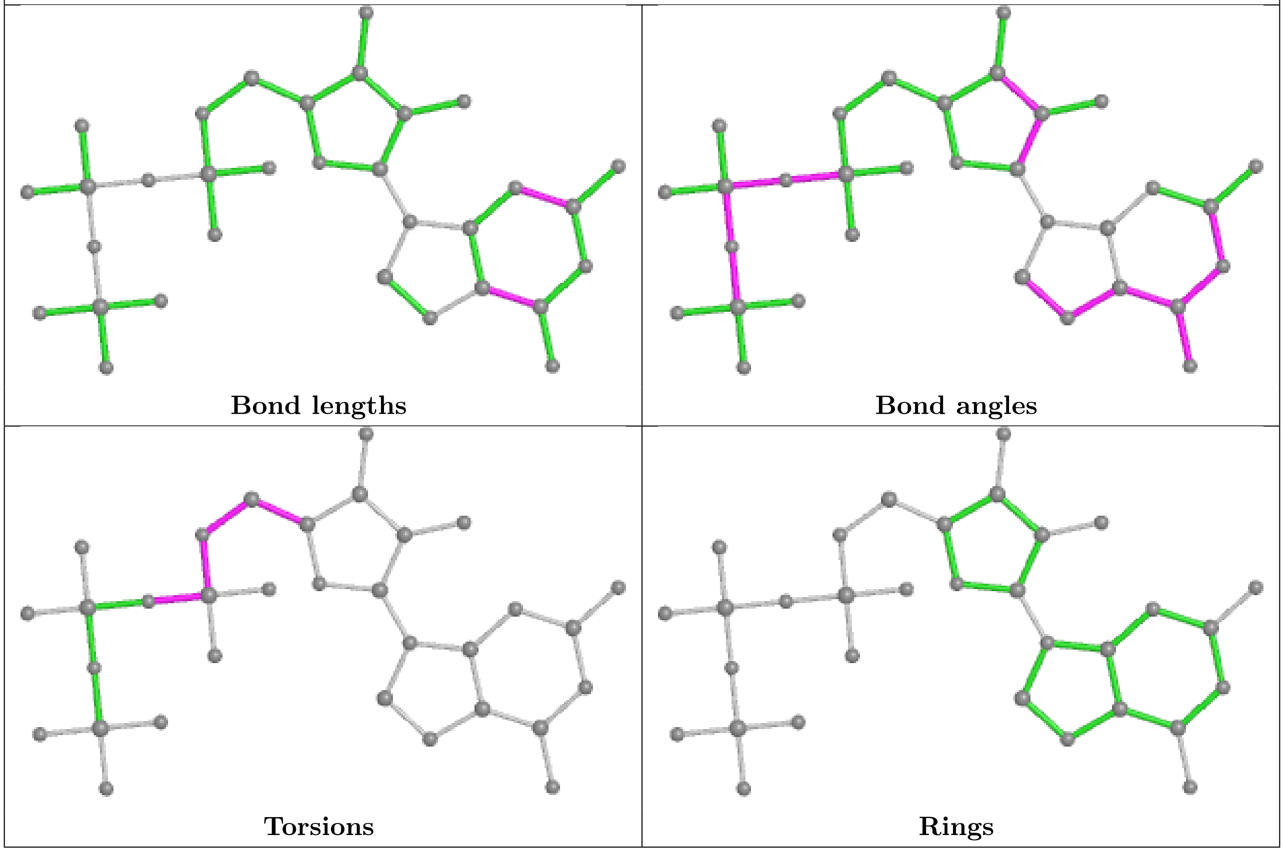


Torsions



Rings

Ligand GTP IK 501



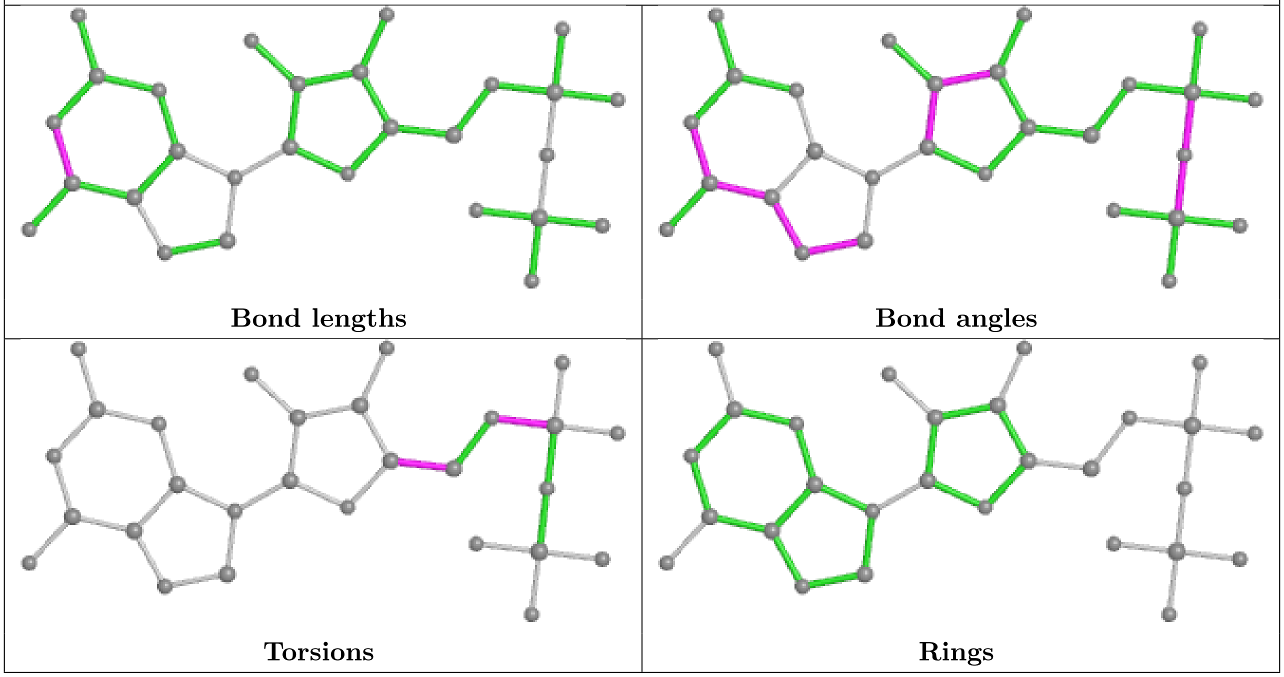
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP OJ 502



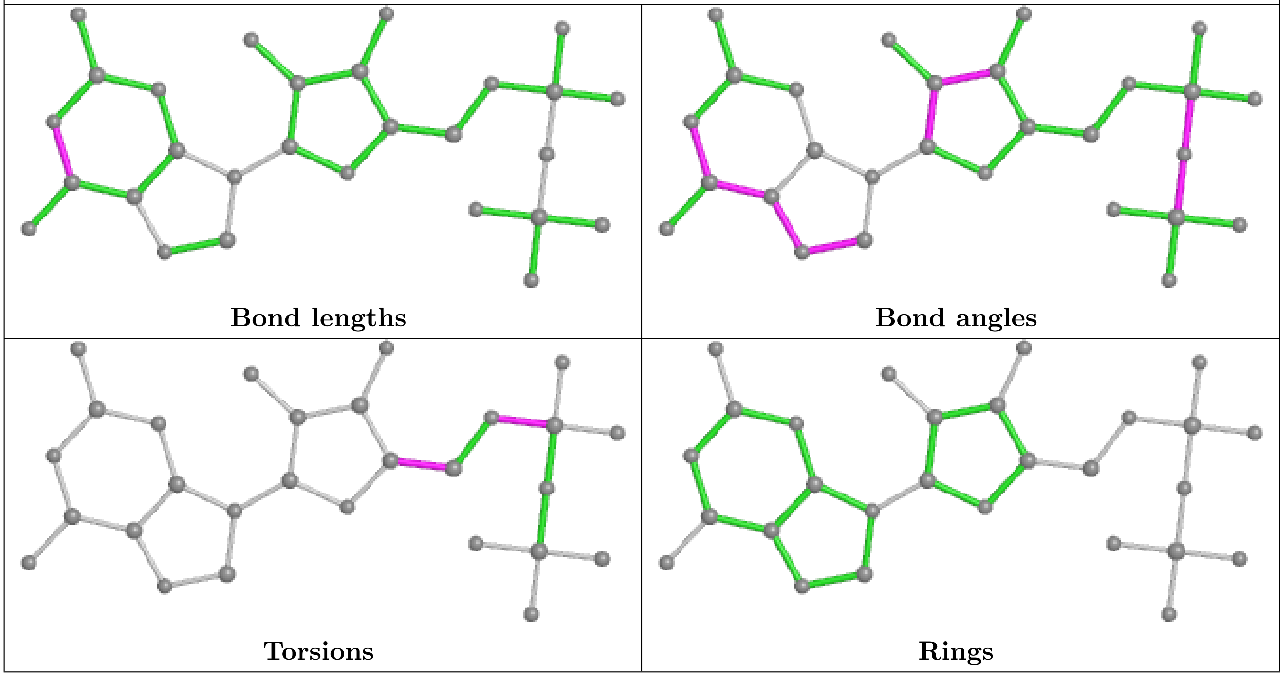
Bond lengths

Bond angles

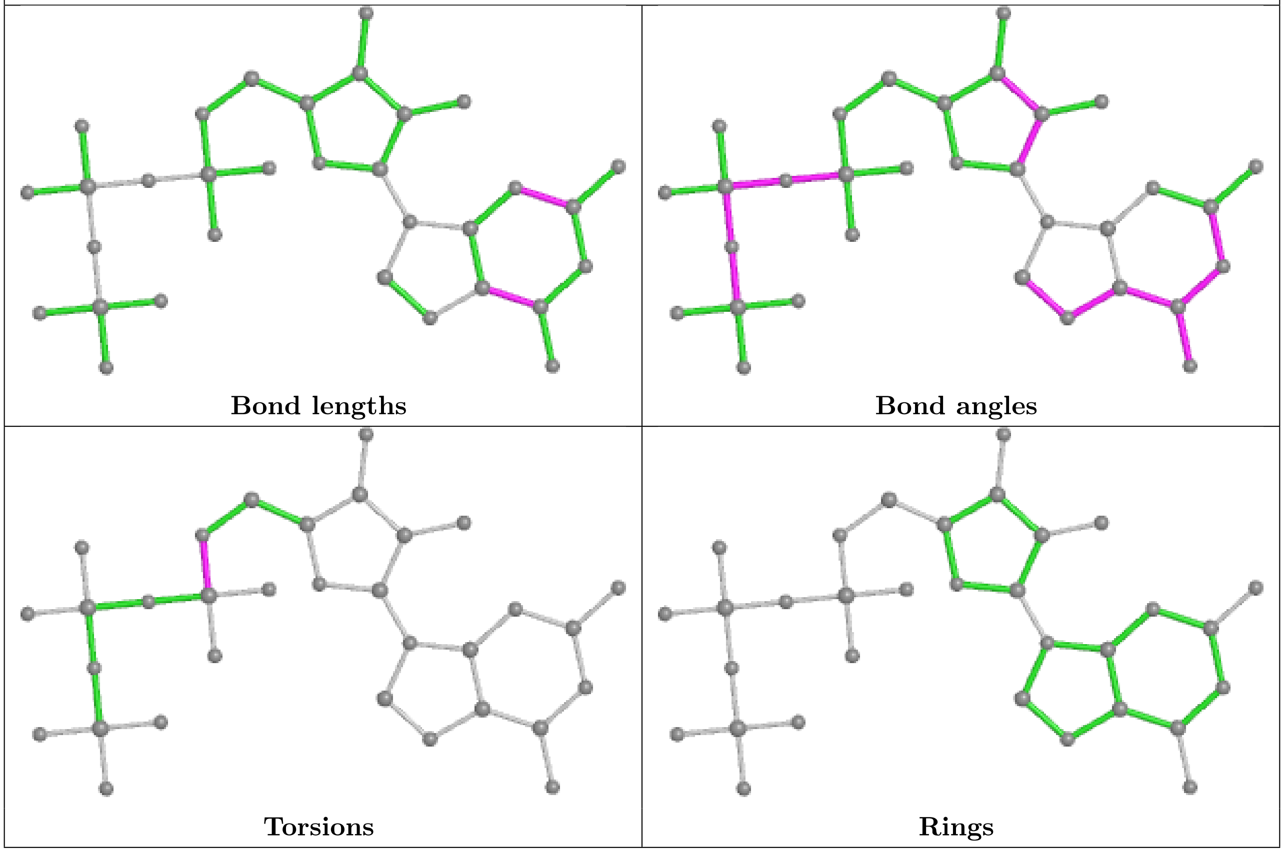
Torsions

Rings

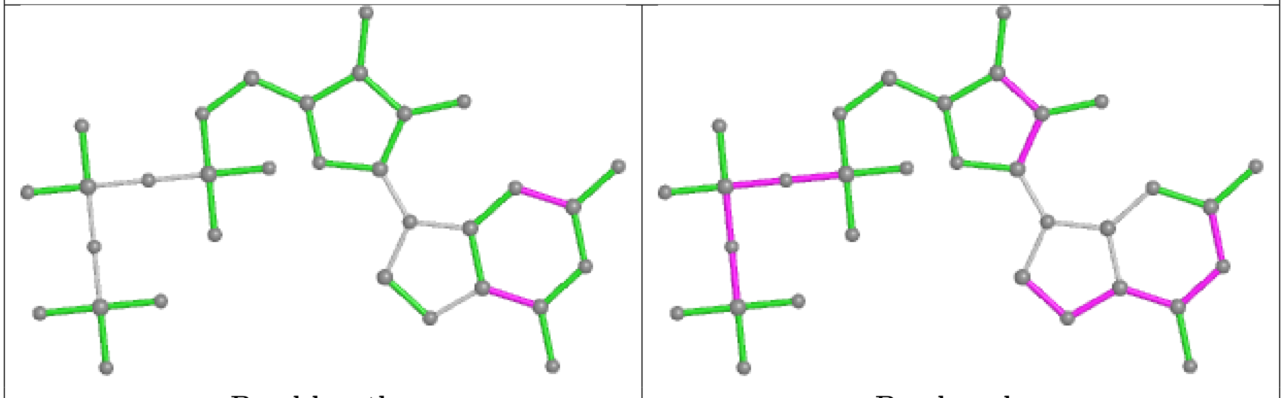
Ligand GDP EL 502



Ligand GTP JE 501

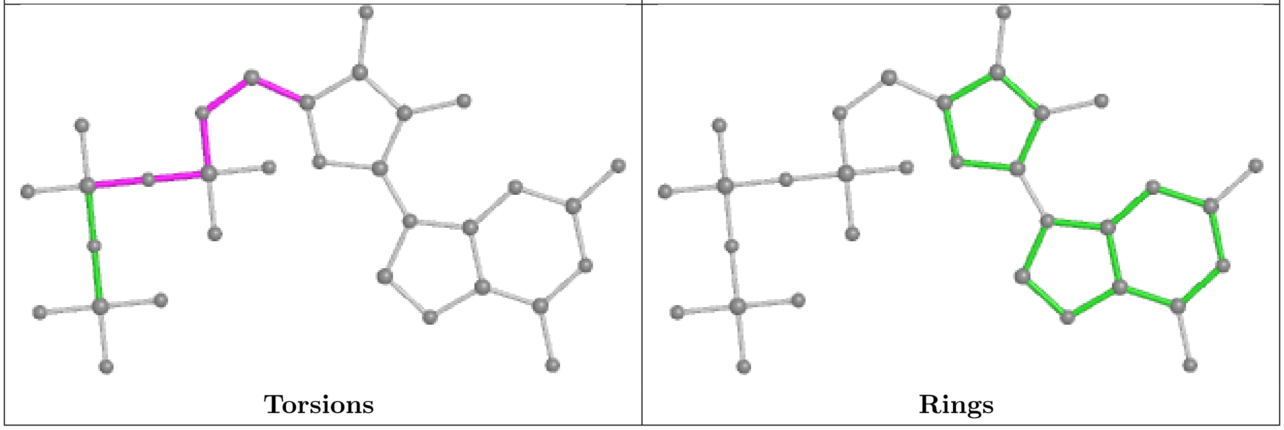


Ligand GTP WM 501



Bond lengths

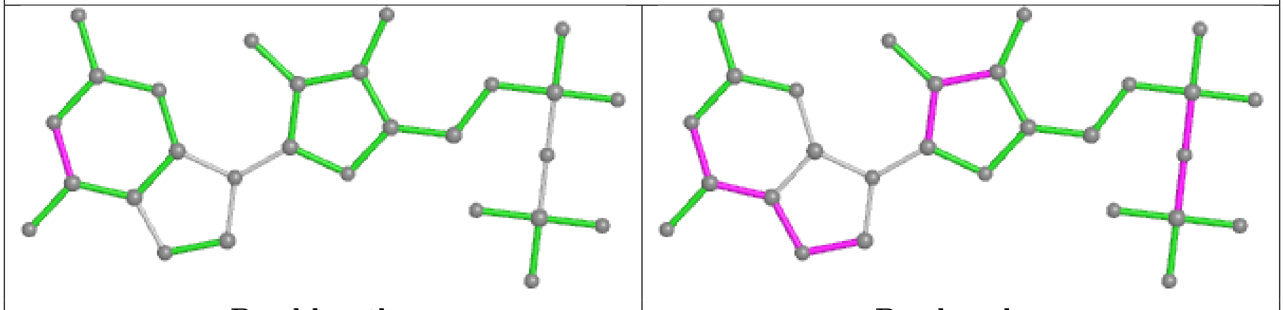
Bond angles



Torsions

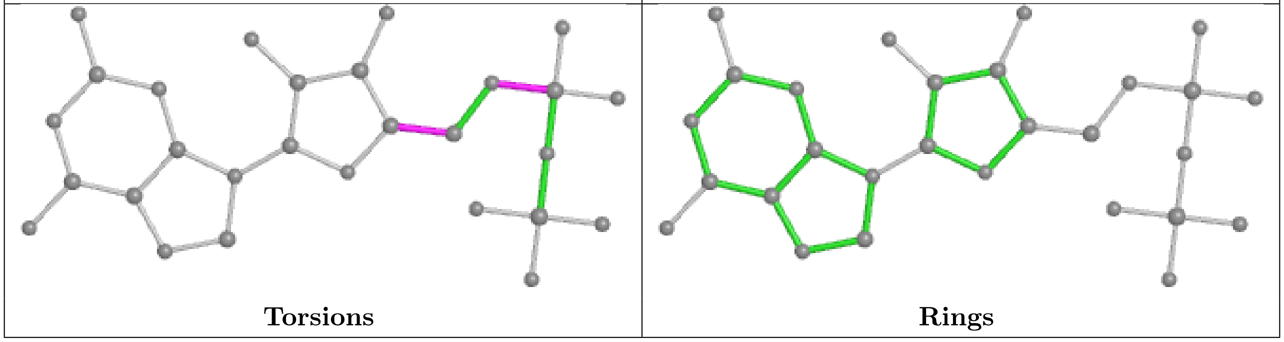
Rings

Ligand GDP LL 502



Bond lengths

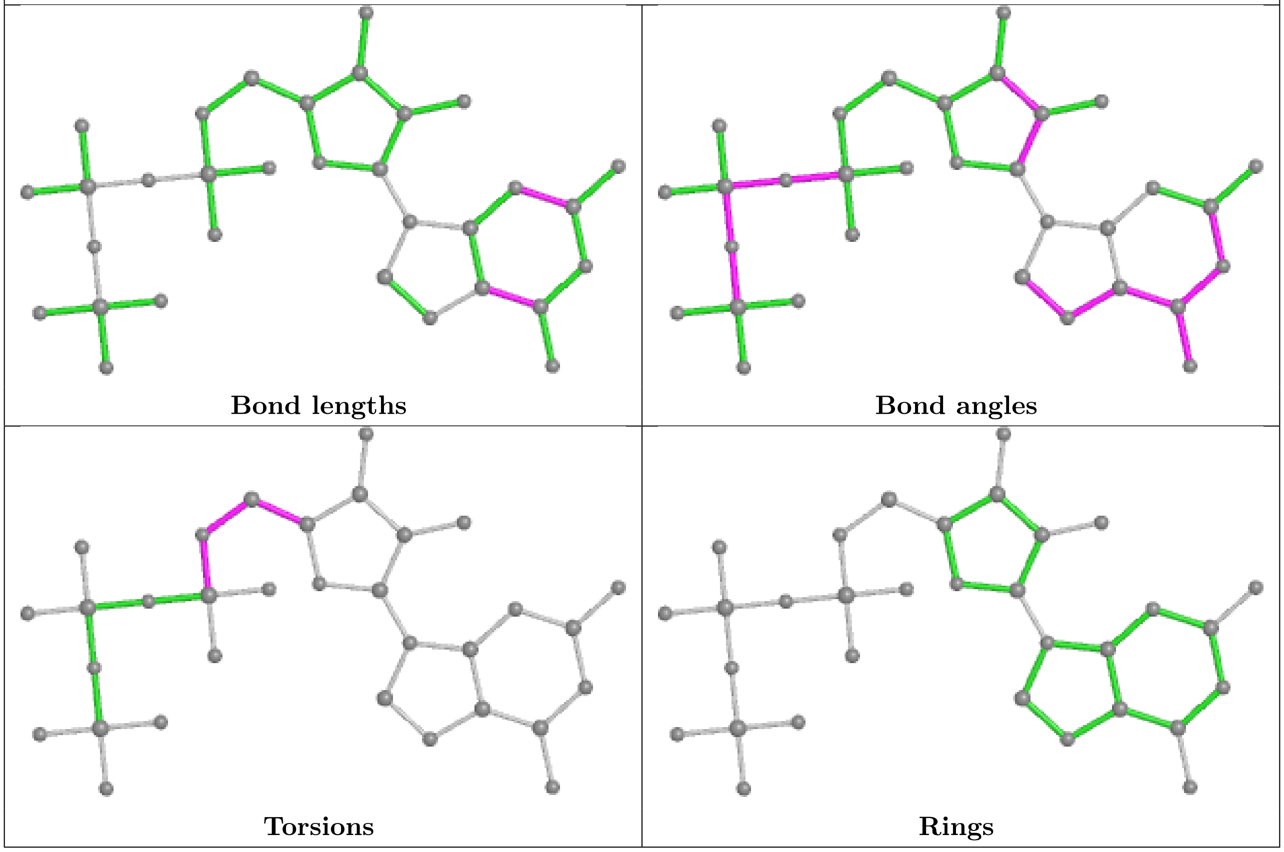
Bond angles



Torsions

Rings

Ligand GTP VI 501



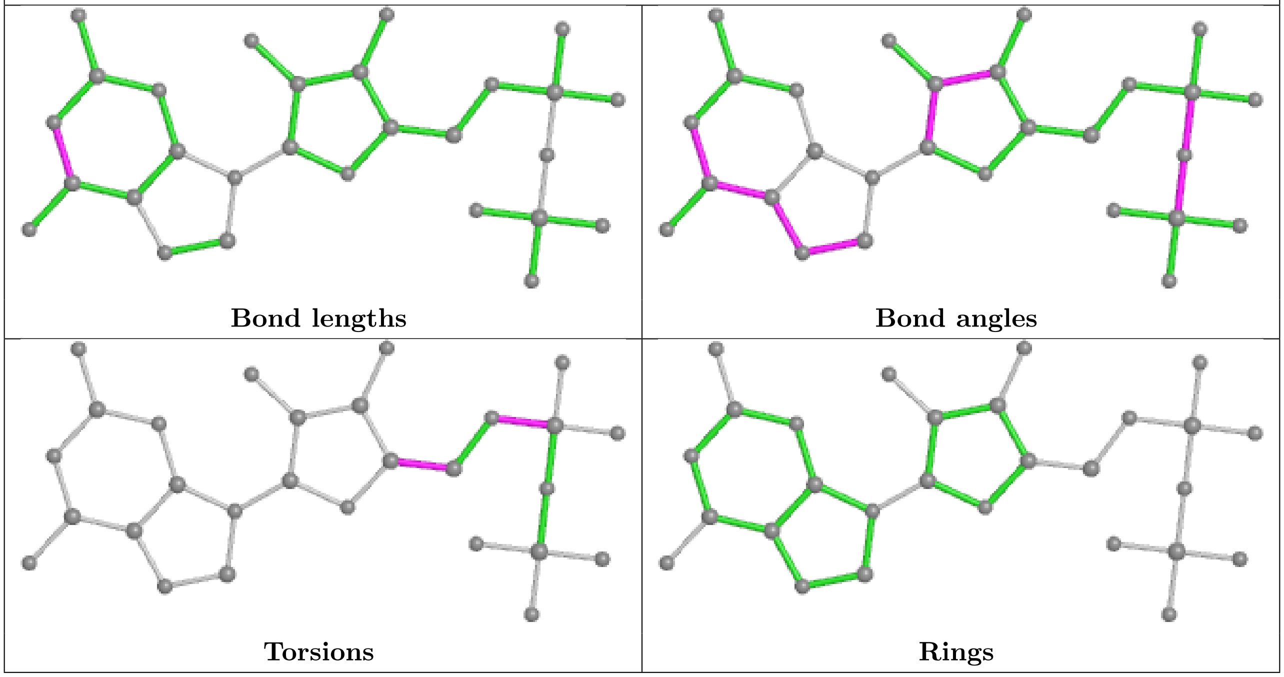
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP PH 502



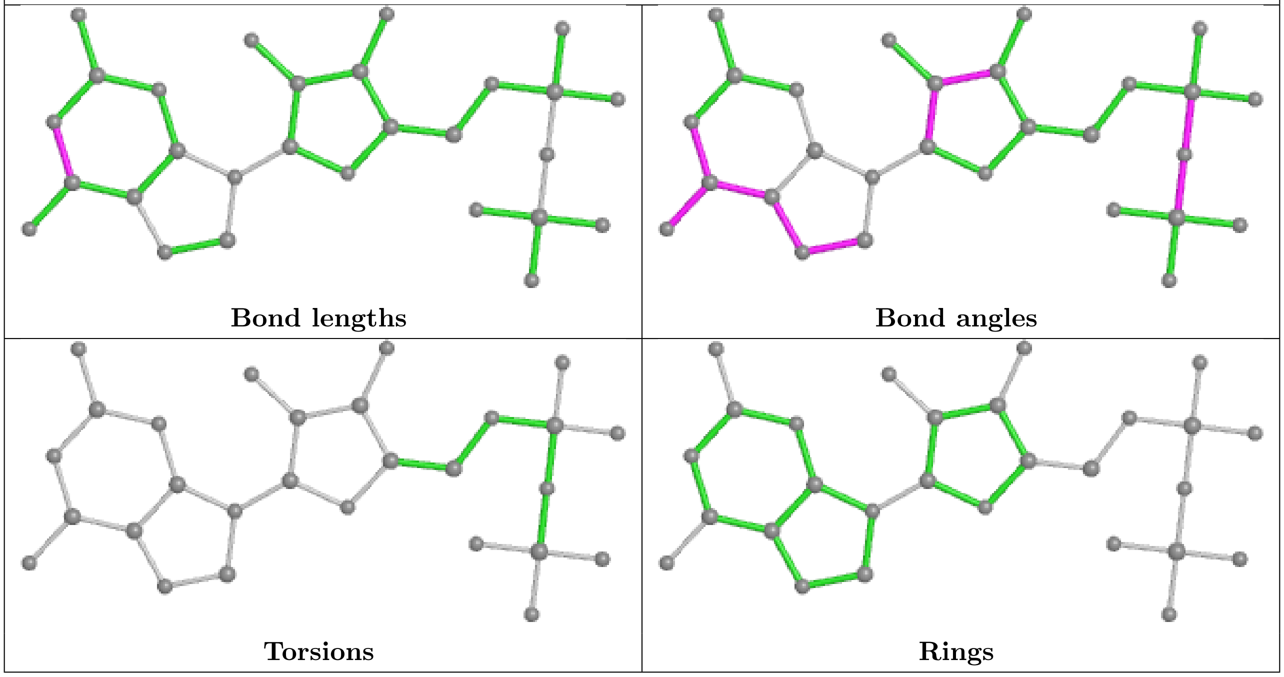
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP SJ 502



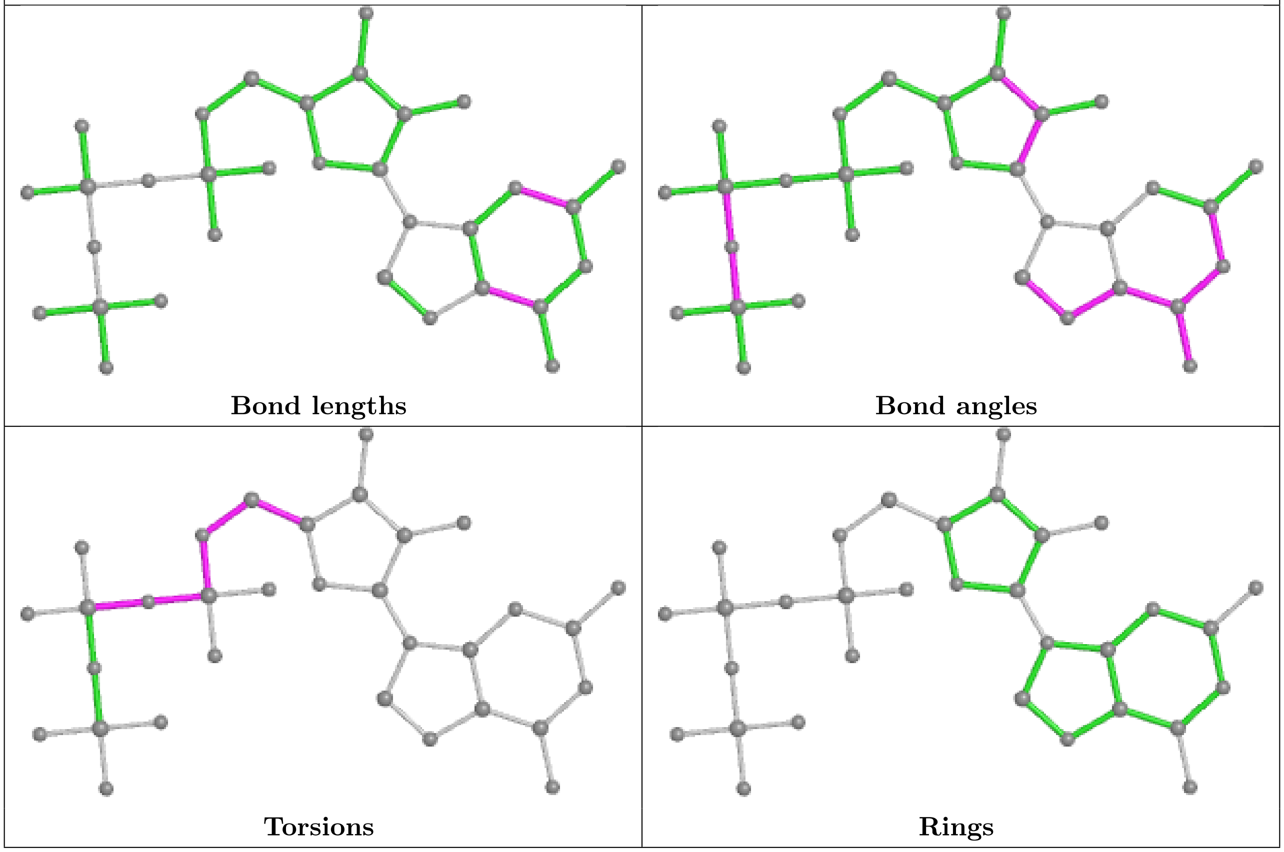
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP QK 501



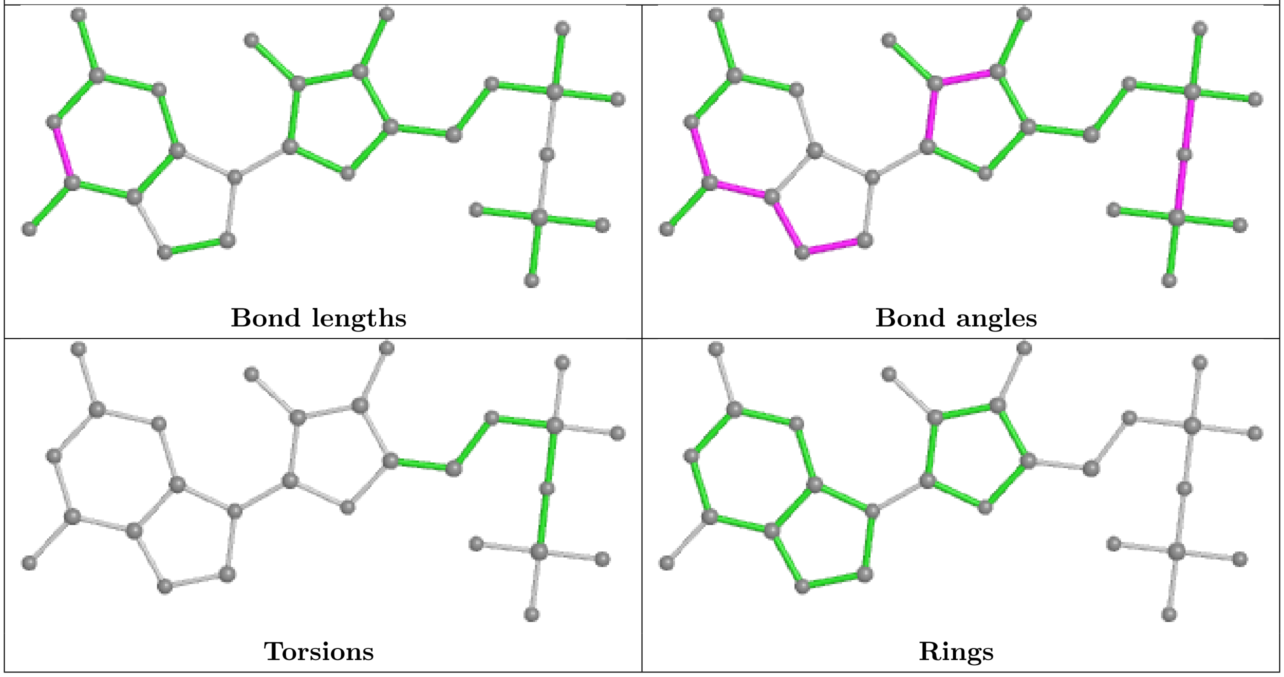
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP HF 502



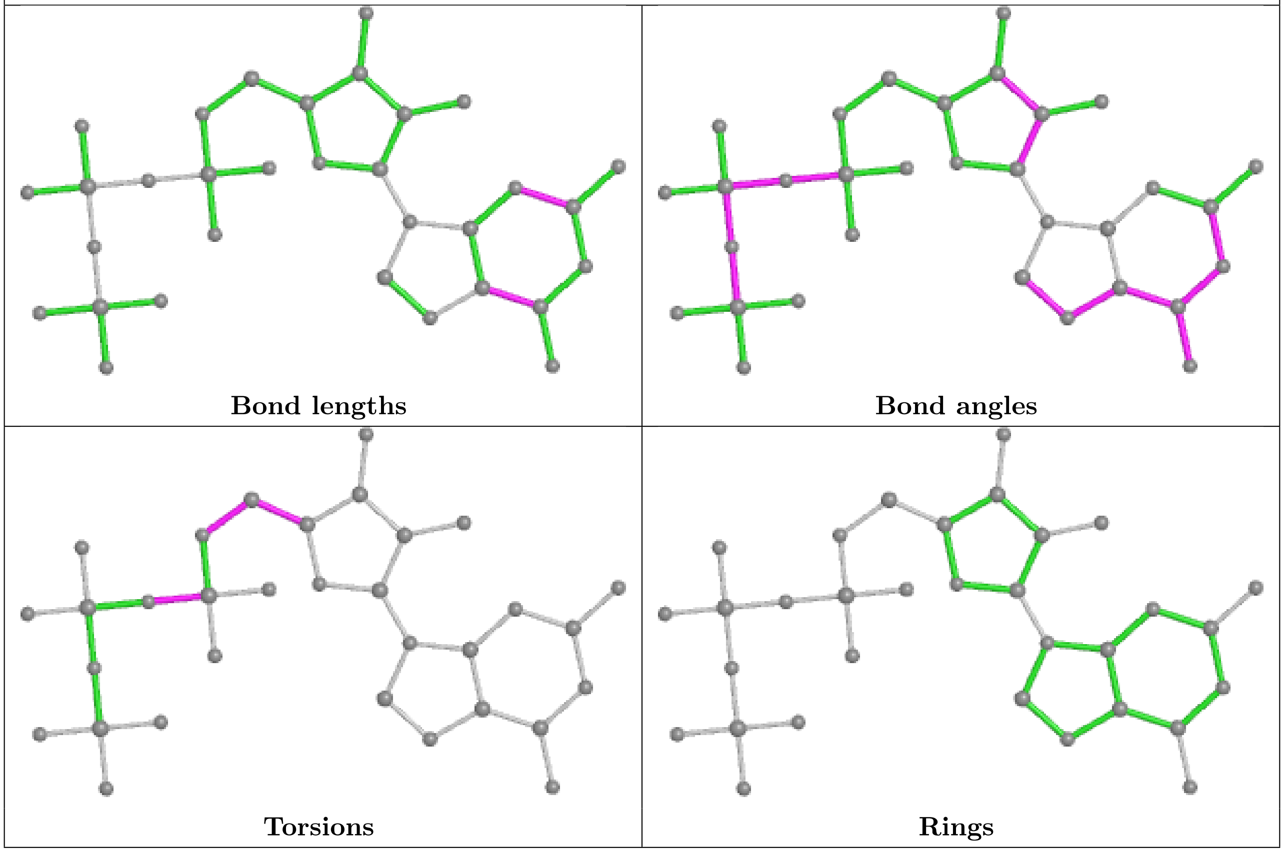
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP HE 501



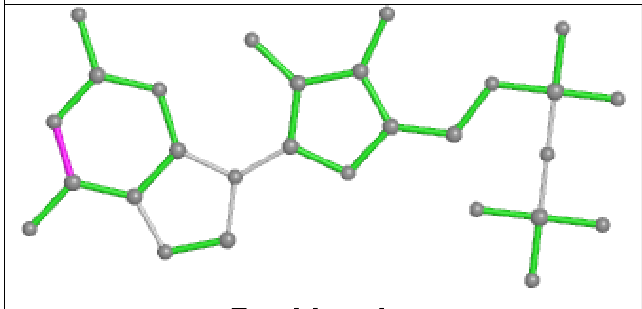
Bond lengths

Bond angles

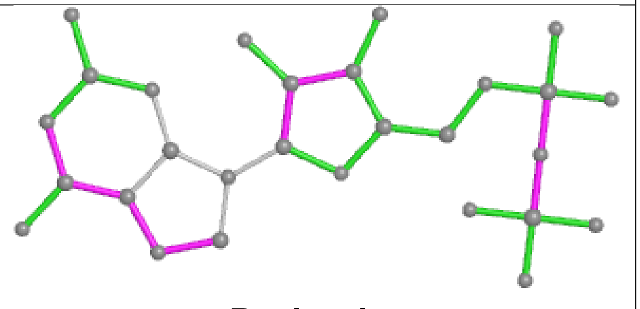
Torsions

Rings

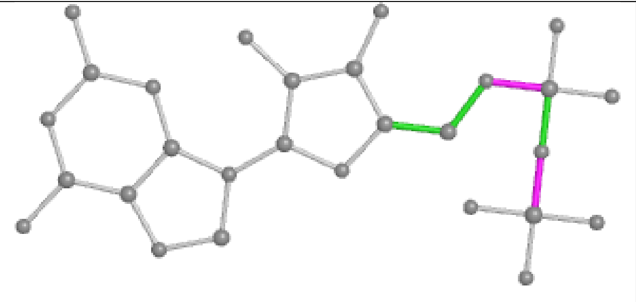
Ligand GDP BL 502



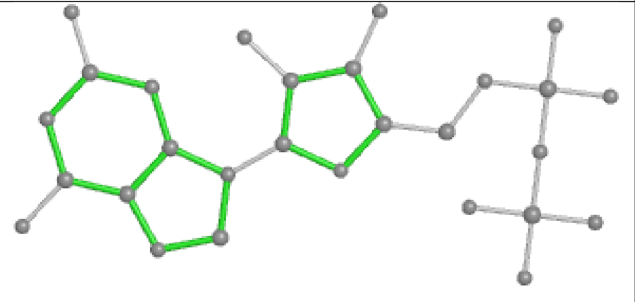
Bond lengths



Bond angles

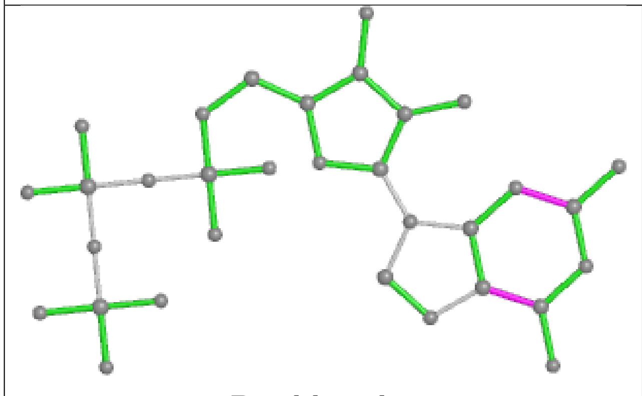


Torsions

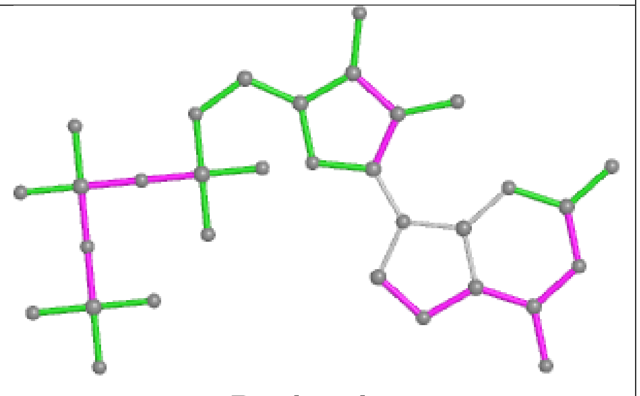


Rings

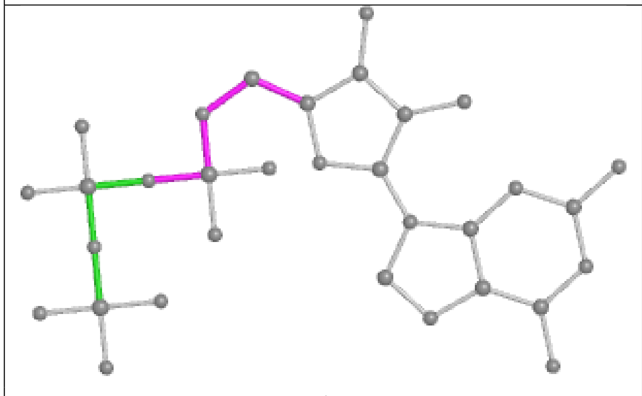
Ligand GTP UG 501



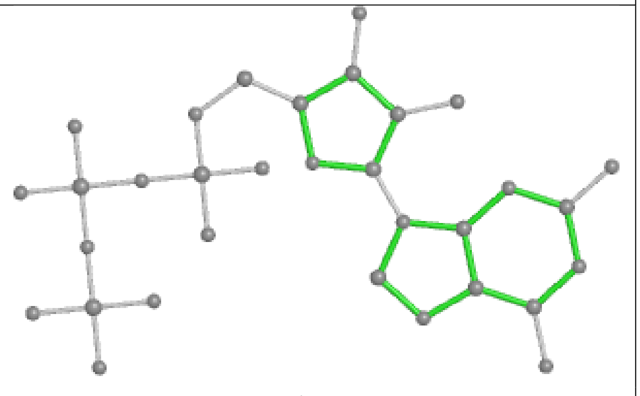
Bond lengths



Bond angles

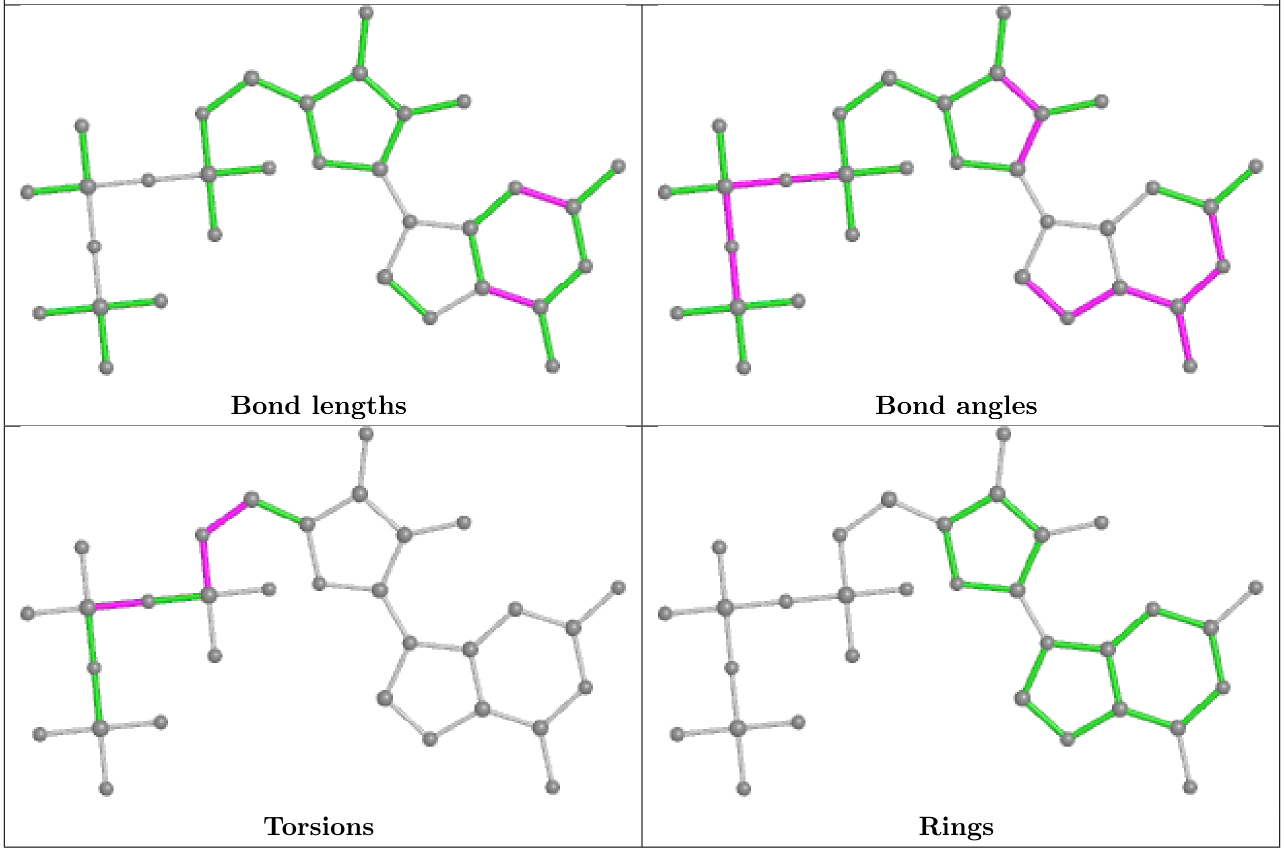


Torsions



Rings

Ligand GTP FG 501



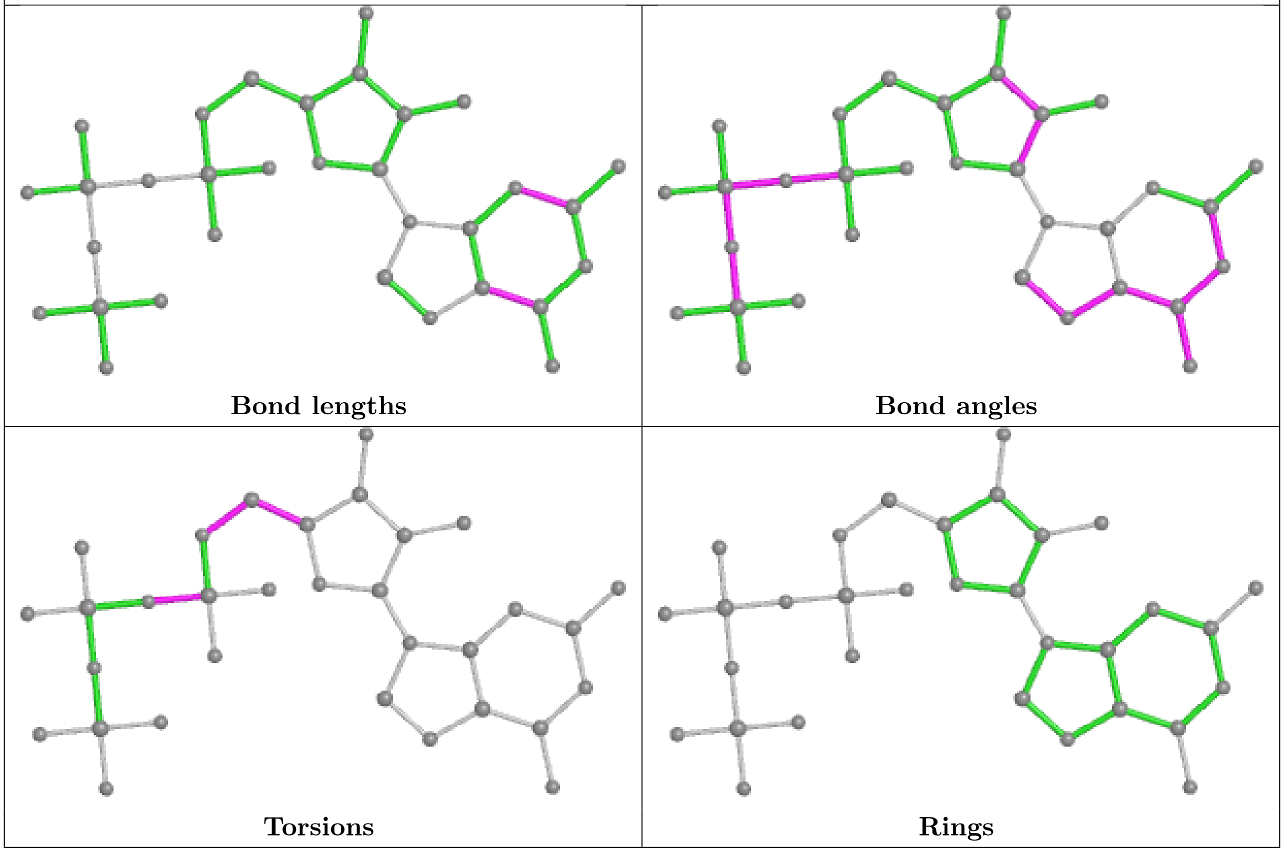
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP HK 501



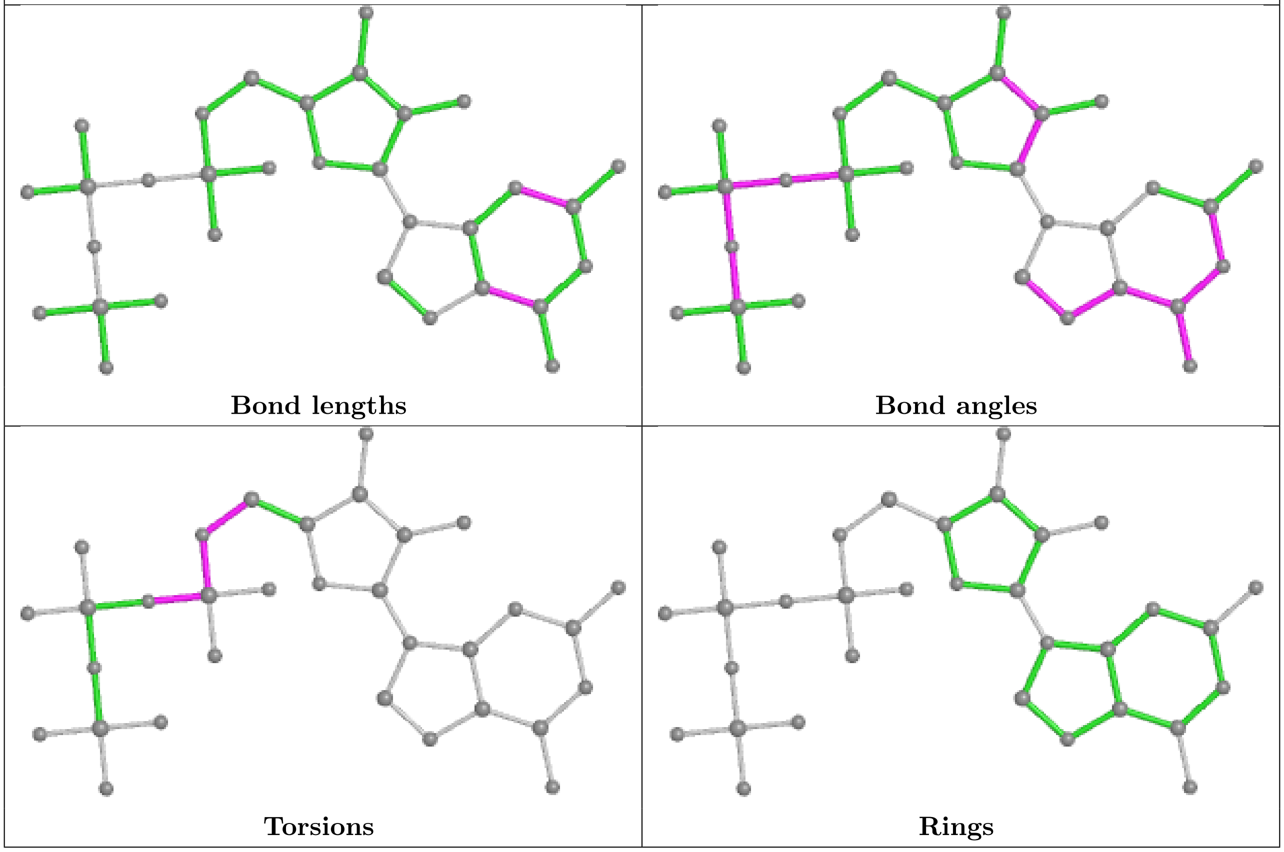
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP EI 501



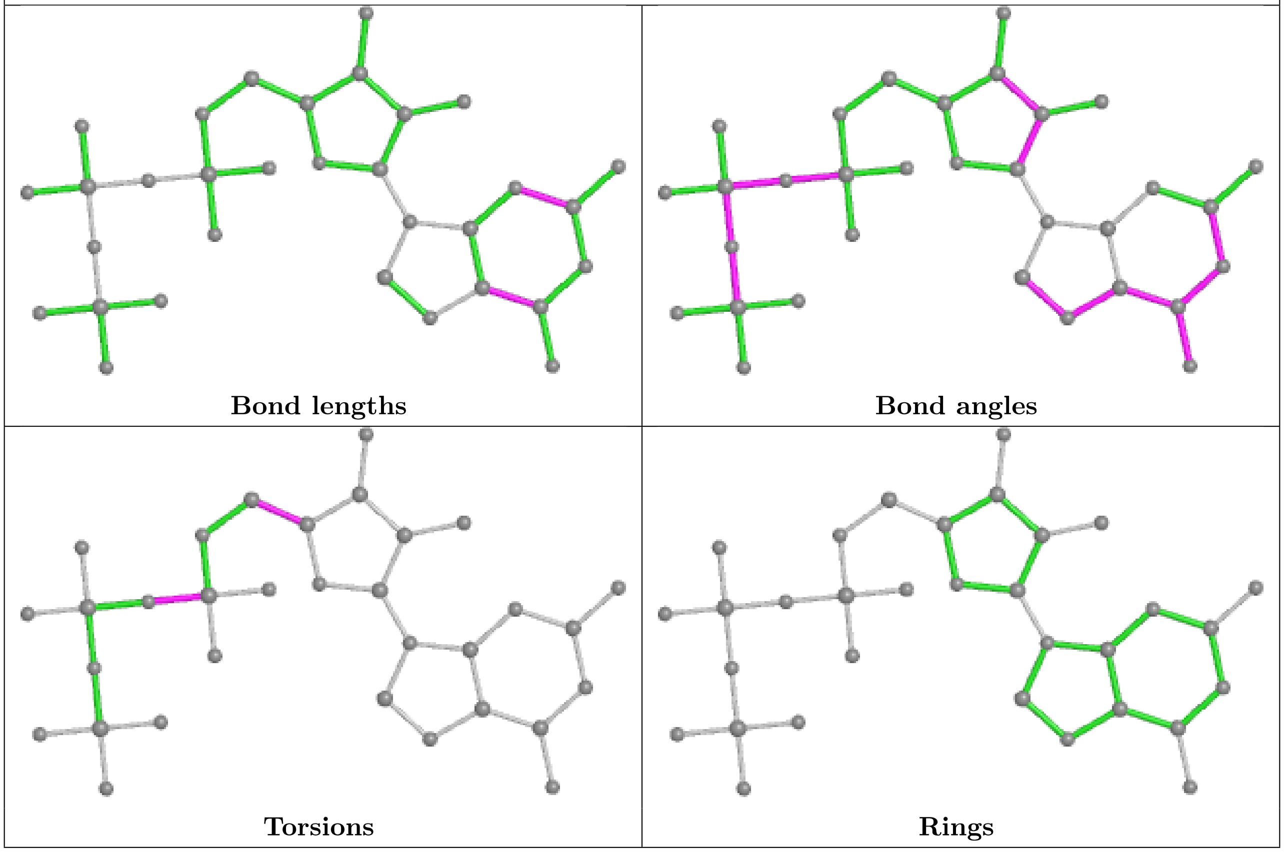
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP AE 501



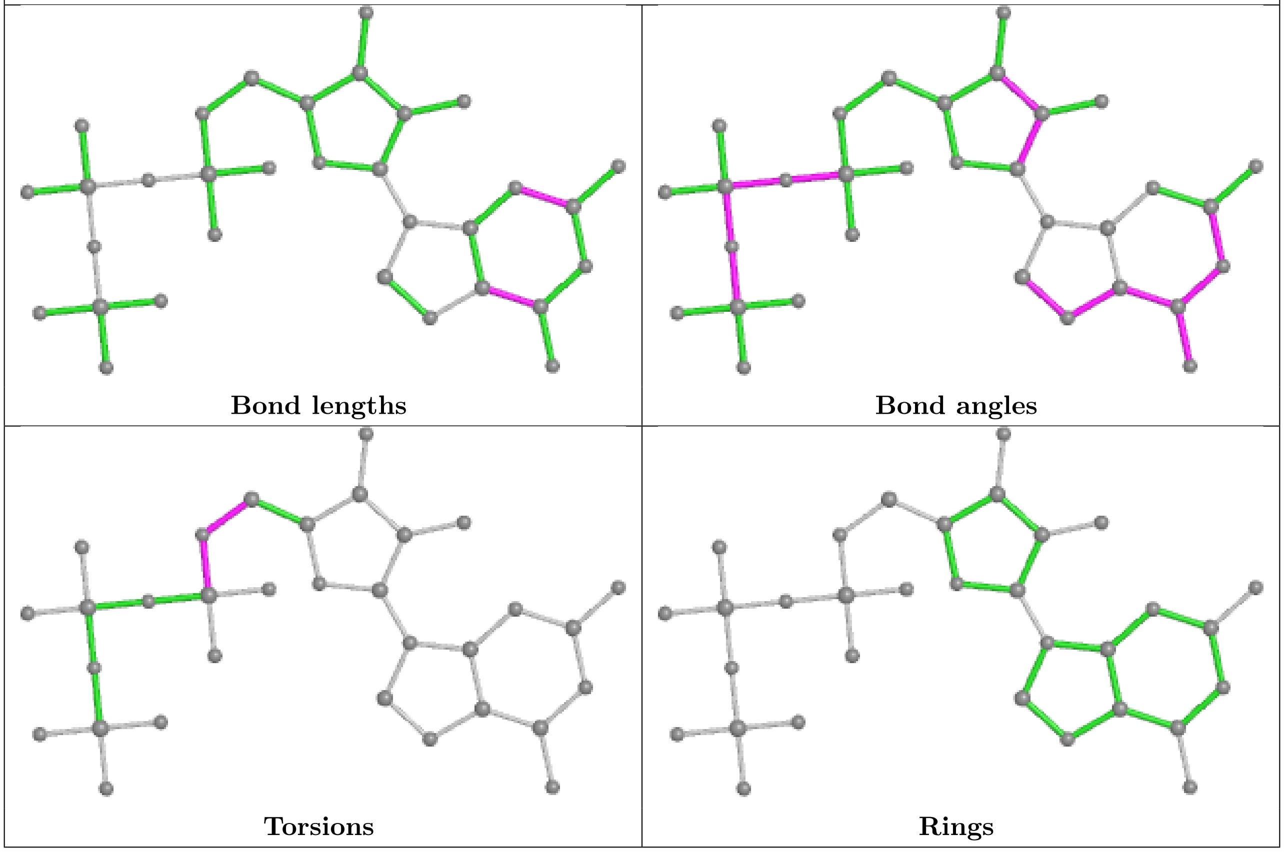
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP PI 501



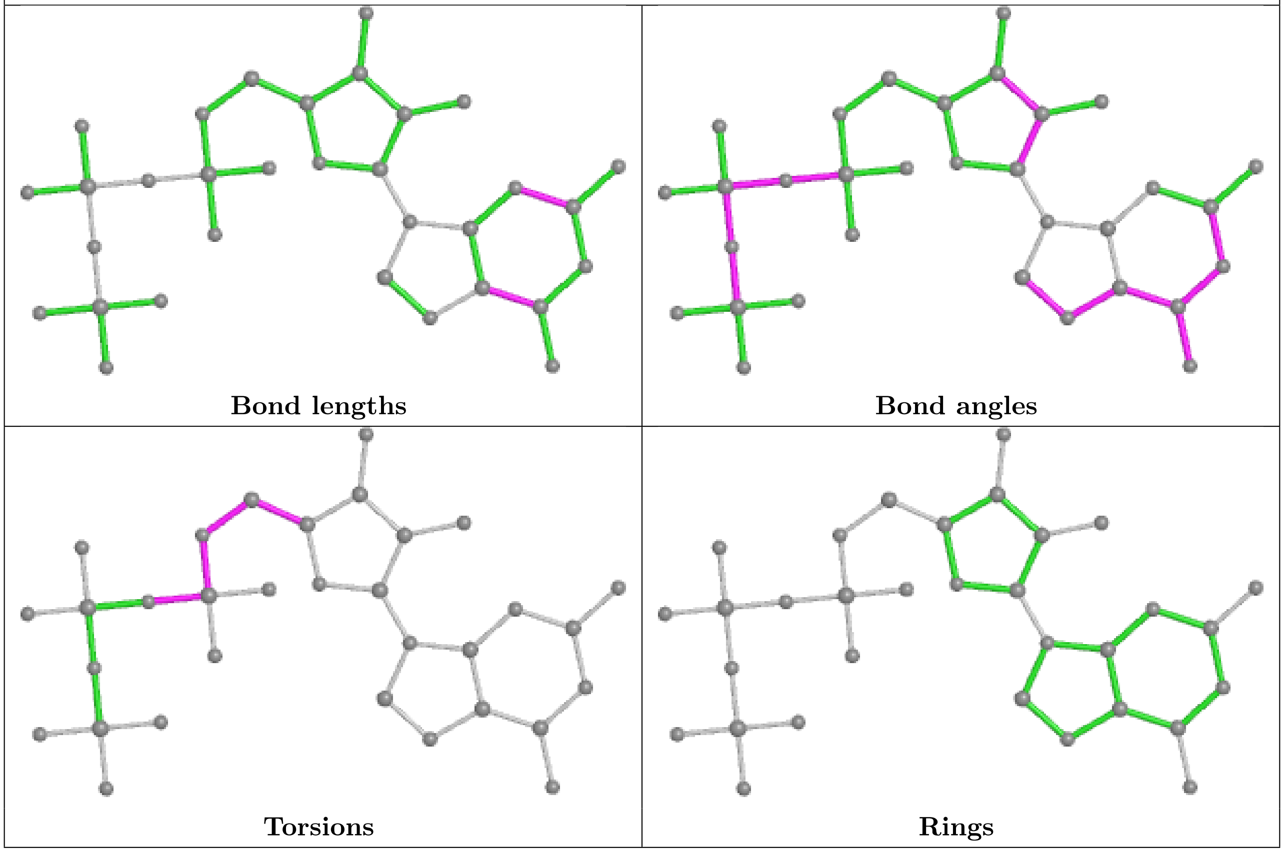
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP UM 501



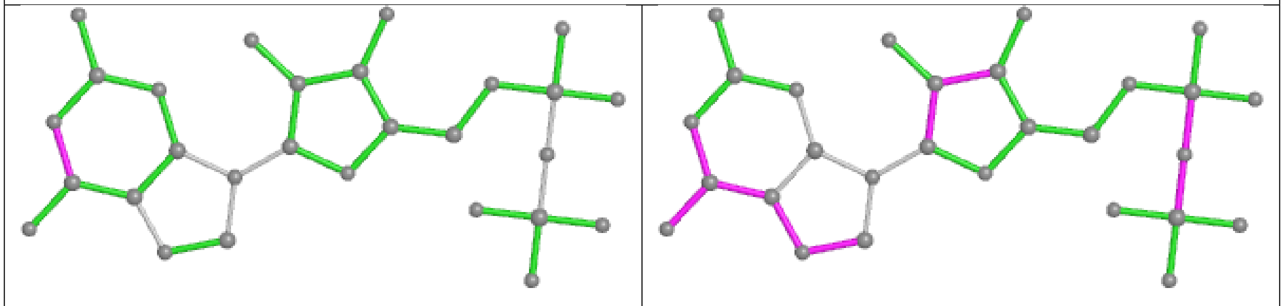
Bond lengths

Bond angles

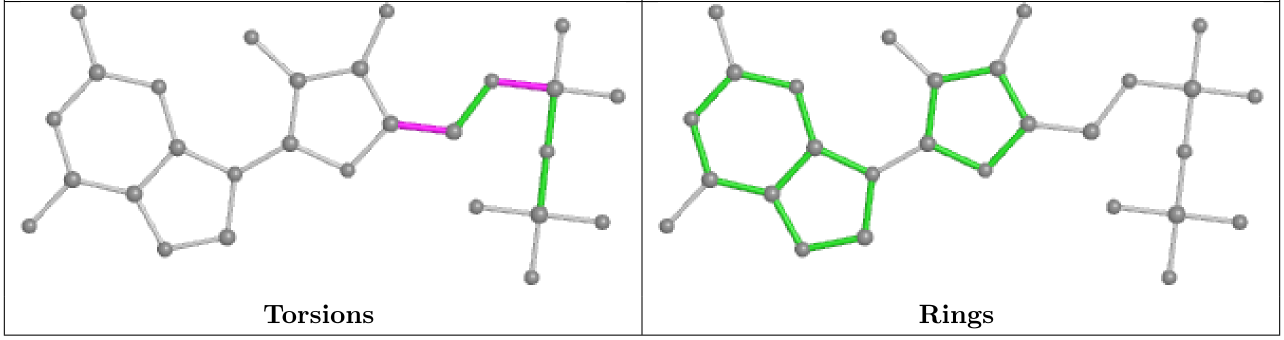
Torsions

Rings

Ligand GDP FD 502

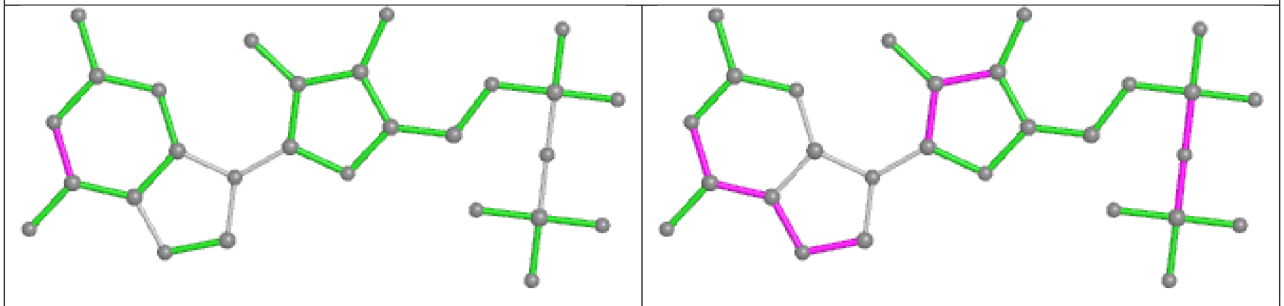


Bond lengths **Bond angles**

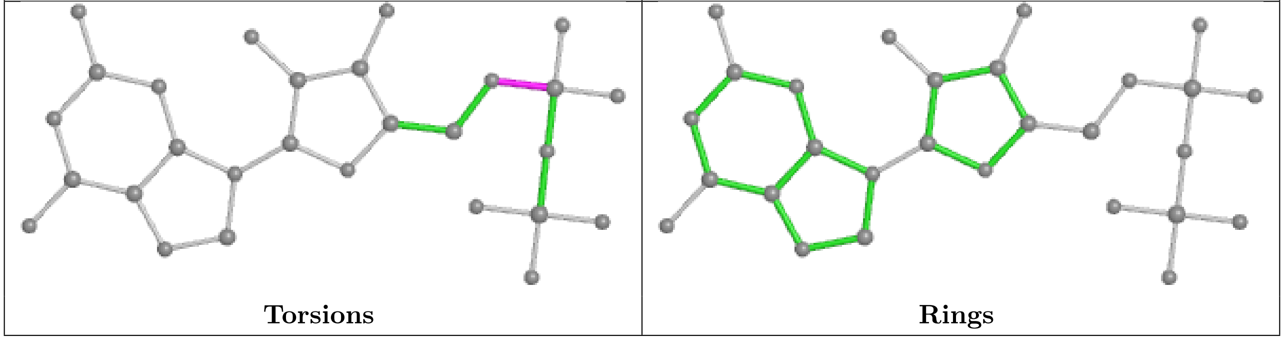


Torsions **Rings**

Ligand GDP JB 502

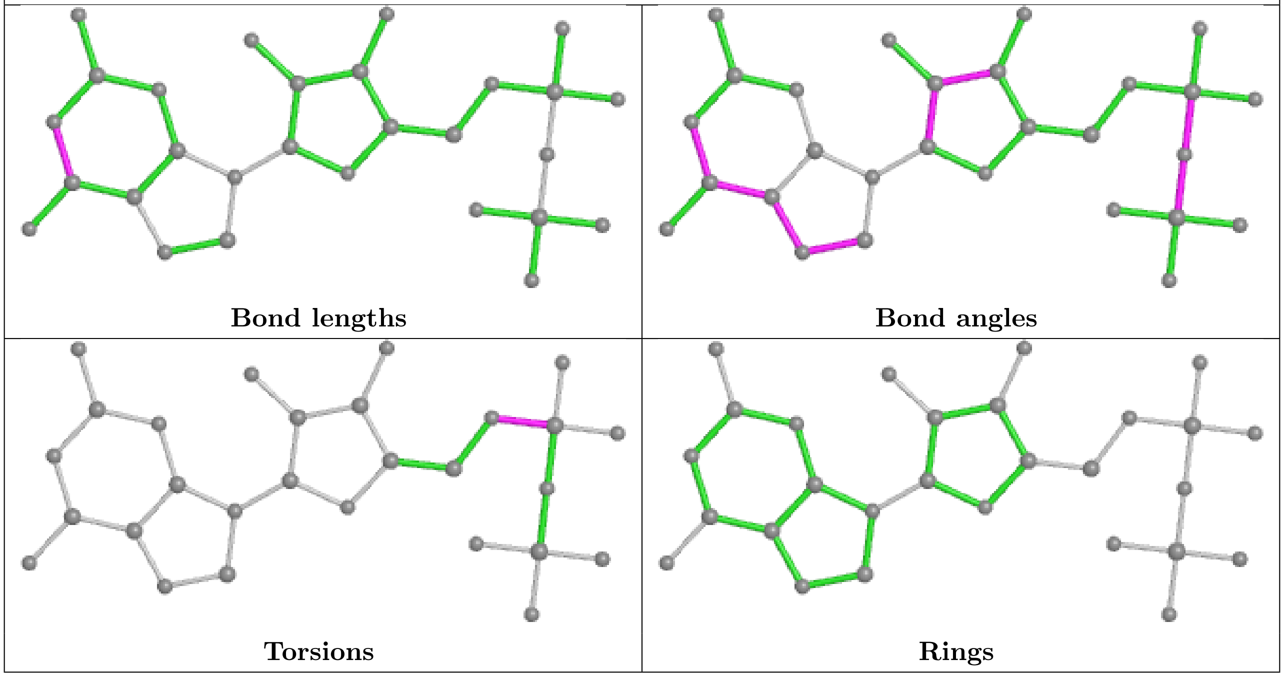


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GDP DF 502



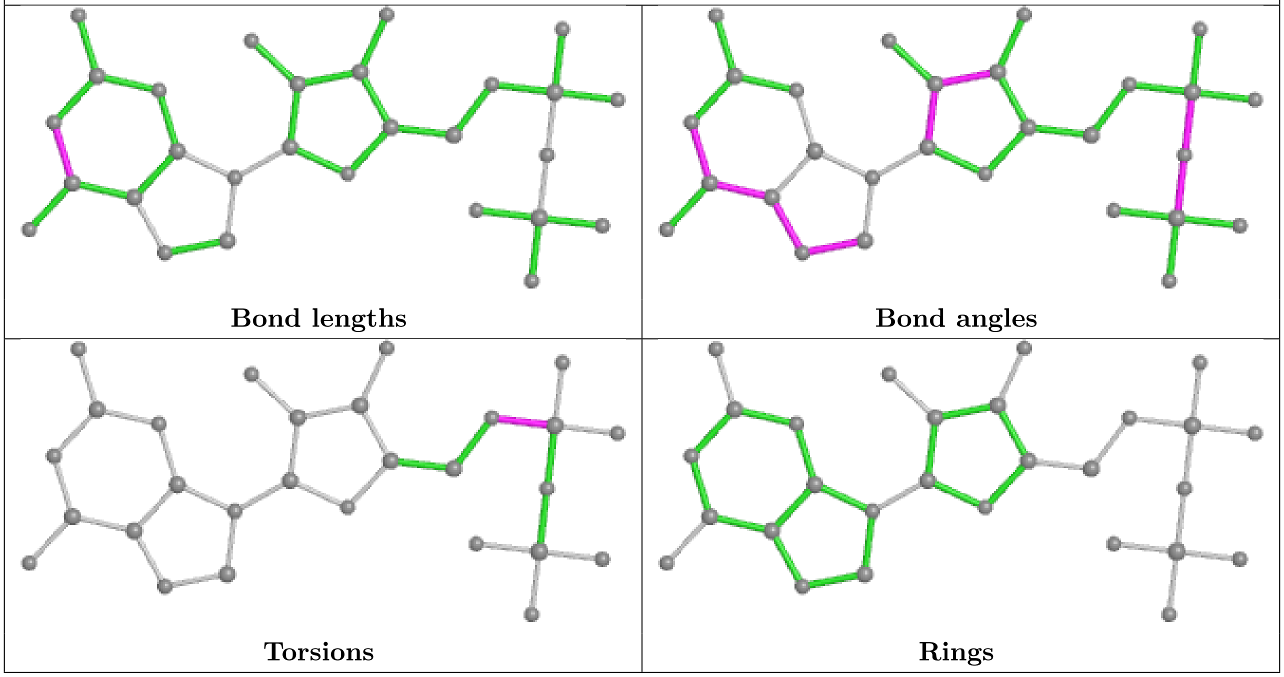
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP FB 502



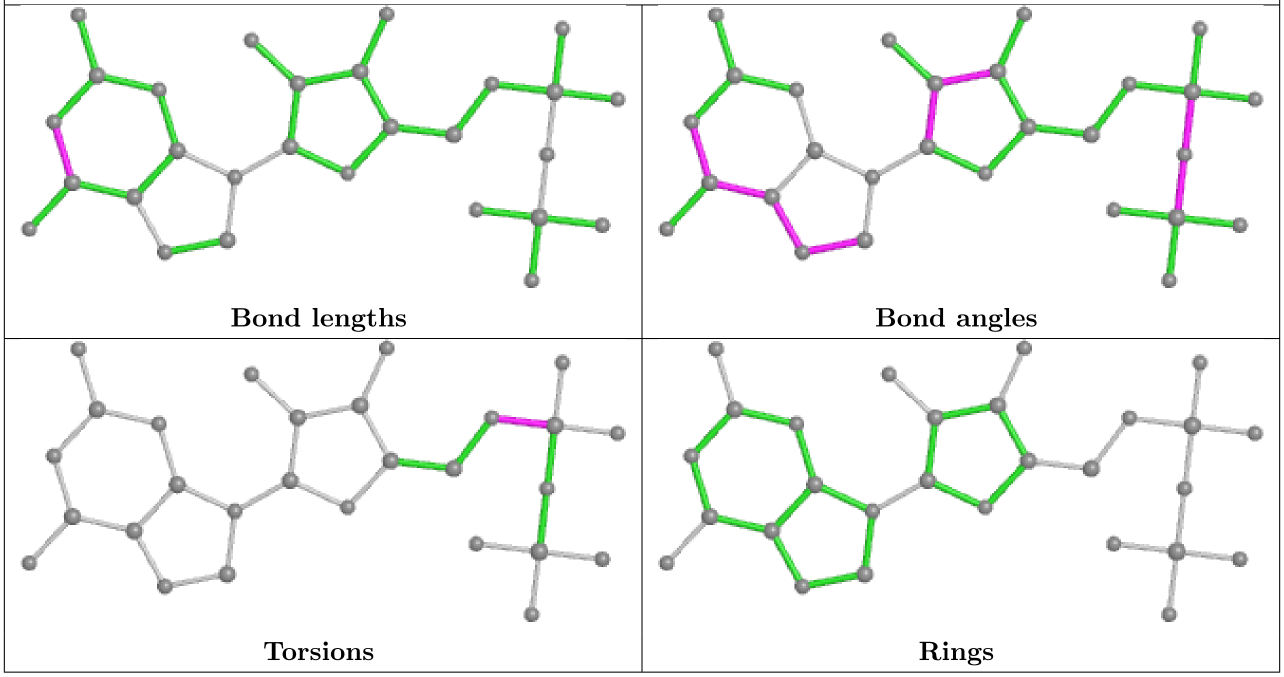
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP FJ 502



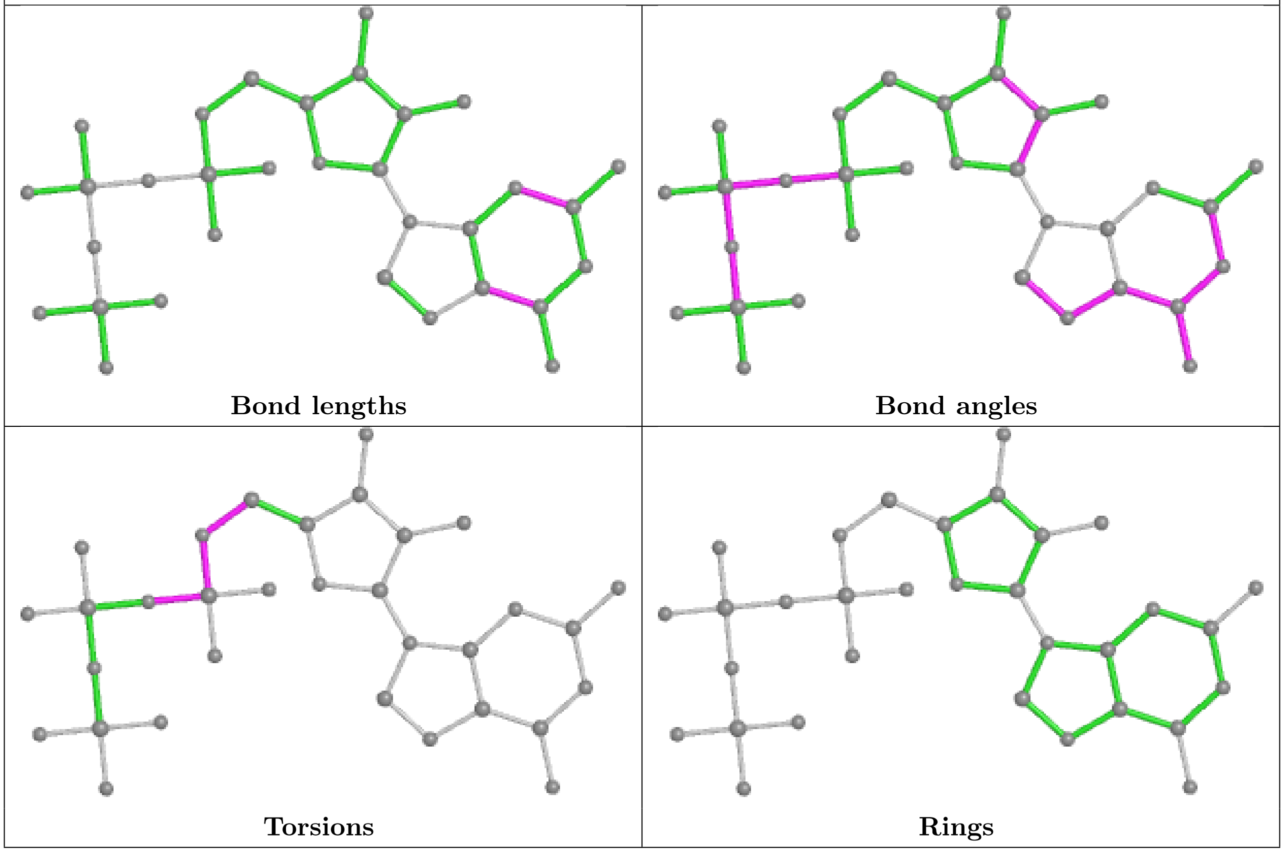
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP QG 501



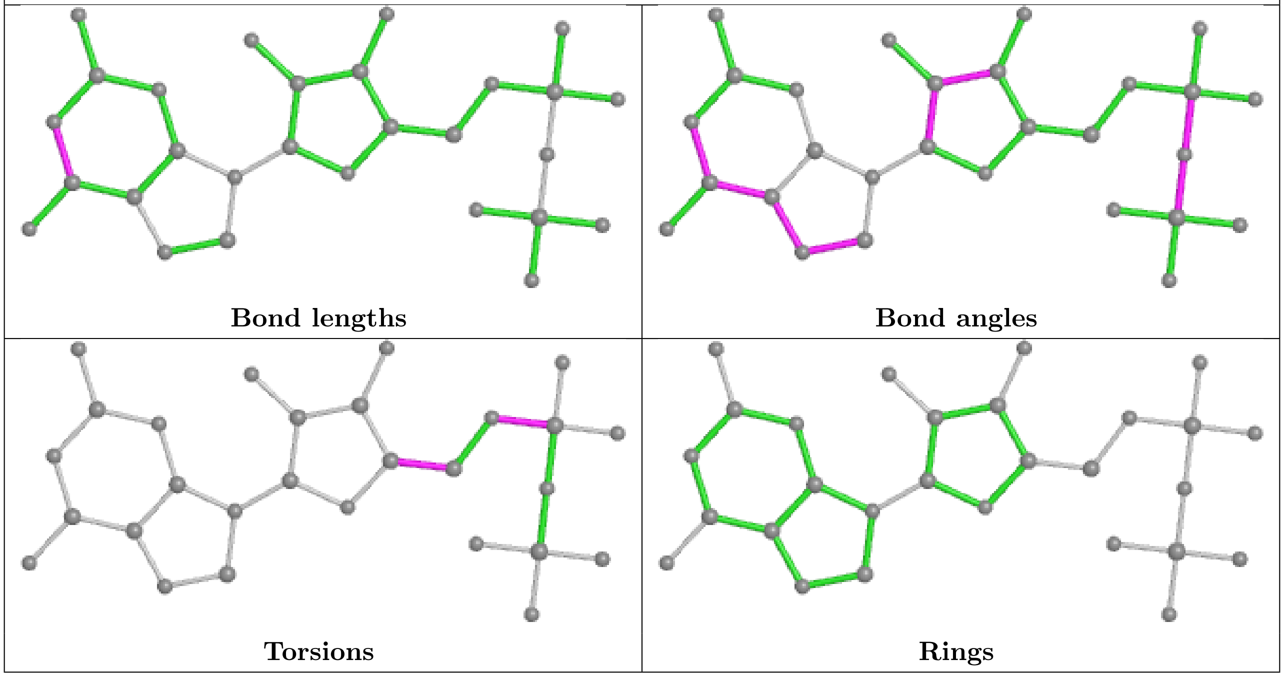
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP TD 502



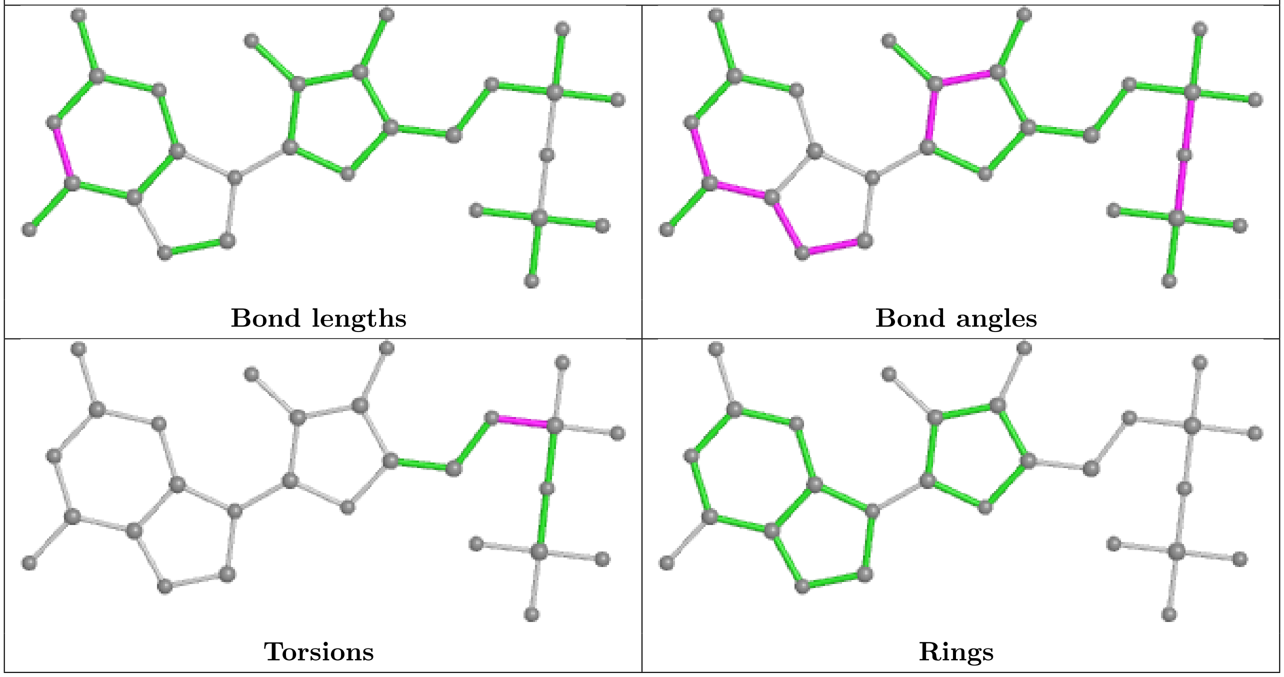
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP MN 502



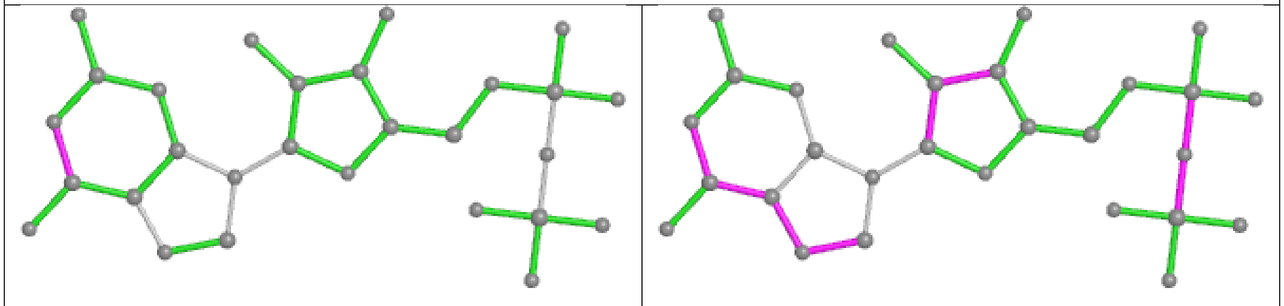
Bond lengths

Bond angles

Torsions

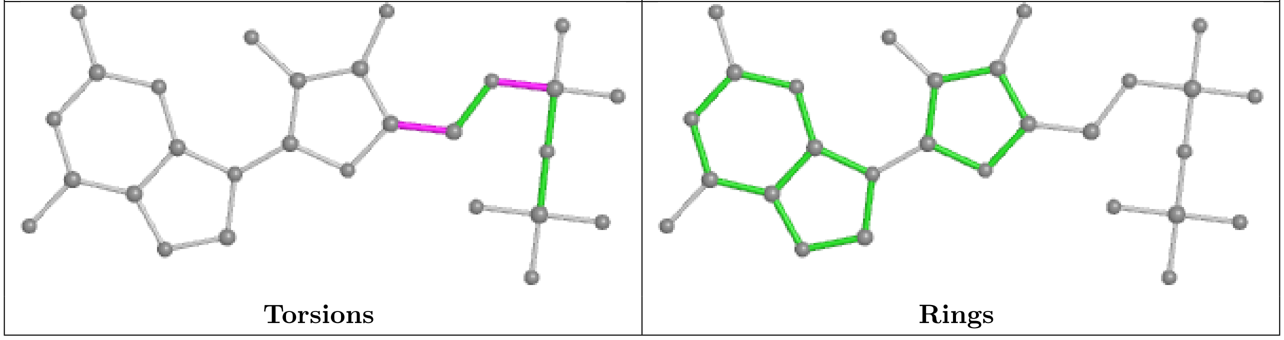
Rings

Ligand GDP QH 502



Bond lengths

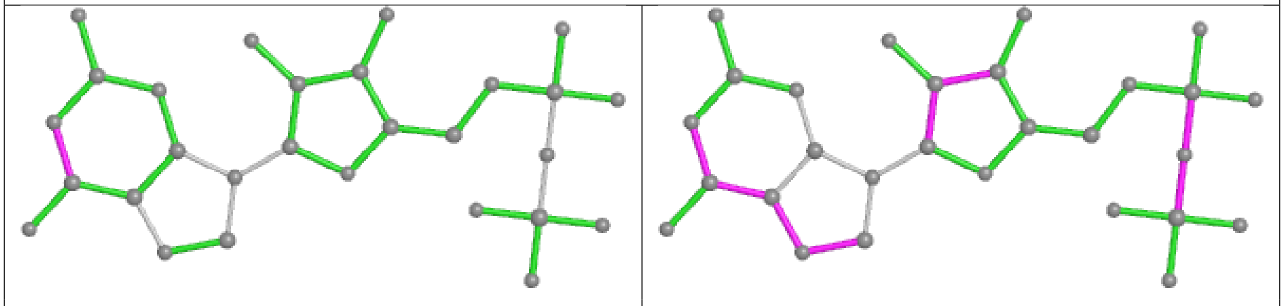
Bond angles



Torsions

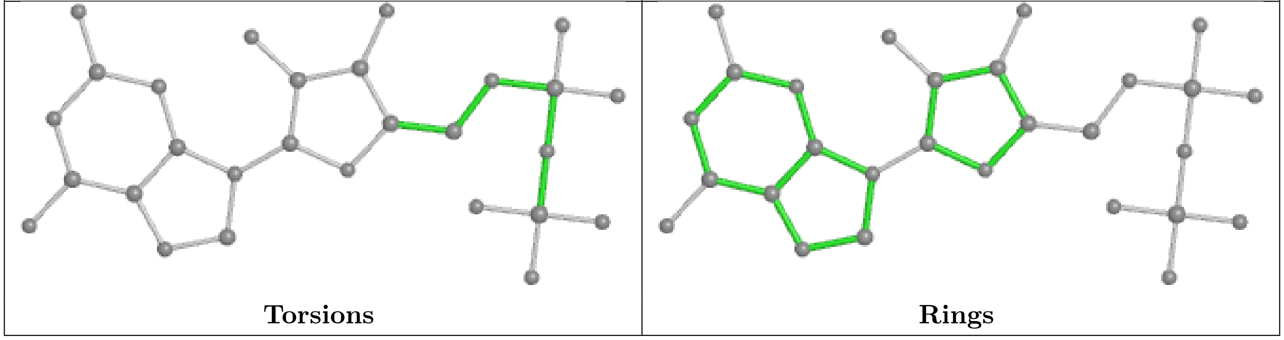
Rings

Ligand GDP HH 502



Bond lengths

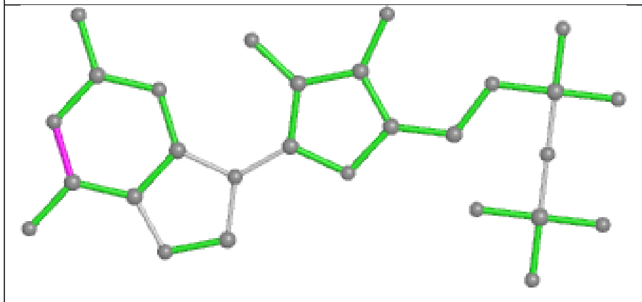
Bond angles



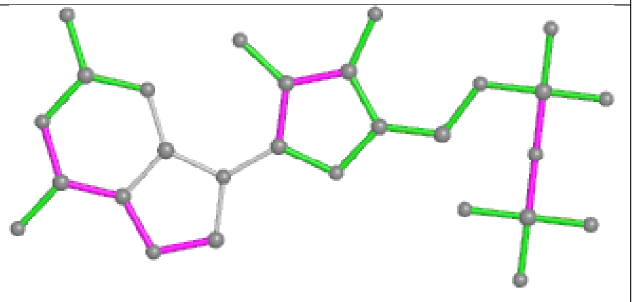
Torsions

Rings

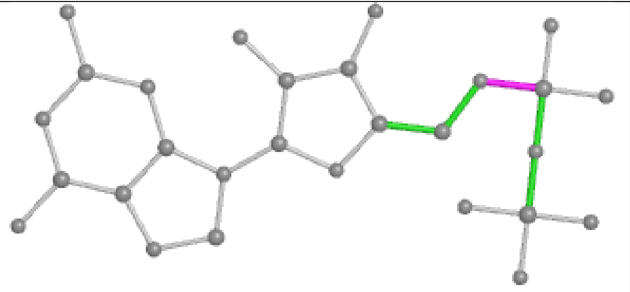
Ligand GDP RN 502



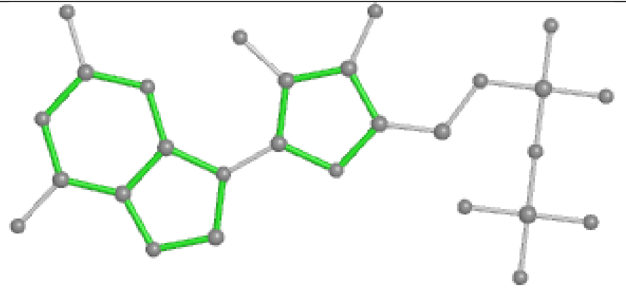
Bond lengths



Bond angles

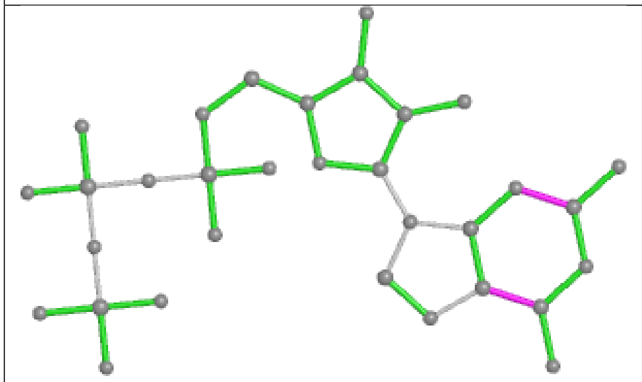


Torsions

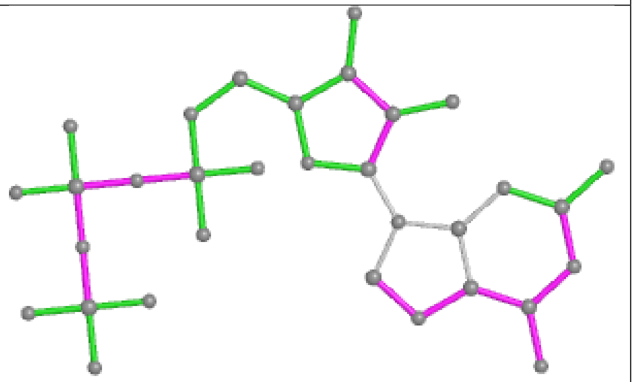


Rings

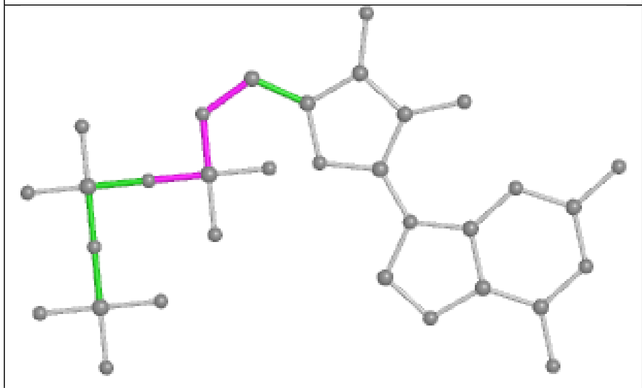
Ligand GTP EG 501



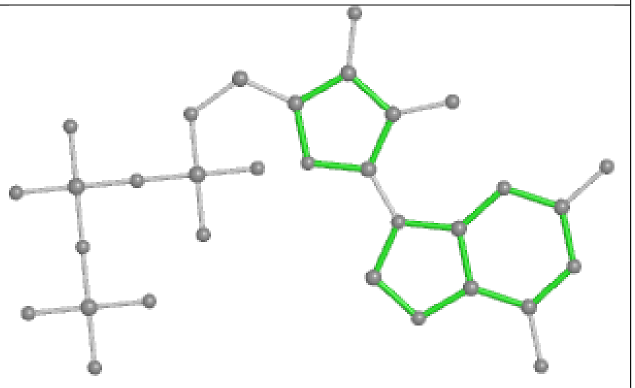
Bond lengths



Bond angles

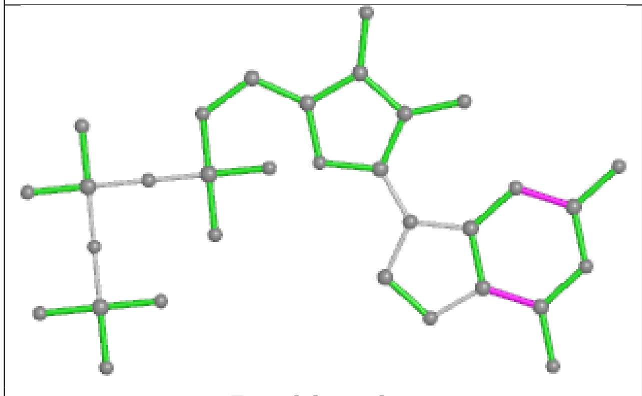


Torsions

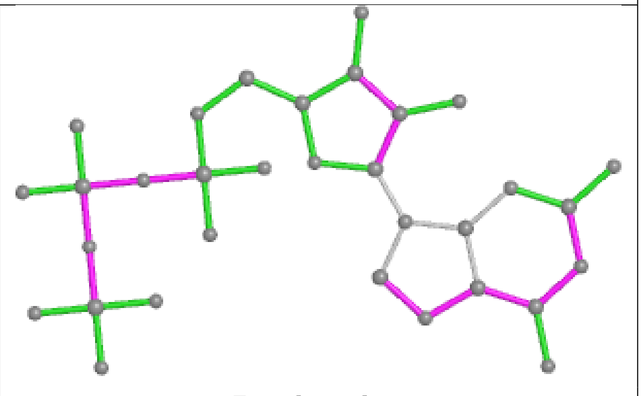


Rings

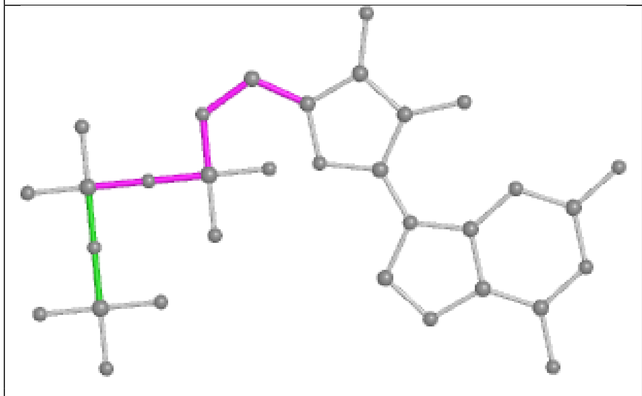
Ligand GTP TE 501



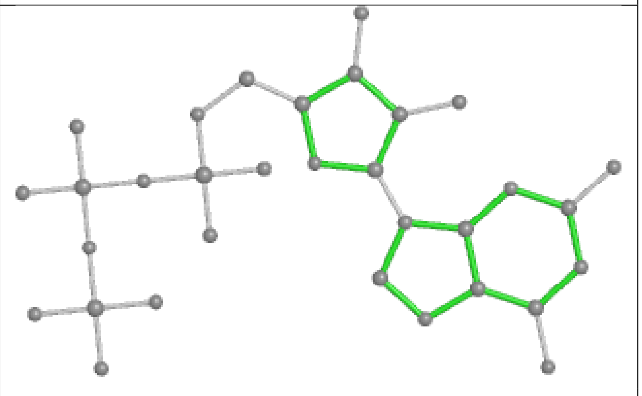
Bond lengths



Bond angles

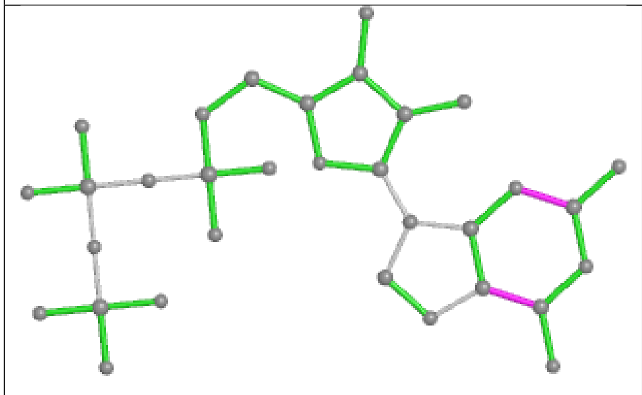


Torsions

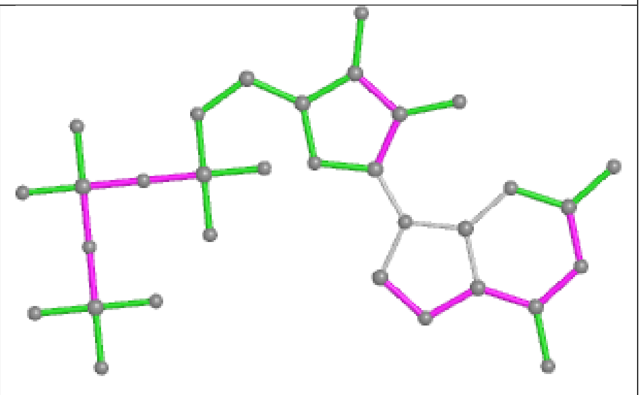


Rings

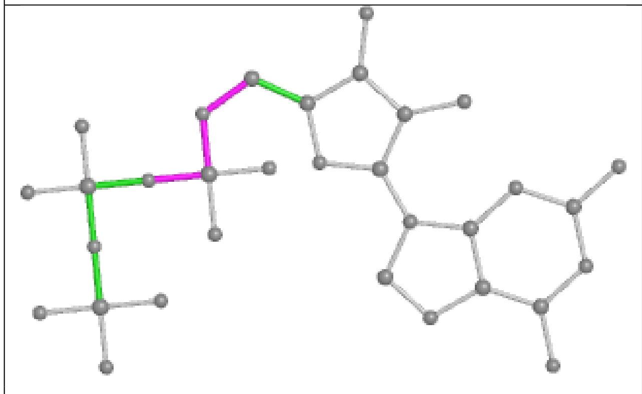
Ligand GTP WK 501



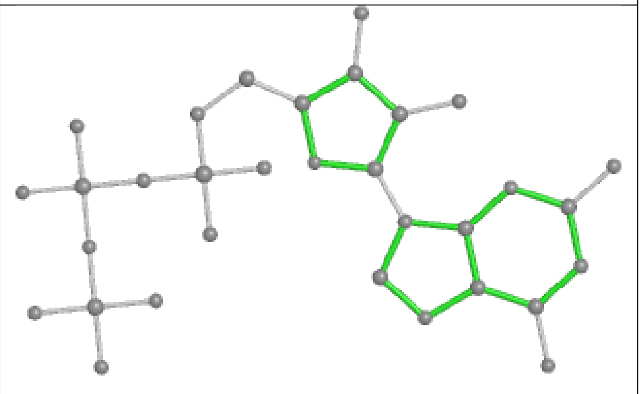
Bond lengths



Bond angles

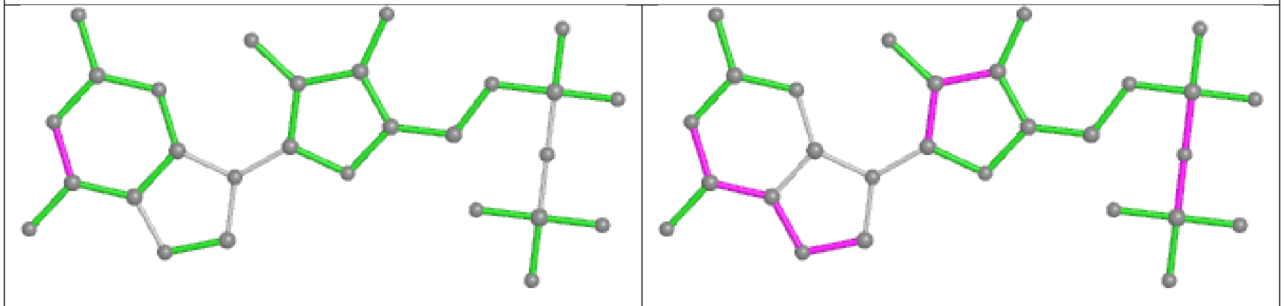


Torsions

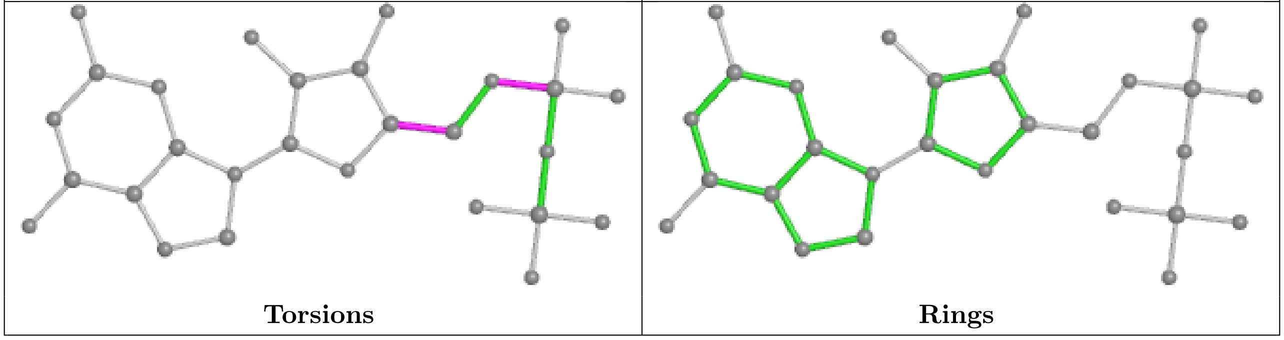


Rings

Ligand GDP KF 502

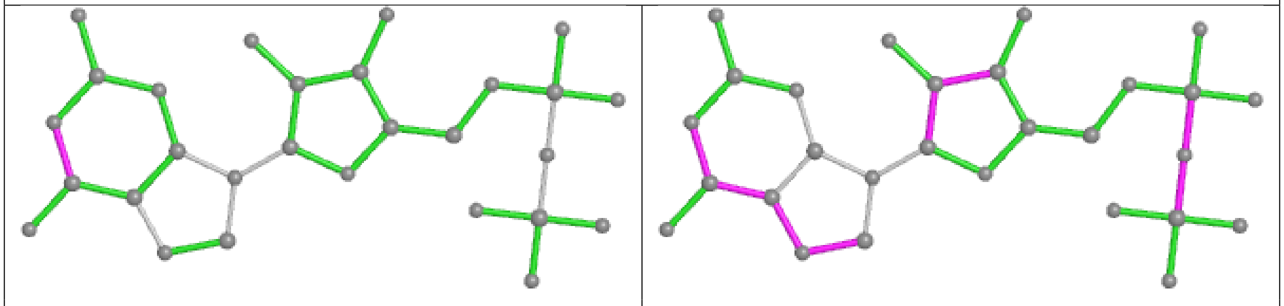


Bond lengths **Bond angles**

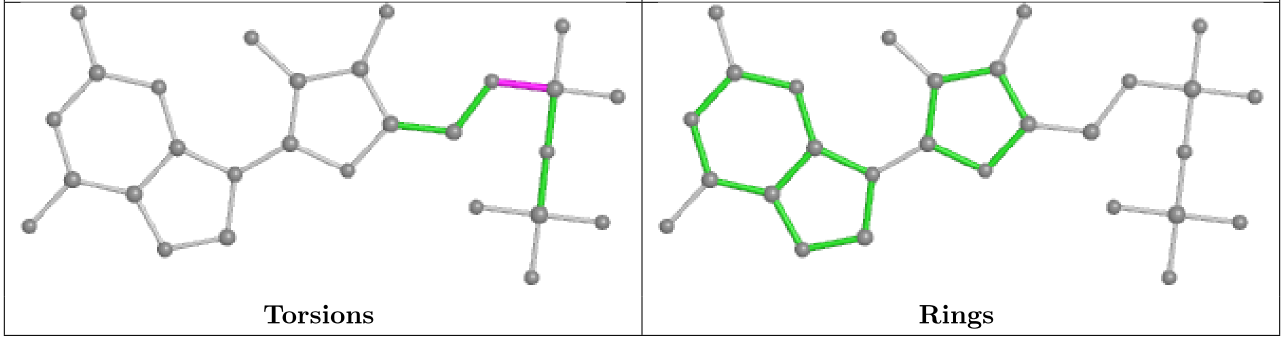


Torsions **Rings**

Ligand GDP VF 502

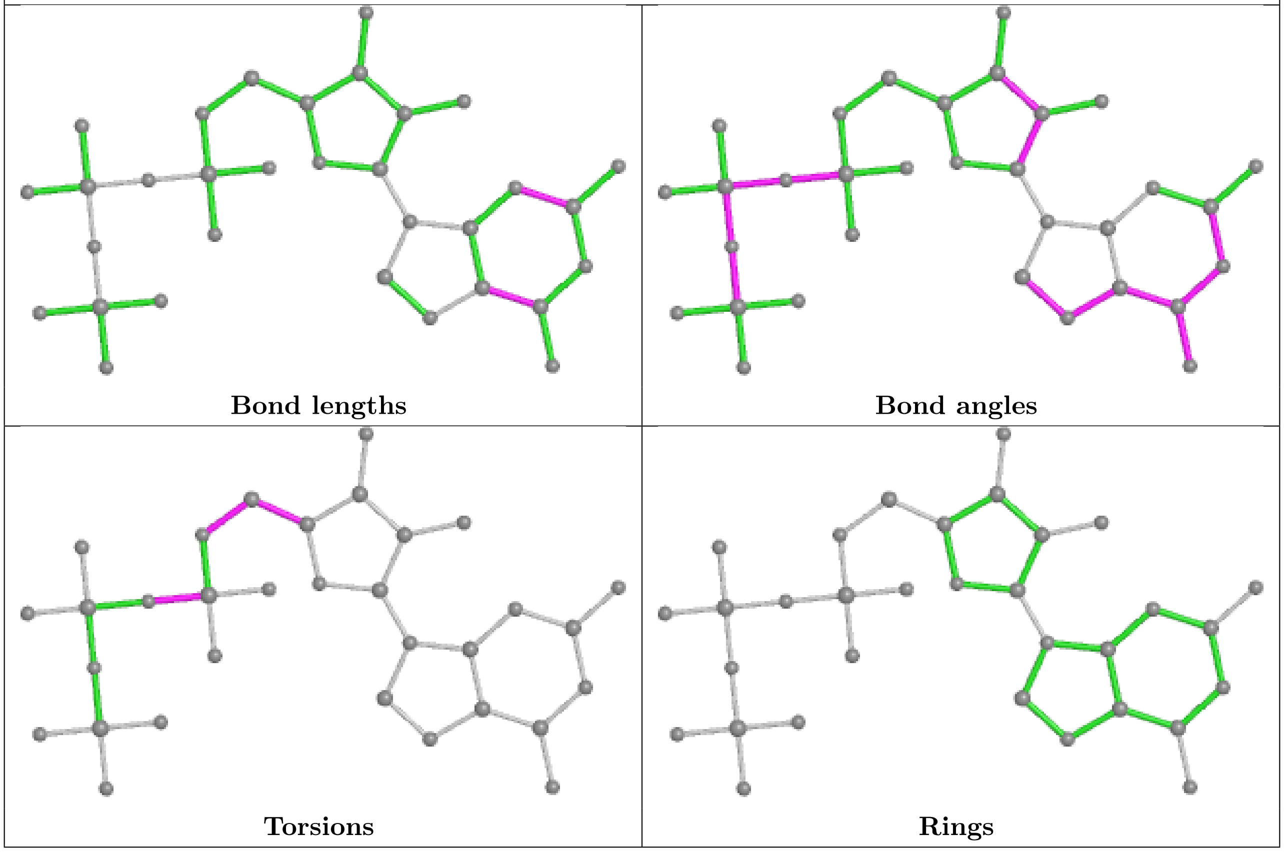


Bond lengths **Bond angles**

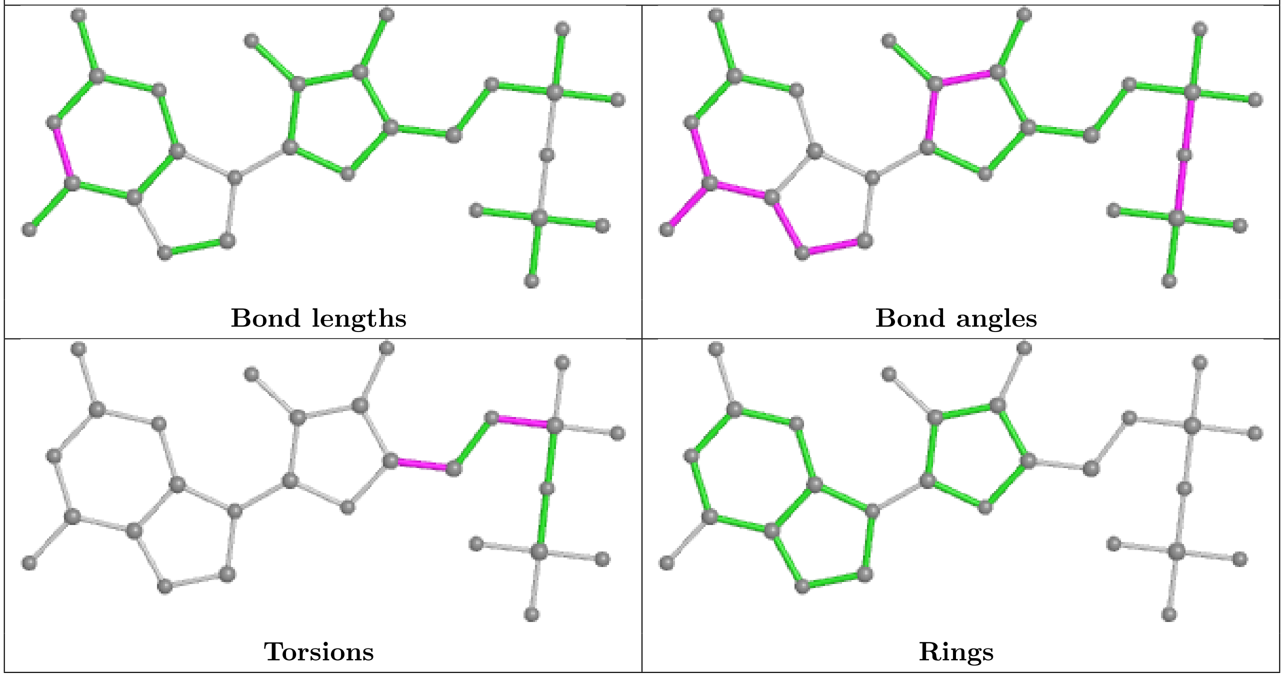


Torsions **Rings**

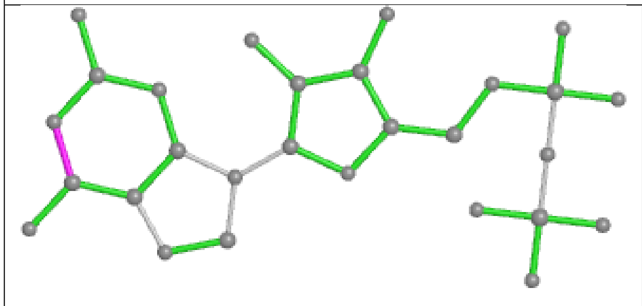
Ligand GTP OE 501



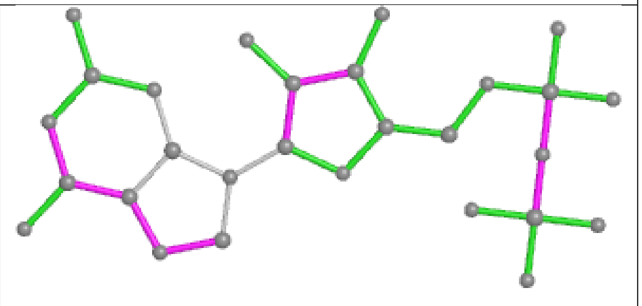
Ligand GDP FL 502



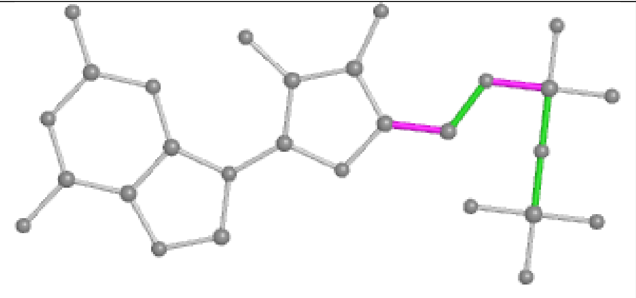
Ligand GDP WD 502



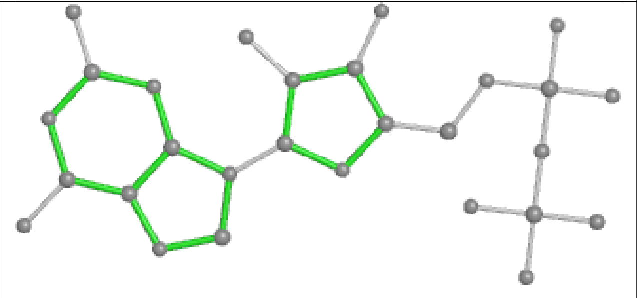
Bond lengths



Bond angles

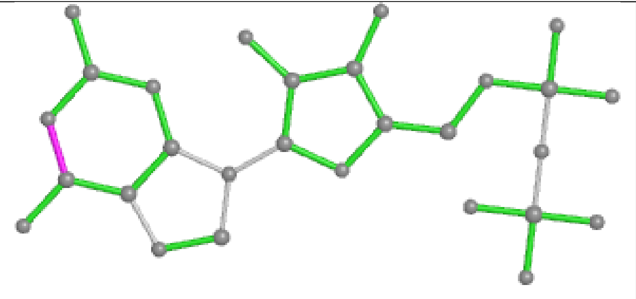


Torsions

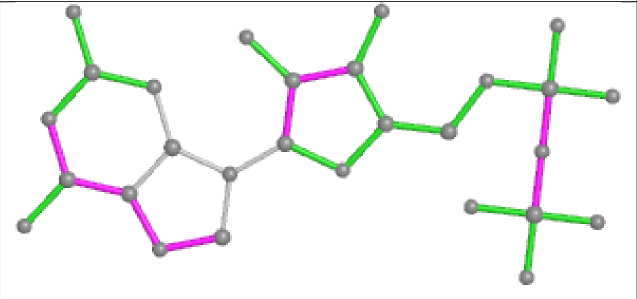


Rings

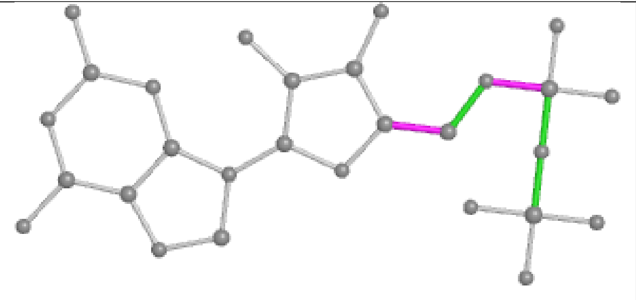
Ligand GDP LJ 502



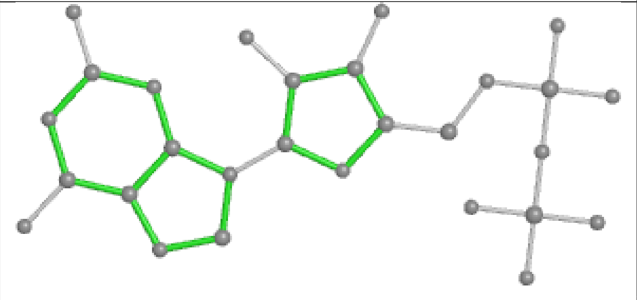
Bond lengths



Bond angles

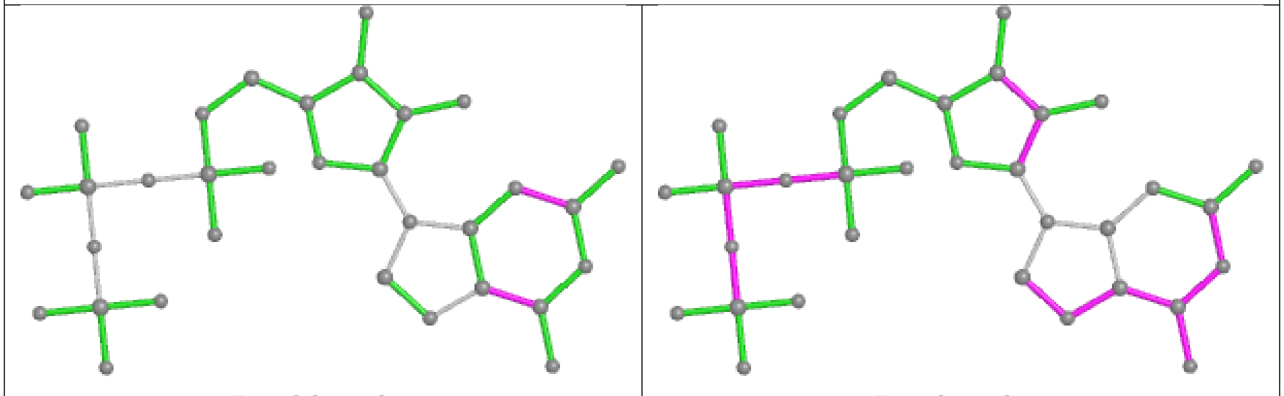


Torsions



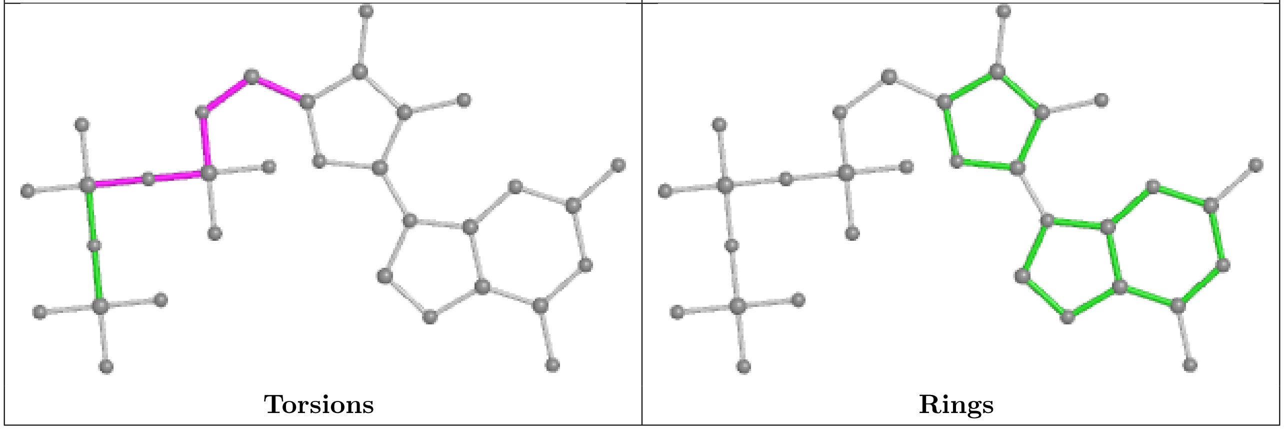
Rings

Ligand GTP CC 501



Bond lengths

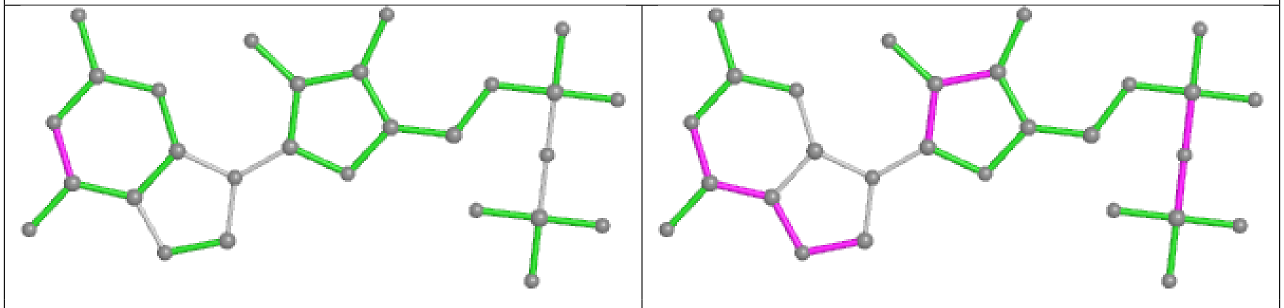
Bond angles



Torsions

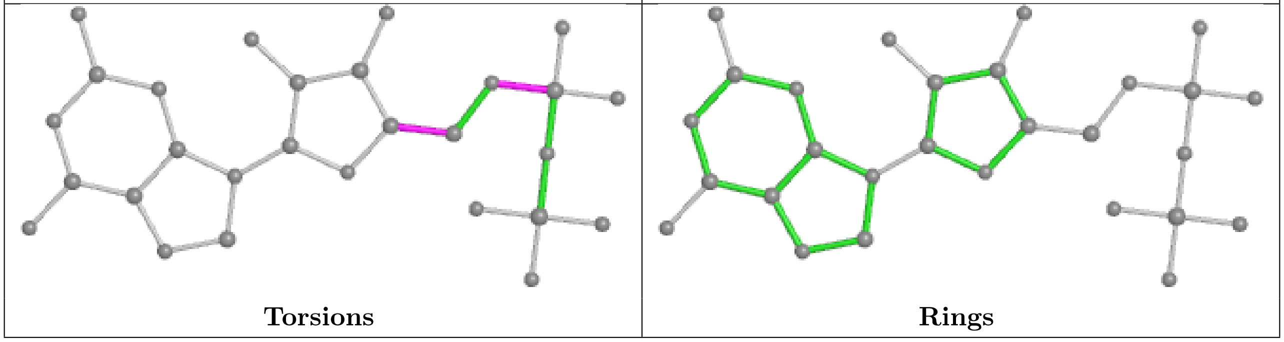
Rings

Ligand GDP GJ 502



Bond lengths

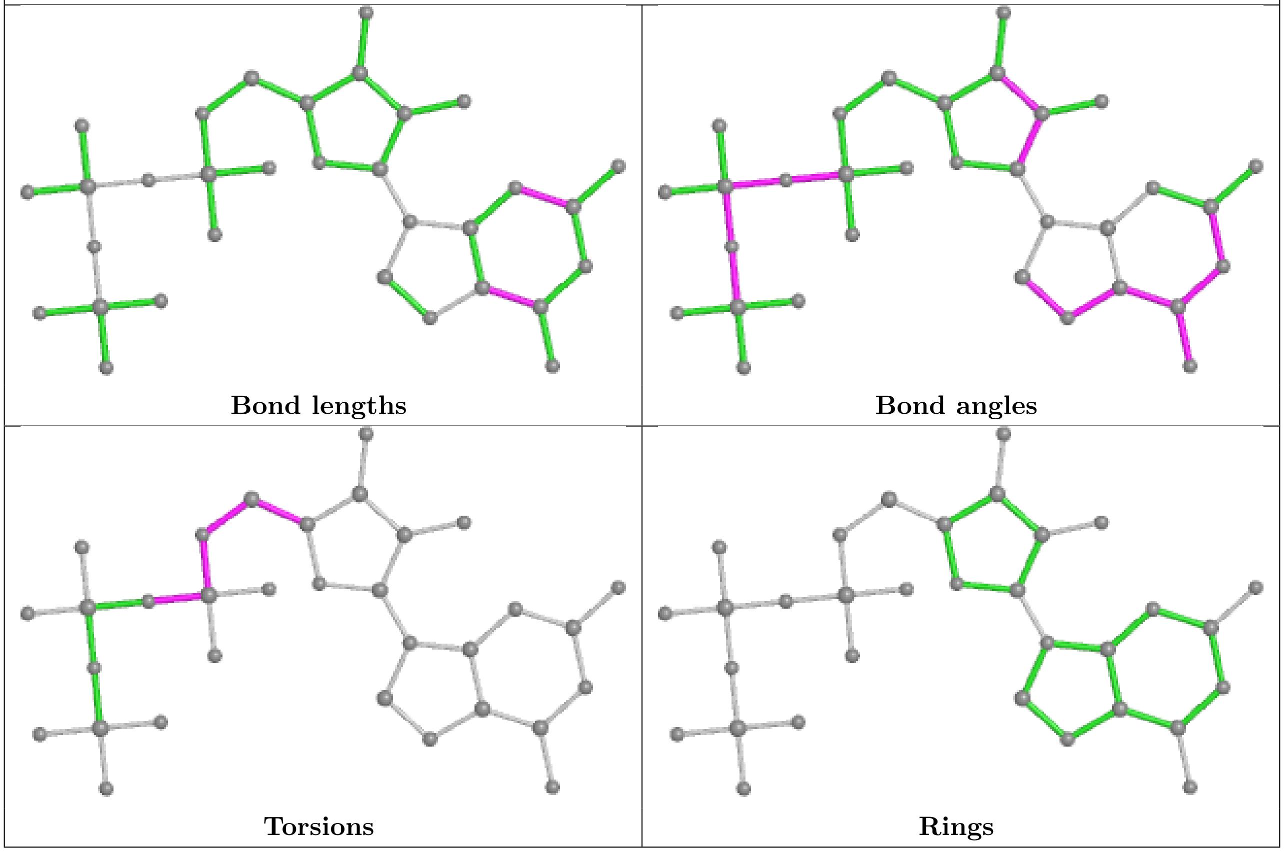
Bond angles



Torsions

Rings

Ligand GTP UI 501



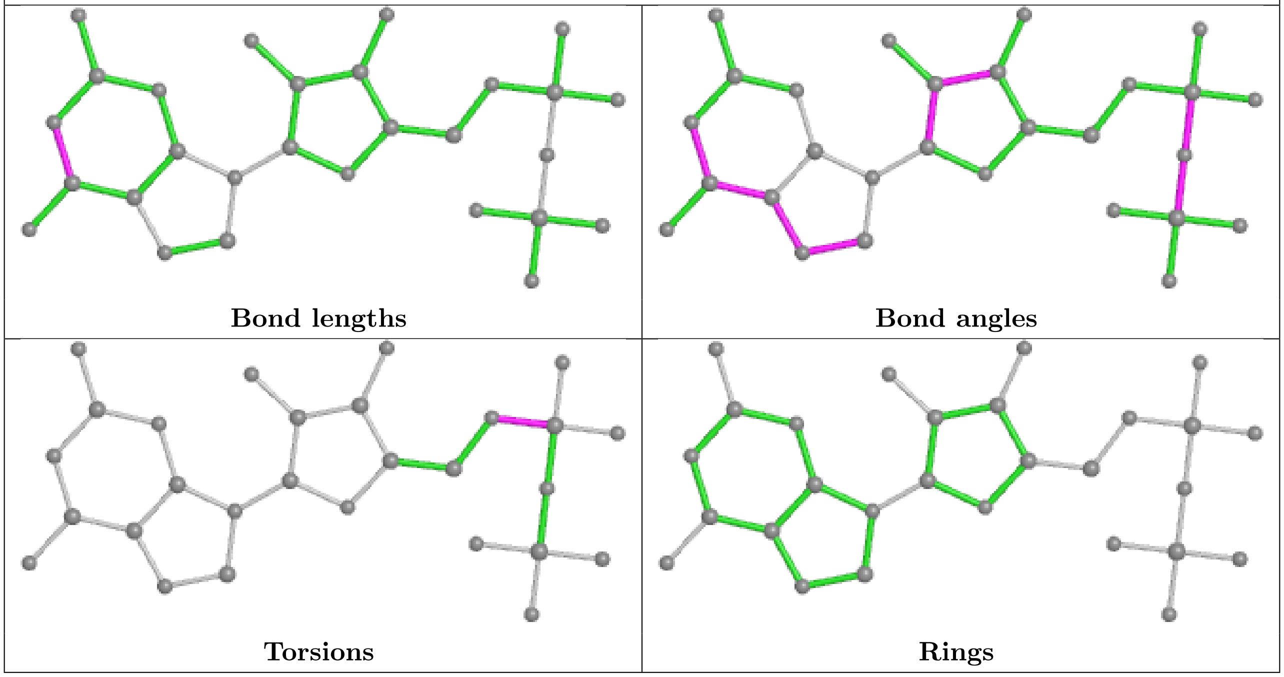
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP HN 502



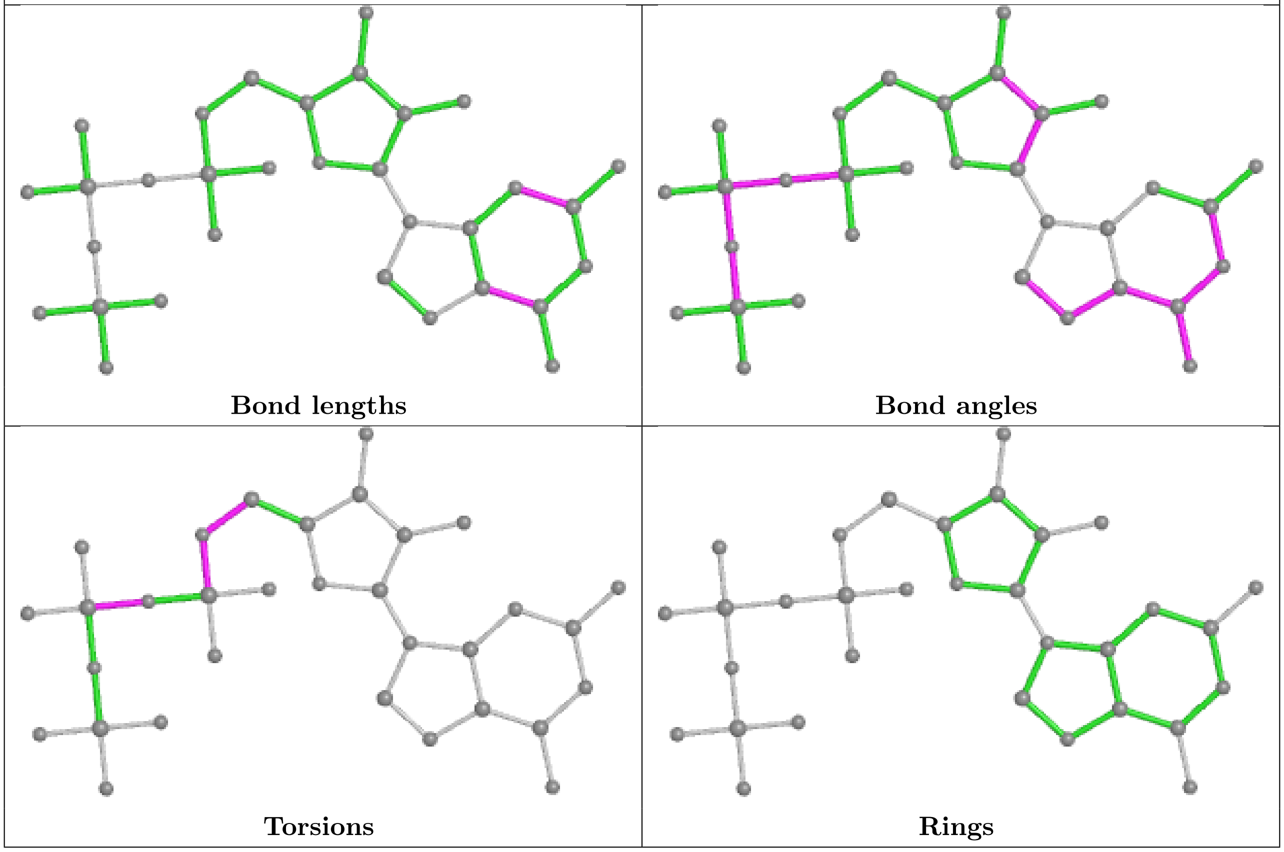
Bond lengths

Bond angles

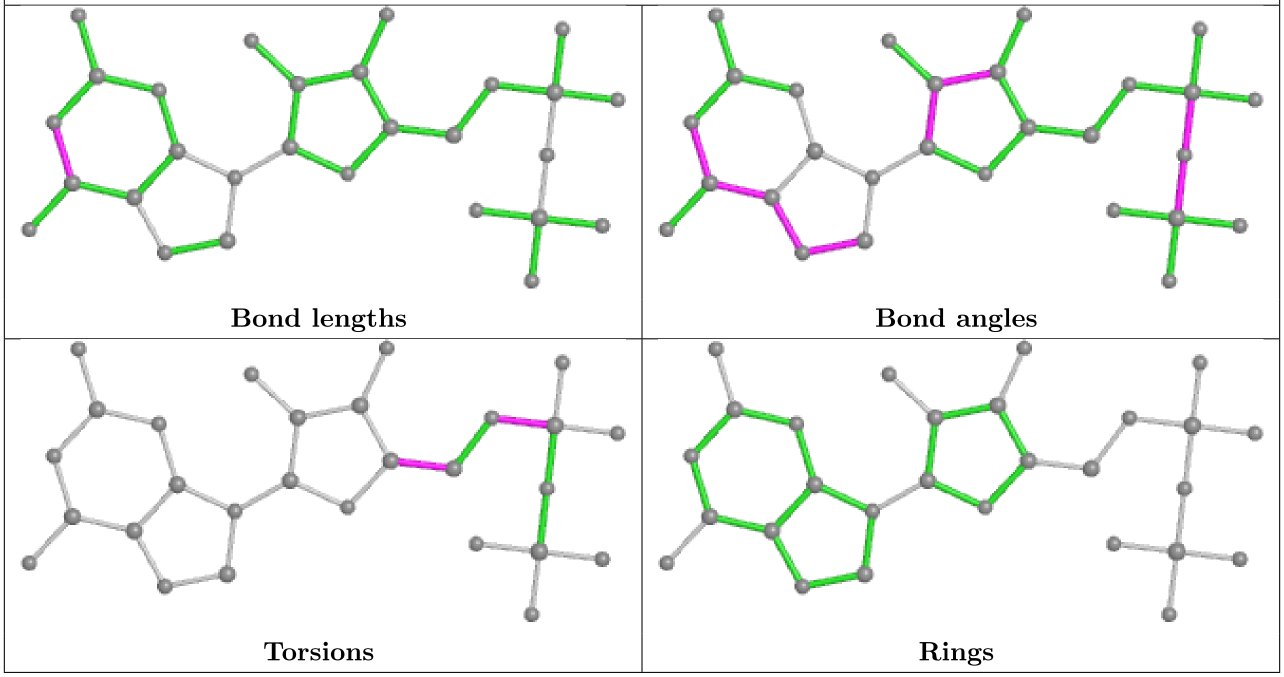
Torsions

Rings

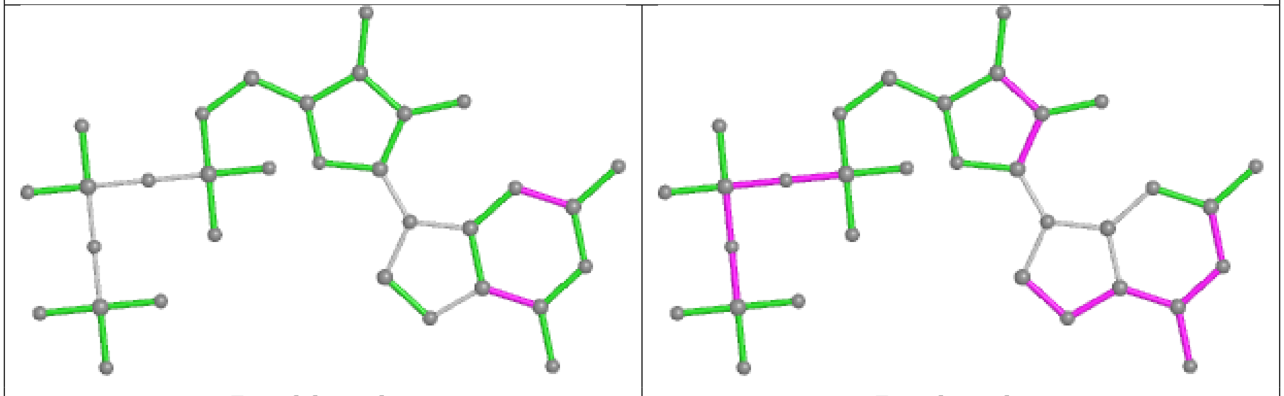
Ligand GTP FC 501



Ligand GDP OL 502

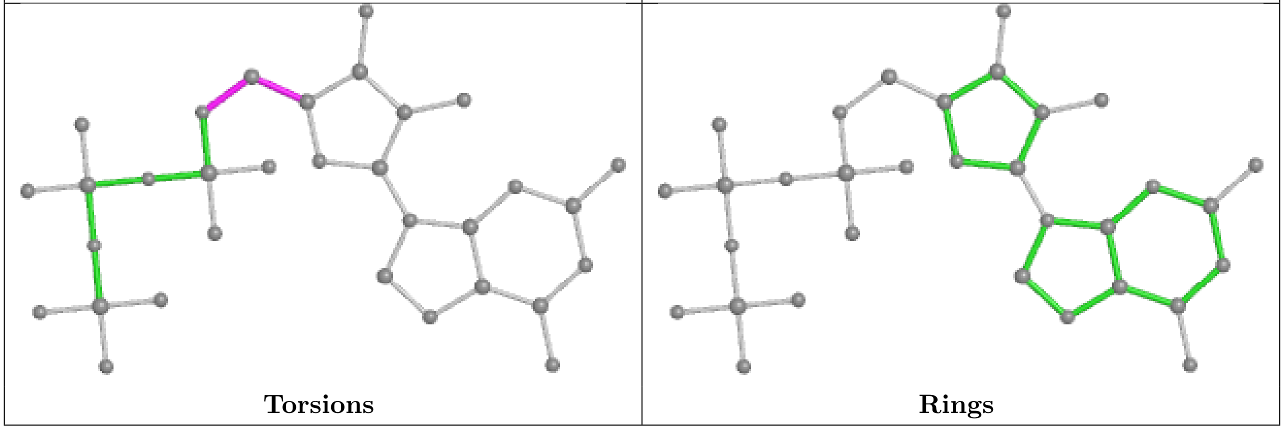


Ligand GTP JI 501



Bond lengths

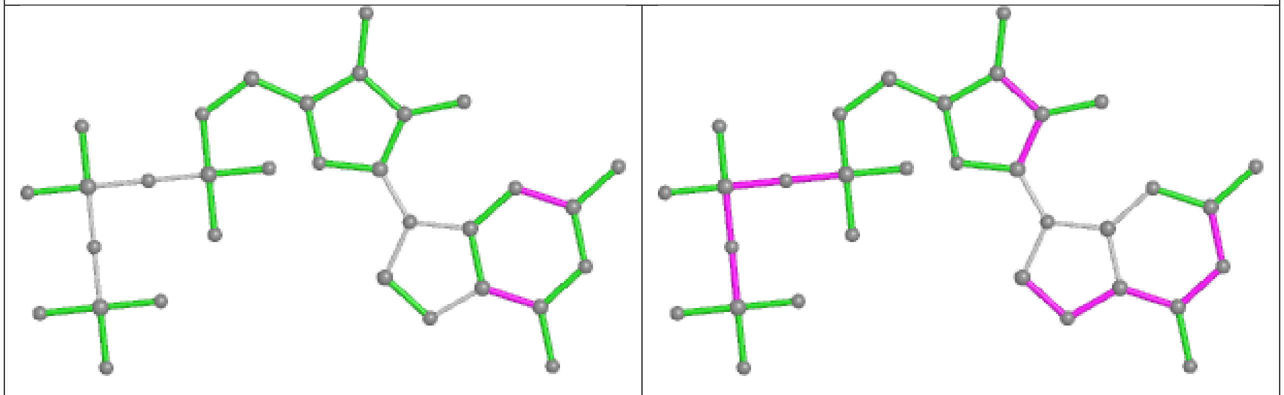
Bond angles



Torsions

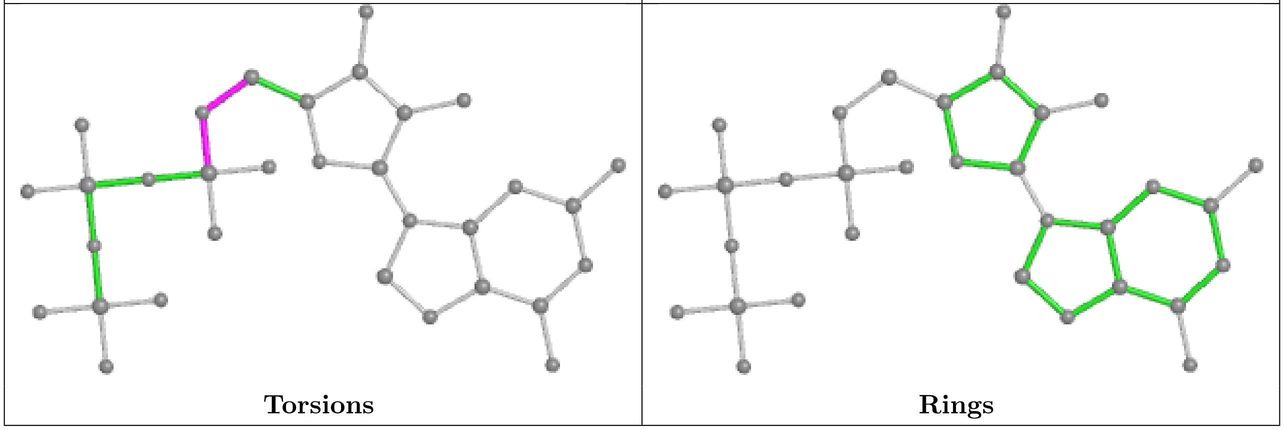
Rings

Ligand GTP DI 501



Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-26624. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal surface views ⓘ

This section was not generated.

6.5 Mask visualisation ⓘ

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 ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.