wwPDB EM Validation Summary Report

Nov 12, 2022 – 02:37 PM EST

PDB ID	:	6VE7
EMDB ID	:	EMD-20858
Title	:	The inner junction complex of Chlamydomonas reinhardtii doublet microtubule
Authors	:	Khalifa, A.A.Z.; Ichikawa, M.; Bui, K.H.
Deposited on	:	2019-12-30
Resolution	:	3.60 Å(reported)

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

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

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

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

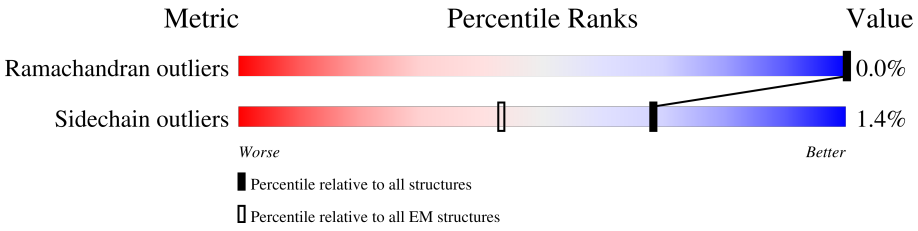
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	22% 74% · 25%
2	B	633	24% 91% 6% ·
2	C	633	19% 91% 6% ·
3	0	451	7% 97% ·
3	1	451	18% 97% ·
3	5	451	6% 96% ·
3	6	451	39% 95% 5%
3	7	451	9% 95% 5%
3	D	451	· 95% 5%

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Mol	Chain	Length	Quality of chain
3	E	451	8% 95% 5%
3	F	451	8% 95% 5%
3	G	451	10% 95% 5%
3	L	451	95%
3	M	451	95% 5%
3	P	451	5% 95% 5%
3	S	451	6% 95% 5%
3	X	451	6% 95% 5%
3	Y	451	13% 95% 5%
3	Z	451	7% 96%
3	e	451	17% 97%
3	f	451	95%
3	h	451	10% 95% 5%
3	k	451	95%
3	m	451	97%
3	o	451	8% 97%
3	s	451	15% 95% 5%
3	y	451	6% 96%
4	H	137	7% 97%
5	4	443	19% 97%
5	8	443	9% 96%
5	9	443	7% 97%
5	I	443	96%
5	J	443	6% 97%
5	K	443	97%

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Mol	Chain	Length	Quality of chain
5	N	443	6% 97%
5	O	443	96%
5	Q	443	7% 96%
5	R	443	97%
5	T	443	96%
5	U	443	97%
5	V	443	18% 97%
5	a	443	20% 97%
5	b	443	12% 96%
5	i	443	7% 97%
5	j	443	9% 96%
5	p	443	6% 98%
5	q	443	5% 98%
5	r	443	5% 99%
5	t	443	12% 98%
5	u	443	6% 96%
5	v	443	15% 97%
5	w	443	7% 96%
6	W	86	35% 90% 10%
6	x	86	37% 90% 10%
7	3	190	91% 8%
7	c	190	6% 91% 8%
7	g	190	91% 8%
7	z	190	6% 91% 8%
8	2	307	19% 86% 8% 6%

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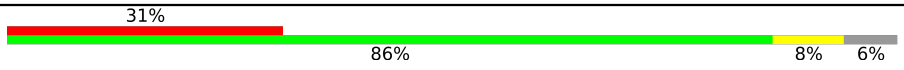
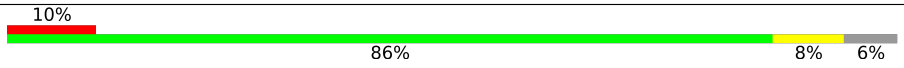
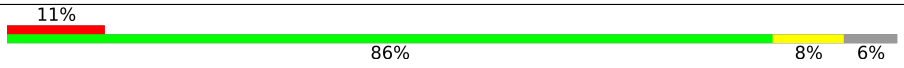
Mol	Chain	Length	Quality of chain
8	d	307	
8	l	307	
8	n	307	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 192224 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 Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	179	Total	C	N	O	S	0	0
			1391	881	249	256	5		

- Molecule 2 is a protein called FAP52.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	619	Total	C	N	O	S	0	0
			4707	2963	820	898	26		
2	C	619	Total	C	N	O	S	0	0
			4707	2963	820	898	26		

- Molecule 3 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	E	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	F	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	G	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	L	431	Total	C	N	O	S	0	0
			3349	2120	569	638	22		
3	M	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	P	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	S	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	X	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	Y	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	436	Total	C	N	O	S	0	0
			3379	2138	575	644	22		
3	e	436	Total	C	N	O	S	0	0
			3379	2138	575	644	22		
3	f	431	Total	C	N	O	S	0	0
			3349	2120	569	638	22		
3	h	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	k	431	Total	C	N	O	S	0	0
			3349	2120	569	638	22		
3	m	436	Total	C	N	O	S	0	0
			3379	2138	575	644	22		
3	o	436	Total	C	N	O	S	0	0
			3379	2138	575	644	22		
3	s	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	y	436	Total	C	N	O	S	0	0
			3379	2138	575	644	22		
3	0	436	Total	C	N	O	S	0	0
			3379	2138	575	644	22		
3	1	436	Total	C	N	O	S	0	0
			3379	2138	575	644	22		
3	5	436	Total	C	N	O	S	0	0
			3379	2138	575	644	22		
3	6	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		
3	7	428	Total	C	N	O	S	0	0
			3329	2109	566	632	22		

- Molecule 4 is a protein called Protein Flattop homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		

- Molecule 5 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	J	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	N	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	O	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	Q	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	R	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	T	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	U	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	V	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	b	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	i	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	j	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	p	437	Total	C	N	O	S	0	0
			3430	2152	585	663	30		
5	q	437	Total	C	N	O	S	0	0
			3430	2152	585	663	30		
5	r	437	Total	C	N	O	S	0	0
			3430	2152	585	663	30		
5	t	437	Total	C	N	O	S	0	0
			3430	2152	585	663	30		
5	u	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	v	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	w	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	4	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
5	8	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		

- Molecule 6 is a protein called FAP276.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	86	Total	C	N	O	S	0	0
			701	438	131	129	3		
6	x	86	Total	C	N	O	S	0	0
			701	438	131	129	3		

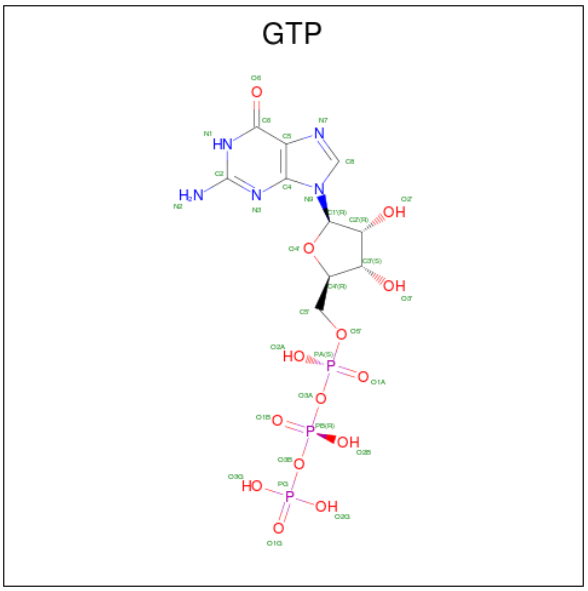
- Molecule 7 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	187	Total	C	N	O	S	0	0
			1538	988	267	276	7		
7	g	187	Total	C	N	O	S	0	0
			1538	988	267	276	7		
7	z	187	Total	C	N	O	S	0	0
			1538	988	267	276	7		
7	3	187	Total	C	N	O	S	0	0
			1538	988	267	276	7		

- Molecule 8 is a protein called PACRG.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	290	Total	C	N	O	S	0	0
			2271	1453	391	420	7		
8	l	290	Total	C	N	O	S	0	0
			2271	1453	391	420	7		
8	n	290	Total	C	N	O	S	0	0
			2271	1453	391	420	7		
8	2	290	Total	C	N	O	S	0	0
			2271	1453	391	420	7		

- Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
9	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	P	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	S	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	X	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	Y	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	e	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	f	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	h	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
9	k	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	m	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	o	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	s	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	y	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	1	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	5	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	
10	G	1	Total	Mg	0
			1	1	
10	L	1	Total	Mg	0
			1	1	
10	M	1	Total	Mg	0
			1	1	
10	P	1	Total	Mg	0
			1	1	
10	S	1	Total	Mg	0
			1	1	
10	X	1	Total	Mg	0
			1	1	

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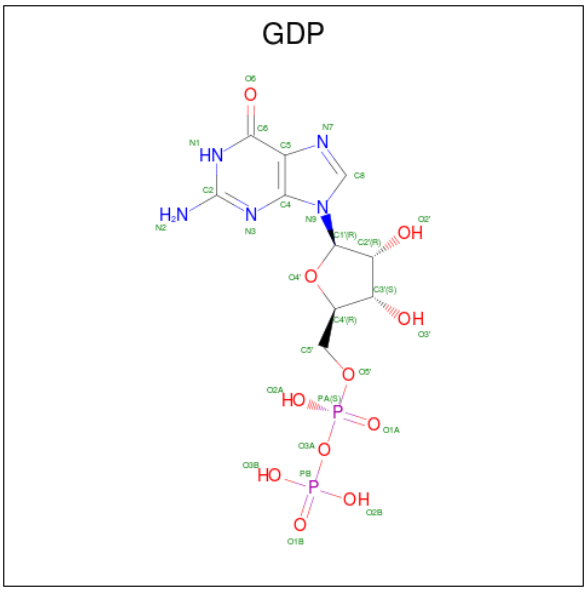
Mol	Chain	Residues	Atoms	AltConf
10	Y	1	Total Mg 1 1	0
10	Z	1	Total Mg 1 1	0
10	e	1	Total Mg 1 1	0
10	f	1	Total Mg 1 1	0
10	h	1	Total Mg 1 1	0
10	k	1	Total Mg 1 1	0
10	m	1	Total Mg 1 1	0
10	o	1	Total Mg 1 1	0
10	p	1	Total Mg 1 1	0
10	s	1	Total Mg 1 1	0
10	0	1	Total Mg 1 1	0
10	1	1	Total Mg 1 1	0
10	5	1	Total Mg 1 1	0
10	6	1	Total Mg 1 1	0
10	7	1	Total Mg 1 1	0

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



Mol	Chain	Residues	Atoms					AltConf
11	I	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	J	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	K	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	N	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	O	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	R	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	T	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	U	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	V	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	a	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	j	1	Total	C	N	O	P	0
			28	10	5	11	2	

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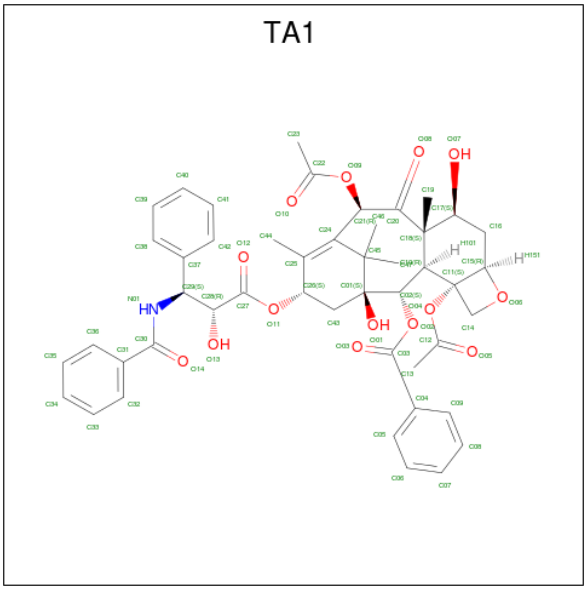
Mol	Chain	Residues	Atoms					AltConf
11	p	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	q	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	r	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	t	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	u	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	v	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	w	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	4	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	8	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	9	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 12 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



Mol	Chain	Residues	Atoms				AltConf
12	J	1	Total	C	N	O	0
			62	47	1	14	

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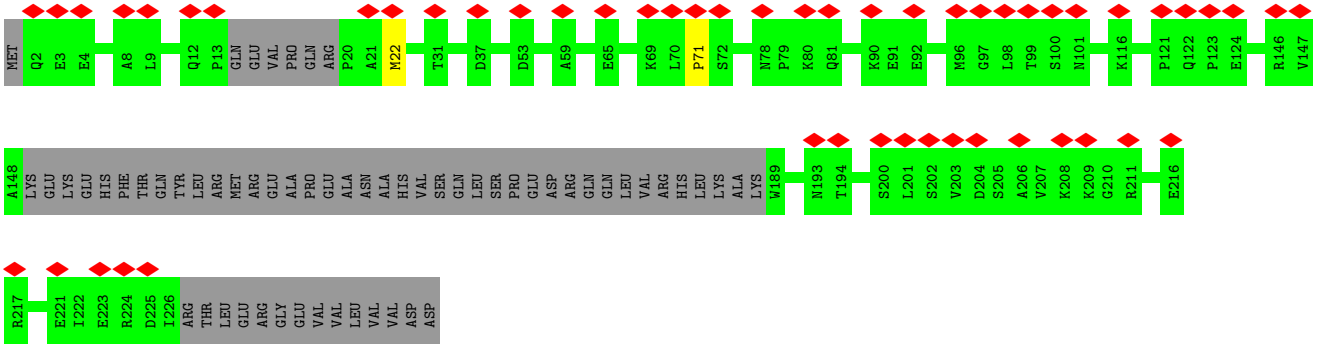
Mol	Chain	Residues	Atoms				AltConf
12	V	1	Total	C	N	O	0
			62	47	1	14	
12	a	1	Total	C	N	O	0
			62	47	1	14	
12	b	1	Total	C	N	O	0
			62	47	1	14	
12	i	1	Total	C	N	O	0
			62	47	1	14	
12	j	1	Total	C	N	O	0
			62	47	1	14	
12	p	1	Total	C	N	O	0
			62	47	1	14	
12	q	1	Total	C	N	O	0
			62	47	1	14	
12	r	1	Total	C	N	O	0
			62	47	1	14	
12	t	1	Total	C	N	O	0
			62	47	1	14	
12	u	1	Total	C	N	O	0
			62	47	1	14	
12	v	1	Total	C	N	O	0
			62	47	1	14	
12	w	1	Total	C	N	O	0
			62	47	1	14	
12	4	1	Total	C	N	O	0
			62	47	1	14	
12	8	1	Total	C	N	O	0
			62	47	1	14	
12	9	1	Total	C	N	O	0
			62	47	1	14	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

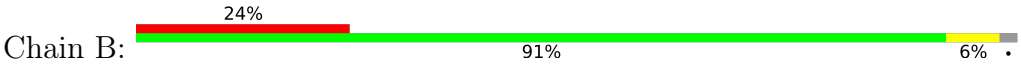
• Molecule 1: Flagellar associated protein

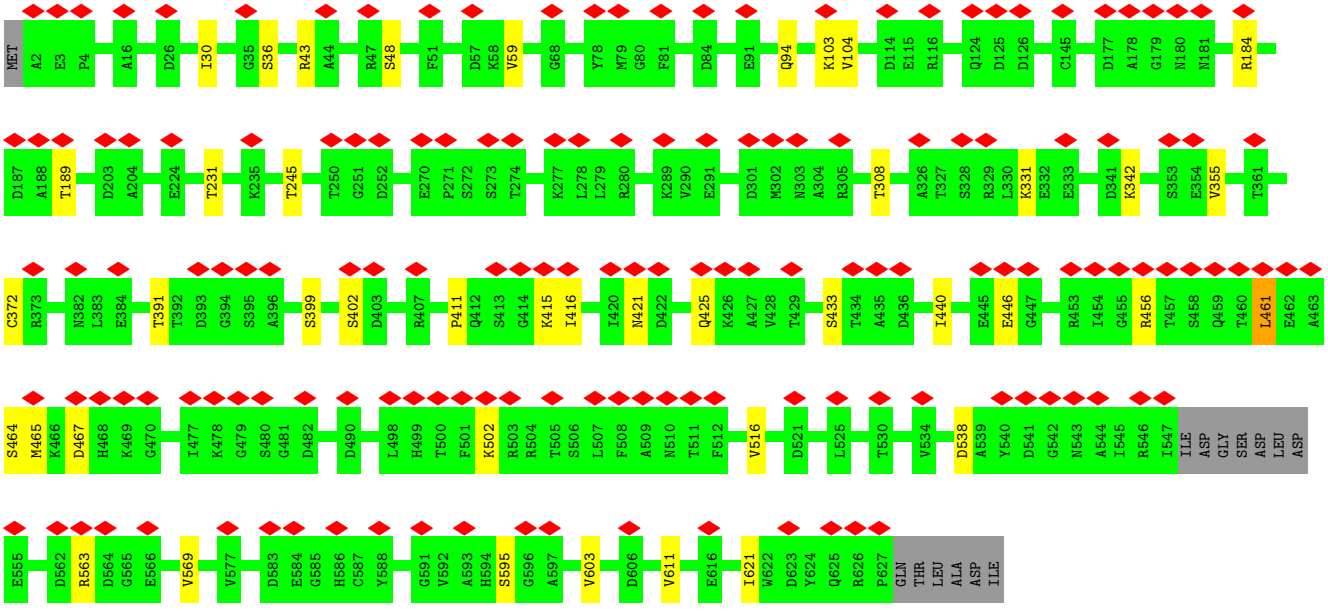
Chain A:



• Molecule 2: FAP52

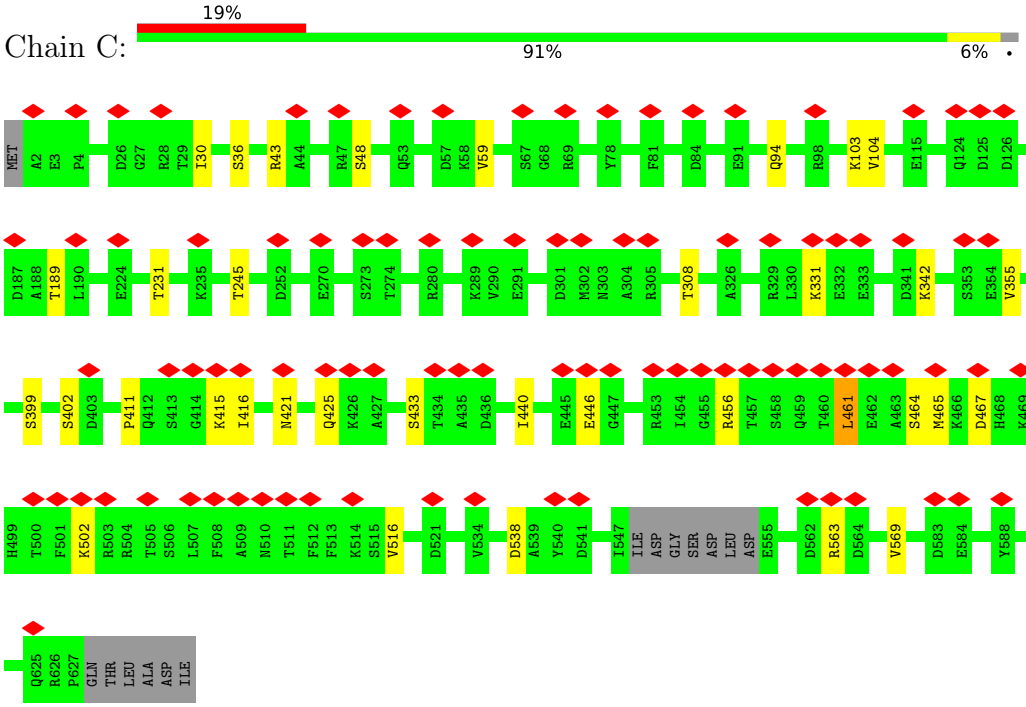
Chain B:





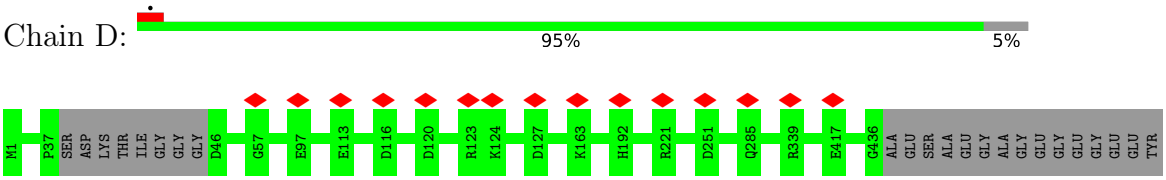
• Molecule 2: FAP52

Chain C:



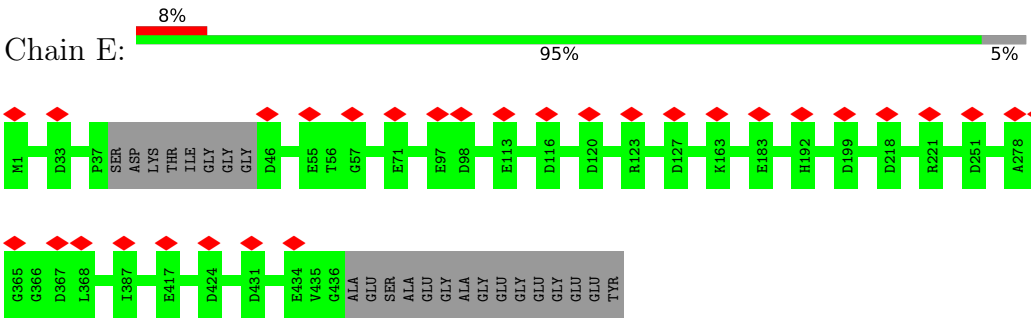
• Molecule 3: Tubulin alpha

Chain D:



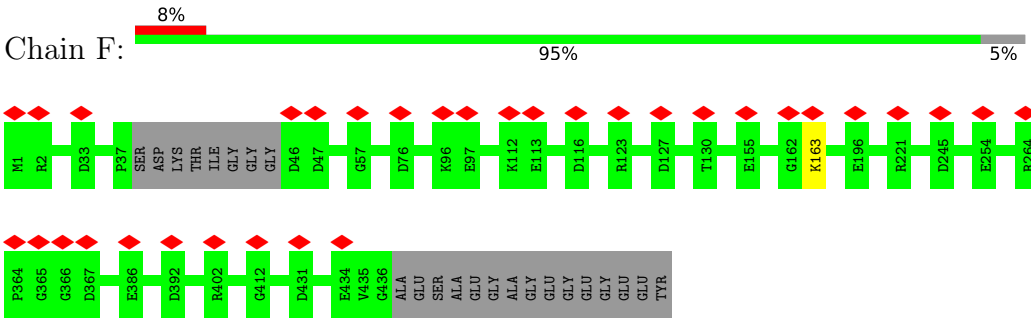
• Molecule 3: Tubulin alpha

Chain E:



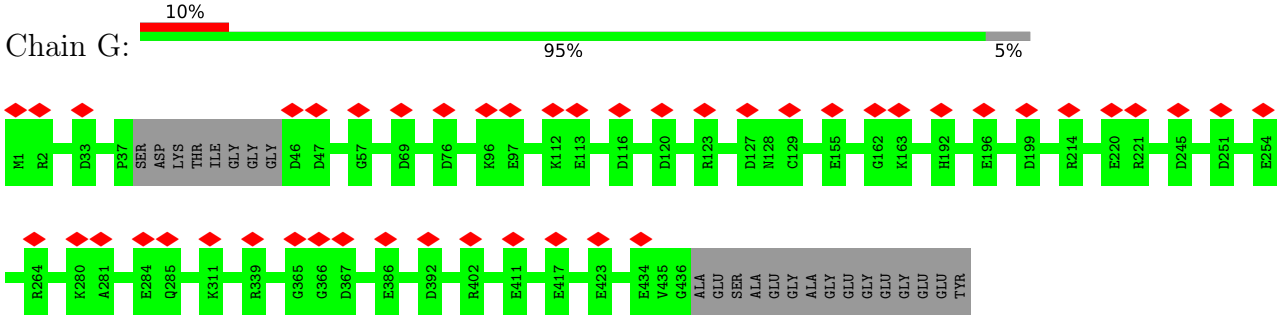
• Molecule 3: Tubulin alpha

Chain F:



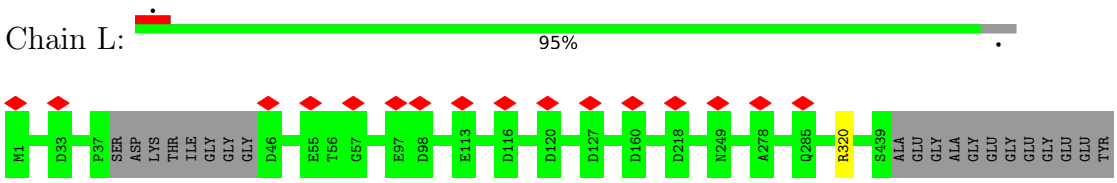
• Molecule 3: Tubulin alpha

Chain G:



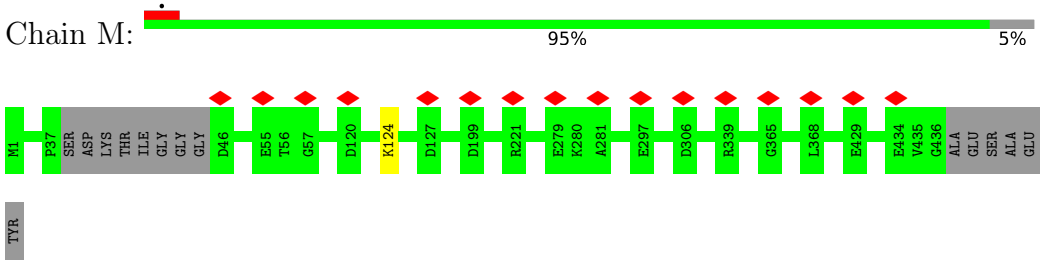
• Molecule 3: Tubulin alpha

Chain L:



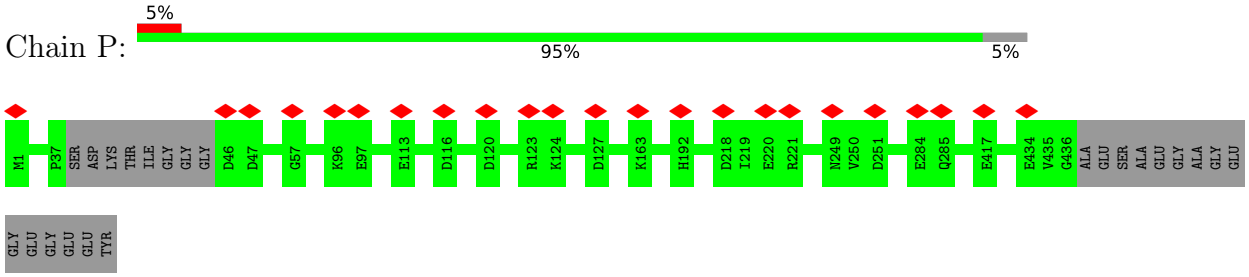
• Molecule 3: Tubulin alpha

Chain M:



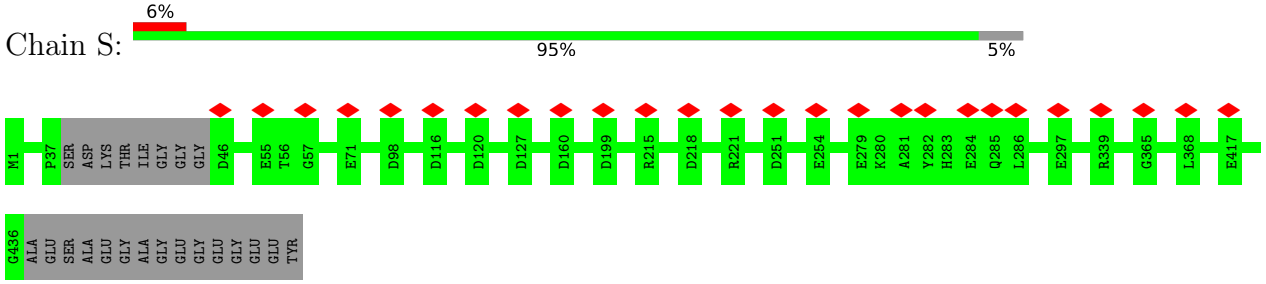
• Molecule 3: Tubulin alpha

Chain P:



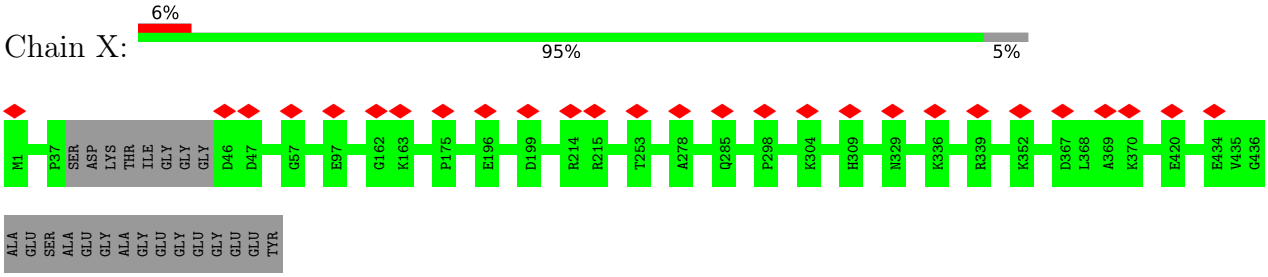
• Molecule 3: Tubulin alpha

Chain S:



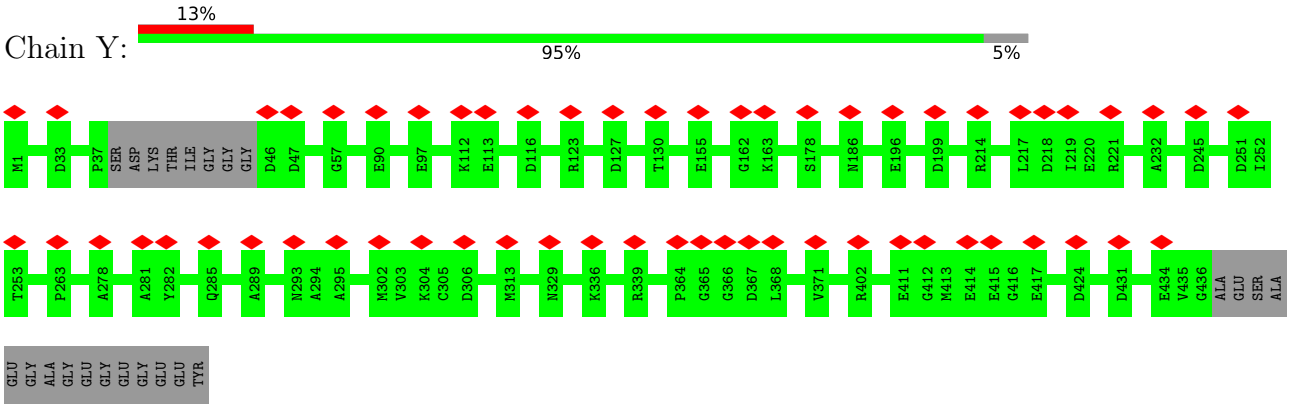
• Molecule 3: Tubulin alpha

Chain X:



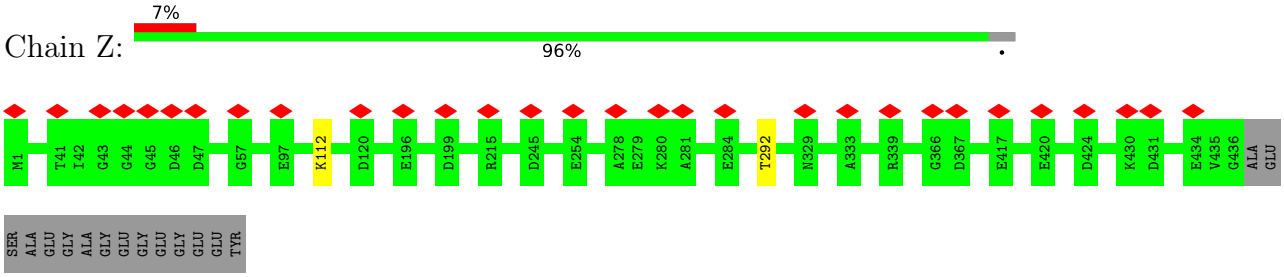
• Molecule 3: Tubulin alpha

Chain Y:



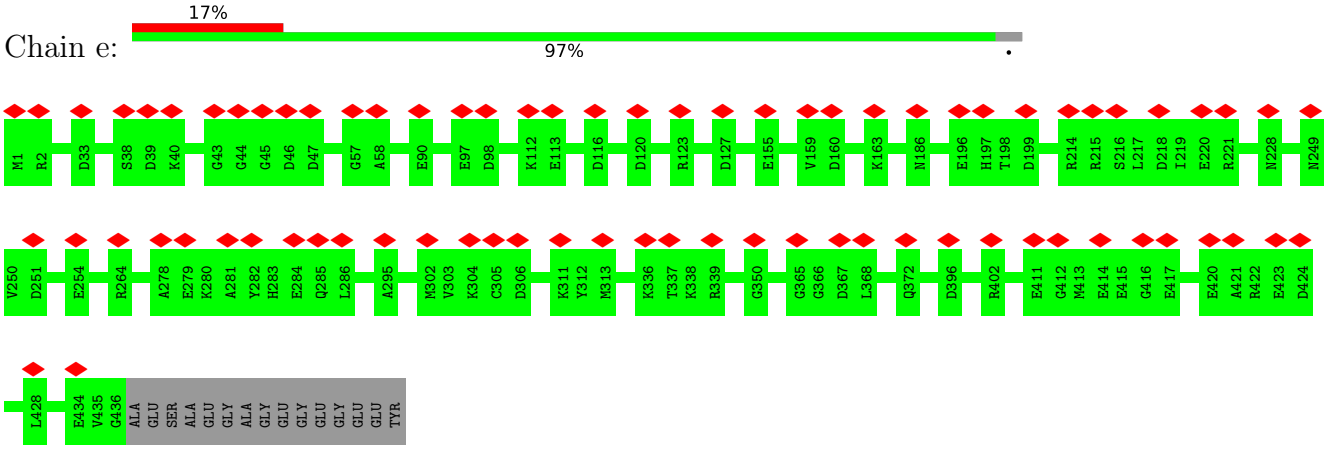
• Molecule 3: Tubulin alpha

Chain Z:



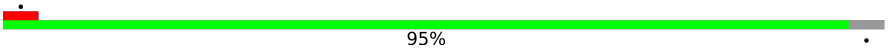
• Molecule 3: Tubulin alpha

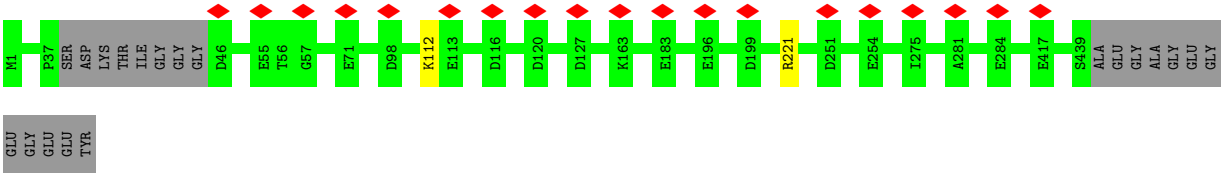
Chain e:



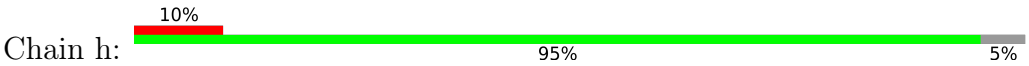
• Molecule 3: Tubulin alpha

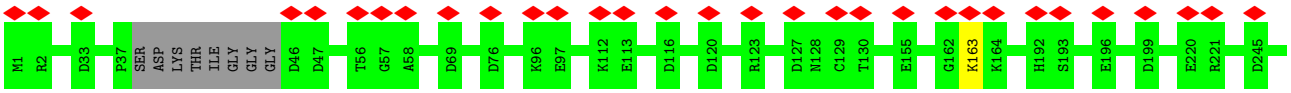
Chain f:

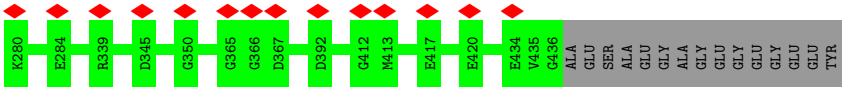




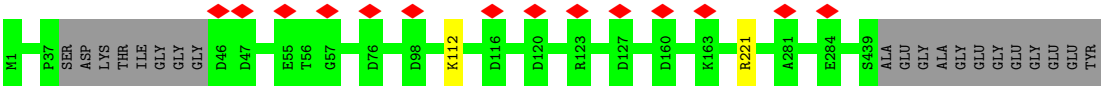
• Molecule 3: Tubulin alpha



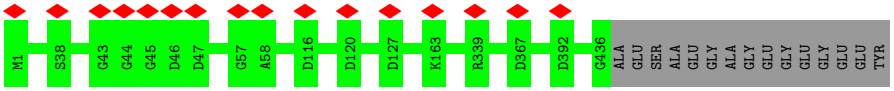




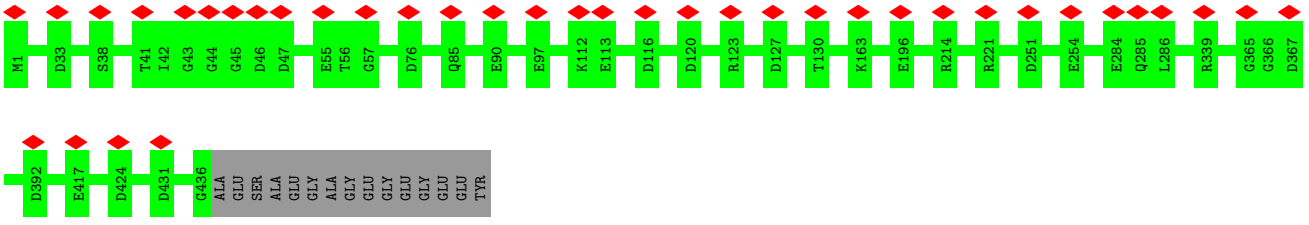
• Molecule 3: Tubulin alpha



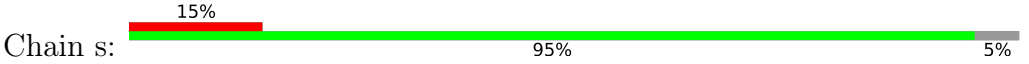
• Molecule 3: Tubulin alpha

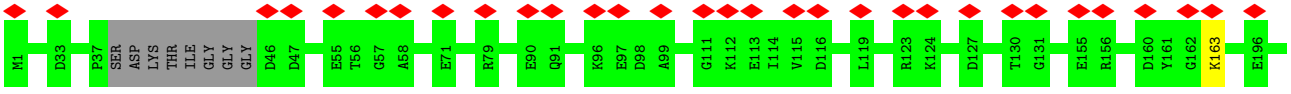


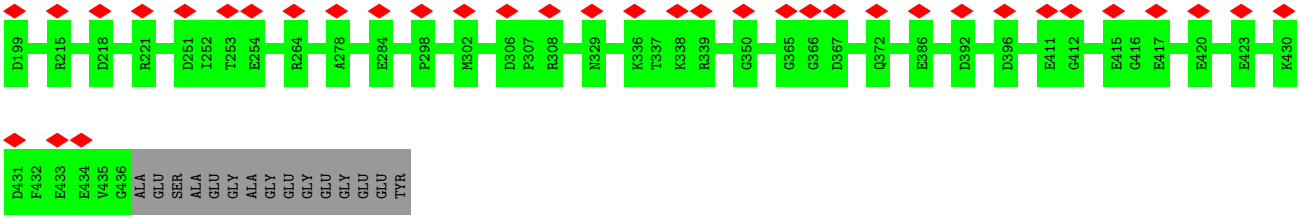
• Molecule 3: Tubulin alpha



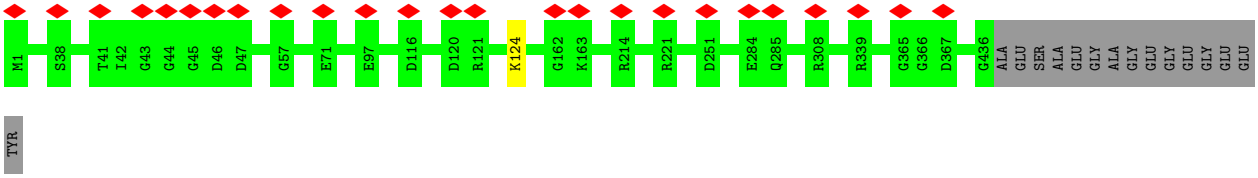
• Molecule 3: Tubulin alpha







• Molecule 3: Tubulin alpha



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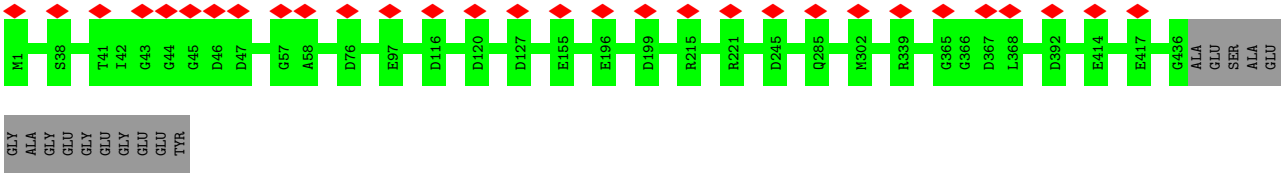
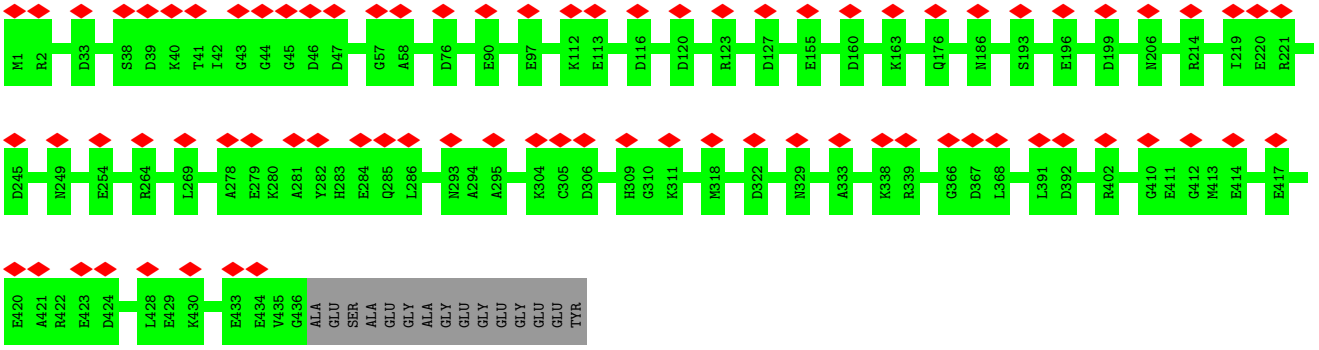
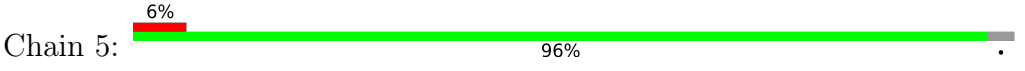
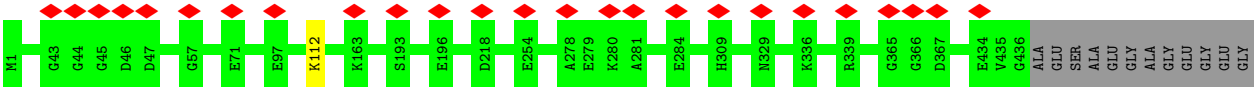


• Molecule 3: Tubulin alpha



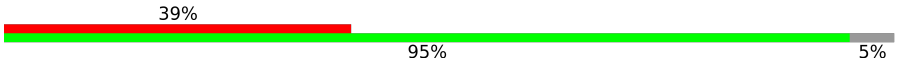
• Molecule 3: Tubulin alpha

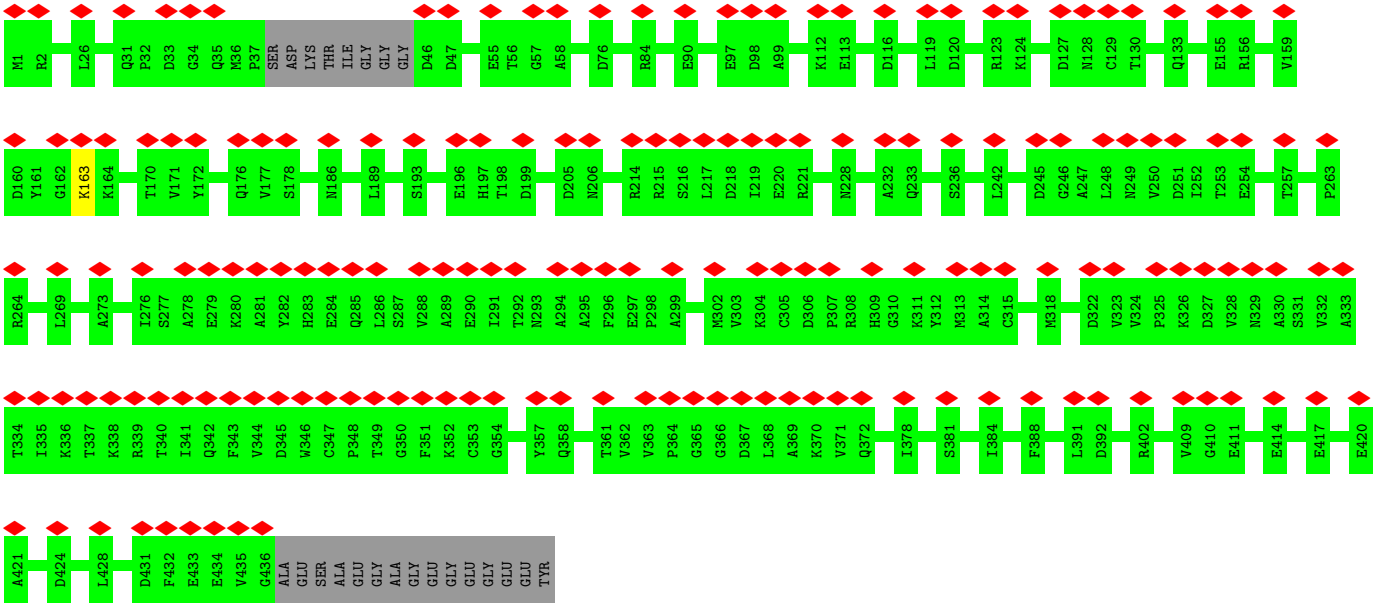




• Molecule 3: Tubulin alpha

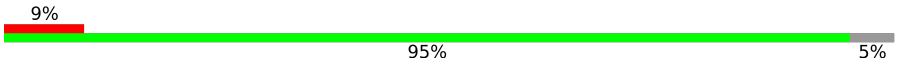
Chain 6:

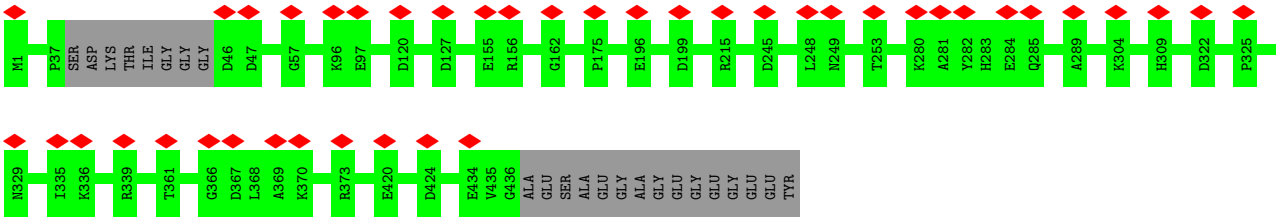




• Molecule 3: Tubulin alpha

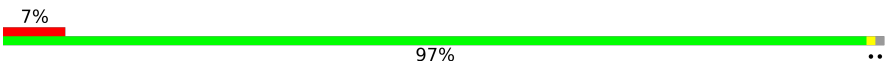
Chain 7:

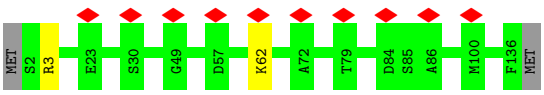




• Molecule 4: Protein Flattop homolog

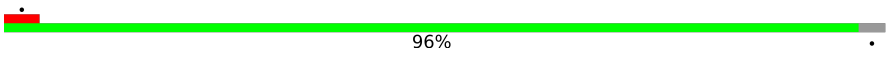
Chain H:

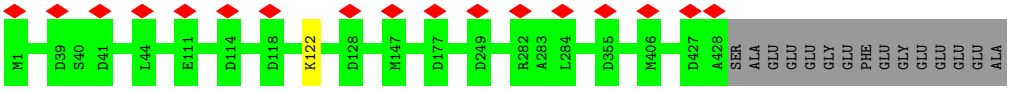




• Molecule 5: Tubulin beta

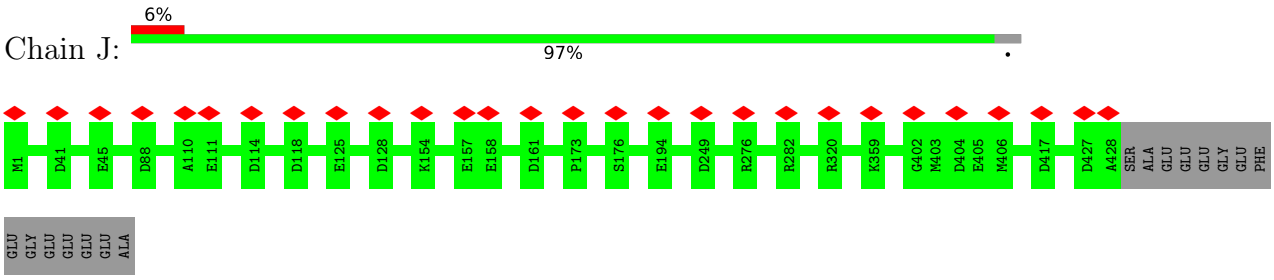
Chain I:





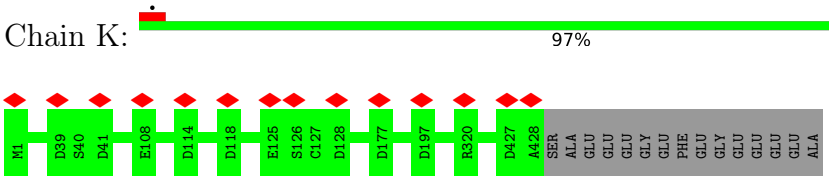
• Molecule 5: Tubulin beta

Chain J:



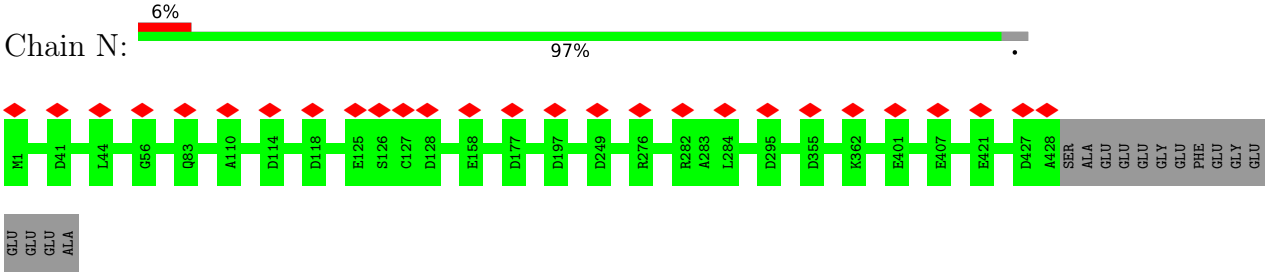
• Molecule 5: Tubulin beta

Chain K:



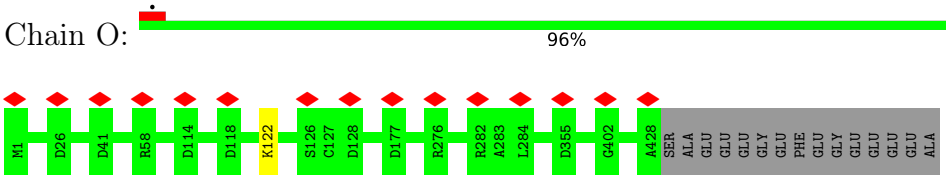
• Molecule 5: Tubulin beta

Chain N:



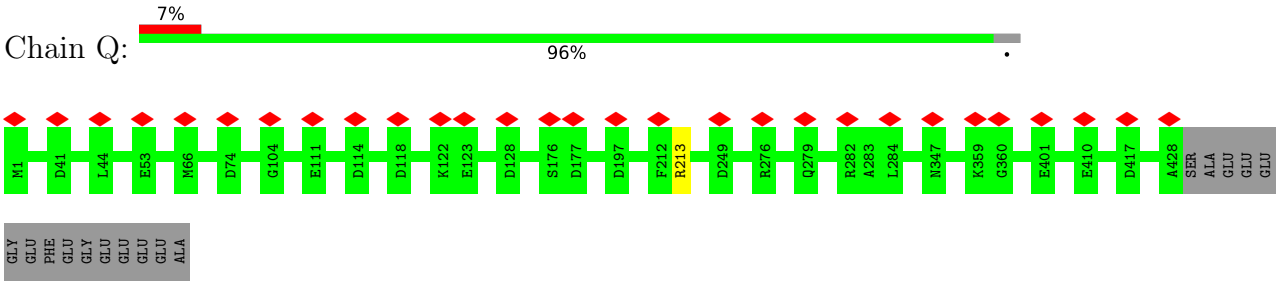
• Molecule 5: Tubulin beta

Chain O:



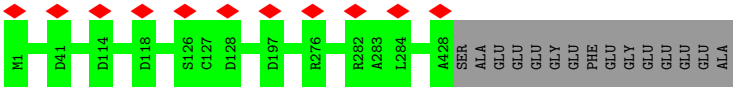
• Molecule 5: Tubulin beta

Chain Q:



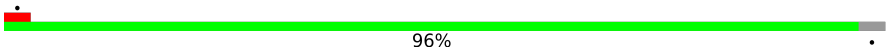
• Molecule 5: Tubulin beta

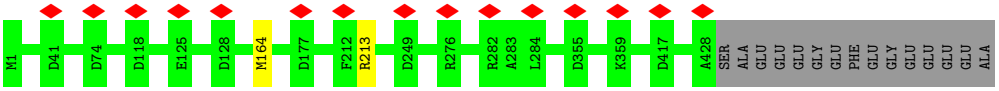
Chain R:



• Molecule 5: Tubulin beta

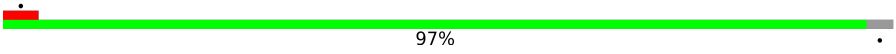
Chain T:

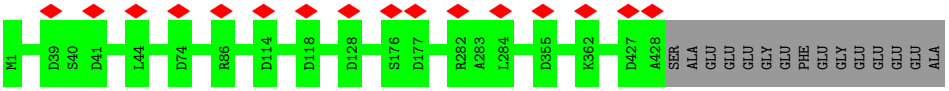




• Molecule 5: Tubulin beta

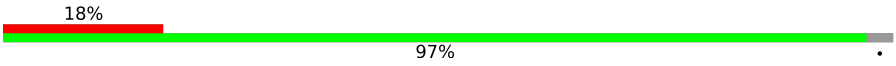
Chain U:

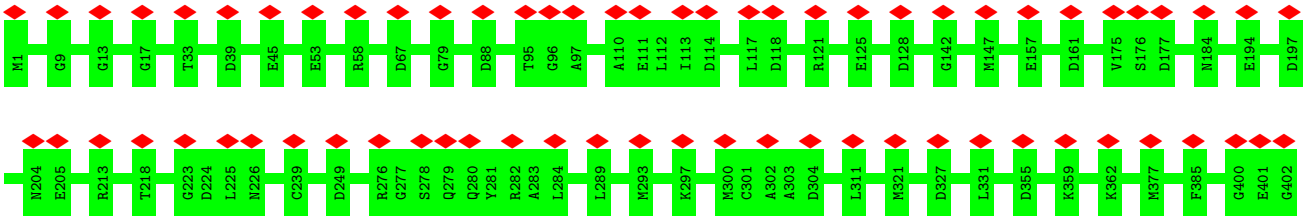




• Molecule 5: Tubulin beta

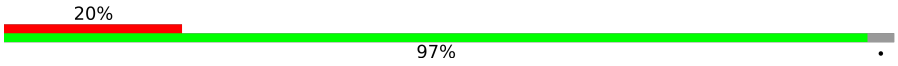
Chain V:

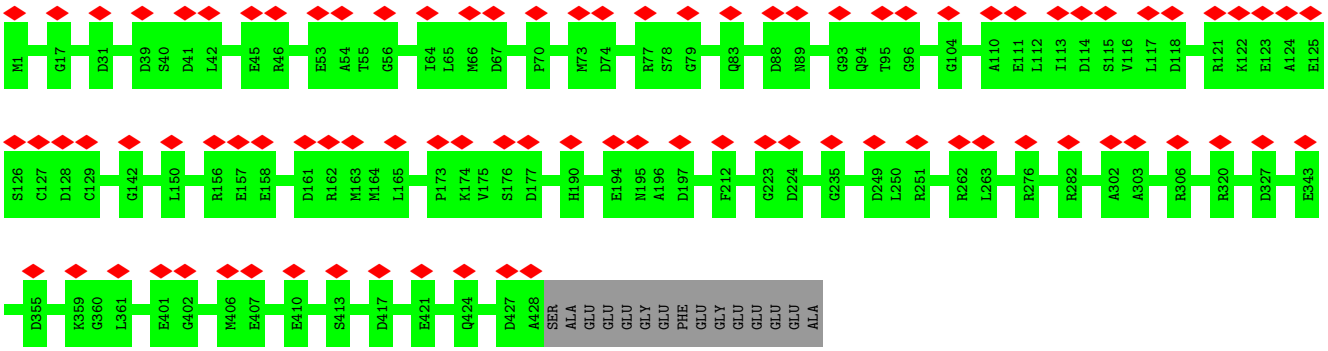




• Molecule 5: Tubulin beta

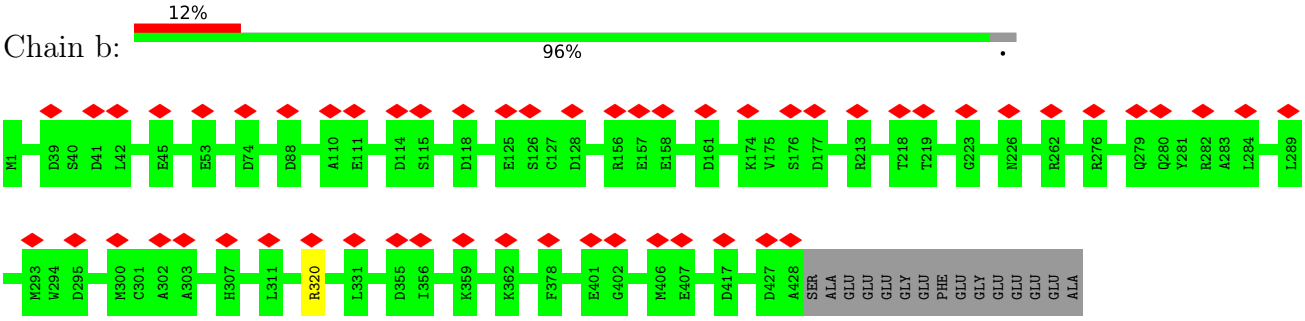
Chain a:





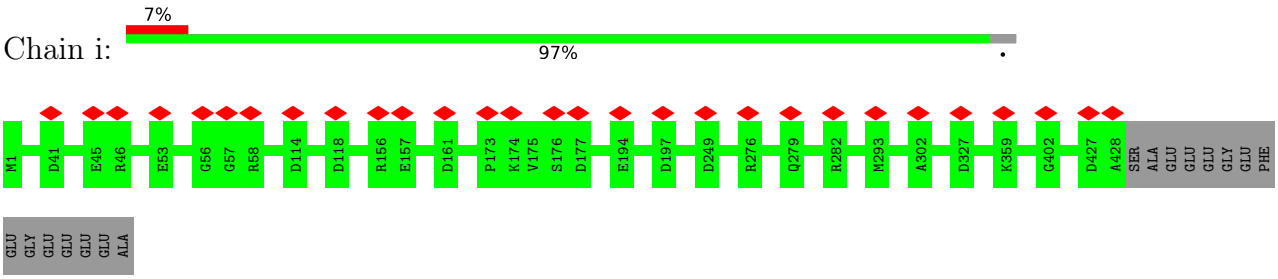
• Molecule 5: Tubulin beta

Chain b:



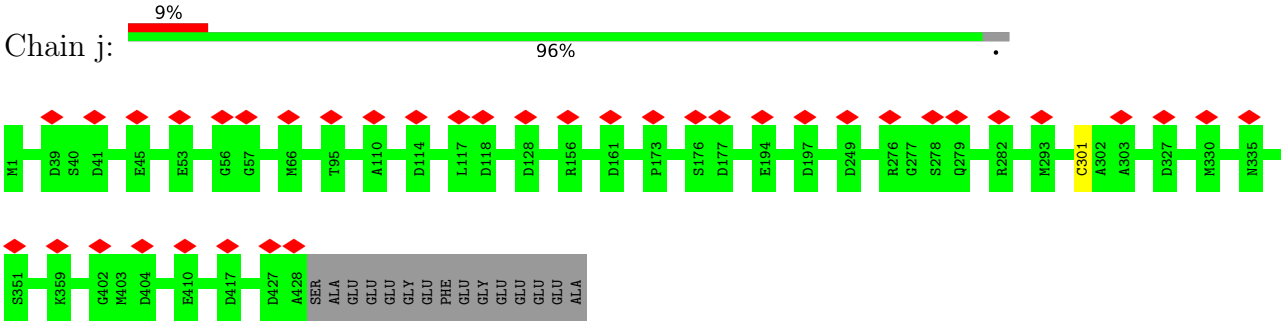
• Molecule 5: Tubulin beta

Chain i:



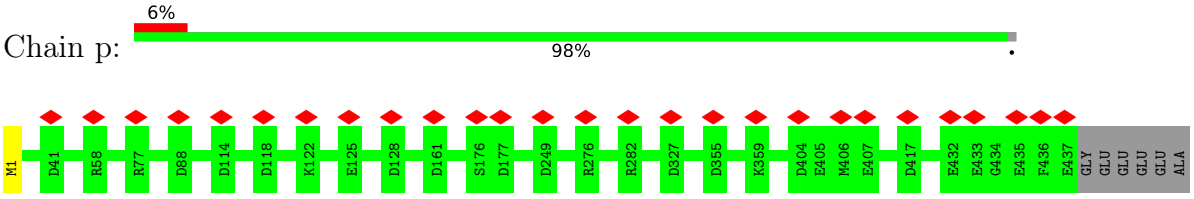
• Molecule 5: Tubulin beta

Chain j:



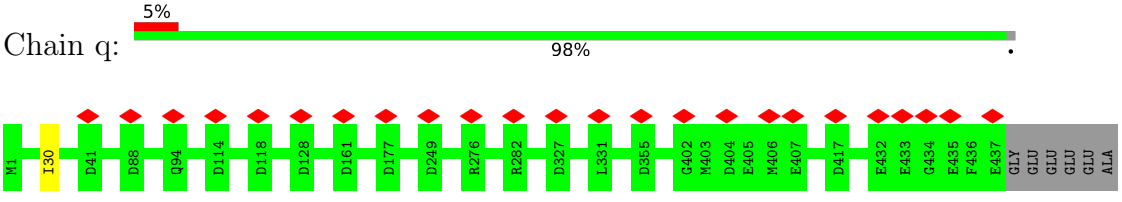
• Molecule 5: Tubulin beta

Chain p:



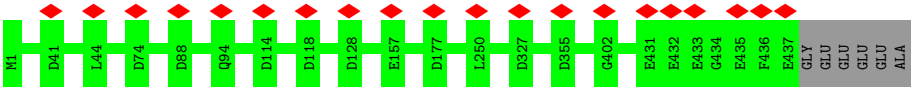
• Molecule 5: Tubulin beta

Chain q:



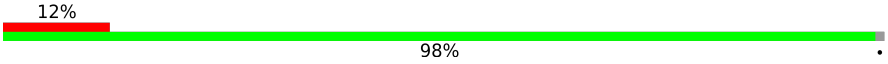
• Molecule 5: Tubulin beta

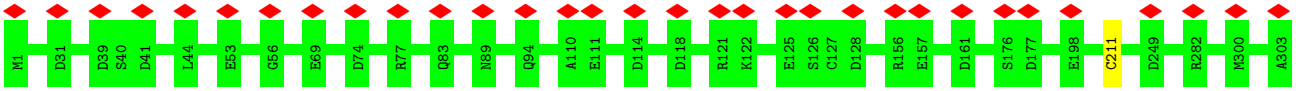
Chain r:

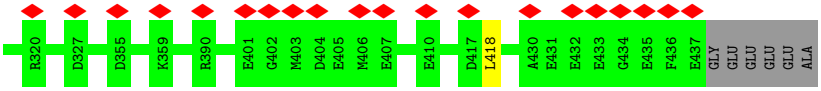


• Molecule 5: Tubulin beta

Chain t:

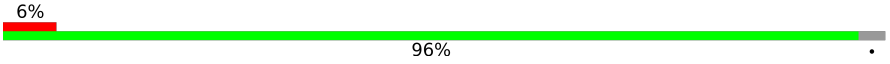


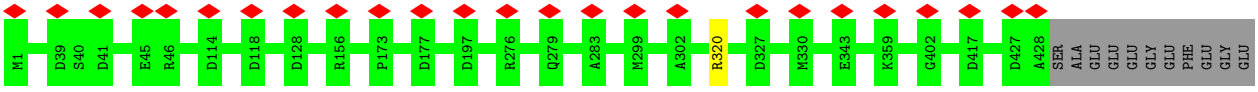




• Molecule 5: Tubulin beta

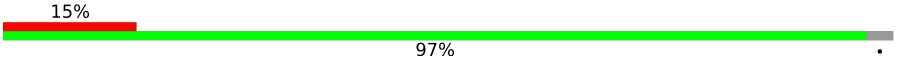
Chain u:

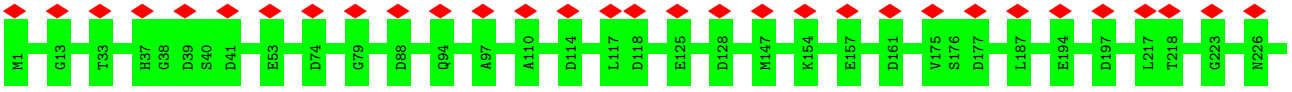


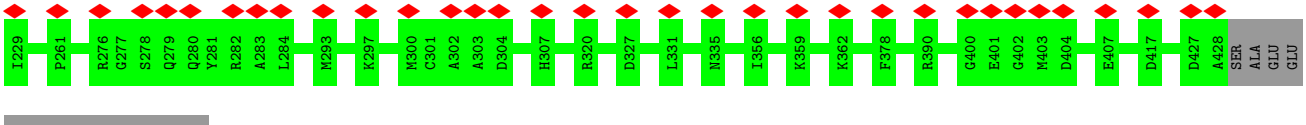


• Molecule 5: Tubulin beta

Chain v:

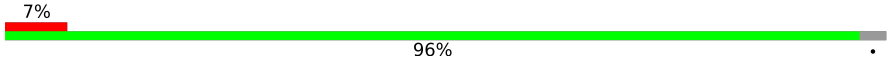


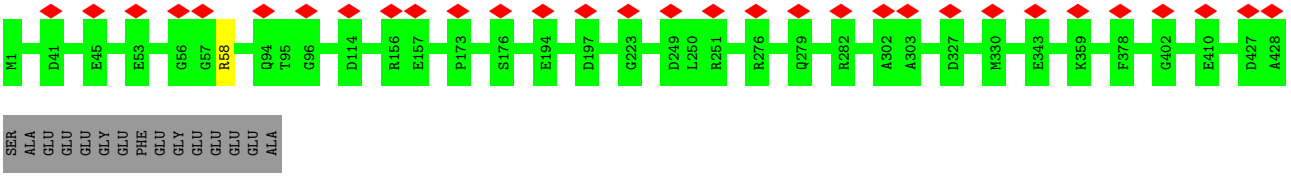




• Molecule 5: Tubulin beta

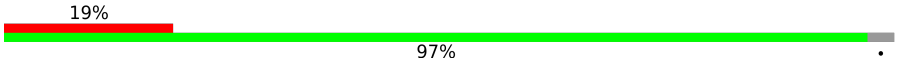
Chain w:

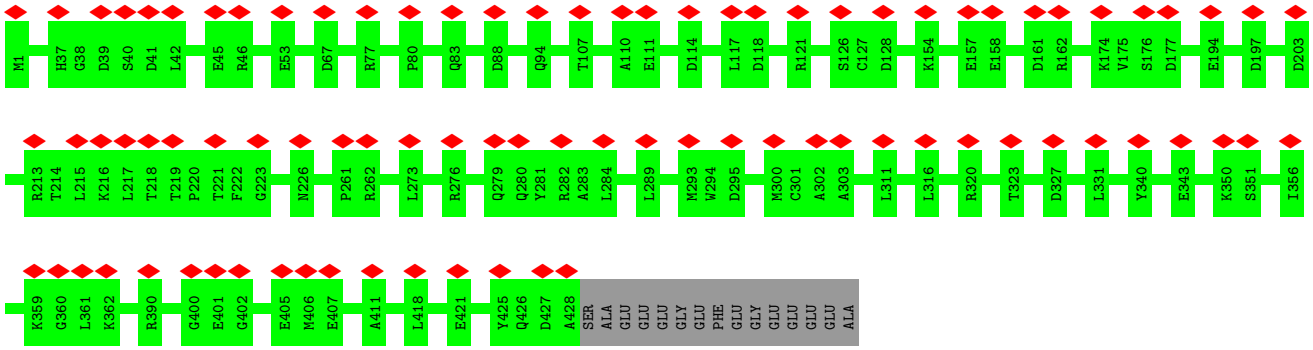




• Molecule 5: Tubulin beta

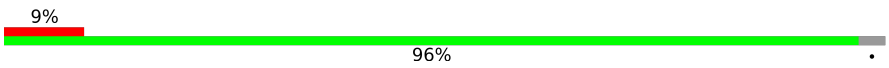
Chain 4:

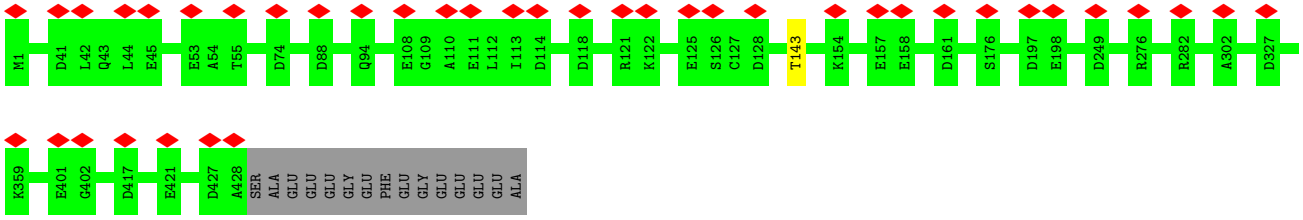




• Molecule 5: Tubulin beta

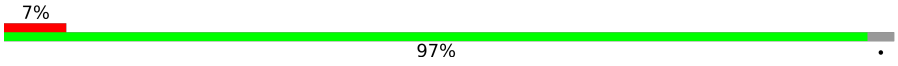
Chain 8:

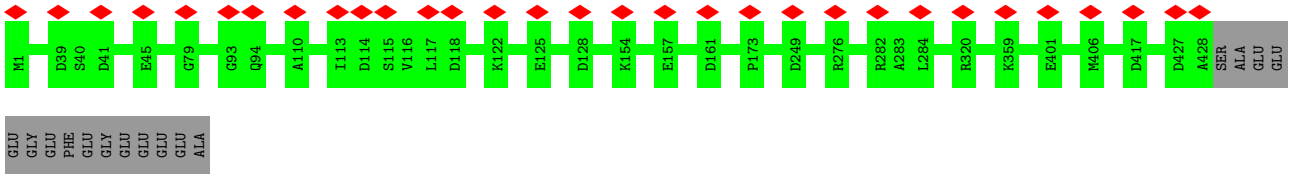




• Molecule 5: Tubulin beta

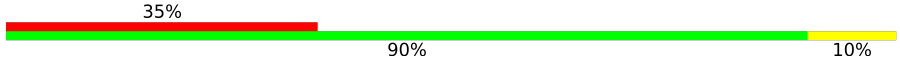
Chain 9:

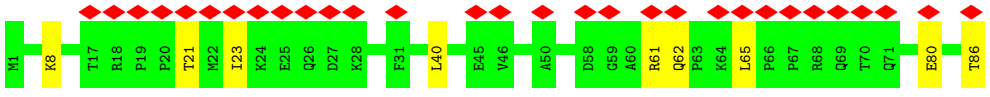




• Molecule 6: FAP276

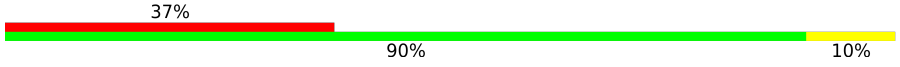
Chain W:

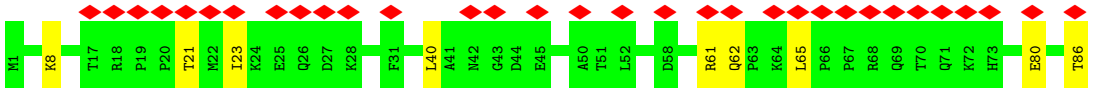




• Molecule 6: FAP276

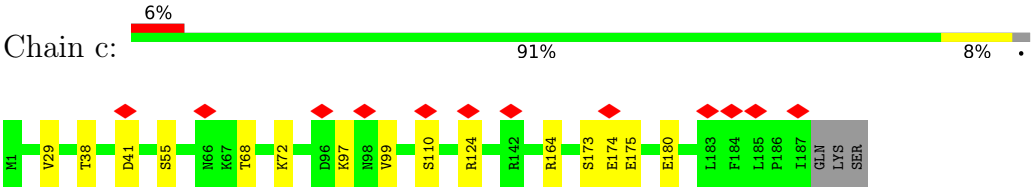
Chain x:





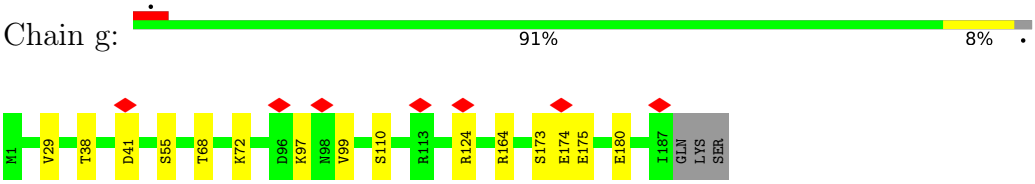
• Molecule 7: Cilia- and flagella-associated protein 20

Chain c:



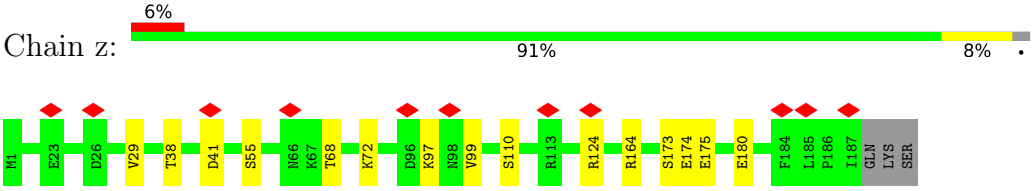
• Molecule 7: Cilia- and flagella-associated protein 20

Chain g:



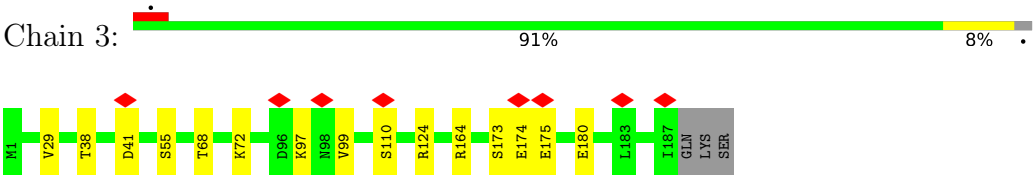
• Molecule 7: Cilia- and flagella-associated protein 20

Chain z:



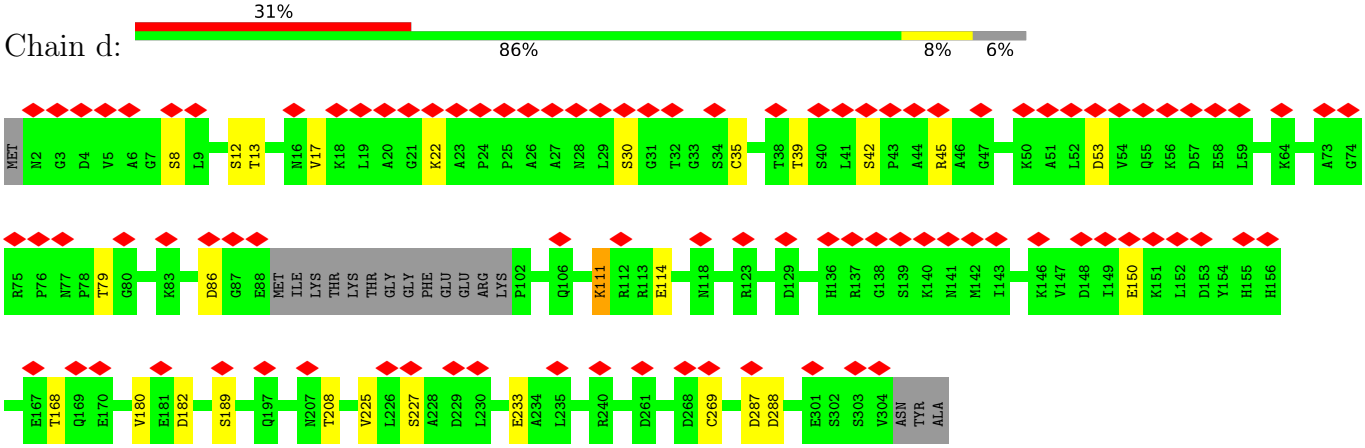
• Molecule 7: Cilia- and flagella-associated protein 20

Chain 3:



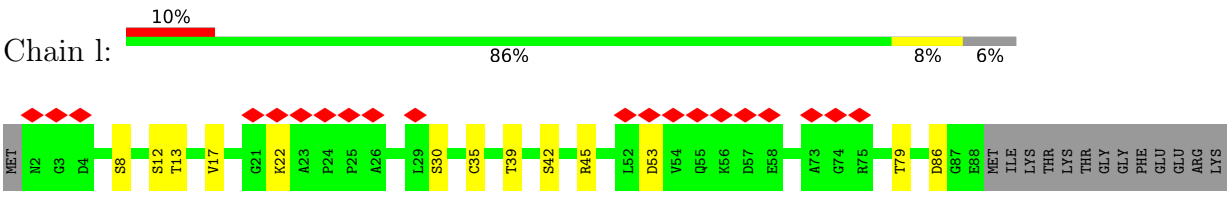
• Molecule 8: PACRG

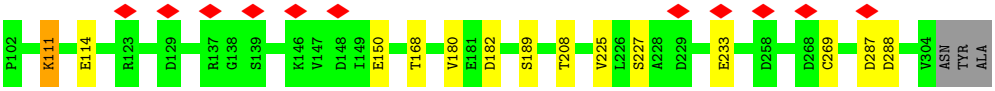
Chain d:



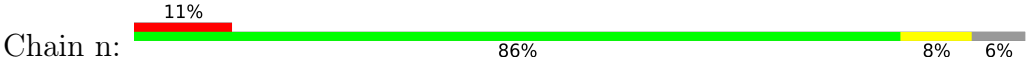
• Molecule 8: PACRG

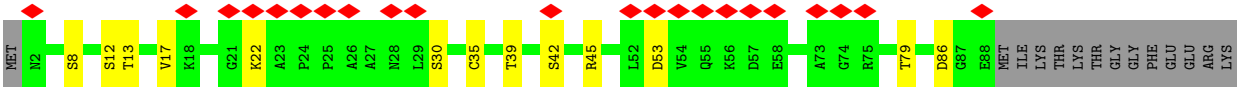
Chain l:



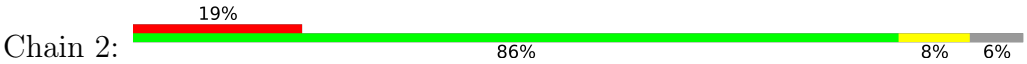


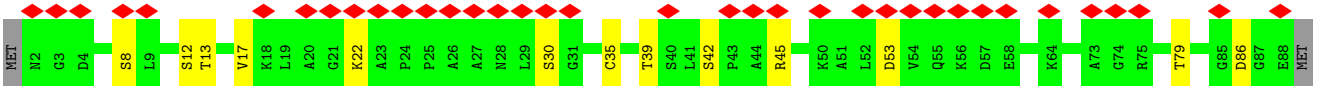
• Molecule 8: PACRG

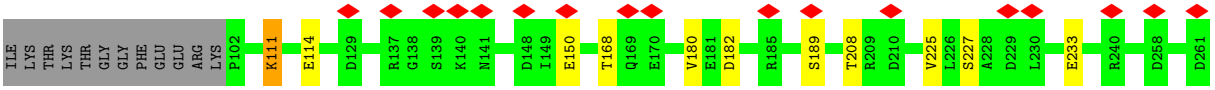


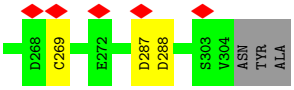


• Molecule 8: PACRG









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	270713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	237.125, 204.75, 393.75	wwPDB
Map dimensions	450, 234, 271	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.875, 0.875, 0.875	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, TA1, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.29	0/1429	0.45	0/1933
2	B	0.31	0/4800	0.54	1/6511 (0.0%)
2	C	0.31	0/4800	0.54	1/6511 (0.0%)
3	0	0.31	0/3451	0.45	0/4678
3	1	0.29	0/3451	0.45	0/4678
3	5	0.33	0/3451	0.51	0/4678
3	6	0.27	0/3400	0.44	0/4609
3	7	0.28	0/3400	0.44	0/4609
3	D	0.33	0/3400	0.46	0/4609
3	E	0.34	0/3400	0.52	0/4609
3	F	0.29	0/3400	0.44	0/4609
3	G	0.30	0/3400	0.44	0/4609
3	L	0.32	0/3420	0.46	0/4636
3	M	0.32	0/3400	0.47	0/4609
3	P	0.31	0/3400	0.46	0/4609
3	S	0.31	0/3400	0.45	0/4609
3	X	0.31	0/3400	0.48	0/4609
3	Y	0.29	0/3400	0.45	0/4609
3	Z	0.29	0/3451	0.46	0/4678
3	e	0.28	0/3451	0.45	0/4678
3	f	0.31	0/3420	0.47	0/4636
3	h	0.29	0/3400	0.45	0/4609
3	k	0.33	0/3420	0.50	0/4636
3	m	0.31	0/3451	0.45	0/4678
3	o	0.31	0/3451	0.45	0/4678
3	s	0.29	0/3400	0.44	0/4609
3	y	0.33	0/3451	0.46	0/4678
4	H	0.30	0/1098	0.51	0/1490
5	4	0.28	0/3433	0.45	0/4646
5	8	0.34	0/3433	0.52	0/4646
5	9	0.29	0/3433	0.44	0/4646
5	I	0.31	0/3433	0.45	0/4646

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	J	0.30	0/3433	0.44	0/4646
5	K	0.31	0/3433	0.46	0/4646
5	N	0.29	0/3433	0.44	0/4646
5	O	0.31	0/3433	0.45	0/4646
5	Q	0.29	0/3433	0.45	0/4646
5	R	0.31	0/3433	0.45	0/4646
5	T	0.32	0/3433	0.48	0/4646
5	U	0.31	0/3433	0.45	0/4646
5	V	0.28	0/3433	0.44	0/4646
5	a	0.28	0/3433	0.43	0/4646
5	b	0.28	0/3433	0.45	0/4646
5	i	0.29	0/3433	0.44	0/4646
5	j	0.29	0/3433	0.44	0/4646
5	p	0.32	0/3505	0.45	0/4742
5	q	0.32	0/3505	0.46	1/4742 (0.0%)
5	r	0.31	0/3505	0.44	0/4742
5	t	0.32	0/3505	0.49	0/4742
5	u	0.30	0/3433	0.45	0/4646
5	v	0.28	0/3433	0.44	0/4646
5	w	0.29	0/3433	0.44	0/4646
6	W	0.31	0/717	0.54	1/967 (0.1%)
6	x	0.31	0/717	0.54	1/967 (0.1%)
7	3	0.34	0/1572	0.50	0/2124
7	c	0.34	0/1572	0.50	0/2124
7	g	0.34	0/1572	0.50	0/2124
7	z	0.34	0/1572	0.50	0/2124
8	2	0.31	0/2325	0.51	1/3151 (0.0%)
8	d	0.31	0/2325	0.51	1/3151 (0.0%)
8	l	0.31	0/2325	0.51	1/3151 (0.0%)
8	n	0.31	0/2325	0.51	1/3151 (0.0%)
All	All	0.31	0/193897	0.47	9/262616 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	l	111	LYS	CD-CE-NZ	9.43	133.39	111.70
8	2	111	LYS	CD-CE-NZ	9.42	133.37	111.70
8	d	111	LYS	CD-CE-NZ	9.41	133.35	111.70
8	n	111	LYS	CD-CE-NZ	9.40	133.33	111.70
5	q	30	ILE	C-N-CA	6.37	137.61	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	173/240 (72%)	150 (87%)	21 (12%)	2 (1%)	13	51
2	B	615/633 (97%)	541 (88%)	72 (12%)	2 (0%)	41	75
2	C	615/633 (97%)	541 (88%)	72 (12%)	2 (0%)	41	75
3	0	434/451 (96%)	408 (94%)	26 (6%)	0	100	100
3	1	434/451 (96%)	409 (94%)	25 (6%)	0	100	100
3	5	434/451 (96%)	402 (93%)	32 (7%)	0	100	100
3	6	424/451 (94%)	398 (94%)	26 (6%)	0	100	100
3	7	424/451 (94%)	401 (95%)	23 (5%)	0	100	100
3	D	424/451 (94%)	396 (93%)	28 (7%)	0	100	100
3	E	424/451 (94%)	393 (93%)	31 (7%)	0	100	100
3	F	424/451 (94%)	395 (93%)	29 (7%)	0	100	100
3	G	424/451 (94%)	400 (94%)	24 (6%)	0	100	100
3	L	427/451 (95%)	399 (93%)	28 (7%)	0	100	100
3	M	424/451 (94%)	394 (93%)	30 (7%)	0	100	100
3	P	424/451 (94%)	394 (93%)	30 (7%)	0	100	100
3	S	424/451 (94%)	389 (92%)	35 (8%)	0	100	100
3	X	424/451 (94%)	398 (94%)	26 (6%)	0	100	100
3	Y	424/451 (94%)	393 (93%)	31 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Z	434/451 (96%)	406 (94%)	28 (6%)	0	100	100
3	e	434/451 (96%)	411 (95%)	23 (5%)	0	100	100
3	f	427/451 (95%)	397 (93%)	30 (7%)	0	100	100
3	h	424/451 (94%)	399 (94%)	25 (6%)	0	100	100
3	k	427/451 (95%)	391 (92%)	36 (8%)	0	100	100
3	m	434/451 (96%)	408 (94%)	26 (6%)	0	100	100
3	o	434/451 (96%)	407 (94%)	27 (6%)	0	100	100
3	s	424/451 (94%)	398 (94%)	26 (6%)	0	100	100
3	y	434/451 (96%)	413 (95%)	21 (5%)	0	100	100
4	H	133/137 (97%)	115 (86%)	18 (14%)	0	100	100
5	4	426/443 (96%)	400 (94%)	26 (6%)	0	100	100
5	8	426/443 (96%)	400 (94%)	25 (6%)	1 (0%)	47	79
5	9	426/443 (96%)	399 (94%)	27 (6%)	0	100	100
5	I	426/443 (96%)	404 (95%)	22 (5%)	0	100	100
5	J	426/443 (96%)	404 (95%)	22 (5%)	0	100	100
5	K	426/443 (96%)	398 (93%)	28 (7%)	0	100	100
5	N	426/443 (96%)	403 (95%)	23 (5%)	0	100	100
5	O	426/443 (96%)	405 (95%)	21 (5%)	0	100	100
5	Q	426/443 (96%)	397 (93%)	29 (7%)	0	100	100
5	R	426/443 (96%)	396 (93%)	30 (7%)	0	100	100
5	T	426/443 (96%)	400 (94%)	26 (6%)	0	100	100
5	U	426/443 (96%)	396 (93%)	30 (7%)	0	100	100
5	V	426/443 (96%)	396 (93%)	30 (7%)	0	100	100
5	a	426/443 (96%)	406 (95%)	20 (5%)	0	100	100
5	b	426/443 (96%)	398 (93%)	28 (7%)	0	100	100
5	i	426/443 (96%)	397 (93%)	29 (7%)	0	100	100
5	j	426/443 (96%)	399 (94%)	27 (6%)	0	100	100
5	p	435/443 (98%)	414 (95%)	21 (5%)	0	100	100
5	q	435/443 (98%)	415 (95%)	20 (5%)	0	100	100
5	r	435/443 (98%)	418 (96%)	17 (4%)	0	100	100
5	t	435/443 (98%)	416 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	u	426/443 (96%)	395 (93%)	31 (7%)	0	100	100
5	v	426/443 (96%)	393 (92%)	33 (8%)	0	100	100
5	w	426/443 (96%)	405 (95%)	21 (5%)	0	100	100
6	W	84/86 (98%)	69 (82%)	15 (18%)	0	100	100
6	x	84/86 (98%)	69 (82%)	15 (18%)	0	100	100
7	3	185/190 (97%)	170 (92%)	15 (8%)	0	100	100
7	c	185/190 (97%)	170 (92%)	15 (8%)	0	100	100
7	g	185/190 (97%)	170 (92%)	15 (8%)	0	100	100
7	z	185/190 (97%)	170 (92%)	15 (8%)	0	100	100
8	2	286/307 (93%)	268 (94%)	18 (6%)	0	100	100
8	d	286/307 (93%)	268 (94%)	18 (6%)	0	100	100
8	l	286/307 (93%)	268 (94%)	18 (6%)	0	100	100
8	n	286/307 (93%)	267 (93%)	19 (7%)	0	100	100
All	All	24113/25259 (96%)	22489 (93%)	1617 (7%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	372	CYS
2	C	372	CYS
5	8	143	THR
1	A	22	MET
2	B	411	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/206 (73%)	150 (100%)	0	100	100
2	B	505/517 (98%)	465 (92%)	40 (8%)	12	44
2	C	505/517 (98%)	465 (92%)	40 (8%)	12	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	0	366/374 (98%)	366 (100%)	0	100	100
3	1	366/374 (98%)	366 (100%)	0	100	100
3	5	366/374 (98%)	365 (100%)	1 (0%)	92	97
3	6	361/374 (96%)	360 (100%)	1 (0%)	92	97
3	7	361/374 (96%)	361 (100%)	0	100	100
3	D	361/374 (96%)	361 (100%)	0	100	100
3	E	361/374 (96%)	361 (100%)	0	100	100
3	F	361/374 (96%)	360 (100%)	1 (0%)	92	97
3	G	361/374 (96%)	361 (100%)	0	100	100
3	L	363/374 (97%)	362 (100%)	1 (0%)	92	97
3	M	361/374 (96%)	360 (100%)	1 (0%)	92	97
3	P	361/374 (96%)	361 (100%)	0	100	100
3	S	361/374 (96%)	361 (100%)	0	100	100
3	X	361/374 (96%)	361 (100%)	0	100	100
3	Y	361/374 (96%)	361 (100%)	0	100	100
3	Z	366/374 (98%)	364 (100%)	2 (0%)	88	95
3	e	366/374 (98%)	366 (100%)	0	100	100
3	f	363/374 (97%)	361 (99%)	2 (1%)	86	94
3	h	361/374 (96%)	360 (100%)	1 (0%)	92	97
3	k	363/374 (97%)	361 (99%)	2 (1%)	86	94
3	m	366/374 (98%)	366 (100%)	0	100	100
3	o	366/374 (98%)	366 (100%)	0	100	100
3	s	361/374 (96%)	360 (100%)	1 (0%)	92	97
3	y	366/374 (98%)	365 (100%)	1 (0%)	92	97
4	H	119/121 (98%)	117 (98%)	2 (2%)	60	82
5	4	368/379 (97%)	368 (100%)	0	100	100
5	8	368/379 (97%)	368 (100%)	0	100	100
5	9	368/379 (97%)	368 (100%)	0	100	100
5	I	368/379 (97%)	367 (100%)	1 (0%)	92	97
5	J	368/379 (97%)	368 (100%)	0	100	100
5	K	368/379 (97%)	368 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	N	368/379 (97%)	368 (100%)	0	100 100
5	O	368/379 (97%)	367 (100%)	1 (0%)	92 97
5	Q	368/379 (97%)	367 (100%)	1 (0%)	92 97
5	R	368/379 (97%)	368 (100%)	0	100 100
5	T	368/379 (97%)	366 (100%)	2 (0%)	88 95
5	U	368/379 (97%)	368 (100%)	0	100 100
5	V	368/379 (97%)	368 (100%)	0	100 100
5	a	368/379 (97%)	368 (100%)	0	100 100
5	b	368/379 (97%)	367 (100%)	1 (0%)	92 97
5	i	368/379 (97%)	368 (100%)	0	100 100
5	j	368/379 (97%)	367 (100%)	1 (0%)	92 97
5	p	375/379 (99%)	374 (100%)	1 (0%)	92 97
5	q	375/379 (99%)	375 (100%)	0	100 100
5	r	375/379 (99%)	375 (100%)	0	100 100
5	t	375/379 (99%)	373 (100%)	2 (0%)	88 95
5	u	368/379 (97%)	367 (100%)	1 (0%)	92 97
5	v	368/379 (97%)	368 (100%)	0	100 100
5	w	368/379 (97%)	367 (100%)	1 (0%)	92 97
6	W	77/77 (100%)	69 (90%)	8 (10%)	7 33
6	x	77/77 (100%)	69 (90%)	8 (10%)	7 33
7	3	173/176 (98%)	158 (91%)	15 (9%)	10 41
7	c	173/176 (98%)	158 (91%)	15 (9%)	10 41
7	g	173/176 (98%)	158 (91%)	15 (9%)	10 41
7	z	173/176 (98%)	158 (91%)	15 (9%)	10 41
8	2	244/258 (95%)	217 (89%)	27 (11%)	6 31
8	d	244/258 (95%)	217 (89%)	27 (11%)	6 31
8	l	244/258 (95%)	217 (89%)	27 (11%)	6 31
8	n	244/258 (95%)	217 (89%)	27 (11%)	6 31
All	All	20671/21323 (97%)	20379 (99%)	292 (1%)	68 85

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	x	86	THR
7	3	173	SER
7	z	72	LYS
8	2	86	ASP
6	W	86	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 268 such sidechains are listed below:

Mol	Chain	Res	Type
8	2	28	ASN
5	4	291	GLN
5	9	105	HIS
5	U	37	HIS
5	T	335	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 88 ligands modelled in this entry, 24 are monoatomic - leaving 64 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	$\#\|Z\|>2$
12	TA1	t	502	-	68,68,68	0.77	2 (2%)	105,105,105	0.82	4 (3%)
12	TA1	9	502	-	68,68,68	0.59	2 (2%)	105,105,105	0.77	4 (3%)
9	GTP	k	501	10	26,34,34	5.15	11 (42%)	32,54,54	1.64	7 (21%)
12	TA1	b	502	-	68,68,68	0.68	1 (1%)	105,105,105	0.76	4 (3%)
12	TA1	q	502	-	68,68,68	0.84	2 (2%)	105,105,105	0.87	3 (2%)
9	GTP	Y	501	10	26,34,34	5.19	11 (42%)	32,54,54	1.55	7 (21%)
12	TA1	j	502	-	68,68,68	0.61	1 (1%)	105,105,105	0.82	4 (3%)
9	GTP	0	501	10	26,34,34	5.17	11 (42%)	32,54,54	1.58	6 (18%)
11	GDP	J	501	-	24,30,30	3.83	12 (50%)	30,47,47	1.60	6 (20%)
12	TA1	v	502	-	68,68,68	0.39	0	105,105,105	0.80	4 (3%)
9	GTP	Z	501	10	26,34,34	5.16	11 (42%)	32,54,54	1.55	7 (21%)
11	GDP	K	501	-	24,30,30	3.85	12 (50%)	30,47,47	1.79	6 (20%)
11	GDP	v	501	-	24,30,30	3.82	12 (50%)	30,47,47	1.59	7 (23%)
9	GTP	5	501	10	26,34,34	5.16	11 (42%)	32,54,54	1.59	6 (18%)
9	GTP	e	501	10	26,34,34	5.15	11 (42%)	32,54,54	1.59	7 (21%)
11	GDP	w	501	-	24,30,30	3.83	12 (50%)	30,47,47	1.49	5 (16%)
9	GTP	G	501	10	26,34,34	5.16	11 (42%)	32,54,54	1.57	6 (18%)
9	GTP	S	501	10	26,34,34	5.15	12 (46%)	32,54,54	1.57	6 (18%)
11	GDP	T	501	-	24,30,30	3.82	12 (50%)	30,47,47	1.65	6 (20%)
9	GTP	X	501	10	26,34,34	5.17	11 (42%)	32,54,54	1.53	6 (18%)
11	GDP	r	501	-	24,30,30	3.83	12 (50%)	30,47,47	1.53	6 (20%)
12	TA1	p	502	-	68,68,68	0.58	2 (2%)	105,105,105	0.78	3 (2%)
9	GTP	1	501	10	26,34,34	5.16	11 (42%)	32,54,54	1.53	7 (21%)
11	GDP	R	501	-	24,30,30	3.89	13 (54%)	30,47,47	1.73	6 (20%)
11	GDP	p	501	-	24,30,30	3.82	12 (50%)	30,47,47	1.51	6 (20%)
9	GTP	m	501	10	26,34,34	5.18	11 (42%)	32,54,54	1.59	6 (18%)
11	GDP	a	501	-	24,30,30	3.84	12 (50%)	30,47,47	1.55	7 (23%)
11	GDP	q	501	-	24,30,30	3.83	12 (50%)	30,47,47	1.59	6 (20%)
11	GDP	I	501	-	24,30,30	3.84	12 (50%)	30,47,47	1.71	6 (20%)
9	GTP	P	501	10	26,34,34	5.17	11 (42%)	32,54,54	1.62	7 (21%)
11	GDP	U	501	-	24,30,30	3.82	12 (50%)	30,47,47	1.62	6 (20%)
11	GDP	9	501	-	24,30,30	3.85	12 (50%)	30,47,47	1.50	6 (20%)
11	GDP	b	501	-	24,30,30	3.84	12 (50%)	30,47,47	1.59	6 (20%)
9	GTP	D	501	10	26,34,34	5.15	11 (42%)	32,54,54	1.69	7 (21%)
11	GDP	8	501	-	24,30,30	3.82	12 (50%)	30,47,47	1.62	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	GTP	L	501	10	26,34,34	5.15	11 (42%)	32,54,54	1.67	7 (21%)
9	GTP	y	501	10	26,34,34	5.17	11 (42%)	32,54,54	1.62	7 (21%)
11	GDP	O	501	-	24,30,30	3.83	12 (50%)	30,47,47	1.63	6 (20%)
11	GDP	j	501	-	24,30,30	3.86	12 (50%)	30,47,47	1.63	6 (20%)
12	TA1	V	502	-	68,68,68	0.51	1 (1%)	105,105,105	0.75	3 (2%)
12	TA1	r	502	-	68,68,68	0.60	1 (1%)	105,105,105	0.80	4 (3%)
9	GTP	F	501	10	26,34,34	5.14	11 (42%)	32,54,54	1.61	6 (18%)
9	GTP	o	501	10	26,34,34	5.15	11 (42%)	32,54,54	1.66	7 (21%)
9	GTP	f	501	10	26,34,34	5.16	11 (42%)	32,54,54	1.64	7 (21%)
9	GTP	s	501	10	26,34,34	5.15	11 (42%)	32,54,54	1.55	7 (21%)
11	GDP	N	501	-	24,30,30	3.82	12 (50%)	30,47,47	1.75	6 (20%)
9	GTP	7	501	10	26,34,34	5.17	11 (42%)	32,54,54	1.53	6 (18%)
9	GTP	M	501	10	26,34,34	5.17	11 (42%)	32,54,54	1.59	6 (18%)
12	TA1	J	502	-	68,68,68	0.55	1 (1%)	105,105,105	0.75	3 (2%)
9	GTP	E	501	10	26,34,34	5.18	11 (42%)	32,54,54	1.59	6 (18%)
9	GTP	6	501	10	26,34,34	5.16	11 (42%)	32,54,54	1.60	7 (21%)
11	GDP	u	501	-	24,30,30	3.82	12 (50%)	30,47,47	1.48	5 (16%)
12	TA1	8	502	-	68,68,68	0.56	1 (1%)	105,105,105	0.75	4 (3%)
11	GDP	4	501	-	24,30,30	3.84	12 (50%)	30,47,47	1.66	7 (23%)
12	TA1	4	502	-	68,68,68	0.48	1 (1%)	105,105,105	0.77	5 (4%)
12	TA1	w	502	-	68,68,68	0.53	1 (1%)	105,105,105	0.72	3 (2%)
11	GDP	Q	501	-	24,30,30	3.85	12 (50%)	30,47,47	1.58	6 (20%)
11	GDP	V	501	-	24,30,30	4.01	13 (54%)	30,47,47	1.75	6 (20%)
12	TA1	a	502	-	68,68,68	0.56	1 (1%)	105,105,105	0.78	4 (3%)
12	TA1	i	502	-	68,68,68	0.60	1 (1%)	105,105,105	0.74	4 (3%)
11	GDP	i	501	-	24,30,30	3.83	12 (50%)	30,47,47	1.58	5 (16%)
12	TA1	u	502	-	68,68,68	0.67	1 (1%)	105,105,105	0.77	4 (3%)
11	GDP	t	501	-	24,30,30	3.84	12 (50%)	30,47,47	1.55	6 (20%)
9	GTP	h	501	10	26,34,34	5.16	11 (42%)	32,54,54	1.57	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
12	TA1	t	502	-	-	2/41/127/127	0/7/7/7
12	TA1	9	502	-	-	0/41/127/127	0/7/7/7
9	GTP	k	501	10	-	2/18/38/38	0/3/3/3
12	TA1	b	502	-	-	10/41/127/127	0/7/7/7
12	TA1	q	502	-	-	4/41/127/127	0/7/7/7
9	GTP	Y	501	10	-	5/18/38/38	0/3/3/3
12	TA1	j	502	-	-	11/41/127/127	0/7/7/7
9	GTP	0	501	10	-	5/18/38/38	0/3/3/3
11	GDP	J	501	-	-	5/12/32/32	0/3/3/3
12	TA1	v	502	-	-	5/41/127/127	0/7/7/7
9	GTP	Z	501	10	-	4/18/38/38	0/3/3/3
11	GDP	K	501	-	-	4/12/32/32	0/3/3/3
11	GDP	v	501	-	-	4/12/32/32	0/3/3/3
9	GTP	5	501	10	-	4/18/38/38	0/3/3/3
9	GTP	e	501	10	-	3/18/38/38	0/3/3/3
11	GDP	w	501	-	-	3/12/32/32	0/3/3/3
9	GTP	G	501	10	-	4/18/38/38	0/3/3/3
9	GTP	S	501	10	-	5/18/38/38	0/3/3/3
11	GDP	T	501	-	-	5/12/32/32	0/3/3/3
9	GTP	X	501	10	-	3/18/38/38	0/3/3/3
11	GDP	r	501	-	-	5/12/32/32	0/3/3/3
12	TA1	p	502	-	-	1/41/127/127	0/7/7/7
9	GTP	1	501	10	-	2/18/38/38	0/3/3/3
11	GDP	R	501	-	-	4/12/32/32	0/3/3/3
11	GDP	p	501	-	-	5/12/32/32	0/3/3/3
9	GTP	m	501	10	-	4/18/38/38	0/3/3/3
11	GDP	a	501	-	-	2/12/32/32	0/3/3/3
11	GDP	q	501	-	-	4/12/32/32	0/3/3/3
11	GDP	I	501	-	-	4/12/32/32	0/3/3/3
9	GTP	P	501	10	-	5/18/38/38	0/3/3/3
11	GDP	U	501	-	-	4/12/32/32	0/3/3/3
11	GDP	9	501	-	-	3/12/32/32	0/3/3/3
11	GDP	b	501	-	-	3/12/32/32	0/3/3/3
9	GTP	D	501	10	-	4/18/38/38	0/3/3/3
11	GDP	8	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GTP	L	501	10	-	4/18/38/38	0/3/3/3
9	GTP	y	501	10	-	5/18/38/38	0/3/3/3
11	GDP	O	501	-	-	4/12/32/32	0/3/3/3
11	GDP	j	501	-	-	3/12/32/32	0/3/3/3
12	TA1	V	502	-	-	6/41/127/127	0/7/7/7
12	TA1	r	502	-	-	4/41/127/127	0/7/7/7
9	GTP	F	501	10	-	4/18/38/38	0/3/3/3
9	GTP	o	501	10	-	5/18/38/38	0/3/3/3
9	GTP	f	501	10	-	3/18/38/38	0/3/3/3
9	GTP	s	501	10	-	4/18/38/38	0/3/3/3
11	GDP	N	501	-	-	6/12/32/32	0/3/3/3
9	GTP	7	501	10	-	4/18/38/38	0/3/3/3
9	GTP	M	501	10	-	5/18/38/38	0/3/3/3
12	TA1	J	502	-	-	4/41/127/127	0/7/7/7
9	GTP	E	501	10	-	5/18/38/38	0/3/3/3
9	GTP	6	501	10	-	4/18/38/38	0/3/3/3
11	GDP	u	501	-	-	4/12/32/32	0/3/3/3
12	TA1	8	502	-	-	5/41/127/127	0/7/7/7
11	GDP	4	501	-	-	1/12/32/32	0/3/3/3
12	TA1	4	502	-	-	6/41/127/127	0/7/7/7
12	TA1	w	502	-	-	11/41/127/127	0/7/7/7
11	GDP	Q	501	-	-	4/12/32/32	0/3/3/3
11	GDP	V	501	-	-	4/12/32/32	0/3/3/3
12	TA1	a	502	-	-	2/41/127/127	0/7/7/7
12	TA1	i	502	-	-	8/41/127/127	0/7/7/7
11	GDP	i	501	-	-	6/12/32/32	0/3/3/3
12	TA1	u	502	-	-	14/41/127/127	0/7/7/7
11	GDP	t	501	-	-	3/12/32/32	0/3/3/3
9	GTP	h	501	10	-	2/18/38/38	0/3/3/3

The worst 5 of 574 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	501	GTP	C2'-C1'	-16.61	1.28	1.53
9	Z	501	GTP	C2'-C1'	-16.59	1.28	1.53
9	m	501	GTP	C2'-C1'	-16.57	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	501	GTP	C2'-C1'	-16.53	1.28	1.53
9	L	501	GTP	C2'-C1'	-16.51	1.28	1.53

The worst 5 of 361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	f	501	GTP	PB-O3B-PG	-4.62	116.96	132.83
9	o	501	GTP	PB-O3B-PG	-4.36	117.87	132.83
9	L	501	GTP	PA-O3A-PB	-4.32	118.00	132.83
9	m	501	GTP	PB-O3B-PG	-4.30	118.08	132.83
9	y	501	GTP	PB-O3B-PG	-4.21	118.38	132.83

There are no chirality outliers.

5 of 281 torsion outliers are listed below:

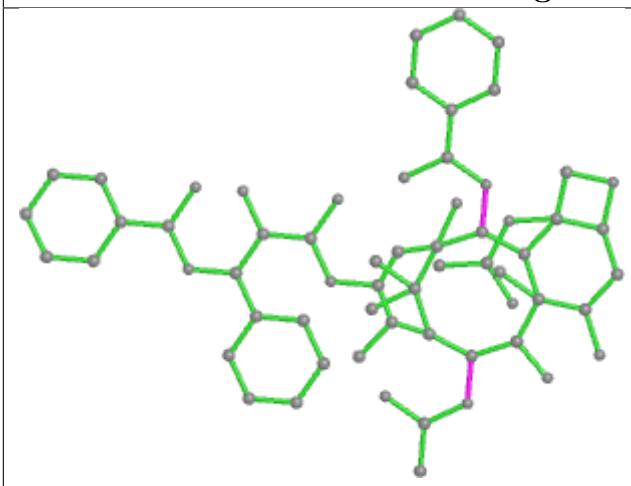
Mol	Chain	Res	Type	Atoms
9	E	501	GTP	C5'-O5'-PA-O3A
9	G	501	GTP	C5'-O5'-PA-O1A
9	L	501	GTP	C5'-O5'-PA-O1A
9	M	501	GTP	C5'-O5'-PA-O3A
9	M	501	GTP	O4'-C4'-C5'-O5'

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 TA1 t 502



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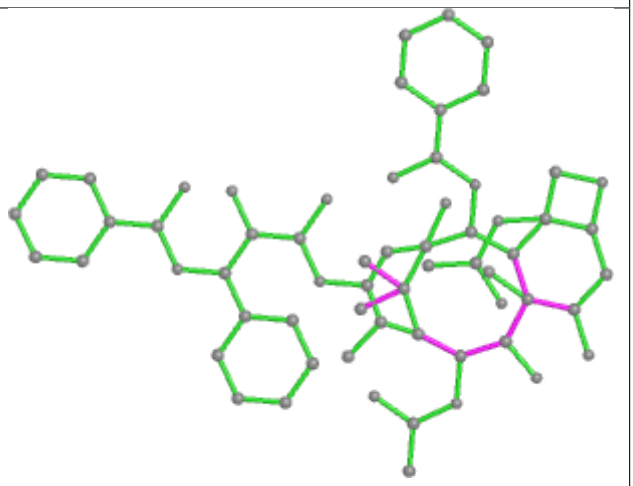
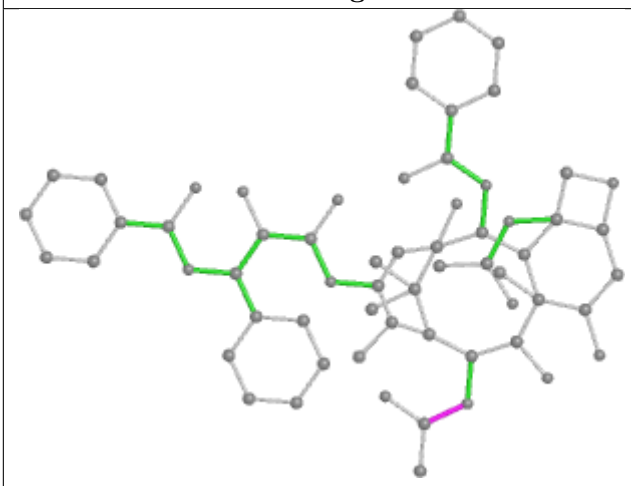
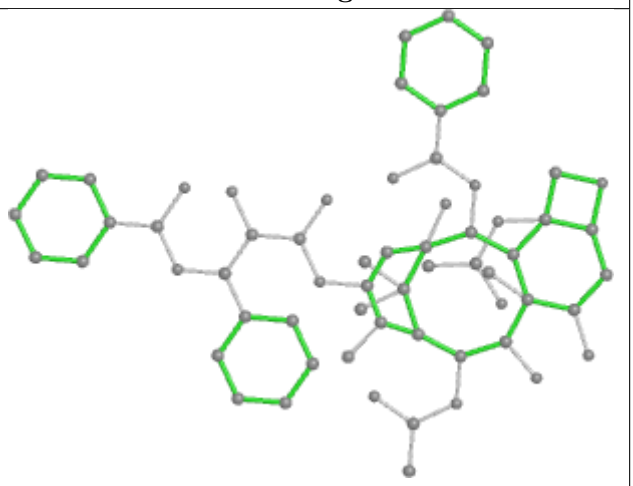


Bond angles

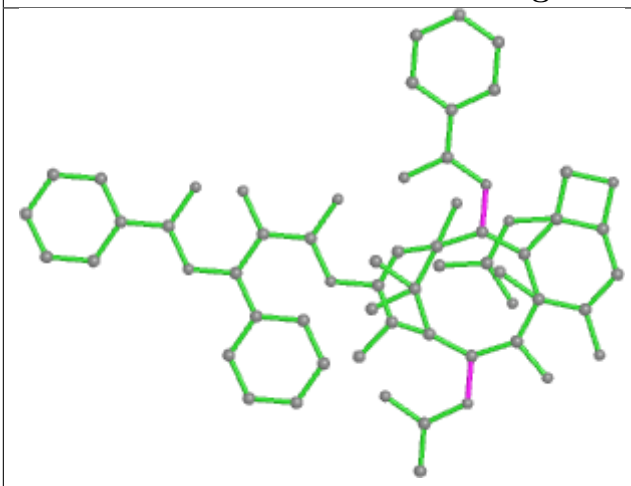


Torsions



Rings

Ligand TA1 9 502



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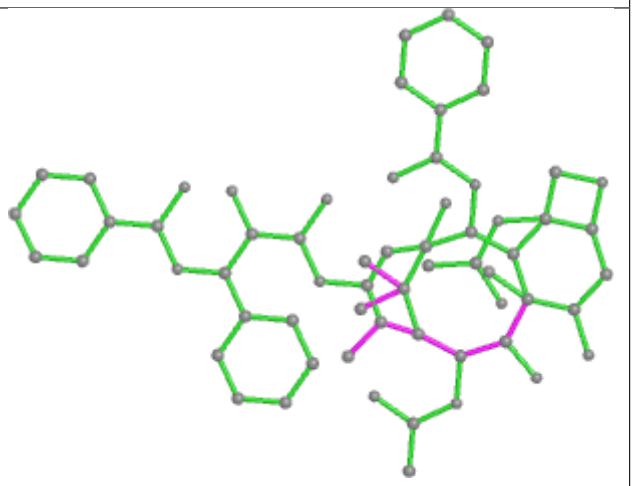

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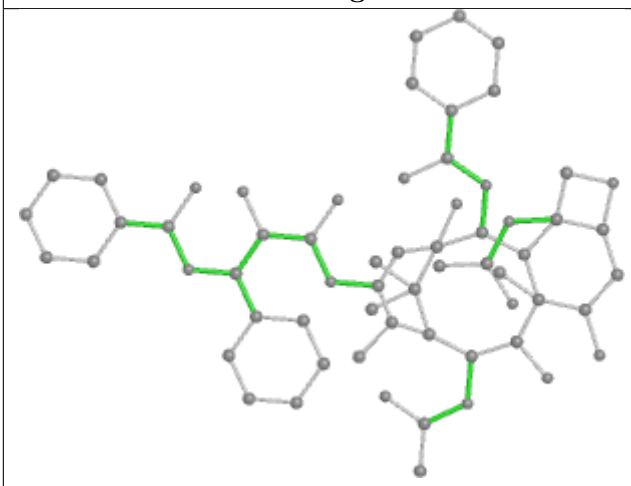

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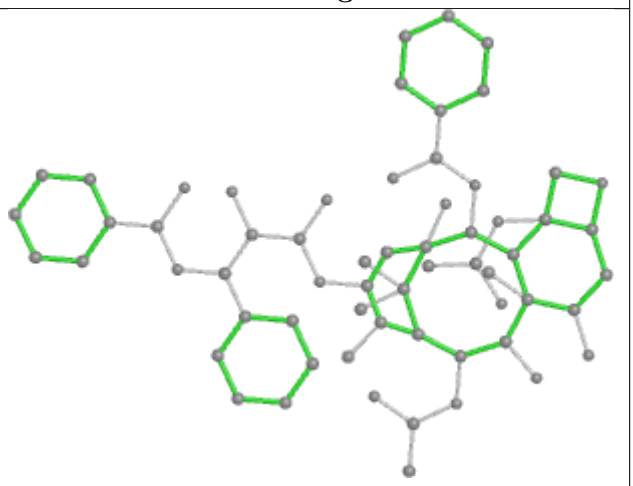
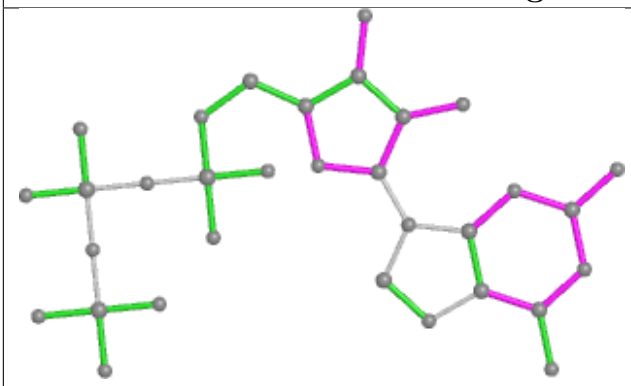


Rings

Ligand GTP k 501



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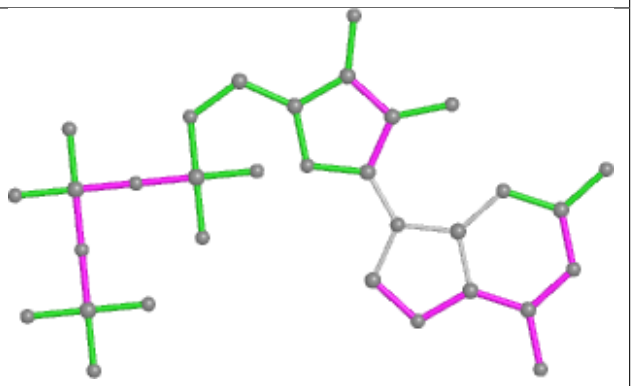

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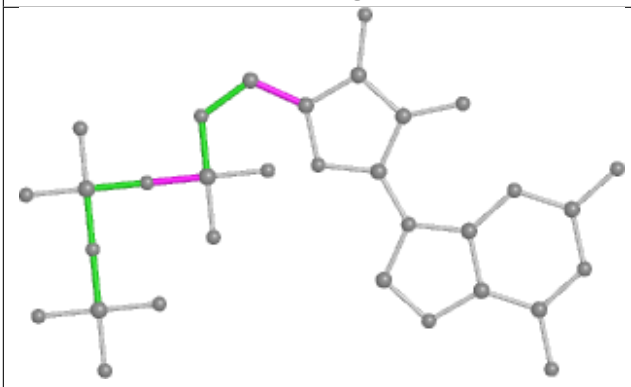

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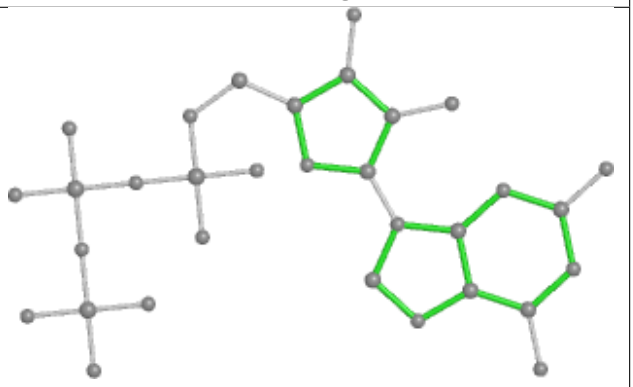
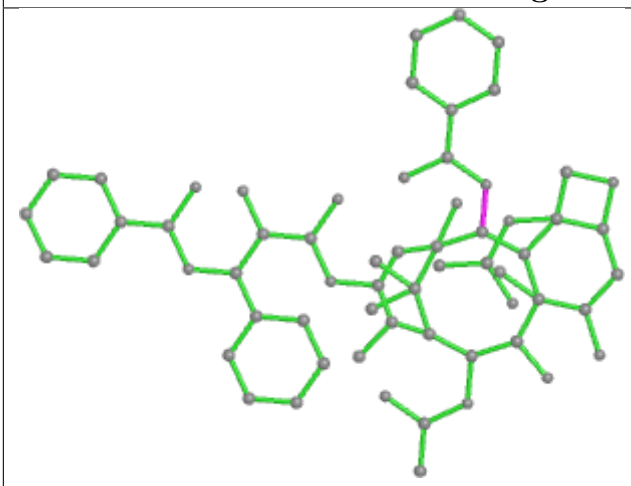


Rings

Ligand TA1 b 502



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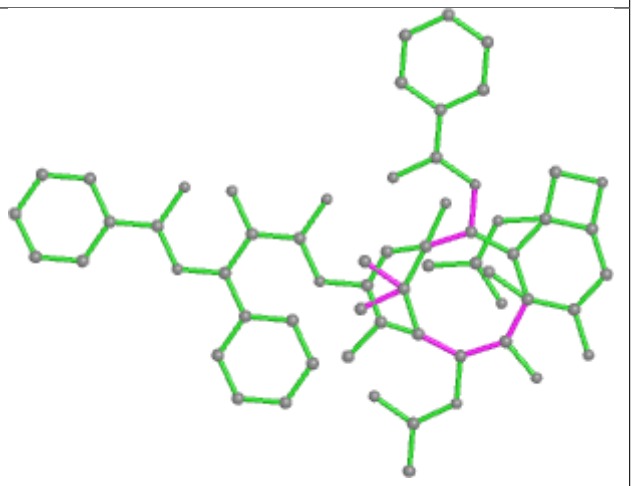

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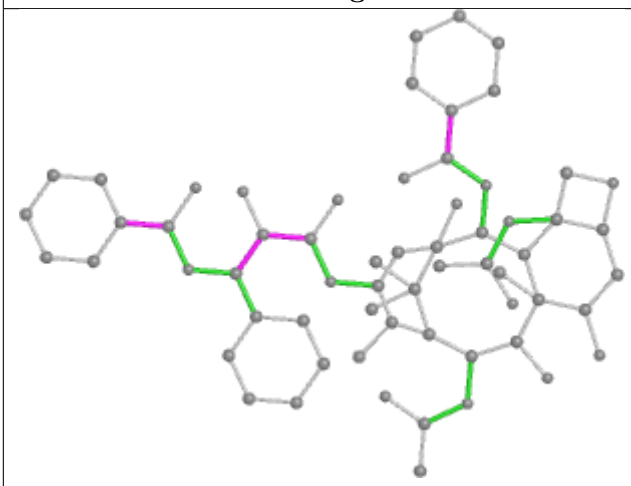

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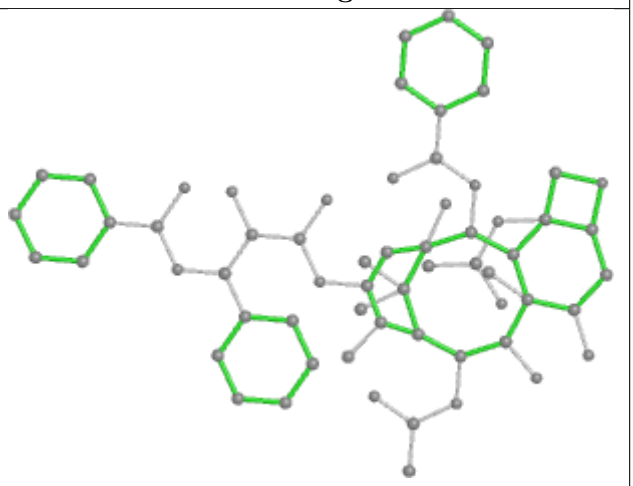
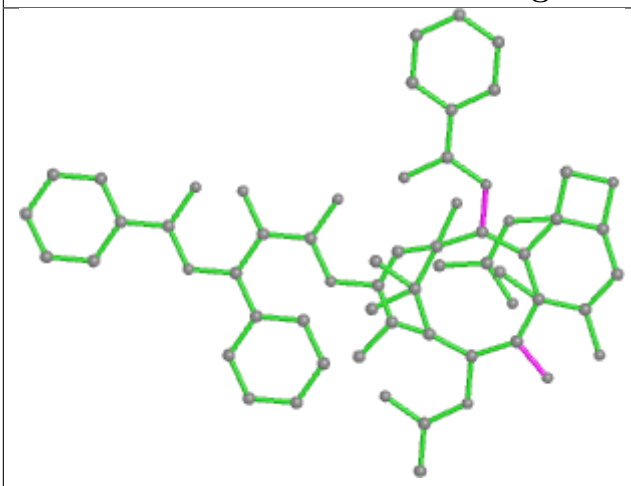


Rings

Ligand TA1 q 502



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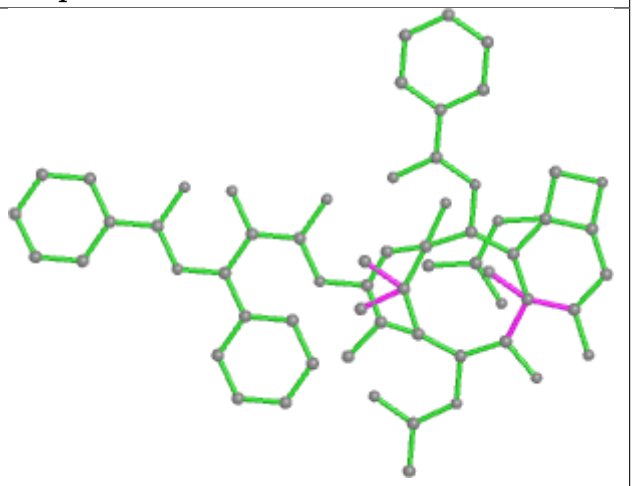

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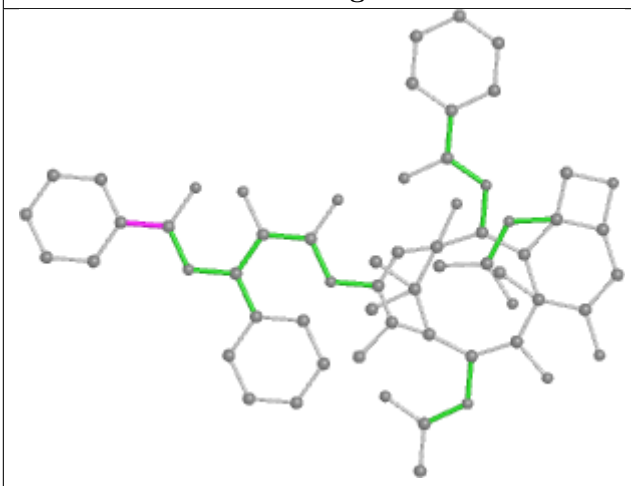

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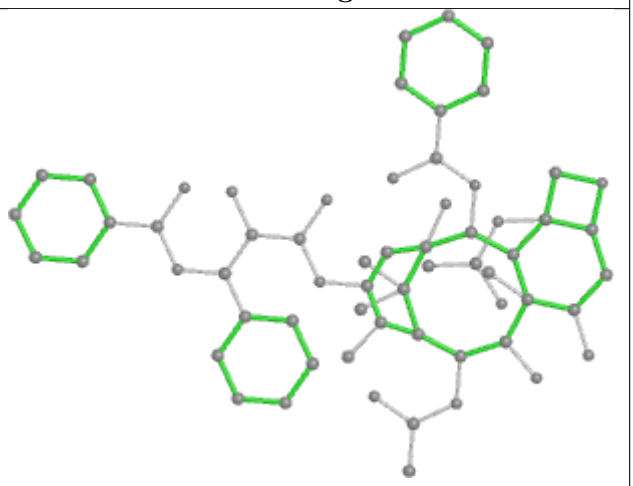
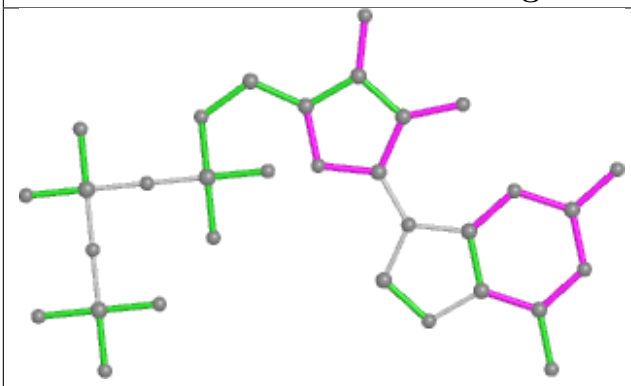


Rings

Ligand GTP Y 501



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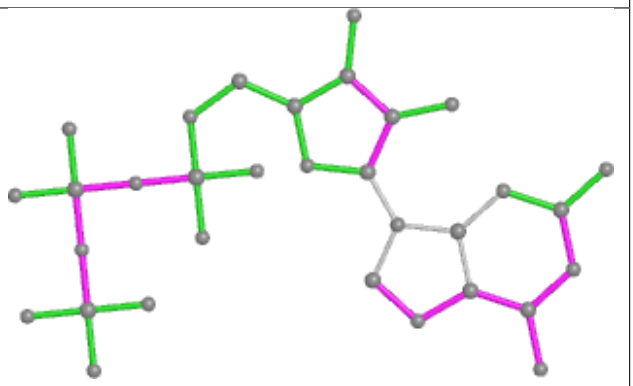

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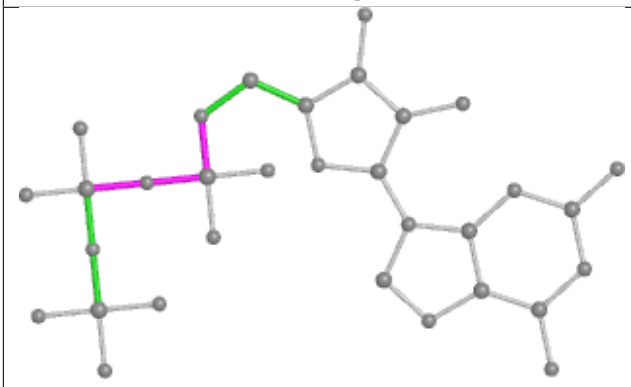

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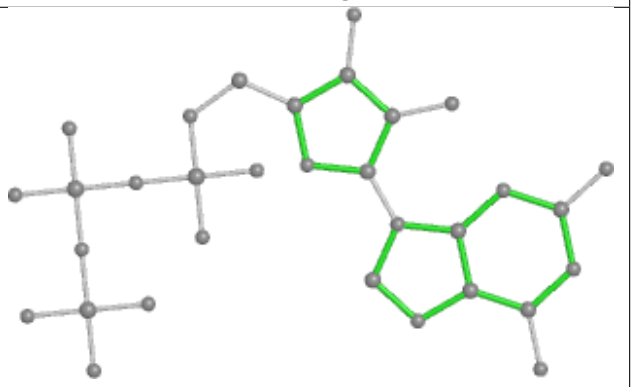
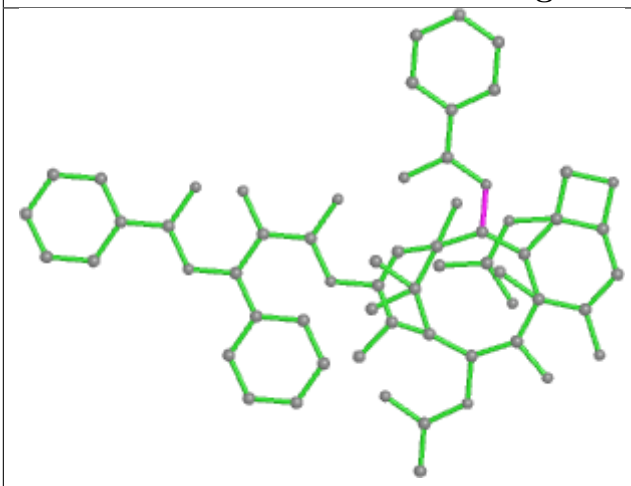


Rings

Ligand TA1 j 502



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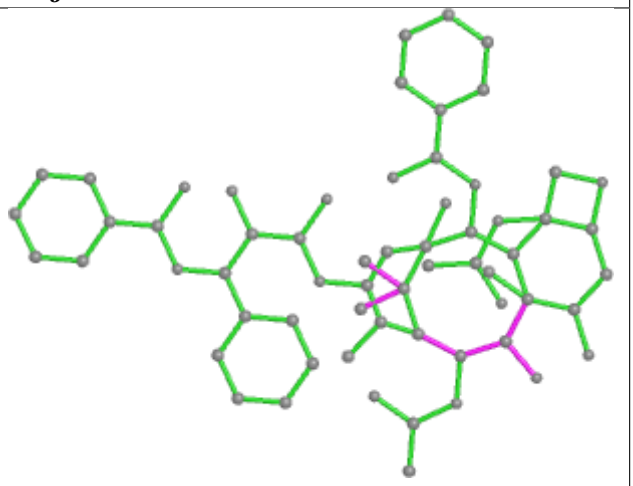

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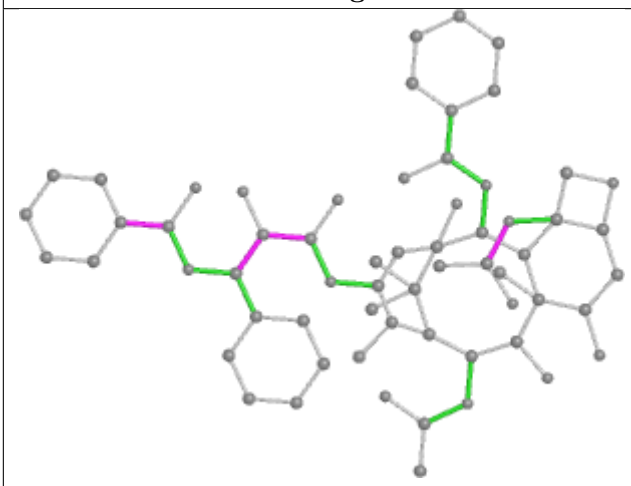

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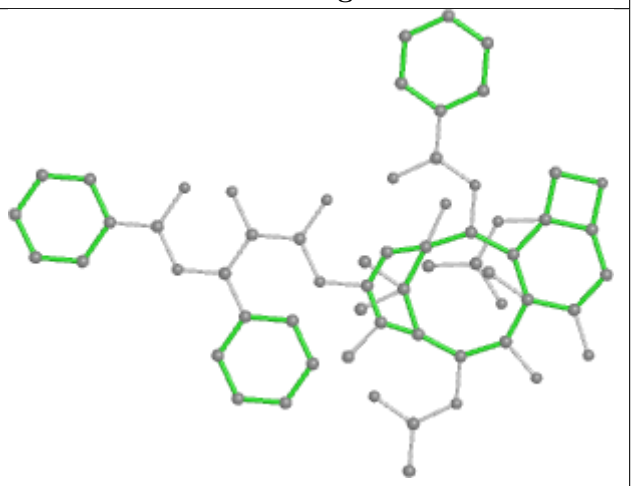
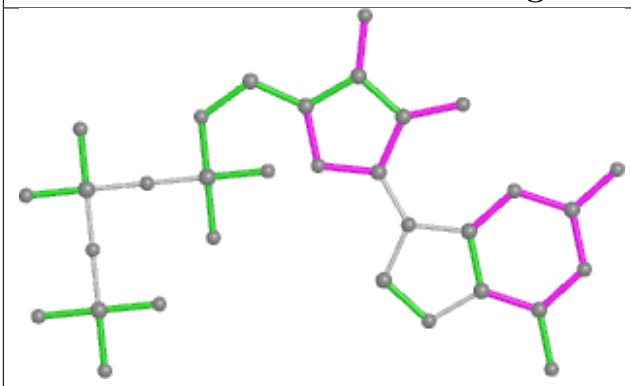


Rings

Ligand GTP 0 501



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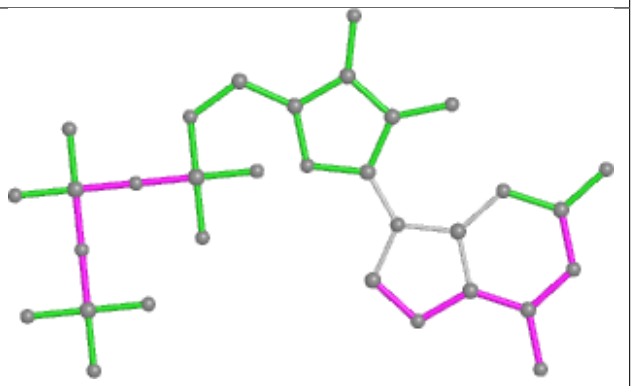

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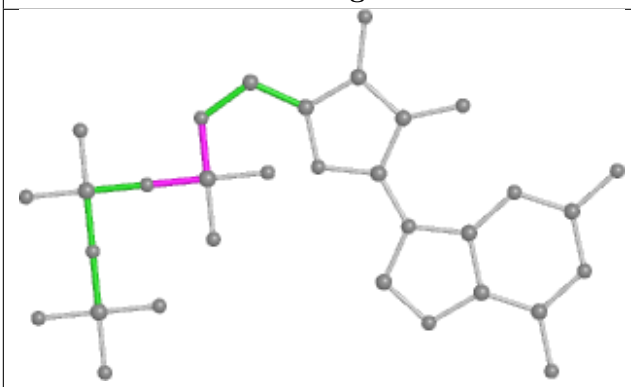

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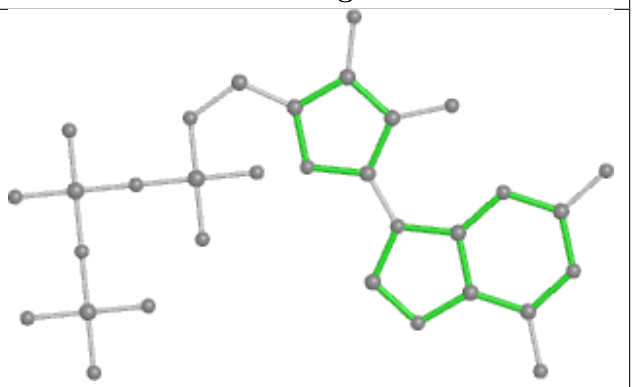
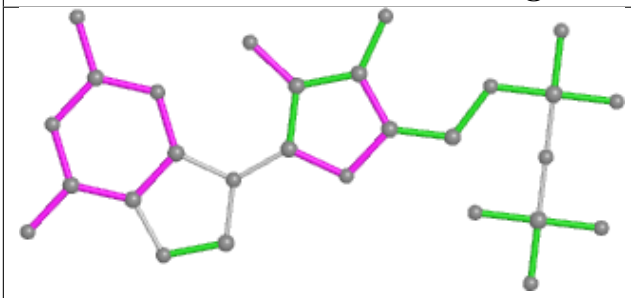


Rings

Ligand GDP J 501



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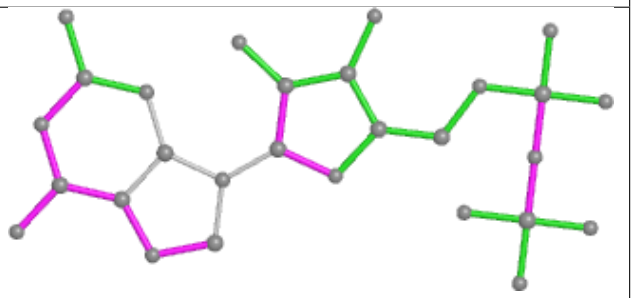

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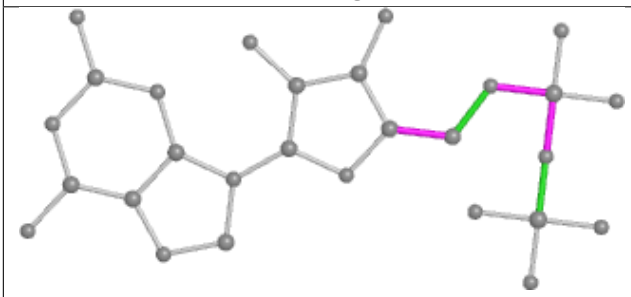

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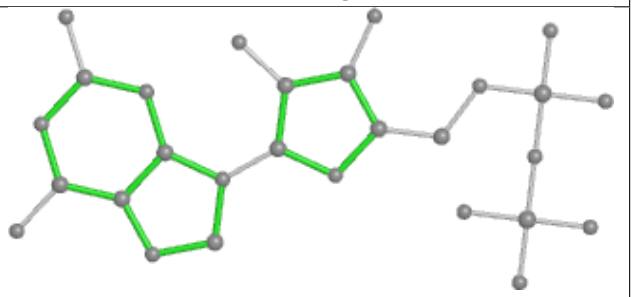
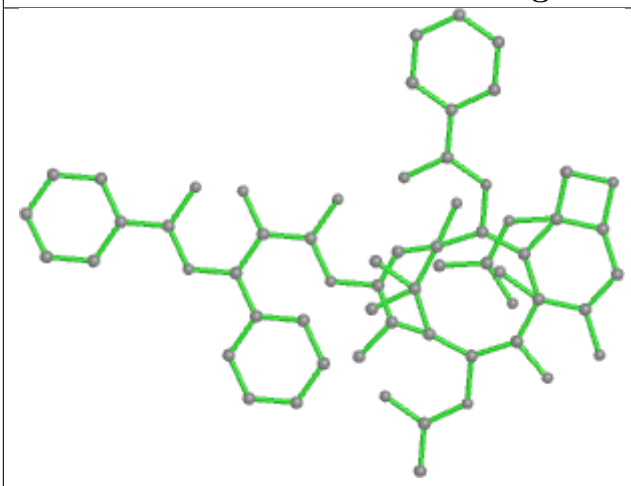


Rings

Ligand TA1 v 502



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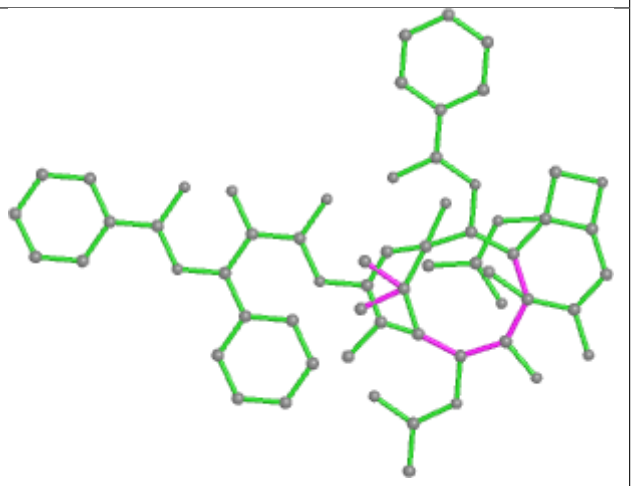

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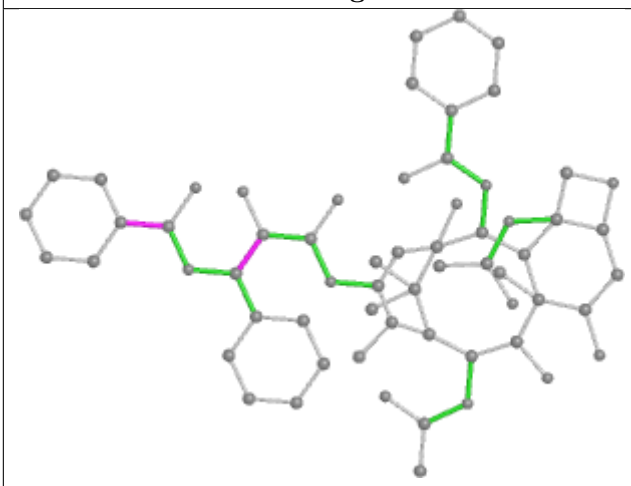

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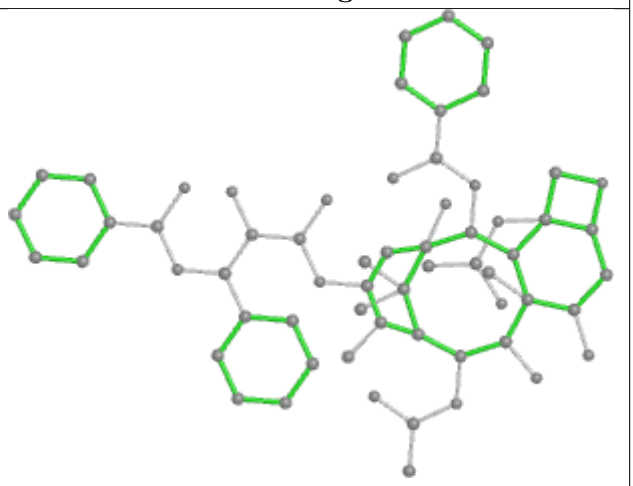
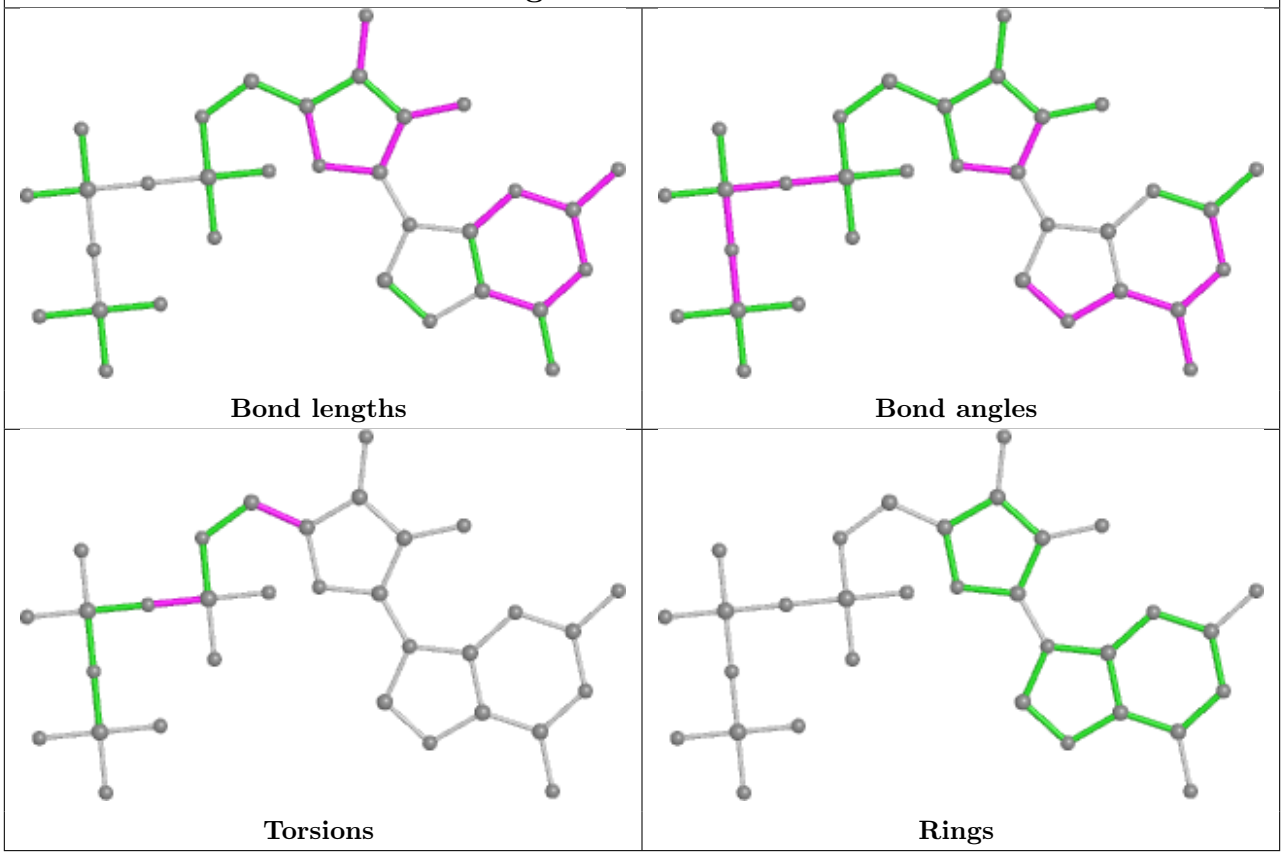


Rings

Ligand GTP Z 501



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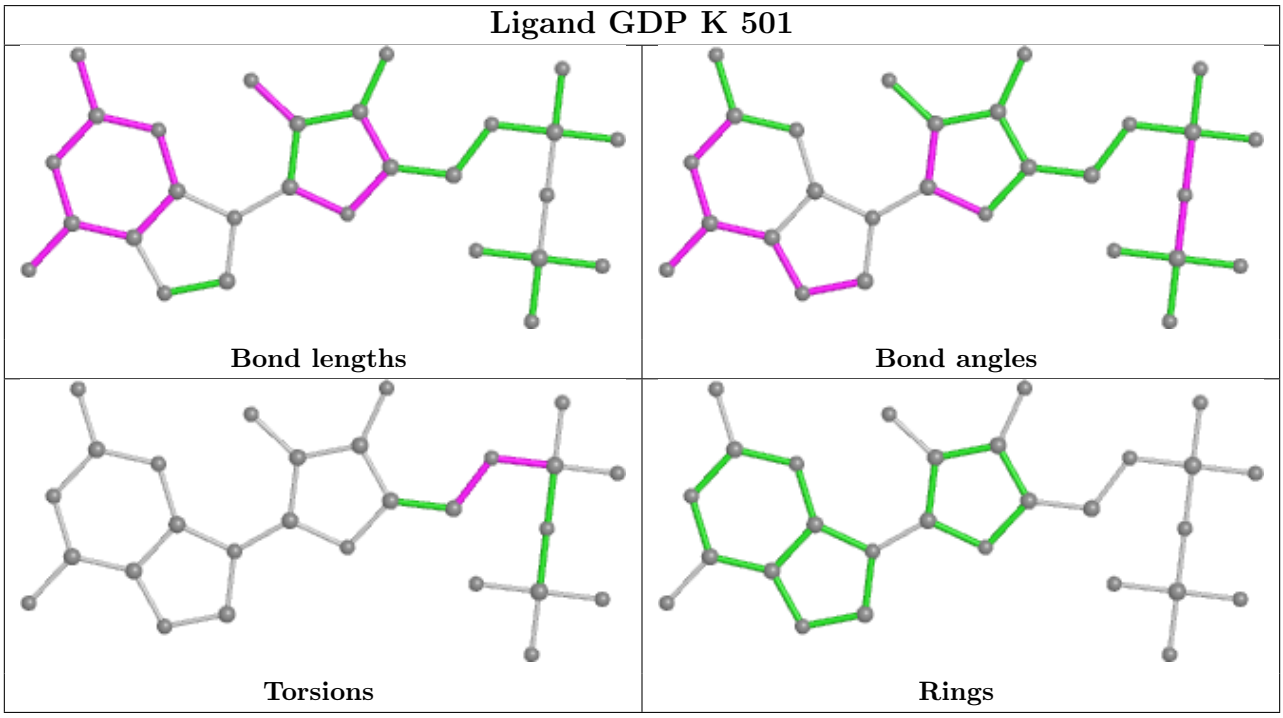

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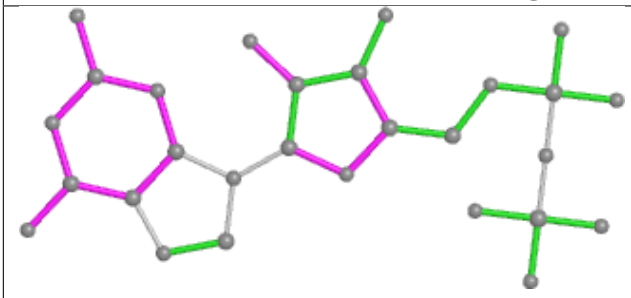

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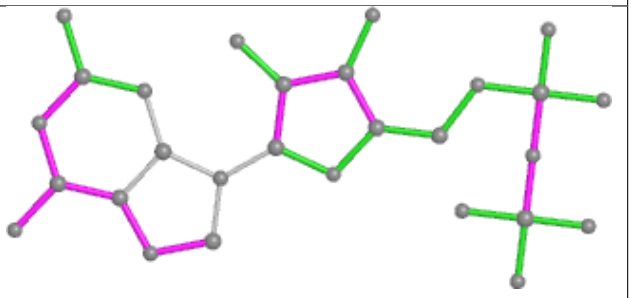

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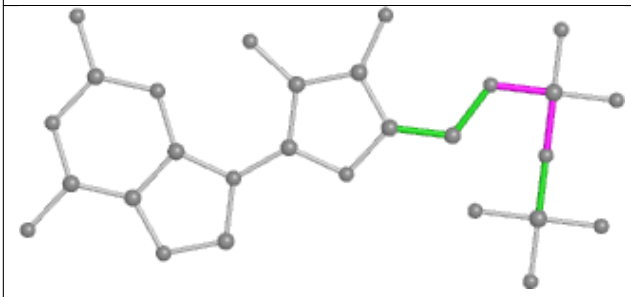

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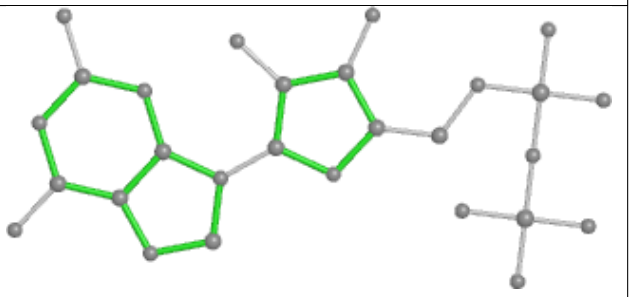
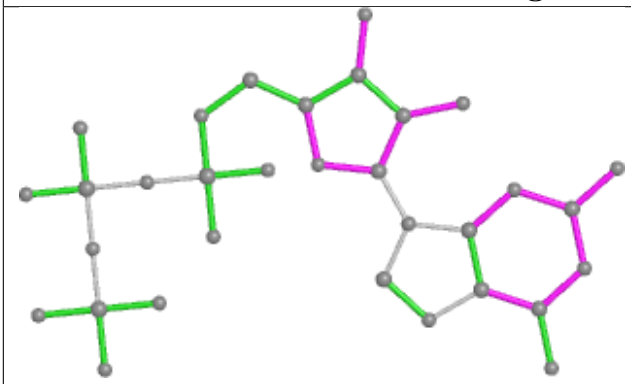
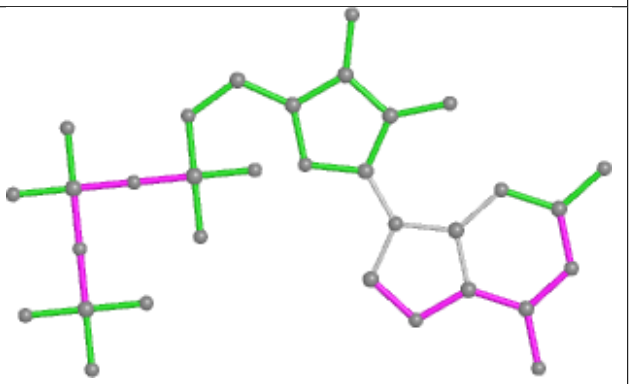


Rings

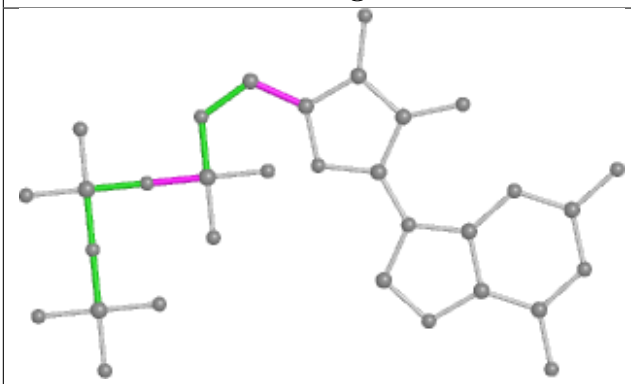
Ligand GTP 5 501



Bond lengths



Bond angles



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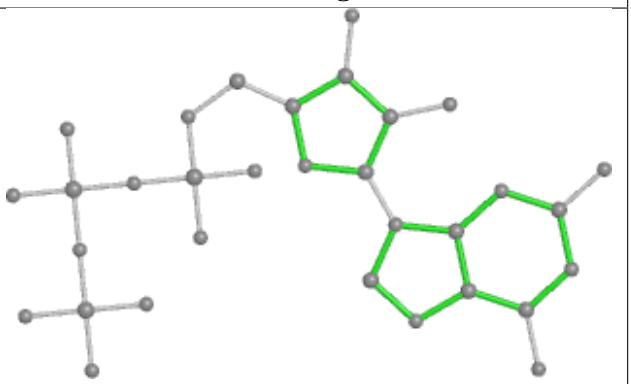
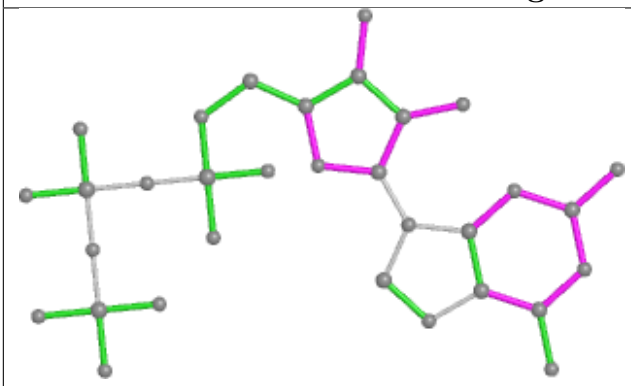
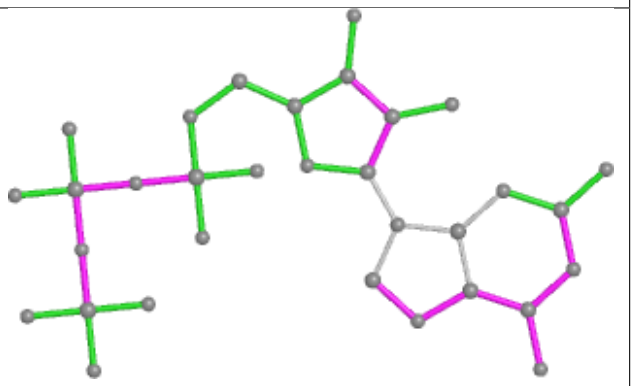


Rings

Ligand GTP e 501



Bond lengths



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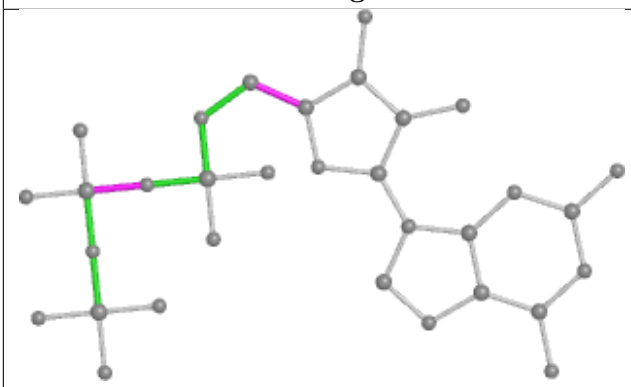

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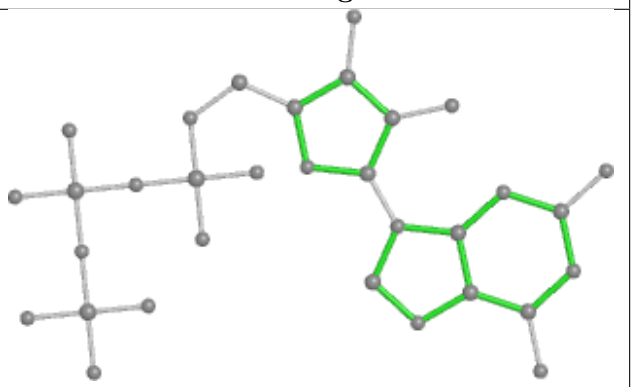

Rings

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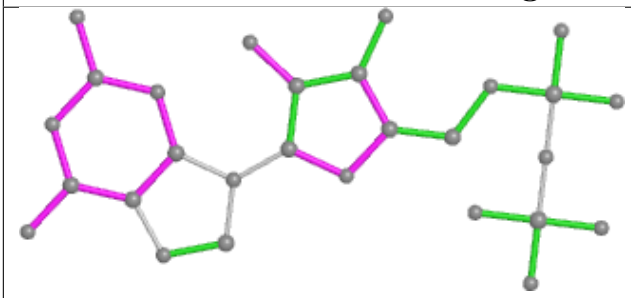

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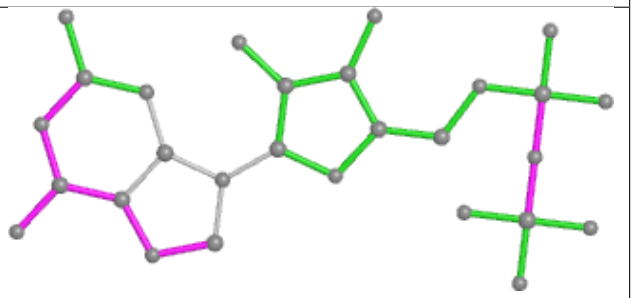

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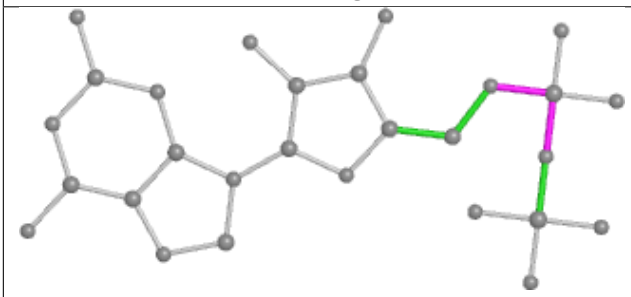

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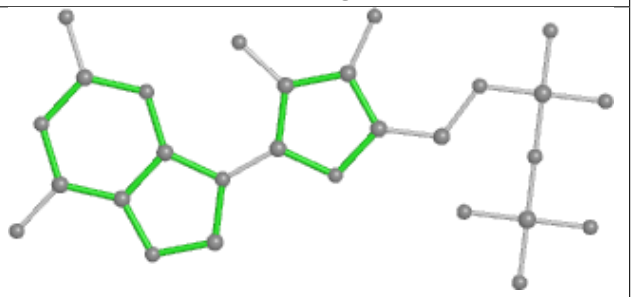

Rings

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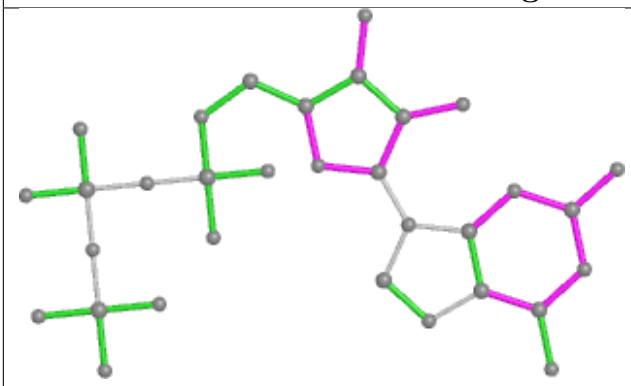

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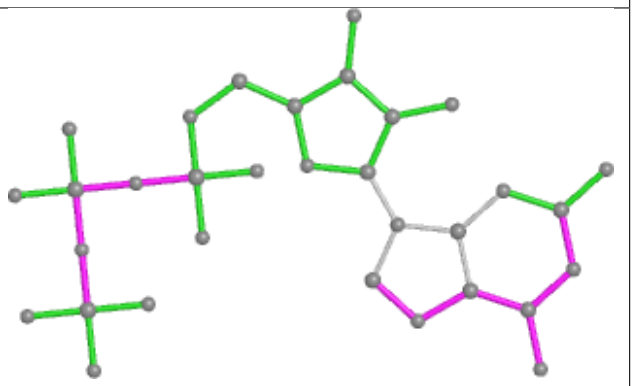

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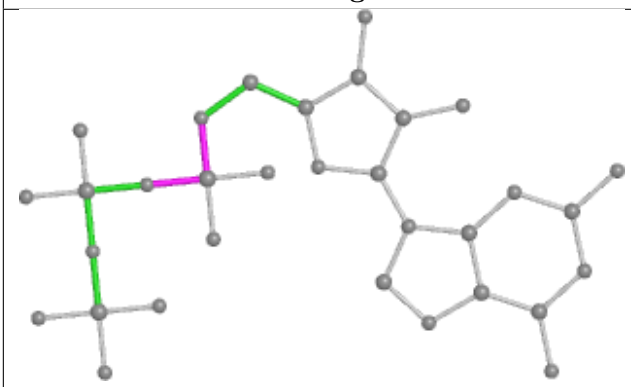

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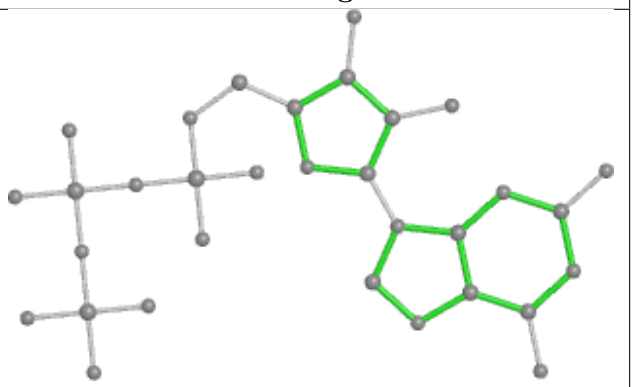

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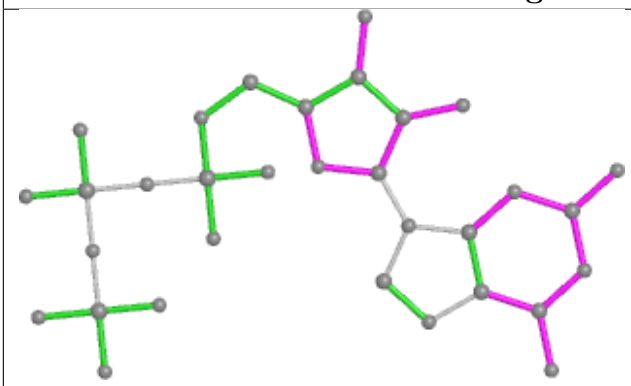

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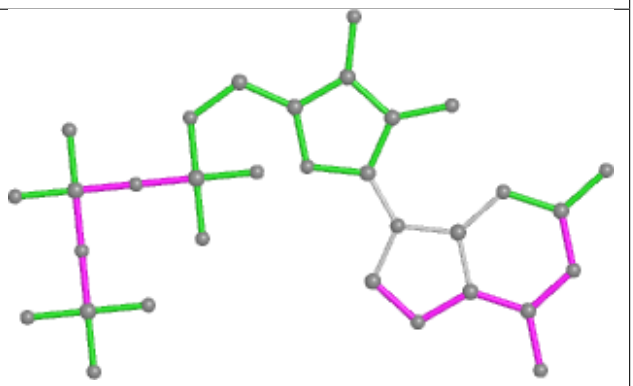

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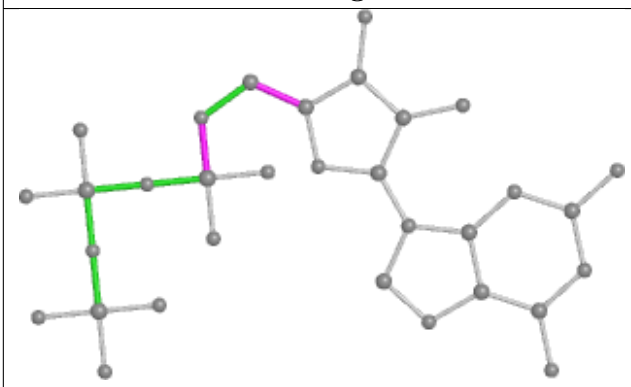

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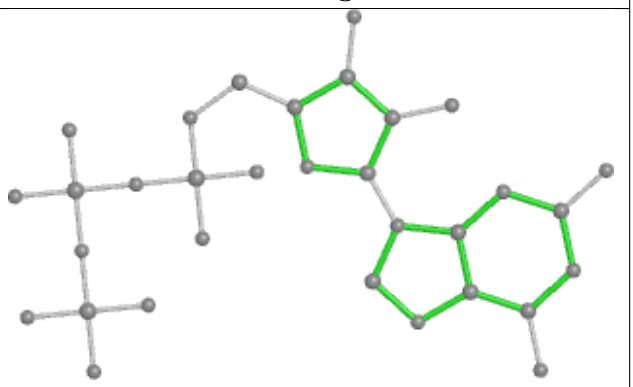

Rings

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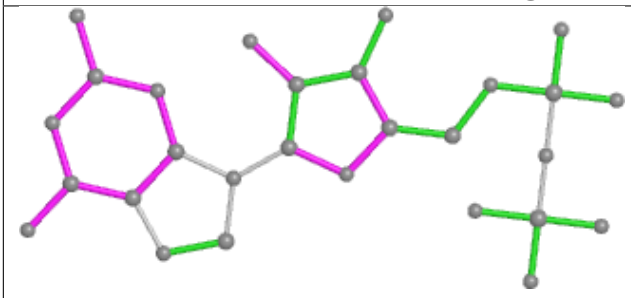

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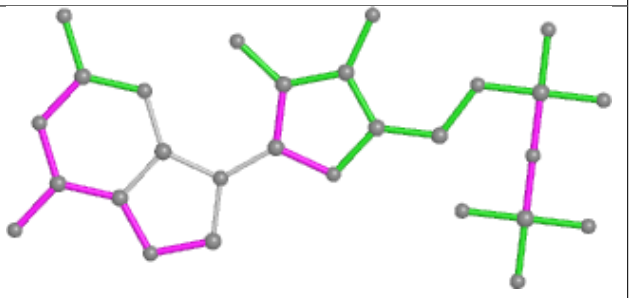

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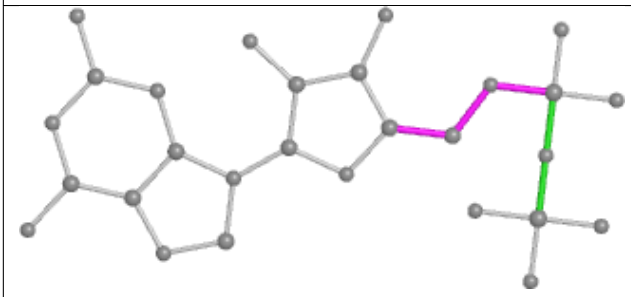

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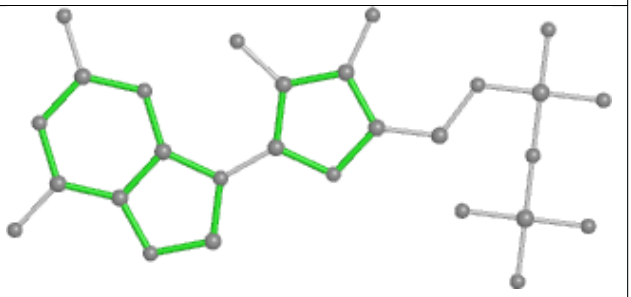

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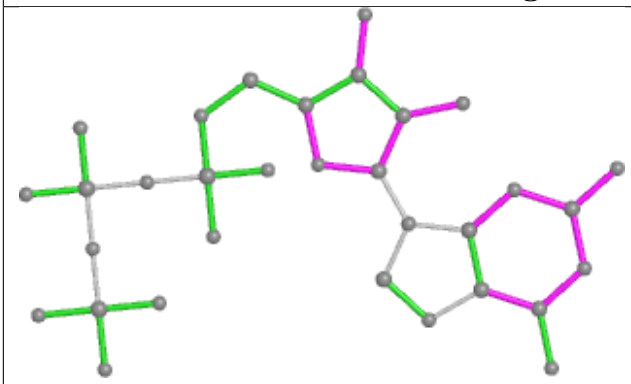

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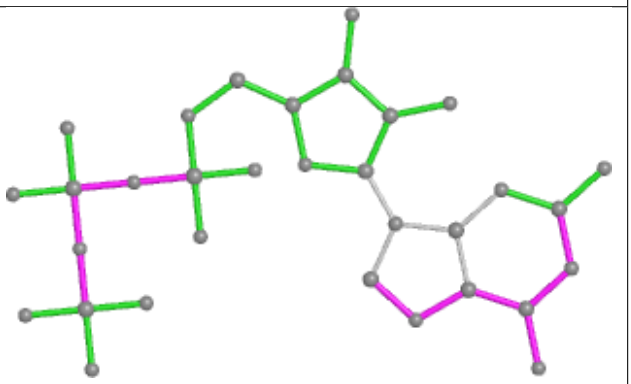

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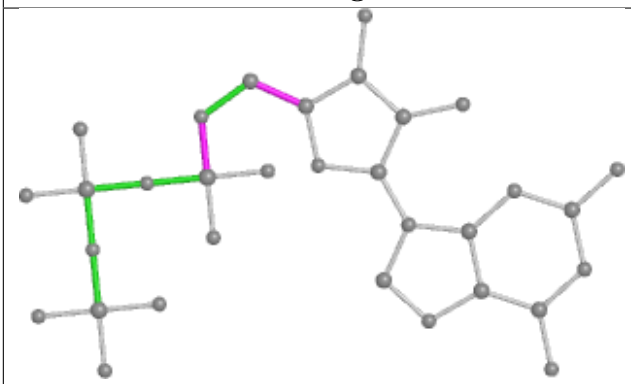

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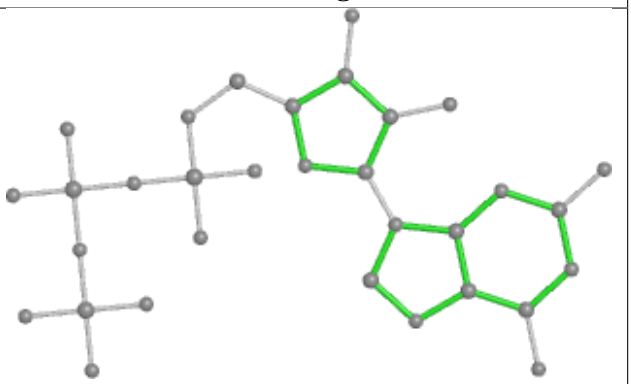
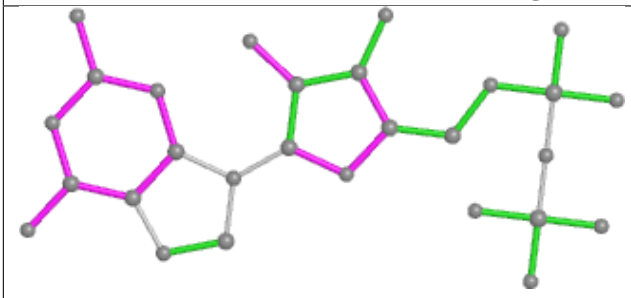


Rings

Ligand GDP r 501



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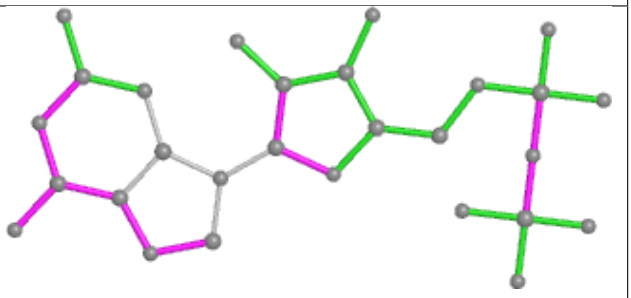

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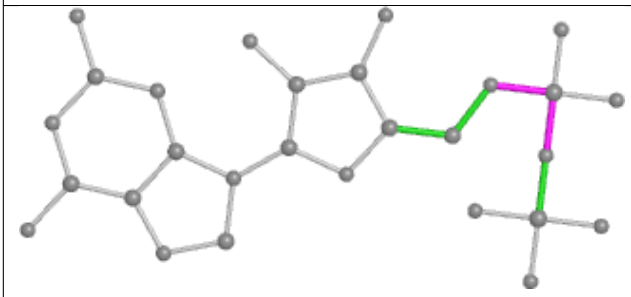

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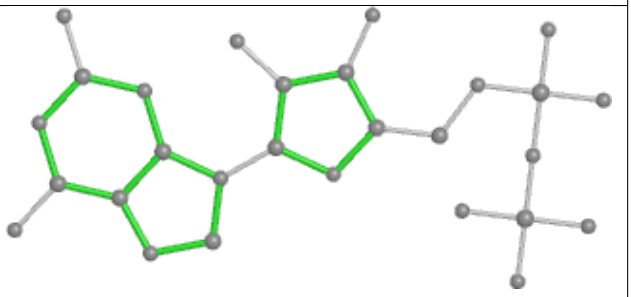

Rings

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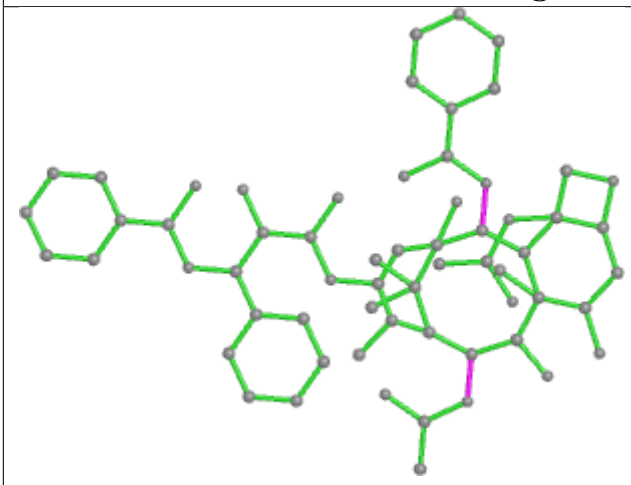

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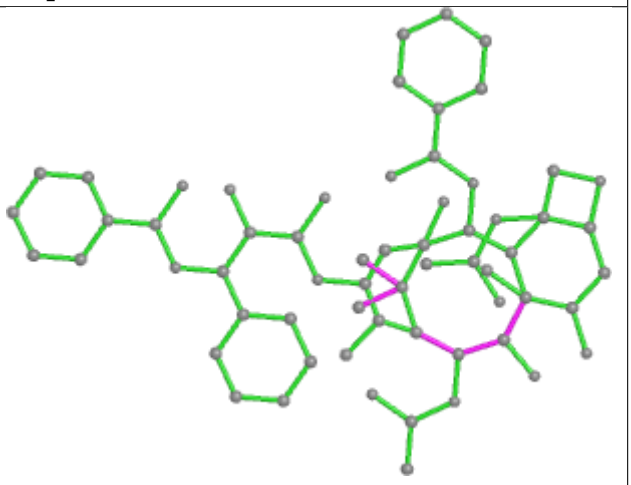

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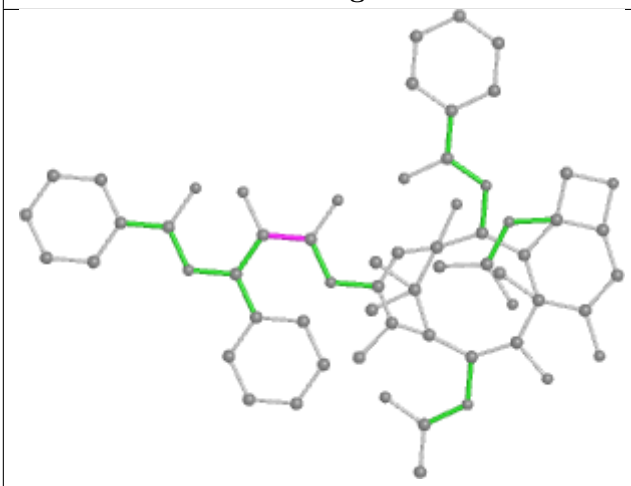

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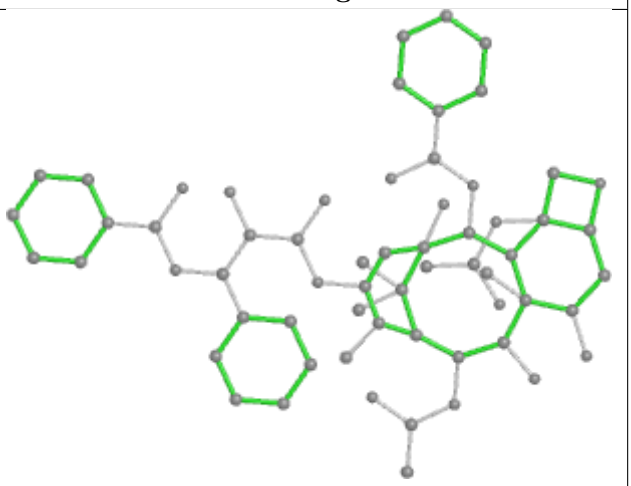

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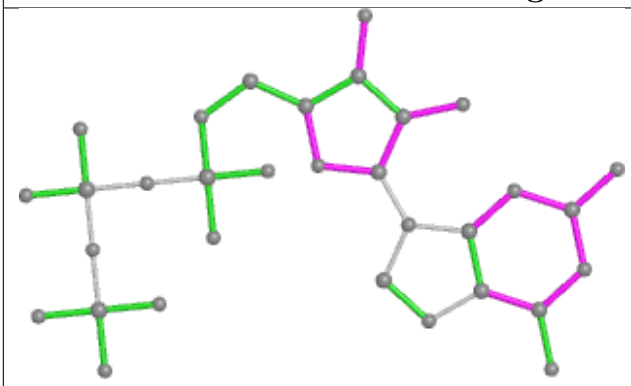

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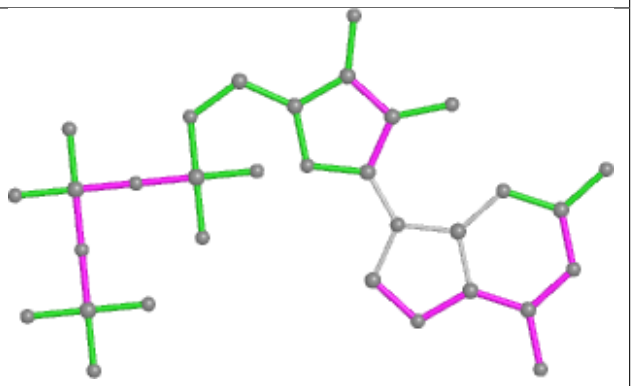

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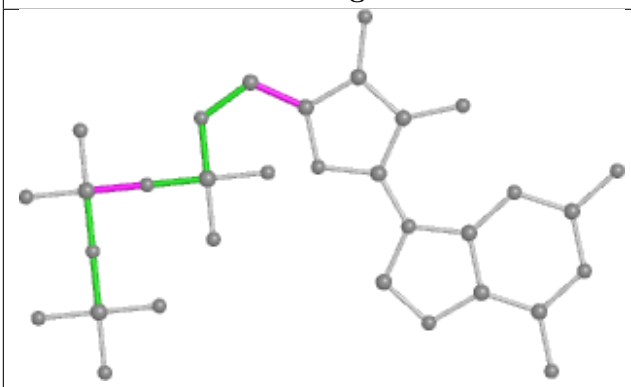

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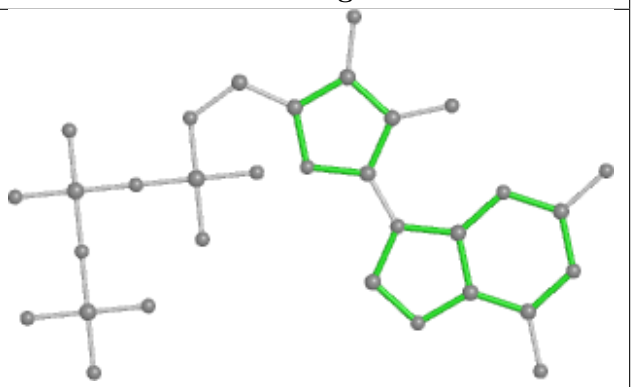

Rings

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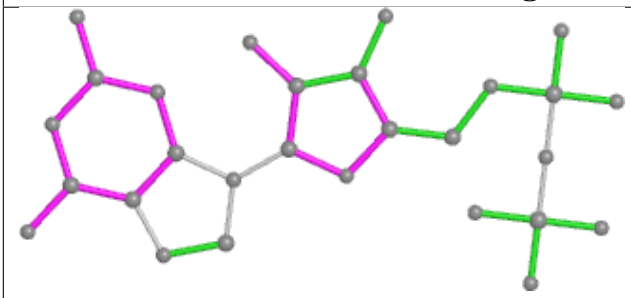

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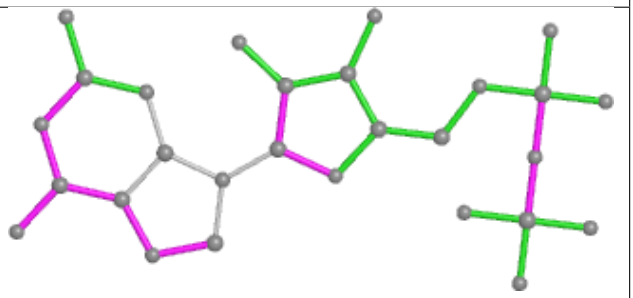

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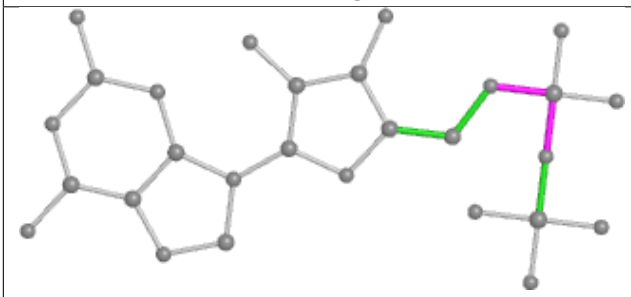

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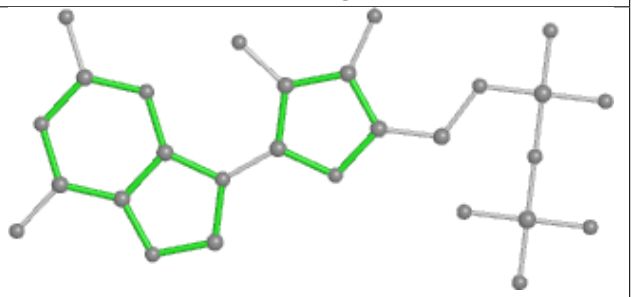

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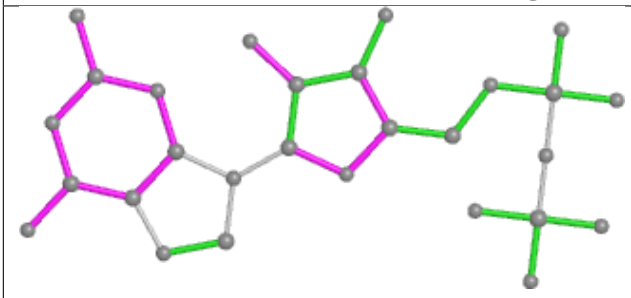

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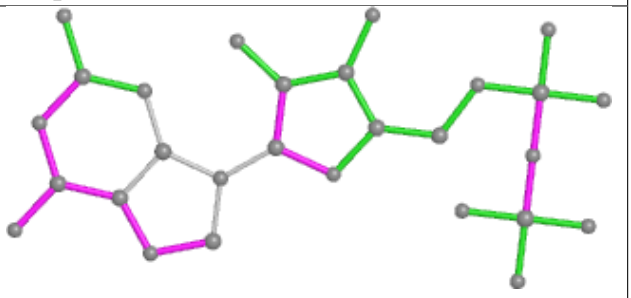

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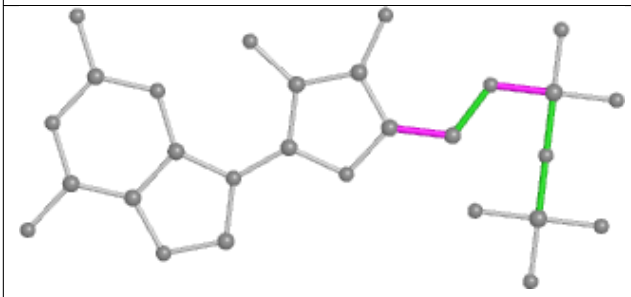

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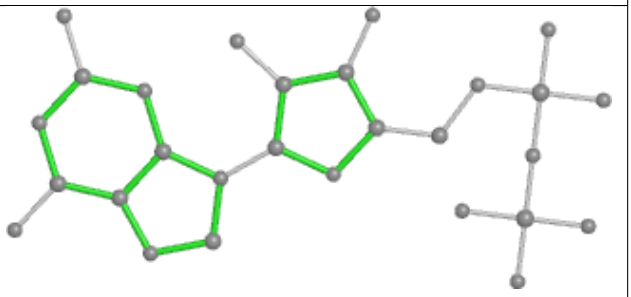

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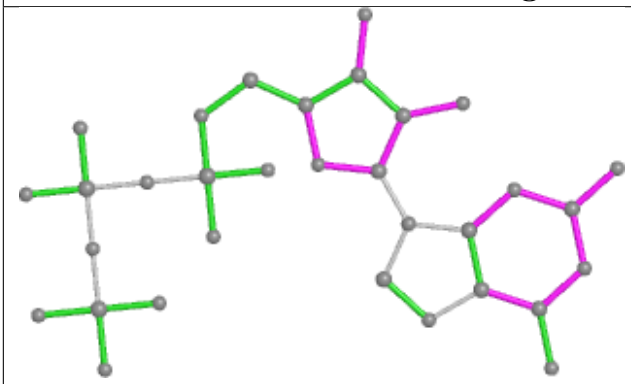

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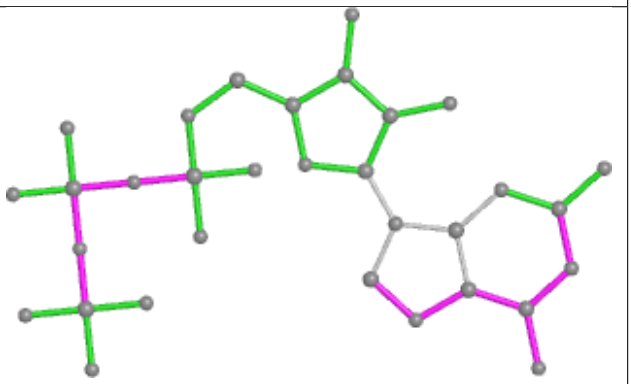

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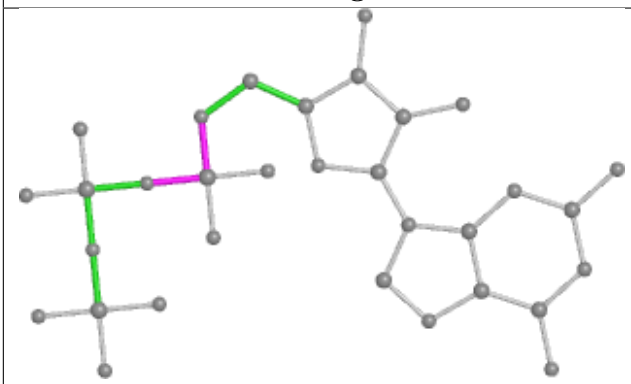

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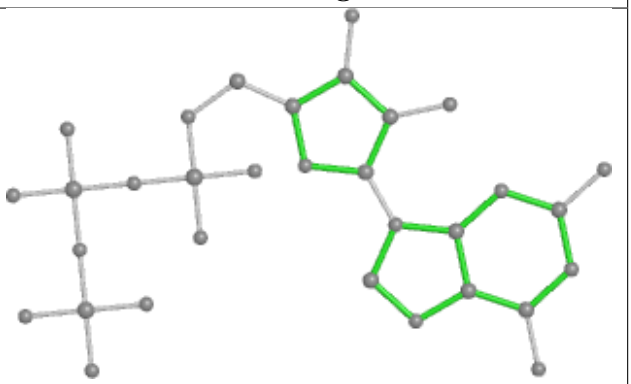

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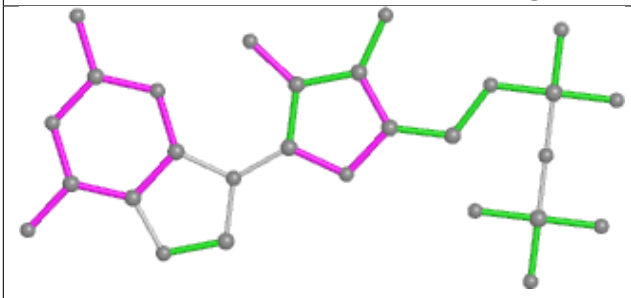
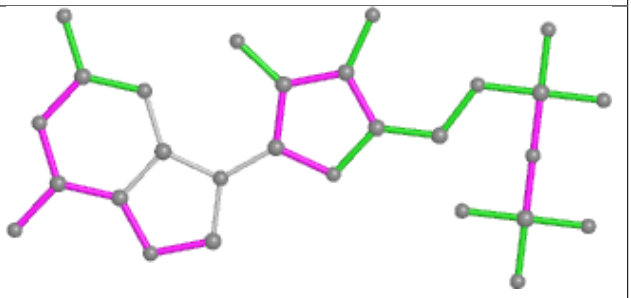
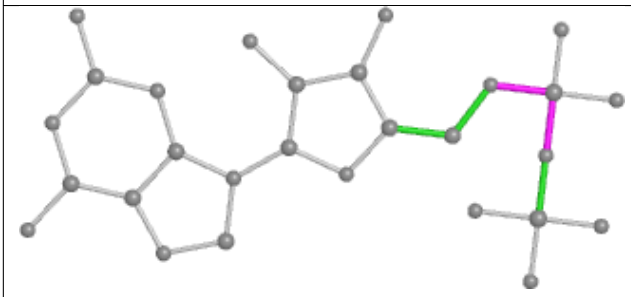
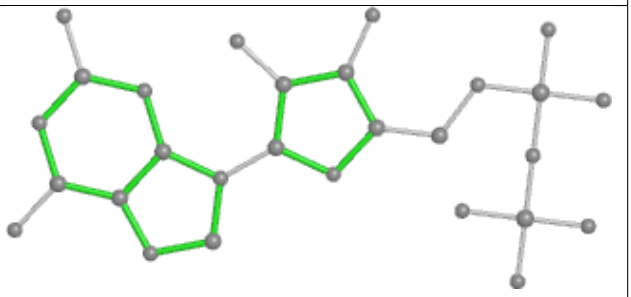
 Bond lengths	 Bond angles
 Torsions	 Rings

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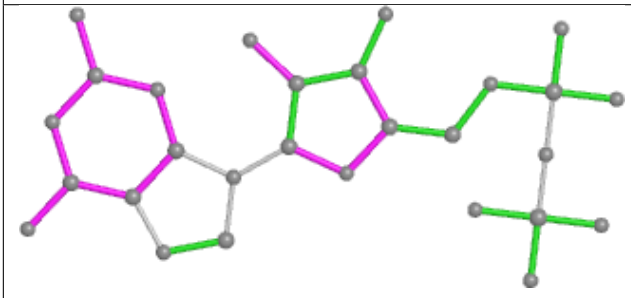
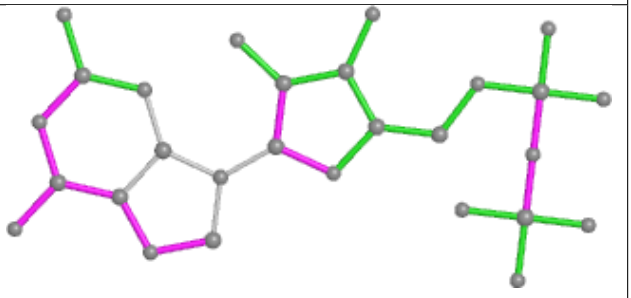
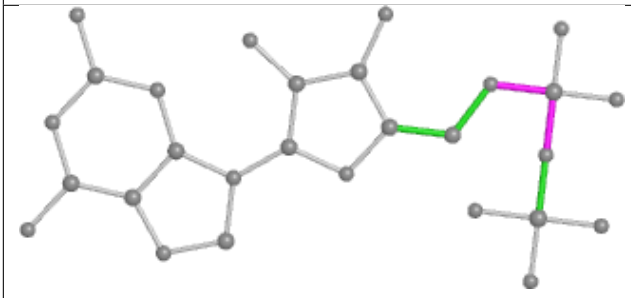
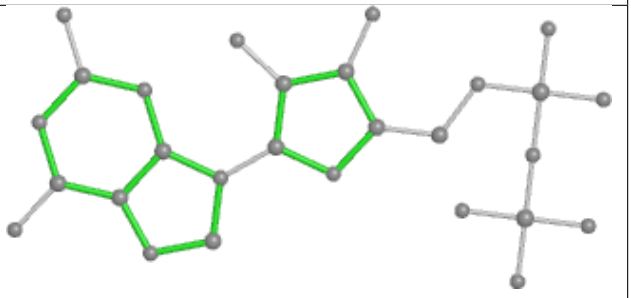
 Bond lengths	 Bond angles
 Torsions	 Rings

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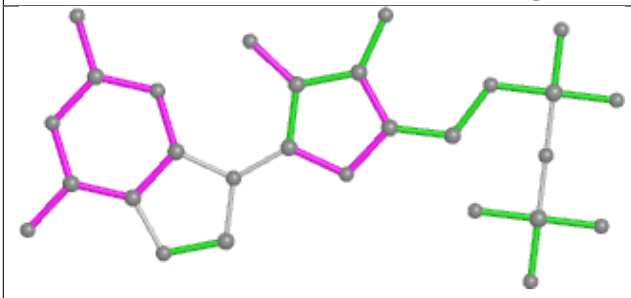
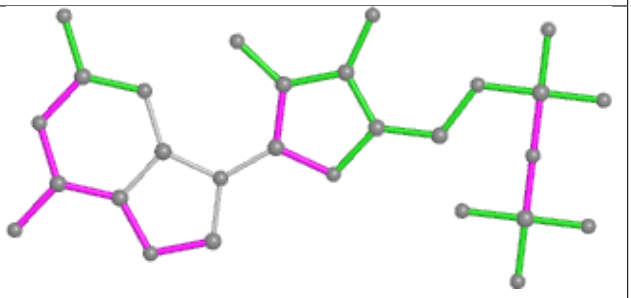
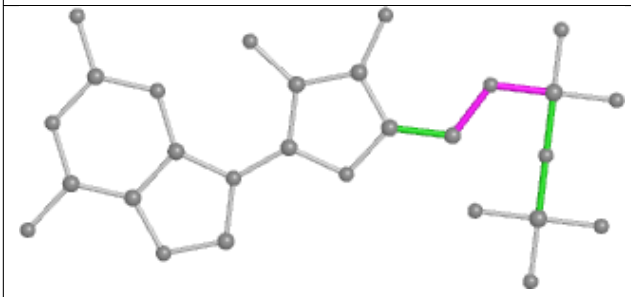
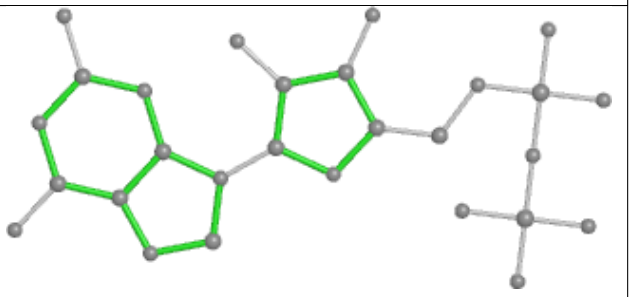
 Bond lengths	 Bond angles
 Torsions	 Rings

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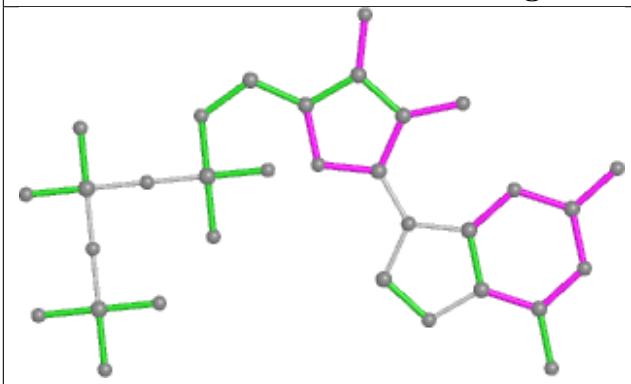
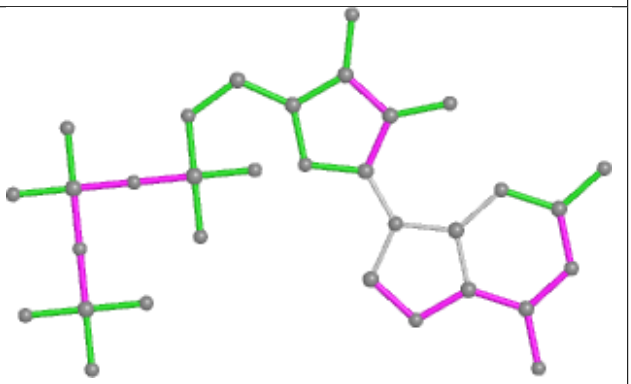
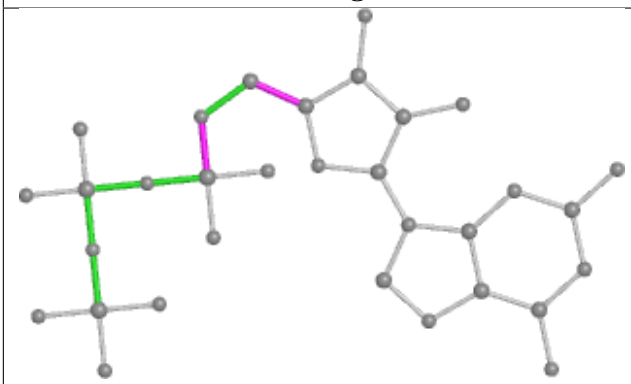
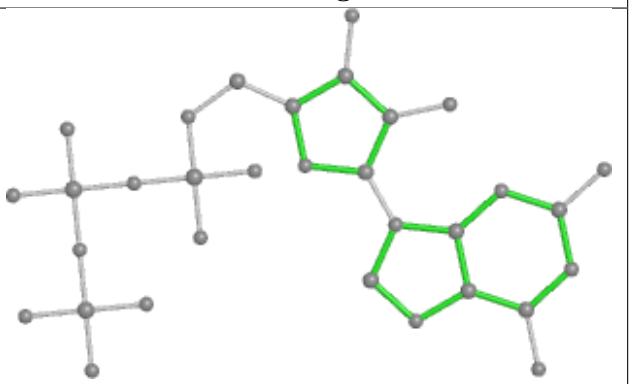
 Bond lengths	 Bond angles
 Torsions	 Rings

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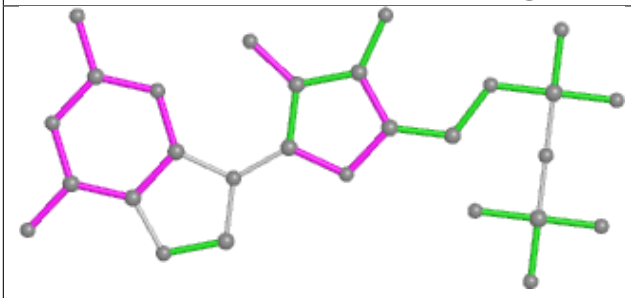
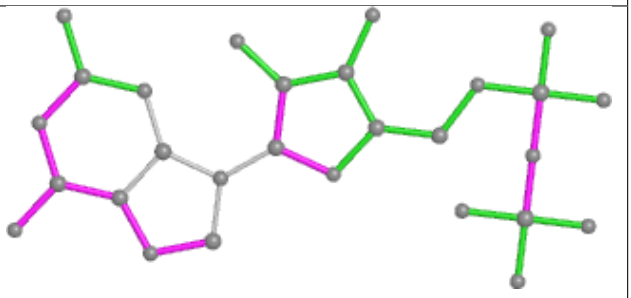
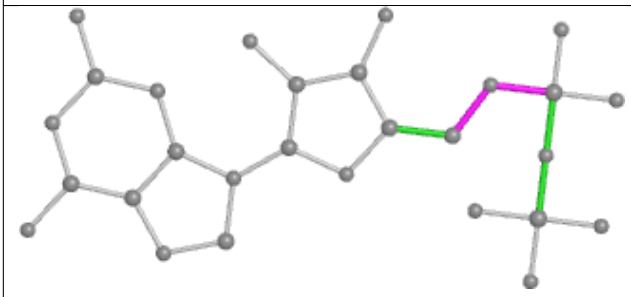
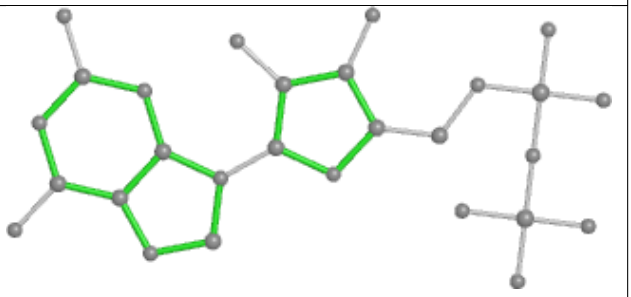
 Bond lengths	 Bond angles
 Torsions	 Rings

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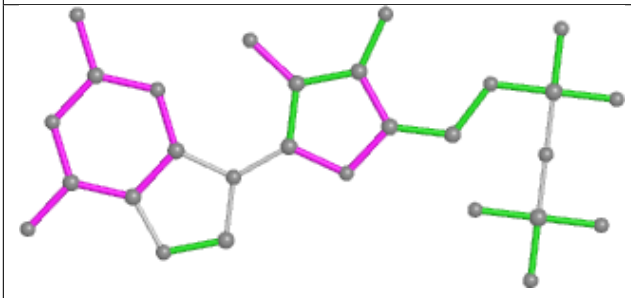
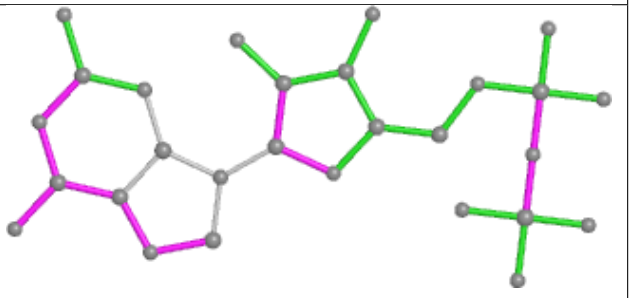
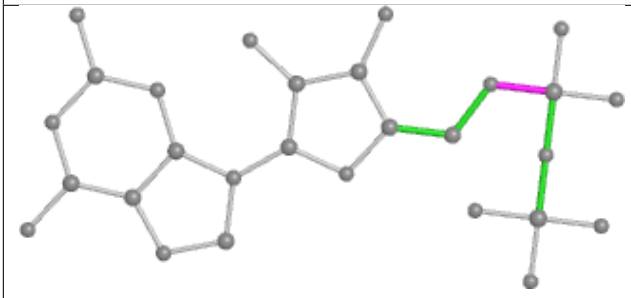
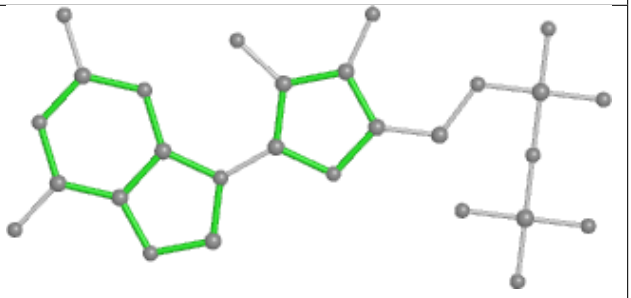
 Bond lengths	 Bond angles
 Torsions	 Rings

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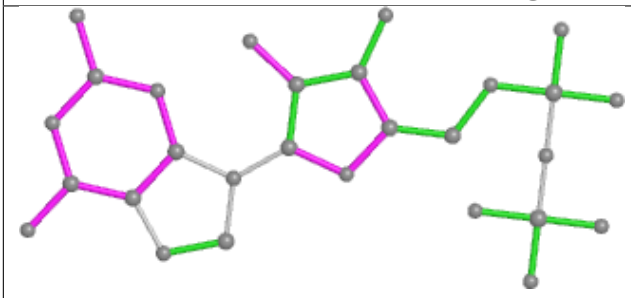

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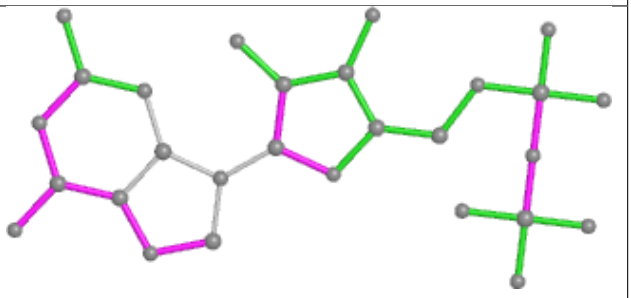

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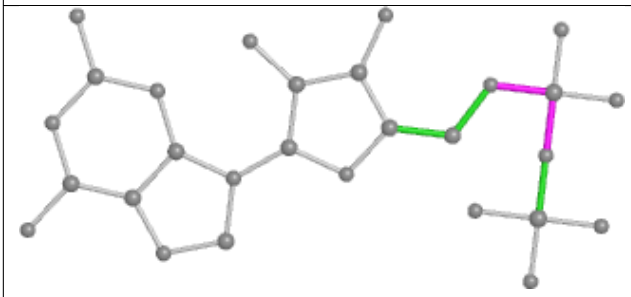

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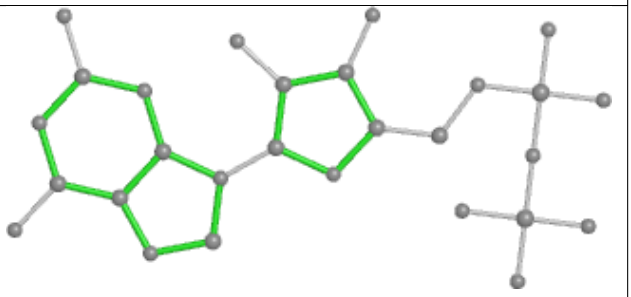

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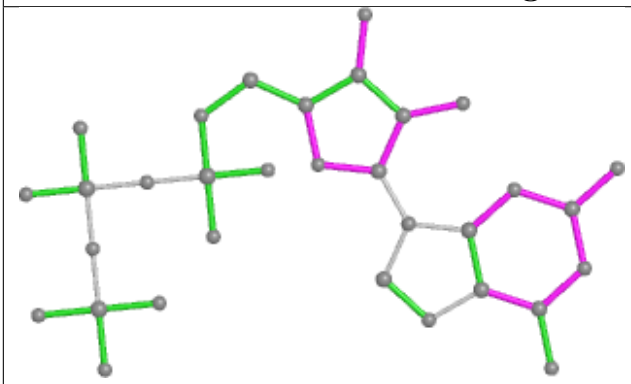

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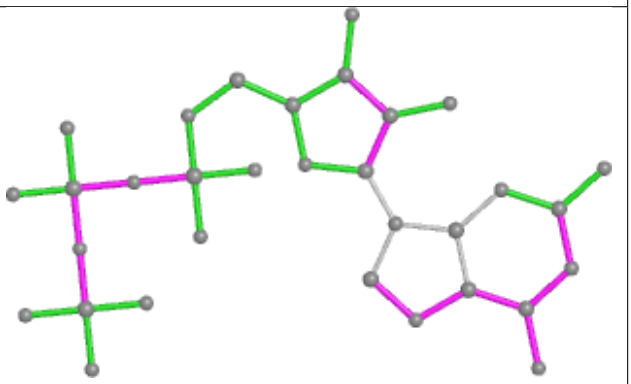

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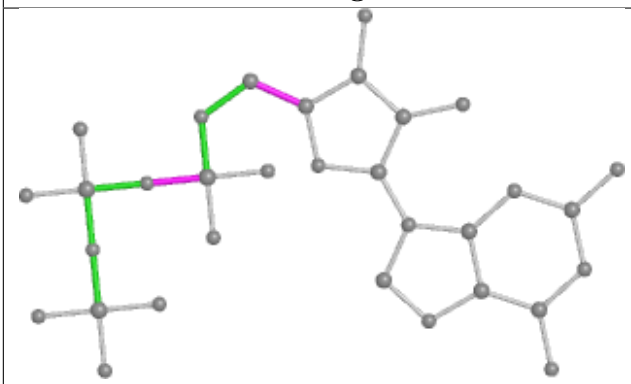

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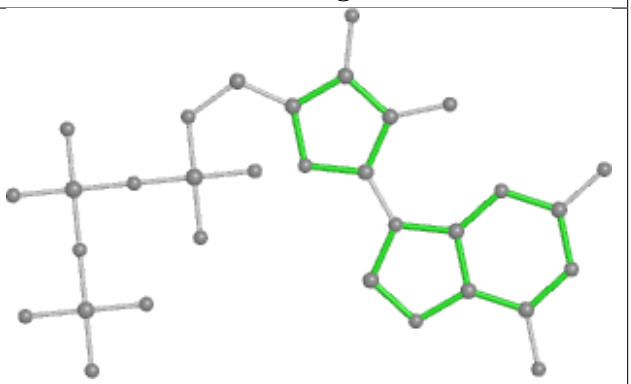

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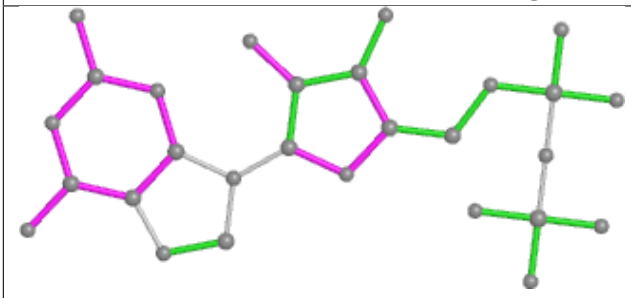

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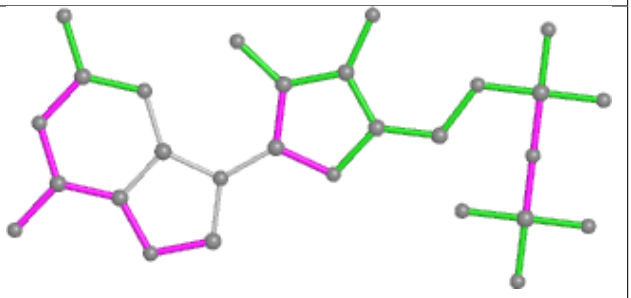

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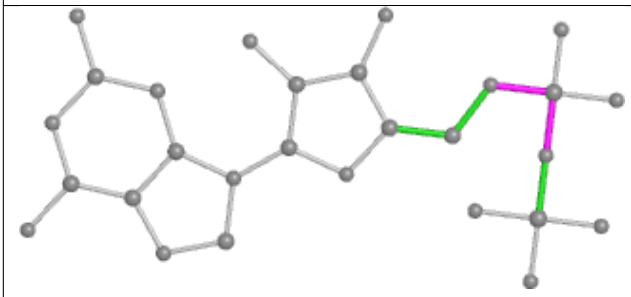

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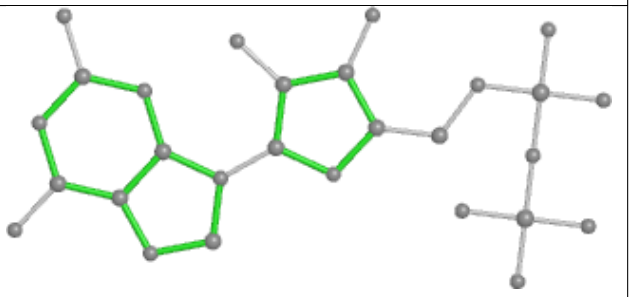

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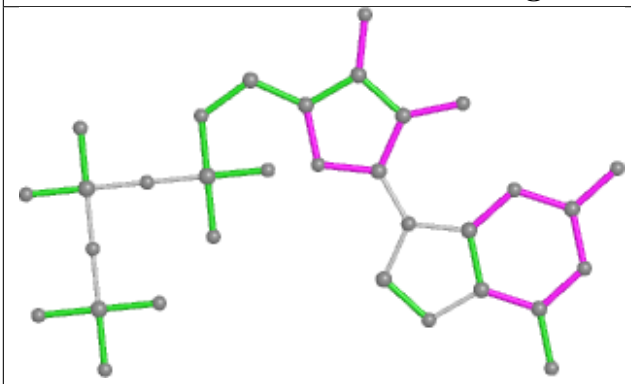

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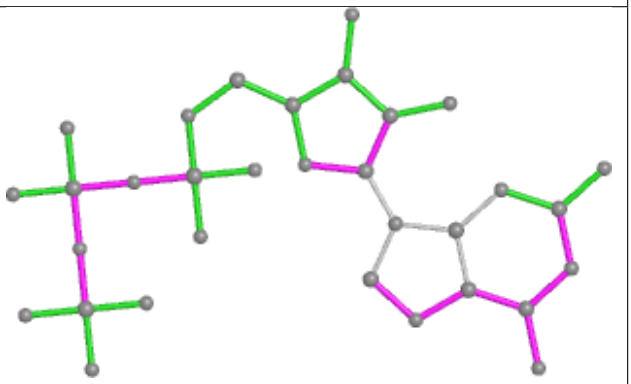

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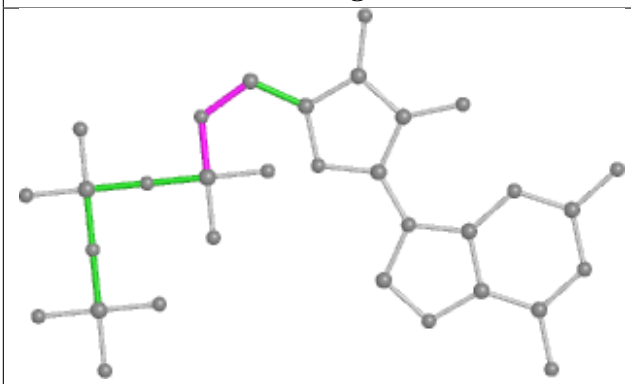

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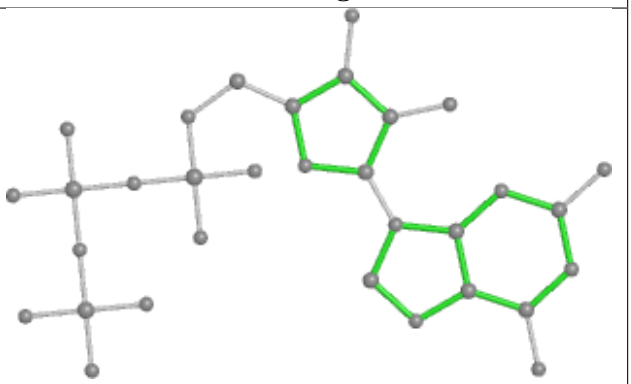

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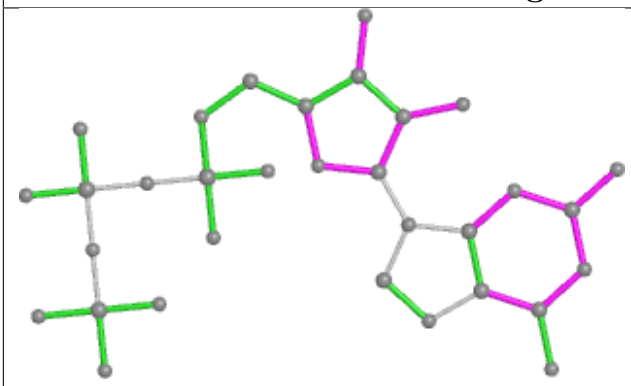

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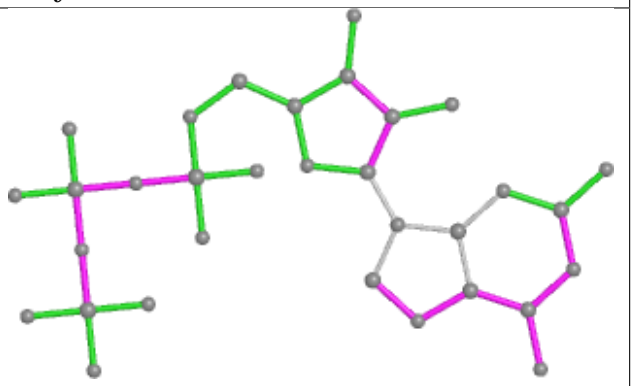

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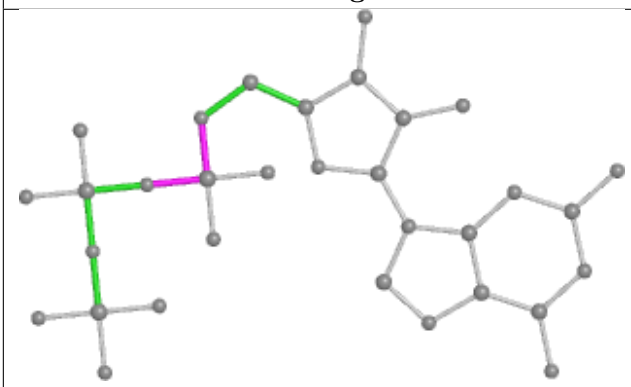

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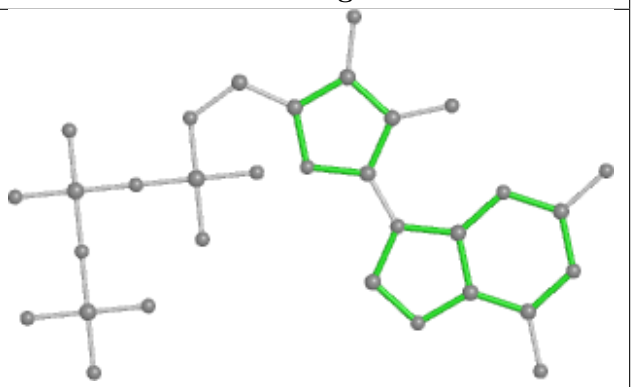

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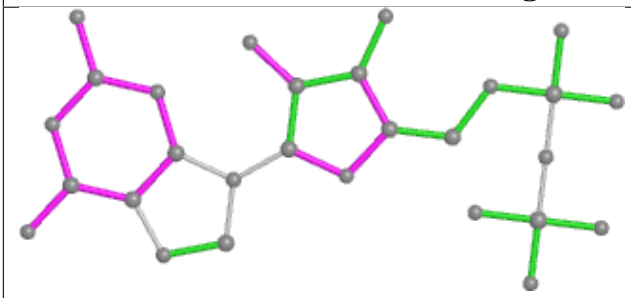

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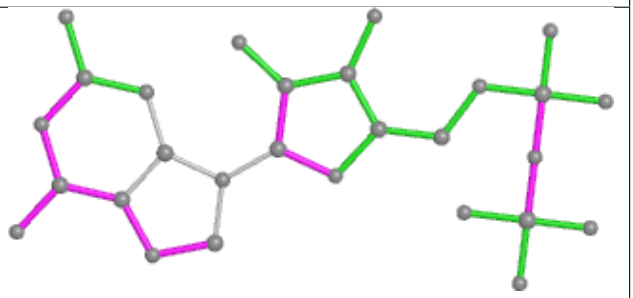

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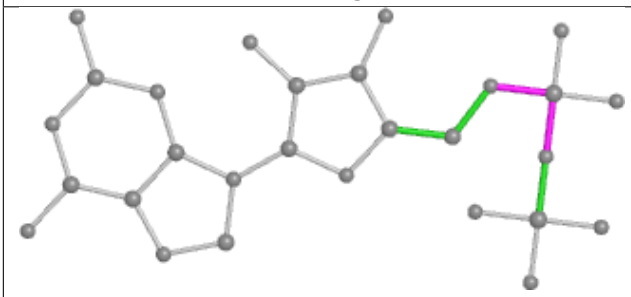

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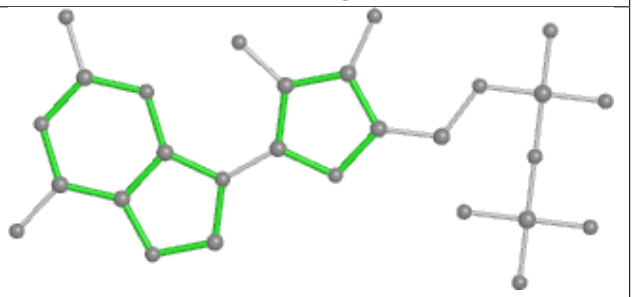

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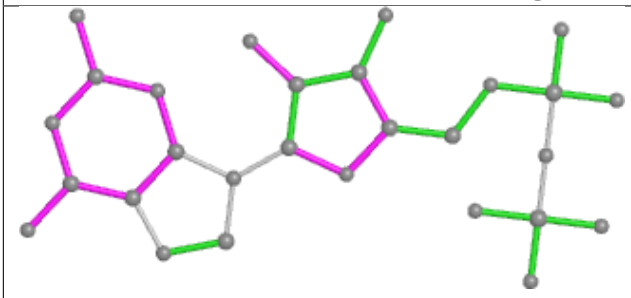

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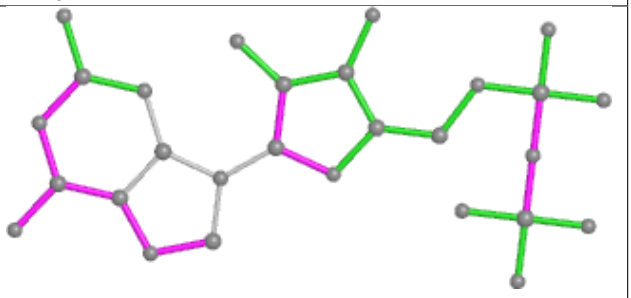

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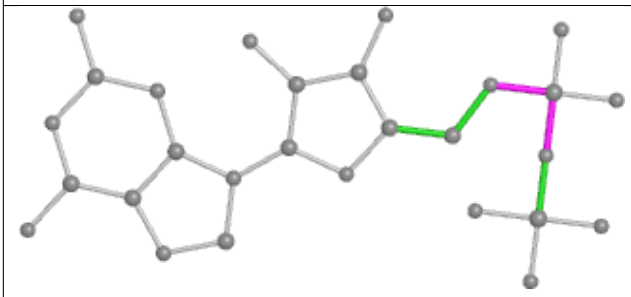

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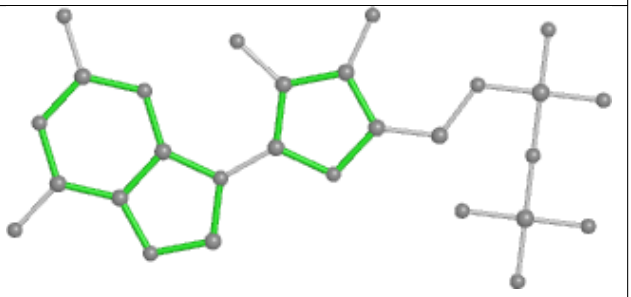

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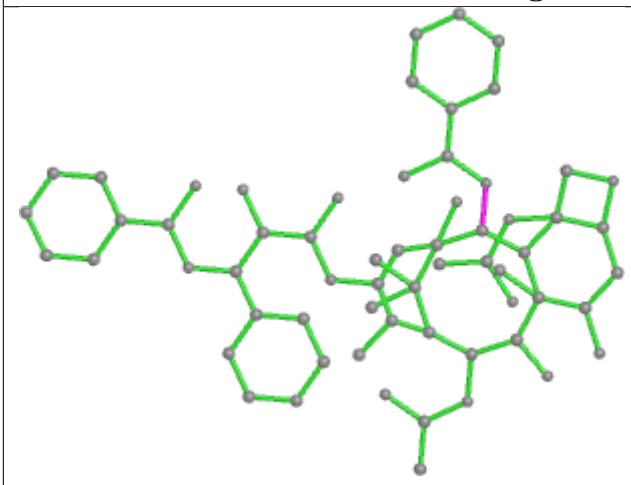

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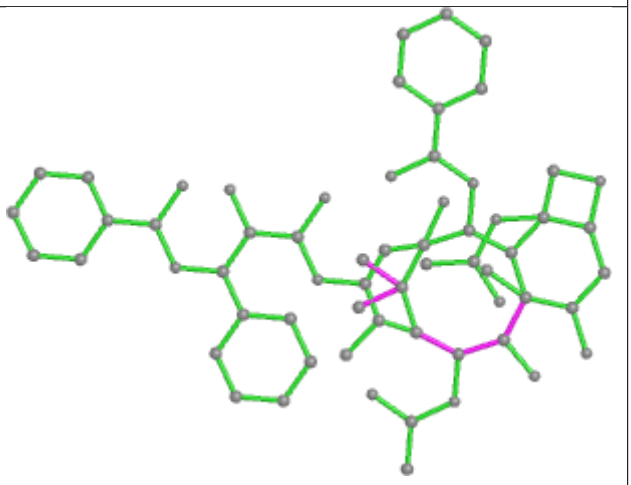

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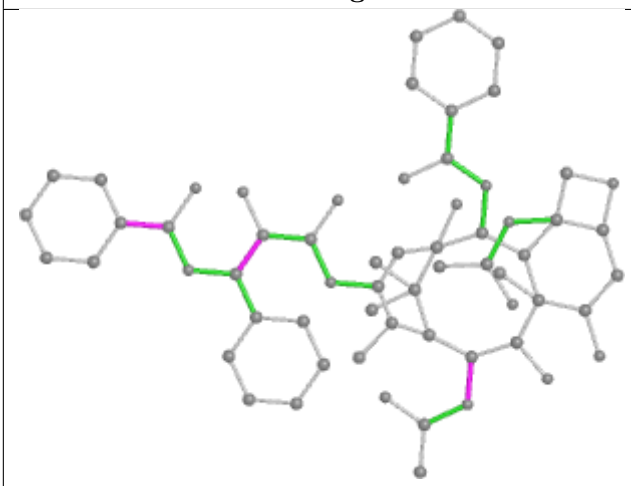

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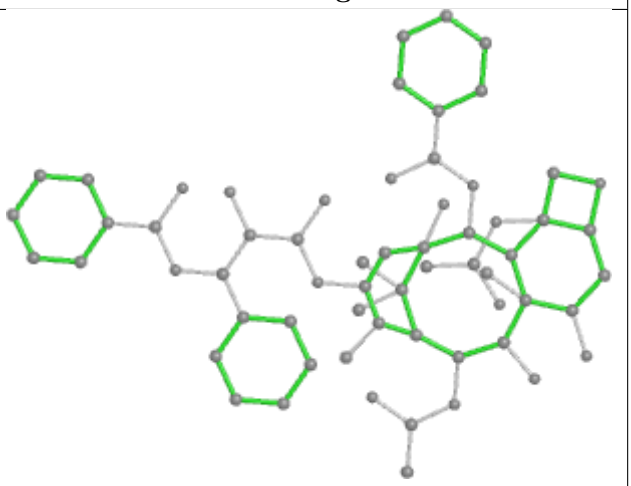

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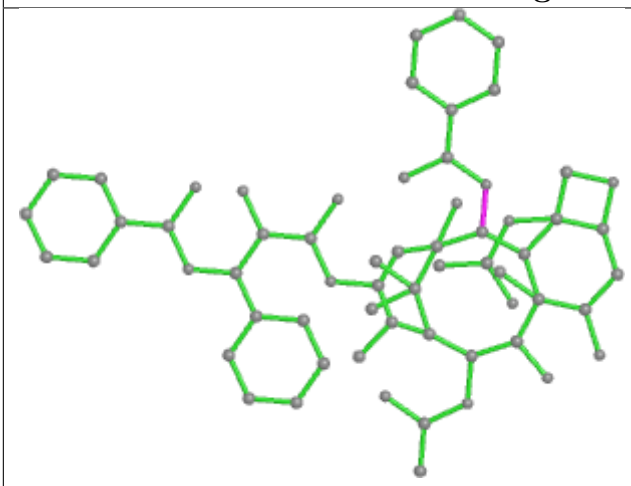

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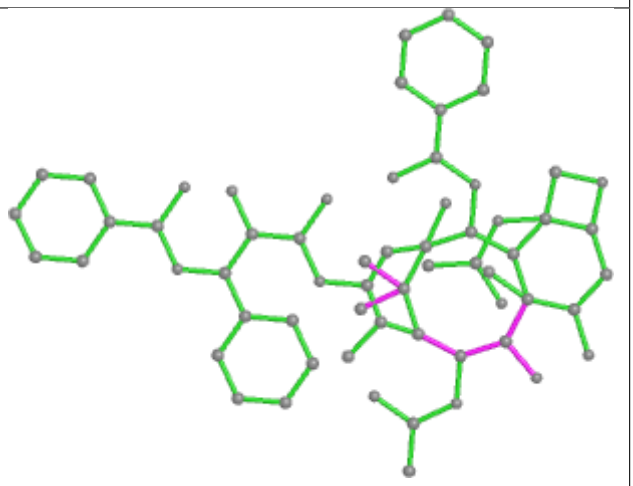

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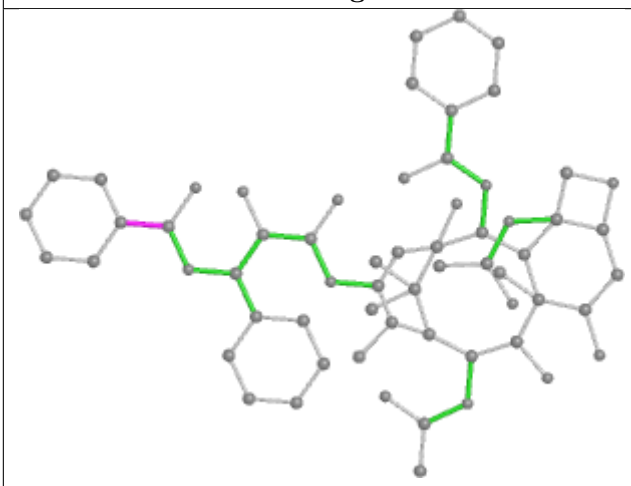

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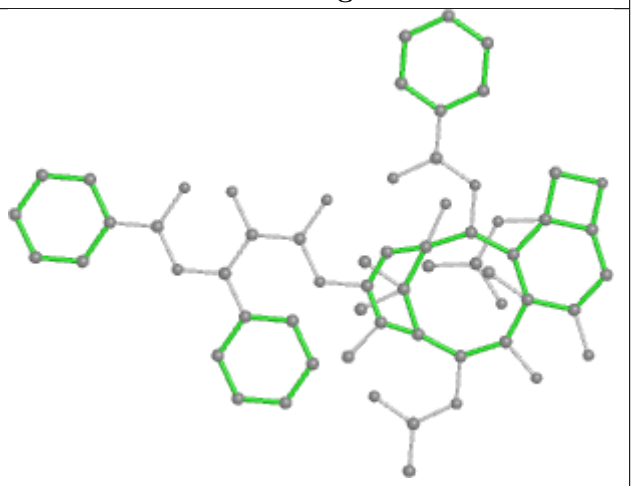

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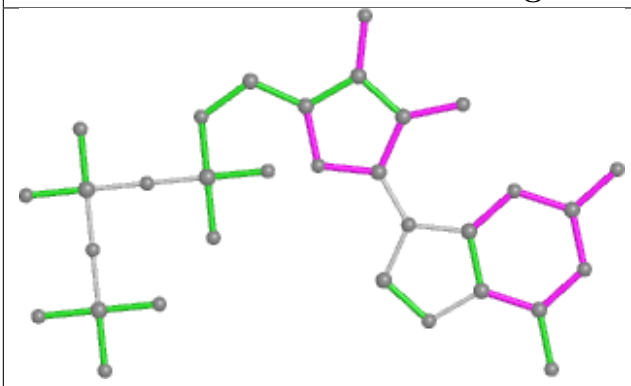

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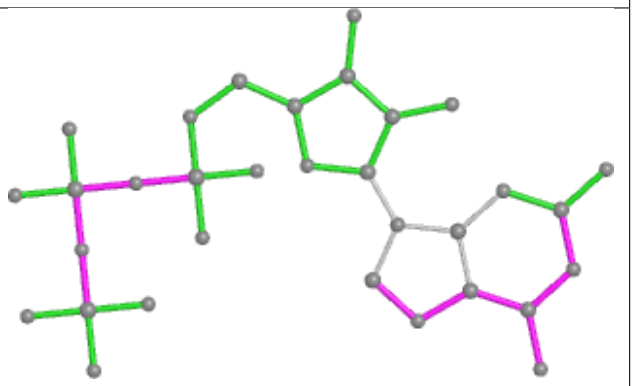

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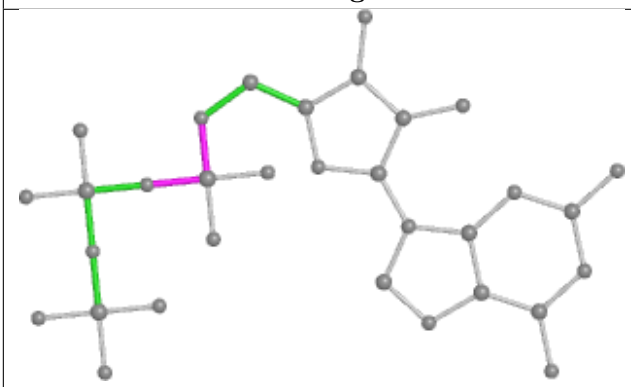

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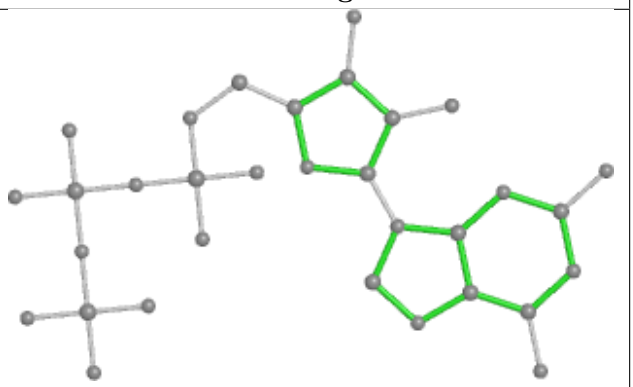

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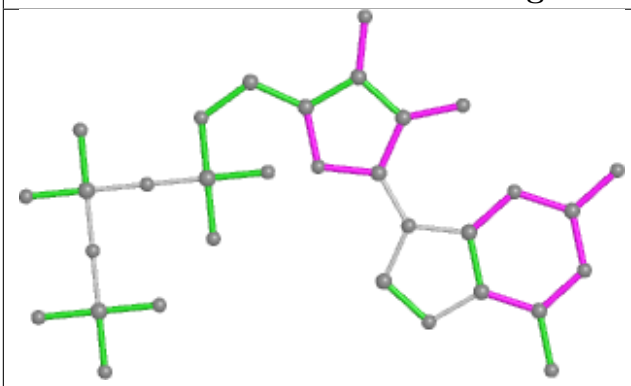

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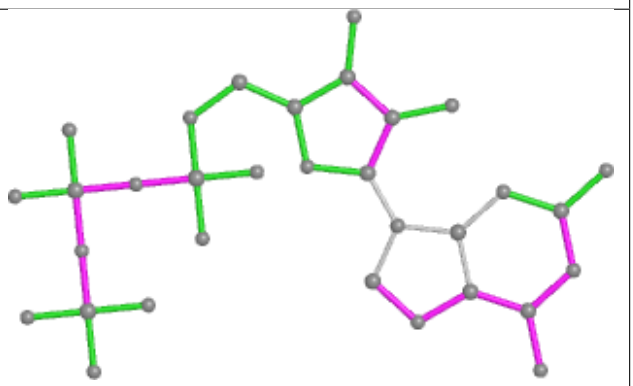

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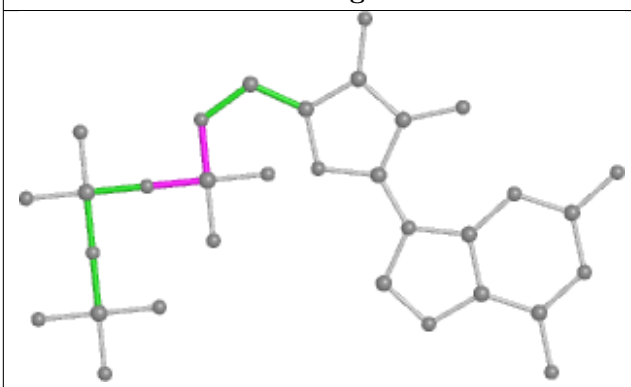
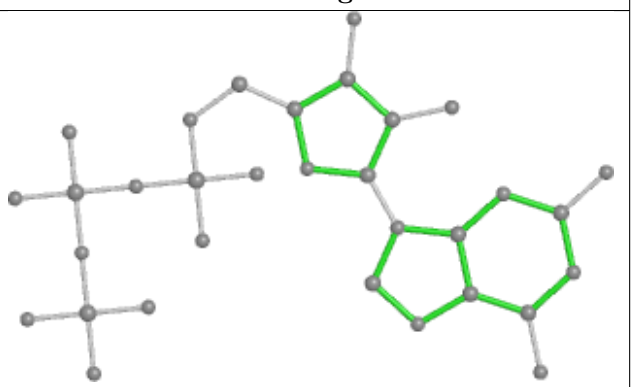
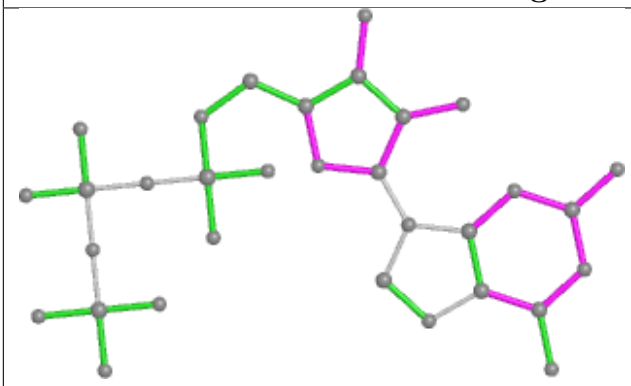


Torsions



Rings

Ligand GTP f 501



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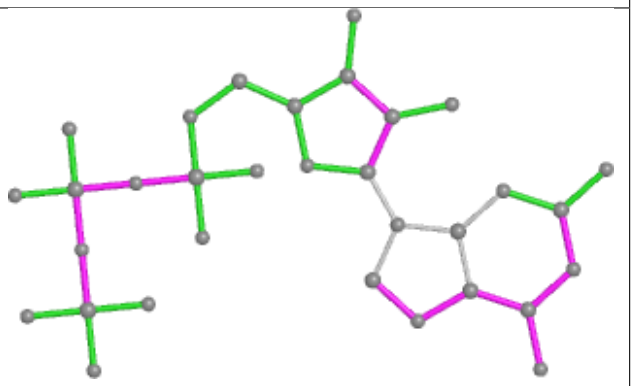
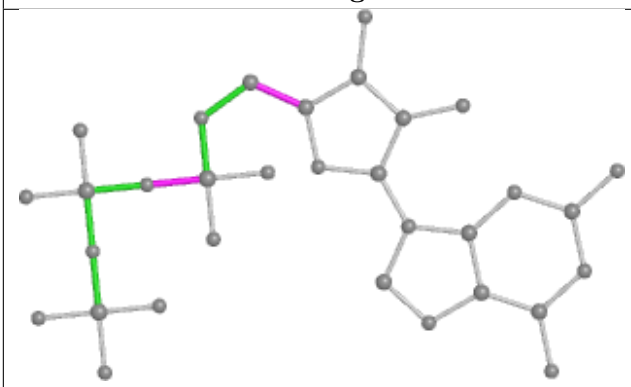


Bond angles



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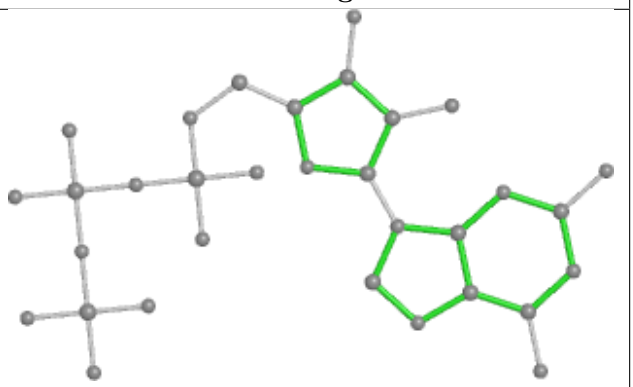
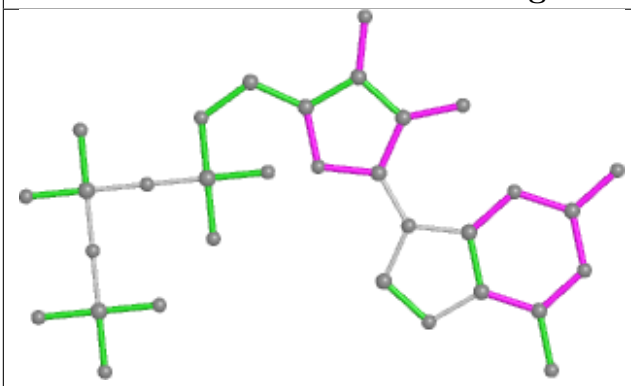


Rings

Ligand GTP s 501



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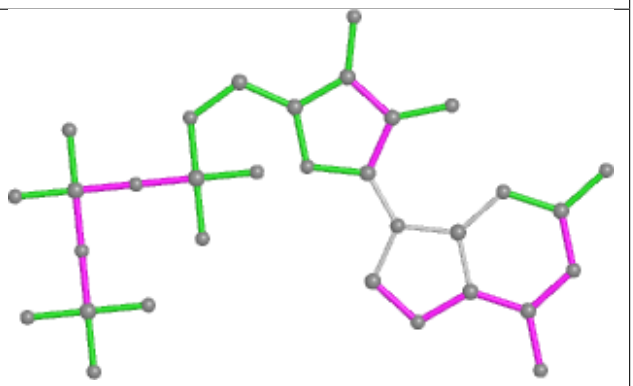

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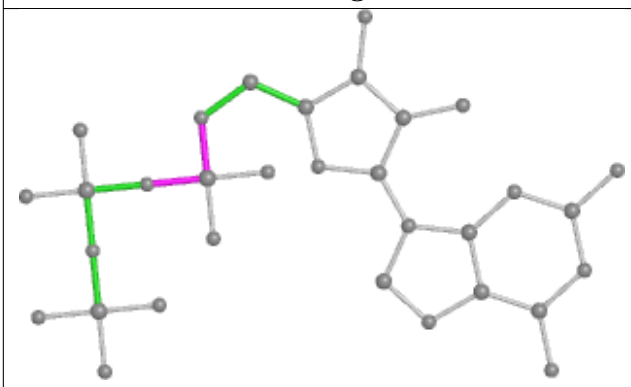

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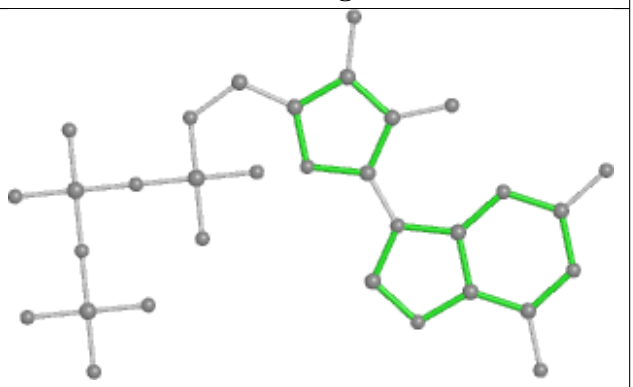
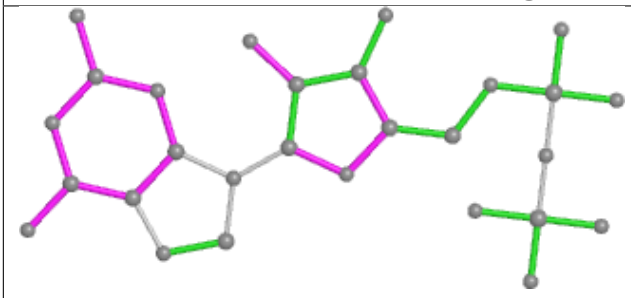
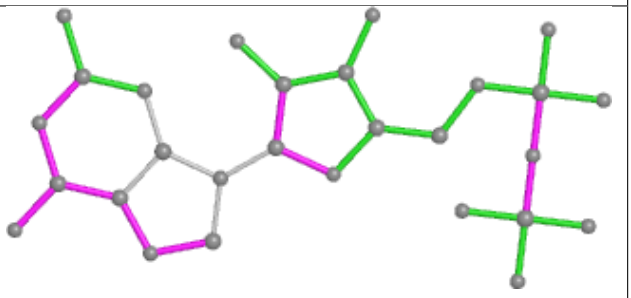
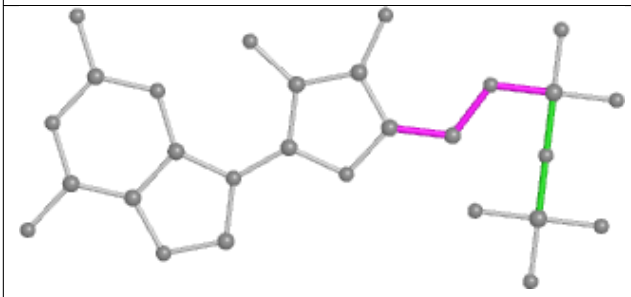
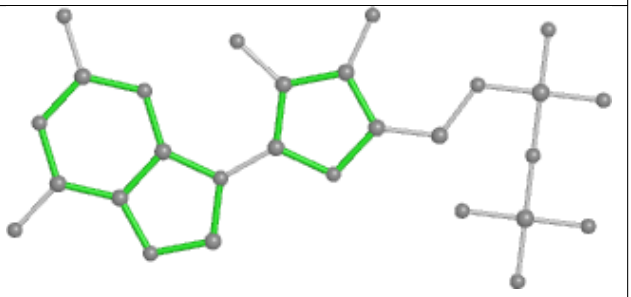
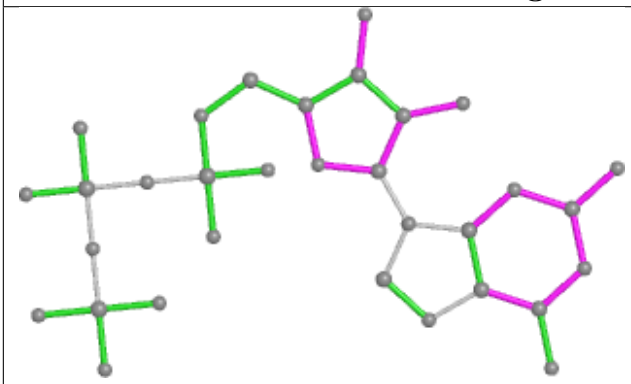
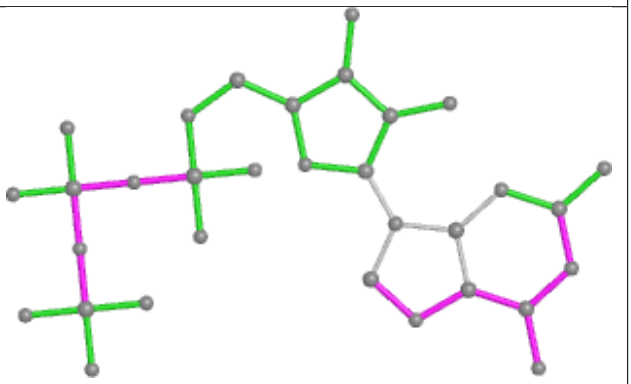
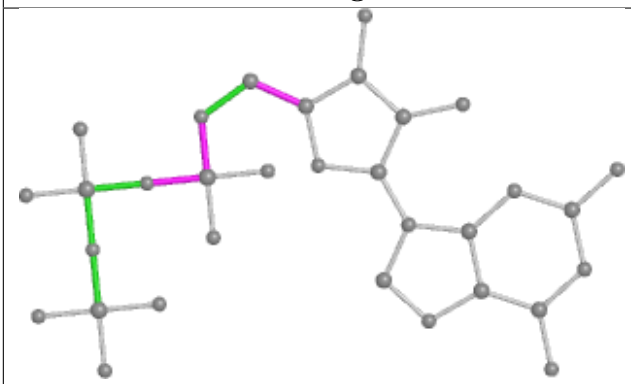
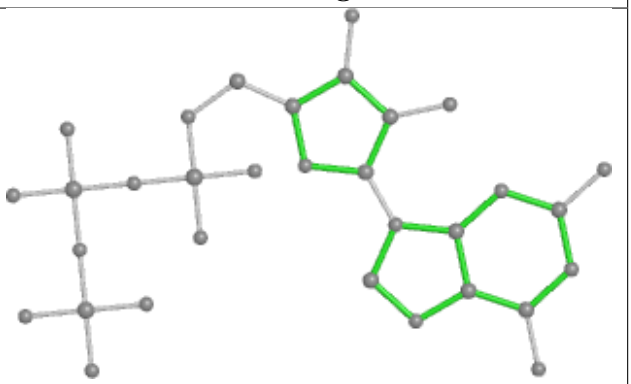
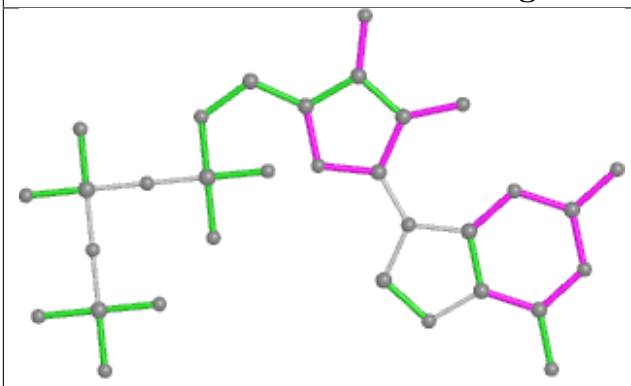


Rings

Ligand GDP N 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP 7 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP M 501



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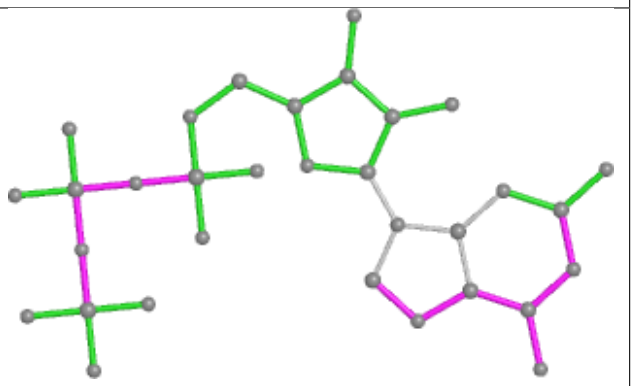

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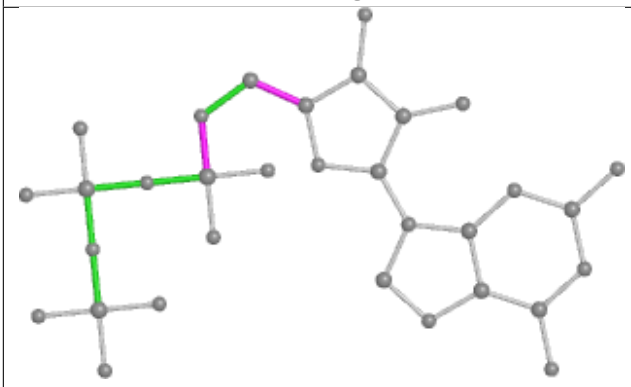

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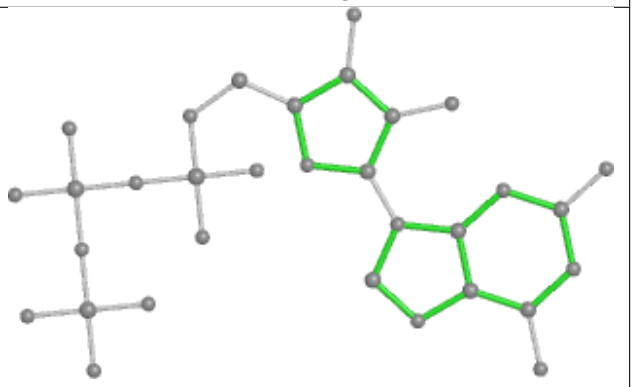
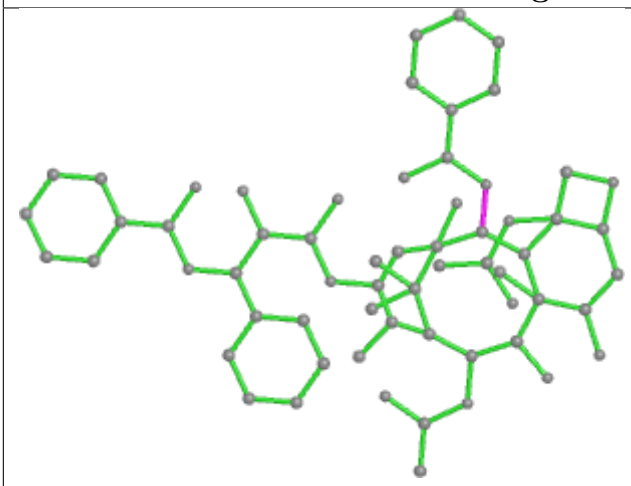


Rings

Ligand TA1 J 502



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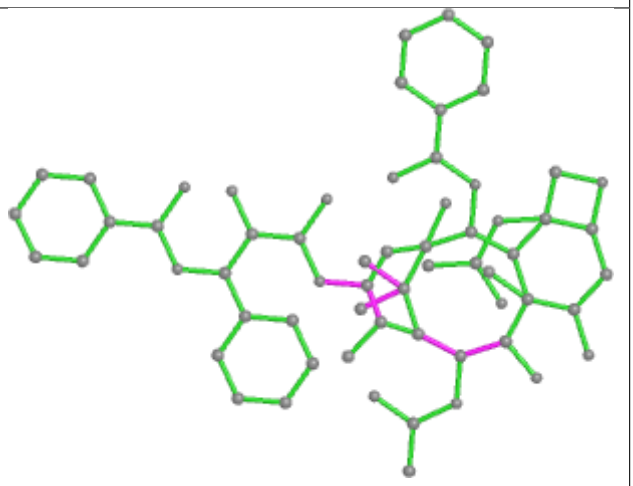

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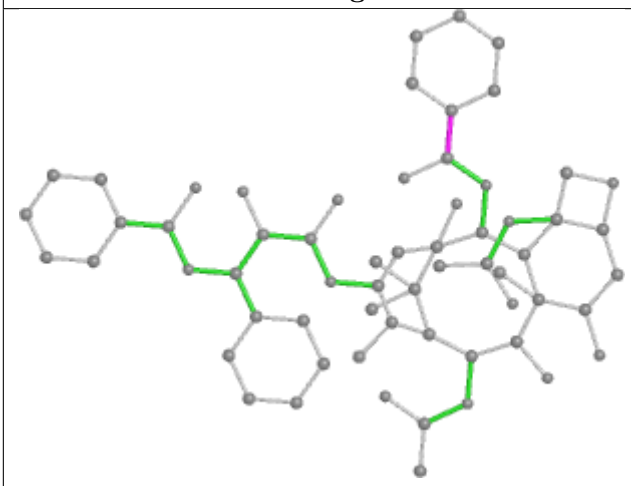

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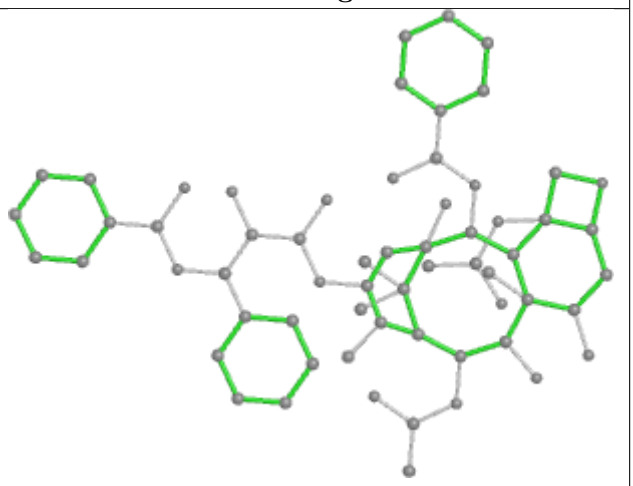
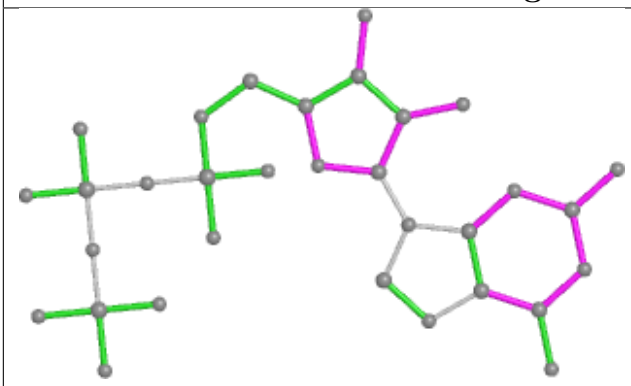


Rings

Ligand GTP E 501



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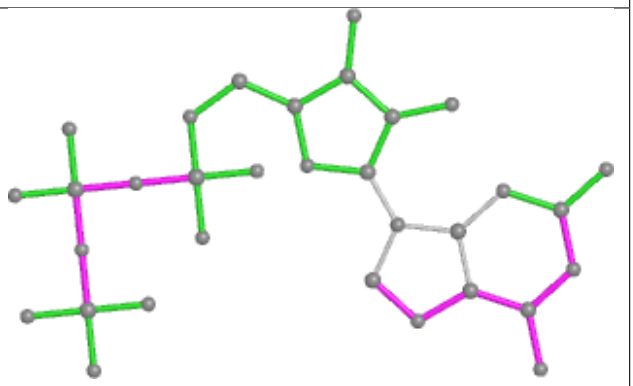

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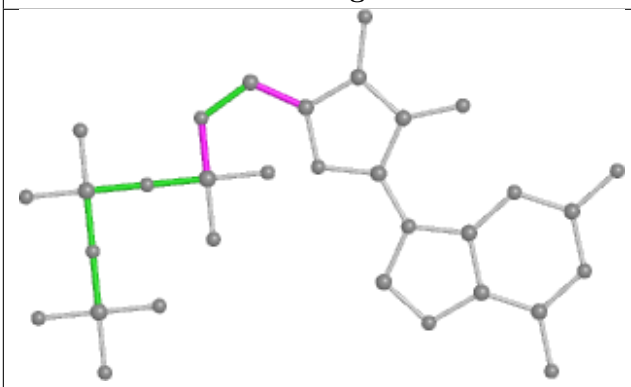

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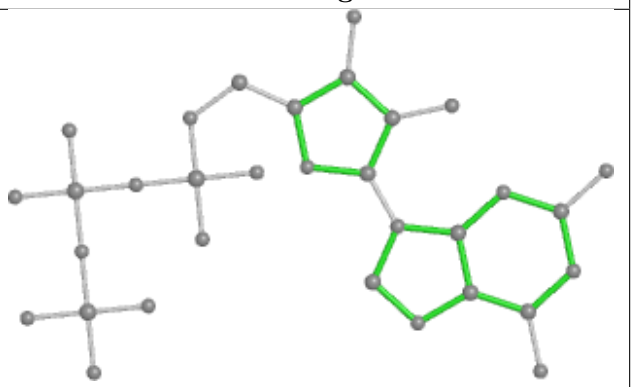

Rings

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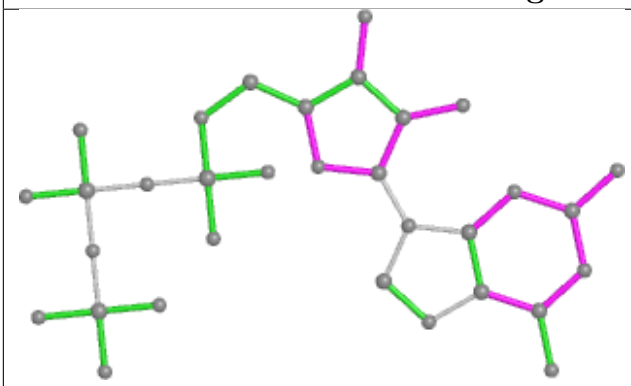

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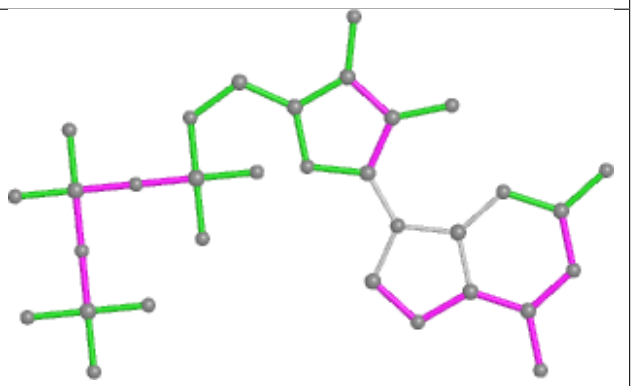

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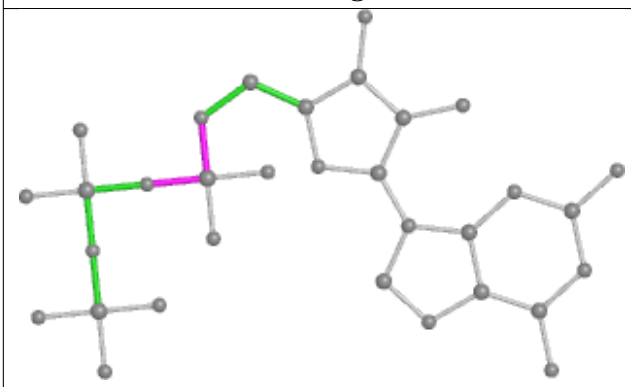

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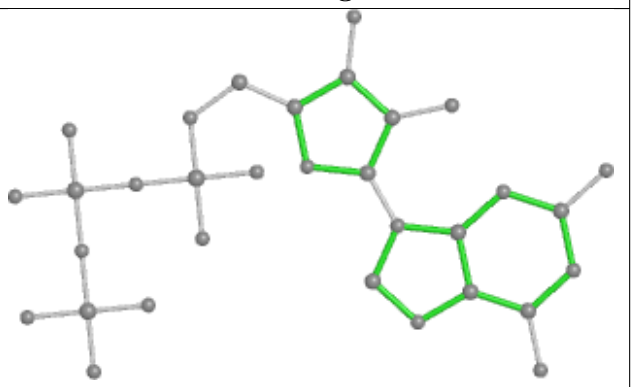
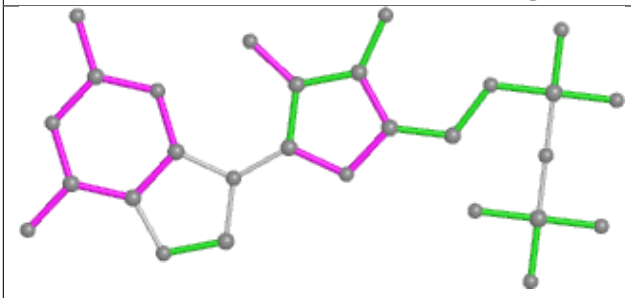


Rings

Ligand GDP u 501



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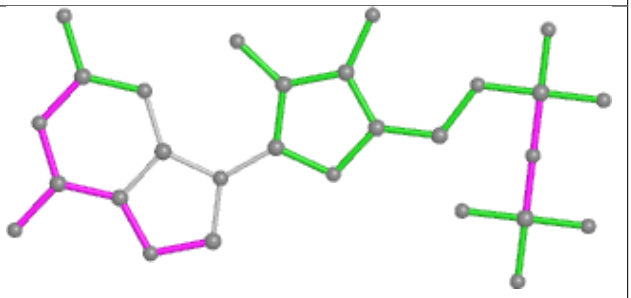

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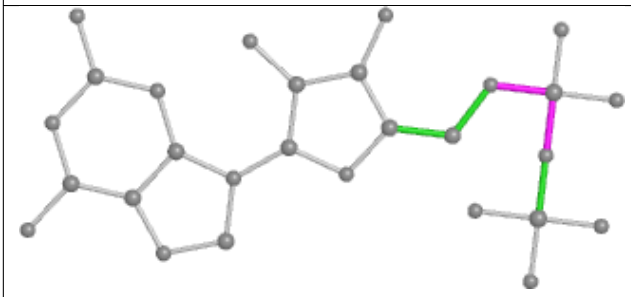

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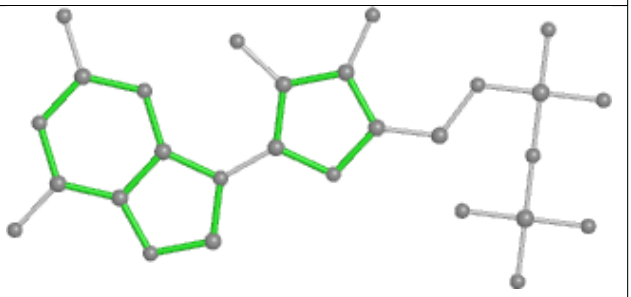
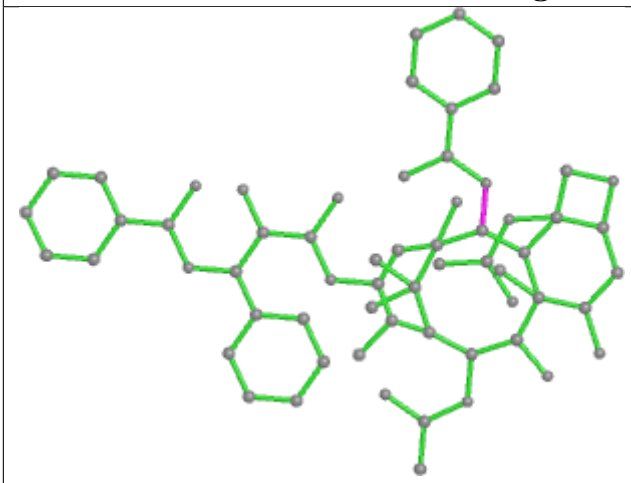


Rings

Ligand TA1 8 502



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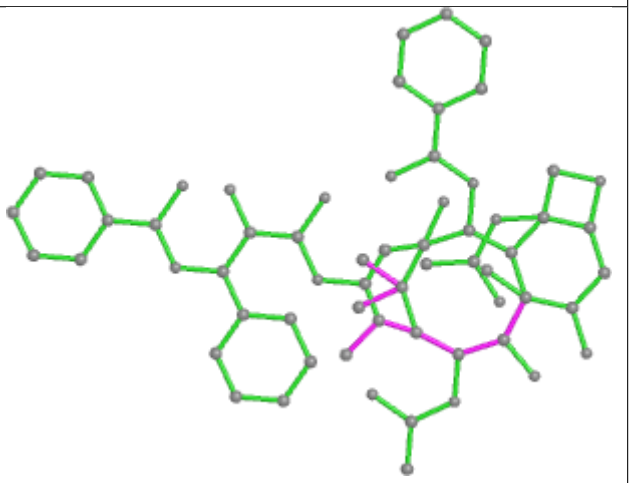

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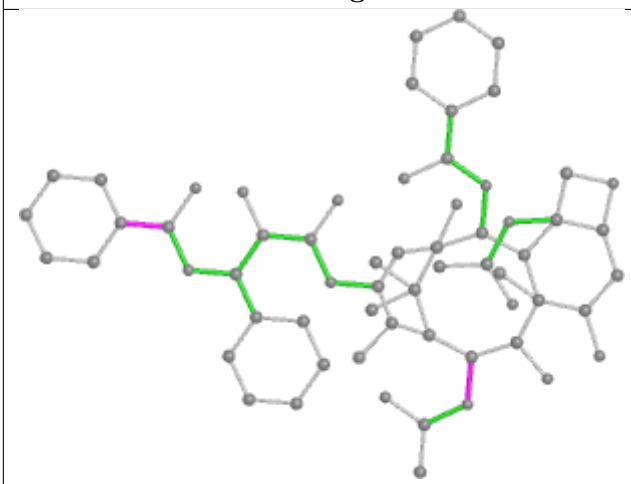

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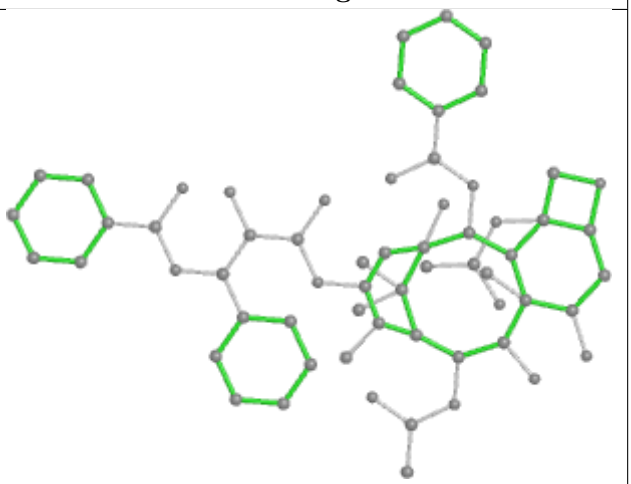
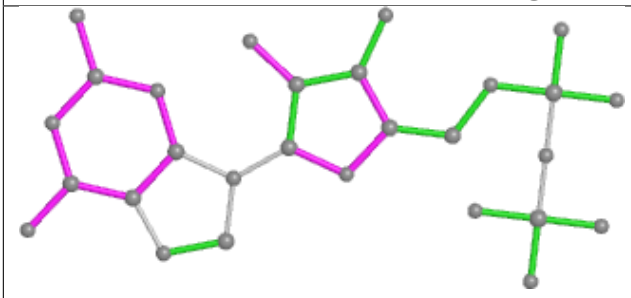


Rings

Ligand GDP 4 501



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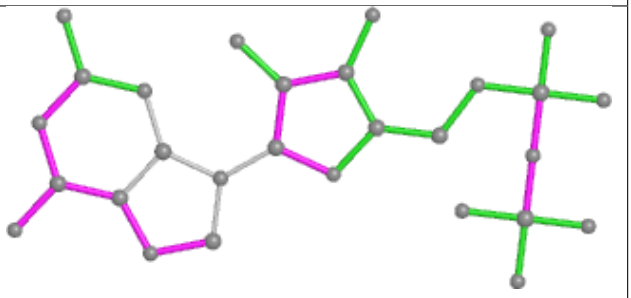

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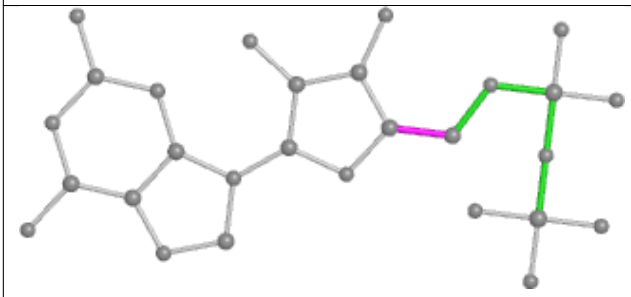

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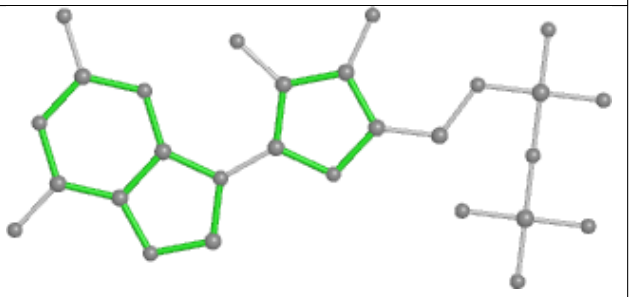
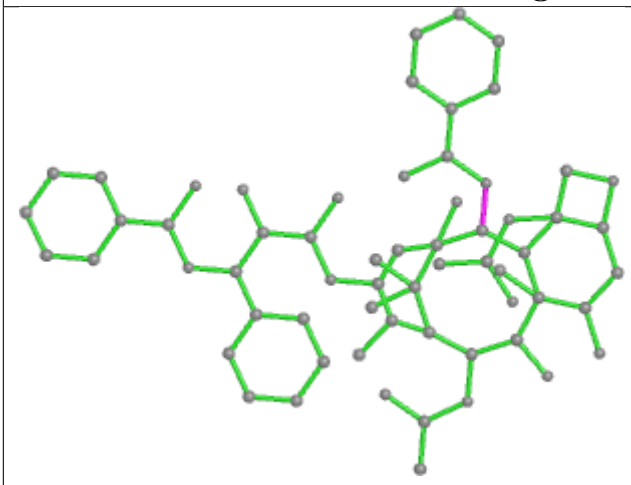


Rings

Ligand TA1 4 502



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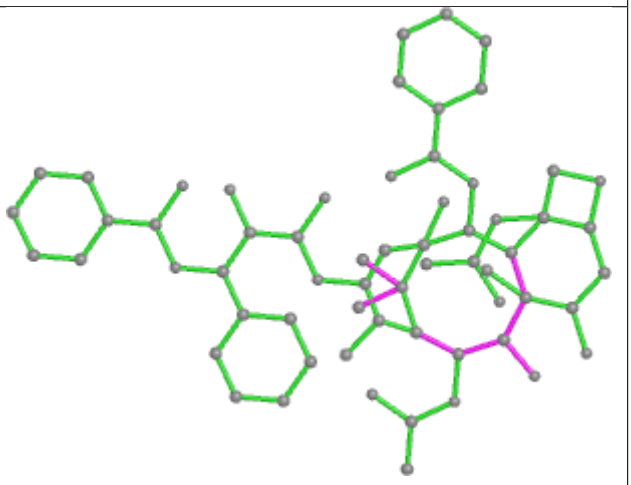

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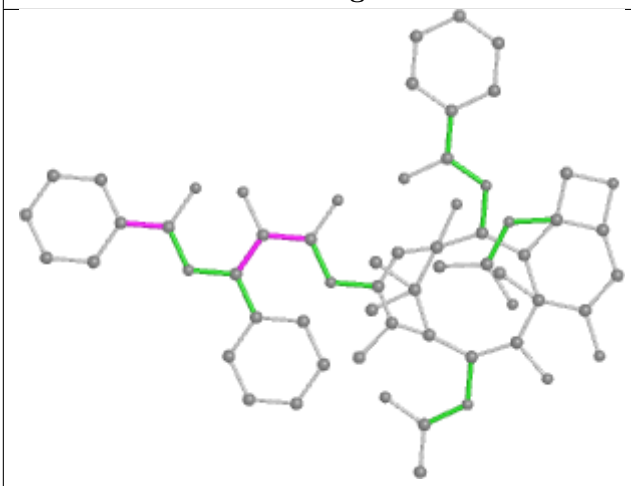

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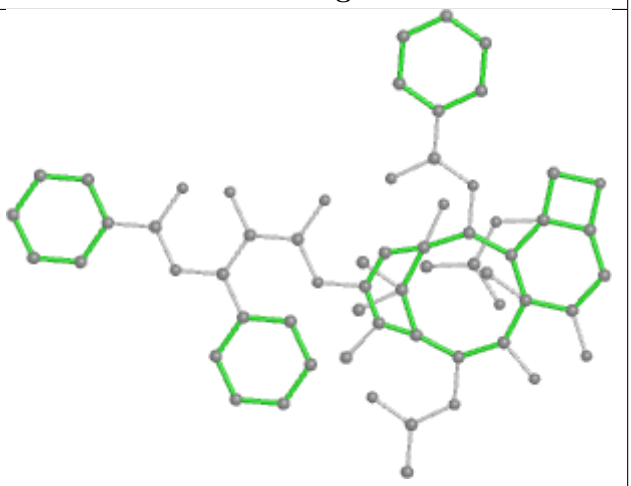
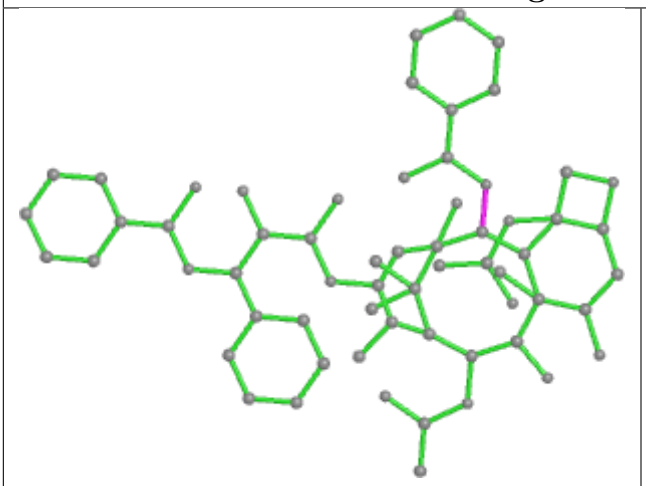


Rings

Ligand TA1 w 502



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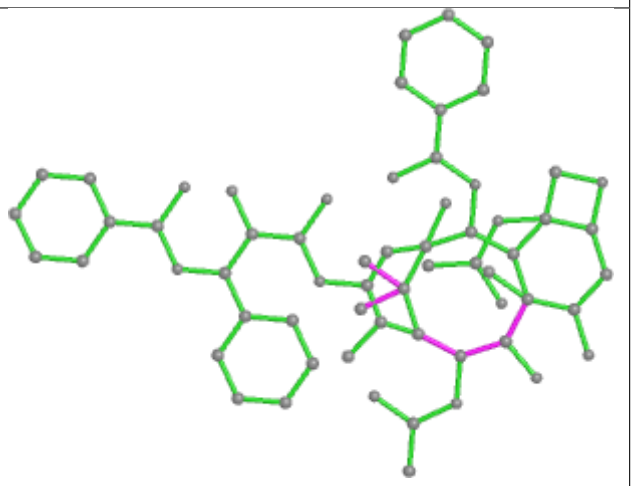

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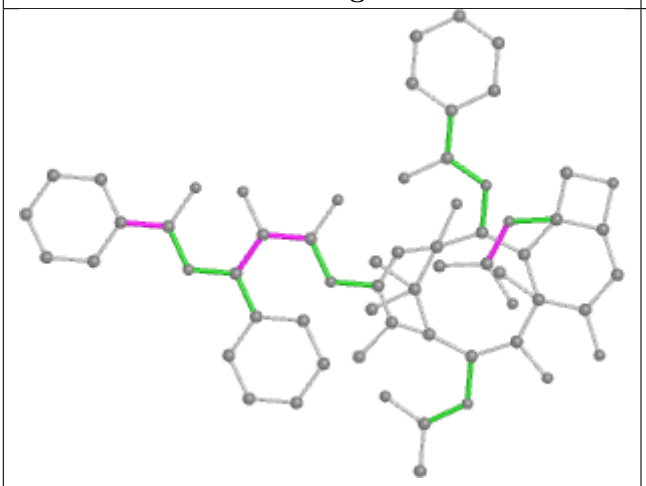

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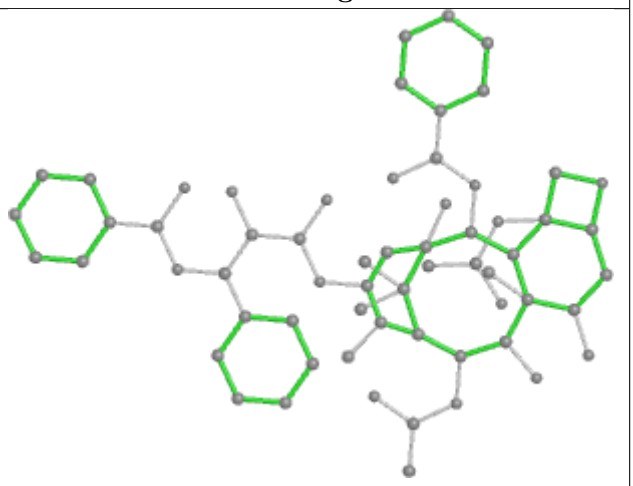
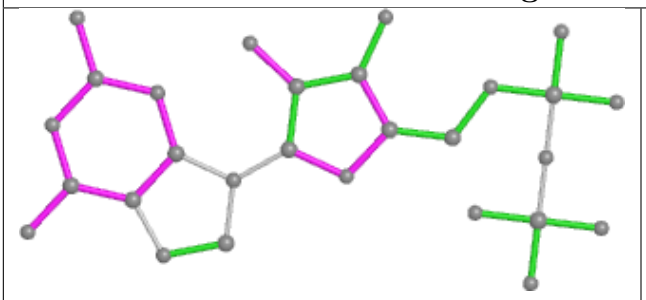


Rings

Ligand GDP Q 501



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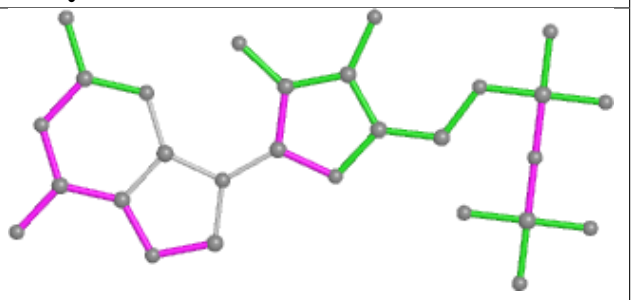
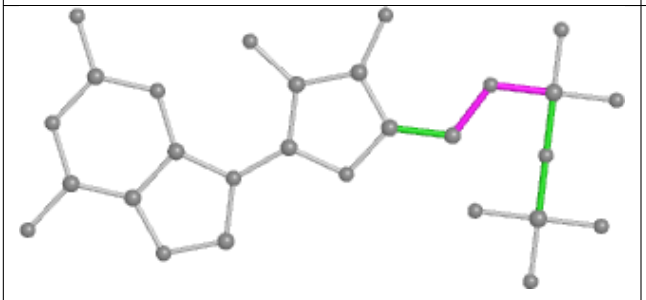


Bond angles



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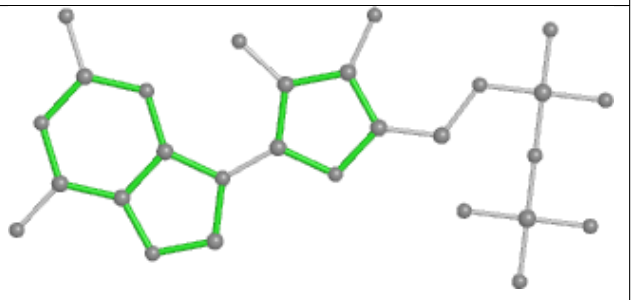
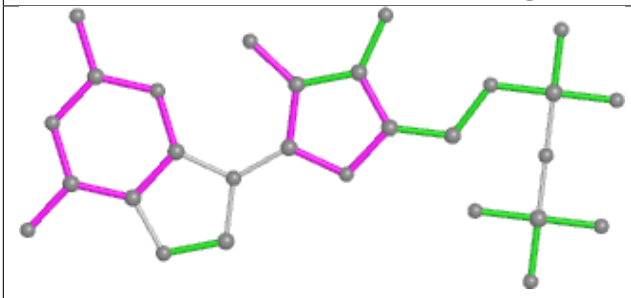
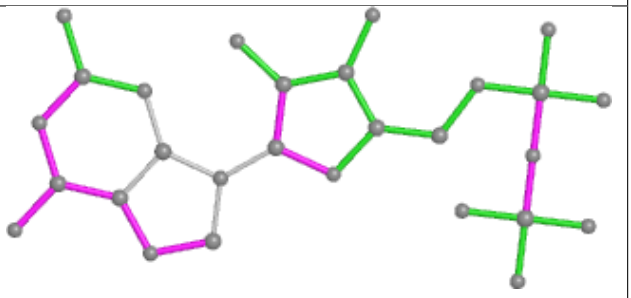


Rings

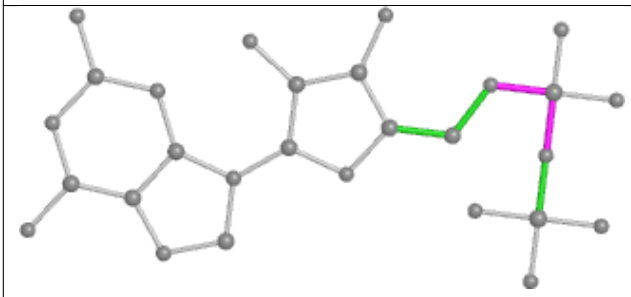
Ligand GDP V 501



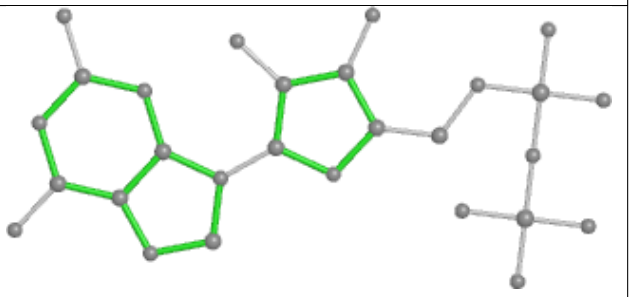
Bond lengths



Bond angles

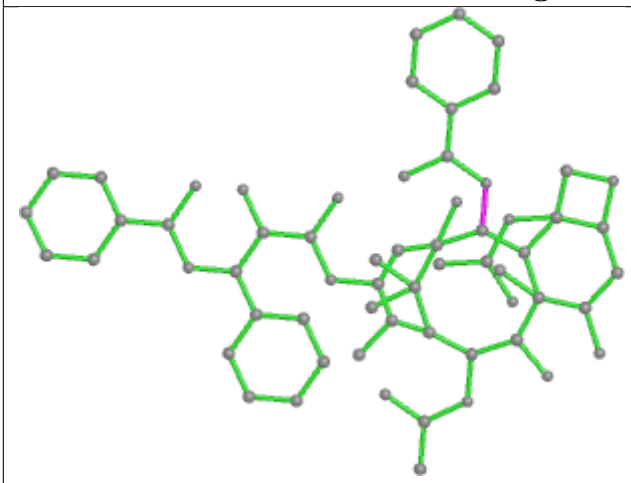


Torsions

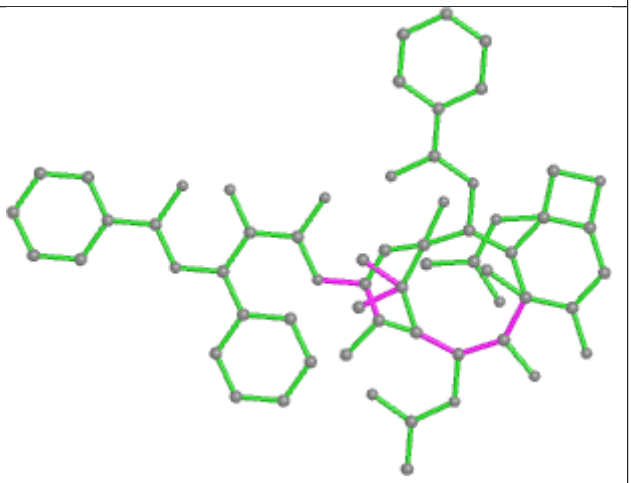


Rings

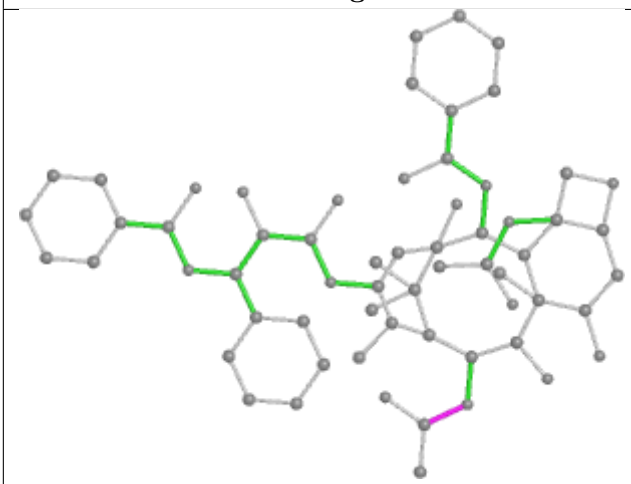
Ligand TA1 a 502



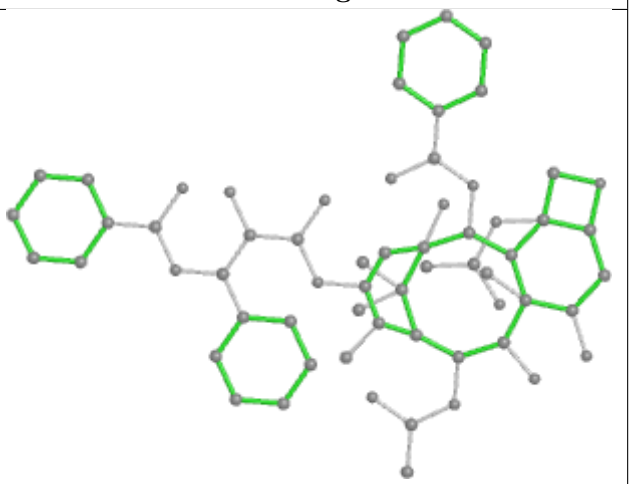
Bond lengths



Bond angles

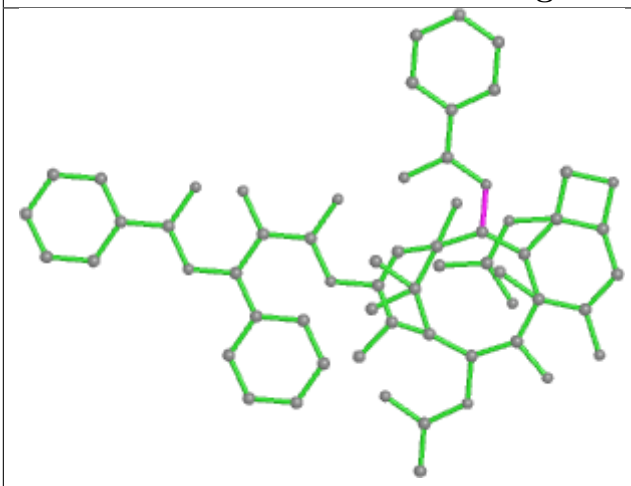


Torsions

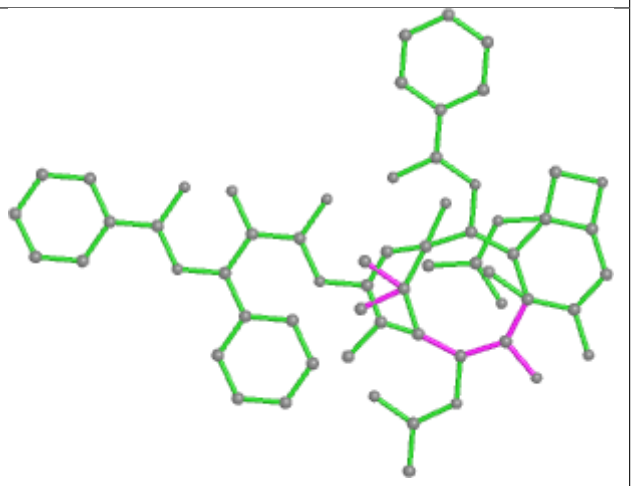


Rings

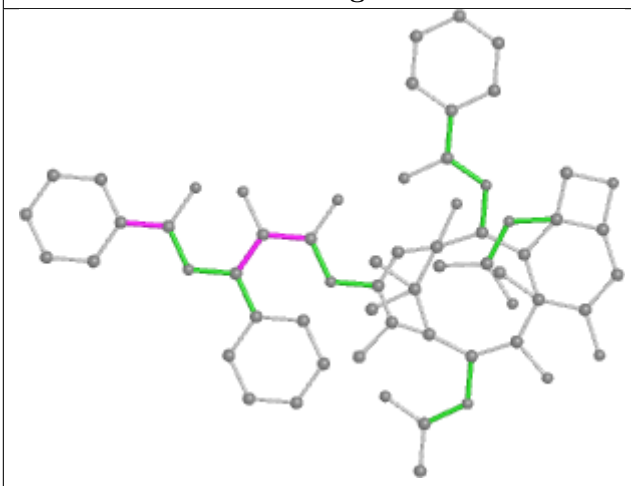
Ligand TA1 i 502



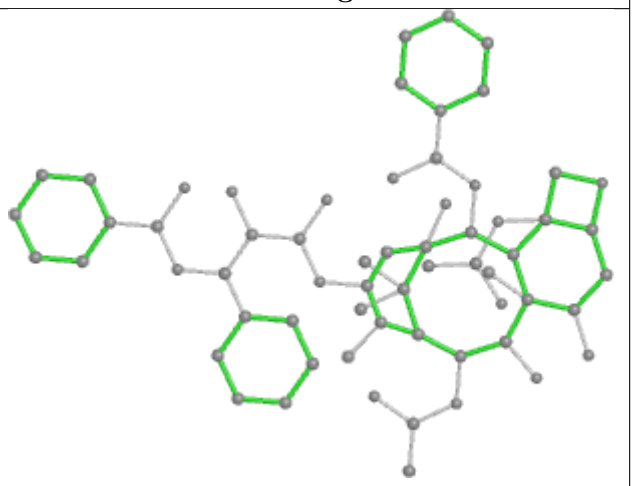
Bond lengths



Bond angles

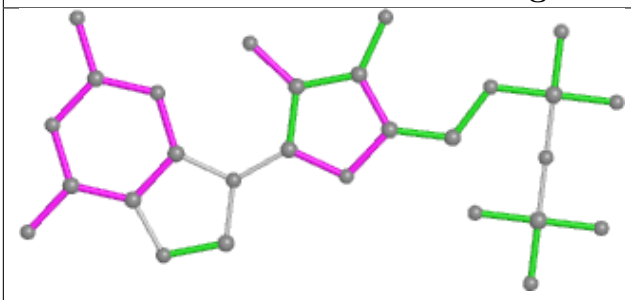


Torsions

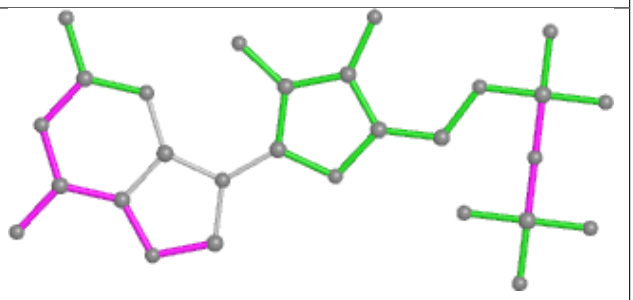


Rings

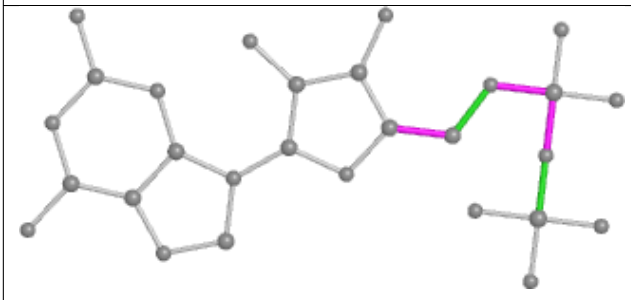
Ligand GDP i 501



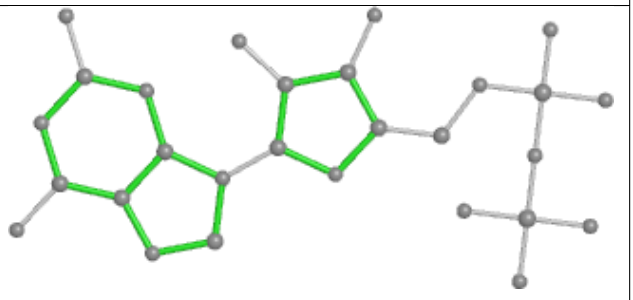
Bond lengths



Bond angles

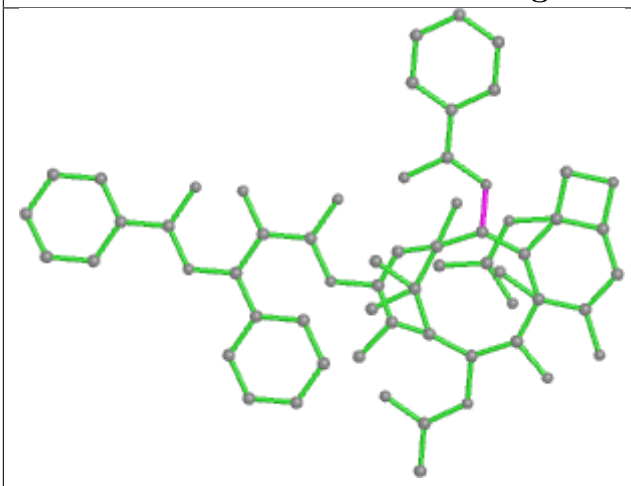


Torsions

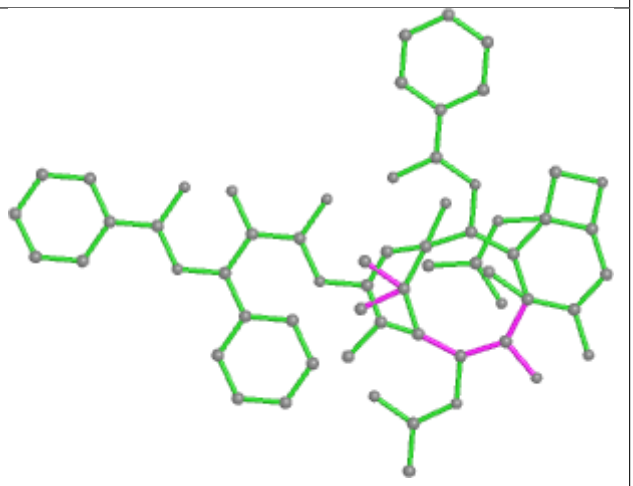


Rings

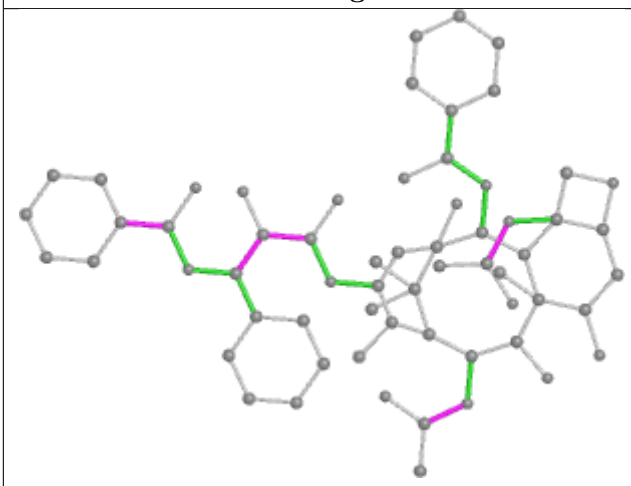
Ligand TA1 u 502



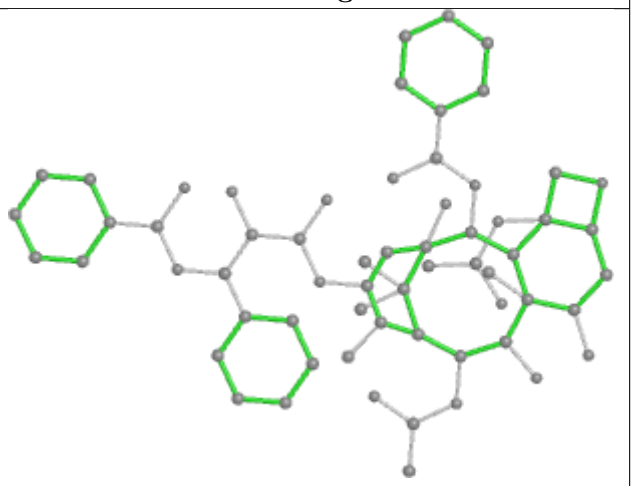
Bond lengths



Bond angles

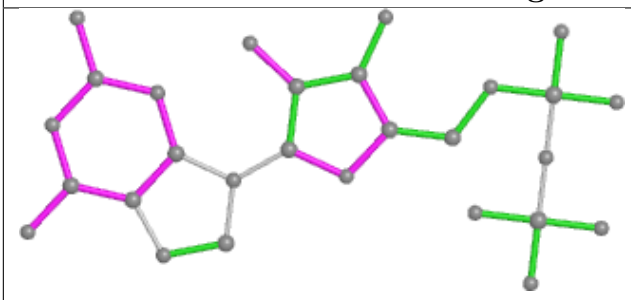


Torsions

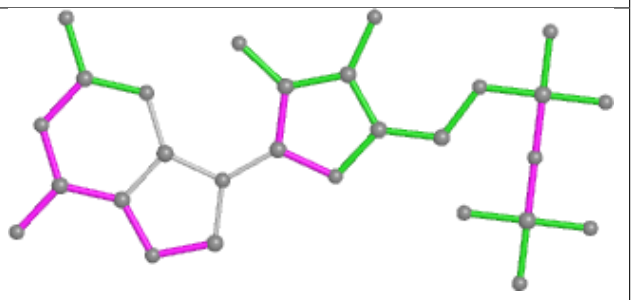


Rings

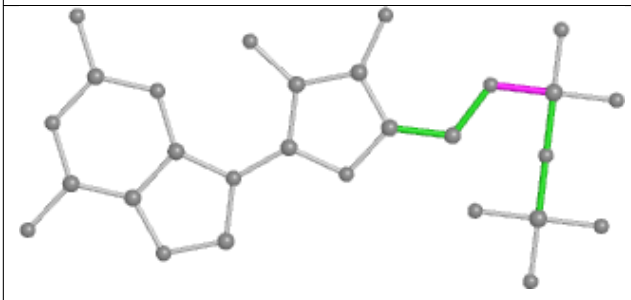
Ligand GDP t 501



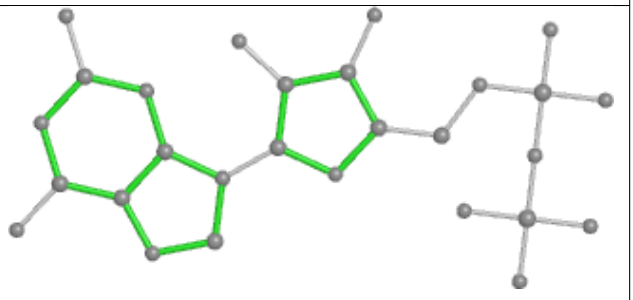
Bond lengths



Bond angles

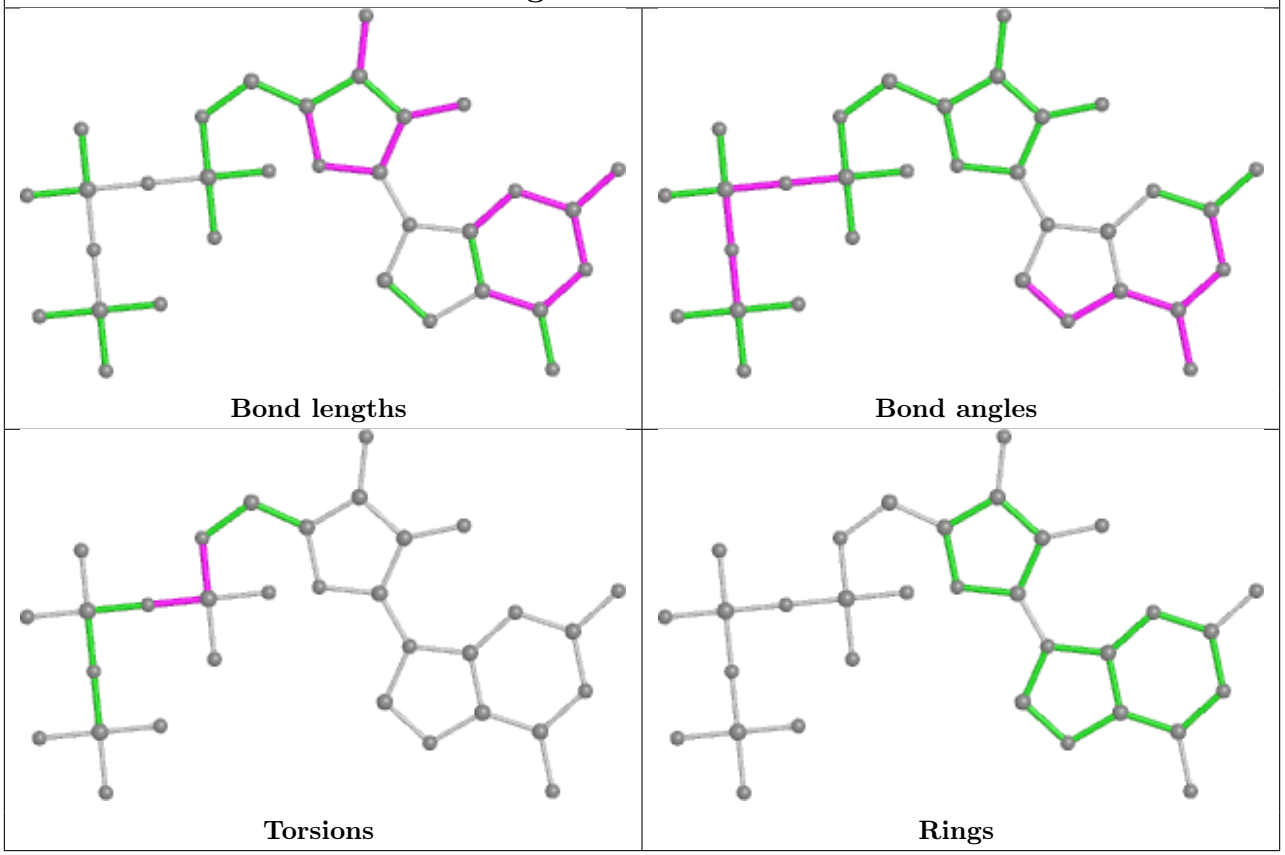


Torsions



Rings

Ligand GTP h 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

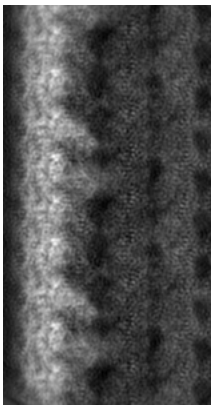
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20858. These allow visual inspection of the internal detail of the map and identification of artifacts.

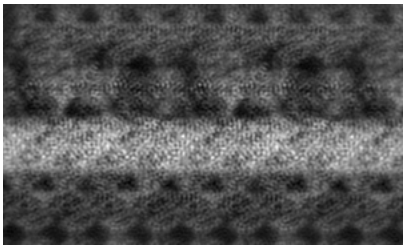
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

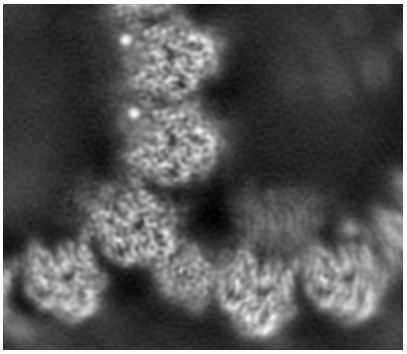
6.1.1 Primary map



X



Y

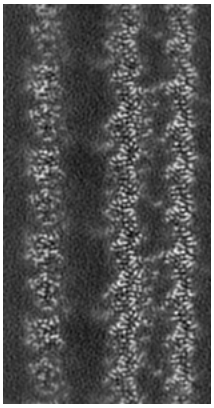


Z

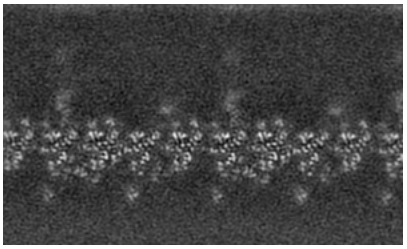
The images above show the map projected in three orthogonal directions.

6.2 Central slices

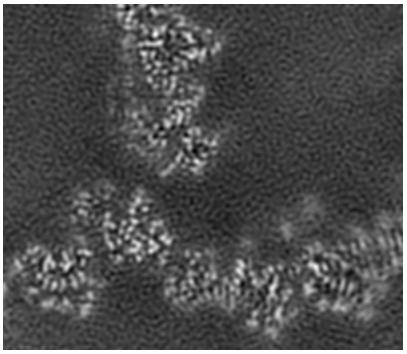
6.2.1 Primary map



X Index: 135



Y Index: 117

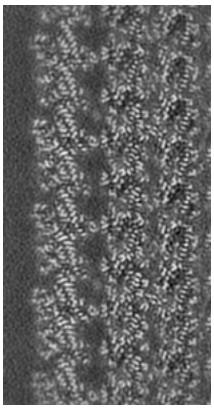


Z Index: 225

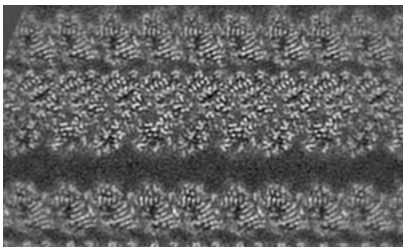
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

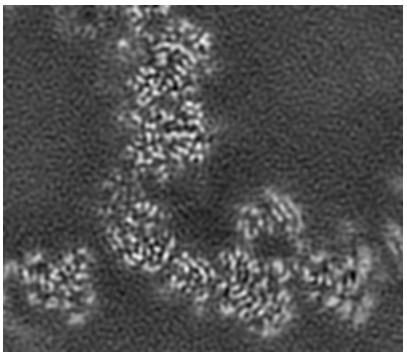
6.3.1 Primary map



X Index: 111



Y Index: 45

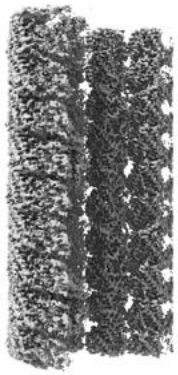


Z Index: 281

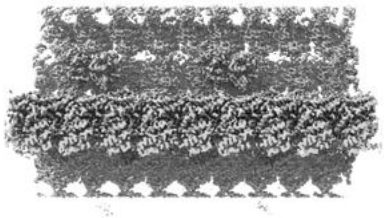
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

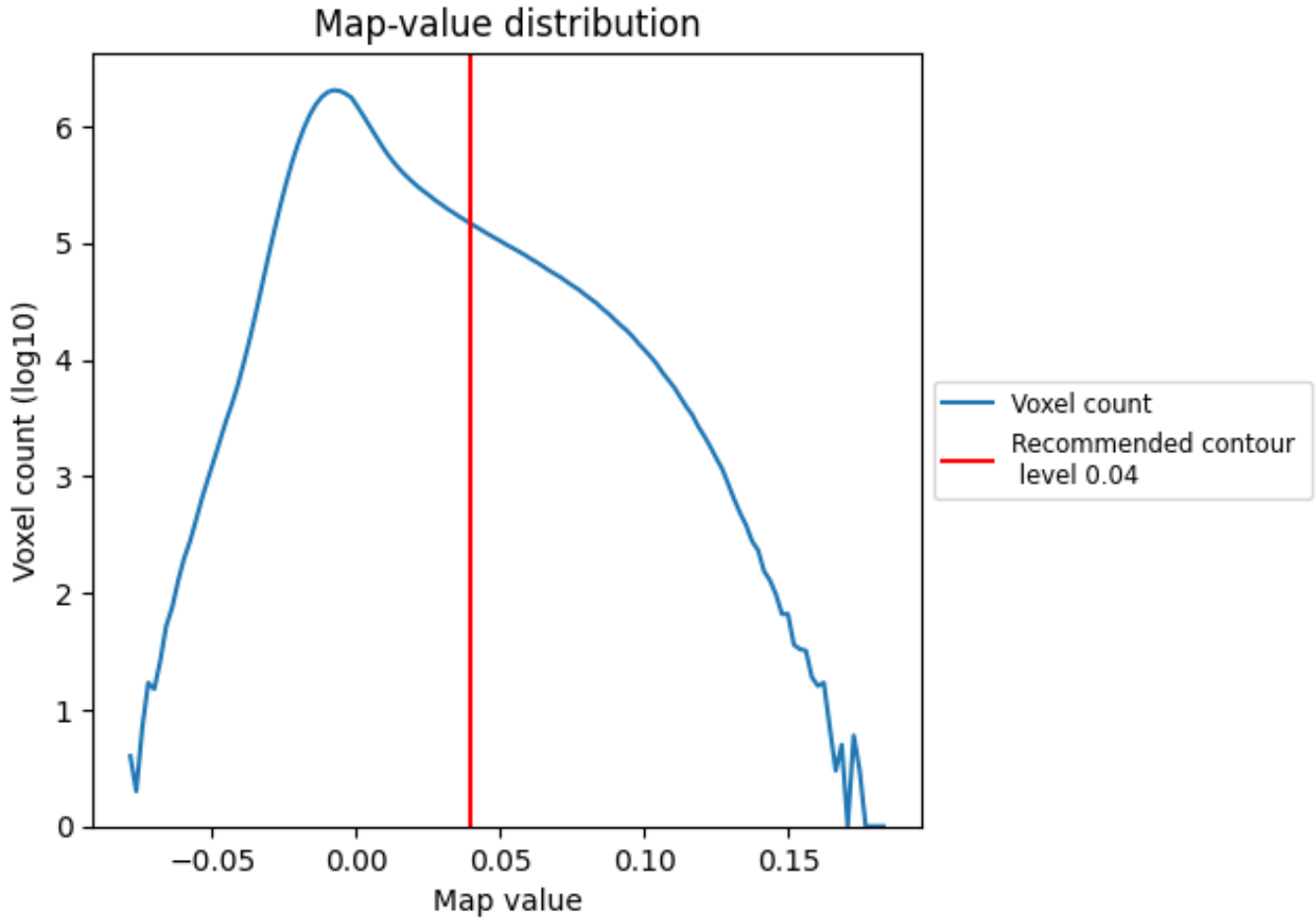
6.5 Mask visualisation (i)

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

7 Map analysis

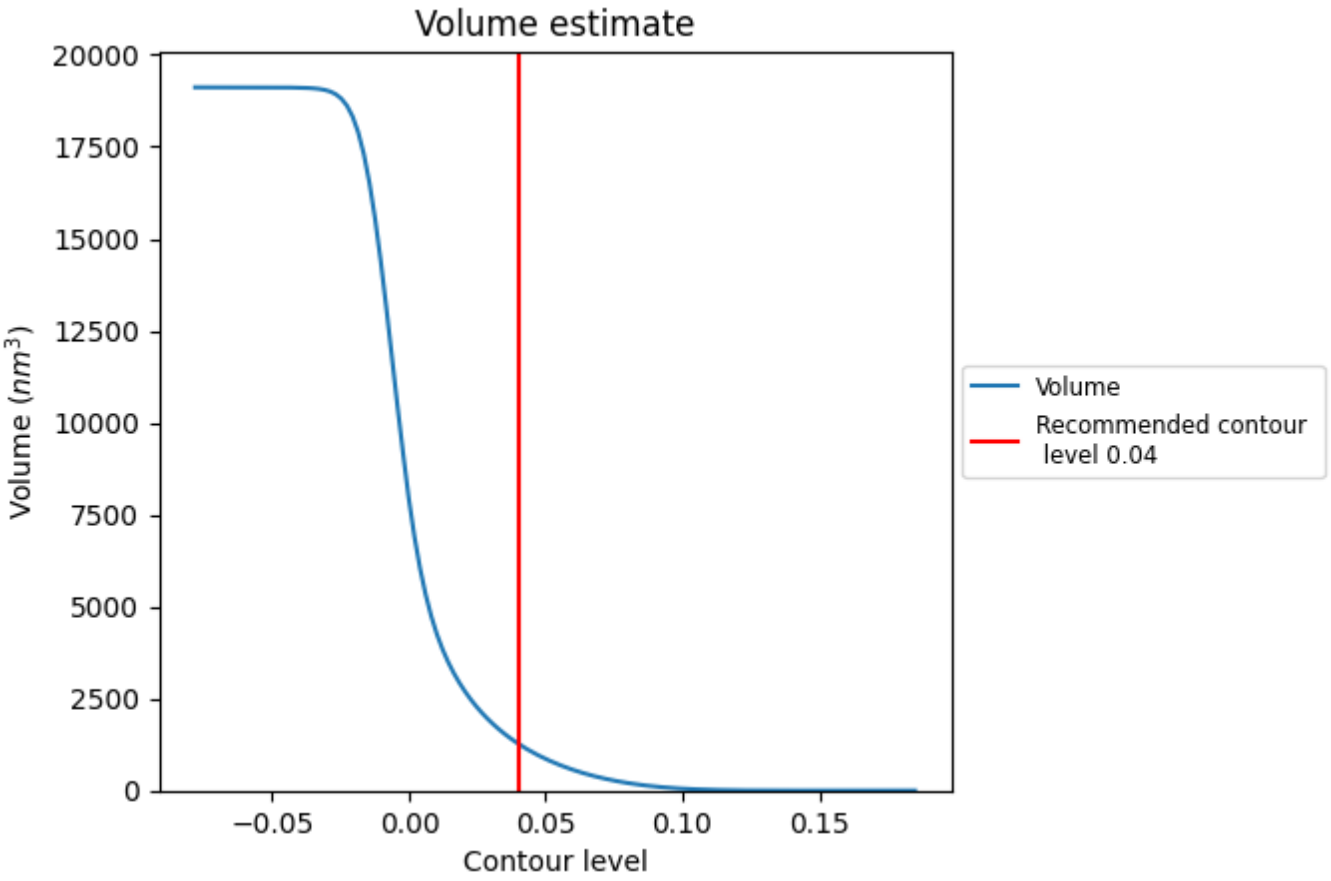
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 1273 nm^3; this corresponds to an approximate mass of 1150 kDa.

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

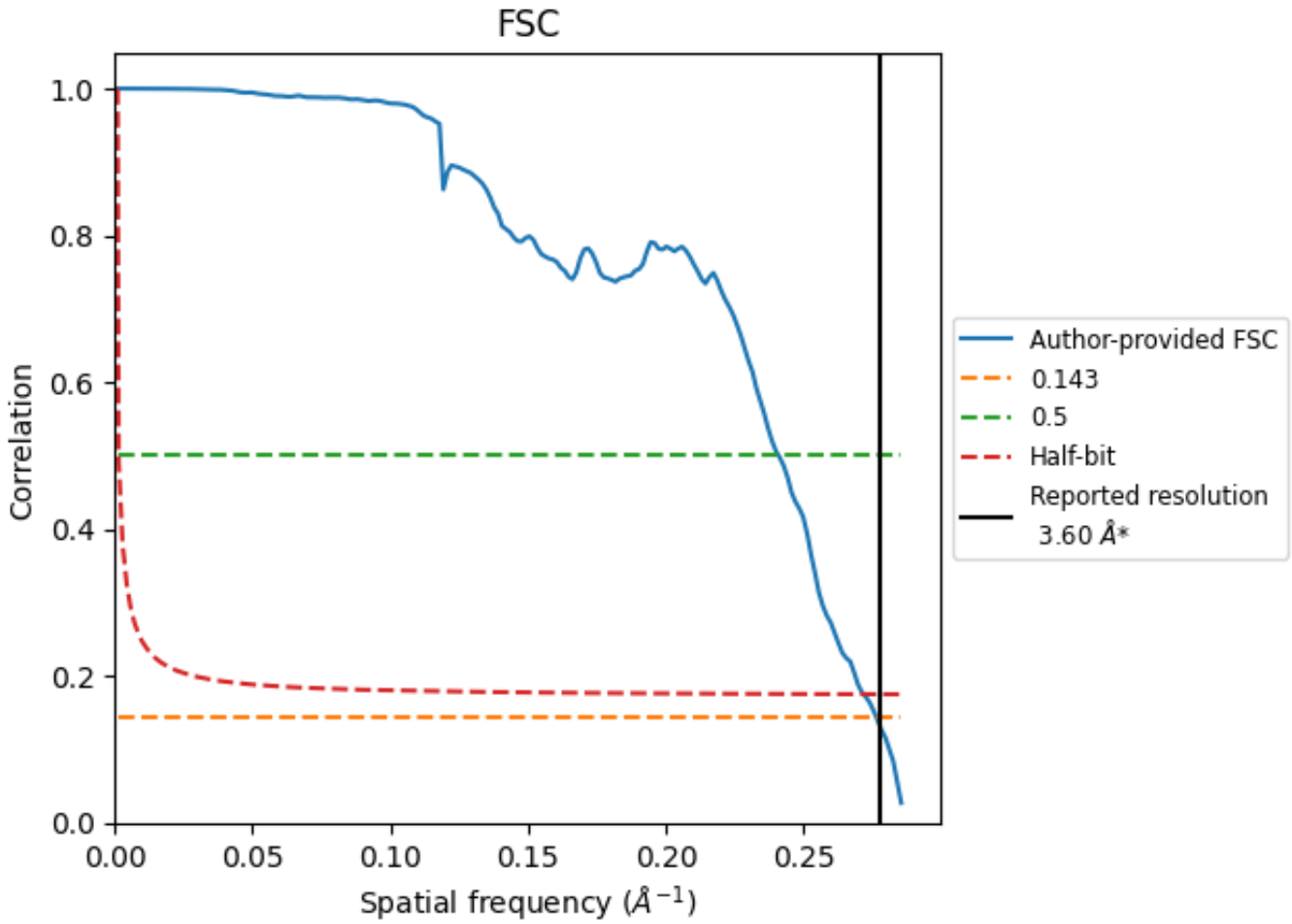
7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

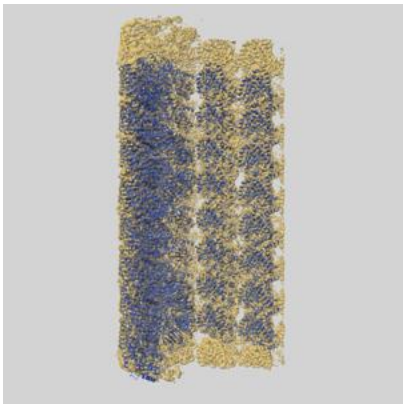
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.62	4.15	3.68
Unmasked-calculated*	-	-	-

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

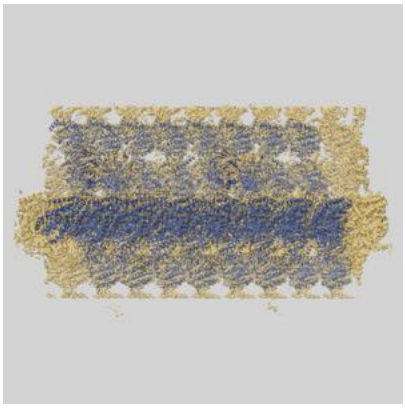
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20858 and PDB model 6VE7. Per-residue inclusion information can be found in section 3 on page 16.

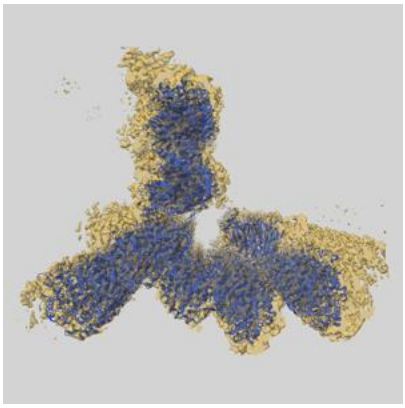
9.1 Map-model overlay



X



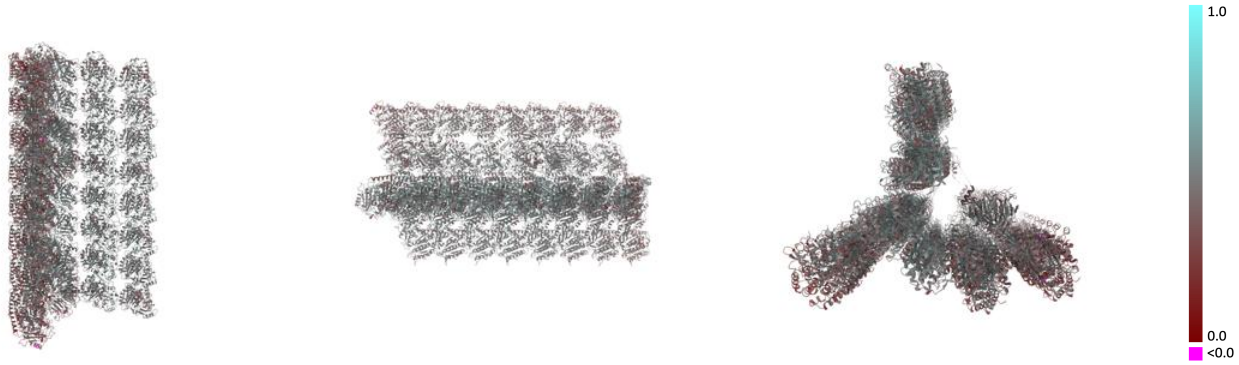
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

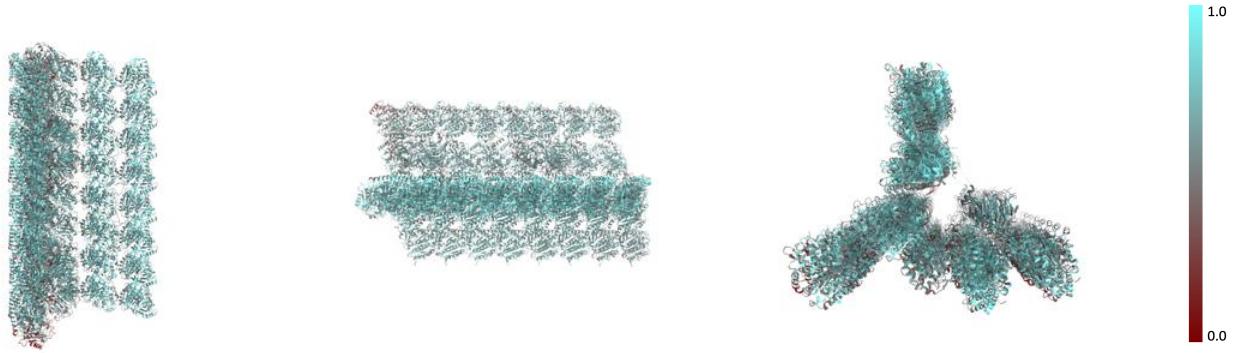
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

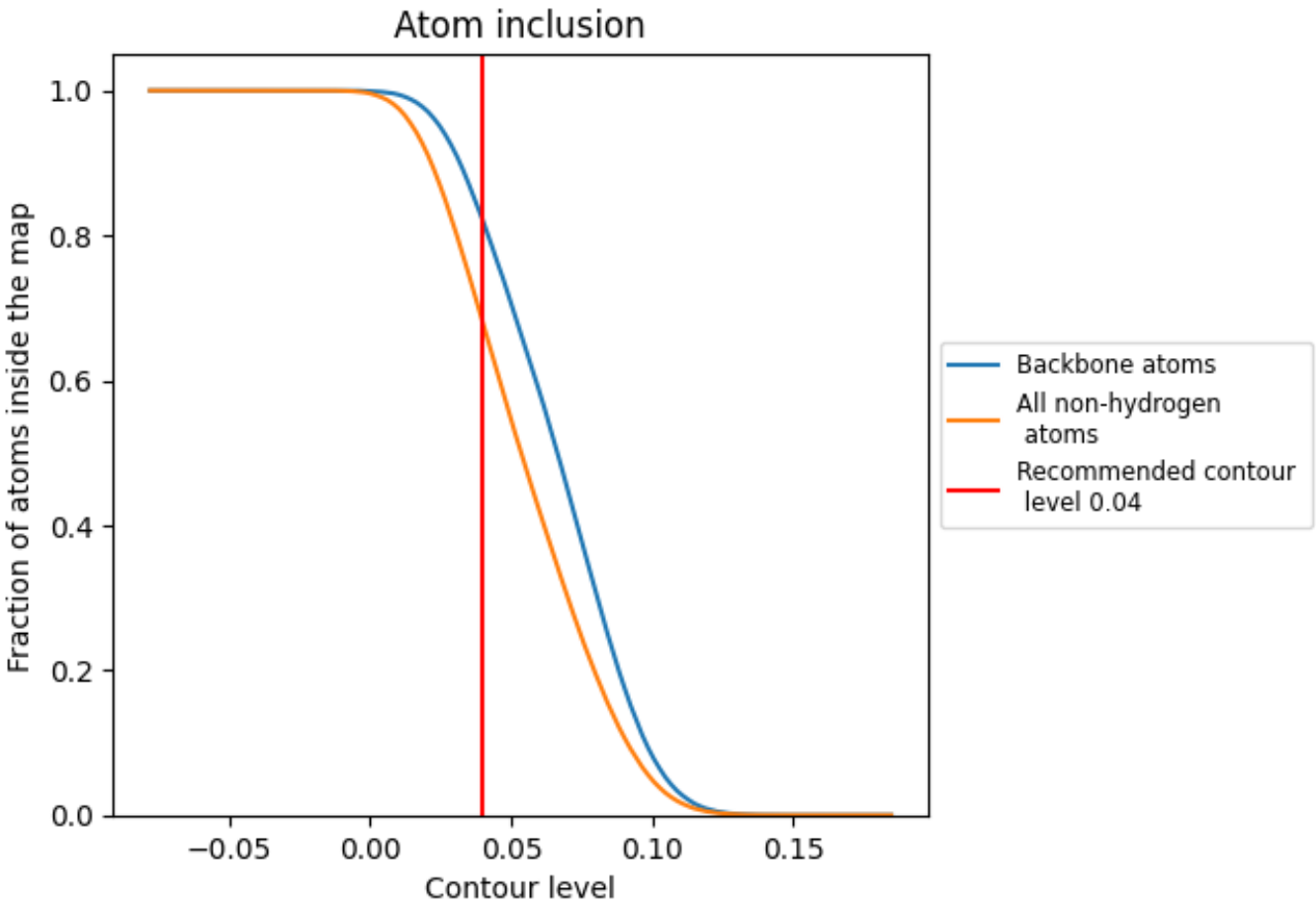
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6792	0.4550
0	0.6968	0.4940
1	0.6243	0.4110
2	0.5899	0.4670
3	0.7393	0.5060
4	0.5818	0.3770
5	0.7120	0.4520
6	0.4705	0.3470
7	0.6556	0.4360
8	0.6680	0.4440
9	0.6875	0.4460
A	0.5733	0.4350
B	0.5519	0.4100
C	0.5970	0.4340
D	0.7483	0.4970
E	0.6892	0.4540
F	0.6895	0.4590
G	0.6783	0.4530
H	0.7073	0.4720
I	0.7298	0.4820
J	0.7082	0.4600
K	0.7455	0.4880
L	0.7395	0.4840
M	0.7437	0.4870
N	0.7013	0.4680
O	0.7470	0.5000
P	0.7168	0.4820
Q	0.6910	0.4490
R	0.7539	0.5030
S	0.7210	0.4680
T	0.7509	0.4900
U	0.7524	0.5030
V	0.5933	0.3600
W	0.5102	0.4170
X	0.7301	0.4640

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.6468	0.4090
Z	0.7064	0.4440
a	0.5718	0.3800
b	0.6465	0.3960
c	0.7220	0.4960
d	0.4852	0.4430
e	0.6252	0.3940
f	0.7329	0.4900
g	0.7433	0.4980
h	0.6416	0.4370
i	0.7330	0.4560
j	0.6931	0.4290
k	0.7456	0.4960
l	0.6893	0.4890
m	0.7308	0.5050
n	0.6763	0.4800
o	0.6855	0.4800
p	0.7261	0.5030
q	0.7183	0.4950
r	0.7084	0.4990
s	0.6128	0.4120
t	0.6468	0.4490
u	0.7336	0.4620
v	0.6421	0.3930
w	0.6991	0.4490
x	0.4649	0.3960
y	0.7266	0.5020
z	0.7100	0.4840