Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 11:26 AM EDT

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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

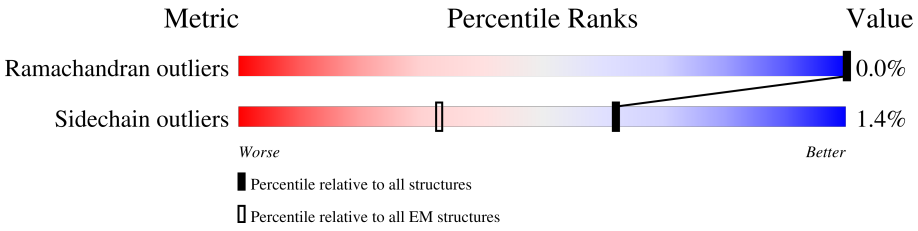
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	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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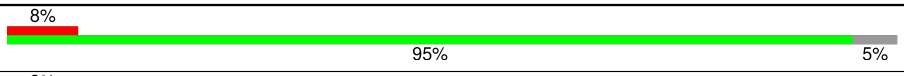
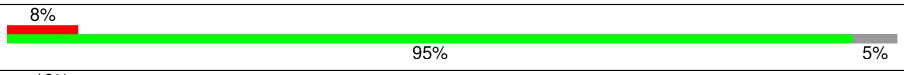
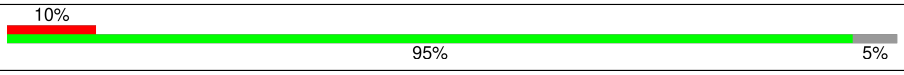
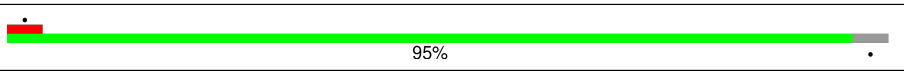
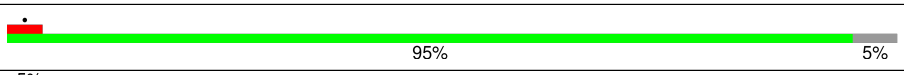
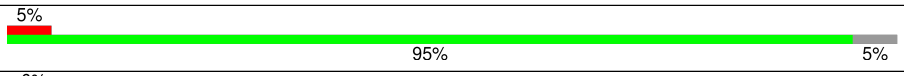
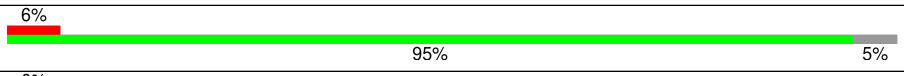
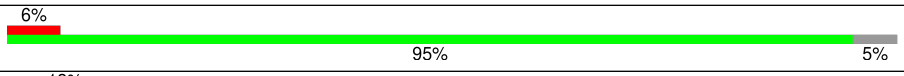
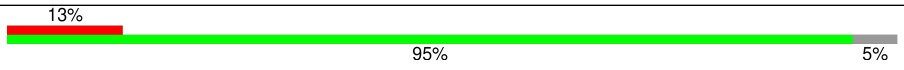
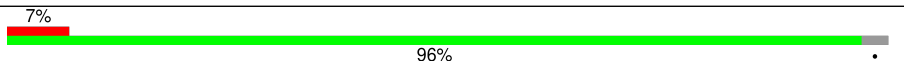
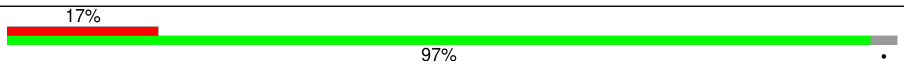
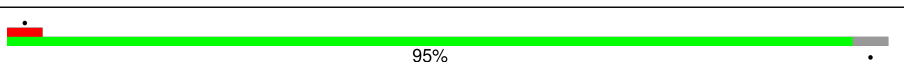
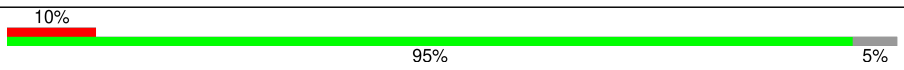
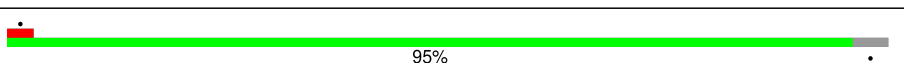
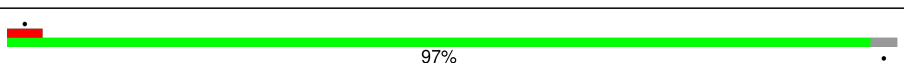
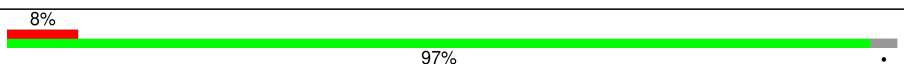
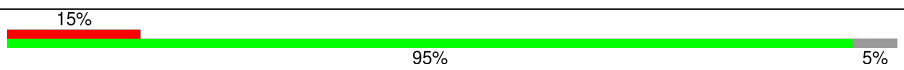
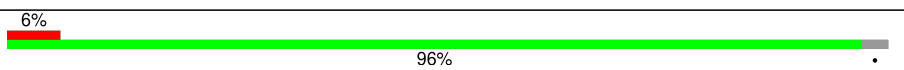
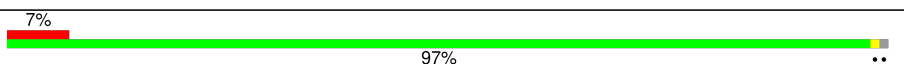
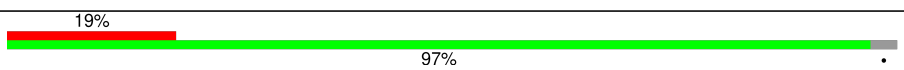
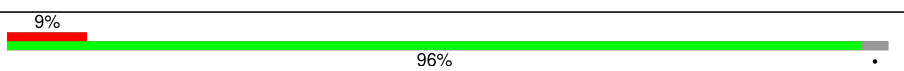
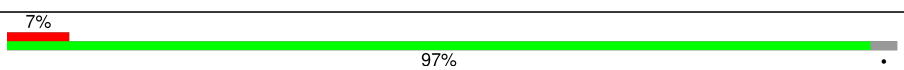
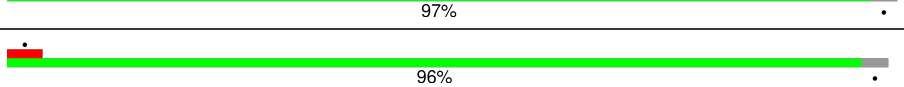
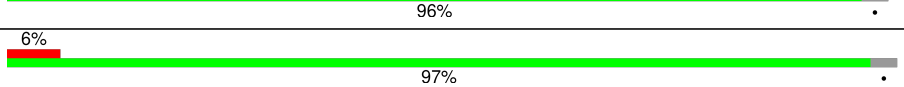
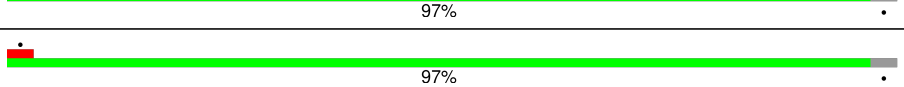
Mol	Chain	Length	Quality of chain
3	E	451	
3	F	451	
3	G	451	
3	L	451	
3	M	451	
3	P	451	
3	S	451	
3	X	451	
3	Y	451	
3	Z	451	
3	e	451	
3	f	451	
3	h	451	
3	k	451	
3	m	451	
3	o	451	
3	s	451	
3	y	451	
4	H	137	
5	4	443	
5	8	443	
5	9	443	
5	I	443	
5	J	443	
5	K	443	

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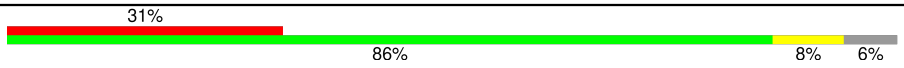
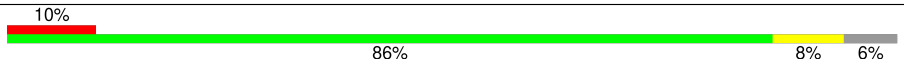
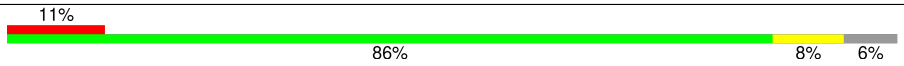
Mol	Chain	Length	Quality of chain
8	d	307	
8	l	307	
8	n	307	

2 Entry composition

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 3359	C 2110	N 576	O 643	S 30	0	0

- Molecule 6 is a protein called FAP276.

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

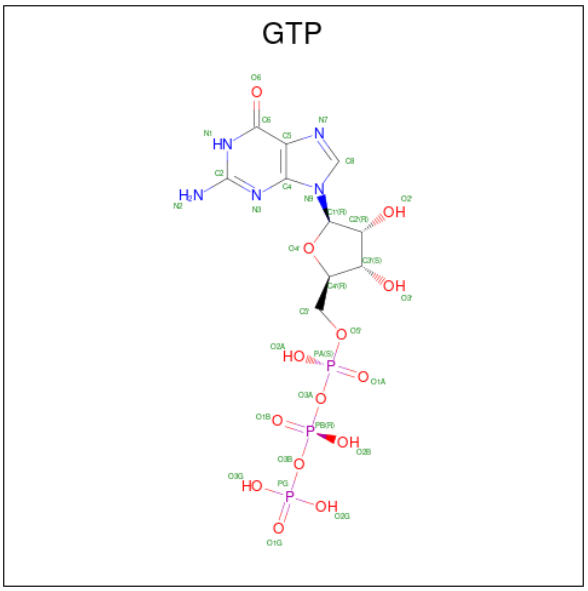
- Molecule 7 is a protein called Cilia- and flagella-associated protein 20.

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

- Molecule 8 is a protein called PACRG.

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

- 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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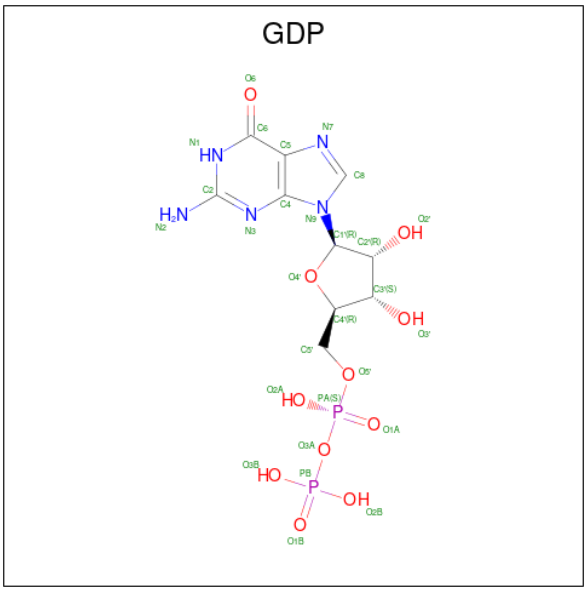
Mol	Chain	Residues	Atoms	AltConf
10	Y	1	Total Mg 1 1	0
10	Z	1	Total Mg 1 1	0
10	e	1	Total Mg 1 1	0
10	f	1	Total Mg 1 1	0
10	h	1	Total Mg 1 1	0
10	k	1	Total Mg 1 1	0
10	m	1	Total Mg 1 1	0
10	o	1	Total Mg 1 1	0
10	p	1	Total Mg 1 1	0
10	s	1	Total Mg 1 1	0
10	0	1	Total Mg 1 1	0
10	1	1	Total Mg 1 1	0
10	5	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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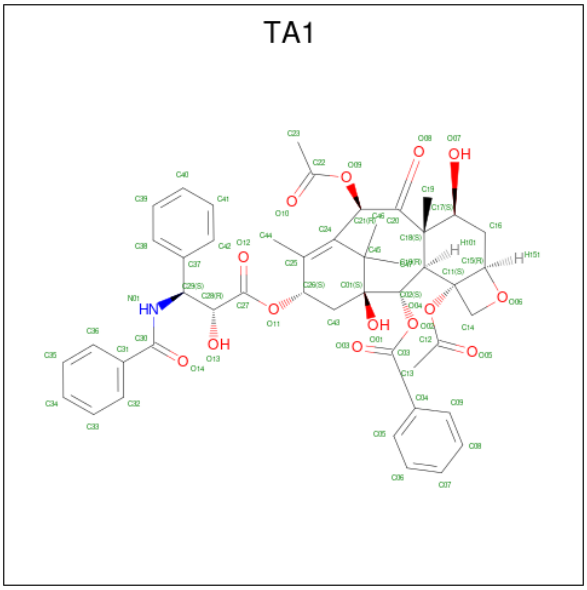
Mol	Chain	Residues	Atoms					AltConf
11	p	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	q	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	r	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	t	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	u	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	v	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	w	1	Total	C	N	O	P	0
			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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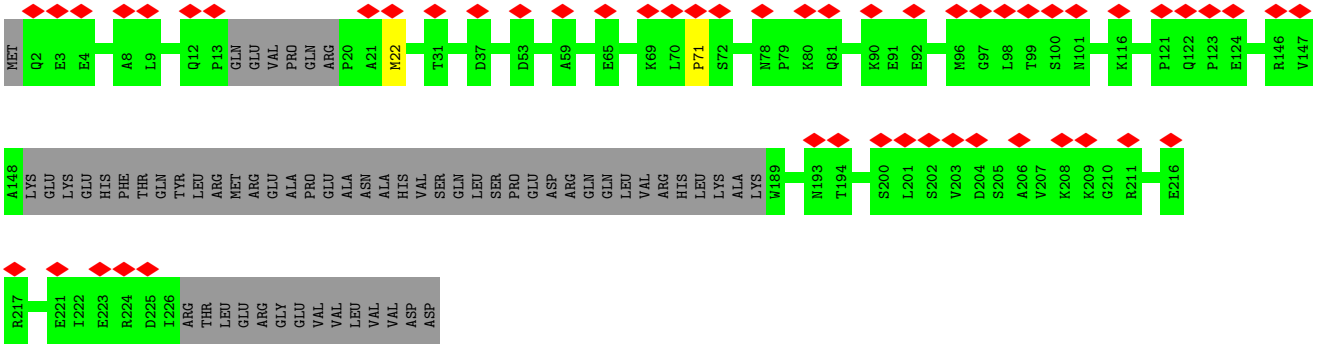
Mol	Chain	Residues	Atoms				AltConf
12	V	1	Total	C	N	O	0
			62	47	1	14	
12	a	1	Total	C	N	O	0
			62	47	1	14	
12	b	1	Total	C	N	O	0
			62	47	1	14	
12	i	1	Total	C	N	O	0
			62	47	1	14	
12	j	1	Total	C	N	O	0
			62	47	1	14	
12	p	1	Total	C	N	O	0
			62	47	1	14	
12	q	1	Total	C	N	O	0
			62	47	1	14	
12	r	1	Total	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.

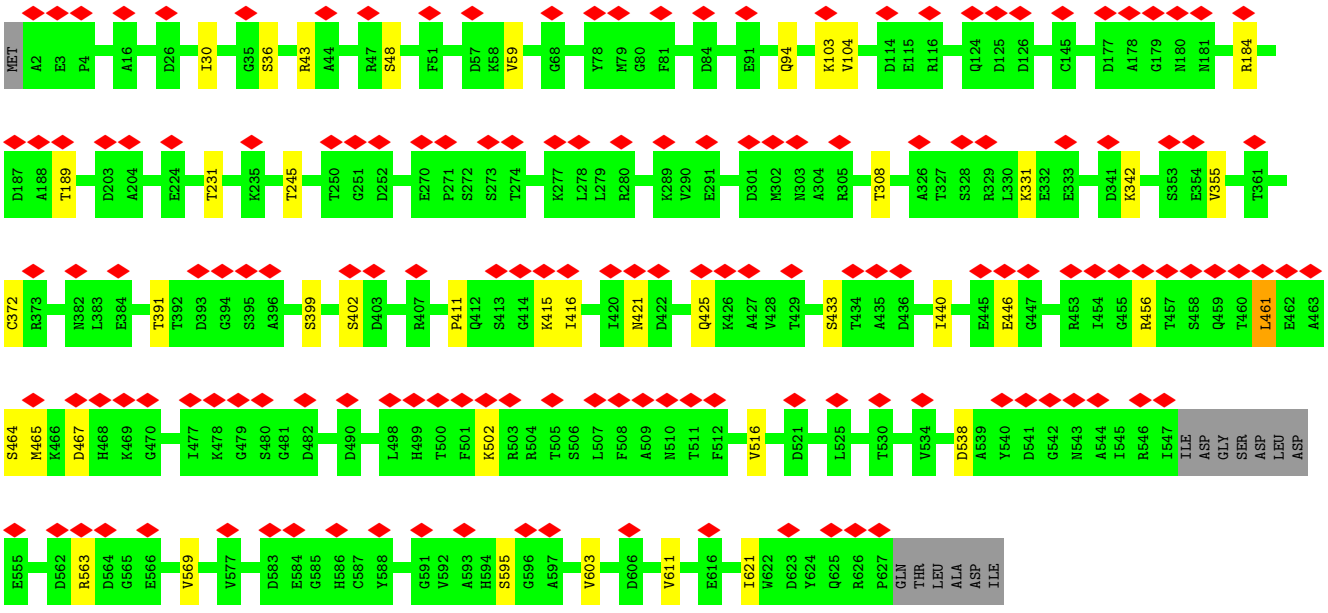
• Molecule 1: Flagellar associated protein

Chain A:



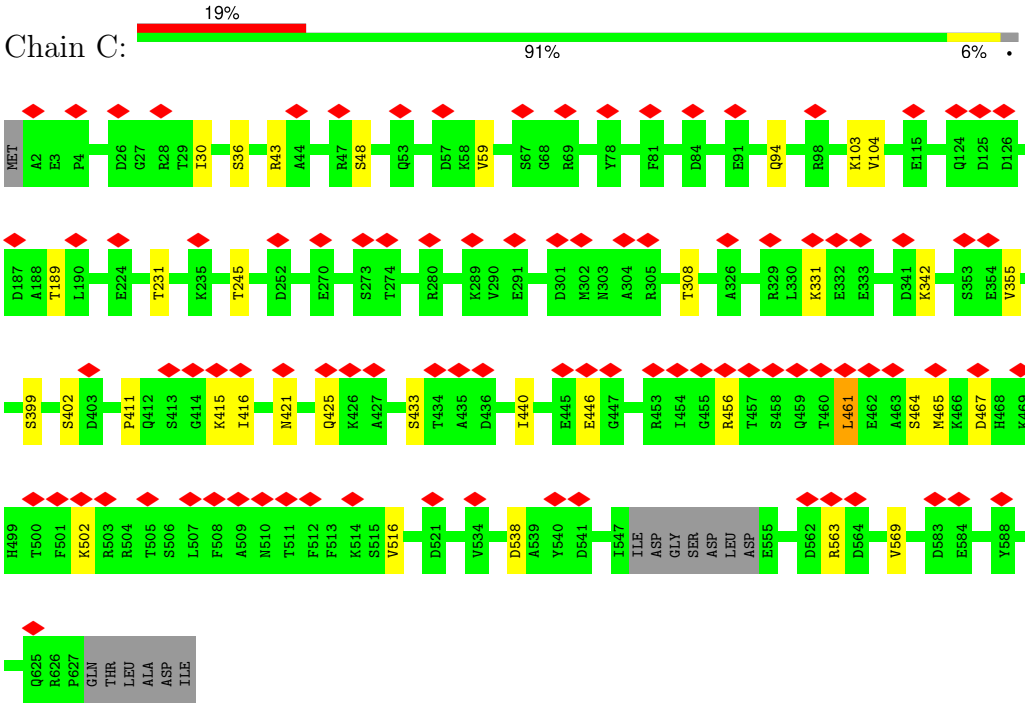
• Molecule 2: FAP52

Chain B:



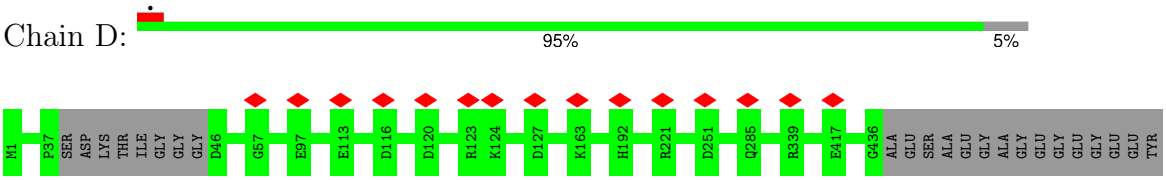
• Molecule 2: FAP52

Chain C:



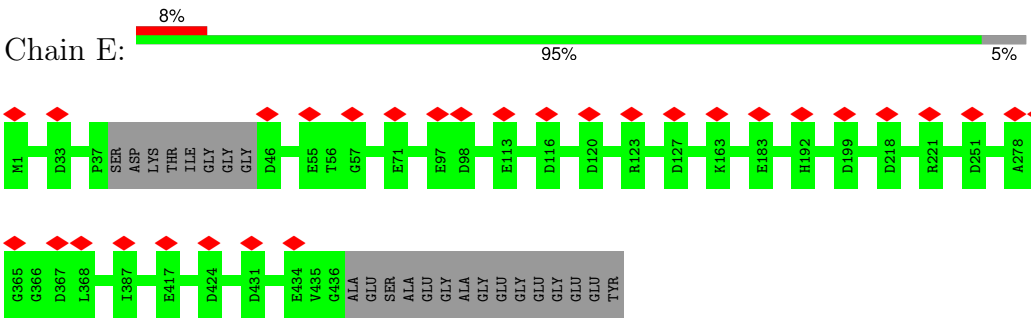
• Molecule 3: Tubulin alpha

Chain D:



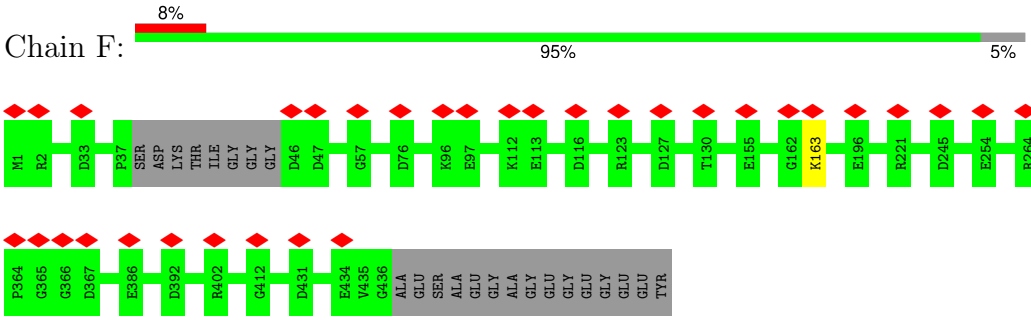
• Molecule 3: Tubulin alpha

Chain E:



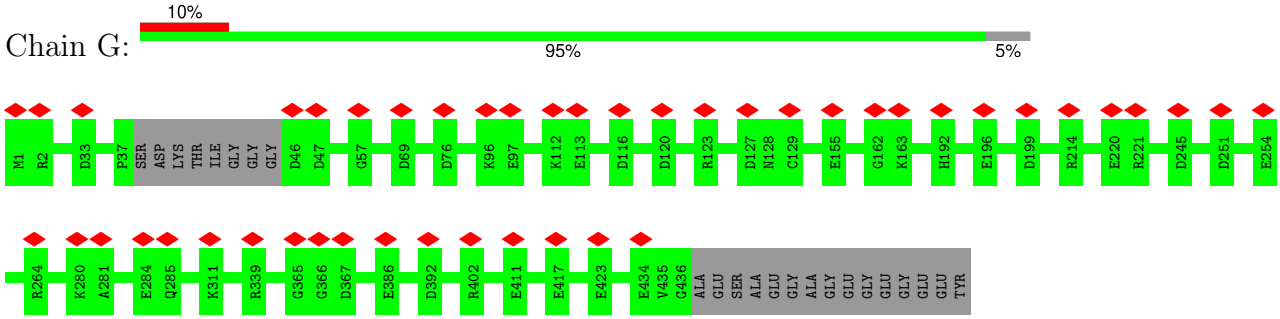
• Molecule 3: Tubulin alpha

Chain F:



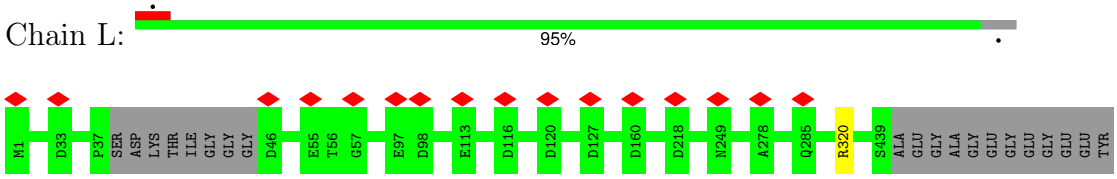
• Molecule 3: Tubulin alpha

Chain G:



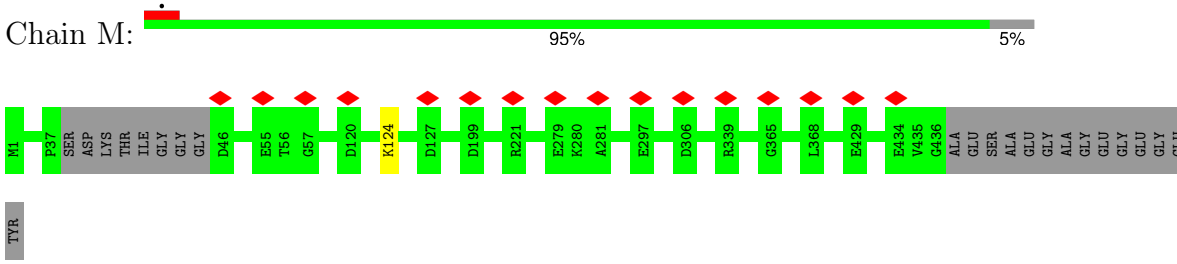
• Molecule 3: Tubulin alpha

Chain L:



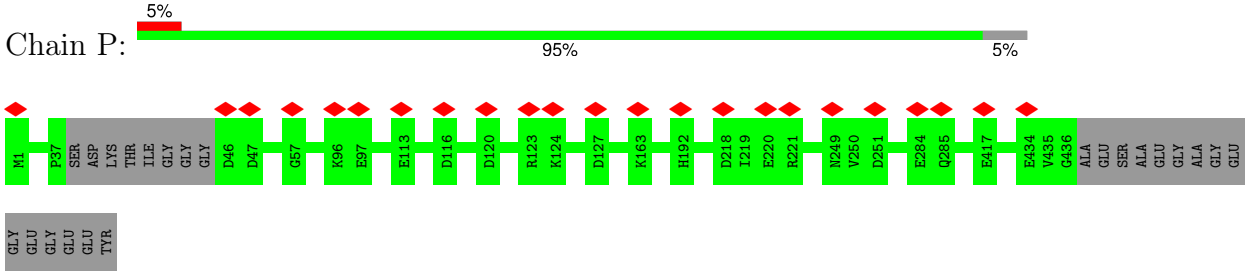
• Molecule 3: Tubulin alpha

Chain M:



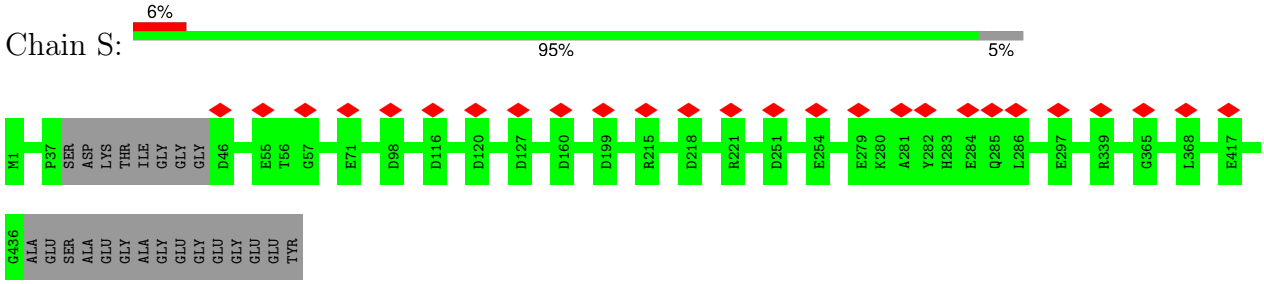
• Molecule 3: Tubulin alpha

Chain P:



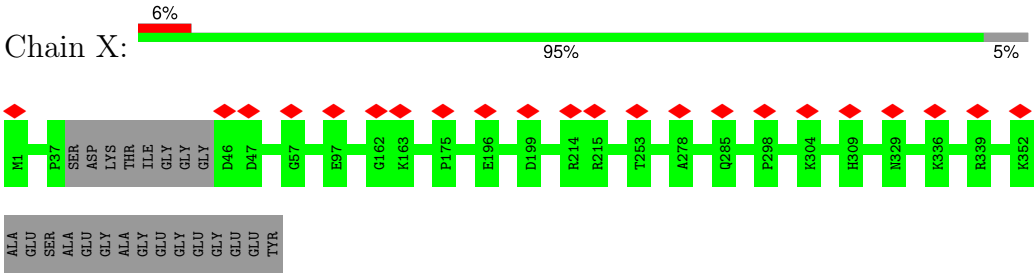
• Molecule 3: Tubulin alpha

Chain S:



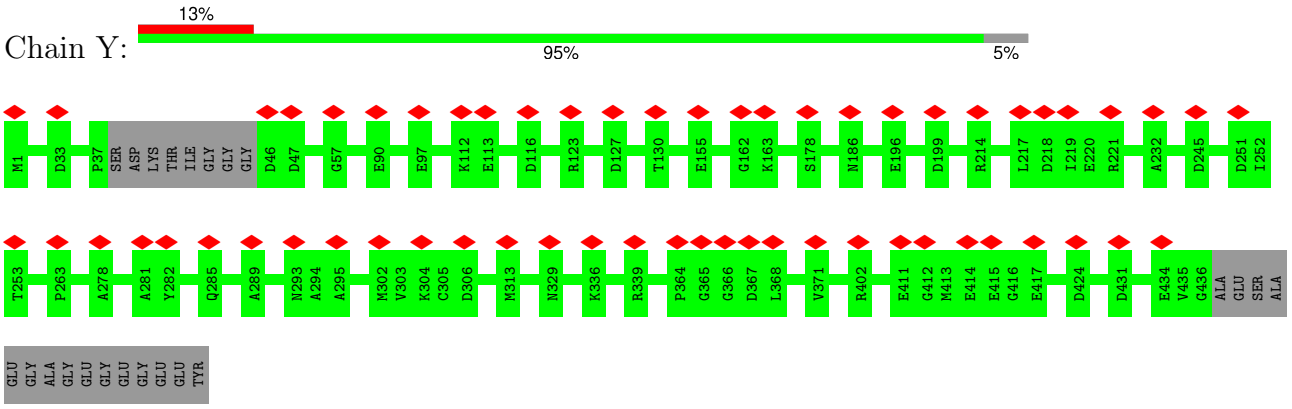
• Molecule 3: Tubulin alpha

Chain X:



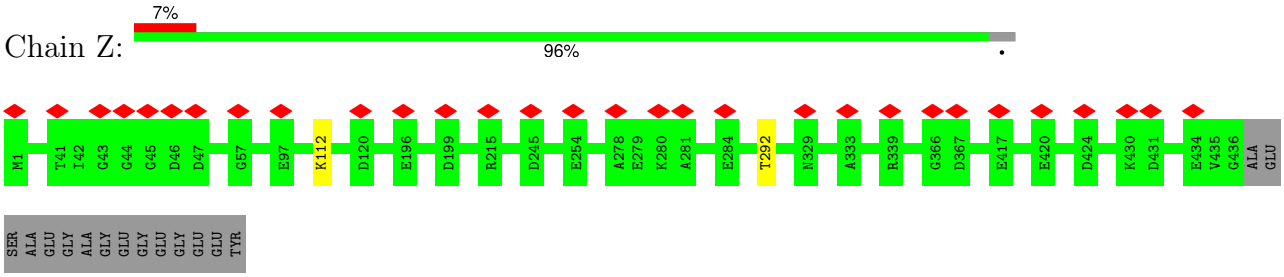
• Molecule 3: Tubulin alpha

Chain Y:



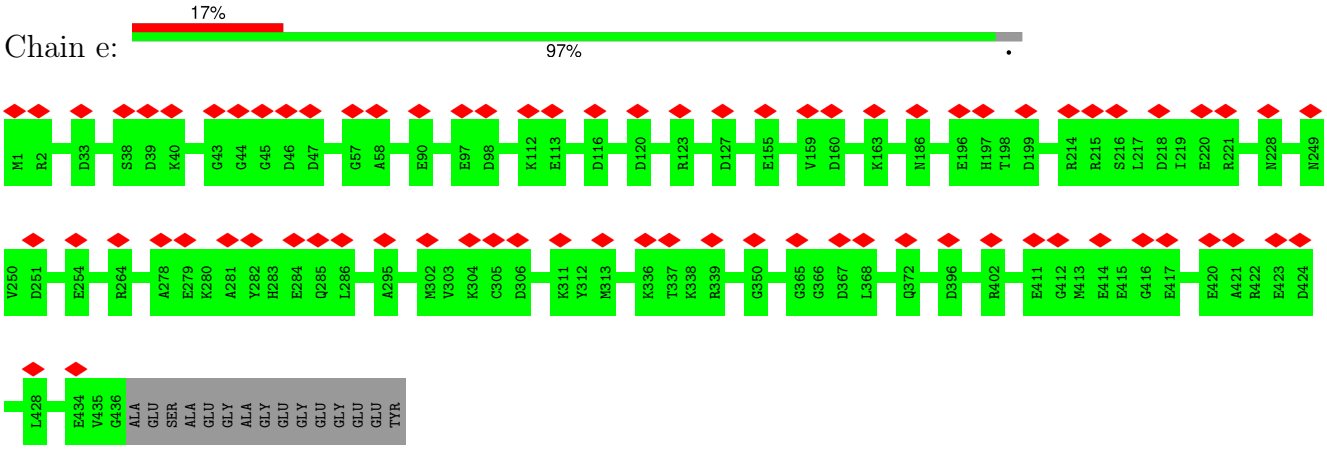
• Molecule 3: Tubulin alpha

Chain Z:



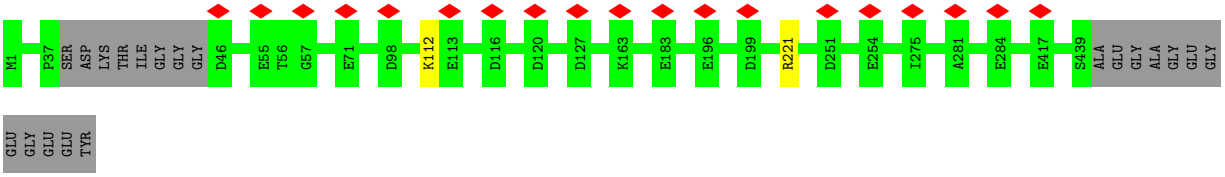
• Molecule 3: Tubulin alpha

Chain e:

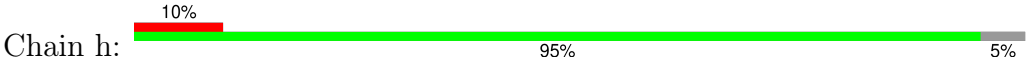


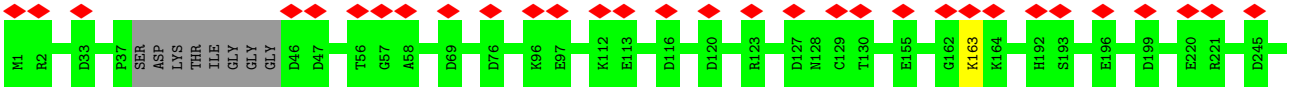
• Molecule 3: Tubulin alpha

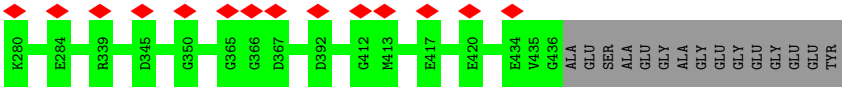
Chain f:



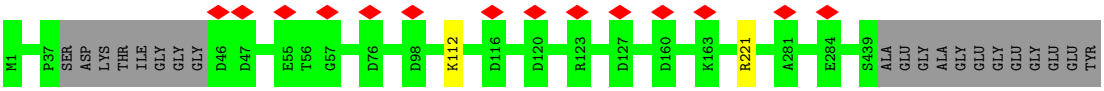
• Molecule 3: Tubulin alpha



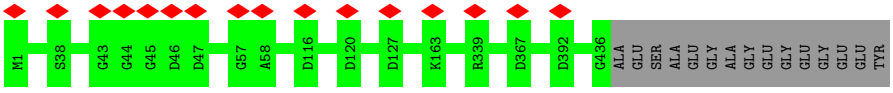




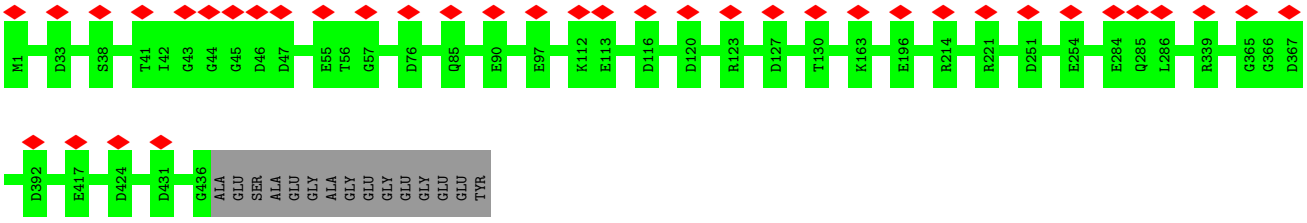
• Molecule 3: Tubulin alpha



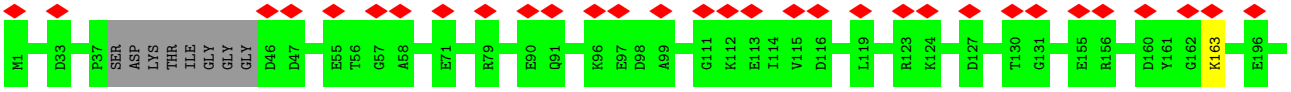
• Molecule 3: Tubulin alpha

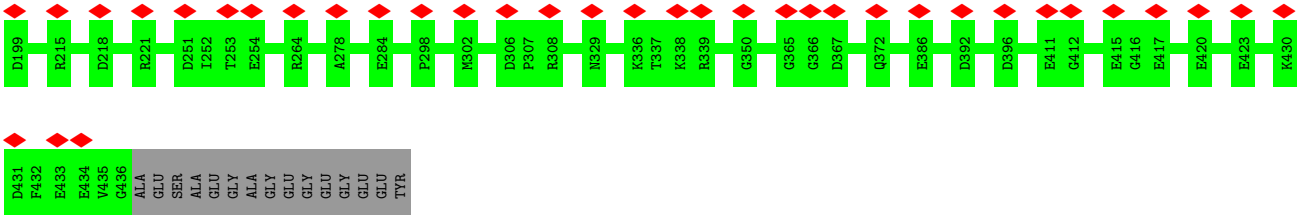


• Molecule 3: Tubulin alpha

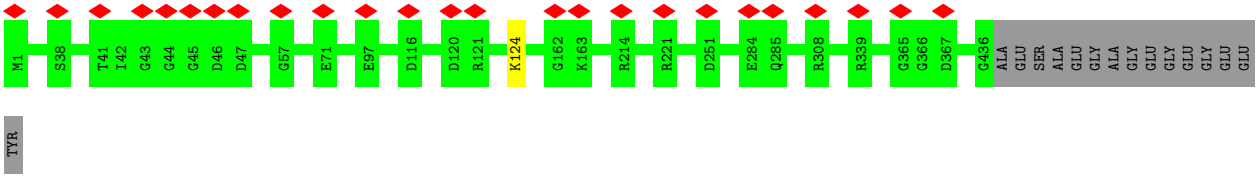


• Molecule 3: Tubulin alpha

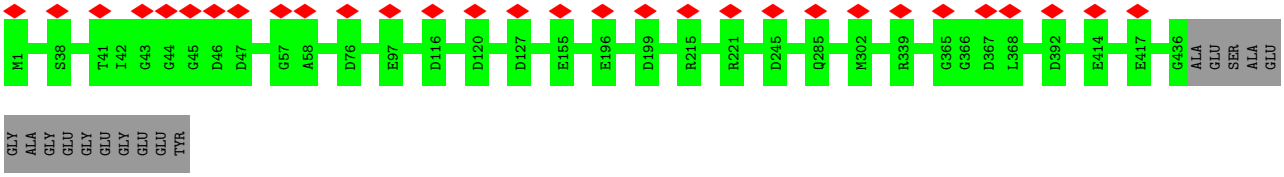




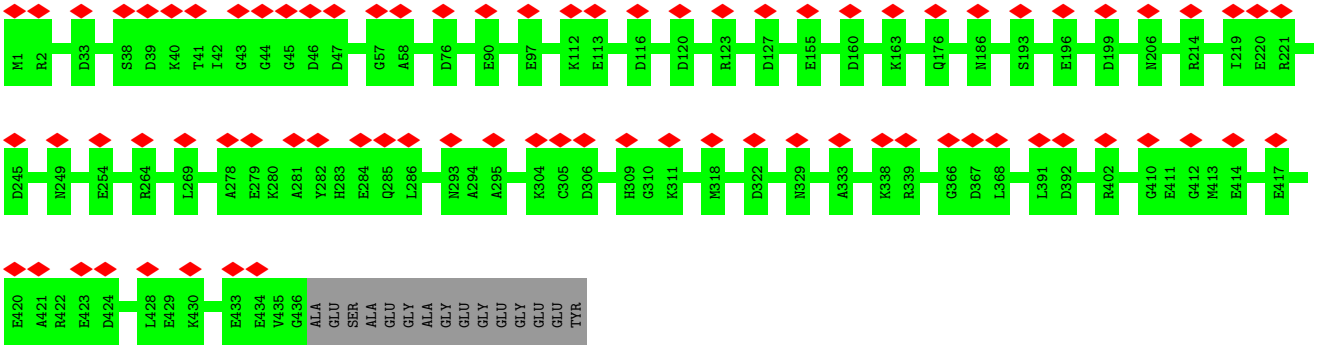
• Molecule 3: Tubulin alpha



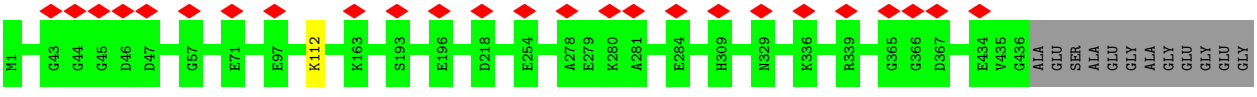
• Molecule 3: Tubulin alpha



• Molecule 3: Tubulin alpha

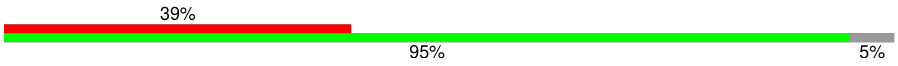


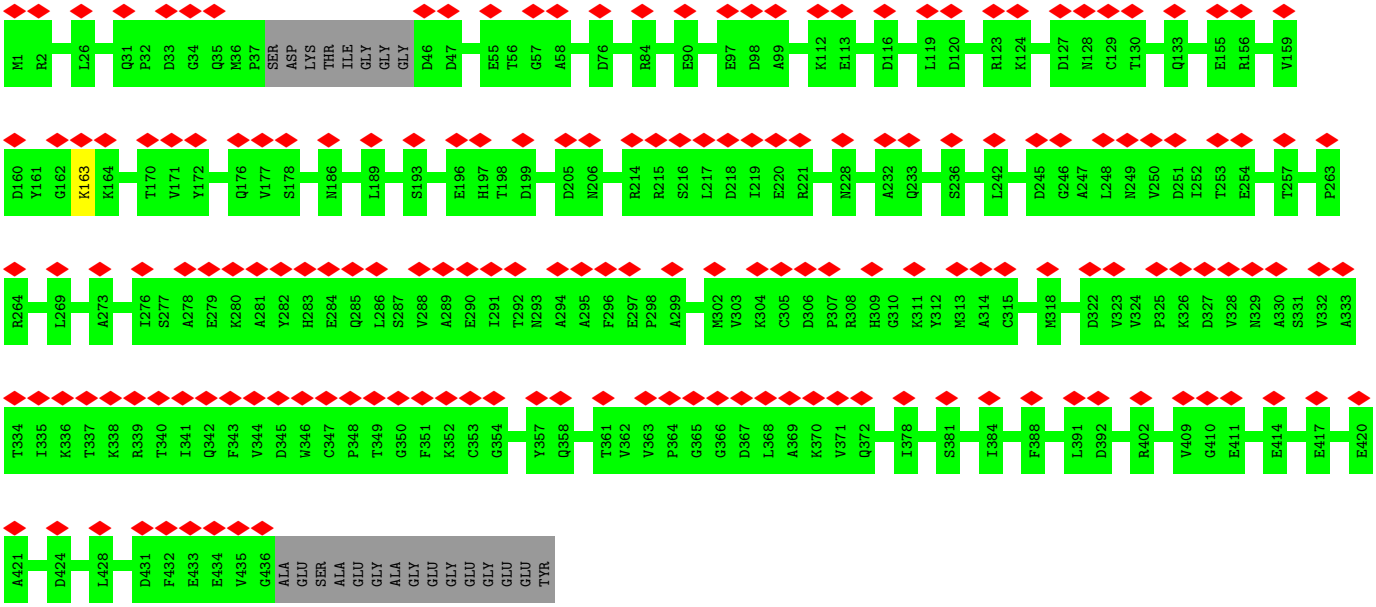
• Molecule 3: Tubulin alpha



• Molecule 3: Tubulin alpha

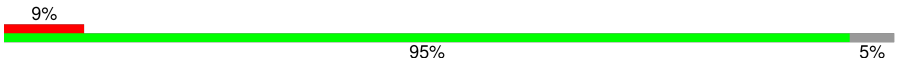
Chain 6:

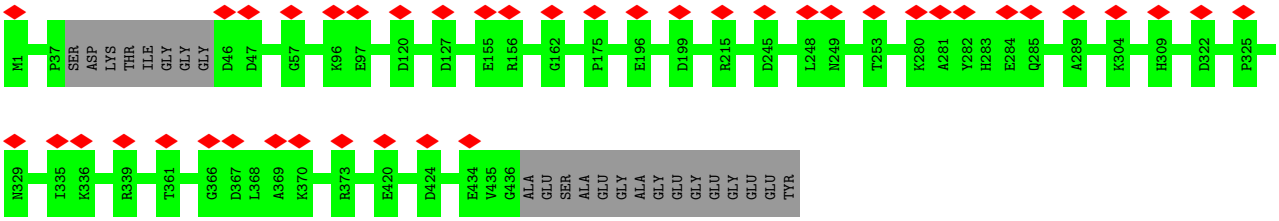




• Molecule 3: Tubulin alpha

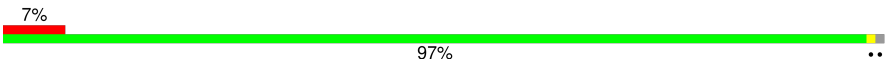
Chain 7:

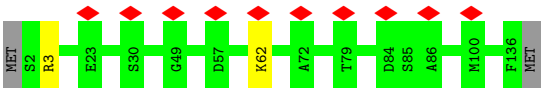




• Molecule 4: Protein Flattop homolog

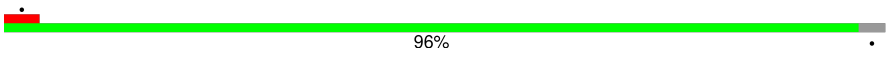
Chain H:

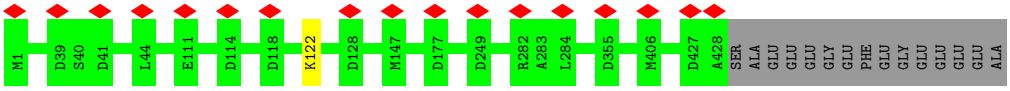




• Molecule 5: Tubulin beta

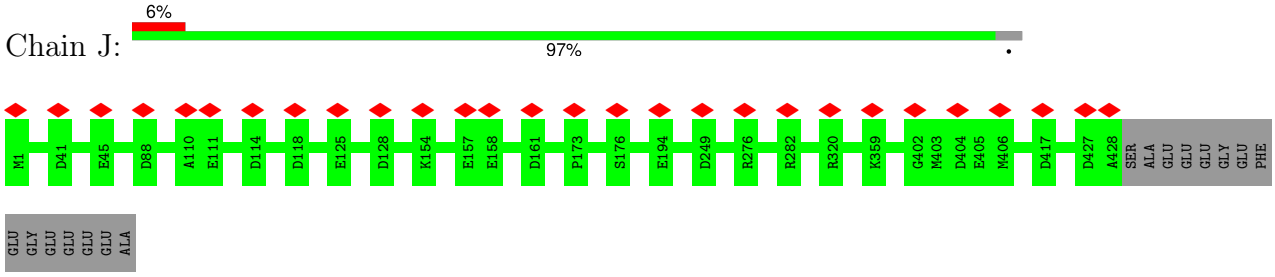
Chain I:





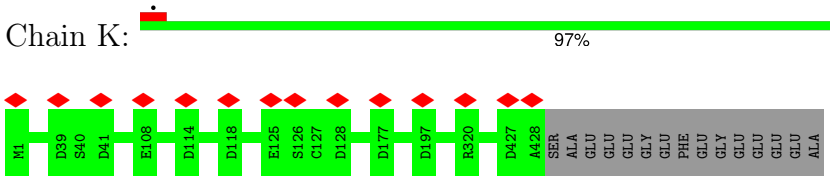
• Molecule 5: Tubulin beta

Chain J:



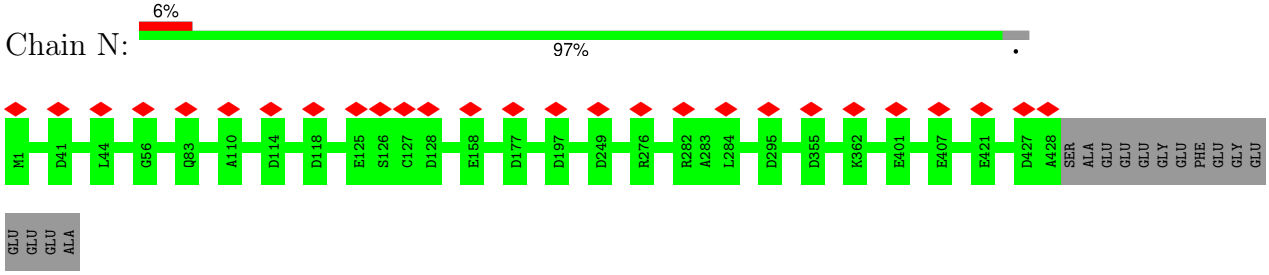
• Molecule 5: Tubulin beta

Chain K:



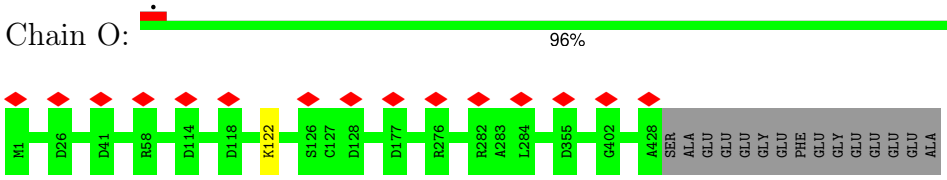
• Molecule 5: Tubulin beta

Chain N:



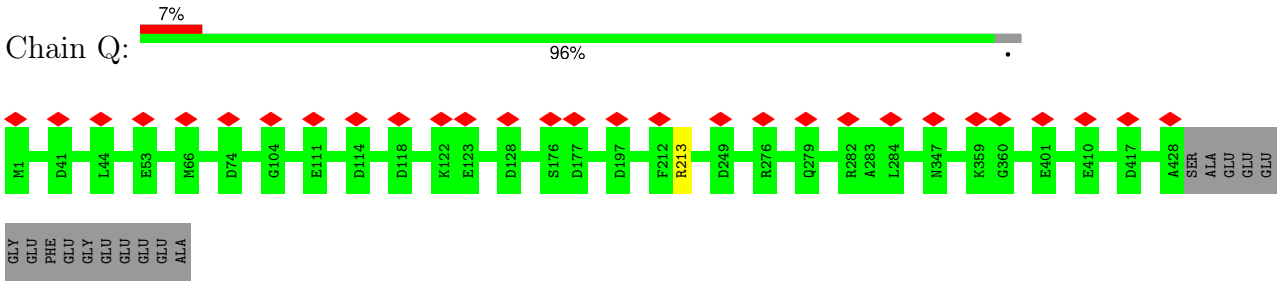
• Molecule 5: Tubulin beta

Chain O:



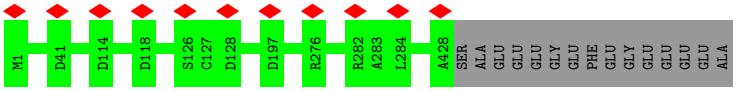
• Molecule 5: Tubulin beta

Chain Q:



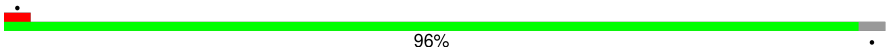
• Molecule 5: Tubulin beta

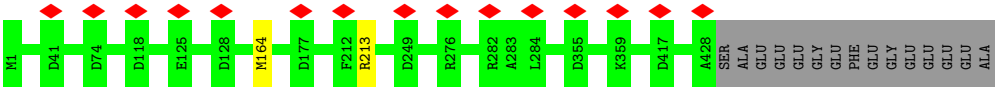
Chain R:



• Molecule 5: Tubulin beta

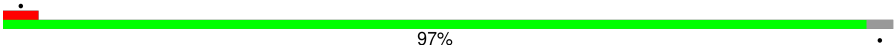
Chain T:

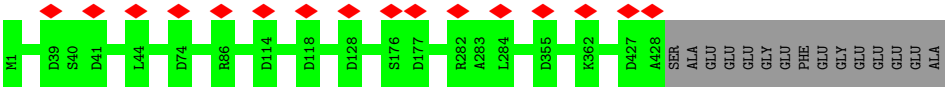




• Molecule 5: Tubulin beta

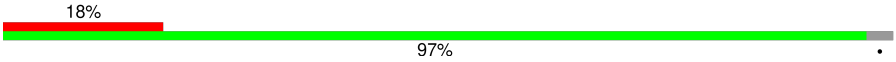
Chain U:

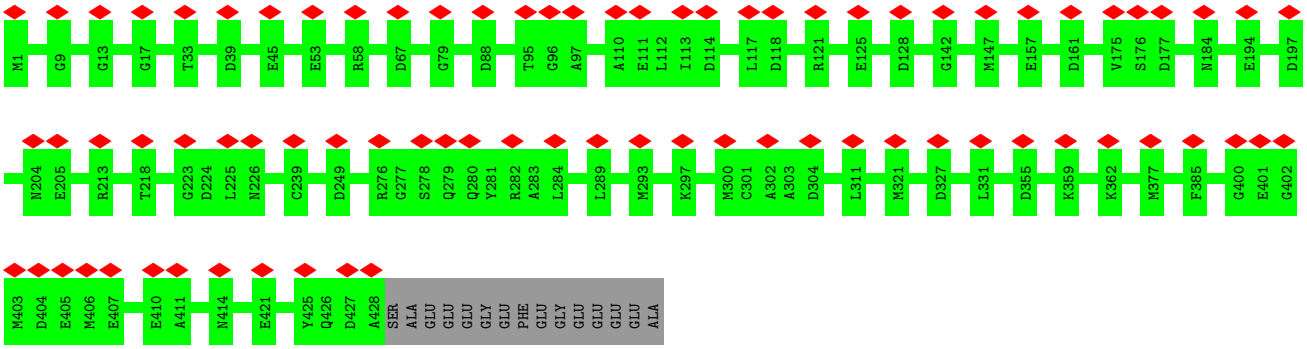




• Molecule 5: Tubulin beta

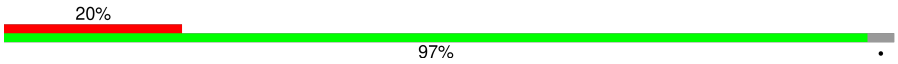
Chain V:

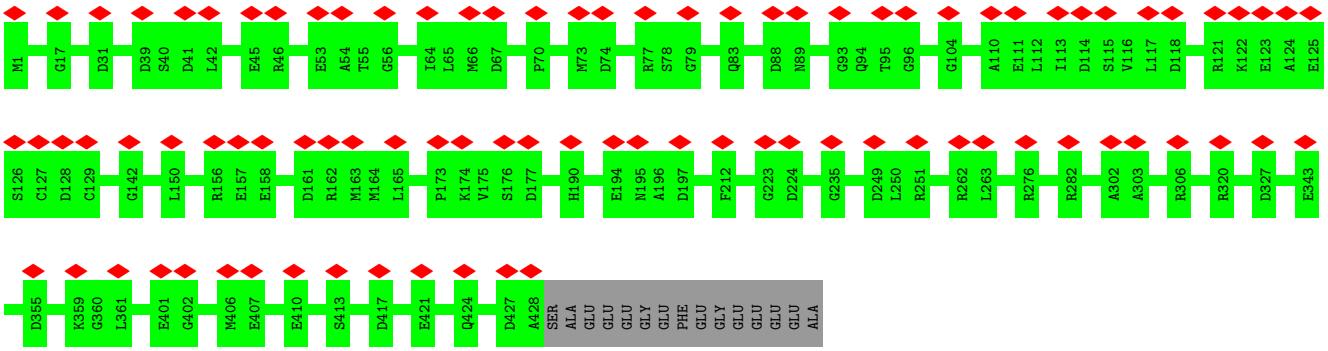




• Molecule 5: Tubulin beta

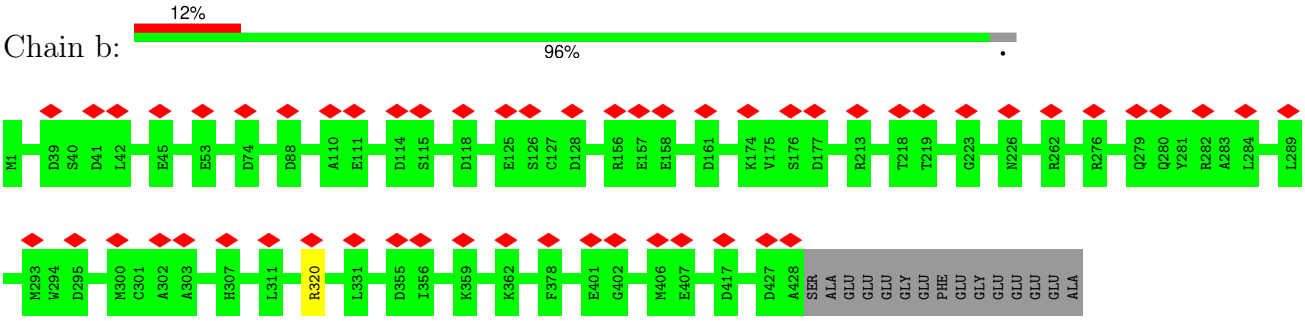
Chain a:





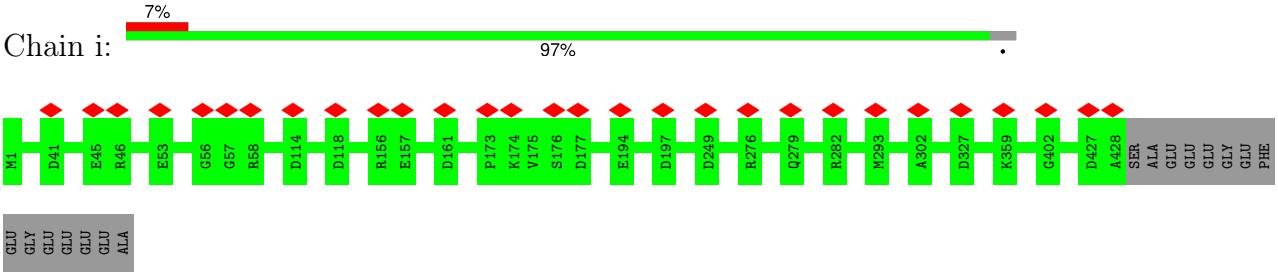
• Molecule 5: Tubulin beta

Chain b:



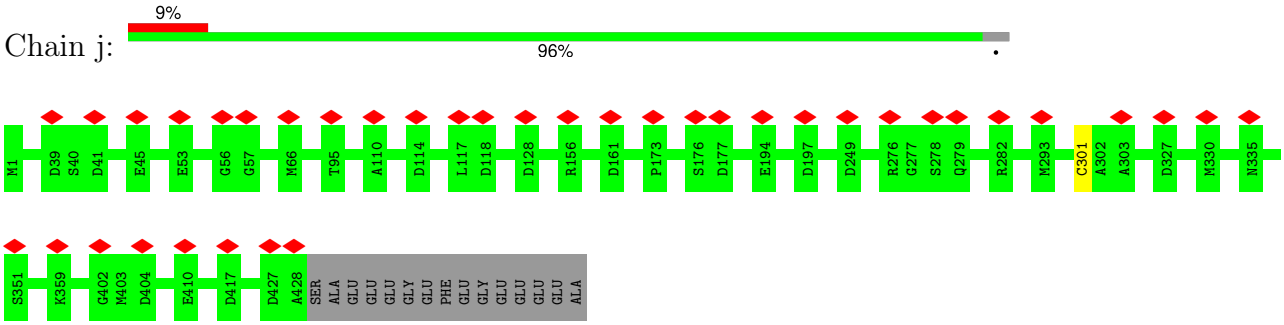
• Molecule 5: Tubulin beta

Chain i:



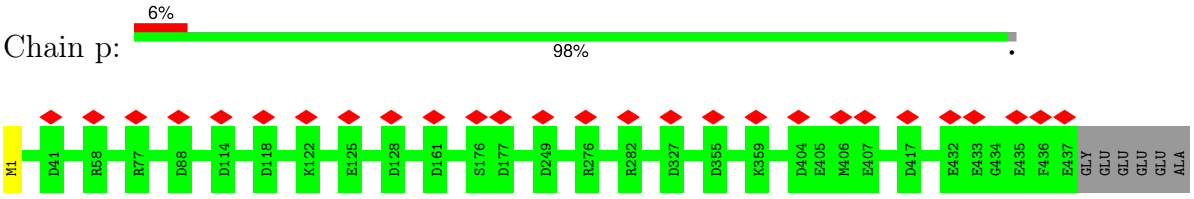
• Molecule 5: Tubulin beta

Chain j:



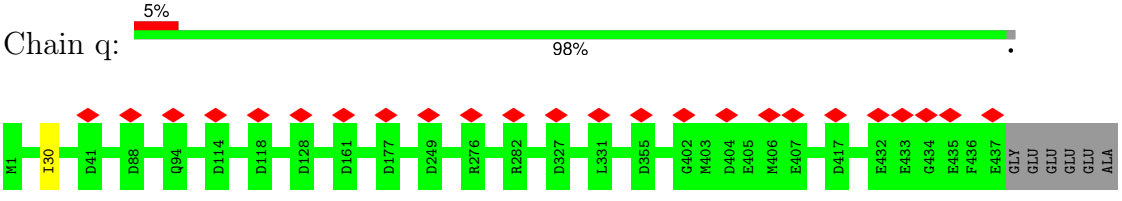
• Molecule 5: Tubulin beta

Chain p:



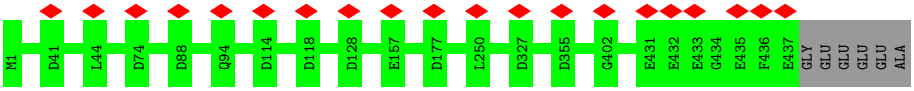
• Molecule 5: Tubulin beta

Chain q:



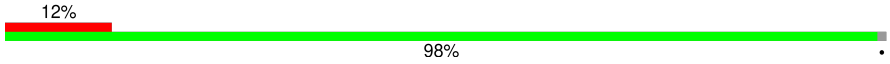
• Molecule 5: Tubulin beta

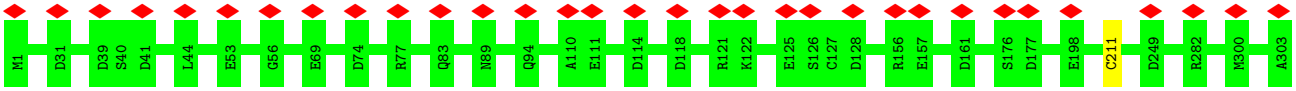
Chain r:

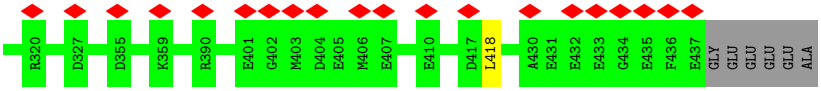


• Molecule 5: Tubulin beta

Chain t:

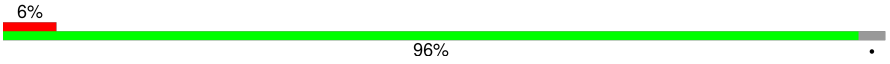


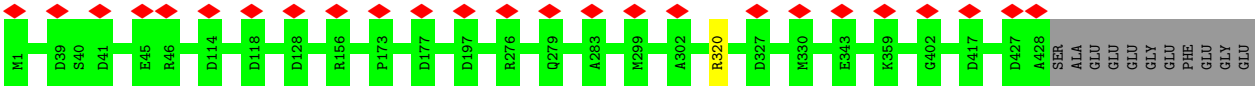




• Molecule 5: Tubulin beta

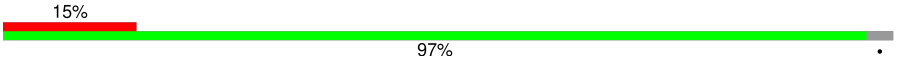
Chain u:

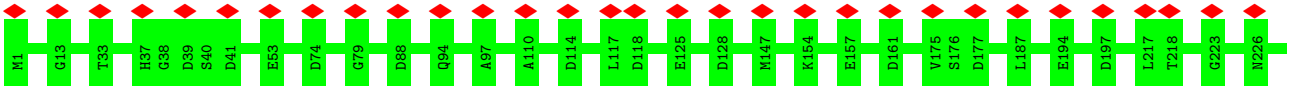


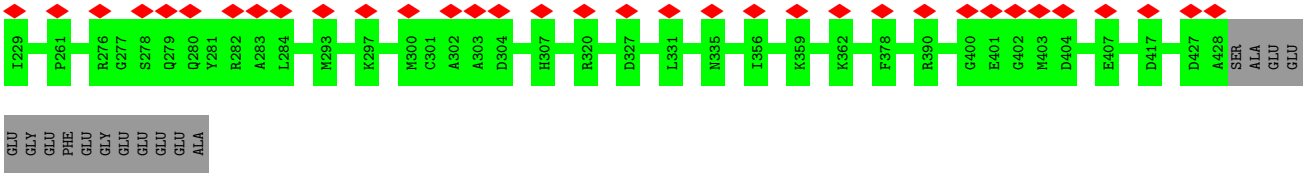


• Molecule 5: Tubulin beta

Chain v:

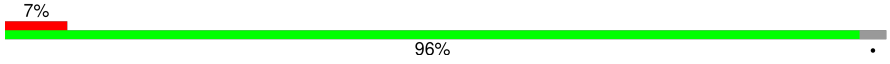


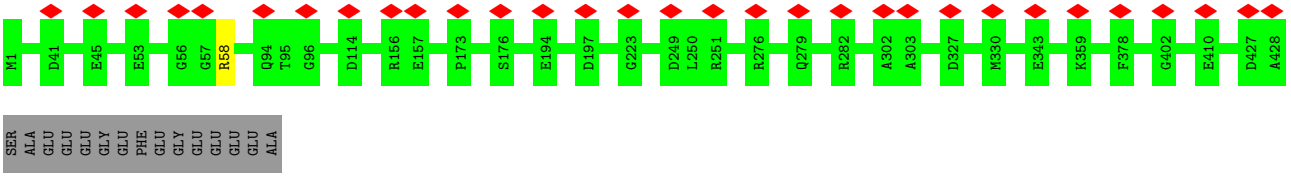




• Molecule 5: Tubulin beta

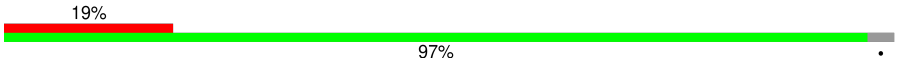
Chain w:

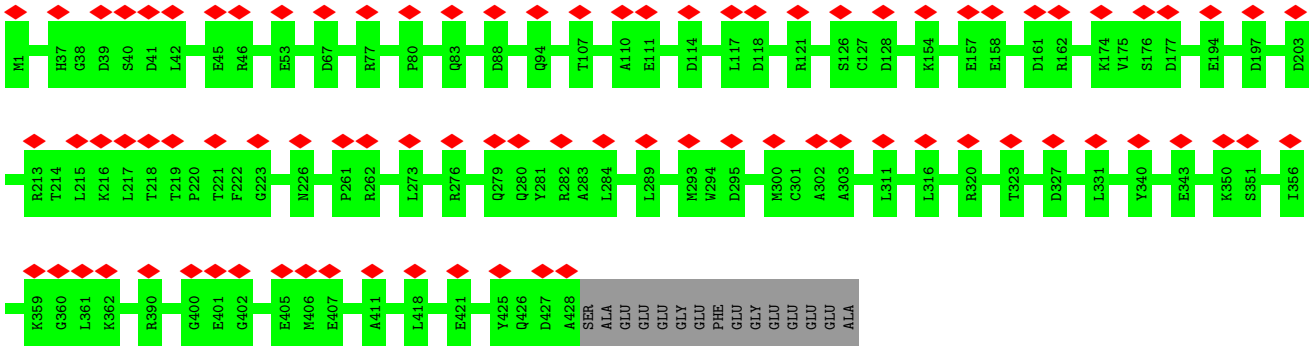




• Molecule 5: Tubulin beta

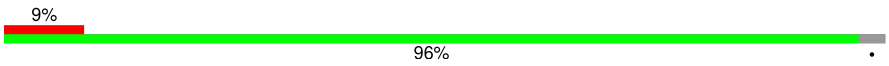
Chain 4:

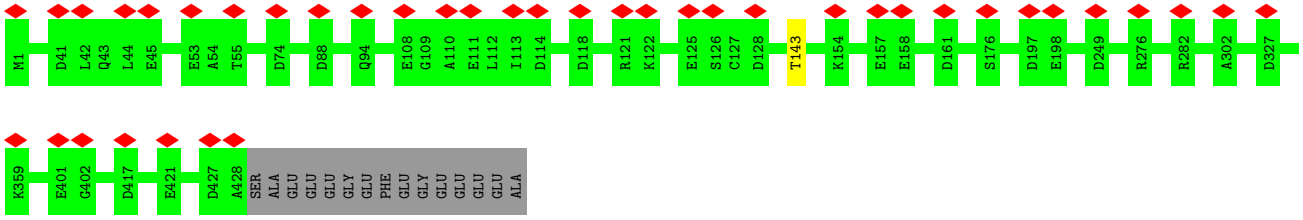




• Molecule 5: Tubulin beta

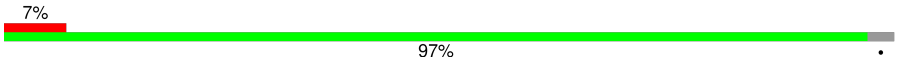
Chain 8:

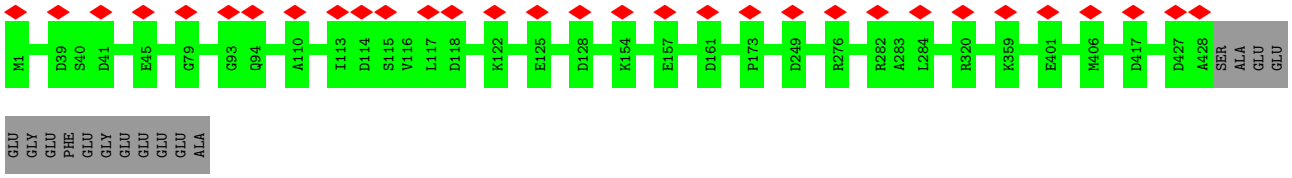




• Molecule 5: Tubulin beta

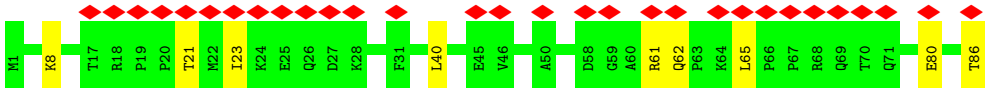
Chain 9:





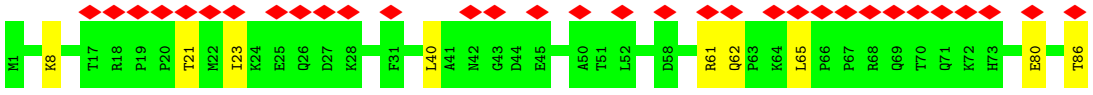
• Molecule 6: FAP276

Chain W:



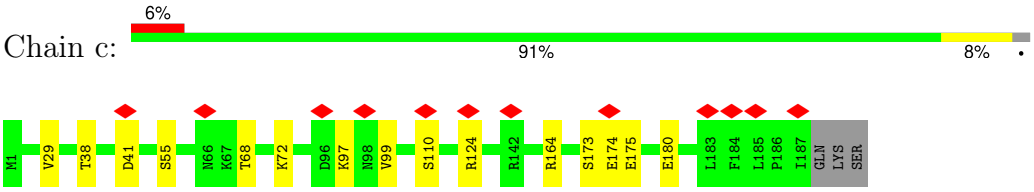
• Molecule 6: FAP276

Chain x:



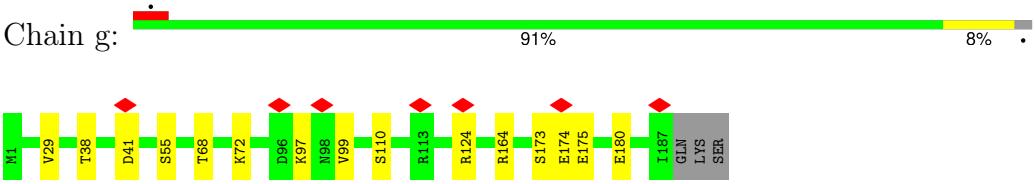
• Molecule 7: Cilia- and flagella-associated protein 20

Chain c:



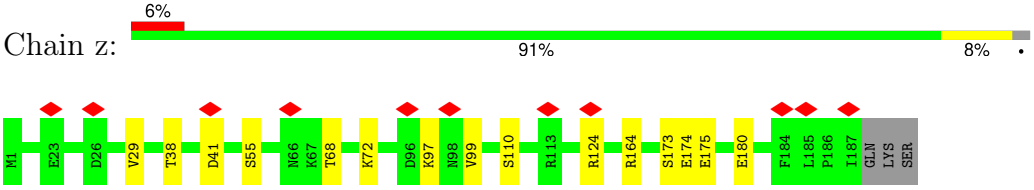
• Molecule 7: Cilia- and flagella-associated protein 20

Chain g:



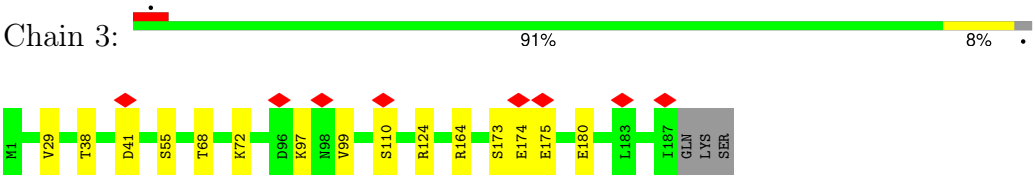
• Molecule 7: Cilia- and flagella-associated protein 20

Chain z:



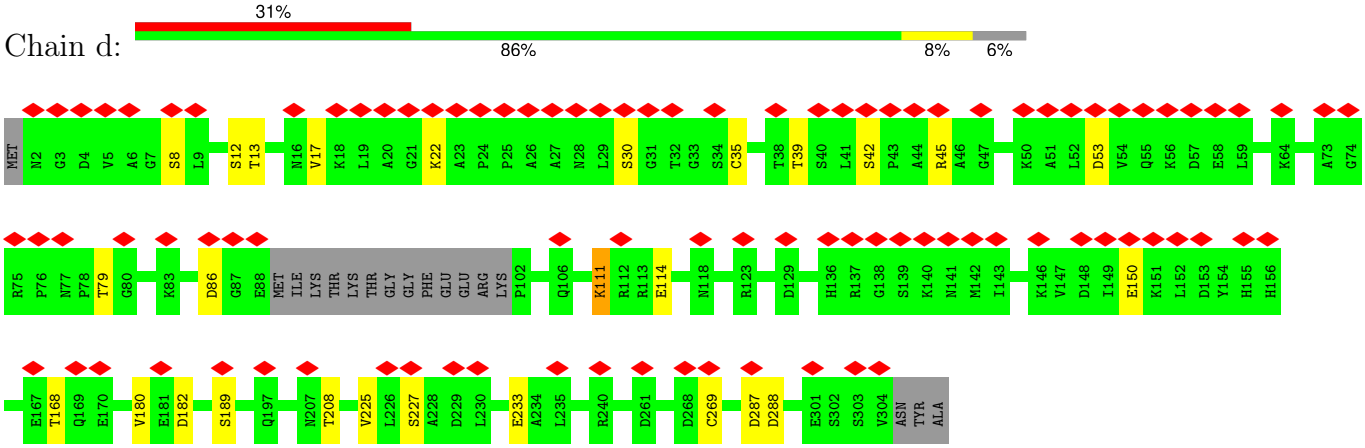
• Molecule 7: Cilia- and flagella-associated protein 20

Chain 3:



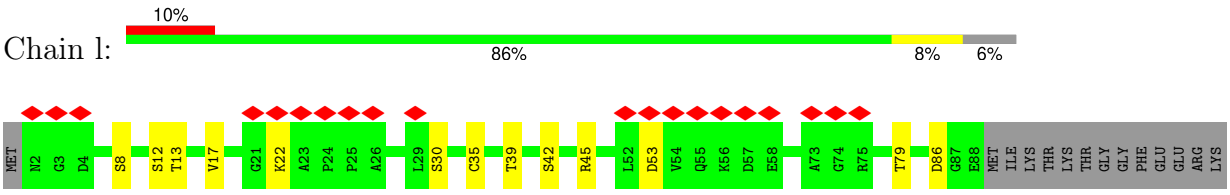
• Molecule 8: PACRG

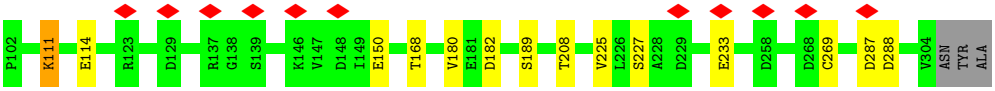
Chain d:



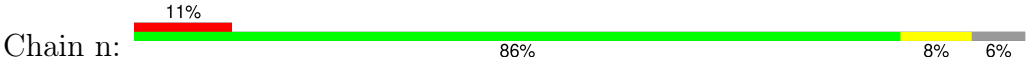
• Molecule 8: PACRG

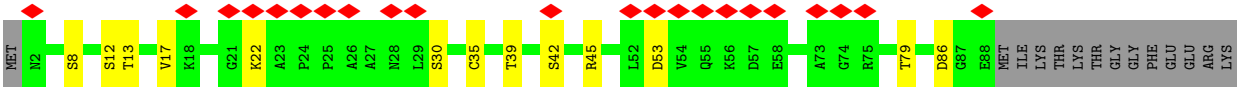
Chain l:



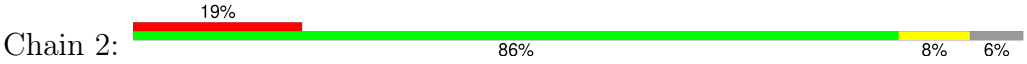


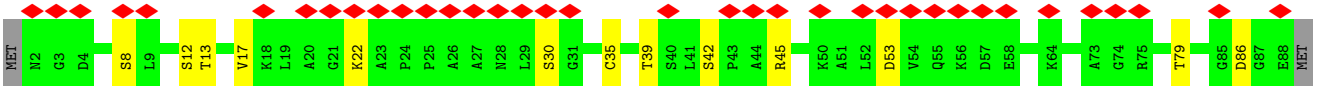
• Molecule 8: PACRG

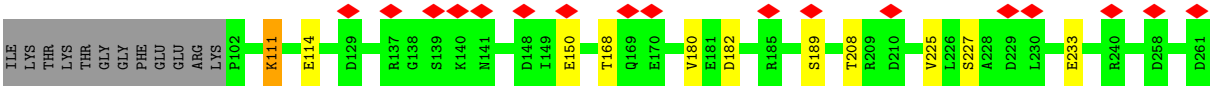


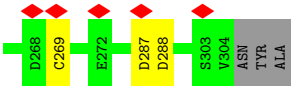


• Molecule 8: PACRG









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, GTP, TA1, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	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.

All (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
2	B	461	LEU	CA-CB-CG	6.12	129.38	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	461	LEU	CA-CB-CG	6.11	129.35	115.30
6	x	61	ARG	NE-CZ-NH1	-5.09	117.75	120.30
6	W	61	ARG	NE-CZ-NH1	-5.03	117.79	120.30

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%)	11 43
2	B	615/633 (97%)	541 (88%)	72 (12%)	2 (0%)	37 67
2	C	615/633 (97%)	541 (88%)	72 (12%)	2 (0%)	37 67
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	44	73
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
2	C	411	PRO
1	A	71	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%)	10 35
2	C	505/517 (98%)	465 (92%)	40 (8%)	10 35
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%)	91 96
3	6	361/374 (96%)	360 (100%)	1 (0%)	91 96
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%)	91 96
3	G	361/374 (96%)	361 (100%)	0	100 100
3	L	363/374 (97%)	362 (100%)	1 (0%)	91 96
3	M	361/374 (96%)	360 (100%)	1 (0%)	91 96
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%)	86 93
3	e	366/374 (98%)	366 (100%)	0	100 100
3	f	363/374 (97%)	361 (99%)	2 (1%)	84 92
3	h	361/374 (96%)	360 (100%)	1 (0%)	91 96
3	k	363/374 (97%)	361 (99%)	2 (1%)	84 92
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%)	91 96
3	y	366/374 (98%)	365 (100%)	1 (0%)	91 96
4	H	119/121 (98%)	117 (98%)	2 (2%)	56 75
5	4	368/379 (97%)	368 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	91 96
5	J	368/379 (97%)	368 (100%)	0	100 100
5	K	368/379 (97%)	368 (100%)	0	100 100
5	N	368/379 (97%)	368 (100%)	0	100 100
5	O	368/379 (97%)	367 (100%)	1 (0%)	91 96
5	Q	368/379 (97%)	367 (100%)	1 (0%)	91 96
5	R	368/379 (97%)	368 (100%)	0	100 100
5	T	368/379 (97%)	366 (100%)	2 (0%)	86 93
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%)	91 96
5	i	368/379 (97%)	368 (100%)	0	100 100
5	j	368/379 (97%)	367 (100%)	1 (0%)	91 96
5	p	375/379 (99%)	374 (100%)	1 (0%)	91 96
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%)	86 93
5	u	368/379 (97%)	367 (100%)	1 (0%)	91 96
5	v	368/379 (97%)	368 (100%)	0	100 100
5	w	368/379 (97%)	367 (100%)	1 (0%)	91 96
6	W	77/77 (100%)	69 (90%)	8 (10%)	5 26
6	x	77/77 (100%)	69 (90%)	8 (10%)	5 26
7	3	173/176 (98%)	158 (91%)	15 (9%)	8 33
7	c	173/176 (98%)	158 (91%)	15 (9%)	8 33
7	g	173/176 (98%)	158 (91%)	15 (9%)	8 33
7	z	173/176 (98%)	158 (91%)	15 (9%)	8 33
8	2	244/258 (95%)	217 (89%)	27 (11%)	5 25
8	d	244/258 (95%)	217 (89%)	27 (11%)	5 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	l	244/258 (95%)	217 (89%)	27 (11%)	5 25
8	n	244/258 (95%)	217 (89%)	27 (11%)	5 25
All	All	20671/21323 (97%)	20379 (99%)	292 (1%)	62 79

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	30	ILE
2	B	36	SER
2	B	43	ARG
2	B	48	SER
2	B	59	VAL
2	B	94	GLN
2	B	103	LYS
2	B	104	VAL
2	B	184	ARG
2	B	189	THR
2	B	231	THR
2	B	245	THR
2	B	308	THR
2	B	331	LYS
2	B	342	LYS
2	B	355	VAL
2	B	391	THR
2	B	399	SER
2	B	402	SER
2	B	415	LYS
2	B	416	ILE
2	B	421	ASN
2	B	425	GLN
2	B	433	SER
2	B	440	ILE
2	B	446	GLU
2	B	456	ARG
2	B	461	LEU
2	B	464	SER
2	B	465	MET
2	B	467	ASP
2	B	502	LYS
2	B	516	VAL
2	B	538	ASP

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Mol	Chain	Res	Type
2	B	563	ARG
2	B	569	VAL
2	B	595	SER
2	B	603	VAL
2	B	611	VAL
2	B	621	ILE
2	C	30	ILE
2	C	36	SER
2	C	43	ARG
2	C	48	SER
2	C	59	VAL
2	C	94	GLN
2	C	103	LYS
2	C	104	VAL
2	C	184	ARG
2	C	189	THR
2	C	231	THR
2	C	245	THR
2	C	308	THR
2	C	331	LYS
2	C	342	LYS
2	C	355	VAL
2	C	391	THR
2	C	399	SER
2	C	402	SER
2	C	415	LYS
2	C	416	ILE
2	C	421	ASN
2	C	425	GLN
2	C	433	SER
2	C	440	ILE
2	C	446	GLU
2	C	456	ARG
2	C	461	LEU
2	C	464	SER
2	C	465	MET
2	C	467	ASP
2	C	502	LYS
2	C	516	VAL
2	C	538	ASP
2	C	563	ARG
2	C	569	VAL

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Mol	Chain	Res	Type
2	C	595	SER
2	C	603	VAL
2	C	611	VAL
2	C	621	ILE
3	F	163	LYS
4	H	3	ARG
4	H	62	LYS
5	I	122	LYS
3	L	320	ARG
3	M	124	LYS
5	O	122	LYS
5	Q	213	ARG
5	T	164	MET
5	T	213	ARG
6	W	8	LYS
6	W	21	THR
6	W	23	ILE
6	W	40	LEU
6	W	62	GLN
6	W	65	LEU
6	W	80	GLU
6	W	86	THR
3	Z	112	LYS
3	Z	292	THR
5	b	320	ARG
7	c	29	VAL
7	c	38	THR
7	c	41	ASP
7	c	55	SER
7	c	68	THR
7	c	72	LYS
7	c	97	LYS
7	c	99	VAL
7	c	110	SER
7	c	124	ARG
7	c	164	ARG
7	c	173	SER
7	c	174	GLU
7	c	175	GLU
7	c	180	GLU
8	d	8	SER
8	d	12	SER

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Mol	Chain	Res	Type
8	d	13	THR
8	d	17	VAL
8	d	22	LYS
8	d	30	SER
8	d	35	CYS
8	d	39	THR
8	d	42	SER
8	d	45	ARG
8	d	53	ASP
8	d	79	THR
8	d	86	ASP
8	d	111	LYS
8	d	114	GLU
8	d	150	GLU
8	d	168	THR
8	d	180	VAL
8	d	182	ASP
8	d	189	SER
8	d	208	THR
8	d	225	VAL
8	d	227	SER
8	d	233	GLU
8	d	269	CYS
8	d	287	ASP
8	d	288	ASP
3	f	112	LYS
3	f	221	ARG
7	g	29	VAL
7	g	38	THR
7	g	41	ASP
7	g	55	SER
7	g	68	THR
7	g	72	LYS
7	g	97	LYS
7	g	99	VAL
7	g	110	SER
7	g	124	ARG
7	g	164	ARG
7	g	173	SER
7	g	174	GLU
7	g	175	GLU
7	g	180	GLU

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Mol	Chain	Res	Type
3	h	163	LYS
5	j	301	CYS
3	k	112	LYS
3	k	221	ARG
8	l	8	SER
8	l	12	SER
8	l	13	THR
8	l	17	VAL
8	l	22	LYS
8	l	30	SER
8	l	35	CYS
8	l	39	THR
8	l	42	SER
8	l	45	ARG
8	l	53	ASP
8	l	79	THR
8	l	86	ASP
8	l	111	LYS
8	l	114	GLU
8	l	150	GLU
8	l	168	THR
8	l	180	VAL
8	l	182	ASP
8	l	189	SER
8	l	208	THR
8	l	225	VAL
8	l	227	SER
8	l	233	GLU
8	l	269	CYS
8	l	287	ASP
8	l	288	ASP
8	n	8	SER
8	n	12	SER
8	n	13	THR
8	n	17	VAL
8	n	22	LYS
8	n	30	SER
8	n	35	CYS
8	n	39	THR
8	n	42	SER
8	n	45	ARG
8	n	53	ASP

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Mol	Chain	Res	Type
8	n	79	THR
8	n	86	ASP
8	n	111	LYS
8	n	114	GLU
8	n	150	GLU
8	n	168	THR
8	n	180	VAL
8	n	182	ASP
8	n	189	SER
8	n	208	THR
8	n	225	VAL
8	n	227	SER
8	n	233	GLU
8	n	269	CYS
8	n	287	ASP
8	n	288	ASP
5	p	1	MET
3	s	163	LYS
5	t	211	CYS
5	t	418	LEU
5	u	320	ARG
5	w	58	ARG
6	x	8	LYS
6	x	21	THR
6	x	23	ILE
6	x	40	LEU
6	x	62	GLN
6	x	65	LEU
6	x	80	GLU
6	x	86	THR
3	y	124	LYS
7	z	29	VAL
7	z	38	THR
7	z	41	ASP
7	z	55	SER
7	z	68	THR
7	z	72	LYS
7	z	97	LYS
7	z	99	VAL
7	z	110	SER
7	z	124	ARG
7	z	164	ARG

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Mol	Chain	Res	Type
7	z	173	SER
7	z	174	GLU
7	z	175	GLU
7	z	180	GLU
8	2	8	SER
8	2	12	SER
8	2	13	THR
8	2	17	VAL
8	2	22	LYS
8	2	30	SER
8	2	35	CYS
8	2	39	THR
8	2	42	SER
8	2	45	ARG
8	2	53	ASP
8	2	79	THR
8	2	86	ASP
8	2	111	LYS
8	2	114	GLU
8	2	150	GLU
8	2	168	THR
8	2	180	VAL
8	2	182	ASP
8	2	189	SER
8	2	208	THR
8	2	225	VAL
8	2	227	SER
8	2	233	GLU
8	2	269	CYS
8	2	287	ASP
8	2	288	ASP
7	3	29	VAL
7	3	38	THR
7	3	41	ASP
7	3	55	SER
7	3	68	THR
7	3	72	LYS
7	3	97	LYS
7	3	99	VAL
7	3	110	SER
7	3	124	ARG
7	3	164	ARG

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Mol	Chain	Res	Type
7	3	173	SER
7	3	174	GLU
7	3	175	GLU
7	3	180	GLU
3	5	112	LYS
3	6	163	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (268) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	40	GLN
1	A	78	ASN
1	A	122	GLN
1	A	193	ASN
1	A	197	GLN
2	B	157	ASN
2	B	170	ASN
2	B	412	GLN
2	B	459	GLN
2	B	468	HIS
2	B	557	ASN
2	C	157	ASN
2	C	170	ASN
2	C	412	GLN
2	C	459	GLN
2	C	468	HIS
2	C	557	ASN
3	D	8	HIS
3	D	11	GLN
3	D	31	GLN
3	D	329	ASN
3	E	107	HIS
3	F	226	ASN
3	G	256	GLN
3	G	356	ASN
4	H	9	GLN
4	H	133	ASN
5	I	6	HIS
5	I	11	GLN
5	I	14	ASN
5	I	94	GLN

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Mol	Chain	Res	Type
5	I	131	GLN
5	I	195	ASN
5	J	100	ASN
5	J	245	GLN
5	J	416	ASN
5	K	8	GLN
5	K	11	GLN
5	K	14	ASN
5	K	279	GLN
3	L	8	HIS
3	L	18	ASN
3	L	61	HIS
3	L	91	GLN
3	L	197	HIS
3	L	206	ASN
3	L	329	ASN
3	L	406	HIS
3	M	8	HIS
3	M	91	GLN
3	M	128	ASN
3	M	342	GLN
3	M	380	ASN
5	N	6	HIS
5	N	37	HIS
5	N	226	ASN
5	N	280	GLN
5	N	298	ASN
5	N	329	GLN
5	N	347	ASN
5	O	11	GLN
5	O	14	ASN
5	O	37	HIS
5	O	89	ASN
5	O	204	ASN
5	O	256	ASN
5	O	298	ASN
3	P	31	GLN
3	P	50	ASN
3	P	61	HIS
3	P	88	HIS
3	P	283	HIS
3	P	329	ASN

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Mol	Chain	Res	Type
5	Q	14	ASN
5	Q	137	HIS
5	Q	298	ASN
5	Q	347	ASN
5	R	14	ASN
5	R	89	ASN
5	R	131	GLN
5	R	204	ASN
5	R	256	ASN
5	R	337	ASN
5	R	426	GLN
3	S	8	HIS
3	S	91	GLN
3	S	206	ASN
3	S	342	GLN
3	S	380	ASN
5	T	6	HIS
5	T	14	ASN
5	T	195	ASN
5	T	298	ASN
5	T	335	ASN
5	T	347	ASN
5	U	6	HIS
5	U	37	HIS
5	U	131	GLN
5	U	256	ASN
5	U	264	HIS
5	U	280	GLN
5	U	298	ASN
5	U	329	GLN
5	V	8	GLN
5	V	89	ASN
5	V	137	HIS
5	V	195	ASN
5	V	291	GLN
5	V	298	ASN
5	V	334	GLN
5	V	335	ASN
6	W	62	GLN
3	X	8	HIS
3	X	256	GLN
3	X	406	HIS

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Mol	Chain	Res	Type
3	Y	8	HIS
3	Y	11	GLN
3	Y	342	GLN
3	Y	356	ASN
3	Y	406	HIS
3	Z	31	GLN
3	Z	249	ASN
5	a	14	ASN
5	a	137	HIS
5	a	227	HIS
5	a	298	ASN
5	a	347	ASN
5	b	8	GLN
5	b	256	ASN
5	b	264	HIS
5	b	335	ASN
5	b	416	ASN
7	c	31	ASN
8	d	28	ASN
8	d	155	HIS
8	d	197	GLN
8	d	247	ASN
3	e	293	ASN
3	e	329	ASN
3	e	356	ASN
3	e	380	ASN
3	f	11	GLN
3	f	91	GLN
7	g	53	ASN
7	g	66	ASN
3	h	18	ASN
3	h	35	GLN
3	h	206	ASN
3	h	283	HIS
5	i	6	HIS
5	i	423	GLN
5	i	426	GLN
5	j	334	GLN
5	j	423	GLN
3	k	11	GLN
3	k	18	ASN
3	k	61	HIS

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Mol	Chain	Res	Type
3	k	91	GLN
3	k	266	HIS
3	k	293	ASN
3	k	309	HIS
8	l	28	ASN
8	l	155	HIS
8	l	197	GLN
8	l	247	ASN
3	m	8	HIS
3	m	31	GLN
3	m	249	ASN
3	m	256	GLN
8	n	28	ASN
8	n	155	HIS
8	n	197	GLN
8	n	247	ASN
3	o	8	HIS
3	o	35	GLN
3	o	107	HIS
3	o	249	ASN
3	o	283	HIS
5	p	256	ASN
5	p	291	GLN
5	p	424	GLN
5	q	14	ASN
5	q	99	ASN
5	q	190	HIS
5	q	298	ASN
5	q	424	GLN
5	r	8	GLN
5	r	37	HIS
5	r	99	ASN
5	r	195	ASN
5	r	298	ASN
5	r	424	GLN
3	s	256	GLN
3	s	293	ASN
5	t	6	HIS
5	t	8	GLN
5	t	105	HIS
5	t	137	HIS
5	t	247	ASN

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Mol	Chain	Res	Type
5	t	256	ASN
5	t	291	GLN
5	t	298	ASN
5	t	424	GLN
5	u	264	HIS
5	u	280	GLN
5	u	298	ASN
5	u	396	HIS
5	v	14	ASN
5	v	83	GLN
5	v	291	GLN
5	v	334	GLN
5	v	335	ASN
5	v	416	ASN
5	w	6	HIS
5	w	8	GLN
5	w	334	GLN
5	w	335	ASN
5	w	347	ASN
5	w	348	ASN
3	y	8	HIS
3	y	35	GLN
7	z	31	ASN
7	z	53	ASN
7	z	66	ASN
3	0	8	HIS
3	0	61	HIS
3	0	249	ASN
3	0	293	ASN
3	1	356	ASN
3	1	406	HIS
8	2	28	ASN
8	2	155	HIS
8	2	197	GLN
8	2	247	ASN
5	4	8	GLN
5	4	37	HIS
5	4	137	HIS
5	4	291	GLN
5	4	298	ASN
5	4	335	ASN
5	4	416	ASN

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Mol	Chain	Res	Type
3	6	8	HIS
3	6	11	GLN
3	6	133	GLN
3	6	380	ASN
3	7	50	ASN
3	7	266	HIS
3	7	380	ASN
5	8	6	HIS
5	8	94	GLN
5	8	137	HIS
5	8	195	ASN
5	8	279	GLN
5	8	298	ASN
5	8	416	ASN
5	9	6	HIS
5	9	37	HIS
5	9	94	GLN
5	9	100	ASN
5	9	105	HIS
5	9	245	GLN
5	9	279	GLN
5	9	280	GLN
5	9	298	ASN
5	9	347	ASN
5	9	348	ASN
5	9	416	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
11	GDP	N	501	-	25,30,30	4.01	13 (52%)	30,47,47	2.28	6 (20%)
12	TA1	t	502	-	68,68,68	0.84	2 (2%)	105,105,105	0.86	4 (3%)
9	GTP	f	501	10	29,34,34	4.33	13 (44%)	35,54,54	1.35	5 (14%)
12	TA1	b	502	-	68,68,68	0.72	1 (1%)	105,105,105	0.80	4 (3%)
11	GDP	J	501	-	25,30,30	4.00	13 (52%)	30,47,47	1.62	5 (16%)
12	TA1	q	502	-	68,68,68	0.89	2 (2%)	105,105,105	0.89	6 (5%)
9	GTP	e	501	10	29,34,34	4.45	13 (44%)	35,54,54	1.41	5 (14%)
12	TA1	r	502	-	68,68,68	0.64	1 (1%)	105,105,105	0.84	4 (3%)
11	GDP	p	501	-	25,30,30	3.98	13 (52%)	30,47,47	1.63	5 (16%)
9	GTP	D	501	10	29,34,34	4.37	13 (44%)	35,54,54	1.34	5 (14%)
11	GDP	q	501	-	25,30,30	4.01	13 (52%)	30,47,47	1.65	5 (16%)
12	TA1	i	502	-	68,68,68	0.64	1 (1%)	105,105,105	0.79	4 (3%)
11	GDP	b	501	-	25,30,30	4.04	13 (52%)	30,47,47	1.69	5 (16%)
12	TA1	4	502	-	68,68,68	0.52	1 (1%)	105,105,105	0.82	5 (4%)
9	GTP	F	501	10	29,34,34	4.36	13 (44%)	35,54,54	1.54	5 (14%)
9	GTP	P	501	10	29,34,34	4.43	13 (44%)	35,54,54	1.35	5 (14%)
12	TA1	8	502	-	68,68,68	0.59	1 (1%)	105,105,105	0.79	4 (3%)
9	GTP	7	501	10	29,34,34	4.47	13 (44%)	35,54,54	1.31	5 (14%)
9	GTP	L	501	10	29,34,34	4.36	13 (44%)	35,54,54	1.46	5 (14%)
9	GTP	5	501	10	29,34,34	4.36	13 (44%)	35,54,54	1.40	5 (14%)
11	GDP	Q	501	-	25,30,30	4.04	13 (52%)	30,47,47	1.72	6 (20%)
9	GTP	0	501	10	29,34,34	4.40	13 (44%)	35,54,54	1.32	5 (14%)
11	GDP	r	501	-	25,30,30	4.03	13 (52%)	30,47,47	1.62	5 (16%)
12	TA1	J	502	-	68,68,68	0.58	1 (1%)	105,105,105	0.78	4 (3%)
9	GTP	M	501	10	29,34,34	4.42	13 (44%)	35,54,54	1.33	5 (14%)
11	GDP	8	501	-	25,30,30	4.00	13 (52%)	30,47,47	1.74	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	GDP	t	501	-	25,30,30	4.02	13 (52%)	30,47,47	1.60	5 (16%)
9	GTP	6	501	10	29,34,34	4.45	13 (44%)	35,54,54	1.37	5 (14%)
9	GTP	y	501	10	29,34,34	4.39	13 (44%)	35,54,54	1.30	5 (14%)
11	GDP	U	501	-	25,30,30	3.99	13 (52%)	30,47,47	1.83	5 (16%)
12	TA1	u	502	-	68,68,68	0.71	2 (2%)	105,105,105	0.81	4 (3%)
12	TA1	v	502	-	68,68,68	0.42	0	105,105,105	0.84	5 (4%)
9	GTP	E	501	10	29,34,34	4.43	13 (44%)	35,54,54	1.44	5 (14%)
12	TA1	9	502	-	68,68,68	0.64	2 (2%)	105,105,105	0.82	4 (3%)
9	GTP	o	501	10	29,34,34	4.39	13 (44%)	35,54,54	1.34	5 (14%)
9	GTP	S	501	10	29,34,34	4.44	13 (44%)	35,54,54	1.35	5 (14%)
9	GTP	X	501	10	29,34,34	4.44	13 (44%)	35,54,54	1.33	5 (14%)
11	GDP	I	501	-	25,30,30	4.02	13 (52%)	30,47,47	1.92	5 (16%)
12	TA1	j	502	-	68,68,68	0.65	1 (1%)	105,105,105	0.87	4 (3%)
9	GTP	1	501	10	29,34,34	4.47	13 (44%)	35,54,54	1.35	5 (14%)
11	GDP	O	501	-	25,30,30	4.01	13 (52%)	30,47,47	1.67	5 (16%)
12	TA1	V	502	-	68,68,68	0.56	2 (2%)	105,105,105	0.79	3 (2%)
12	TA1	a	502	-	68,68,68	0.60	2 (2%)	105,105,105	0.82	4 (3%)
11	GDP	u	501	-	25,30,30	4.00	13 (52%)	30,47,47	1.43	5 (16%)
11	GDP	9	501	-	25,30,30	4.04	13 (52%)	30,47,47	1.51	5 (16%)
9	GTP	Y	501	10	29,34,34	4.45	13 (44%)	35,54,54	1.48	5 (14%)
12	TA1	p	502	-	68,68,68	0.63	2 (2%)	105,105,105	0.82	4 (3%)
9	GTP	G	501	10	29,34,34	4.38	13 (44%)	35,54,54	1.52	5 (14%)
11	GDP	j	501	-	25,30,30	4.05	13 (52%)	30,47,47	1.69	5 (16%)
11	GDP	4	501	-	25,30,30	4.05	13 (52%)	30,47,47	1.89	5 (16%)
11	GDP	v	501	-	25,30,30	4.03	13 (52%)	30,47,47	1.60	6 (20%)
11	GDP	V	501	-	25,30,30	4.18	13 (52%)	30,47,47	1.93	5 (16%)
11	GDP	a	501	-	25,30,30	4.06	13 (52%)	30,47,47	1.57	6 (20%)
11	GDP	T	501	-	25,30,30	3.98	13 (52%)	30,47,47	1.81	5 (16%)
12	TA1	w	502	-	68,68,68	0.57	1 (1%)	105,105,105	0.76	4 (3%)
9	GTP	h	501	10	29,34,34	4.39	13 (44%)	35,54,54	1.43	5 (14%)
9	GTP	Z	501	10	29,34,34	4.38	13 (44%)	35,54,54	1.48	6 (17%)
11	GDP	R	501	-	25,30,30	4.05	13 (52%)	30,47,47	1.93	6 (20%)
11	GDP	K	501	-	25,30,30	4.02	13 (52%)	30,47,47	2.10	6 (20%)
11	GDP	i	501	-	25,30,30	4.01	13 (52%)	30,47,47	1.54	5 (16%)
9	GTP	m	501	10	29,34,34	4.39	13 (44%)	35,54,54	1.40	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	GTP	s	501	10	29,34,34	4.42	13 (44%)	35,54,54	1.55	5 (14%)
11	GDP	w	501	-	25,30,30	4.03	13 (52%)	30,47,47	1.48	5 (16%)
9	GTP	k	501	10	29,34,34	4.35	13 (44%)	35,54,54	1.30	5 (14%)

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
11	GDP	N	501	-	-	6/12/32/32	0/3/3/3
12	TA1	t	502	-	-	2/41/127/127	0/7/7/7
9	GTP	f	501	10	-	3/18/38/38	0/3/3/3
12	TA1	b	502	-	-	10/41/127/127	0/7/7/7
11	GDP	J	501	-	-	5/12/32/32	0/3/3/3
12	TA1	q	502	-	-	4/41/127/127	0/7/7/7
9	GTP	e	501	10	-	4/18/38/38	0/3/3/3
12	TA1	r	502	-	-	4/41/127/127	0/7/7/7
11	GDP	p	501	-	-	5/12/32/32	0/3/3/3
9	GTP	D	501	10	-	4/18/38/38	0/3/3/3
11	GDP	q	501	-	-	5/12/32/32	0/3/3/3
12	TA1	i	502	-	-	9/41/127/127	0/7/7/7
11	GDP	b	501	-	-	4/12/32/32	0/3/3/3
12	TA1	4	502	-	-	5/41/127/127	0/7/7/7
9	GTP	F	501	10	-	4/18/38/38	0/3/3/3
9	GTP	P	501	10	-	5/18/38/38	0/3/3/3
12	TA1	8	502	-	-	4/41/127/127	0/7/7/7
9	GTP	7	501	10	-	4/18/38/38	0/3/3/3
9	GTP	L	501	10	-	4/18/38/38	0/3/3/3
9	GTP	5	501	10	-	4/18/38/38	0/3/3/3
11	GDP	Q	501	-	-	5/12/32/32	0/3/3/3
9	GTP	0	501	10	-	5/18/38/38	0/3/3/3
11	GDP	r	501	-	-	5/12/32/32	0/3/3/3
12	TA1	J	502	-	-	4/41/127/127	0/7/7/7
9	GTP	M	501	10	-	5/18/38/38	0/3/3/3
11	GDP	8	501	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GDP	t	501	-	-	4/12/32/32	0/3/3/3
9	GTP	6	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	U	501	-	-	4/12/32/32	0/3/3/3
12	TA1	u	502	-	-	14/41/127/127	0/7/7/7
12	TA1	v	502	-	-	5/41/127/127	0/7/7/7
9	GTP	E	501	10	-	5/18/38/38	0/3/3/3
12	TA1	9	502	-	-	0/41/127/127	0/7/7/7
9	GTP	o	501	10	-	5/18/38/38	0/3/3/3
9	GTP	S	501	10	-	5/18/38/38	0/3/3/3
9	GTP	X	501	10	-	3/18/38/38	0/3/3/3
11	GDP	I	501	-	-	4/12/32/32	0/3/3/3
12	TA1	j	502	-	-	11/41/127/127	0/7/7/7
9	GTP	1	501	10	-	3/18/38/38	0/3/3/3
11	GDP	O	501	-	-	5/12/32/32	0/3/3/3
12	TA1	V	502	-	-	5/41/127/127	0/7/7/7
12	TA1	a	502	-	-	2/41/127/127	0/7/7/7
11	GDP	u	501	-	-	5/12/32/32	0/3/3/3
11	GDP	9	501	-	-	3/12/32/32	0/3/3/3
9	GTP	Y	501	10	-	6/18/38/38	0/3/3/3
12	TA1	p	502	-	-	1/41/127/127	0/7/7/7
9	GTP	G	501	10	-	5/18/38/38	0/3/3/3
11	GDP	j	501	-	-	2/12/32/32	0/3/3/3
11	GDP	4	501	-	-	1/12/32/32	0/3/3/3
11	GDP	v	501	-	-	5/12/32/32	0/3/3/3
11	GDP	V	501	-	-	5/12/32/32	0/3/3/3
11	GDP	a	501	-	-	1/12/32/32	0/3/3/3
11	GDP	T	501	-	-	5/12/32/32	0/3/3/3
12	TA1	w	502	-	-	11/41/127/127	0/7/7/7
9	GTP	h	501	10	-	2/18/38/38	0/3/3/3
9	GTP	Z	501	10	-	4/18/38/38	0/3/3/3
11	GDP	R	501	-	-	5/12/32/32	0/3/3/3
11	GDP	K	501	-	-	4/12/32/32	0/3/3/3
11	GDP	i	501	-	-	6/12/32/32	0/3/3/3
9	GTP	m	501	10	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GTP	s	501	10	-	3/18/38/38	0/3/3/3
11	GDP	w	501	-	-	3/12/32/32	0/3/3/3
9	GTP	k	501	10	-	2/18/38/38	0/3/3/3

All (646) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	7	501	GTP	O4'-C1'	16.10	1.62	1.40
9	0	501	GTP	O4'-C1'	16.02	1.61	1.40
9	X	501	GTP	O4'-C1'	15.96	1.61	1.40
9	M	501	GTP	O4'-C1'	15.95	1.61	1.40
9	y	501	GTP	O4'-C1'	15.93	1.61	1.40
9	P	501	GTP	O4'-C1'	15.92	1.61	1.40
9	m	501	GTP	O4'-C1'	15.92	1.61	1.40
9	S	501	GTP	O4'-C1'	15.84	1.61	1.40
9	D	501	GTP	O4'-C1'	15.81	1.61	1.40
9	k	501	GTP	O4'-C1'	15.79	1.61	1.40
9	E	501	GTP	O4'-C1'	15.79	1.61	1.40
9	h	501	GTP	O4'-C1'	15.79	1.61	1.40
9	o	501	GTP	O4'-C1'	15.79	1.61	1.40
9	6	501	GTP	O4'-C1'	15.78	1.61	1.40
9	1	501	GTP	O4'-C1'	15.75	1.61	1.40
9	Y	501	GTP	O4'-C1'	15.74	1.61	1.40
9	f	501	GTP	O4'-C1'	15.72	1.61	1.40
9	L	501	GTP	O4'-C1'	15.72	1.61	1.40
9	G	501	GTP	O4'-C1'	15.71	1.61	1.40
9	e	501	GTP	O4'-C1'	15.69	1.61	1.40
9	5	501	GTP	O4'-C1'	15.69	1.61	1.40
9	F	501	GTP	O4'-C1'	15.62	1.61	1.40
9	s	501	GTP	O4'-C1'	15.62	1.61	1.40
9	Z	501	GTP	O4'-C1'	15.57	1.61	1.40
11	p	501	GDP	C3'-C4'	-9.18	1.29	1.53
11	J	501	GDP	C3'-C4'	-9.13	1.29	1.53
11	w	501	GDP	C3'-C4'	-9.10	1.29	1.53
11	i	501	GDP	C3'-C4'	-9.07	1.30	1.53
11	R	501	GDP	C3'-C4'	-9.06	1.30	1.53
11	u	501	GDP	C3'-C4'	-9.05	1.30	1.53
11	V	501	GDP	C3'-C4'	-9.04	1.30	1.53
11	j	501	GDP	C3'-C4'	-9.04	1.30	1.53
11	9	501	GDP	C3'-C4'	-9.03	1.30	1.53
11	I	501	GDP	C3'-C4'	-9.02	1.30	1.53
11	r	501	GDP	C3'-C4'	-9.02	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	501	GDP	C3'-C4'	-9.01	1.30	1.53
11	q	501	GDP	C3'-C4'	-8.99	1.30	1.53
11	t	501	GDP	C3'-C4'	-8.99	1.30	1.53
11	O	501	GDP	C3'-C4'	-8.99	1.30	1.53
11	4	501	GDP	C3'-C4'	-8.98	1.30	1.53
11	v	501	GDP	C3'-C4'	-8.98	1.30	1.53
11	K	501	GDP	C3'-C4'	-8.97	1.30	1.53
11	T	501	GDP	C3'-C4'	-8.95	1.30	1.53
11	U	501	GDP	C3'-C4'	-8.95	1.30	1.53
11	N	501	GDP	C3'-C4'	-8.93	1.30	1.53
11	a	501	GDP	C3'-C4'	-8.90	1.30	1.53
11	8	501	GDP	C3'-C4'	-8.90	1.30	1.53
11	b	501	GDP	C3'-C4'	-8.90	1.30	1.53
11	j	501	GDP	O4'-C4'	8.12	1.63	1.45
11	9	501	GDP	O4'-C4'	8.06	1.62	1.45
11	w	501	GDP	O4'-C4'	8.06	1.62	1.45
11	t	501	GDP	O4'-C4'	8.04	1.62	1.45
11	i	501	GDP	O4'-C4'	8.04	1.62	1.45
11	R	501	GDP	O4'-C4'	8.04	1.62	1.45
11	Q	501	GDP	O4'-C4'	8.01	1.62	1.45
11	O	501	GDP	O4'-C4'	7.99	1.62	1.45
11	u	501	GDP	O4'-C4'	7.99	1.62	1.45
11	b	501	GDP	O4'-C4'	7.99	1.62	1.45
11	8	501	GDP	O4'-C4'	7.97	1.62	1.45
11	q	501	GDP	O4'-C4'	7.97	1.62	1.45
11	U	501	GDP	O4'-C4'	7.97	1.62	1.45
11	T	501	GDP	O4'-C4'	7.96	1.62	1.45
11	K	501	GDP	O4'-C4'	7.96	1.62	1.45
11	I	501	GDP	O4'-C4'	7.96	1.62	1.45
11	a	501	GDP	O4'-C4'	7.94	1.62	1.45
11	r	501	GDP	O4'-C4'	7.94	1.62	1.45
11	V	501	GDP	O4'-C4'	7.93	1.62	1.45
11	J	501	GDP	O4'-C4'	7.93	1.62	1.45
11	p	501	GDP	O4'-C4'	7.89	1.62	1.45
11	N	501	GDP	O4'-C4'	7.88	1.62	1.45
11	v	501	GDP	O4'-C4'	7.87	1.62	1.45
11	4	501	GDP	O4'-C4'	7.76	1.62	1.45
11	a	501	GDP	PA-O3A	7.50	1.67	1.59
11	4	501	GDP	PA-O3A	7.33	1.67	1.59
11	v	501	GDP	PA-O3A	7.29	1.67	1.59
11	w	501	GDP	PA-O3A	7.24	1.67	1.59
11	Q	501	GDP	PA-O3A	7.24	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	501	GDP	PA-O3A	7.23	1.67	1.59
11	j	501	GDP	PA-O3A	7.19	1.67	1.59
11	9	501	GDP	PA-O3A	7.17	1.67	1.59
11	r	501	GDP	PA-O3A	7.13	1.67	1.59
11	N	501	GDP	PA-O3A	7.12	1.67	1.59
11	V	501	GDP	PA-O3A	7.12	1.67	1.59
11	8	501	GDP	PA-O3A	7.10	1.67	1.59
11	O	501	GDP	PA-O3A	7.06	1.67	1.59
11	V	501	GDP	C2-N2	7.05	1.50	1.34
11	i	501	GDP	PA-O3A	7.03	1.67	1.59
11	b	501	GDP	C2-N2	7.01	1.50	1.34
11	a	501	GDP	C2-N2	7.00	1.50	1.34
11	q	501	GDP	PA-O3A	6.96	1.67	1.59
11	Q	501	GDP	C2-N2	6.96	1.50	1.34
11	v	501	GDP	C2-N2	6.96	1.50	1.34
11	r	501	GDP	C2-N2	6.94	1.50	1.34
11	K	501	GDP	PA-O3A	6.94	1.67	1.59
11	U	501	GDP	PA-O3A	6.93	1.67	1.59
11	9	501	GDP	C2-N2	6.93	1.50	1.34
11	R	501	GDP	PA-O3A	6.93	1.67	1.59
11	I	501	GDP	PA-O3A	6.93	1.67	1.59
11	t	501	GDP	C2-N2	6.93	1.50	1.34
11	p	501	GDP	C2-N2	6.92	1.50	1.34
11	u	501	GDP	C2-N2	6.92	1.50	1.34
11	J	501	GDP	PA-O3A	6.92	1.67	1.59
11	t	501	GDP	PA-O3A	6.92	1.67	1.59
9	1	501	GTP	PA-O3A	6.91	1.67	1.59
11	q	501	GDP	C2-N2	6.91	1.50	1.34
11	T	501	GDP	C2-N2	6.90	1.50	1.34
11	u	501	GDP	PA-O3A	6.89	1.66	1.59
11	w	501	GDP	C2-N2	6.88	1.50	1.34
9	e	501	GTP	PA-O3A	6.87	1.66	1.59
11	U	501	GDP	C2-N2	6.87	1.50	1.34
11	j	501	GDP	C2-N2	6.85	1.50	1.34
11	8	501	GDP	C2-N2	6.84	1.50	1.34
11	J	501	GDP	C2-N2	6.82	1.50	1.34
11	i	501	GDP	C2-N2	6.80	1.50	1.34
11	4	501	GDP	C2-N2	6.79	1.50	1.34
11	p	501	GDP	PA-O3A	6.78	1.66	1.59
11	I	501	GDP	C2-N2	6.76	1.50	1.34
9	Y	501	GTP	PA-O3A	6.72	1.66	1.59
11	N	501	GDP	C2-N2	6.71	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	501	GDP	C2-N2	6.69	1.49	1.34
9	6	501	GTP	PA-O3A	6.68	1.66	1.59
11	T	501	GDP	PA-O3A	6.68	1.66	1.59
11	K	501	GDP	C2-N2	6.67	1.49	1.34
11	O	501	GDP	C2-N2	6.65	1.49	1.34
9	7	501	GTP	PA-O3A	6.62	1.66	1.59
9	6	501	GTP	C2-N3	6.59	1.49	1.33
9	s	501	GTP	PA-O3A	6.56	1.66	1.59
9	Y	501	GTP	C2-N3	6.55	1.49	1.33
9	S	501	GTP	PA-O3A	6.55	1.66	1.59
9	X	501	GTP	PA-O3A	6.54	1.66	1.59
9	7	501	GTP	C2-N3	6.54	1.49	1.33
9	P	501	GTP	C2-N3	6.53	1.49	1.33
9	e	501	GTP	C2-N3	6.52	1.49	1.33
9	1	501	GTP	C2-N3	6.51	1.49	1.33
9	5	501	GTP	C2-N3	6.51	1.49	1.33
9	X	501	GTP	C2-N3	6.50	1.49	1.33
9	E	501	GTP	C2-N3	6.49	1.49	1.33
9	o	501	GTP	C2-N3	6.48	1.49	1.33
9	s	501	GTP	C2-N3	6.47	1.49	1.33
9	D	501	GTP	C2-N3	6.47	1.49	1.33
9	Z	501	GTP	C2-N3	6.46	1.49	1.33
9	f	501	GTP	C2-N3	6.46	1.49	1.33
9	M	501	GTP	C2-N3	6.46	1.49	1.33
9	h	501	GTP	C2-N3	6.45	1.48	1.33
9	Z	501	GTP	PA-O3A	6.43	1.66	1.59
9	S	501	GTP	C2-N3	6.43	1.48	1.33
9	F	501	GTP	C2-N3	6.43	1.48	1.33
9	G	501	GTP	C2-N3	6.42	1.48	1.33
9	y	501	GTP	C2-N3	6.42	1.48	1.33
9	k	501	GTP	C2-N3	6.42	1.48	1.33
9	L	501	GTP	C2-N3	6.42	1.48	1.33
9	0	501	GTP	C2-N3	6.41	1.48	1.33
9	m	501	GTP	C2-N3	6.39	1.48	1.33
11	V	501	GDP	C6-N1	6.38	1.47	1.37
9	G	501	GTP	PA-O3A	6.36	1.66	1.59
9	E	501	GTP	PA-O3A	6.32	1.66	1.59
9	P	501	GTP	PA-O3A	6.32	1.66	1.59
9	h	501	GTP	PA-O3A	6.31	1.66	1.59
9	M	501	GTP	PA-O3A	6.23	1.66	1.59
9	1	501	GTP	PB-O3A	6.22	1.66	1.59
9	s	501	GTP	O4'-C4'	-6.22	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	501	GTP	O4'-C4'	-6.21	1.31	1.45
9	E	501	GTP	PB-O3B	6.19	1.66	1.59
9	6	501	GTP	O4'-C4'	-6.19	1.31	1.45
9	P	501	GTP	O4'-C4'	-6.18	1.31	1.45
9	D	501	GTP	O4'-C4'	-6.18	1.31	1.45
9	o	501	GTP	PA-O3A	6.17	1.66	1.59
9	m	501	GTP	PA-O3A	6.17	1.66	1.59
9	F	501	GTP	PA-O3A	6.16	1.66	1.59
9	k	501	GTP	O4'-C4'	-6.16	1.31	1.45
9	y	501	GTP	O4'-C4'	-6.15	1.31	1.45
9	e	501	GTP	O4'-C4'	-6.15	1.31	1.45
9	o	501	GTP	O4'-C4'	-6.15	1.31	1.45
9	f	501	GTP	O4'-C4'	-6.14	1.31	1.45
9	e	501	GTP	PB-O3A	6.14	1.66	1.59
9	1	501	GTP	O4'-C4'	-6.14	1.31	1.45
9	h	501	GTP	O4'-C4'	-6.14	1.31	1.45
9	0	501	GTP	PA-O3A	6.14	1.66	1.59
9	G	501	GTP	O4'-C4'	-6.13	1.31	1.45
9	E	501	GTP	O4'-C4'	-6.12	1.31	1.45
9	0	501	GTP	O4'-C4'	-6.12	1.31	1.45
9	5	501	GTP	PA-O3A	6.12	1.66	1.59
9	5	501	GTP	O4'-C4'	-6.11	1.31	1.45
9	S	501	GTP	PB-O3B	6.10	1.66	1.59
9	Y	501	GTP	O4'-C4'	-6.10	1.31	1.45
9	L	501	GTP	O4'-C4'	-6.09	1.31	1.45
9	Z	501	GTP	O4'-C4'	-6.08	1.31	1.45
9	S	501	GTP	O4'-C4'	-6.07	1.31	1.45
9	M	501	GTP	O4'-C4'	-6.07	1.31	1.45
9	S	501	GTP	PB-O3A	6.06	1.66	1.59
9	D	501	GTP	PA-O3A	6.05	1.66	1.59
9	X	501	GTP	O4'-C4'	-6.04	1.31	1.45
9	m	501	GTP	O4'-C4'	-6.02	1.31	1.45
9	y	501	GTP	PA-O3A	6.02	1.66	1.59
9	X	501	GTP	PB-O3A	6.01	1.66	1.59
9	L	501	GTP	PA-O3A	6.01	1.66	1.59
9	7	501	GTP	O4'-C4'	-5.98	1.31	1.45
9	k	501	GTP	PA-O3A	5.97	1.65	1.59
9	f	501	GTP	PA-O3A	5.97	1.65	1.59
12	q	502	TA1	O02-C02	-5.94	1.35	1.45
9	7	501	GTP	PB-O3A	5.94	1.65	1.59
11	V	501	GDP	O4'-C1'	-5.92	1.33	1.40
9	P	501	GTP	PB-O3B	5.91	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	501	GTP	PB-O3B	5.89	1.65	1.59
9	6	501	GTP	PB-O3B	5.87	1.65	1.59
9	1	501	GTP	PB-O3B	5.87	1.65	1.59
9	M	501	GTP	PB-O3A	5.86	1.65	1.59
9	Y	501	GTP	PB-O3A	5.84	1.65	1.59
9	7	501	GTP	PB-O3B	5.79	1.65	1.59
9	6	501	GTP	PB-O3A	5.79	1.65	1.59
9	P	501	GTP	PB-O3A	5.78	1.65	1.59
9	s	501	GTP	PB-O3A	5.78	1.65	1.59
9	L	501	GTP	PB-O3B	5.76	1.65	1.59
9	Y	501	GTP	PB-O3B	5.75	1.65	1.59
11	4	501	GDP	O4'-C1'	-5.74	1.33	1.40
11	K	501	GDP	O4'-C1'	-5.74	1.33	1.40
9	Z	501	GTP	PB-O3A	5.73	1.65	1.59
11	R	501	GDP	O4'-C1'	-5.72	1.33	1.40
9	s	501	GTP	PB-O3B	5.71	1.65	1.59
9	o	501	GTP	PB-O3B	5.68	1.65	1.59
9	e	501	GTP	PB-O3B	5.67	1.65	1.59
9	E	501	GTP	PB-O3A	5.66	1.65	1.59
9	m	501	GTP	PB-O3A	5.66	1.65	1.59
9	o	501	GTP	PB-O3A	5.63	1.65	1.59
9	5	501	GTP	PB-O3A	5.63	1.65	1.59
11	I	501	GDP	O4'-C1'	-5.63	1.33	1.40
9	Z	501	GTP	PB-O3B	5.61	1.65	1.59
11	a	501	GDP	C4-N3	5.61	1.50	1.37
11	O	501	GDP	O4'-C1'	-5.60	1.33	1.40
11	v	501	GDP	C4-N3	5.60	1.50	1.37
11	V	501	GDP	C4-N3	5.58	1.50	1.37
9	m	501	GTP	PB-O3B	5.57	1.65	1.59
11	9	501	GDP	C4-N3	5.57	1.50	1.37
9	X	501	GTP	PB-O3B	5.56	1.65	1.59
11	b	501	GDP	C4-N3	5.56	1.50	1.37
9	y	501	GTP	PB-O3B	5.55	1.65	1.59
11	w	501	GDP	C4-N3	5.55	1.50	1.37
11	t	501	GDP	C4-N3	5.55	1.50	1.37
11	Q	501	GDP	C4-N3	5.54	1.50	1.37
11	q	501	GDP	C4-N3	5.53	1.50	1.37
11	V	501	GDP	C2-N3	5.53	1.46	1.33
9	y	501	GTP	PB-O3A	5.52	1.65	1.59
11	R	501	GDP	C6-N1	5.52	1.46	1.37
9	G	501	GTP	PB-O3A	5.51	1.65	1.59
9	0	501	GTP	PB-O3A	5.51	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	501	GDP	O4'-C1'	-5.51	1.33	1.40
9	G	501	GTP	PB-O3B	5.50	1.65	1.59
9	0	501	GTP	PB-O3B	5.50	1.65	1.59
11	r	501	GDP	C4-N3	5.50	1.50	1.37
9	F	501	GTP	PB-O3A	5.50	1.65	1.59
11	r	501	GDP	O4'-C1'	-5.50	1.33	1.40
11	T	501	GDP	O4'-C1'	-5.50	1.33	1.40
9	h	501	GTP	PB-O3B	5.50	1.65	1.59
11	T	501	GDP	C4-N3	5.50	1.50	1.37
11	j	501	GDP	C4-N3	5.49	1.50	1.37
11	q	501	GDP	O4'-C1'	-5.48	1.33	1.40
9	D	501	GTP	PB-O3B	5.48	1.65	1.59
11	u	501	GDP	C4-N3	5.47	1.50	1.37
9	k	501	GTP	PB-O3A	5.47	1.65	1.59
9	h	501	GTP	PB-O3A	5.47	1.65	1.59
11	I	501	GDP	C4-N3	5.44	1.50	1.37
11	U	501	GDP	C4-N3	5.43	1.50	1.37
11	J	501	GDP	C4-N3	5.41	1.50	1.37
11	i	501	GDP	C4-N3	5.41	1.50	1.37
11	8	501	GDP	C4-N3	5.41	1.50	1.37
9	f	501	GTP	PB-O3A	5.41	1.65	1.59
9	D	501	GTP	PB-O3A	5.39	1.65	1.59
9	5	501	GTP	PB-O3B	5.39	1.65	1.59
11	b	501	GDP	O4'-C1'	-5.37	1.33	1.40
9	k	501	GTP	PB-O3B	5.37	1.65	1.59
11	U	501	GDP	O4'-C1'	-5.36	1.33	1.40
11	t	501	GDP	O4'-C1'	-5.36	1.33	1.40
11	8	501	GDP	O4'-C1'	-5.35	1.33	1.40
9	F	501	GTP	PB-O3B	5.35	1.65	1.59
11	Q	501	GDP	O4'-C1'	-5.35	1.33	1.40
11	a	501	GDP	O4'-C1'	-5.34	1.33	1.40
11	j	501	GDP	O4'-C1'	-5.34	1.33	1.40
11	i	501	GDP	O4'-C1'	-5.34	1.33	1.40
11	p	501	GDP	C4-N3	5.34	1.50	1.37
11	v	501	GDP	O4'-C1'	-5.34	1.33	1.40
11	4	501	GDP	C4-N3	5.33	1.50	1.37
11	K	501	GDP	C4-N3	5.33	1.50	1.37
11	9	501	GDP	O4'-C1'	-5.32	1.33	1.40
9	L	501	GTP	PB-O3A	5.30	1.65	1.59
11	w	501	GDP	O4'-C1'	-5.29	1.33	1.40
11	p	501	GDP	O4'-C1'	-5.29	1.33	1.40
11	O	501	GDP	C4-N3	5.28	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	u	501	GDP	O4'-C1'	-5.27	1.34	1.40
11	R	501	GDP	C4-N3	5.25	1.49	1.37
11	4	501	GDP	C6-N1	5.22	1.45	1.37
11	K	501	GDP	C6-N1	5.22	1.45	1.37
11	N	501	GDP	C4-N3	5.21	1.49	1.37
11	N	501	GDP	C6-N1	5.20	1.45	1.37
11	b	501	GDP	C2-N3	5.16	1.45	1.33
11	J	501	GDP	O4'-C1'	-5.16	1.34	1.40
11	j	501	GDP	C2-N3	5.12	1.45	1.33
11	O	501	GDP	C6-N1	5.12	1.45	1.37
11	v	501	GDP	C2-N3	5.11	1.45	1.33
11	4	501	GDP	C2-N3	5.10	1.45	1.33
11	a	501	GDP	C2-N3	5.10	1.45	1.33
11	j	501	GDP	C6-N1	5.09	1.45	1.37
11	K	501	GDP	C2-N3	5.08	1.45	1.33
11	I	501	GDP	C2-N3	5.08	1.45	1.33
9	Y	501	GTP	C4-N3	5.08	1.49	1.37
11	R	501	GDP	C2-N3	5.07	1.45	1.33
11	Q	501	GDP	C2-N3	5.05	1.45	1.33
11	T	501	GDP	C2-N3	5.04	1.45	1.33
11	t	501	GDP	C2-N3	5.04	1.45	1.33
11	a	501	GDP	C6-N1	5.04	1.45	1.37
11	J	501	GDP	C6-N1	5.03	1.45	1.37
12	b	502	TA1	O02-C02	-5.03	1.36	1.45
11	w	501	GDP	C2-N3	5.02	1.45	1.33
9	6	501	GTP	C4-N3	5.02	1.49	1.37
9	7	501	GTP	C4-N3	5.02	1.49	1.37
11	9	501	GDP	C2-N3	5.01	1.45	1.33
9	P	501	GTP	C4-N3	5.01	1.49	1.37
11	J	501	GDP	C2-N3	5.01	1.45	1.33
11	i	501	GDP	C2-N3	5.01	1.45	1.33
9	Z	501	GTP	C4-N3	5.00	1.49	1.37
9	5	501	GTP	C4-N3	5.00	1.49	1.37
9	Y	501	GTP	C2-N2	4.99	1.45	1.34
9	E	501	GTP	C4-N3	4.99	1.49	1.37
11	8	501	GDP	C2-N3	4.99	1.45	1.33
11	u	501	GDP	C2-N3	4.99	1.45	1.33
9	G	501	GTP	C4-N3	4.99	1.49	1.37
11	q	501	GDP	C2-N3	4.99	1.45	1.33
11	r	501	GDP	C2-N3	4.99	1.45	1.33
11	I	501	GDP	C6-N1	4.99	1.45	1.37
9	k	501	GTP	C4-N3	4.98	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	s	501	GTP	C4-N3	4.97	1.49	1.37
9	f	501	GTP	C4-N3	4.97	1.49	1.37
9	X	501	GTP	C4-N3	4.97	1.49	1.37
9	D	501	GTP	C4-N3	4.96	1.49	1.37
9	o	501	GTP	C4-N3	4.96	1.49	1.37
9	1	501	GTP	C4-N3	4.96	1.49	1.37
9	h	501	GTP	C4-N3	4.94	1.49	1.37
9	0	501	GTP	C4-N3	4.94	1.49	1.37
11	O	501	GDP	C2-N3	4.94	1.45	1.33
9	y	501	GTP	C4-N3	4.94	1.49	1.37
11	Q	501	GDP	C6-N1	4.94	1.45	1.37
9	M	501	GTP	C4-N3	4.93	1.49	1.37
9	e	501	GTP	C4-N3	4.93	1.49	1.37
9	L	501	GTP	C4-N3	4.93	1.49	1.37
9	S	501	GTP	C4-N3	4.93	1.49	1.37
11	U	501	GDP	C6-N1	4.92	1.45	1.37
11	i	501	GDP	C6-N1	4.91	1.45	1.37
11	u	501	GDP	C6-N1	4.91	1.45	1.37
11	N	501	GDP	C2-N3	4.91	1.45	1.33
11	t	501	GDP	C6-N1	4.91	1.45	1.37
11	p	501	GDP	C2-N3	4.91	1.45	1.33
9	m	501	GTP	C4-N3	4.91	1.49	1.37
9	1	501	GTP	C2-N2	4.91	1.45	1.34
9	F	501	GTP	C4-N3	4.90	1.49	1.37
9	7	501	GTP	C2-N2	4.89	1.45	1.34
9	Z	501	GTP	C2-N2	4.89	1.45	1.34
9	s	501	GTP	C2-N2	4.89	1.45	1.34
11	U	501	GDP	C2-N3	4.89	1.45	1.33
9	6	501	GTP	C2-N2	4.88	1.45	1.34
9	m	501	GTP	C2-N2	4.87	1.45	1.34
9	e	501	GTP	C2-N2	4.87	1.45	1.34
9	f	501	GTP	C2-N2	4.87	1.45	1.34
9	h	501	GTP	C2-N2	4.87	1.45	1.34
11	9	501	GDP	C6-N1	4.86	1.45	1.37
11	b	501	GDP	C6-N1	4.86	1.45	1.37
9	Y	501	GTP	C6-N1	4.86	1.45	1.37
11	8	501	GDP	C6-N1	4.85	1.45	1.37
9	G	501	GTP	C2-N2	4.85	1.45	1.34
9	5	501	GTP	C2-N2	4.85	1.45	1.34
9	0	501	GTP	C2-N2	4.84	1.45	1.34
9	P	501	GTP	C2-N2	4.84	1.45	1.34
9	o	501	GTP	C2-N2	4.84	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	501	GTP	C2-N2	4.84	1.45	1.34
9	F	501	GTP	C2-N2	4.83	1.45	1.34
9	M	501	GTP	C2-N2	4.83	1.45	1.34
9	L	501	GTP	C2-N2	4.83	1.45	1.34
9	s	501	GTP	C6-N1	4.83	1.45	1.37
9	S	501	GTP	C2-N2	4.82	1.45	1.34
9	D	501	GTP	C2-N2	4.81	1.45	1.34
11	r	501	GDP	C6-N1	4.81	1.45	1.37
9	X	501	GTP	C2-N2	4.80	1.45	1.34
11	w	501	GDP	C6-N1	4.79	1.45	1.37
11	q	501	GDP	C6-N1	4.78	1.45	1.37
11	v	501	GDP	C6-N1	4.78	1.45	1.37
9	f	501	GTP	PB-O3B	4.78	1.64	1.59
9	k	501	GTP	C2-N2	4.76	1.45	1.34
11	p	501	GDP	C6-N1	4.76	1.45	1.37
9	y	501	GTP	C2-N2	4.75	1.45	1.34
9	y	501	GTP	C6-N1	4.75	1.45	1.37
9	G	501	GTP	C6-N1	4.75	1.45	1.37
9	Z	501	GTP	C6-N1	4.74	1.45	1.37
9	h	501	GTP	C6-N1	4.73	1.45	1.37
9	f	501	GTP	C6-N1	4.72	1.45	1.37
9	k	501	GTP	C6-N1	4.72	1.45	1.37
9	1	501	GTP	C6-N1	4.72	1.45	1.37
9	F	501	GTP	C6-N1	4.69	1.45	1.37
11	T	501	GDP	C6-N1	4.68	1.45	1.37
9	e	501	GTP	C6-N1	4.68	1.45	1.37
9	E	501	GTP	C6-N1	4.67	1.44	1.37
12	t	502	TA1	O02-C02	-4.66	1.37	1.45
9	o	501	GTP	C6-N1	4.66	1.44	1.37
12	u	502	TA1	O02-C02	-4.66	1.37	1.45
9	7	501	GTP	C6-N1	4.66	1.44	1.37
9	5	501	GTP	C6-N1	4.66	1.44	1.37
9	D	501	GTP	C6-N1	4.65	1.44	1.37
9	L	501	GTP	C6-N1	4.65	1.44	1.37
9	X	501	GTP	C6-N1	4.63	1.44	1.37
9	6	501	GTP	C6-N1	4.63	1.44	1.37
9	M	501	GTP	C6-N1	4.61	1.44	1.37
9	0	501	GTP	C6-N1	4.60	1.44	1.37
9	m	501	GTP	C6-N1	4.60	1.44	1.37
9	S	501	GTP	C6-N1	4.59	1.44	1.37
12	i	502	TA1	O02-C02	-4.54	1.37	1.45
9	P	501	GTP	C6-N1	4.53	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	t	502	TA1	O09-C21	4.23	1.54	1.44
12	j	502	TA1	O02-C02	-4.19	1.38	1.45
12	r	502	TA1	O02-C02	-4.17	1.38	1.45
9	6	501	GTP	C5-C6	4.03	1.55	1.47
9	e	501	GTP	C5-C6	4.02	1.55	1.47
9	F	501	GTP	C5-C6	4.00	1.55	1.47
9	1	501	GTP	C5-C6	3.97	1.55	1.47
9	Y	501	GTP	C5-C6	3.96	1.55	1.47
9	s	501	GTP	C5-C6	3.95	1.55	1.47
9	h	501	GTP	C5-C6	3.92	1.55	1.47
9	G	501	GTP	C5-C6	3.91	1.55	1.47
9	o	501	GTP	C5-C6	3.87	1.55	1.47
9	X	501	GTP	C5-C6	3.86	1.55	1.47
9	7	501	GTP	C5-C6	3.83	1.55	1.47
9	Z	501	GTP	C5-C6	3.82	1.55	1.47
9	5	501	GTP	C5-C6	3.82	1.55	1.47
9	y	501	GTP	C5-C6	3.82	1.55	1.47
9	L	501	GTP	C5-C6	3.79	1.54	1.47
9	f	501	GTP	C5-C6	3.78	1.54	1.47
9	E	501	GTP	C5-C6	3.77	1.54	1.47
9	S	501	GTP	C5-C6	3.76	1.54	1.47
9	D	501	GTP	C5-C6	3.73	1.54	1.47
12	8	502	TA1	O02-C02	-3.72	1.39	1.45
9	k	501	GTP	C5-C6	3.70	1.54	1.47
9	0	501	GTP	C5-C6	3.70	1.54	1.47
9	M	501	GTP	C5-C6	3.69	1.54	1.47
9	m	501	GTP	C5-C6	3.69	1.54	1.47
9	P	501	GTP	C5-C6	3.69	1.54	1.47
12	9	502	TA1	O02-C02	-3.58	1.39	1.45
12	J	502	TA1	O02-C02	-3.55	1.39	1.45
11	V	501	GDP	C5-C4	-3.44	1.34	1.43
12	p	502	TA1	O02-C02	-3.35	1.39	1.45
11	R	501	GDP	C5-C4	-3.35	1.34	1.43
11	N	501	GDP	C5-C4	-3.35	1.34	1.43
11	J	501	GDP	C5-C4	-3.34	1.34	1.43
11	K	501	GDP	C5-C4	-3.33	1.34	1.43
11	I	501	GDP	O2'-C2'	-3.27	1.34	1.43
11	4	501	GDP	C5-C4	-3.27	1.35	1.43
11	R	501	GDP	O2'-C2'	-3.26	1.34	1.43
12	w	502	TA1	O02-C02	-3.26	1.39	1.45
11	O	501	GDP	O2'-C2'	-3.25	1.34	1.43
11	i	501	GDP	C5-C4	-3.24	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	501	GDP	O2'-C2'	-3.24	1.34	1.43
11	T	501	GDP	O2'-C2'	-3.24	1.34	1.43
11	8	501	GDP	O2'-C2'	-3.23	1.35	1.43
11	i	501	GDP	O2'-C2'	-3.23	1.35	1.43
11	U	501	GDP	O2'-C2'	-3.22	1.35	1.43
11	O	501	GDP	C5-C4	-3.21	1.35	1.43
11	q	501	GDP	O2'-C2'	-3.20	1.35	1.43
11	K	501	GDP	O2'-C2'	-3.20	1.35	1.43
11	9	501	GDP	O2'-C2'	-3.20	1.35	1.43
11	j	501	GDP	O2'-C2'	-3.20	1.35	1.43
11	I	501	GDP	C5-C4	-3.20	1.35	1.43
11	Q	501	GDP	O2'-C2'	-3.20	1.35	1.43
11	w	501	GDP	O2'-C2'	-3.20	1.35	1.43
11	u	501	GDP	O2'-C2'	-3.19	1.35	1.43
11	8	501	GDP	C5-C4	-3.19	1.35	1.43
11	p	501	GDP	O2'-C2'	-3.18	1.35	1.43
11	j	501	GDP	C5-C4	-3.18	1.35	1.43
11	U	501	GDP	C5-C4	-3.18	1.35	1.43
9	s	501	GTP	C2-N1	3.18	1.45	1.37
11	4	501	GDP	O2'-C2'	-3.17	1.35	1.43
11	r	501	GDP	O2'-C2'	-3.16	1.35	1.43
11	t	501	GDP	O2'-C2'	-3.16	1.35	1.43
11	J	501	GDP	O2'-C2'	-3.15	1.35	1.43
11	p	501	GDP	C5-C4	-3.15	1.35	1.43
9	1	501	GTP	C2-N1	3.15	1.45	1.37
11	b	501	GDP	O2'-C2'	-3.14	1.35	1.43
9	e	501	GTP	C2-N1	3.13	1.45	1.37
12	a	502	TA1	O02-C02	-3.12	1.40	1.45
11	q	501	GDP	C5-C4	-3.12	1.35	1.43
11	a	501	GDP	O2'-C2'	-3.12	1.35	1.43
9	Y	501	GTP	C2-N1	3.12	1.45	1.37
11	9	501	GDP	C5-C4	-3.12	1.35	1.43
11	r	501	GDP	C5-C4	-3.10	1.35	1.43
9	h	501	GTP	C2-N1	3.10	1.45	1.37
11	w	501	GDP	C5-C4	-3.09	1.35	1.43
11	b	501	GDP	C5-C4	-3.09	1.35	1.43
11	v	501	GDP	C5-C4	-3.08	1.35	1.43
11	v	501	GDP	O2'-C2'	-3.08	1.35	1.43
11	t	501	GDP	C5-C4	-3.08	1.35	1.43
9	Z	501	GTP	C2-N1	3.07	1.45	1.37
9	F	501	GTP	C2-N1	3.07	1.45	1.37
9	E	501	GTP	C2-N1	3.07	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	501	GDP	C5-C4	-3.07	1.35	1.43
11	u	501	GDP	C5-C4	-3.07	1.35	1.43
9	o	501	GTP	C2-N1	3.06	1.45	1.37
11	Q	501	GDP	C5-C4	-3.05	1.35	1.43
9	f	501	GTP	C2-N1	3.04	1.45	1.37
9	X	501	GTP	C2-N1	3.04	1.45	1.37
9	k	501	GTP	C2-N1	3.04	1.45	1.37
9	6	501	GTP	C2-N1	3.03	1.45	1.37
9	S	501	GTP	C2-N1	3.03	1.45	1.37
9	G	501	GTP	C2-N1	3.03	1.45	1.37
9	0	501	GTP	C2-N1	3.03	1.45	1.37
9	7	501	GTP	C2-N1	3.02	1.45	1.37
9	m	501	GTP	C2-N1	3.02	1.45	1.37
9	M	501	GTP	C2-N1	3.02	1.45	1.37
11	V	501	GDP	O2'-C2'	-3.01	1.35	1.43
9	y	501	GTP	C2-N1	3.01	1.44	1.37
9	5	501	GTP	C2-N1	3.01	1.44	1.37
9	L	501	GTP	C2-N1	3.00	1.44	1.37
11	a	501	GDP	C5-C4	-2.99	1.35	1.43
9	D	501	GTP	C2-N1	2.98	1.44	1.37
9	P	501	GTP	C2-N1	2.98	1.44	1.37
11	V	501	GDP	C5-C6	2.94	1.53	1.47
12	p	502	TA1	O09-C21	2.90	1.51	1.44
12	V	502	TA1	O02-C02	-2.89	1.40	1.45
12	4	502	TA1	O02-C02	-2.84	1.40	1.45
12	9	502	TA1	O09-C21	2.61	1.50	1.44
11	J	501	GDP	O6-C6	-2.61	1.17	1.23
9	7	501	GTP	O2'-C2'	2.59	1.49	1.43
11	4	501	GDP	C5-C6	2.58	1.52	1.47
9	s	501	GTP	O2'-C2'	2.58	1.49	1.43
9	y	501	GTP	O3'-C3'	-2.57	1.36	1.43
11	8	501	GDP	O6-C6	-2.57	1.17	1.23
9	P	501	GTP	O2'-C2'	2.56	1.49	1.43
9	m	501	GTP	O2'-C2'	2.56	1.49	1.43
9	S	501	GTP	O2'-C2'	2.56	1.49	1.43
9	m	501	GTP	O3'-C3'	-2.55	1.36	1.43
9	1	501	GTP	O2'-C2'	2.55	1.49	1.43
9	F	501	GTP	O2'-C2'	2.55	1.49	1.43
9	o	501	GTP	O3'-C3'	-2.54	1.36	1.43
9	L	501	GTP	O3'-C3'	-2.54	1.36	1.43
9	6	501	GTP	O2'-C2'	2.54	1.49	1.43
9	e	501	GTP	O2'-C2'	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	X	501	GTP	O3'-C3'	-2.54	1.36	1.43
9	E	501	GTP	O2'-C2'	2.53	1.49	1.43
9	Z	501	GTP	O2'-C2'	2.53	1.49	1.43
9	Y	501	GTP	O2'-C2'	2.53	1.49	1.43
9	G	501	GTP	O3'-C3'	-2.53	1.36	1.43
9	f	501	GTP	O3'-C3'	-2.53	1.36	1.43
9	D	501	GTP	O2'-C2'	2.53	1.49	1.43
9	F	501	GTP	O3'-C3'	-2.53	1.36	1.43
9	k	501	GTP	O3'-C3'	-2.53	1.36	1.43
9	o	501	GTP	O2'-C2'	2.52	1.49	1.43
9	h	501	GTP	O3'-C3'	-2.52	1.36	1.43
9	7	501	GTP	O3'-C3'	-2.52	1.36	1.43
9	E	501	GTP	O3'-C3'	-2.52	1.36	1.43
9	0	501	GTP	O2'-C2'	2.52	1.49	1.43
9	D	501	GTP	O3'-C3'	-2.51	1.36	1.43
9	k	501	GTP	O2'-C2'	2.51	1.49	1.43
9	P	501	GTP	O3'-C3'	-2.51	1.36	1.43
9	0	501	GTP	O3'-C3'	-2.51	1.36	1.43
9	5	501	GTP	O3'-C3'	-2.51	1.36	1.43
11	R	501	GDP	C5-C6	2.50	1.52	1.47
9	h	501	GTP	O2'-C2'	2.50	1.49	1.43
9	Y	501	GTP	O3'-C3'	-2.50	1.36	1.43
9	y	501	GTP	O2'-C2'	2.50	1.49	1.43
9	S	501	GTP	O3'-C3'	-2.50	1.36	1.43
9	f	501	GTP	O2'-C2'	2.49	1.49	1.43
9	L	501	GTP	O2'-C2'	2.49	1.49	1.43
9	e	501	GTP	O3'-C3'	-2.49	1.36	1.43
9	X	501	GTP	O2'-C2'	2.49	1.49	1.43
9	6	501	GTP	O3'-C3'	-2.49	1.36	1.43
9	G	501	GTP	O2'-C2'	2.49	1.49	1.43
9	M	501	GTP	O2'-C2'	2.49	1.49	1.43
9	Z	501	GTP	O3'-C3'	-2.49	1.36	1.43
9	M	501	GTP	O3'-C3'	-2.48	1.36	1.43
11	N	501	GDP	O6-C6	-2.48	1.17	1.23
11	T	501	GDP	O6-C6	-2.48	1.17	1.23
9	5	501	GTP	O2'-C2'	2.47	1.49	1.43
11	i	501	GDP	O6-C6	-2.47	1.17	1.23
11	p	501	GDP	O6-C6	-2.47	1.17	1.23
11	b	501	GDP	C2-N1	2.47	1.43	1.37
11	O	501	GDP	C5-C6	2.47	1.52	1.47
11	b	501	GDP	O6-C6	-2.47	1.17	1.23
9	1	501	GTP	O3'-C3'	-2.47	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	9	501	GDP	O6-C6	-2.45	1.17	1.23
9	s	501	GTP	O3'-C3'	-2.45	1.36	1.43
11	r	501	GDP	O6-C6	-2.45	1.17	1.23
11	v	501	GDP	O6-C6	-2.45	1.17	1.23
11	t	501	GDP	O6-C6	-2.44	1.17	1.23
11	q	501	GDP	O6-C6	-2.44	1.17	1.23
11	p	501	GDP	C2-N1	2.44	1.43	1.37
11	j	501	GDP	O6-C6	-2.43	1.17	1.23
11	t	501	GDP	C2-N1	2.43	1.43	1.37
11	t	501	GDP	C5-C6	2.43	1.52	1.47
11	K	501	GDP	O6-C6	-2.42	1.17	1.23
11	u	501	GDP	O6-C6	-2.42	1.17	1.23
11	Q	501	GDP	C2-N1	2.42	1.43	1.37
11	w	501	GDP	O6-C6	-2.42	1.17	1.23
11	a	501	GDP	C2-N1	2.42	1.43	1.37
11	U	501	GDP	O6-C6	-2.41	1.17	1.23
11	a	501	GDP	O6-C6	-2.41	1.17	1.23
11	4	501	GDP	O6-C6	-2.40	1.17	1.23
11	u	501	GDP	C2-N1	2.40	1.43	1.37
11	Q	501	GDP	O6-C6	-2.40	1.17	1.23
11	9	501	GDP	C2-N1	2.39	1.43	1.37
11	r	501	GDP	C2-N1	2.38	1.43	1.37
11	I	501	GDP	O6-C6	-2.38	1.17	1.23
11	9	501	GDP	C5-C6	2.38	1.52	1.47
11	U	501	GDP	C2-N1	2.38	1.43	1.37
11	j	501	GDP	C2-N1	2.38	1.43	1.37
11	N	501	GDP	C2-N1	2.37	1.43	1.37
12	q	502	TA1	O08-C20	2.37	1.25	1.21
11	4	501	GDP	C2-N1	2.37	1.43	1.37
11	V	501	GDP	C2-N1	2.37	1.43	1.37
11	J	501	GDP	C2-N1	2.36	1.43	1.37
11	a	501	GDP	C5-C6	2.36	1.52	1.47
11	r	501	GDP	C5-C6	2.35	1.52	1.47
11	R	501	GDP	C2-N1	2.35	1.43	1.37
11	K	501	GDP	C2-N1	2.35	1.43	1.37
11	8	501	GDP	C2-N1	2.35	1.43	1.37
11	v	501	GDP	C2-N1	2.34	1.43	1.37
11	v	501	GDP	C5-C6	2.33	1.52	1.47
11	w	501	GDP	C2-N1	2.33	1.43	1.37
11	q	501	GDP	C2-N1	2.32	1.43	1.37
11	O	501	GDP	O6-C6	-2.32	1.17	1.23
11	R	501	GDP	O6-C6	-2.30	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	w	501	GDP	C5-C6	2.30	1.52	1.47
11	N	501	GDP	C5-C6	2.30	1.52	1.47
11	I	501	GDP	C2-N1	2.30	1.43	1.37
11	T	501	GDP	C2-N1	2.28	1.43	1.37
11	O	501	GDP	C2-N1	2.28	1.43	1.37
11	i	501	GDP	C5-C6	2.27	1.51	1.47
11	Q	501	GDP	C5-C6	2.26	1.51	1.47
11	b	501	GDP	C5-C6	2.26	1.51	1.47
11	j	501	GDP	C5-C6	2.25	1.51	1.47
11	8	501	GDP	C5-C6	2.25	1.51	1.47
11	q	501	GDP	C5-C6	2.24	1.51	1.47
11	u	501	GDP	C5-C6	2.24	1.51	1.47
11	p	501	GDP	C5-C6	2.24	1.51	1.47
11	T	501	GDP	C5-C6	2.22	1.51	1.47
11	i	501	GDP	C2-N1	2.22	1.43	1.37
11	U	501	GDP	C5-C6	2.22	1.51	1.47
12	V	502	TA1	O09-C21	2.21	1.49	1.44
11	I	501	GDP	C5-C6	2.16	1.51	1.47
11	K	501	GDP	C5-C6	2.16	1.51	1.47
11	J	501	GDP	C5-C6	2.12	1.51	1.47
12	a	502	TA1	O09-C21	2.11	1.49	1.44
12	u	502	TA1	O09-C21	-2.08	1.40	1.44
11	V	501	GDP	O6-C6	-2.02	1.18	1.23

All (314) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	501	GDP	C4'-O4'-C1'	-8.78	101.88	109.92
11	K	501	GDP	C4'-O4'-C1'	-7.37	103.17	109.92
11	I	501	GDP	C4'-O4'-C1'	-6.53	103.95	109.92
11	U	501	GDP	C4'-O4'-C1'	-6.38	104.09	109.92
11	4	501	GDP	C4'-O4'-C1'	-6.26	104.19	109.92
11	T	501	GDP	C4'-O4'-C1'	-6.23	104.22	109.92
11	R	501	GDP	C4'-O4'-C1'	-5.85	104.56	109.92
11	V	501	GDP	C4'-O4'-C1'	-5.69	104.71	109.92
9	s	501	GTP	C4'-O4'-C1'	-5.50	104.89	109.92
11	Q	501	GDP	C4'-O4'-C1'	-5.43	104.95	109.92
11	8	501	GDP	C4'-O4'-C1'	-5.30	105.07	109.92
9	F	501	GTP	C4'-O4'-C1'	-5.25	105.12	109.92
11	b	501	GDP	C4'-O4'-C1'	-5.06	105.29	109.92
11	p	501	GDP	C4'-O4'-C1'	-4.93	105.41	109.92
9	G	501	GTP	C4'-O4'-C1'	-4.84	105.50	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	q	501	GDP	C4'-O4'-C1'	-4.76	105.56	109.92
11	r	501	GDP	C4'-O4'-C1'	-4.65	105.66	109.92
9	Z	501	GTP	C4'-O4'-C1'	-4.51	105.80	109.92
11	j	501	GDP	C4'-O4'-C1'	-4.48	105.83	109.92
12	b	502	TA1	C24-C21-C20	4.42	122.94	113.31
12	u	502	TA1	C24-C21-C20	4.38	122.85	113.31
12	a	502	TA1	C24-C21-C20	4.37	122.84	113.31
11	t	501	GDP	C4'-O4'-C1'	-4.36	105.93	109.92
12	9	502	TA1	C24-C21-C20	4.29	122.65	113.31
12	j	502	TA1	C24-C21-C20	4.28	122.64	113.31
12	w	502	TA1	C24-C21-C20	4.25	122.57	113.31
11	O	501	GDP	C4'-O4'-C1'	-4.15	106.13	109.92
11	v	501	GDP	C4'-O4'-C1'	-4.09	106.18	109.92
12	V	502	TA1	C24-C21-C20	4.08	122.19	113.31
11	V	501	GDP	C8-N7-C5	4.07	109.48	102.55
11	R	501	GDP	C2-N1-C6	-4.07	117.66	125.11
9	Y	501	GTP	C4'-O4'-C1'	-4.07	106.20	109.92
9	E	501	GTP	C4'-O4'-C1'	-4.07	106.20	109.92
11	V	501	GDP	C2-N1-C6	-4.07	117.66	125.11
9	h	501	GTP	C4'-O4'-C1'	-4.06	106.21	109.92
12	v	502	TA1	C24-C21-C20	4.05	122.14	113.31
11	a	501	GDP	C4'-O4'-C1'	-4.04	106.23	109.92
12	J	502	TA1	C24-C21-C20	3.99	122.00	113.31
12	q	502	TA1	C47-C45-C46	-3.97	95.03	106.29
11	4	501	GDP	C2-N1-C6	-3.96	117.85	125.11
12	8	502	TA1	C24-C21-C20	3.95	121.92	113.31
9	L	501	GTP	C4'-O4'-C1'	-3.95	106.31	109.92
11	K	501	GDP	C2-N1-C6	-3.95	117.88	125.11
12	4	502	TA1	C24-C21-C20	3.83	121.66	113.31
11	J	501	GDP	C4'-O4'-C1'	-3.83	106.42	109.92
11	R	501	GDP	C8-N7-C5	3.80	109.01	102.55
11	N	501	GDP	C2-N1-C6	-3.79	118.17	125.11
11	O	501	GDP	C2-N1-C6	-3.78	118.20	125.11
12	i	502	TA1	C24-C21-C20	3.74	121.46	113.31
11	I	501	GDP	C2-N1-C6	-3.74	118.27	125.11
11	4	501	GDP	C8-N7-C5	3.72	108.89	102.55
11	9	501	GDP	C4'-O4'-C1'	-3.71	106.53	109.92
11	j	501	GDP	C2-N1-C6	-3.71	118.32	125.11
9	5	501	GTP	C4'-O4'-C1'	-3.71	106.53	109.92
11	V	501	GDP	O6-C6-C5	-3.70	116.98	124.32
11	N	501	GDP	C8-N7-C5	3.69	108.84	102.55
11	J	501	GDP	C2-N1-C6	-3.68	118.37	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	O	501	GDP	C8-N7-C5	3.66	108.78	102.55
9	e	501	GTP	C4'-O4'-C1'	-3.64	106.59	109.92
11	K	501	GDP	C8-N7-C5	3.61	108.69	102.55
12	p	502	TA1	C24-C21-C20	3.61	121.16	113.31
11	t	501	GDP	C8-N7-C5	3.60	108.68	102.55
11	i	501	GDP	C2-N1-C6	-3.58	118.56	125.11
11	J	501	GDP	C5-C6-N1	3.57	120.89	114.07
11	r	501	GDP	C8-N7-C5	3.57	108.63	102.55
11	p	501	GDP	C8-N7-C5	3.56	108.61	102.55
12	r	502	TA1	C24-C21-C20	3.55	121.05	113.31
11	K	501	GDP	C5-C6-N1	3.55	120.85	114.07
12	j	502	TA1	C18-C20-C21	3.55	128.98	121.38
11	q	501	GDP	C8-N7-C5	3.54	108.58	102.55
12	t	502	TA1	C24-C21-C20	3.54	121.02	113.31
11	U	501	GDP	C8-N7-C5	3.54	108.57	102.55
11	b	501	GDP	C8-N7-C5	3.53	108.55	102.55
11	N	501	GDP	C5-C6-N1	3.52	120.80	114.07
11	I	501	GDP	C8-N7-C5	3.51	108.53	102.55
11	R	501	GDP	C5-C6-N1	3.51	120.76	114.07
11	v	501	GDP	C8-N7-C5	3.51	108.52	102.55
11	9	501	GDP	C8-N7-C5	3.51	108.52	102.55
11	u	501	GDP	C8-N7-C5	3.50	108.51	102.55
11	Q	501	GDP	C8-N7-C5	3.50	108.50	102.55
11	T	501	GDP	C8-N7-C5	3.49	108.49	102.55
11	4	501	GDP	C5-C6-N1	3.49	120.72	114.07
11	a	501	GDP	C8-N7-C5	3.49	108.48	102.55
11	8	501	GDP	C8-N7-C5	3.48	108.47	102.55
11	K	501	GDP	O6-C6-C5	-3.48	117.43	124.32
11	I	501	GDP	C5-C6-N1	3.47	120.69	114.07
11	j	501	GDP	C5-C6-N1	3.47	120.68	114.07
11	w	501	GDP	C8-N7-C5	3.44	108.41	102.55
11	i	501	GDP	C8-N7-C5	3.44	108.41	102.55
11	i	501	GDP	C5-C6-N1	3.42	120.61	114.07
11	j	501	GDP	C8-N7-C5	3.42	108.37	102.55
11	J	501	GDP	C8-N7-C5	3.40	108.34	102.55
11	O	501	GDP	C5-C6-N1	3.40	120.56	114.07
11	8	501	GDP	C5-C6-N1	3.36	120.48	114.07
11	8	501	GDP	C2-N1-C6	-3.34	118.99	125.11
9	e	501	GTP	C8-N7-C5	3.34	108.23	102.55
9	F	501	GTP	C8-N7-C5	3.33	108.22	102.55
9	G	501	GTP	C8-N7-C5	3.32	108.20	102.55
9	m	501	GTP	C8-N7-C5	3.32	108.20	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	V	501	GDP	C5-C6-N1	3.32	120.40	114.07
9	1	501	GTP	C8-N7-C5	3.30	108.17	102.55
9	0	501	GTP	C8-N7-C5	3.30	108.17	102.55
9	1	501	GTP	C4'-O4'-C1'	-3.30	106.90	109.92
9	6	501	GTP	C8-N7-C5	3.30	108.17	102.55
9	L	501	GTP	C2-N1-C6	-3.28	119.10	125.11
9	X	501	GTP	C8-N7-C5	3.28	108.14	102.55
9	M	501	GTP	C2-N1-C6	-3.28	119.11	125.11
9	L	501	GTP	C8-N7-C5	3.27	108.12	102.55
9	Y	501	GTP	C8-N7-C5	3.27	108.11	102.55
9	6	501	GTP	C4'-O4'-C1'	-3.26	106.94	109.92
9	h	501	GTP	C8-N7-C5	3.26	108.09	102.55
9	s	501	GTP	C8-N7-C5	3.26	108.09	102.55
11	R	501	GDP	O6-C6-C5	-3.25	117.87	124.32
9	o	501	GTP	C8-N7-C5	3.25	108.08	102.55
9	m	501	GTP	C4'-O4'-C1'	-3.25	106.95	109.92
9	7	501	GTP	C8-N7-C5	3.24	108.06	102.55
9	M	501	GTP	C8-N7-C5	3.23	108.04	102.55
9	E	501	GTP	C8-N7-C5	3.22	108.04	102.55
11	b	501	GDP	C2-N1-C6	-3.22	119.21	125.11
9	y	501	GTP	C8-N7-C5	3.22	108.03	102.55
11	b	501	GDP	C5-C6-N1	3.22	120.21	114.07
9	Y	501	GTP	C5-C6-N1	3.21	120.20	114.07
9	S	501	GTP	C8-N7-C5	3.21	108.02	102.55
9	P	501	GTP	C2-N1-C6	-3.21	119.23	125.11
9	X	501	GTP	C2-N1-C6	-3.21	119.23	125.11
9	L	501	GTP	C5-C6-N1	3.21	120.20	114.07
9	E	501	GTP	C2-N1-C6	-3.21	119.23	125.11
11	v	501	GDP	C5-C6-N1	3.20	120.18	114.07
11	N	501	GDP	O6-C6-C5	-3.20	117.98	124.32
9	5	501	GTP	C8-N7-C5	3.20	107.99	102.55
9	M	501	GTP	C5-C6-N1	3.20	120.17	114.07
9	f	501	GTP	C8-N7-C5	3.20	107.99	102.55
9	6	501	GTP	C2-N1-C6	-3.20	119.26	125.11
9	D	501	GTP	C2-N1-C6	-3.20	119.26	125.11
9	7	501	GTP	C2-N1-C6	-3.18	119.28	125.11
9	S	501	GTP	C5-C6-N1	3.18	120.14	114.07
9	Z	501	GTP	C8-N7-C5	3.18	107.96	102.55
9	1	501	GTP	C2-N1-C6	-3.17	119.30	125.11
9	P	501	GTP	C5-C6-N1	3.17	120.12	114.07
9	D	501	GTP	C8-N7-C5	3.17	107.95	102.55
9	S	501	GTP	C2-N1-C6	-3.17	119.31	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	X	501	GTP	C5-C6-N1	3.15	120.09	114.07
9	o	501	GTP	C2-N1-C6	-3.15	119.34	125.11
9	o	501	GTP	C5-C6-N1	3.15	120.09	114.07
9	5	501	GTP	C5-C6-N1	3.15	120.08	114.07
11	a	501	GDP	C5-C6-N1	3.14	120.07	114.07
11	w	501	GDP	C5-C6-N1	3.14	120.07	114.07
9	P	501	GTP	C8-N7-C5	3.14	107.90	102.55
9	D	501	GTP	C5-C6-N1	3.14	120.06	114.07
9	E	501	GTP	C5-C6-N1	3.14	120.06	114.07
9	m	501	GTP	C2-N1-C6	-3.14	119.36	125.11
11	9	501	GDP	C5-C6-N1	3.14	120.05	114.07
9	7	501	GTP	C5-C6-N1	3.13	120.05	114.07
9	k	501	GTP	C2-N1-C6	-3.13	119.38	125.11
9	5	501	GTP	C2-N1-C6	-3.13	119.38	125.11
9	0	501	GTP	C2-N1-C6	-3.13	119.39	125.11
11	T	501	GDP	C5-C6-N1	3.12	120.03	114.07
9	f	501	GTP	C2-N1-C6	-3.11	119.41	125.11
12	q	502	TA1	C17-C18-C20	3.11	109.55	102.58
9	m	501	GTP	C5-C6-N1	3.10	119.99	114.07
9	y	501	GTP	C2-N1-C6	-3.10	119.43	125.11
9	k	501	GTP	C8-N7-C5	3.10	107.83	102.55
11	q	501	GDP	C5-C6-N1	3.10	119.99	114.07
9	f	501	GTP	C5-C6-N1	3.10	119.98	114.07
11	U	501	GDP	C5-C6-N1	3.10	119.98	114.07
9	Z	501	GTP	C5-C6-N1	3.09	119.97	114.07
9	k	501	GTP	C5-C6-N1	3.09	119.97	114.07
9	6	501	GTP	C5-C6-N1	3.09	119.96	114.07
12	4	502	TA1	C18-C20-C21	3.09	127.99	121.38
11	T	501	GDP	C2-N1-C6	-3.08	119.46	125.11
12	J	502	TA1	C47-C45-C46	-3.08	97.55	106.29
11	v	501	GDP	C2-N1-C6	-3.07	119.48	125.11
11	w	501	GDP	C2-N1-C6	-3.07	119.49	125.11
11	I	501	GDP	O6-C6-C5	-3.07	118.24	124.32
9	e	501	GTP	C2-N1-C6	-3.07	119.50	125.11
11	9	501	GDP	C2-N1-C6	-3.06	119.51	125.11
9	F	501	GTP	C5-C6-N1	3.06	119.91	114.07
11	J	501	GDP	O6-C6-C5	-3.06	118.26	124.32
11	Q	501	GDP	C5-C6-N1	3.06	119.91	114.07
9	0	501	GTP	C5-C6-N1	3.06	119.90	114.07
9	G	501	GTP	C5-C6-N1	3.06	119.90	114.07
11	u	501	GDP	C2-N1-C6	-3.06	119.52	125.11
11	r	501	GDP	C5-C6-N1	3.05	119.89	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	U	501	GDP	C2-N1-C6	-3.05	119.53	125.11
9	F	501	GTP	C2-N1-C6	-3.05	119.53	125.11
9	y	501	GTP	C5-C6-N1	3.05	119.89	114.07
9	Z	501	GTP	C2-N1-C6	-3.05	119.53	125.11
11	t	501	GDP	C5-C6-N1	3.04	119.88	114.07
11	t	501	GDP	C2-N1-C6	-3.04	119.55	125.11
9	h	501	GTP	C2-N1-C6	-3.04	119.55	125.11
9	G	501	GTP	C2-N1-C6	-3.03	119.56	125.11
11	u	501	GDP	C5-C6-N1	3.03	119.85	114.07
11	w	501	GDP	C4'-O4'-C1'	-3.02	107.16	109.92
11	r	501	GDP	C2-N1-C6	-3.02	119.59	125.11
11	p	501	GDP	C5-C6-N1	3.02	119.82	114.07
11	a	501	GDP	C2-N1-C6	-3.01	119.60	125.11
11	q	501	GDP	C2-N1-C6	-3.01	119.60	125.11
11	Q	501	GDP	C2-N1-C6	-3.01	119.60	125.11
9	h	501	GTP	C5-C6-N1	3.01	119.81	114.07
9	e	501	GTP	C5-C6-N1	3.00	119.79	114.07
9	1	501	GTP	C5-C6-N1	2.99	119.77	114.07
11	j	501	GDP	O6-C6-C5	-2.98	118.41	124.32
9	s	501	GTP	C5-C6-N1	2.98	119.75	114.07
11	p	501	GDP	C2-N1-C6	-2.98	119.66	125.11
12	j	502	TA1	O08-C20-C21	-2.97	115.71	119.28
12	8	502	TA1	C47-C45-C46	-2.97	97.87	106.29
9	s	501	GTP	C2-N1-C6	-2.96	119.69	125.11
9	Y	501	GTP	C2-N1-C6	-2.95	119.71	125.11
12	r	502	TA1	C47-C45-C46	-2.95	97.93	106.29
12	r	502	TA1	C18-C20-C21	2.92	127.63	121.38
11	4	501	GDP	O6-C6-C5	-2.91	118.54	124.32
11	i	501	GDP	C4'-O4'-C1'	-2.85	107.31	109.92
9	P	501	GTP	C4'-O4'-C1'	-2.85	107.31	109.92
11	u	501	GDP	C4'-O4'-C1'	-2.81	107.35	109.92
9	X	501	GTP	C4'-O4'-C1'	-2.81	107.35	109.92
12	9	502	TA1	C18-C20-C21	2.79	127.35	121.38
12	t	502	TA1	C10-C18-C17	-2.78	101.27	106.55
12	p	502	TA1	C47-C45-C46	-2.78	98.40	106.29
12	t	502	TA1	C47-C45-C46	-2.77	98.44	106.29
12	9	502	TA1	C47-C45-C46	-2.76	98.45	106.29
12	a	502	TA1	C47-C45-C46	-2.76	98.46	106.29
12	v	502	TA1	C18-C20-C21	2.75	127.28	121.38
9	f	501	GTP	C4'-O4'-C1'	-2.75	107.41	109.92
11	O	501	GDP	O6-C6-C5	-2.75	118.88	124.32
12	i	502	TA1	C18-C20-C21	2.73	127.22	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	u	502	TA1	C18-C20-C21	2.72	127.22	121.38
12	a	502	TA1	O11-C26-C25	2.71	116.28	109.85
12	p	502	TA1	C18-C20-C21	2.69	127.15	121.38
12	w	502	TA1	C18-C20-C21	2.67	127.10	121.38
11	i	501	GDP	O6-C6-C5	-2.66	119.05	124.32
9	S	501	GTP	C4'-O4'-C1'	-2.65	107.50	109.92
12	i	502	TA1	C47-C45-C46	-2.65	98.77	106.29
11	N	501	GDP	O4'-C1'-N9	2.63	112.23	108.75
12	q	502	TA1	C19-C18-C20	-2.62	99.77	106.56
12	b	502	TA1	C47-C45-C46	-2.60	98.91	106.29
12	t	502	TA1	C18-C20-C21	2.56	126.87	121.38
11	b	501	GDP	O6-C6-C5	-2.53	119.31	124.32
12	b	502	TA1	C18-C20-C21	2.52	126.78	121.38
9	0	501	GTP	C4'-O4'-C1'	-2.51	107.62	109.92
11	8	501	GDP	O6-C6-C5	-2.51	119.35	124.32
9	7	501	GTP	C4'-O4'-C1'	-2.50	107.64	109.92
12	4	502	TA1	C47-C45-C46	-2.49	99.22	106.29
12	V	502	TA1	C47-C45-C46	-2.49	99.22	106.29
12	a	502	TA1	C18-C20-C21	2.49	126.71	121.38
9	M	501	GTP	O6-C6-C5	-2.44	119.48	124.32
9	D	501	GTP	C4'-O4'-C1'	-2.43	107.70	109.92
12	4	502	TA1	O08-C20-C21	-2.43	116.36	119.28
12	r	502	TA1	O08-C20-C21	-2.42	116.37	119.28
11	R	501	GDP	O4'-C1'-N9	2.42	111.95	108.75
9	P	501	GTP	O6-C6-C5	-2.41	119.54	124.32
11	U	501	GDP	O6-C6-C5	-2.37	119.63	124.32
9	o	501	GTP	C4'-O4'-C1'	-2.36	107.77	109.92
9	E	501	GTP	O6-C6-C5	-2.36	119.65	124.32
9	D	501	GTP	O6-C6-C5	-2.34	119.68	124.32
9	L	501	GTP	O6-C6-C5	-2.34	119.69	124.32
9	k	501	GTP	O6-C6-C5	-2.33	119.71	124.32
11	Q	501	GDP	O6-C6-C5	-2.33	119.71	124.32
9	S	501	GTP	O6-C6-C5	-2.32	119.72	124.32
11	T	501	GDP	O6-C6-C5	-2.32	119.72	124.32
11	w	501	GDP	O6-C6-C5	-2.31	119.73	124.32
11	u	501	GDP	O6-C6-C5	-2.30	119.75	124.32
9	7	501	GTP	O6-C6-C5	-2.29	119.79	124.32
12	i	502	TA1	O08-C20-C21	-2.28	116.54	119.28
12	v	502	TA1	C47-C45-C46	-2.28	99.81	106.29
11	a	501	GDP	O6-C6-C5	-2.28	119.80	124.32
11	v	501	GDP	O6-C6-C5	-2.28	119.80	124.32
9	o	501	GTP	O6-C6-C5	-2.27	119.81	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	v	501	GDP	C2'-C3'-C4'	2.27	107.00	102.61
12	8	502	TA1	C18-C20-C21	2.27	126.24	121.38
9	m	501	GTP	O6-C6-C5	-2.27	119.82	124.32
11	9	501	GDP	O6-C6-C5	-2.26	119.83	124.32
12	j	502	TA1	C47-C45-C46	-2.26	99.89	106.29
9	0	501	GTP	O6-C6-C5	-2.24	119.87	124.32
9	f	501	GTP	O6-C6-C5	-2.24	119.88	124.32
9	5	501	GTP	O6-C6-C5	-2.23	119.90	124.32
12	V	502	TA1	C18-C20-C21	2.23	126.15	121.38
12	w	502	TA1	C47-C45-C46	-2.23	99.97	106.29
11	p	501	GDP	O6-C6-C5	-2.22	119.91	124.32
9	y	501	GTP	O6-C6-C5	-2.22	119.92	124.32
9	M	501	GTP	C4'-O4'-C1'	-2.21	107.90	109.92
12	9	502	TA1	C44-C25-C24	-2.21	122.69	125.32
12	u	502	TA1	C47-C45-C46	-2.21	100.02	106.29
11	q	501	GDP	O6-C6-C5	-2.20	119.95	124.32
9	X	501	GTP	O6-C6-C5	-2.20	119.97	124.32
12	v	502	TA1	C10-C18-C20	2.18	119.89	116.30
12	u	502	TA1	O08-C20-C21	-2.17	116.67	119.28
9	Z	501	GTP	O6-C6-C5	-2.15	120.06	124.32
11	K	501	GDP	O4'-C1'-N9	2.15	111.60	108.75
12	v	502	TA1	O08-C20-C21	-2.14	116.70	119.28
12	8	502	TA1	C44-C25-C24	-2.14	122.78	125.32
9	k	501	GTP	C4'-O4'-C1'	-2.14	107.97	109.92
11	t	501	GDP	O6-C6-C5	-2.13	120.10	124.32
9	Y	501	GTP	O6-C6-C5	-2.12	120.12	124.32
12	4	502	TA1	C10-C18-C20	2.11	119.78	116.30
11	r	501	GDP	O6-C6-C5	-2.11	120.14	124.32
12	b	502	TA1	O02-C02-C01	-2.10	100.39	104.74
9	h	501	GTP	O6-C6-C5	-2.09	120.17	124.32
12	w	502	TA1	O08-C20-C21	-2.09	116.77	119.28
12	J	502	TA1	C18-C20-C21	2.09	125.85	121.38
9	y	501	GTP	C4'-O4'-C1'	-2.08	108.02	109.92
9	Z	501	GTP	O4'-C1'-N9	2.08	111.51	108.75
11	a	501	GDP	C2'-C3'-C4'	2.08	106.64	102.61
9	1	501	GTP	O6-C6-C5	-2.08	120.20	124.32
9	s	501	GTP	O6-C6-C5	-2.05	120.25	124.32
12	q	502	TA1	C44-C25-C24	-2.05	122.88	125.32
9	G	501	GTP	O6-C6-C5	-2.05	120.26	124.32
9	6	501	GTP	O6-C6-C5	-2.05	120.26	124.32
12	p	502	TA1	O08-C20-C21	-2.04	116.83	119.28
12	J	502	TA1	O11-C26-C25	2.04	114.69	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	e	501	GTP	O6-C6-C5	-2.03	120.31	124.32
9	F	501	GTP	O6-C6-C5	-2.02	120.32	124.32
11	Q	501	GDP	C2'-C3'-C4'	2.01	106.48	102.61
12	q	502	TA1	C18-C20-C21	2.00	125.67	121.38
12	q	502	TA1	C47-C45-C24	2.00	120.78	112.78

There are no chirality outliers.

All (291) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	501	GTP	C5'-O5'-PA-O2A
9	G	501	GTP	C5'-O5'-PA-O3A
9	G	501	GTP	C5'-O5'-PA-O1A
9	L	501	GTP	C5'-O5'-PA-O3A
9	L	501	GTP	C5'-O5'-PA-O1A
9	M	501	GTP	O4'-C4'-C5'-O5'
9	P	501	GTP	C5'-O5'-PA-O2A
9	S	501	GTP	O4'-C4'-C5'-O5'
9	X	501	GTP	O4'-C4'-C5'-O5'
9	Y	501	GTP	C5'-O5'-PA-O3A
9	Y	501	GTP	C5'-O5'-PA-O1A
9	Y	501	GTP	C5'-O5'-PA-O2A
9	m	501	GTP	C5'-O5'-PA-O3A
9	m	501	GTP	C5'-O5'-PA-O1A
9	o	501	GTP	C5'-O5'-PA-O1A
9	y	501	GTP	C5'-O5'-PA-O3A
9	y	501	GTP	C5'-O5'-PA-O1A
9	0	501	GTP	C5'-O5'-PA-O3A
9	0	501	GTP	C5'-O5'-PA-O1A
9	6	501	GTP	C5'-O5'-PA-O3A
9	6	501	GTP	C5'-O5'-PA-O1A
11	I	501	GDP	C5'-O5'-PA-O2A
11	J	501	GDP	C5'-O5'-PA-O3A
11	J	501	GDP	C5'-O5'-PA-O1A
11	J	501	GDP	C5'-O5'-PA-O2A
11	K	501	GDP	C5'-O5'-PA-O3A
11	K	501	GDP	C5'-O5'-PA-O1A
11	K	501	GDP	C5'-O5'-PA-O2A
11	N	501	GDP	C5'-O5'-PA-O3A
11	N	501	GDP	C5'-O5'-PA-O2A
11	O	501	GDP	C5'-O5'-PA-O3A
11	O	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
11	O	501	GDP	C5'-O5'-PA-O2A
11	Q	501	GDP	C5'-O5'-PA-O3A
11	Q	501	GDP	C5'-O5'-PA-O1A
11	Q	501	GDP	C5'-O5'-PA-O2A
11	R	501	GDP	C5'-O5'-PA-O3A
11	R	501	GDP	C5'-O5'-PA-O1A
11	R	501	GDP	C5'-O5'-PA-O2A
11	U	501	GDP	C5'-O5'-PA-O3A
11	U	501	GDP	C5'-O5'-PA-O1A
11	U	501	GDP	C5'-O5'-PA-O2A
11	V	501	GDP	C5'-O5'-PA-O3A
11	V	501	GDP	C5'-O5'-PA-O2A
11	i	501	GDP	C5'-O5'-PA-O3A
11	i	501	GDP	C5'-O5'-PA-O1A
11	i	501	GDP	C5'-O5'-PA-O2A
11	p	501	GDP	C5'-O5'-PA-O3A
11	p	501	GDP	C5'-O5'-PA-O2A
11	q	501	GDP	C5'-O5'-PA-O3A
11	q	501	GDP	C5'-O5'-PA-O1A
11	q	501	GDP	C5'-O5'-PA-O2A
11	r	501	GDP	C5'-O5'-PA-O3A
11	r	501	GDP	C5'-O5'-PA-O1A
11	r	501	GDP	C5'-O5'-PA-O2A
11	t	501	GDP	C5'-O5'-PA-O3A
11	t	501	GDP	C5'-O5'-PA-O1A
11	t	501	GDP	C5'-O5'-PA-O2A
11	u	501	GDP	C5'-O5'-PA-O3A
11	u	501	GDP	C5'-O5'-PA-O2A
11	v	501	GDP	C5'-O5'-PA-O2A
11	9	501	GDP	C5'-O5'-PA-O3A
11	9	501	GDP	C5'-O5'-PA-O1A
11	9	501	GDP	C5'-O5'-PA-O2A
12	j	502	TA1	C27-C28-C29-N01
12	u	502	TA1	C27-C28-C29-N01
12	w	502	TA1	C27-C28-C29-N01
12	w	502	TA1	O13-C28-C29-C37
12	V	502	TA1	O14-C30-C31-C32
12	b	502	TA1	O14-C30-C31-C32
12	b	502	TA1	O14-C30-C31-C36
12	r	502	TA1	O14-C30-C31-C32
12	4	502	TA1	O14-C30-C31-C32
12	V	502	TA1	O14-C30-C31-C36

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Mol	Chain	Res	Type	Atoms
12	r	502	TA1	O14-C30-C31-C36
12	4	502	TA1	O14-C30-C31-C36
12	V	502	TA1	N01-C30-C31-C36
12	4	502	TA1	N01-C30-C31-C36
12	V	502	TA1	N01-C30-C31-C32
12	b	502	TA1	N01-C30-C31-C32
12	b	502	TA1	N01-C30-C31-C36
12	q	502	TA1	N01-C30-C31-C36
12	r	502	TA1	N01-C30-C31-C32
12	r	502	TA1	N01-C30-C31-C36
12	v	502	TA1	N01-C30-C31-C32
12	4	502	TA1	N01-C30-C31-C32
12	q	502	TA1	O14-C30-C31-C32
12	q	502	TA1	O14-C30-C31-C36
12	v	502	TA1	O14-C30-C31-C32
12	v	502	TA1	O14-C30-C31-C36
12	q	502	TA1	N01-C30-C31-C32
12	v	502	TA1	N01-C30-C31-C36
12	w	502	TA1	O14-C30-C31-C32
12	i	502	TA1	N01-C30-C31-C32
12	w	502	TA1	N01-C30-C31-C32
12	i	502	TA1	O14-C30-C31-C32
12	w	502	TA1	O14-C30-C31-C36
12	j	502	TA1	N01-C30-C31-C32
12	w	502	TA1	N01-C30-C31-C36
9	E	501	GTP	O4'-C4'-C5'-O5'
9	M	501	GTP	C3'-C4'-C5'-O5'
9	P	501	GTP	O4'-C4'-C5'-O5'
9	S	501	GTP	C3'-C4'-C5'-O5'
9	X	501	GTP	C3'-C4'-C5'-O5'
9	7	501	GTP	O4'-C4'-C5'-O5'
9	7	501	GTP	C3'-C4'-C5'-O5'
11	p	501	GDP	C3'-C4'-C5'-O5'
12	i	502	TA1	N01-C30-C31-C36
12	i	502	TA1	O14-C30-C31-C36
12	j	502	TA1	O14-C30-C31-C32
12	j	502	TA1	N01-C30-C31-C36
12	u	502	TA1	N01-C30-C31-C32
12	j	502	TA1	O14-C30-C31-C36
12	w	502	TA1	C13-C12-O04-C11
12	u	502	TA1	O14-C30-C31-C32
12	J	502	TA1	O02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
12	j	502	TA1	C13-C12-O04-C11
12	w	502	TA1	O05-C12-O04-C11
12	u	502	TA1	O14-C30-C31-C36
12	u	502	TA1	N01-C30-C31-C36
12	J	502	TA1	O02-C03-C04-C09
12	j	502	TA1	O05-C12-O04-C11
12	u	502	TA1	C13-C12-O04-C11
9	P	501	GTP	C3'-C4'-C5'-O5'
9	e	501	GTP	C3'-C4'-C5'-O5'
12	u	502	TA1	O05-C12-O04-C11
9	D	501	GTP	C3'-C4'-C5'-O5'
9	E	501	GTP	C3'-C4'-C5'-O5'
12	J	502	TA1	O03-C03-C04-C05
12	J	502	TA1	O03-C03-C04-C09
11	p	501	GDP	O4'-C4'-C5'-O5'
12	t	502	TA1	C23-C22-O09-C21
9	f	501	GTP	C3'-C4'-C5'-O5'
11	T	501	GDP	C3'-C4'-C5'-O5'
9	e	501	GTP	O4'-C4'-C5'-O5'
12	b	502	TA1	O13-C28-C29-C37
12	i	502	TA1	O13-C28-C29-C37
12	j	502	TA1	O13-C28-C29-C37
12	u	502	TA1	O13-C28-C29-C37
12	w	502	TA1	O13-C28-C29-N01
9	Z	501	GTP	C3'-C4'-C5'-O5'
12	i	502	TA1	C27-C28-C29-N01
9	5	501	GTP	C3'-C4'-C5'-O5'
9	Y	501	GTP	PA-O3A-PB-O1B
9	k	501	GTP	PB-O3A-PA-O2A
11	O	501	GDP	PB-O3A-PA-O1A
11	R	501	GDP	PB-O3A-PA-O1A
11	V	501	GDP	PB-O3A-PA-O1A
11	b	501	GDP	PB-O3A-PA-O1A
11	i	501	GDP	PB-O3A-PA-O1A
11	j	501	GDP	PB-O3A-PA-O1A
11	r	501	GDP	PB-O3A-PA-O1A
11	u	501	GDP	PB-O3A-PA-O1A
11	v	501	GDP	PB-O3A-PA-O1A
11	N	501	GDP	C3'-C4'-C5'-O5'
12	u	502	TA1	C23-C22-O09-C21
9	D	501	GTP	O4'-C4'-C5'-O5'
11	T	501	GDP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
9	E	501	GTP	C5'-O5'-PA-O3A
9	E	501	GTP	C5'-O5'-PA-O1A
9	F	501	GTP	C5'-O5'-PA-O3A
9	F	501	GTP	C5'-O5'-PA-O2A
9	G	501	GTP	C5'-O5'-PA-O2A
9	L	501	GTP	C5'-O5'-PA-O2A
9	M	501	GTP	C5'-O5'-PA-O3A
9	M	501	GTP	C5'-O5'-PA-O1A
9	M	501	GTP	C5'-O5'-PA-O2A
9	P	501	GTP	C5'-O5'-PA-O3A
9	P	501	GTP	C5'-O5'-PA-O1A
9	S	501	GTP	C5'-O5'-PA-O3A
9	S	501	GTP	C5'-O5'-PA-O1A
9	S	501	GTP	C5'-O5'-PA-O2A
9	X	501	GTP	C5'-O5'-PA-O1A
9	m	501	GTP	C5'-O5'-PA-O2A
9	o	501	GTP	C5'-O5'-PA-O3A
9	o	501	GTP	C5'-O5'-PA-O2A
9	s	501	GTP	C5'-O5'-PA-O2A
9	y	501	GTP	C5'-O5'-PA-O2A
9	0	501	GTP	C5'-O5'-PA-O2A
9	6	501	GTP	C5'-O5'-PA-O2A
9	7	501	GTP	C5'-O5'-PA-O1A
11	I	501	GDP	C5'-O5'-PA-O3A
11	I	501	GDP	C5'-O5'-PA-O1A
11	N	501	GDP	C5'-O5'-PA-O1A
11	T	501	GDP	C5'-O5'-PA-O3A
11	T	501	GDP	C5'-O5'-PA-O1A
11	V	501	GDP	C5'-O5'-PA-O1A
11	b	501	GDP	C5'-O5'-PA-O3A
11	b	501	GDP	C5'-O5'-PA-O1A
11	p	501	GDP	C5'-O5'-PA-O1A
11	u	501	GDP	C5'-O5'-PA-O1A
11	v	501	GDP	C5'-O5'-PA-O3A
11	v	501	GDP	C5'-O5'-PA-O1A
11	w	501	GDP	C5'-O5'-PA-O1A
11	8	501	GDP	C5'-O5'-PA-O3A
11	8	501	GDP	C5'-O5'-PA-O1A
11	N	501	GDP	C4'-C5'-O5'-PA
12	t	502	TA1	O10-C22-O09-C21
11	J	501	GDP	C3'-C4'-C5'-O5'
12	a	502	TA1	C23-C22-O09-C21

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Mol	Chain	Res	Type	Atoms
9	D	501	GTP	PB-O3A-PA-O2A
9	F	501	GTP	PB-O3A-PA-O2A
9	G	501	GTP	PB-O3A-PA-O2A
9	e	501	GTP	PA-O3A-PB-O1B
9	h	501	GTP	PB-O3A-PA-O2A
9	o	501	GTP	PB-O3A-PA-O2A
9	s	501	GTP	PB-O3A-PA-O2A
9	y	501	GTP	PB-O3A-PA-O2A
9	0	501	GTP	PB-O3A-PA-O2A
9	5	501	GTP	PB-O3A-PA-O2A
11	q	501	GDP	PB-O3A-PA-O1A
12	w	502	TA1	O11-C27-C28-O13
12	8	502	TA1	O14-C30-C31-C36
11	T	501	GDP	C4'-C5'-O5'-PA
12	8	502	TA1	N01-C30-C31-C36
12	j	502	TA1	O13-C28-C29-N01
12	u	502	TA1	O13-C28-C29-N01
9	f	501	GTP	O4'-C4'-C5'-O5'
11	4	501	GDP	C3'-C4'-C5'-O5'
12	i	502	TA1	O11-C27-C28-O13
9	1	501	GTP	PA-O3A-PB-O1B
9	6	501	GTP	PB-O3A-PA-O2A
11	w	501	GDP	PB-O3A-PA-O1A
11	8	501	GDP	PB-O3A-PA-O1A
11	K	501	GDP	C4'-C5'-O5'-PA
11	Q	501	GDP	C4'-C5'-O5'-PA
12	u	502	TA1	O10-C22-O09-C21
9	Z	501	GTP	O4'-C4'-C5'-O5'
12	V	502	TA1	C27-C28-C29-N01
12	b	502	TA1	O11-C27-C28-O13
12	b	502	TA1	C27-C28-C29-N01
12	u	502	TA1	O11-C27-C28-O13
12	v	502	TA1	C27-C28-C29-N01
12	j	502	TA1	O11-C27-C28-C29
12	j	502	TA1	O12-C27-C28-C29
11	I	501	GDP	C4'-C5'-O5'-PA
9	5	501	GTP	O4'-C4'-C5'-O5'
11	N	501	GDP	O4'-C4'-C5'-O5'
12	a	502	TA1	O10-C22-O09-C21
9	k	501	GTP	C3'-C4'-C5'-O5'
9	1	501	GTP	C3'-C4'-C5'-O5'
9	D	501	GTP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
9	F	501	GTP	PB-O3A-PA-O1A
9	Y	501	GTP	PB-O3A-PA-O2A
9	Z	501	GTP	PB-O3A-PA-O1A
9	Z	501	GTP	PB-O3A-PA-O2A
9	f	501	GTP	PB-O3A-PA-O2A
9	m	501	GTP	PB-O3A-PA-O2A
9	o	501	GTP	PB-O3A-PA-O1A
9	s	501	GTP	PB-O3A-PA-O1A
9	y	501	GTP	PB-O3A-PA-O1A
9	0	501	GTP	PB-O3A-PA-O1A
9	5	501	GTP	PB-O3A-PA-O1A
9	7	501	GTP	PB-O3A-PA-O2A
11	J	501	GDP	PB-O3A-PA-O1A
11	a	501	GDP	PB-O3A-PA-O1A
11	i	501	GDP	PB-O3A-PA-O2A
11	r	501	GDP	PB-O3A-PA-O2A
12	8	502	TA1	O14-C30-C31-C32
12	b	502	TA1	O12-C27-C28-O13
9	L	501	GTP	C4'-C5'-O5'-PA
12	8	502	TA1	N01-C30-C31-C32
11	i	501	GDP	C3'-C4'-C5'-O5'
11	U	501	GDP	C4'-C5'-O5'-PA
12	u	502	TA1	O12-C27-C28-O13
12	b	502	TA1	O02-C03-C04-C05
12	b	502	TA1	O11-C27-C28-C29
12	i	502	TA1	O11-C27-C28-C29
12	p	502	TA1	O11-C27-C28-C29
12	u	502	TA1	O11-C27-C28-C29
12	4	502	TA1	O11-C27-C28-C29
12	i	502	TA1	O12-C27-C28-O13
12	w	502	TA1	O12-C27-C28-O13
9	G	501	GTP	PB-O3A-PA-O1A
9	Y	501	GTP	PA-O3A-PB-O2B
9	e	501	GTP	PA-O3A-PB-O2B
9	h	501	GTP	PB-O3A-PA-O1A
9	m	501	GTP	PB-O3A-PA-O1A
9	1	501	GTP	PA-O3A-PB-O2B
11	O	501	GDP	PB-O3A-PA-O2A
11	R	501	GDP	PB-O3A-PA-O2A
11	V	501	GDP	PB-O3A-PA-O2A
11	b	501	GDP	PB-O3A-PA-O2A
11	j	501	GDP	PB-O3A-PA-O2A

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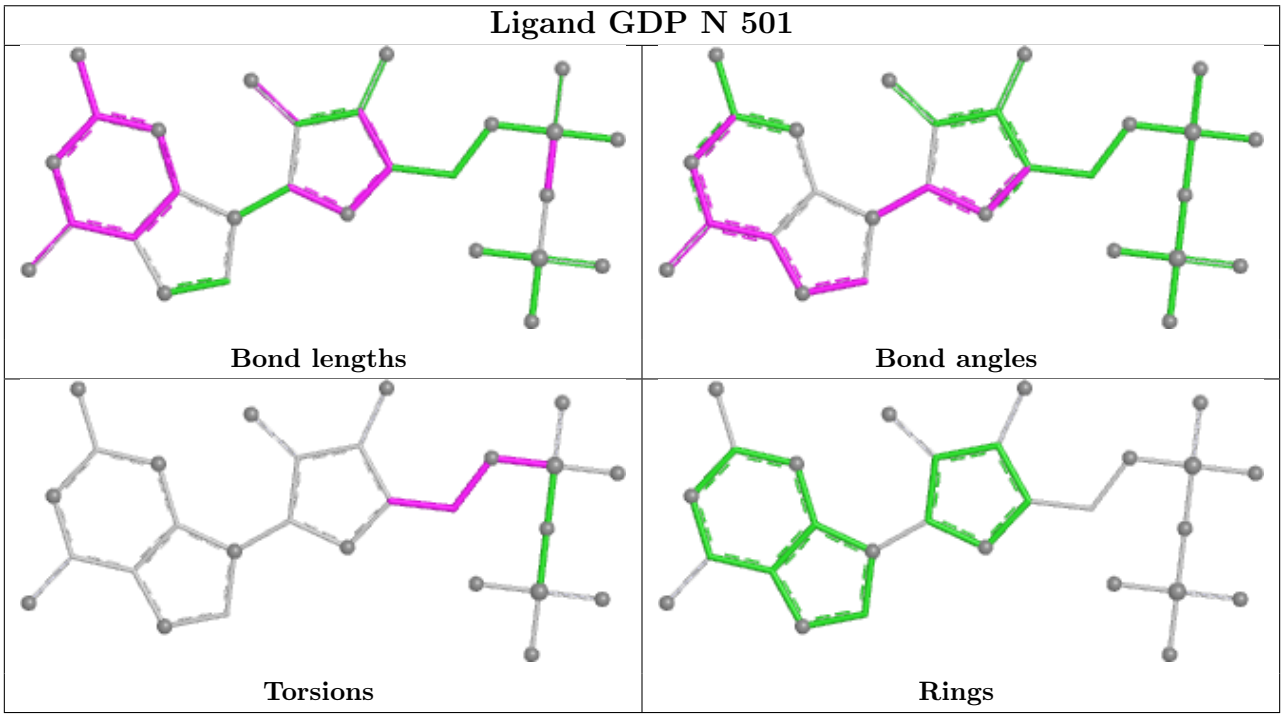
Mol	Chain	Res	Type	Atoms
11	q	501	GDP	PB-O3A-PA-O2A
11	t	501	GDP	PB-O3A-PA-O1A
11	u	501	GDP	PB-O3A-PA-O2A
11	v	501	GDP	PB-O3A-PA-O2A
11	w	501	GDP	PB-O3A-PA-O2A
11	8	501	GDP	PB-O3A-PA-O2A
11	Q	501	GDP	C3'-C4'-C5'-O5'

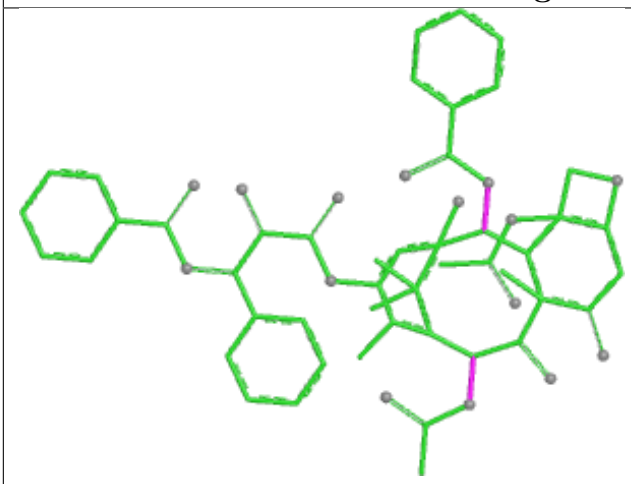
There are no ring outliers.

No monomer is involved in short contacts.

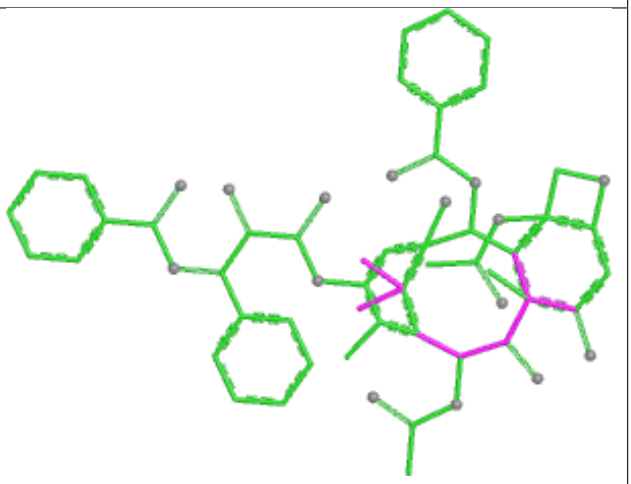
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



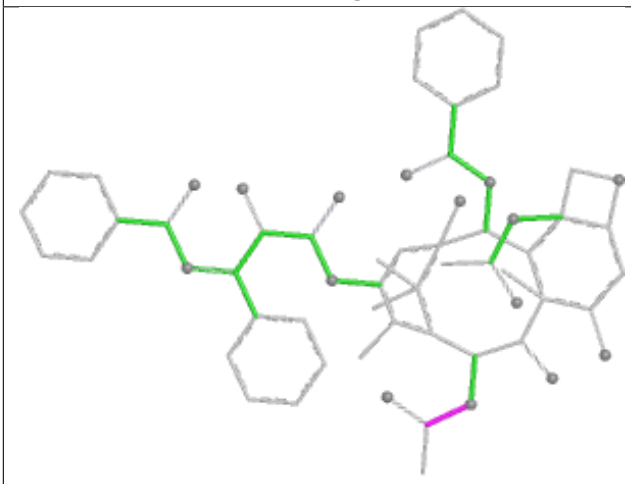
Ligand TA1 t 502



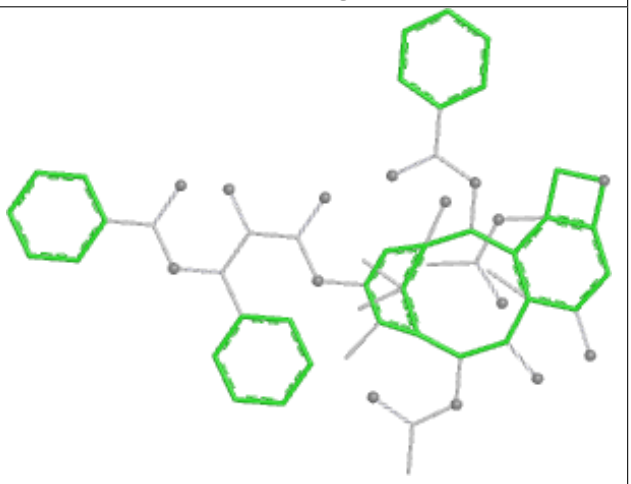
Bond lengths



Bond angles

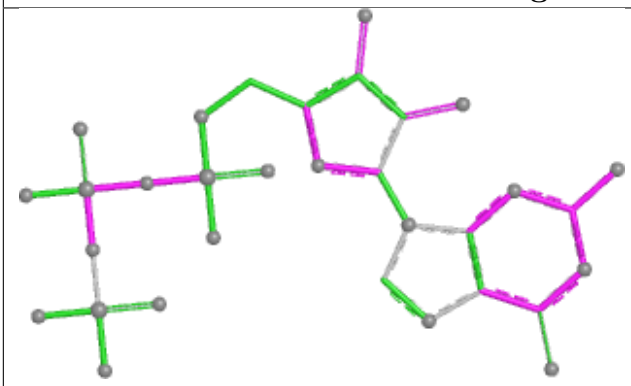


Torsions

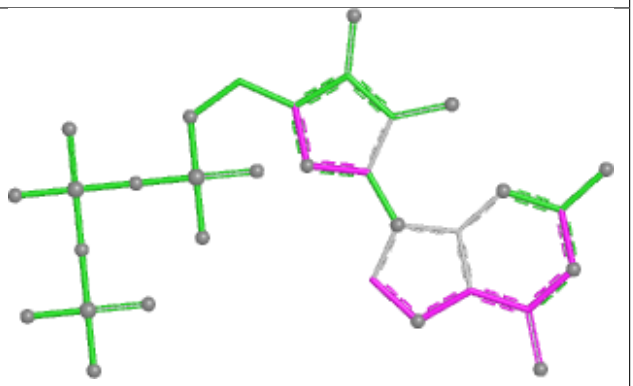


Rings

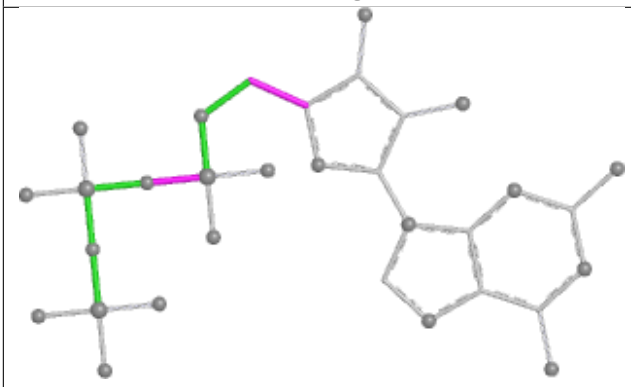
Ligand GTP f 501



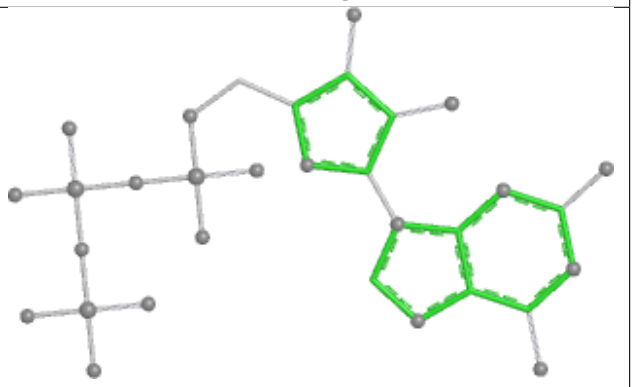
Bond lengths



Bond angles

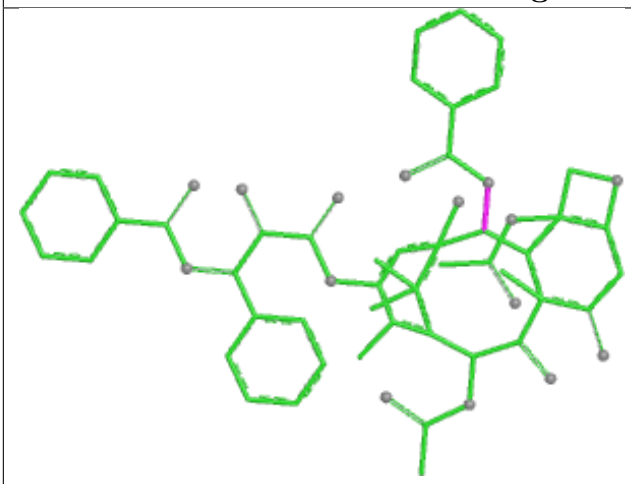


Torsions

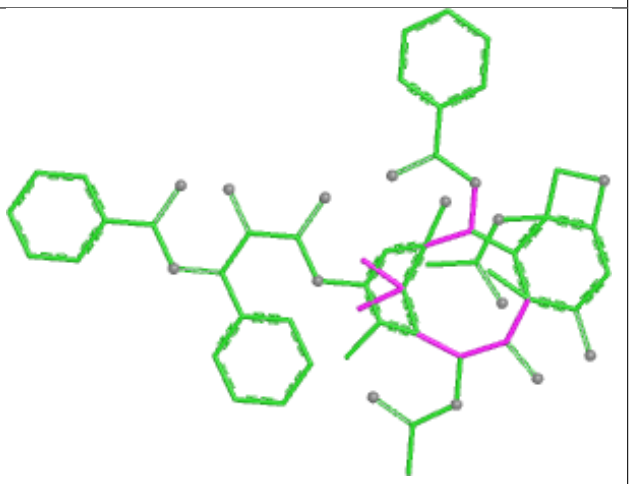


Rings

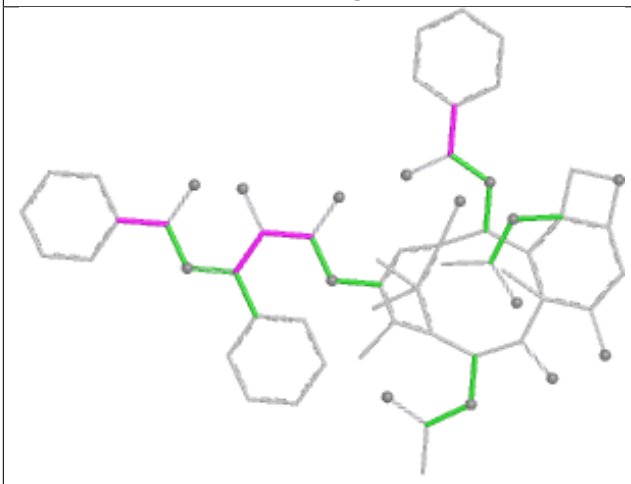
Ligand TA1 b 502



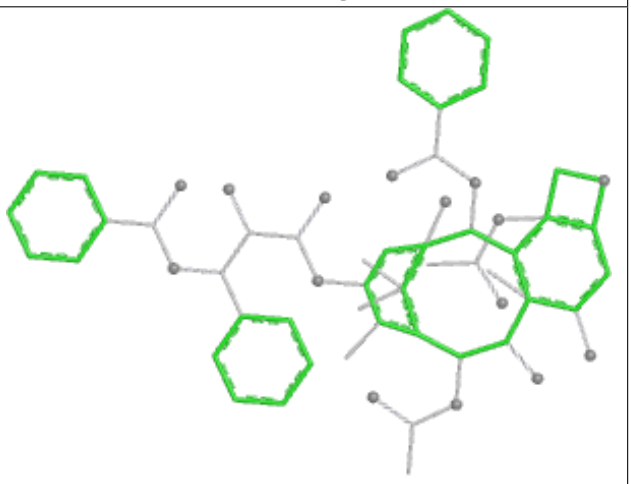
Bond lengths



Bond angles

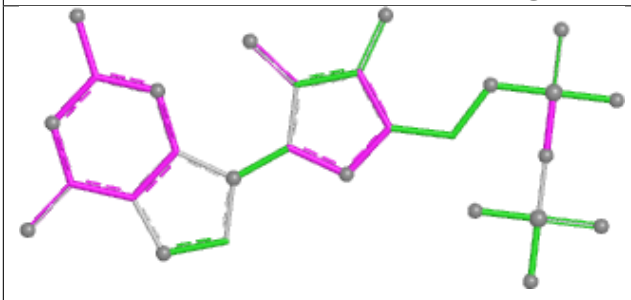


Torsions

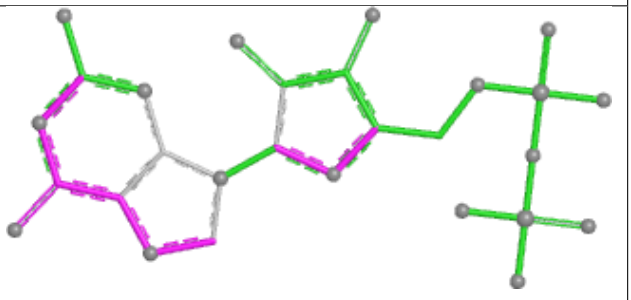


Rings

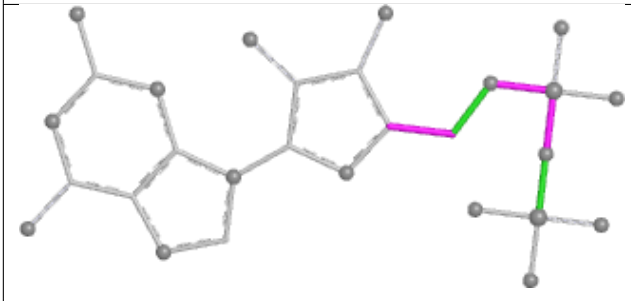
Ligand GDP J 501



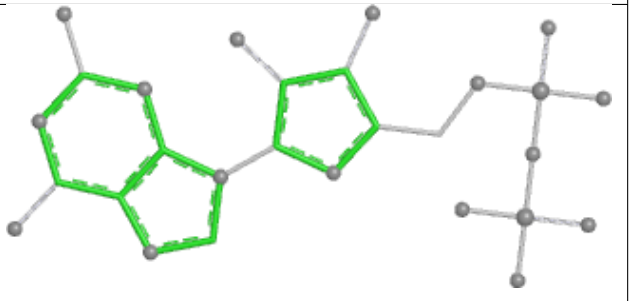
Bond lengths



Bond angles

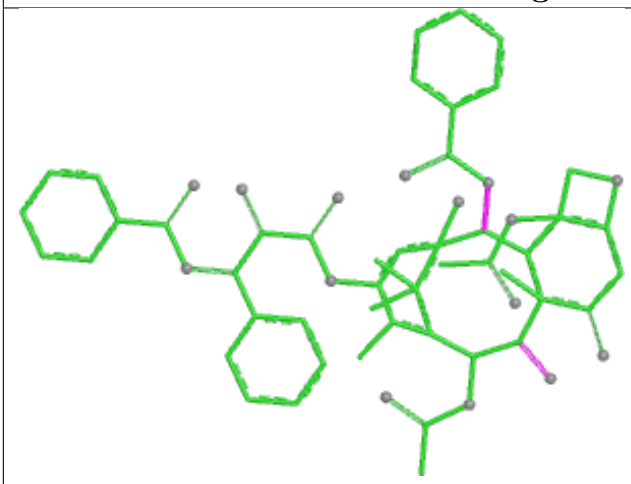


Torsions



Rings

Ligand TA1 q 502



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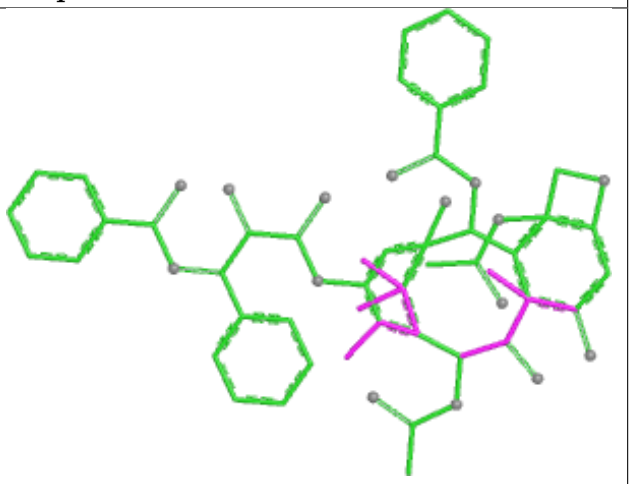

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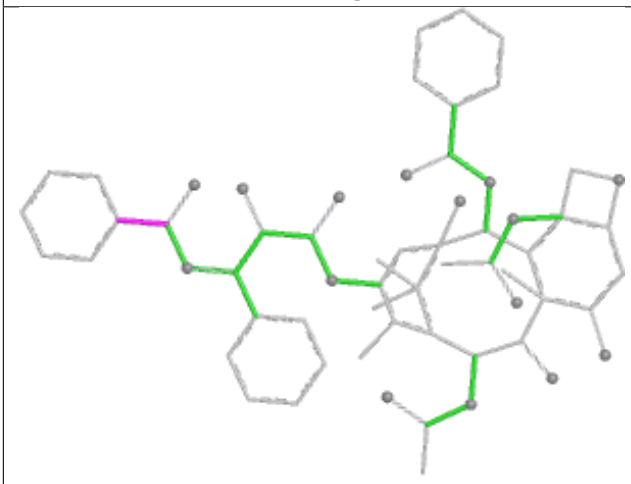
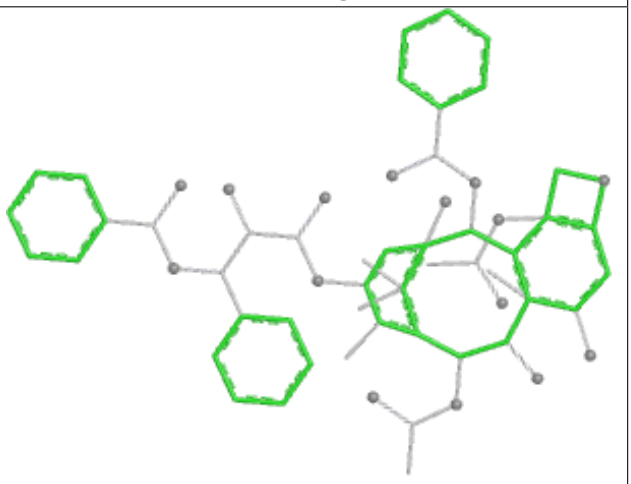
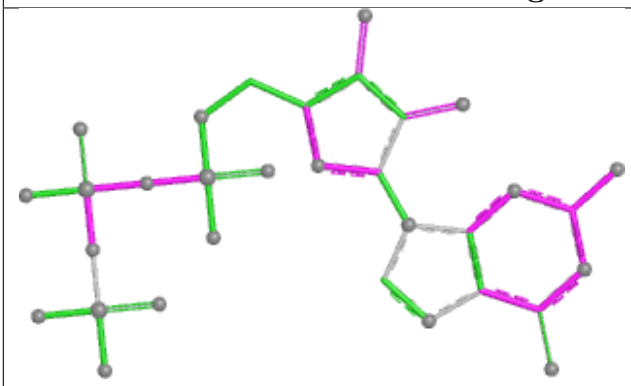


Torsions



Rings

Ligand GTP e 501



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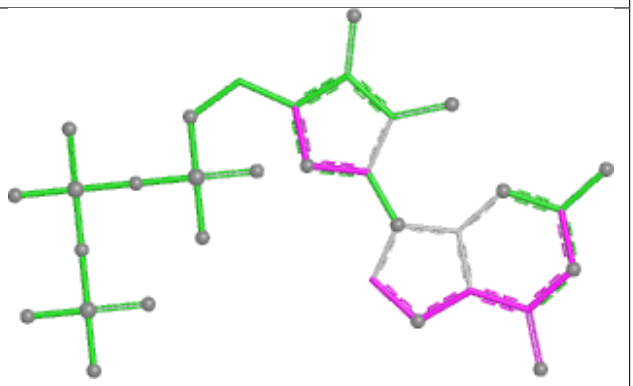

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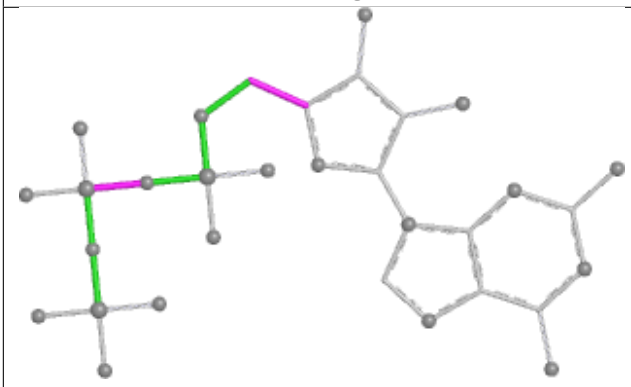

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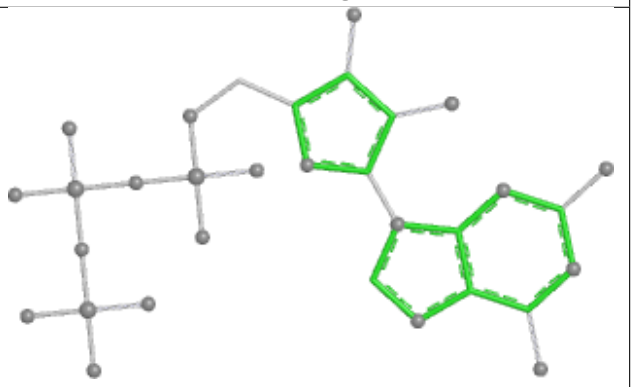
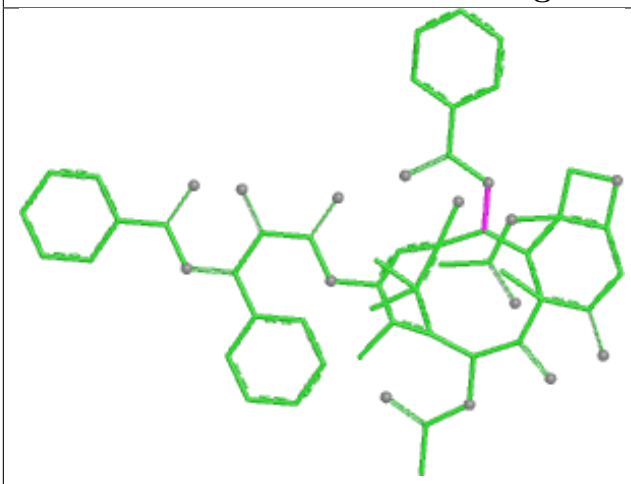


Rings

Ligand TA1 r 502



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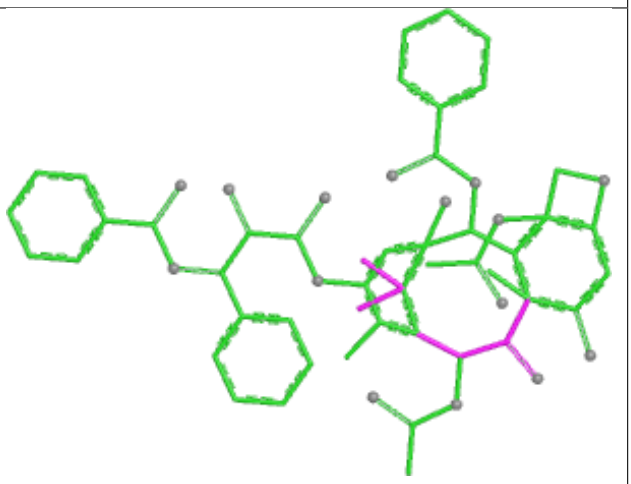

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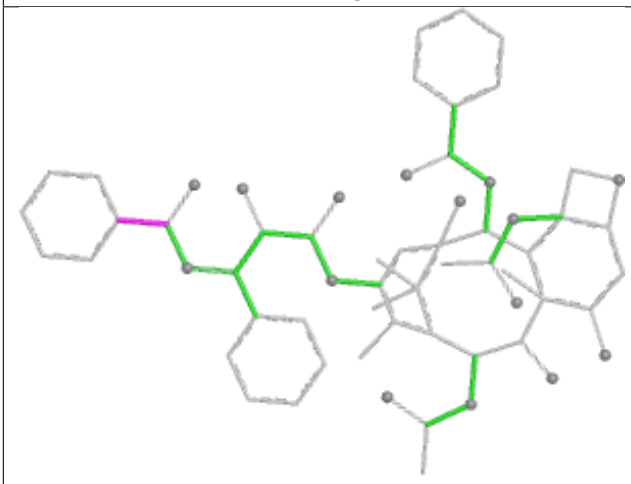

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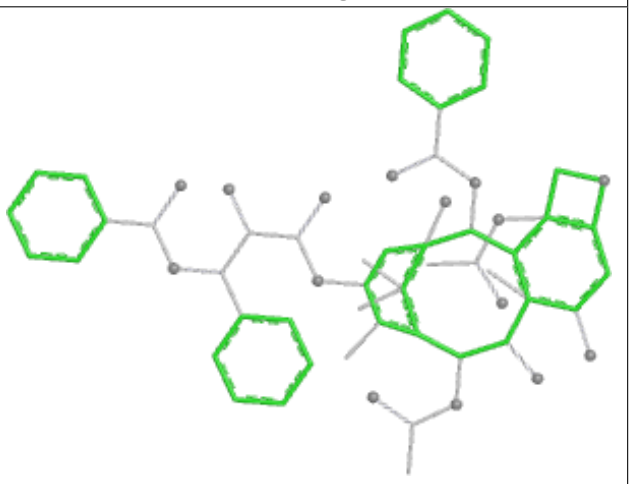
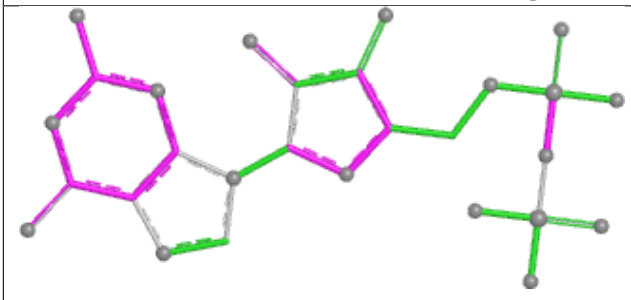


Rings

Ligand GDP p 501



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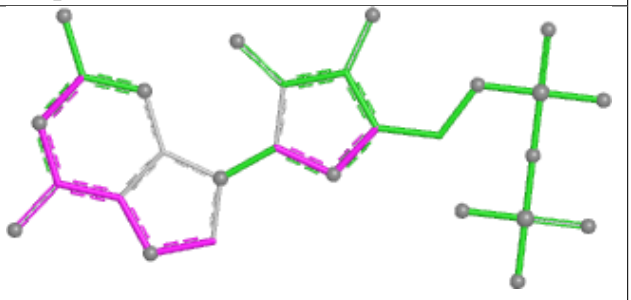

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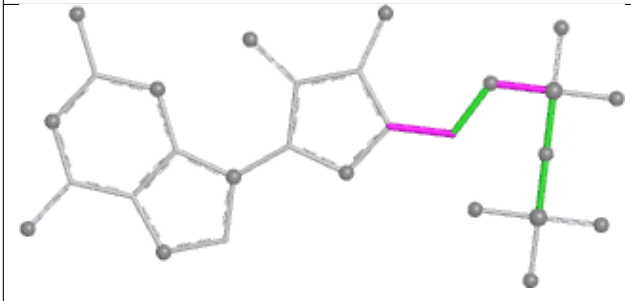

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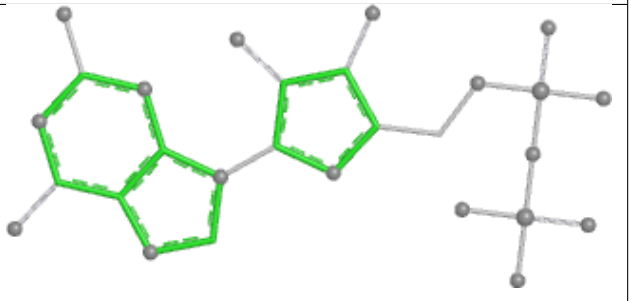
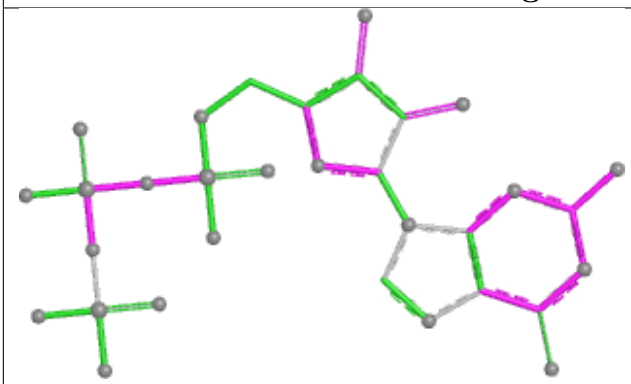


Rings

Ligand GTP D 501



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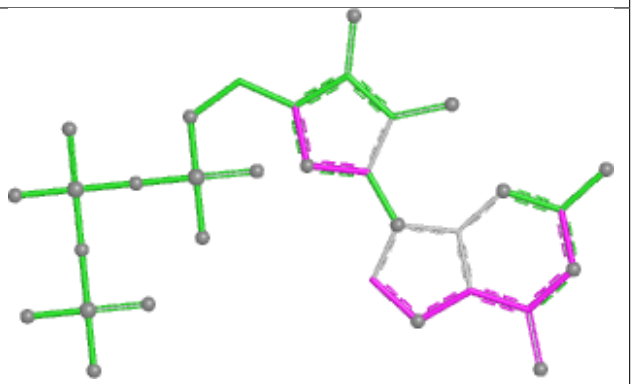

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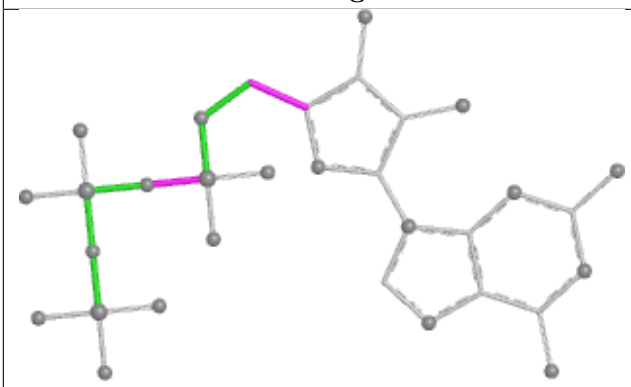

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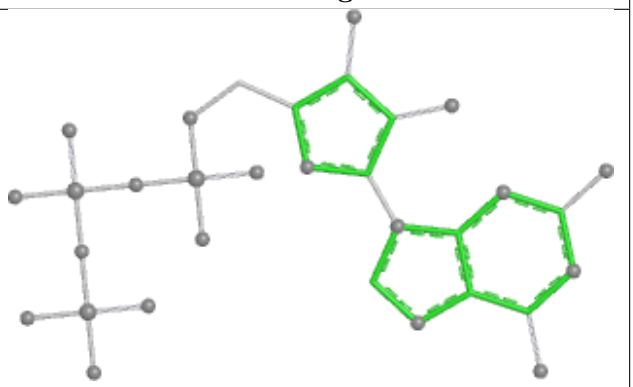

Rings

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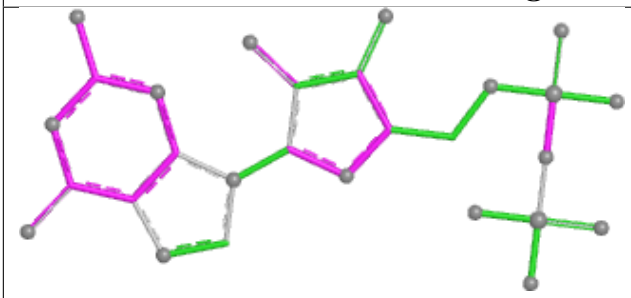

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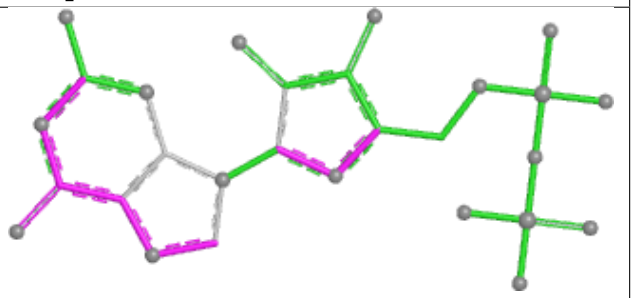

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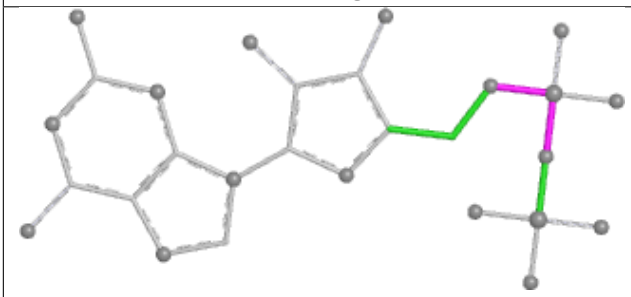

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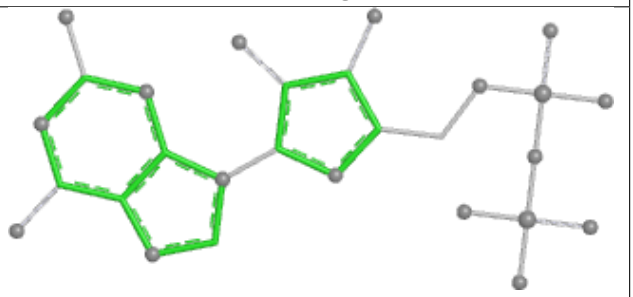

Rings

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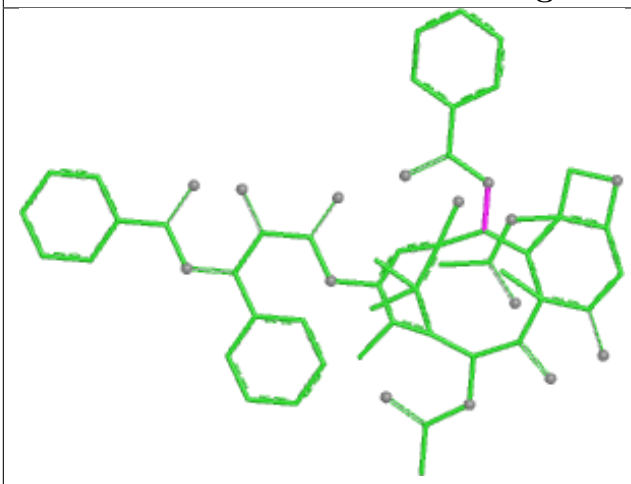

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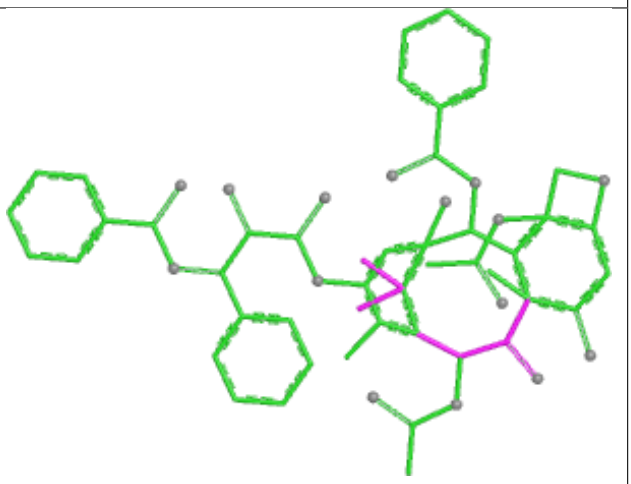

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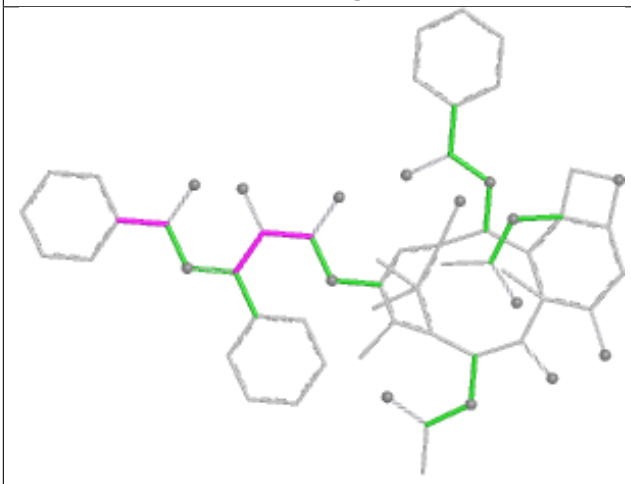

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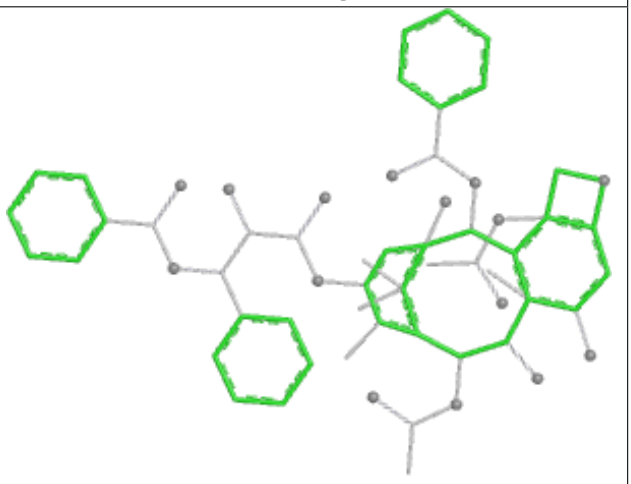

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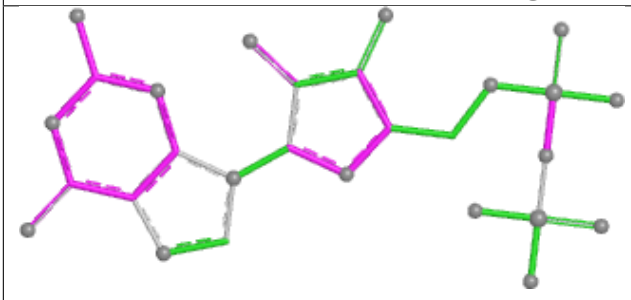

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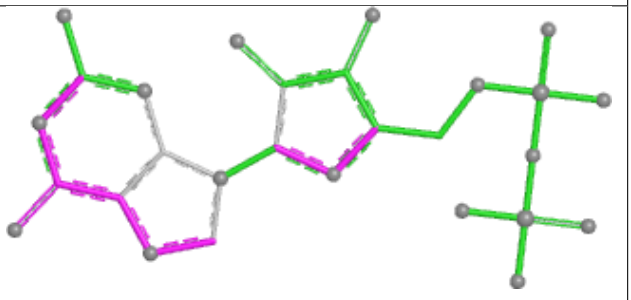

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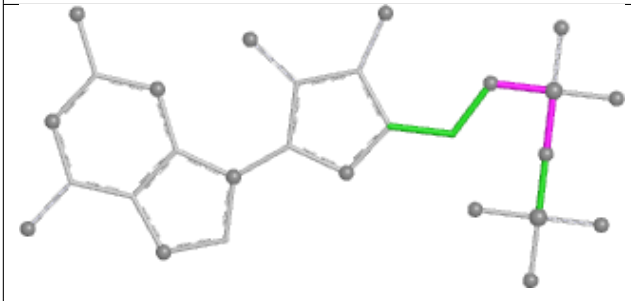

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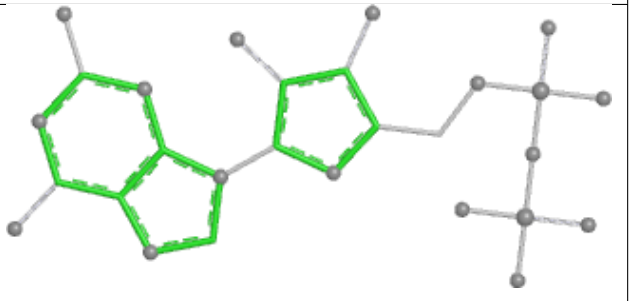

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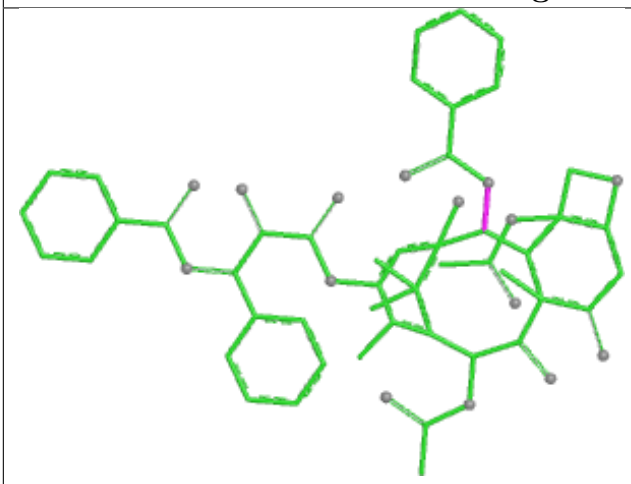

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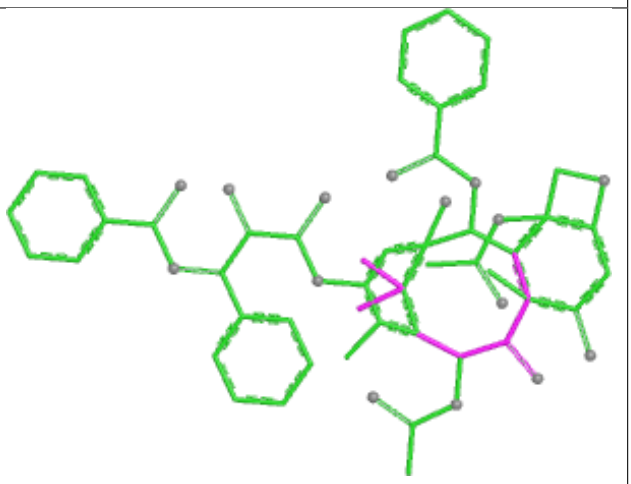

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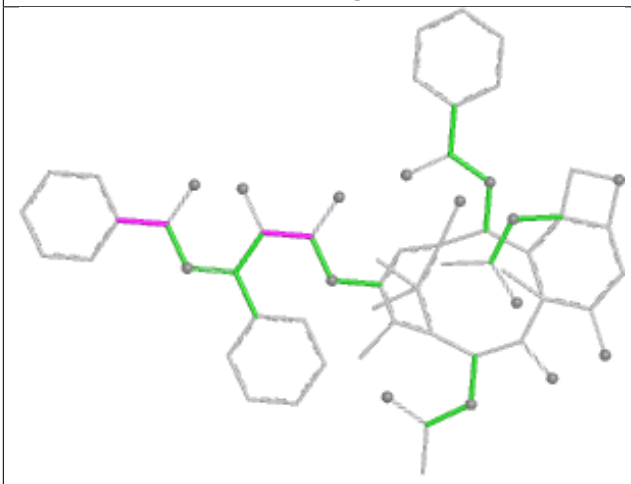

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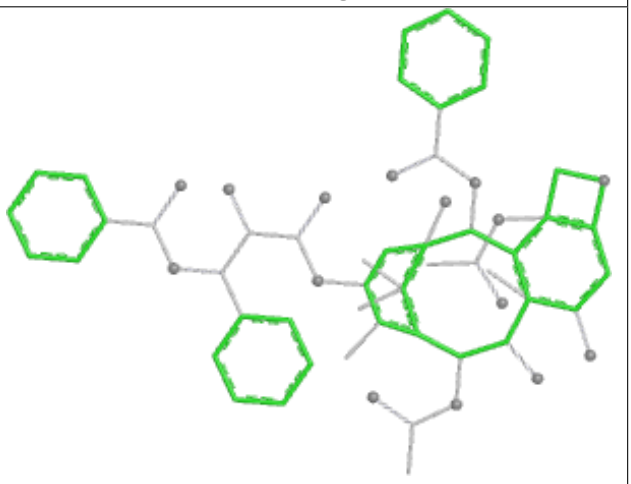
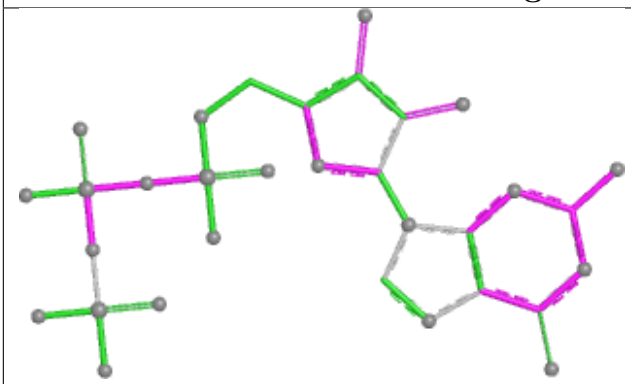


Rings

Ligand GTP F 501



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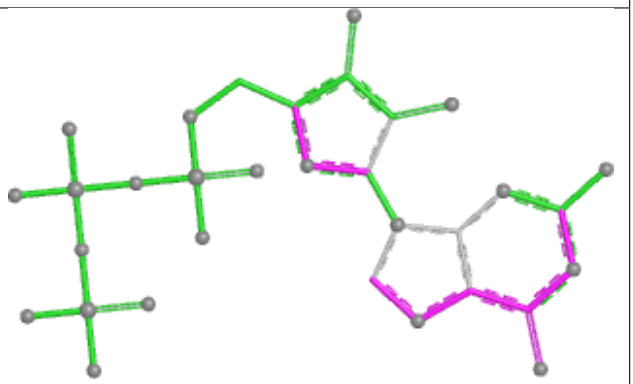

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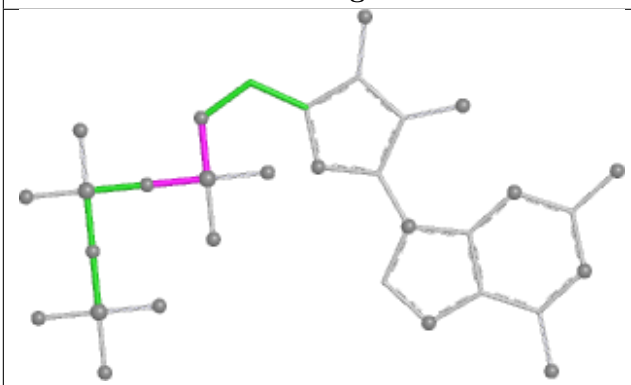

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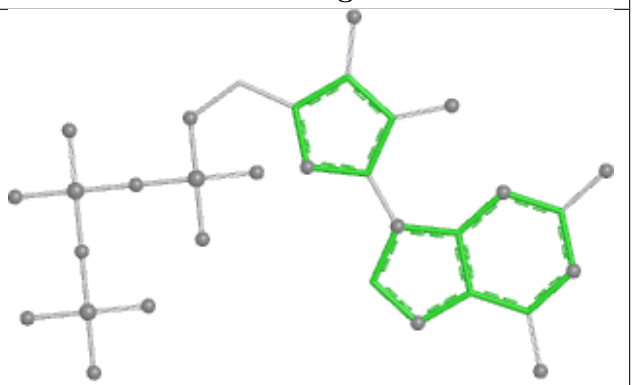

Rings

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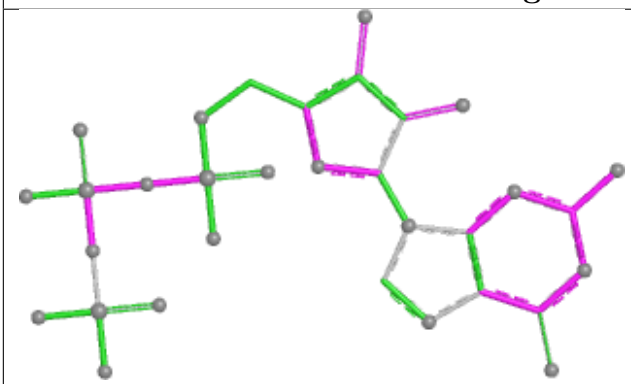

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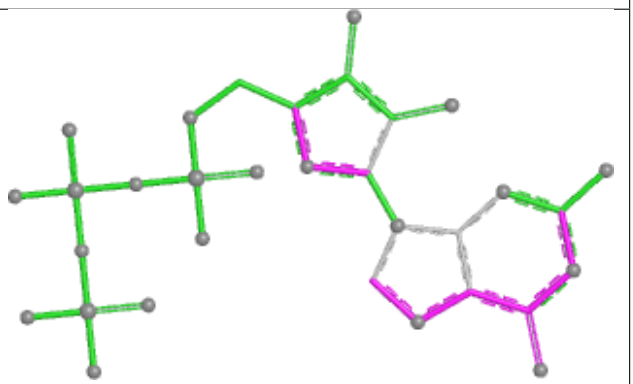

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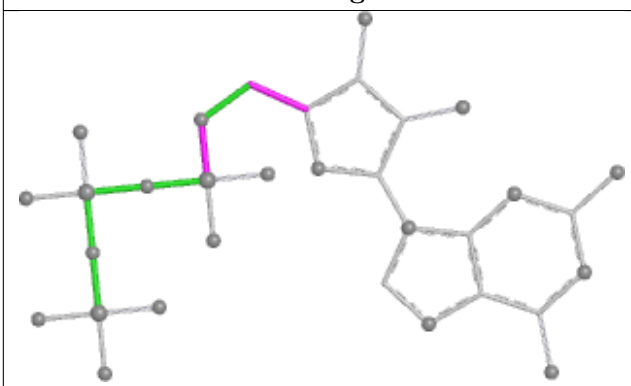

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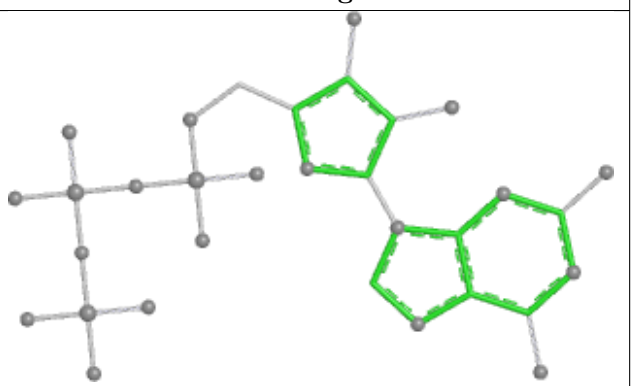

Rings

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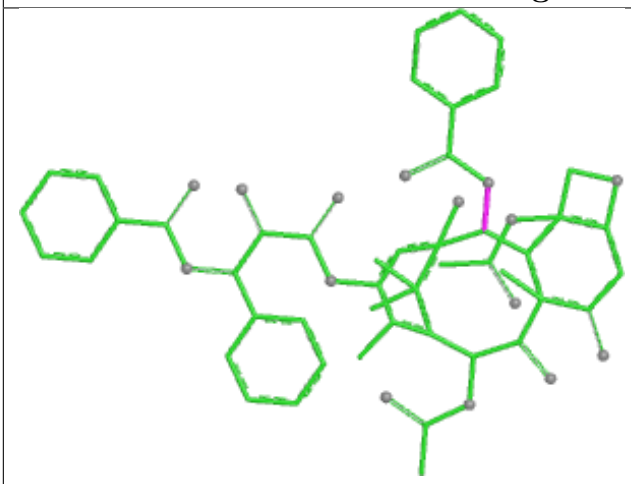

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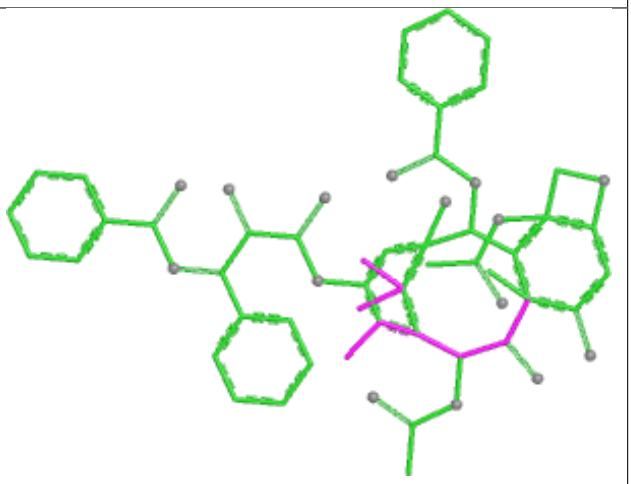

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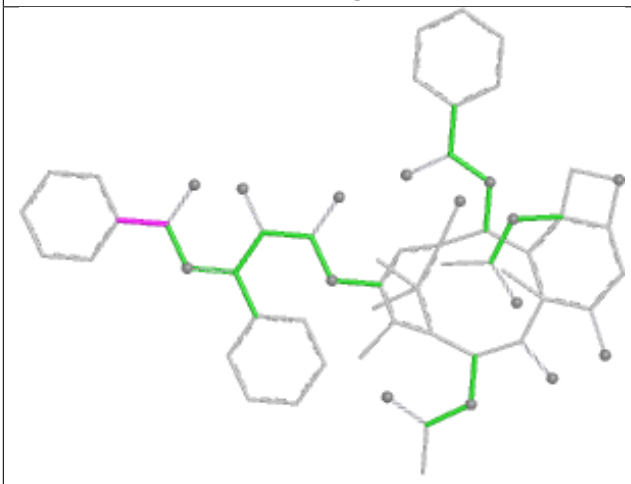

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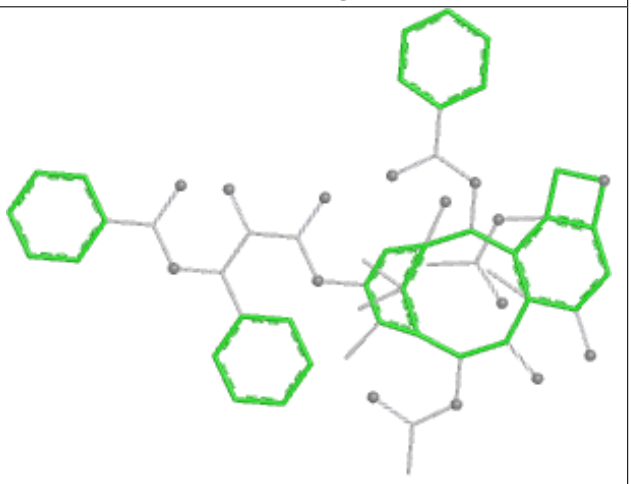
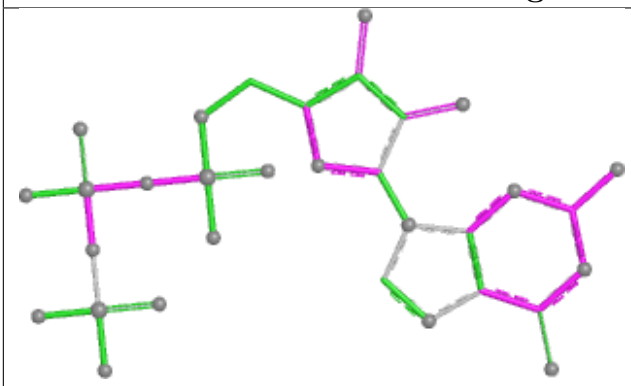


Rings

Ligand GTP 7 501



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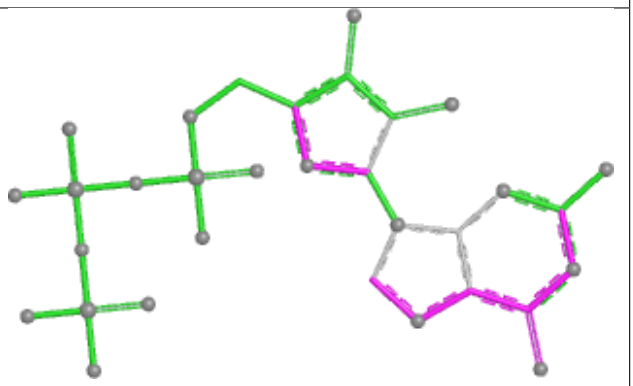

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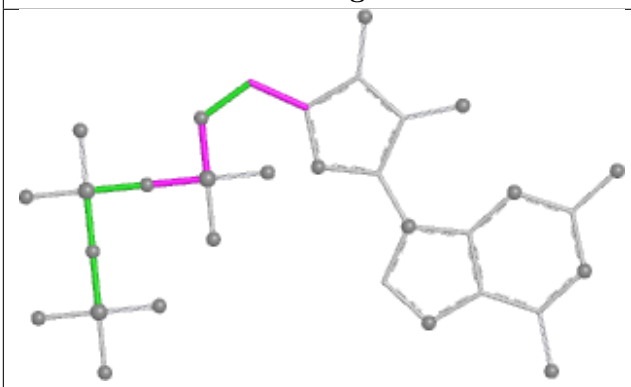

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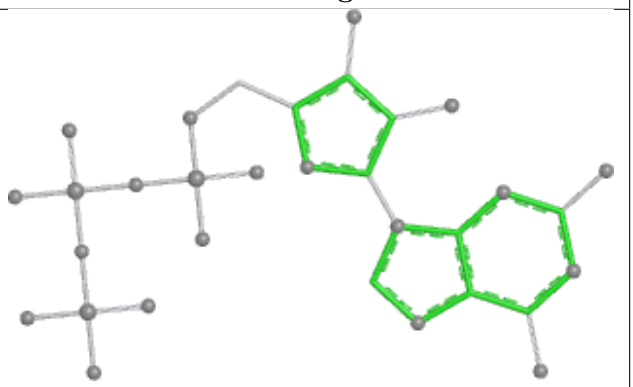
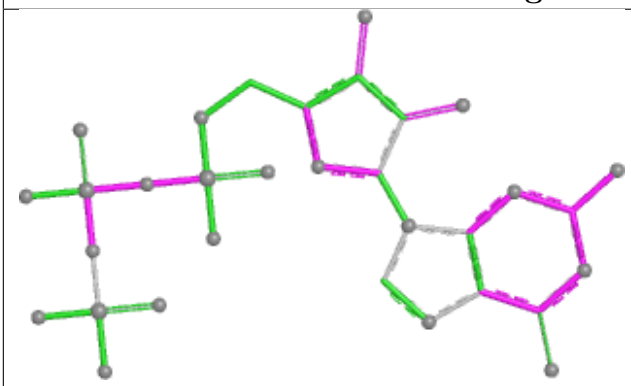


Rings

Ligand GTP L 501



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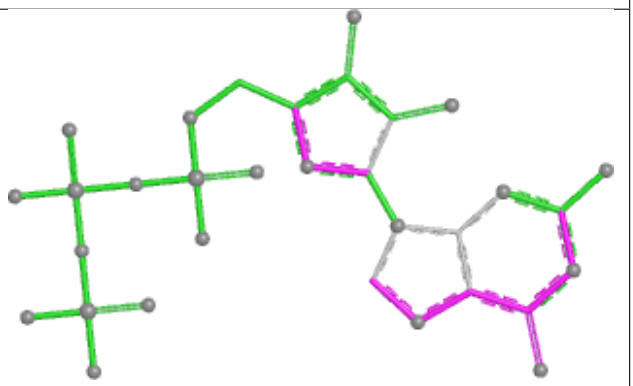

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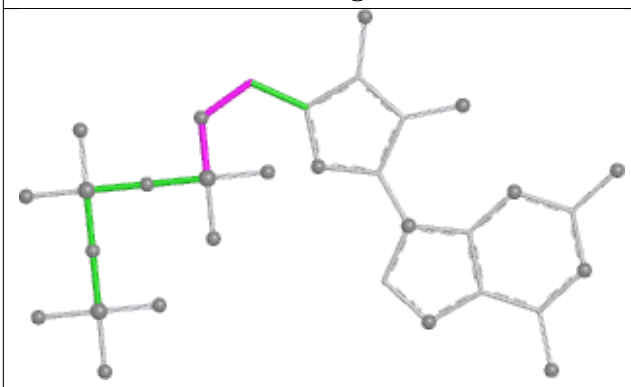
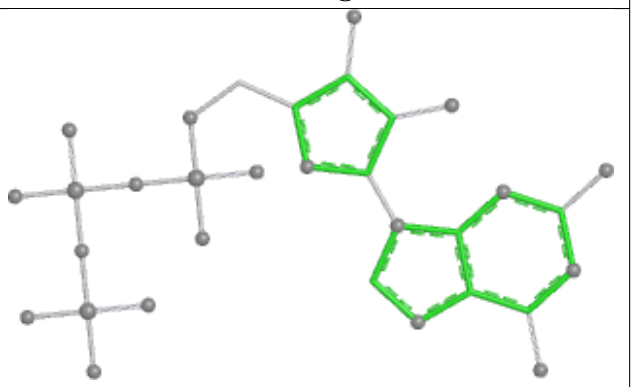
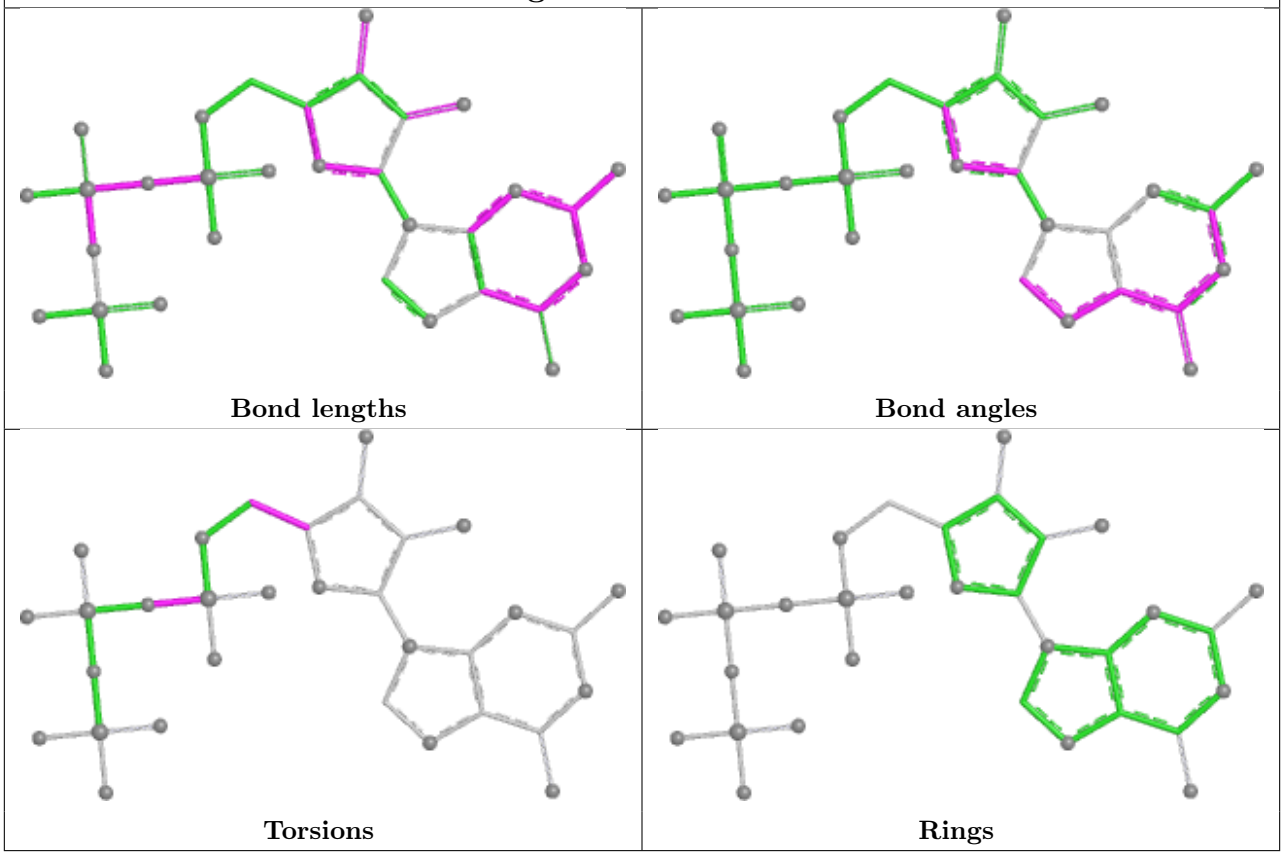


Torsions



Rings

Ligand GTP 5 501



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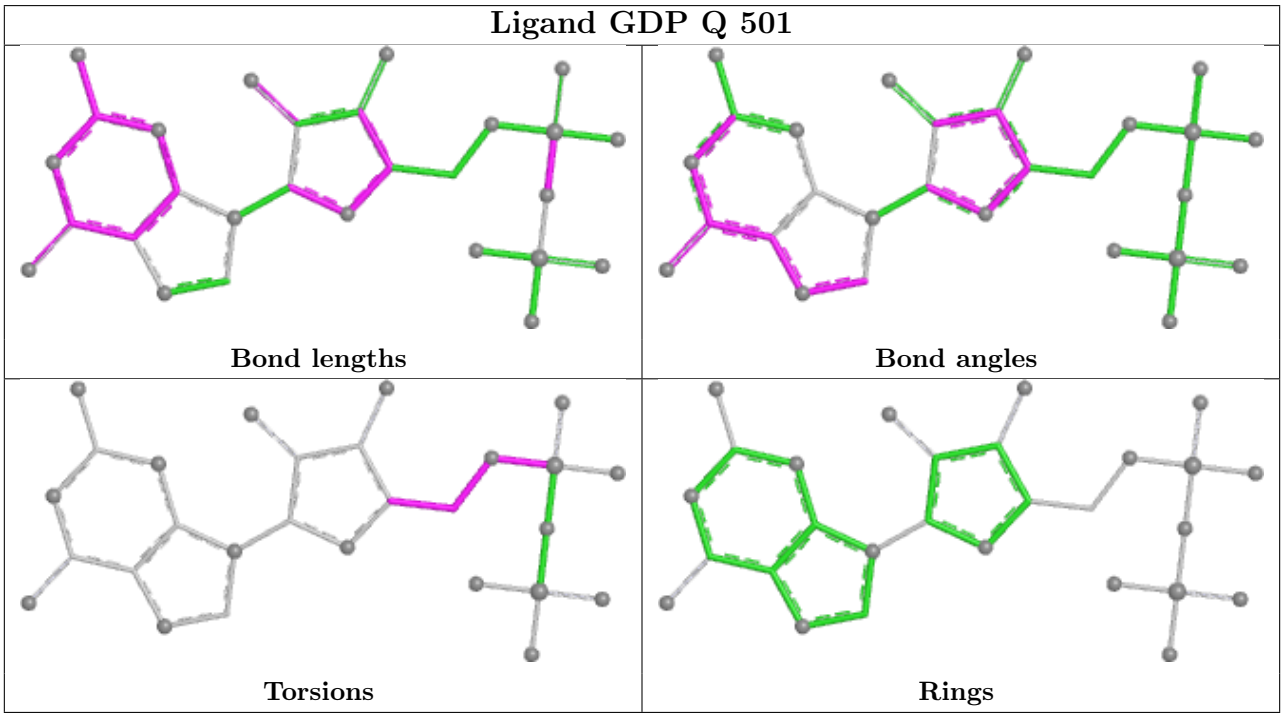

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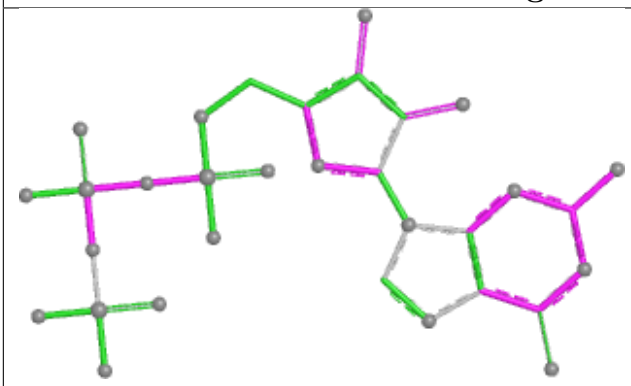

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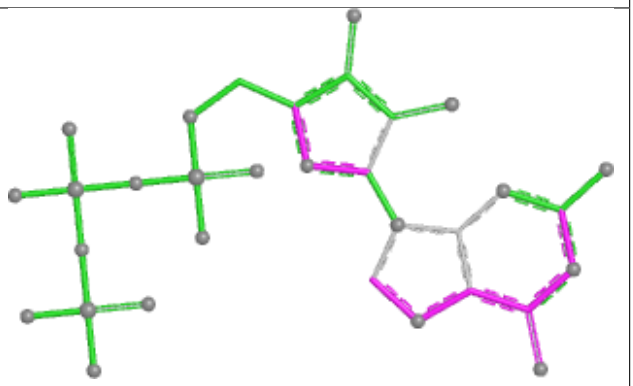

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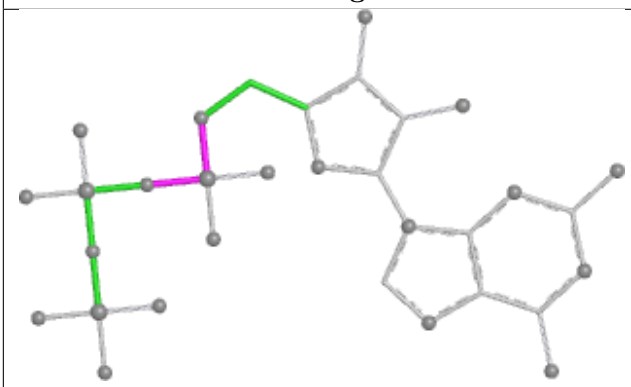

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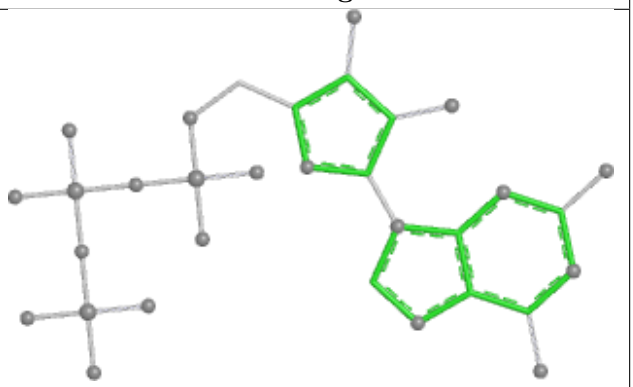

Rings

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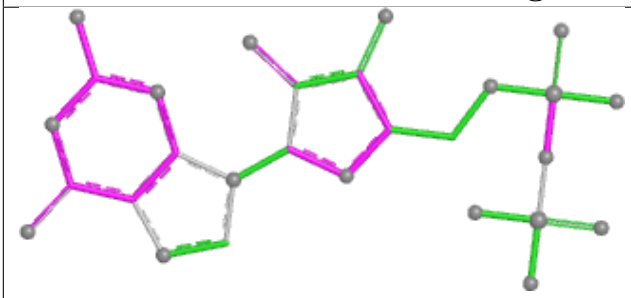

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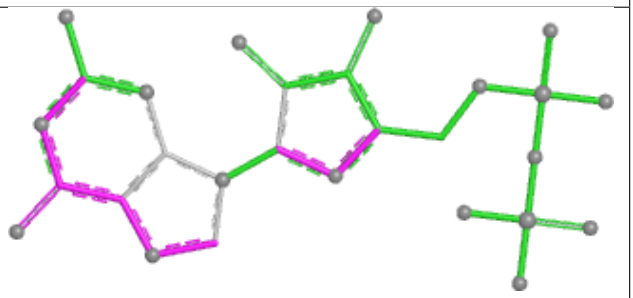

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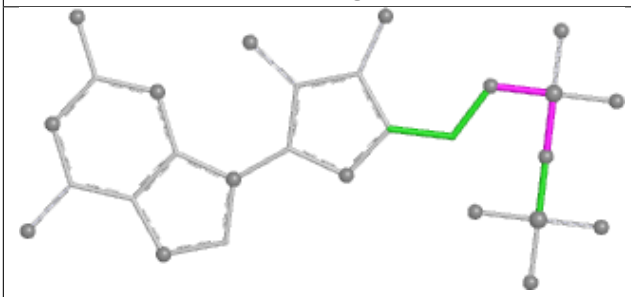

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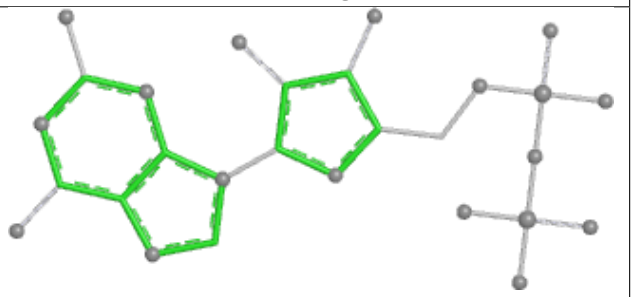

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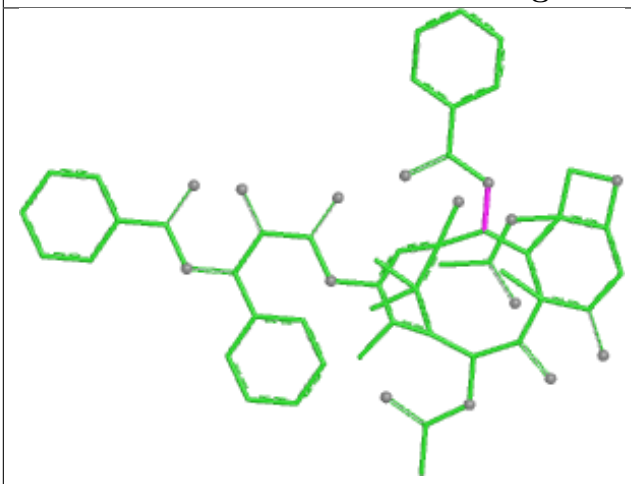

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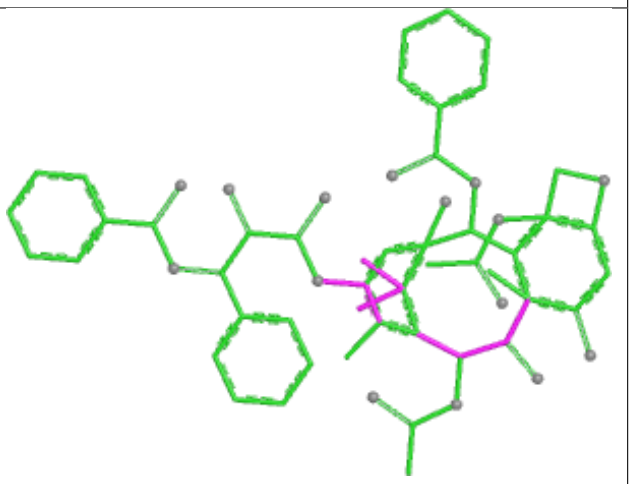

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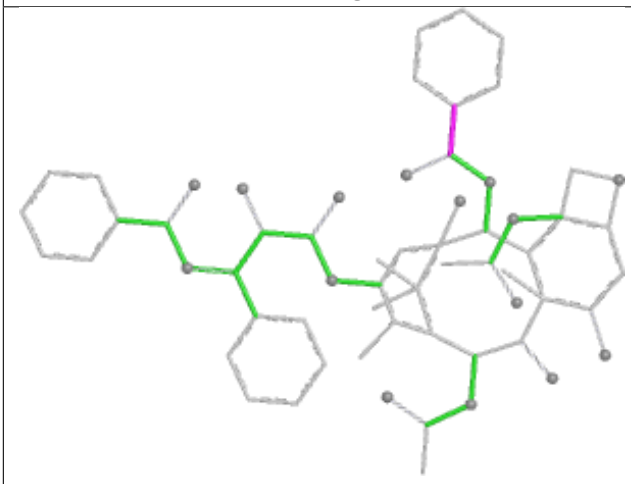

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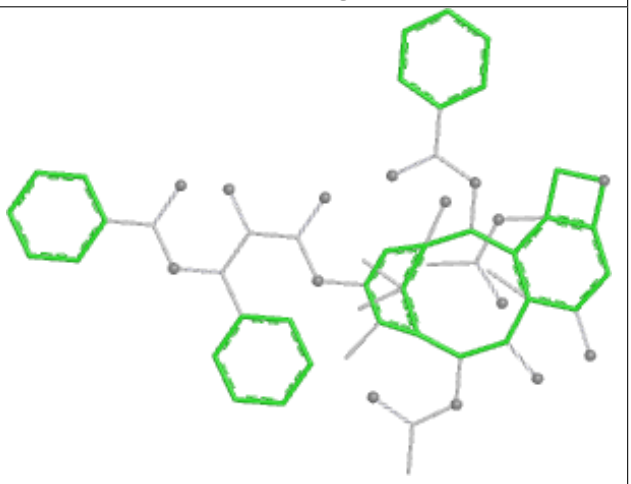

Rings

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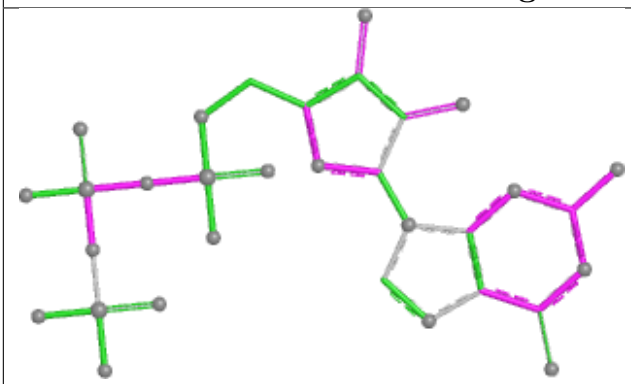

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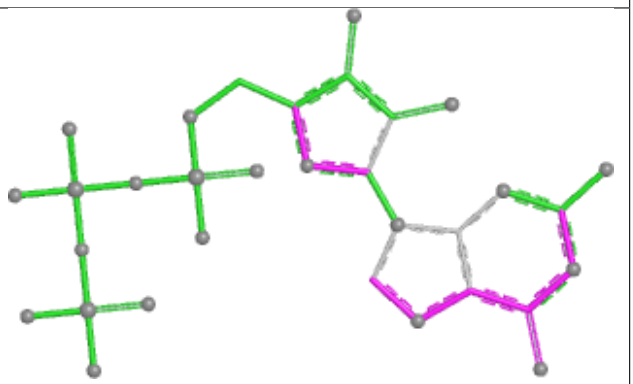

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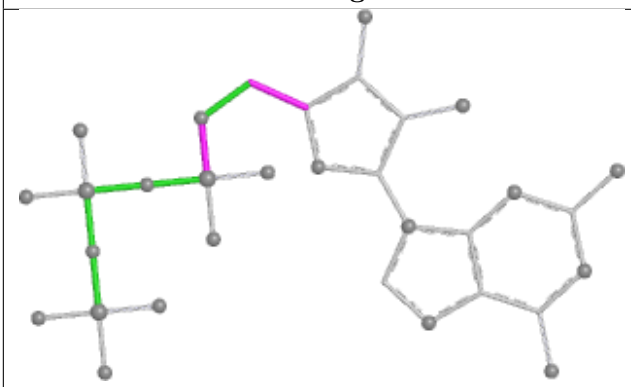

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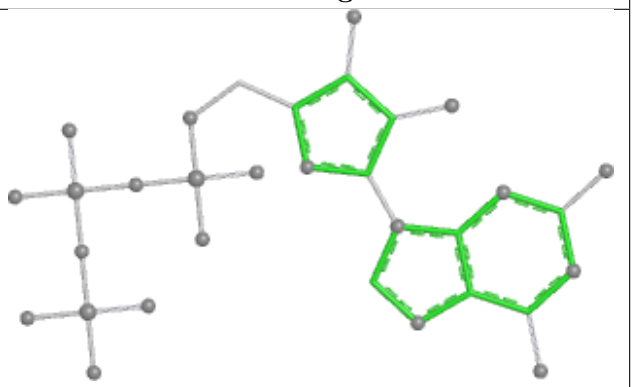

Rings

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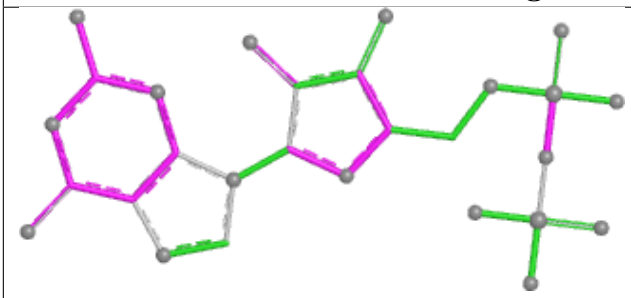

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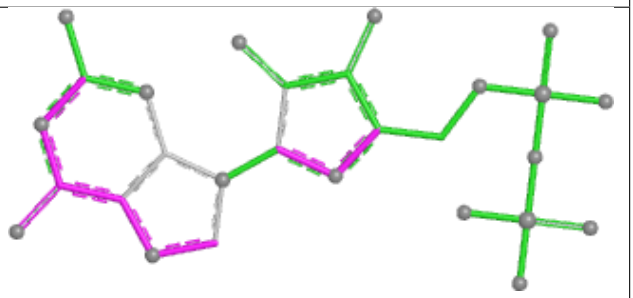

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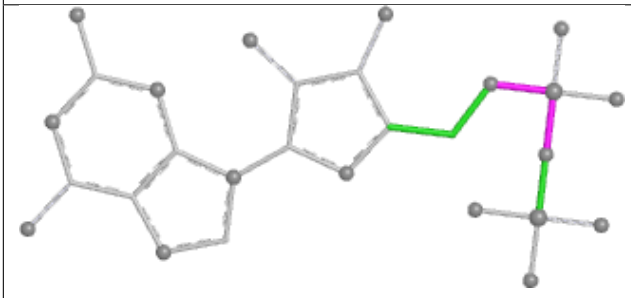

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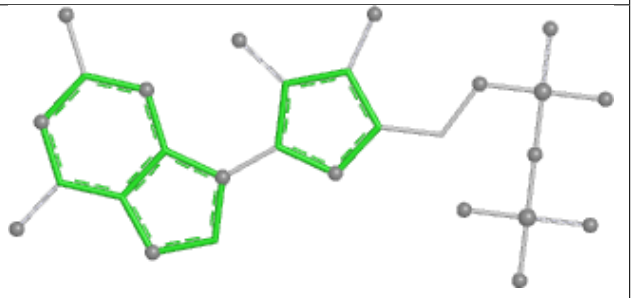

Rings

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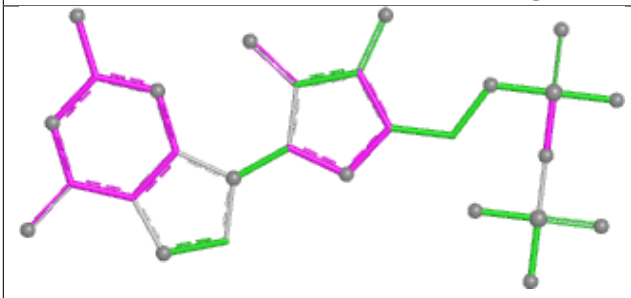
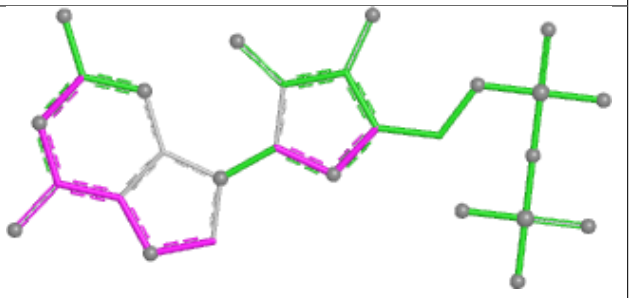
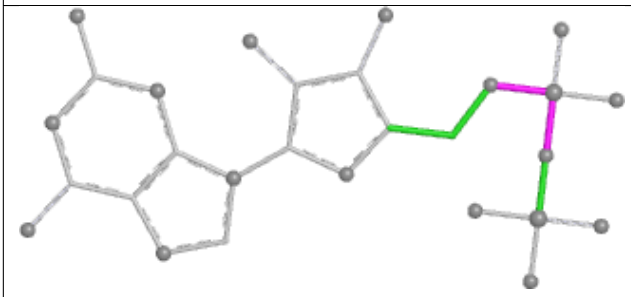
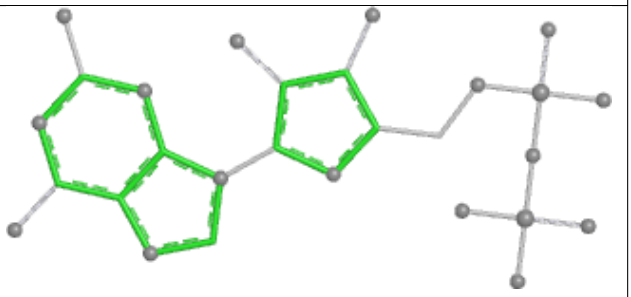
 Bond lengths	 Bond angles
 Torsions	 Rings

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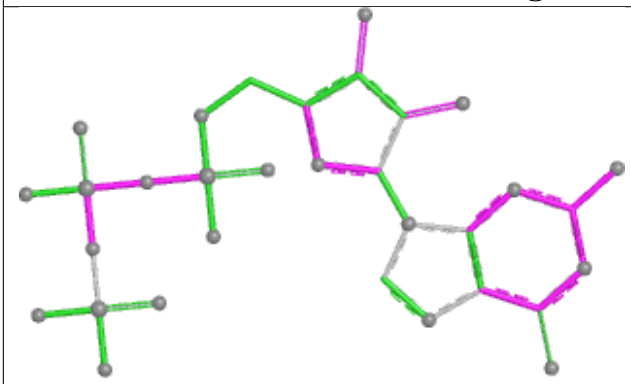
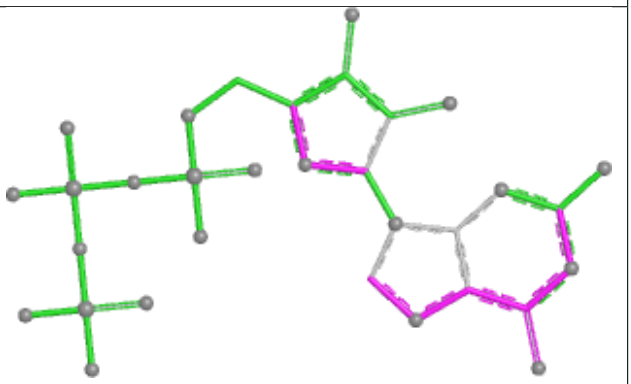
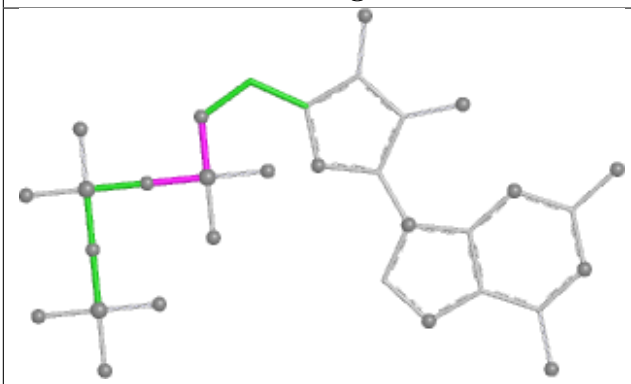
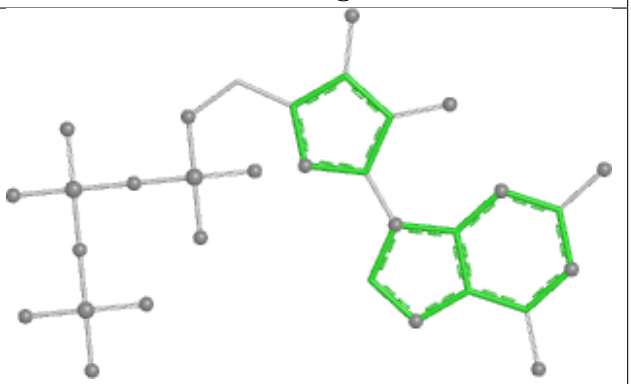
 Bond lengths	 Bond angles
 Torsions	 Rings

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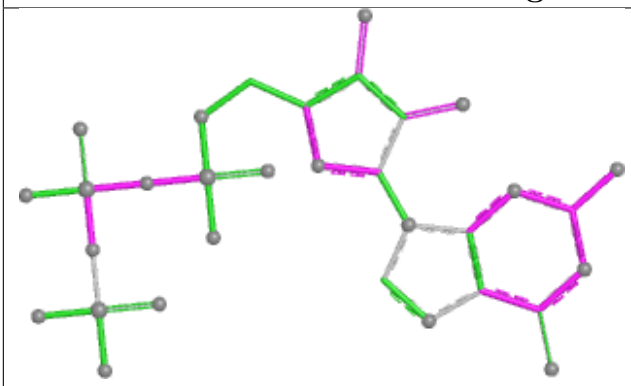

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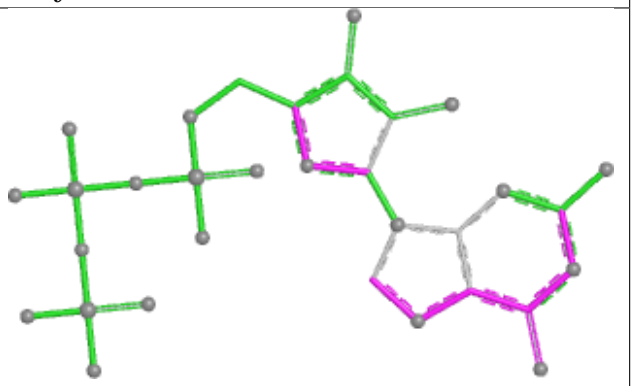

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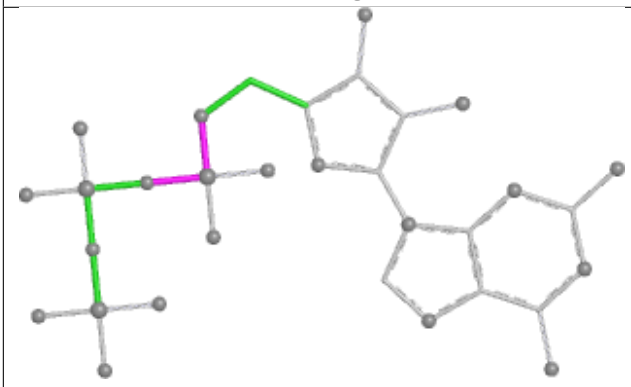

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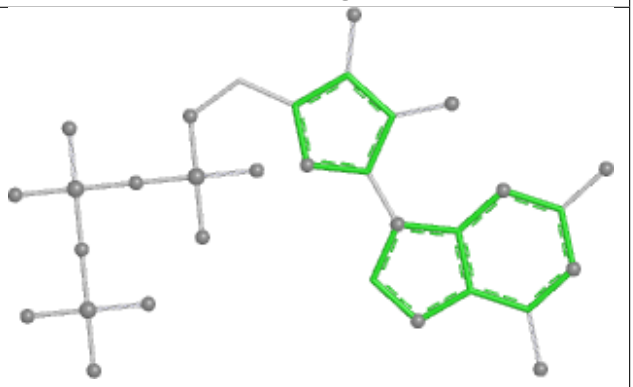

Rings

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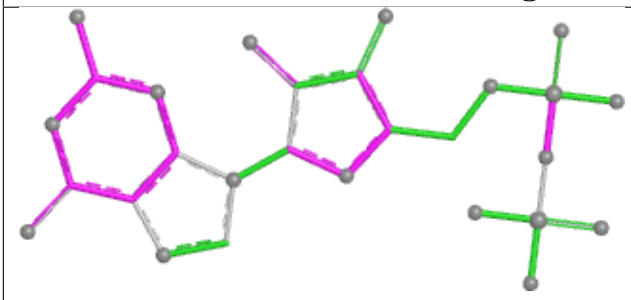

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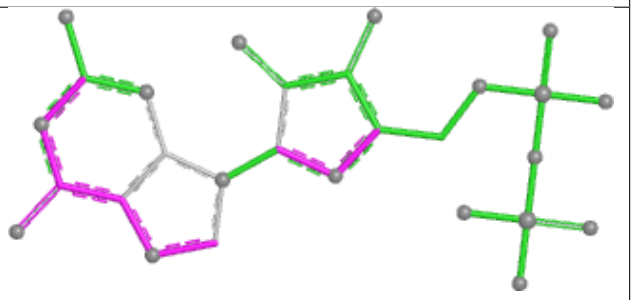

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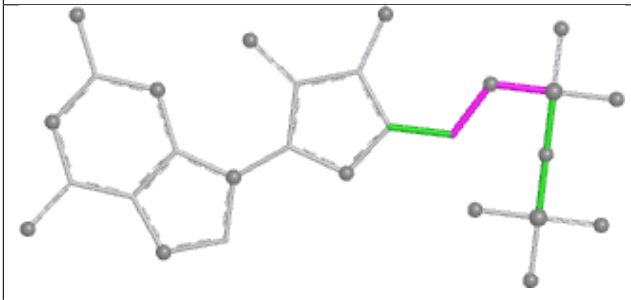

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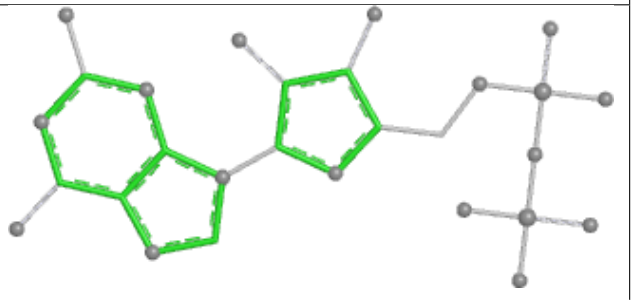

Rings

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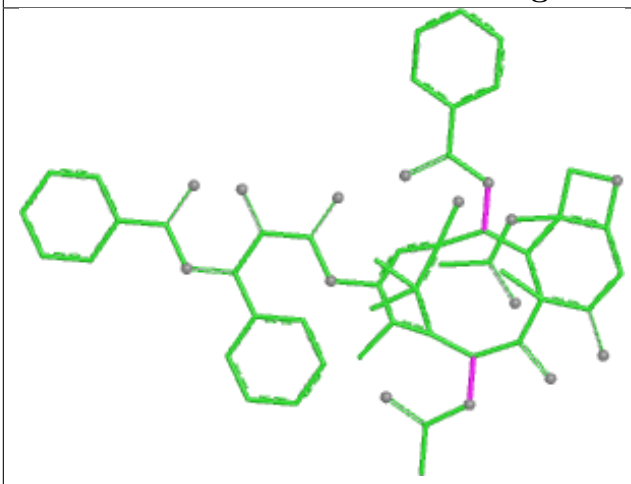

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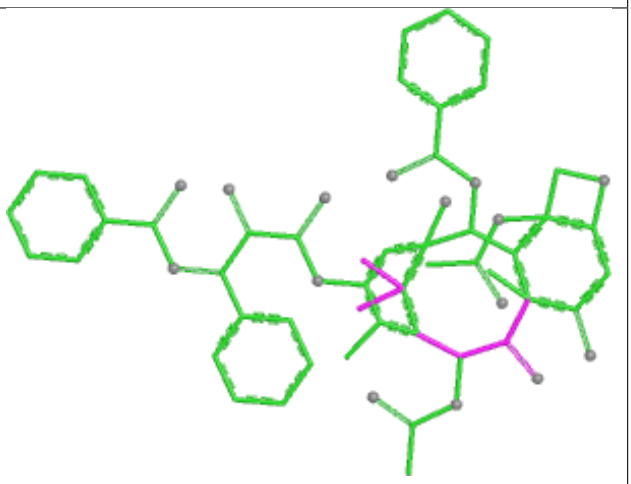

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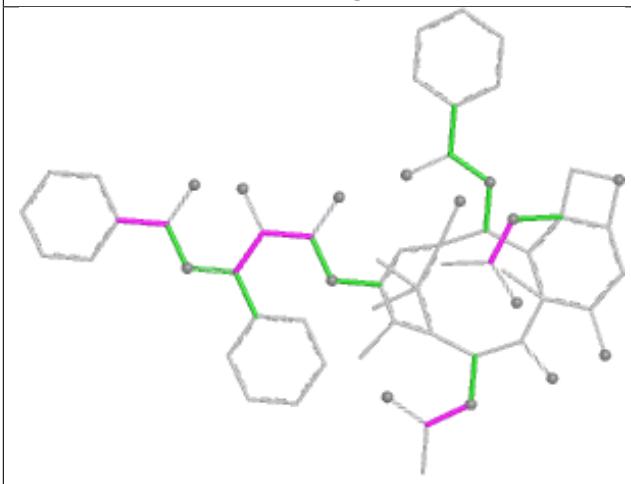

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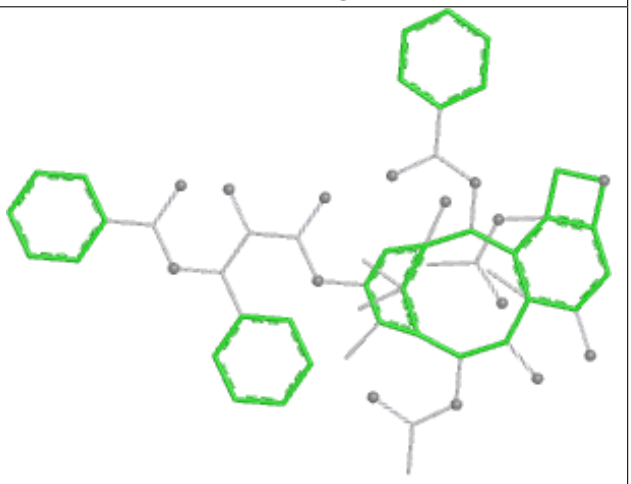

Rings

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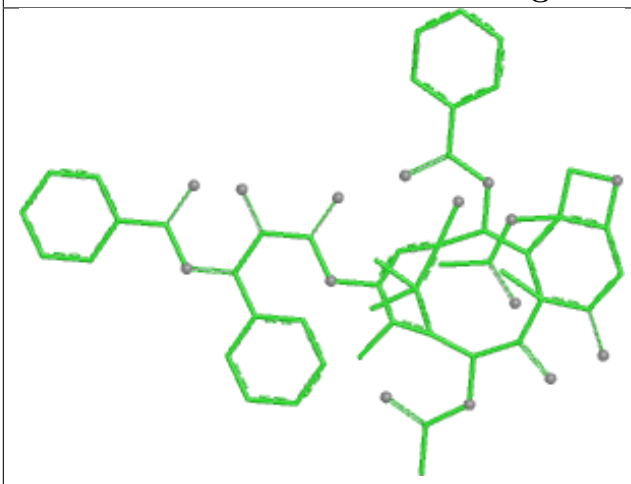

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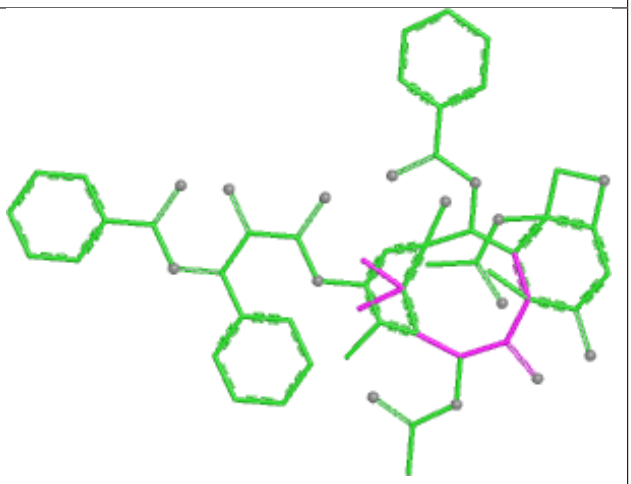

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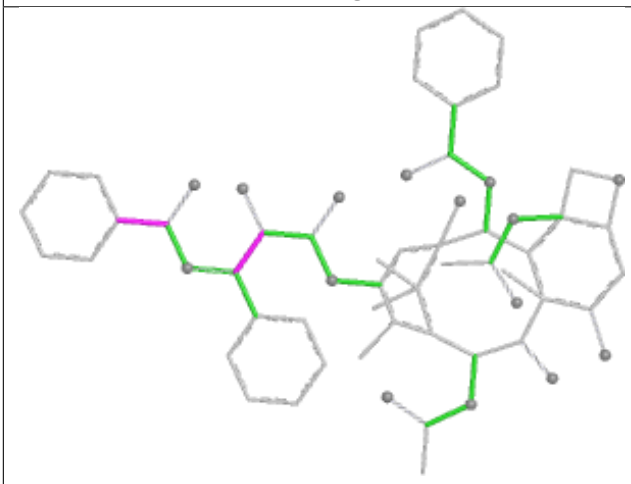

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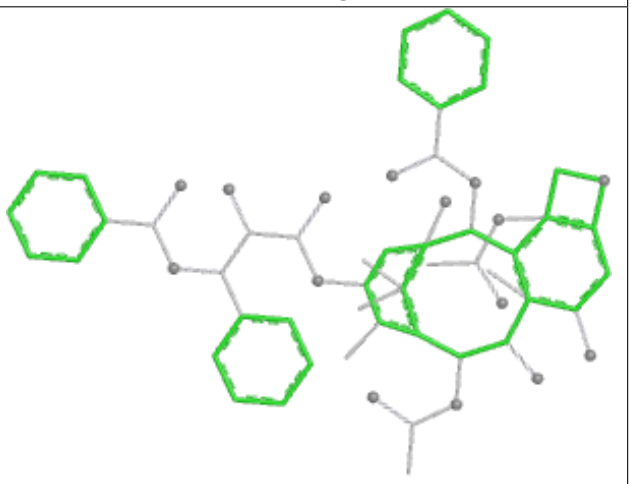
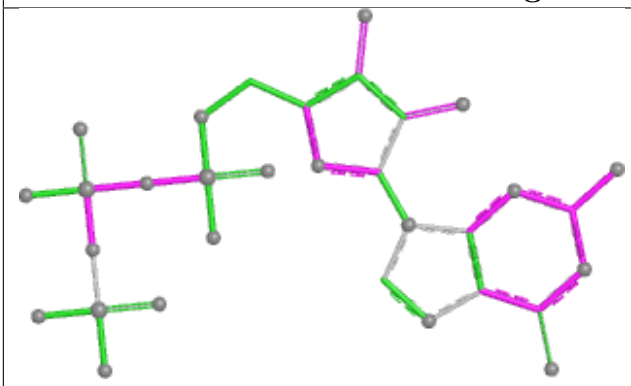


Rings

Ligand GTP E 501



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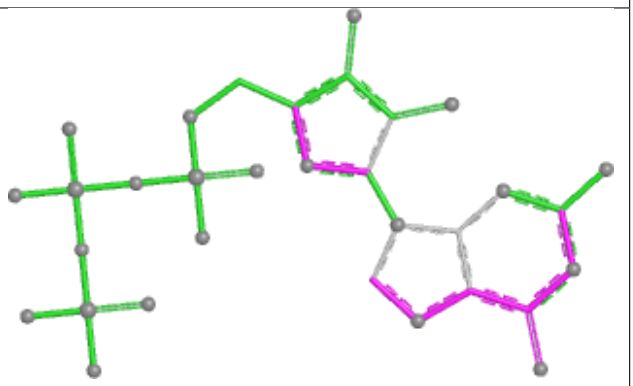

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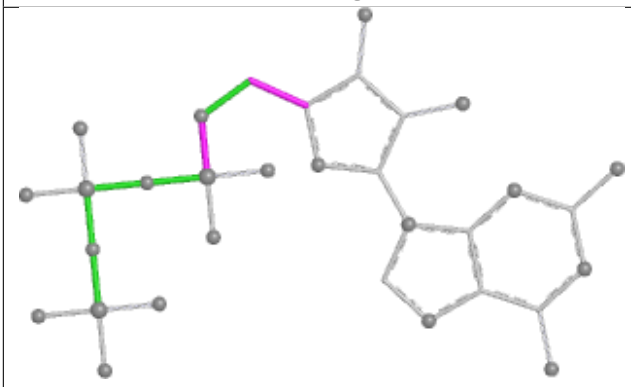

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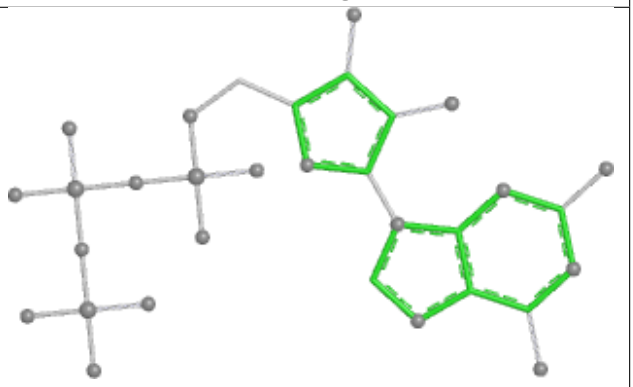

Rings

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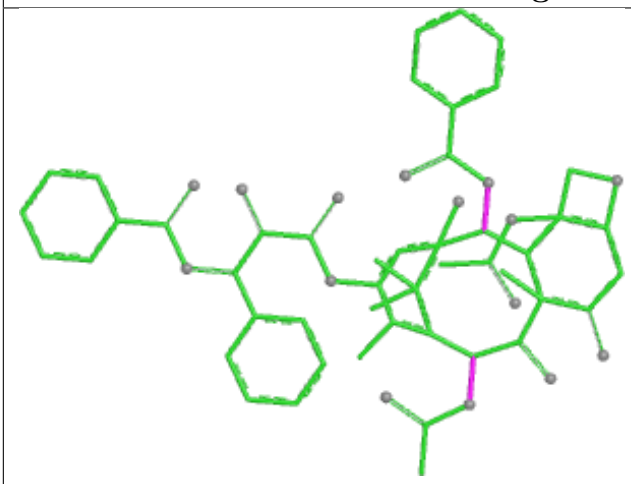

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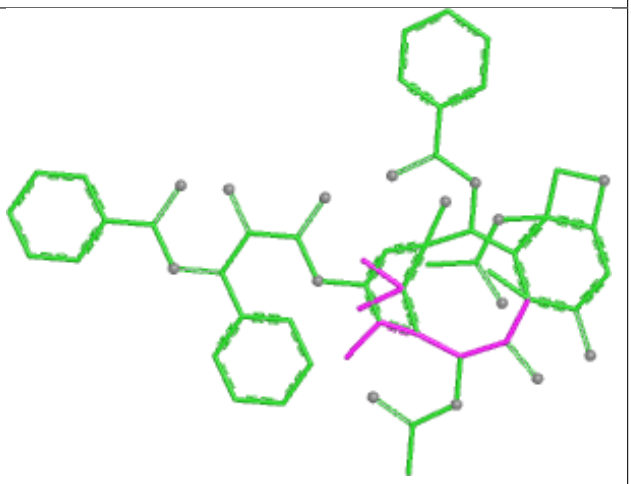

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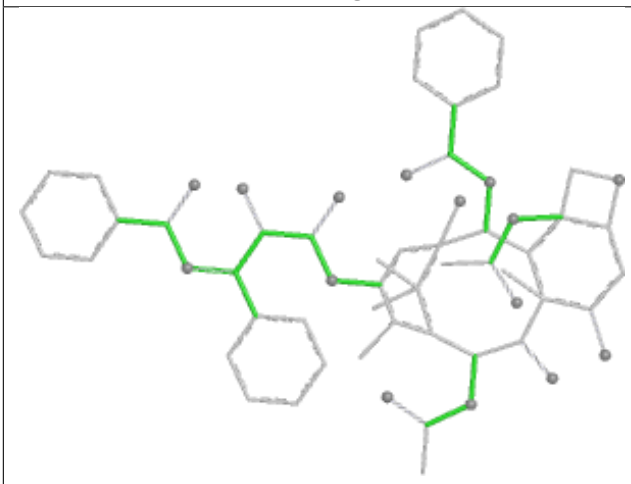
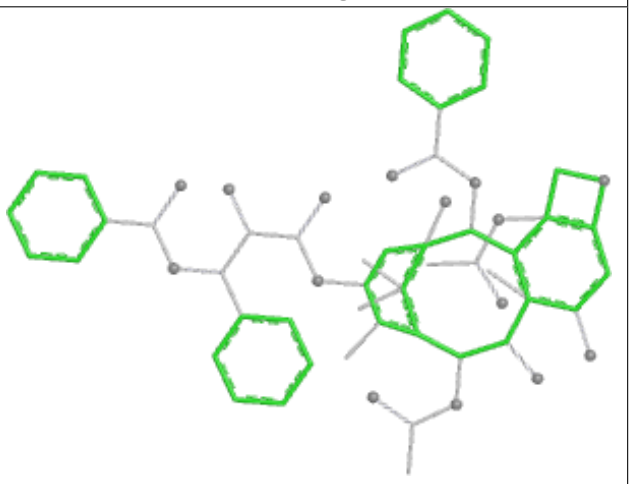
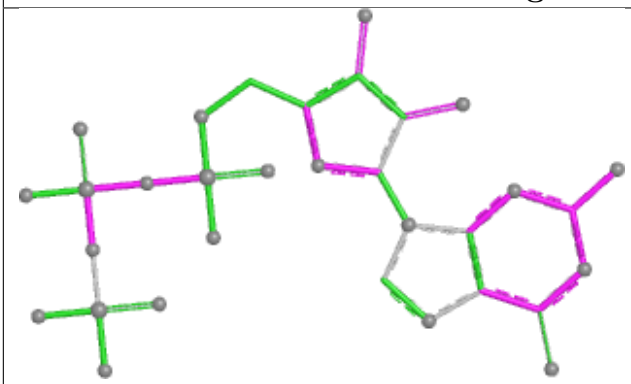


Torsions



Rings

Ligand GTP o 501



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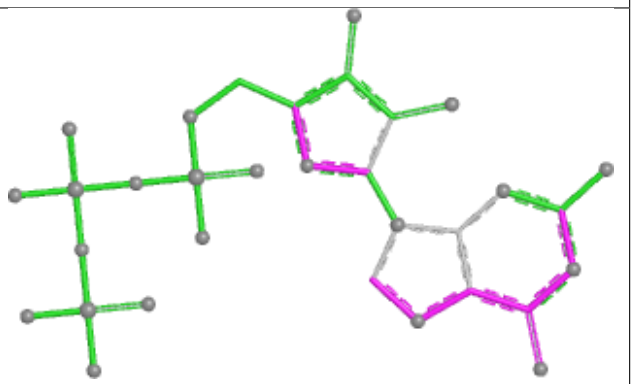

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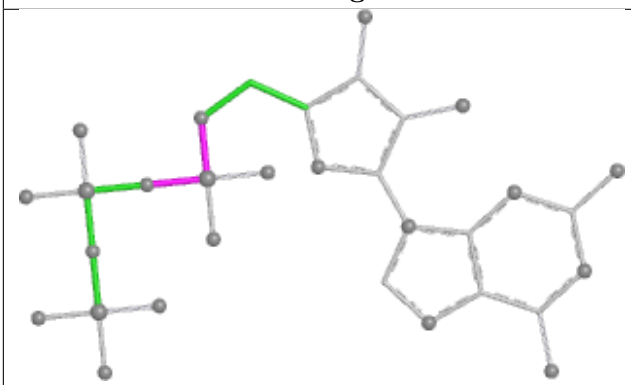

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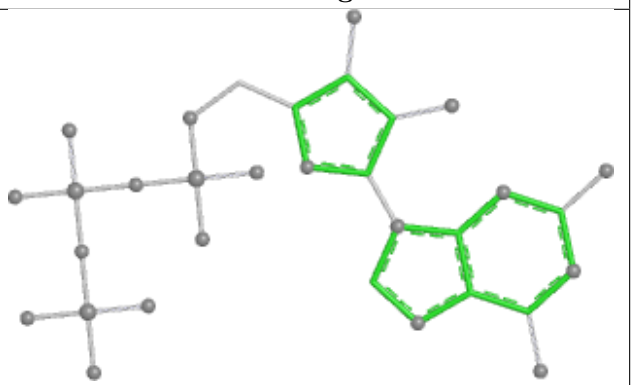

Rings

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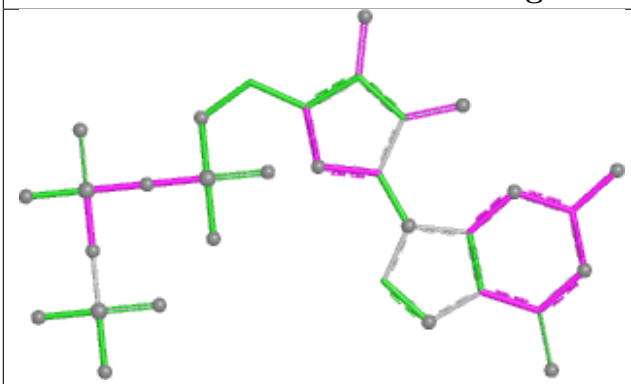

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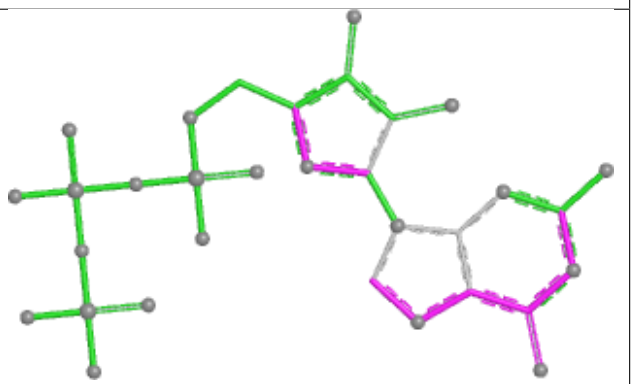

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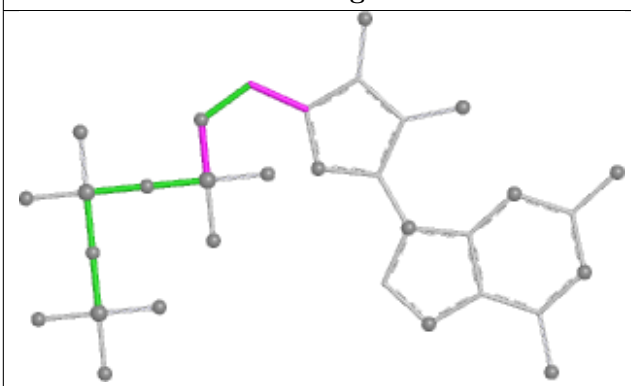

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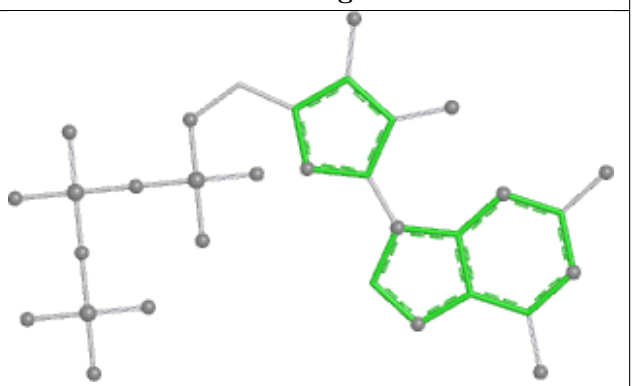

Rings

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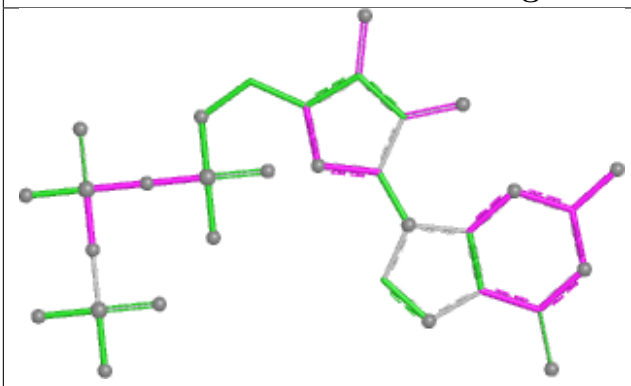

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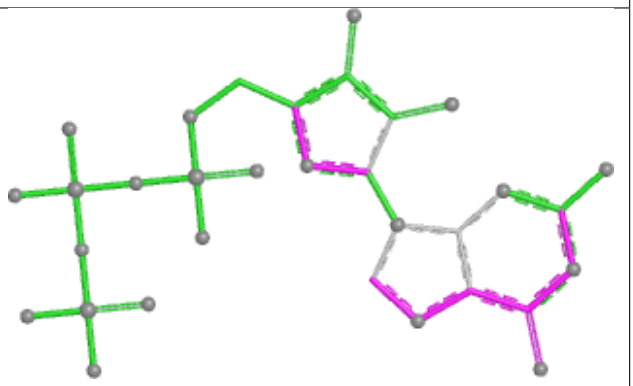

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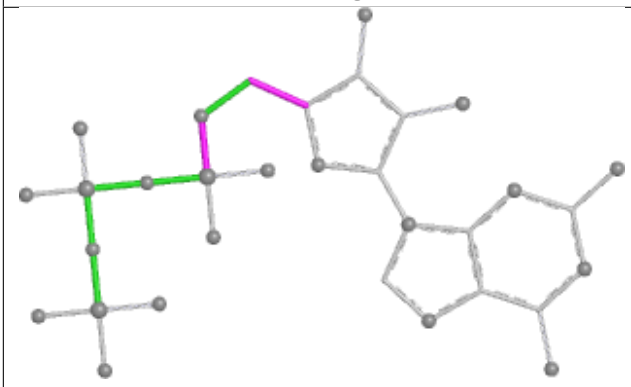

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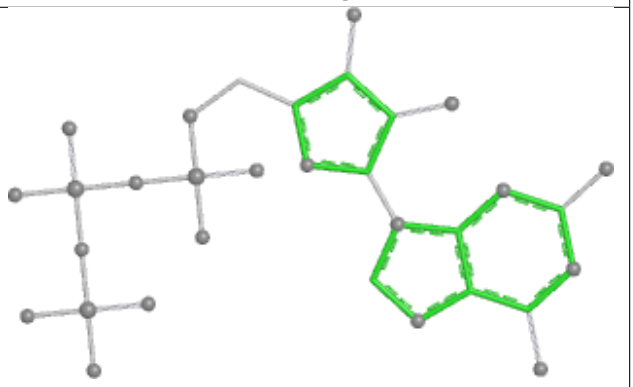

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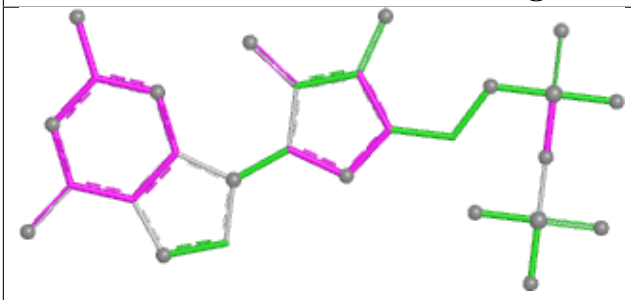

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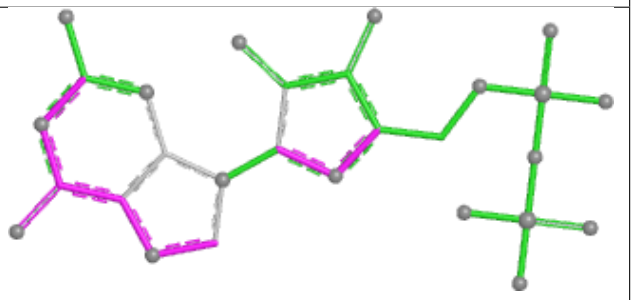

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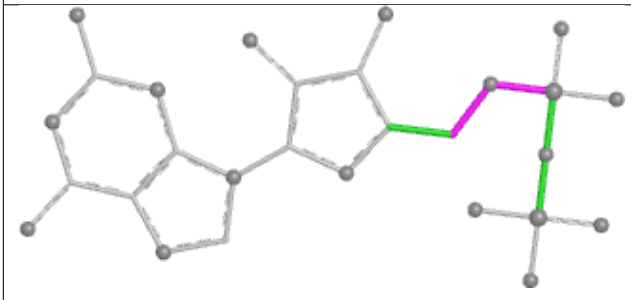

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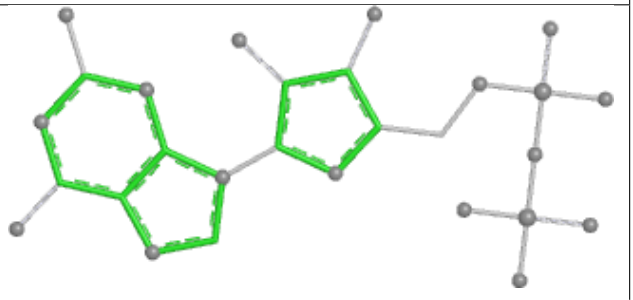

Rings

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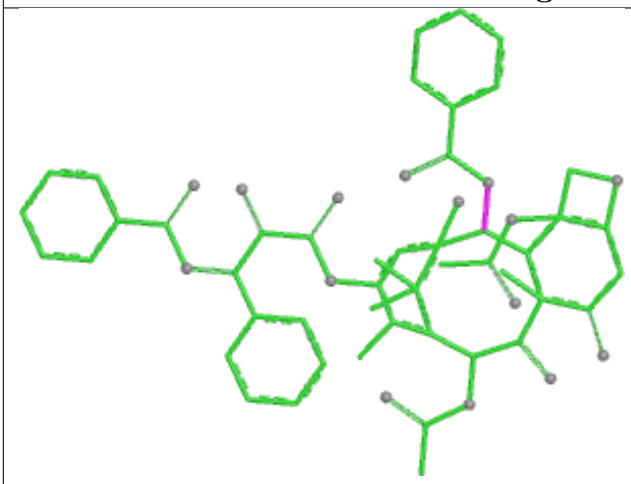

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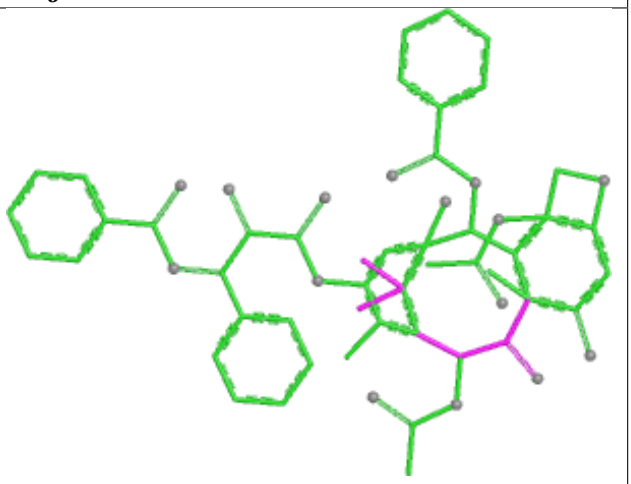

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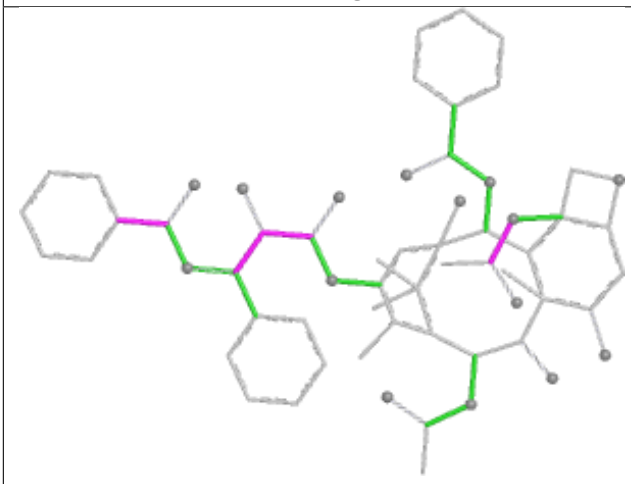

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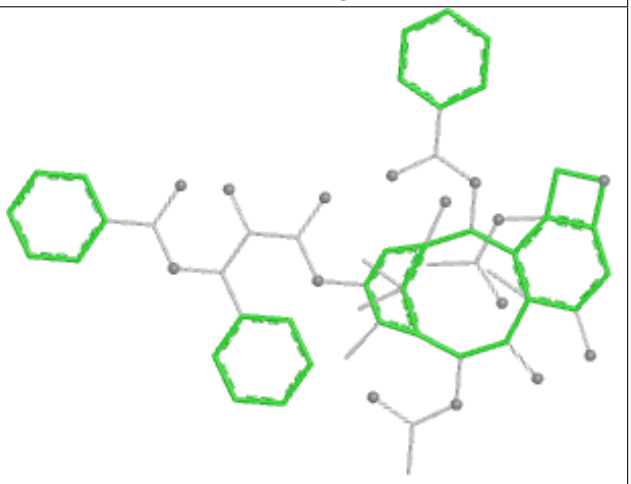

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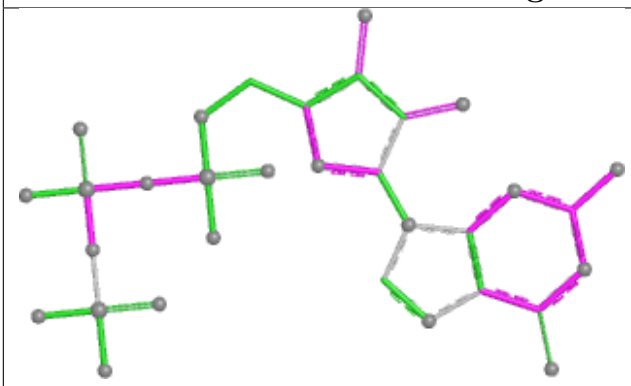

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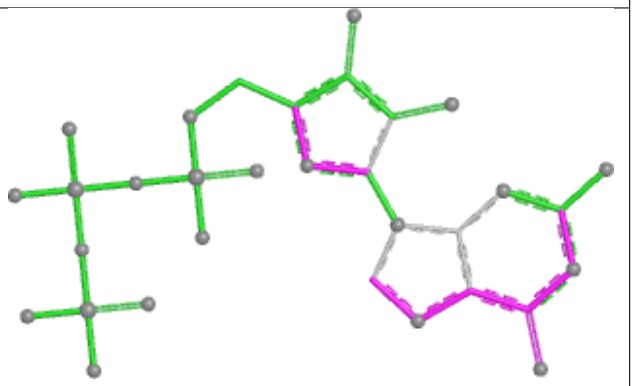

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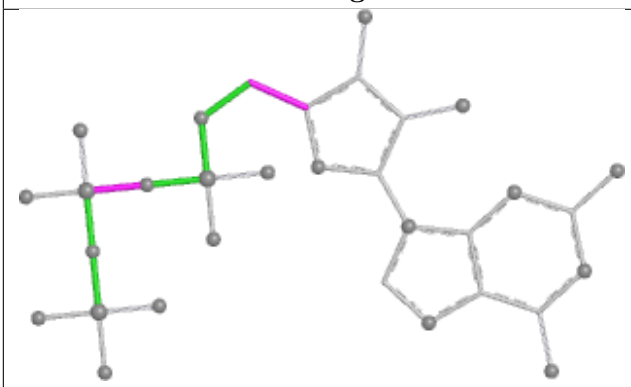

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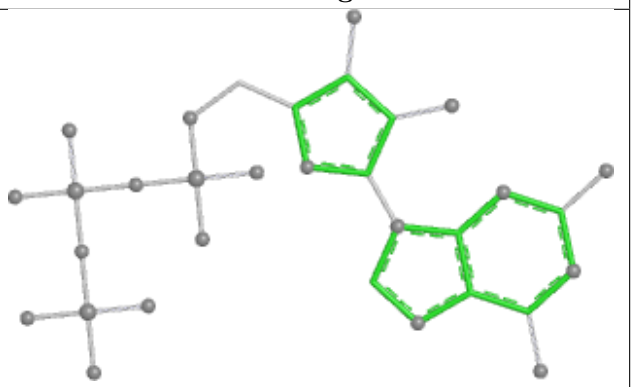

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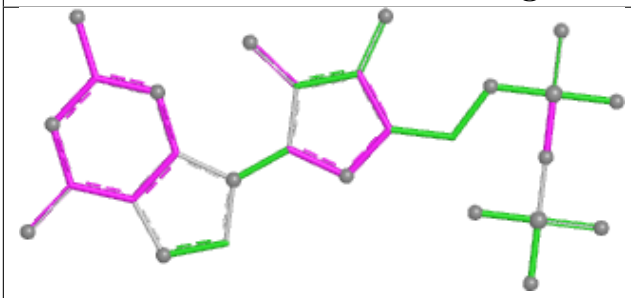

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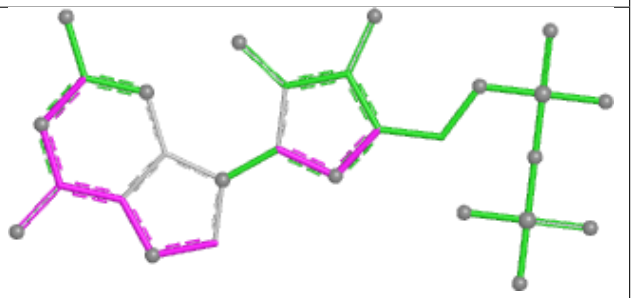

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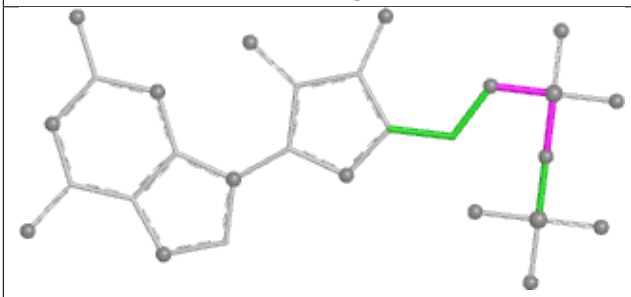

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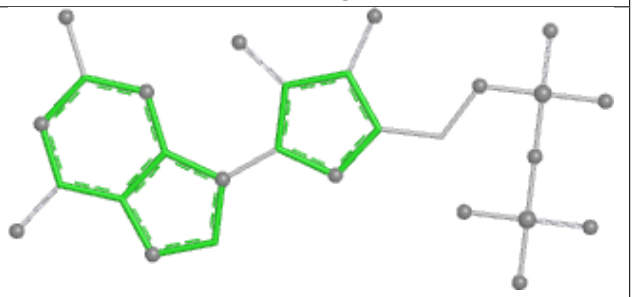

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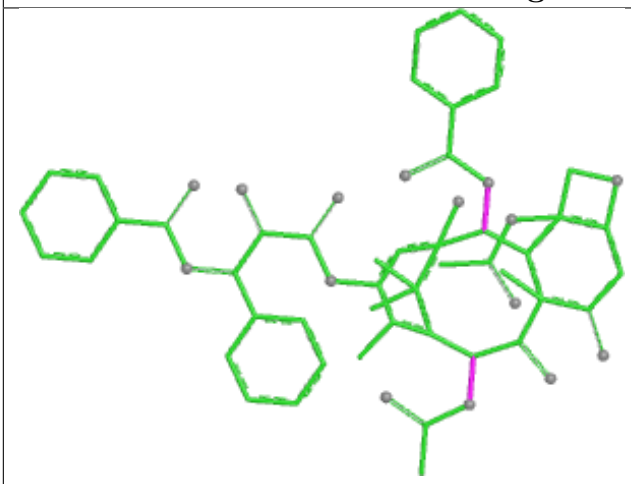

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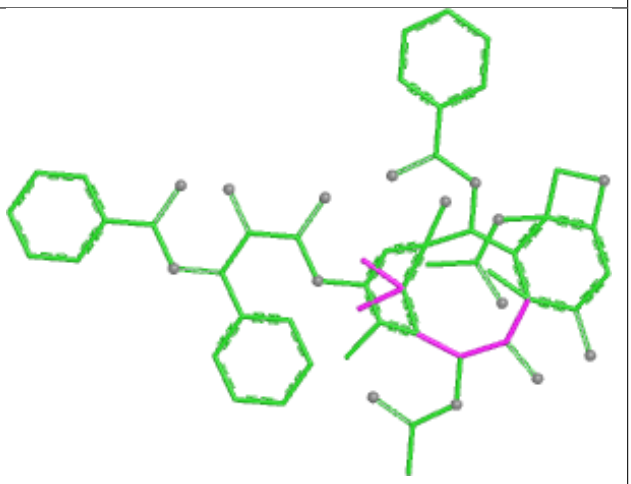

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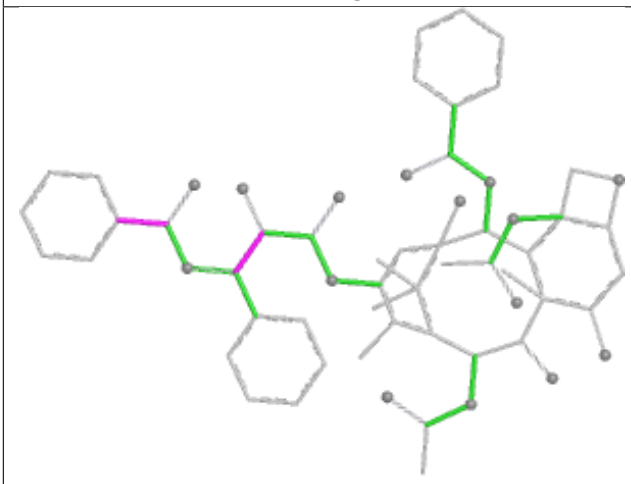

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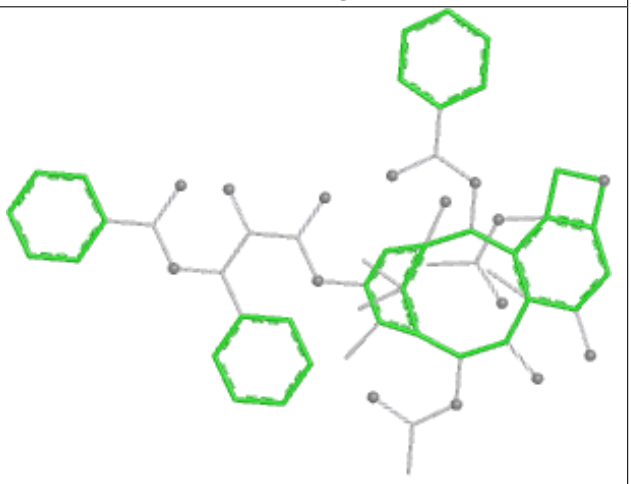

Rings

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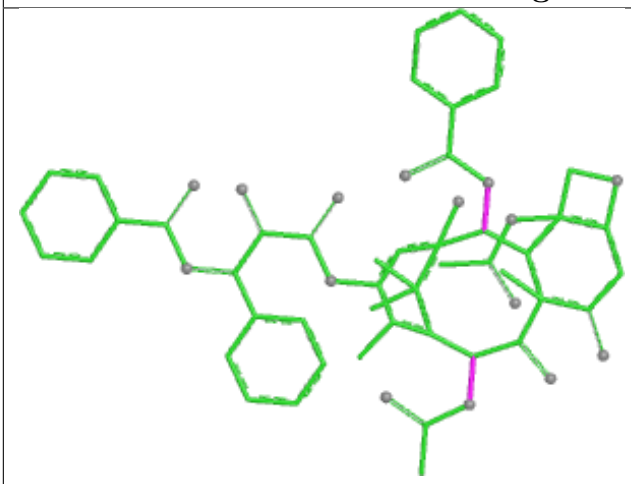

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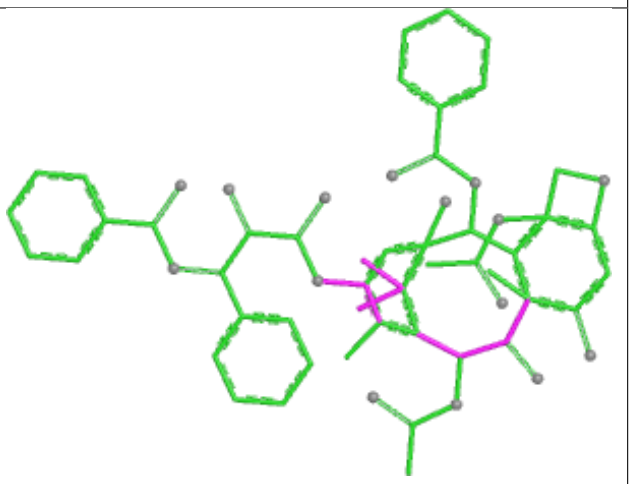

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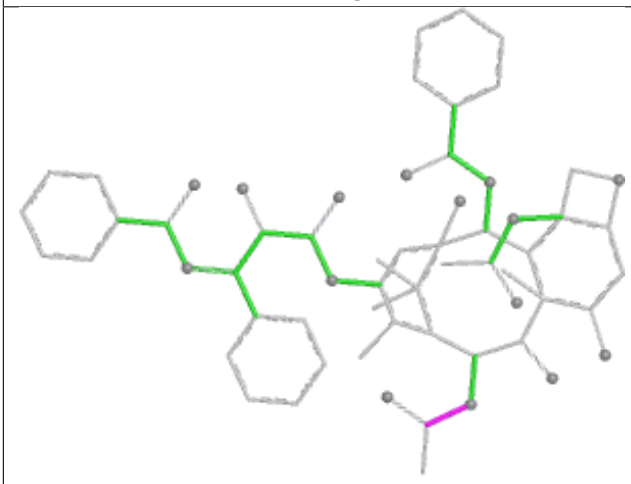

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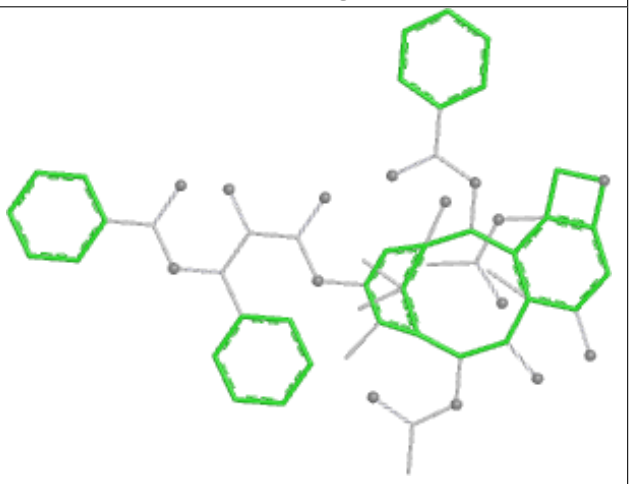

Rings

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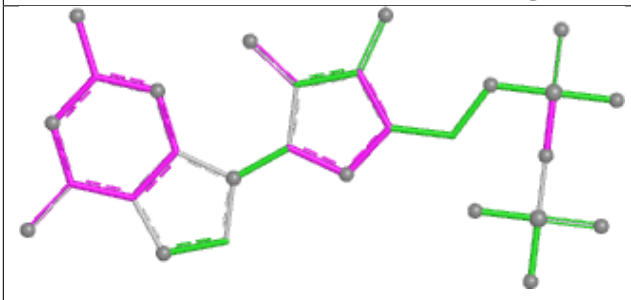

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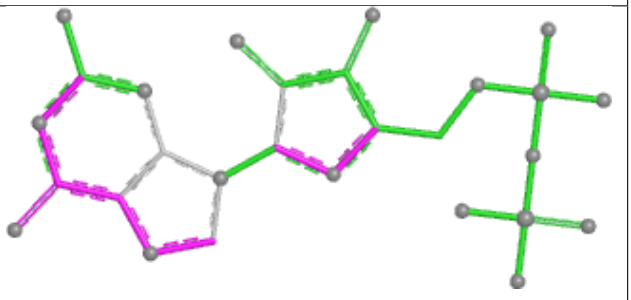

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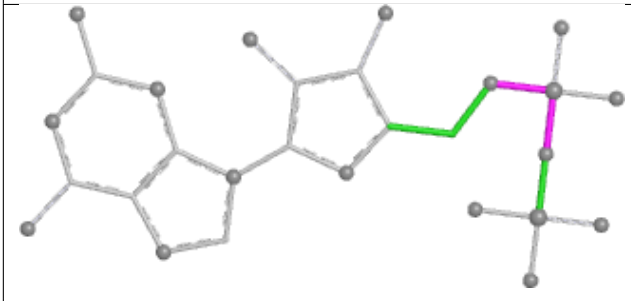

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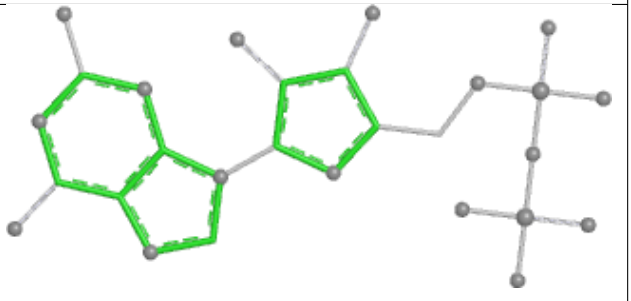

Rings

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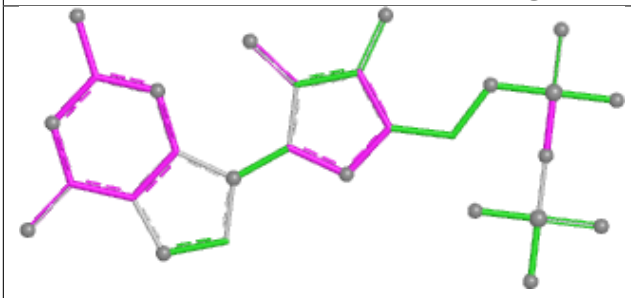
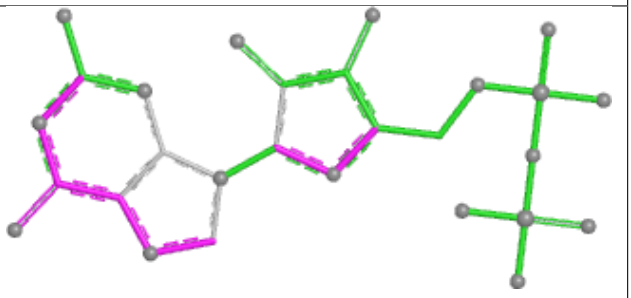
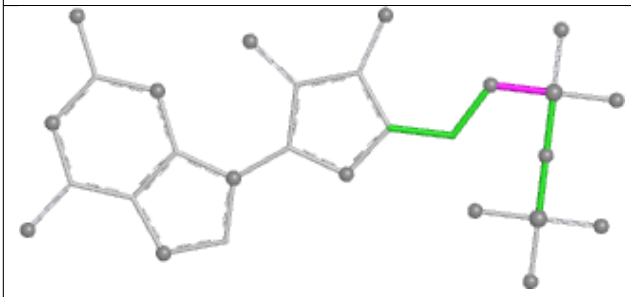
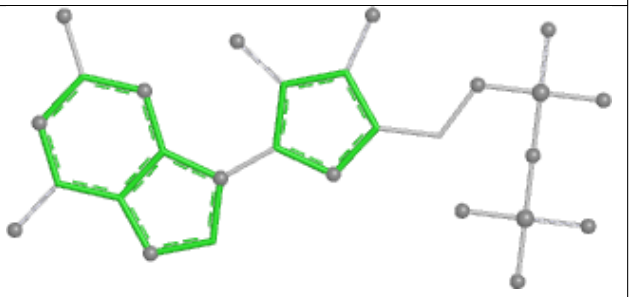
 Bond lengths	 Bond angles
 Torsions	 Rings

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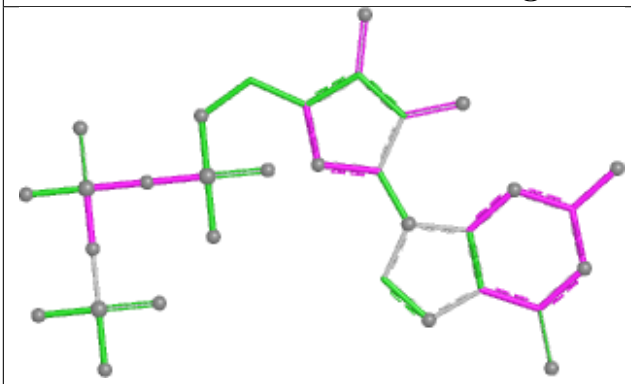
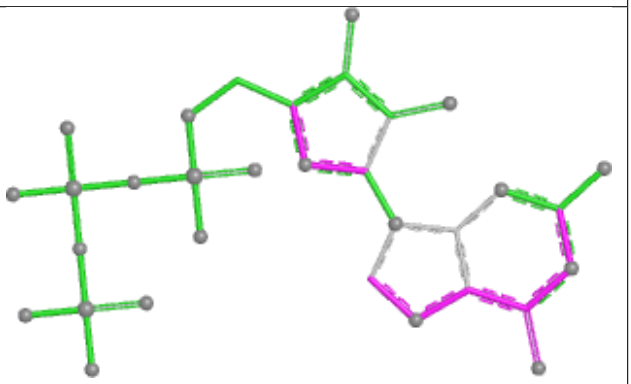
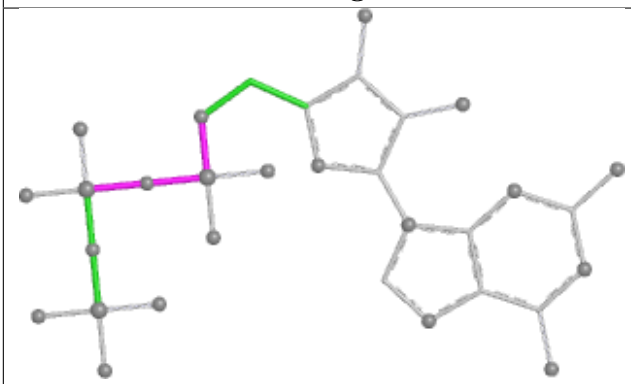
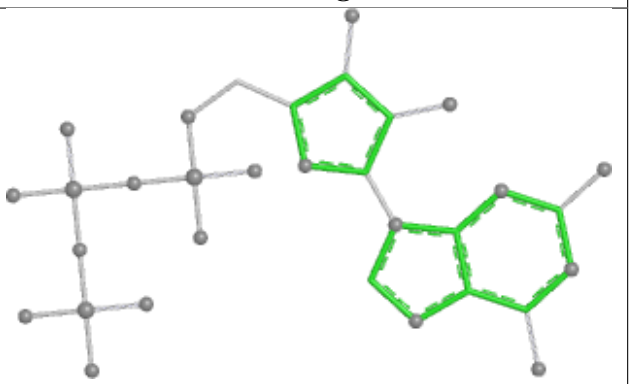
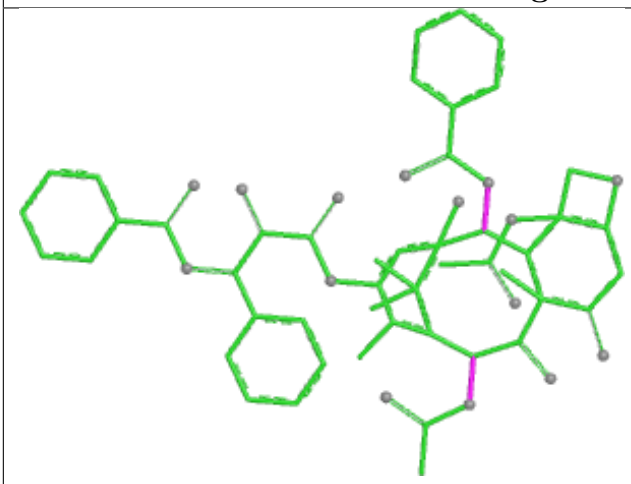
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TA1 p 502



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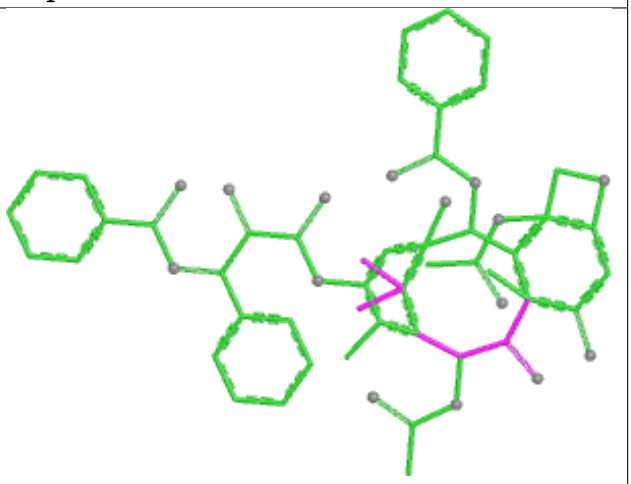

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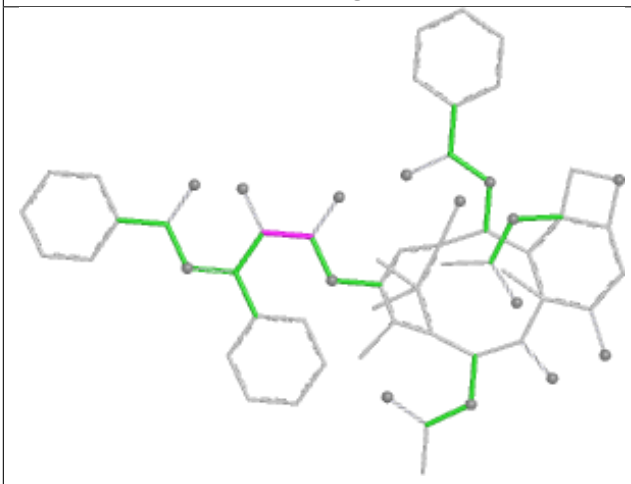

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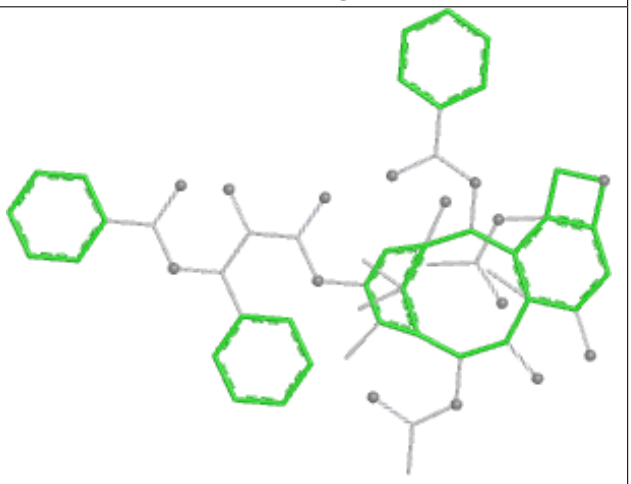
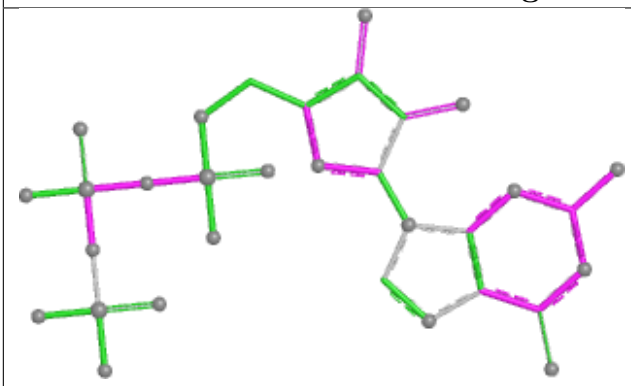


Rings

Ligand GTP G 501



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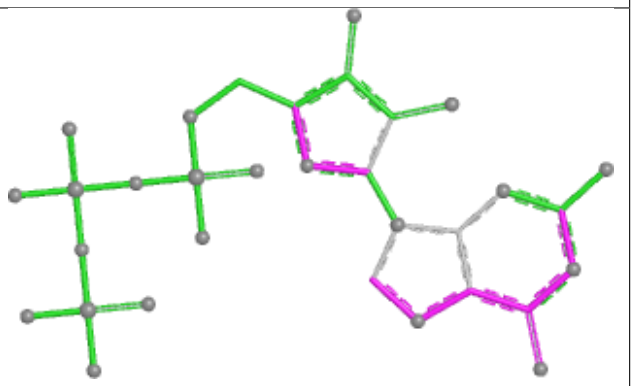

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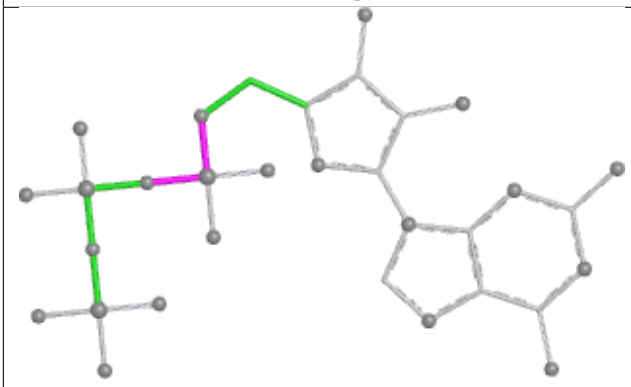

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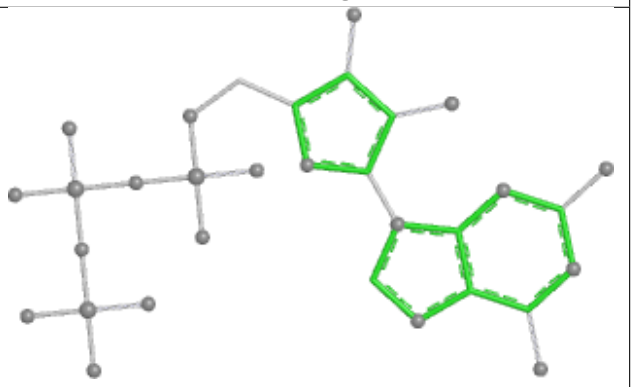
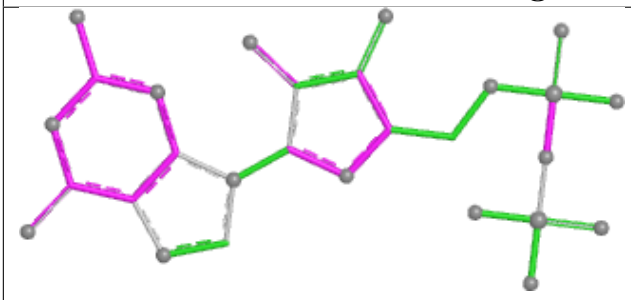


Rings

Ligand GDP j 501



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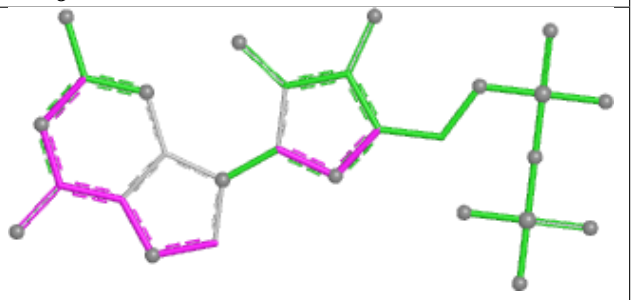

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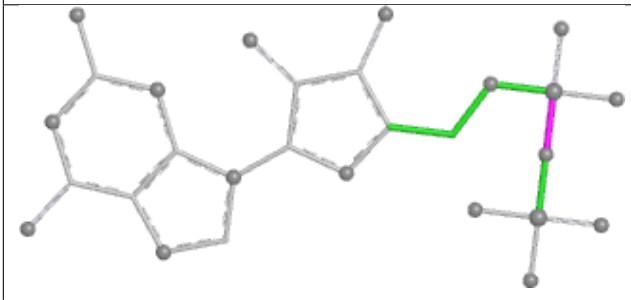

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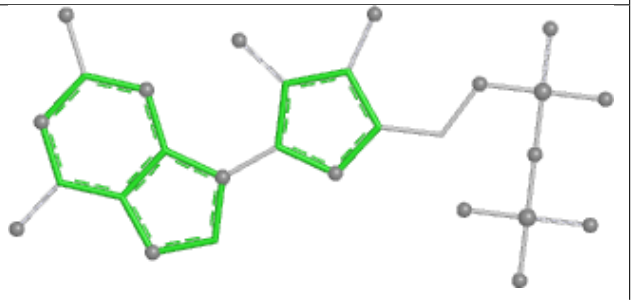

Rings

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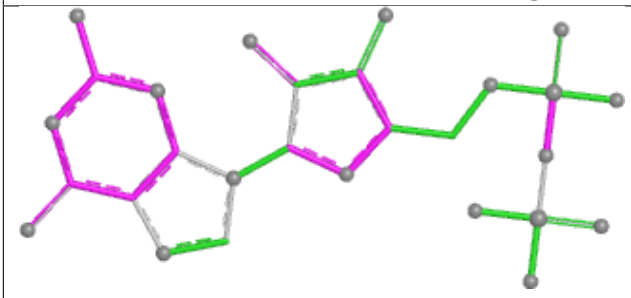
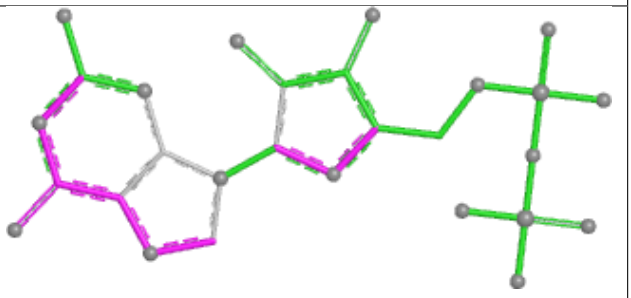
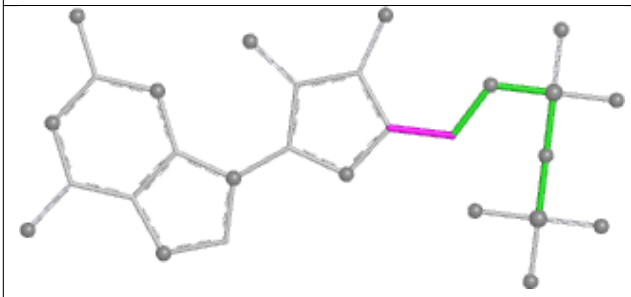
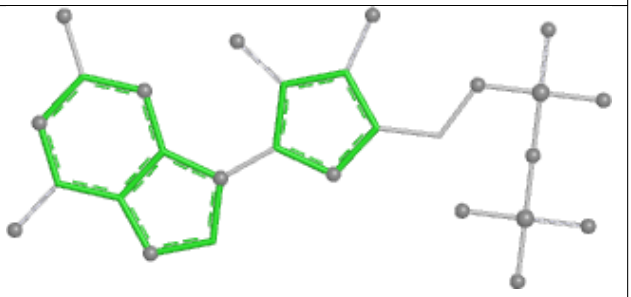
 Bond lengths	 Bond angles
 Torsions	 Rings

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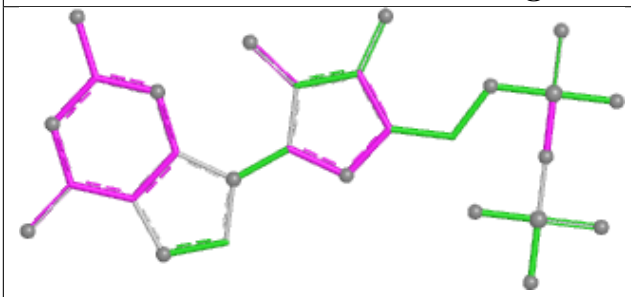
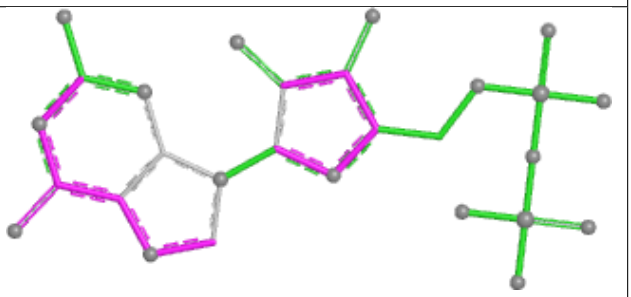
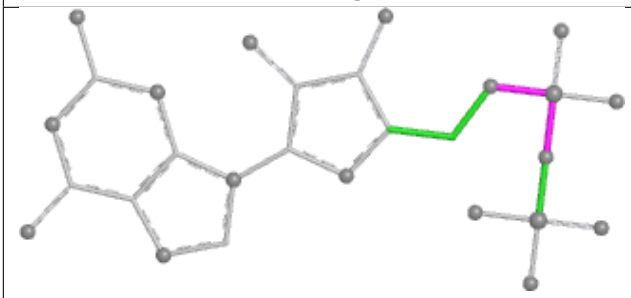
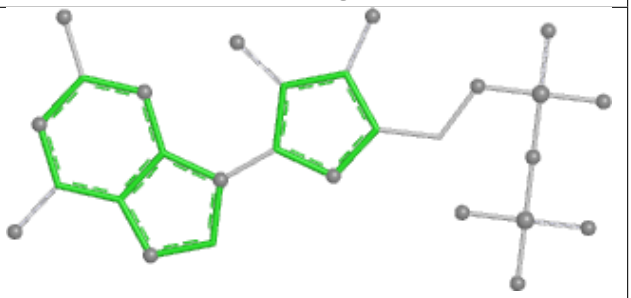
 Bond lengths	 Bond angles
 Torsions	 Rings

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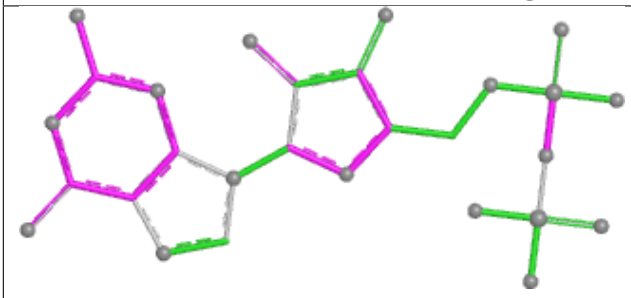
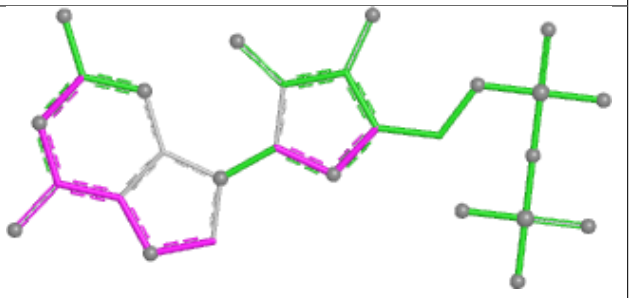
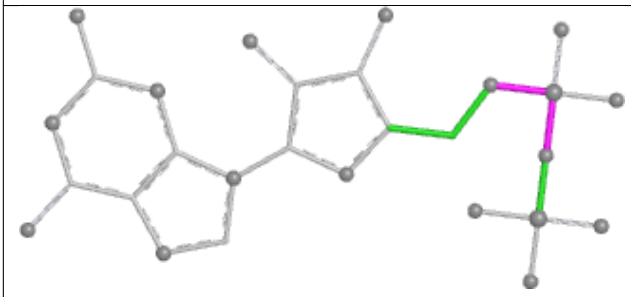
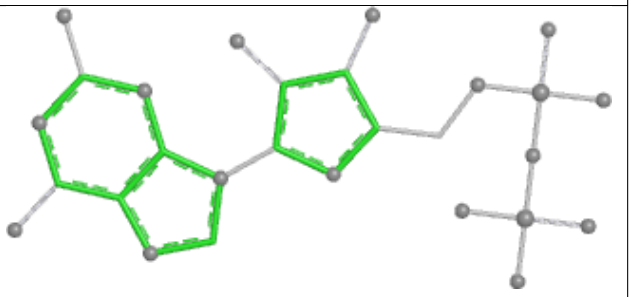
 Bond lengths	 Bond angles
 Torsions	 Rings

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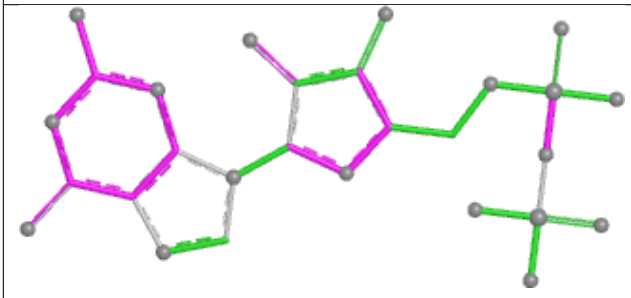
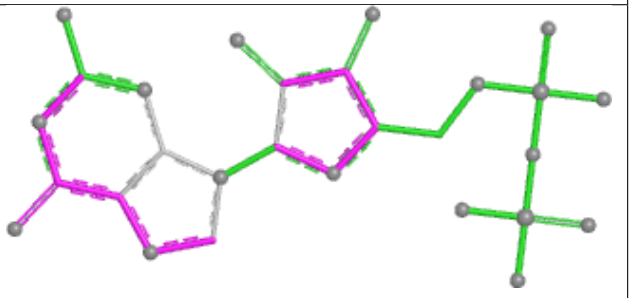
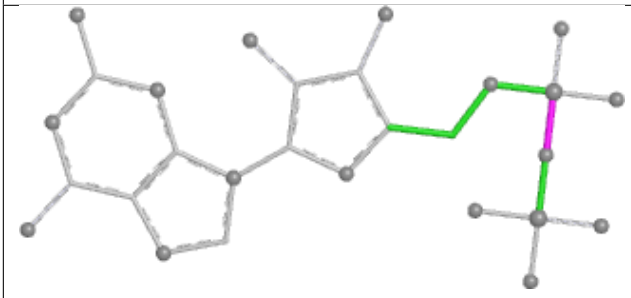
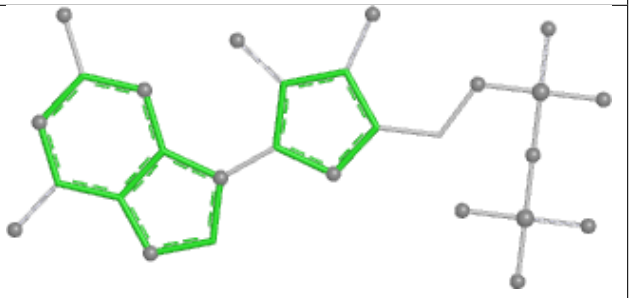
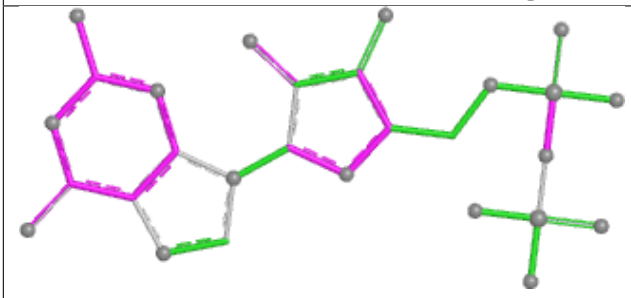
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP T 501



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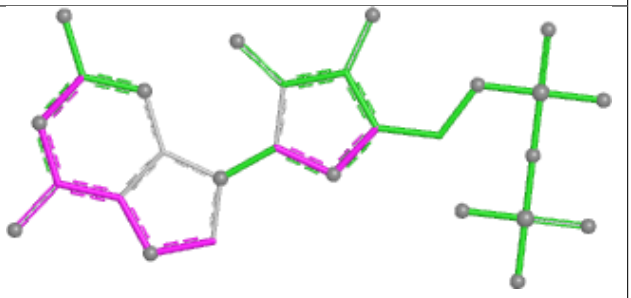

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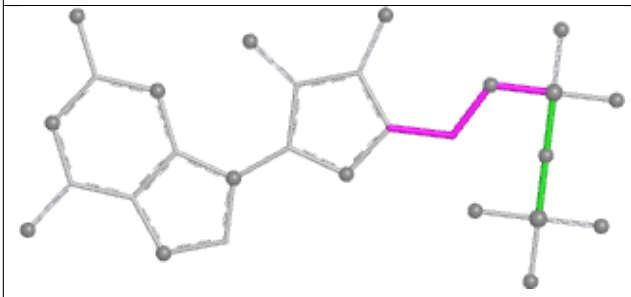

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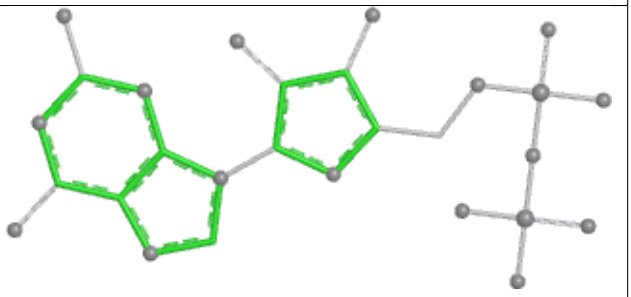
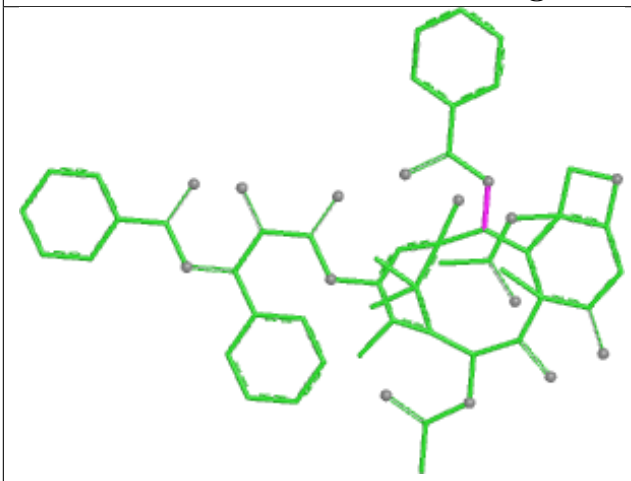


Rings

Ligand TA1 w 502



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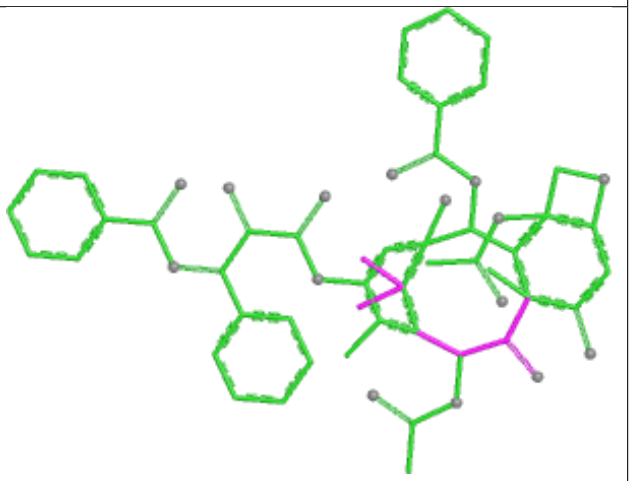

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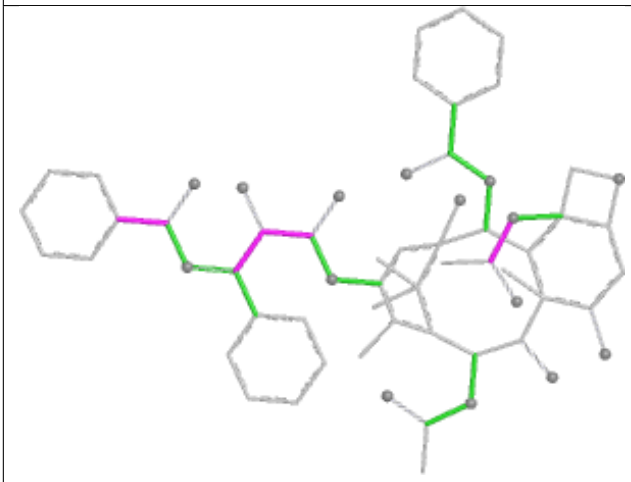

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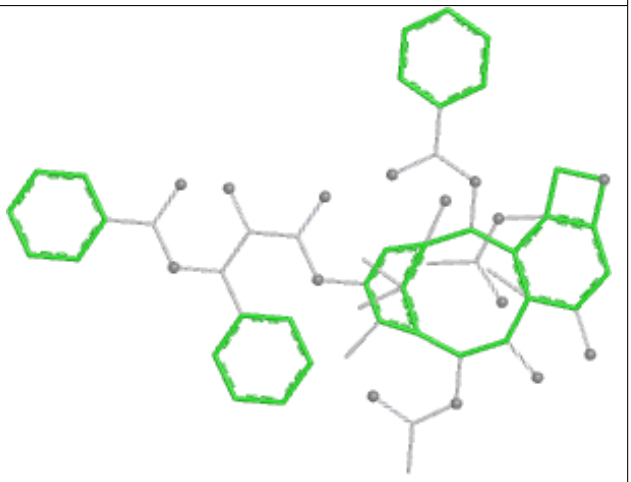

Rings

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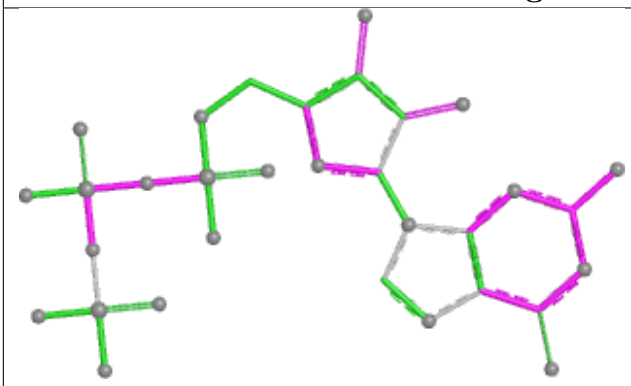

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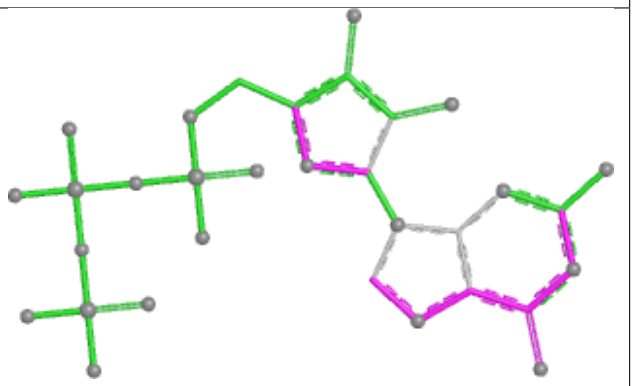

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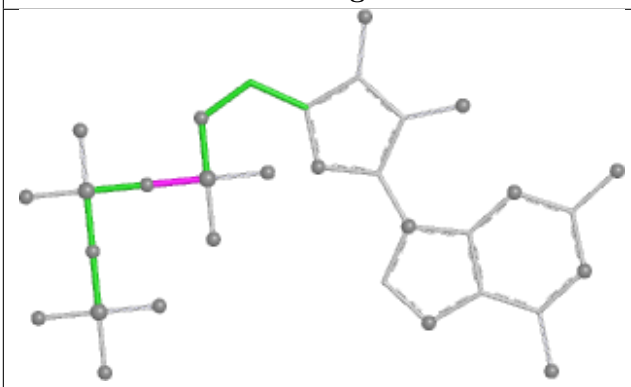

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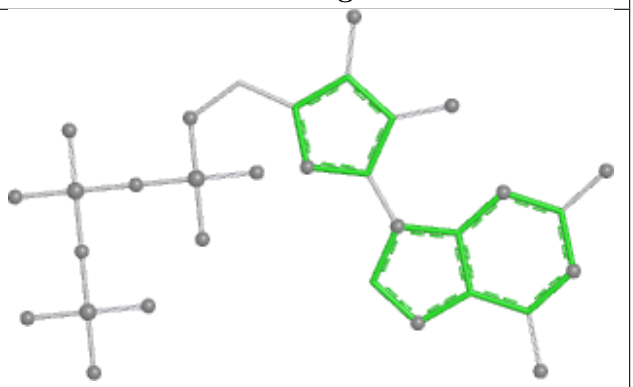

Rings

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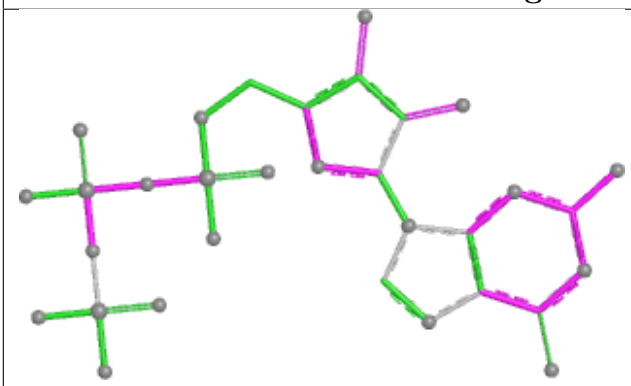

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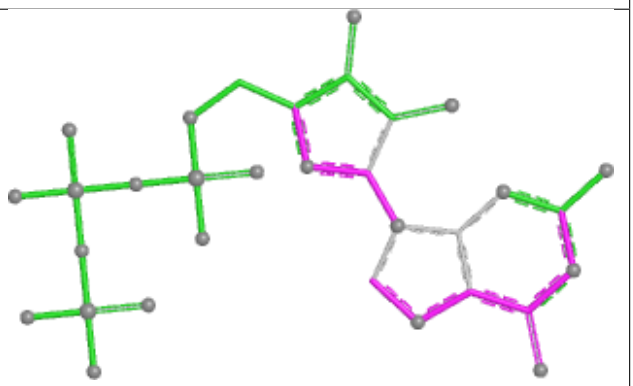

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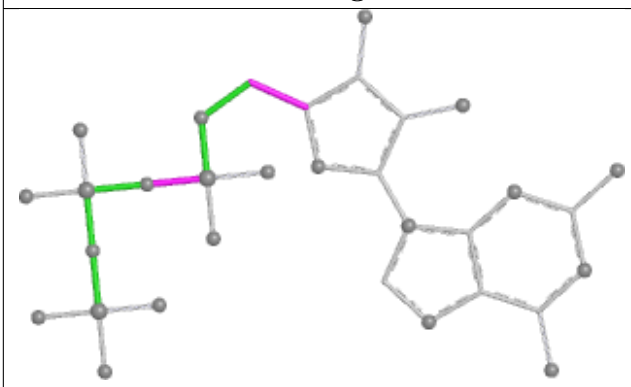

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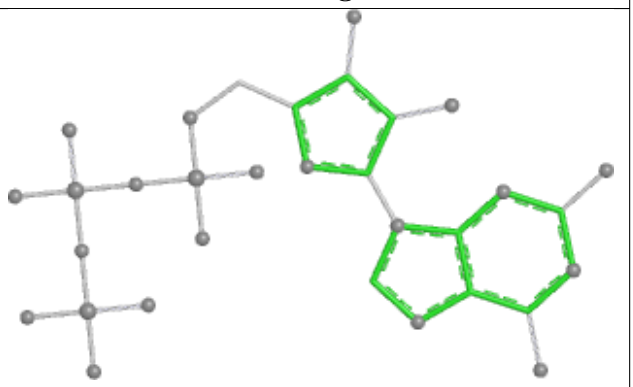

Rings

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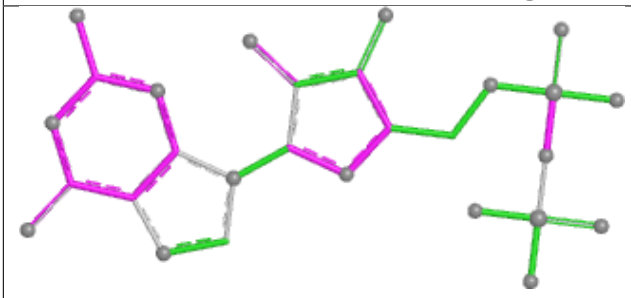
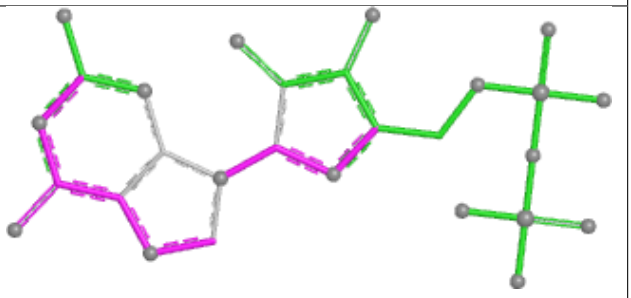
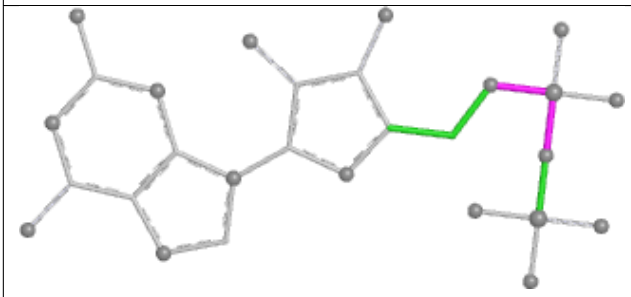
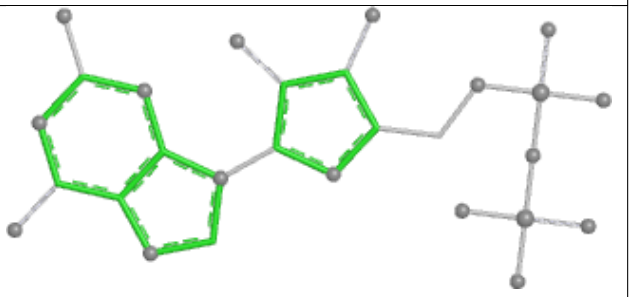
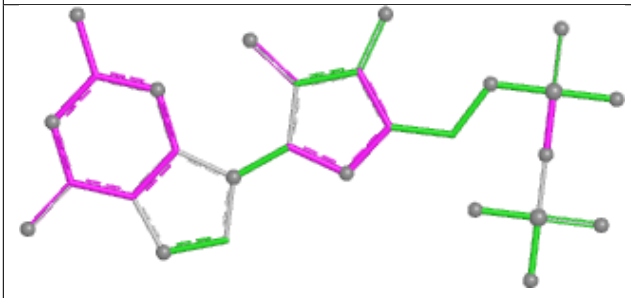
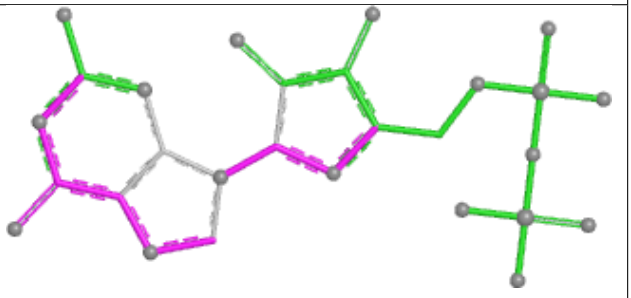
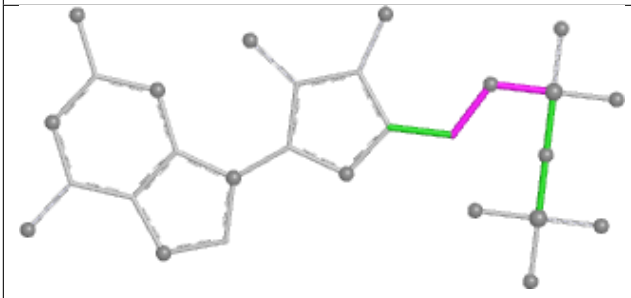
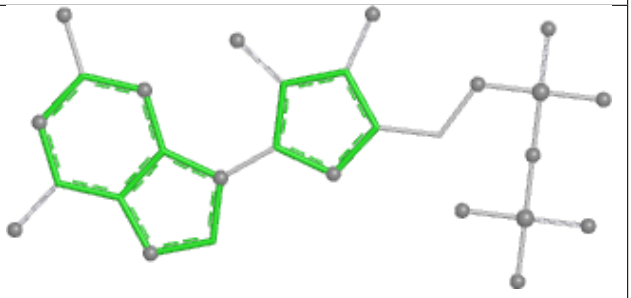
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP K 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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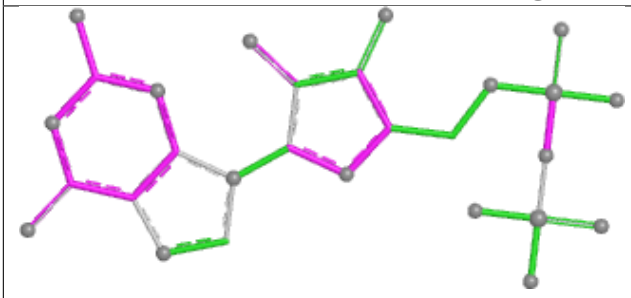
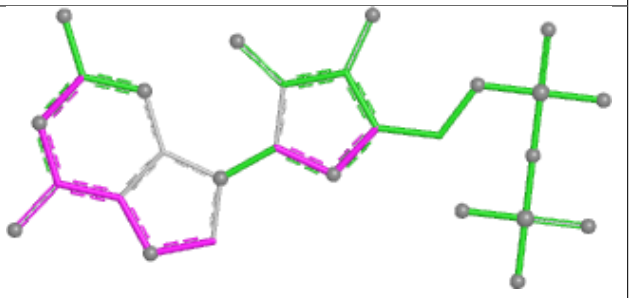
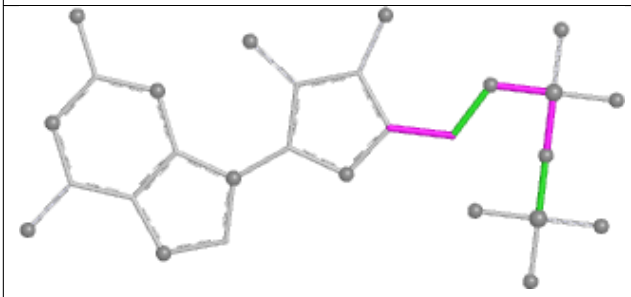
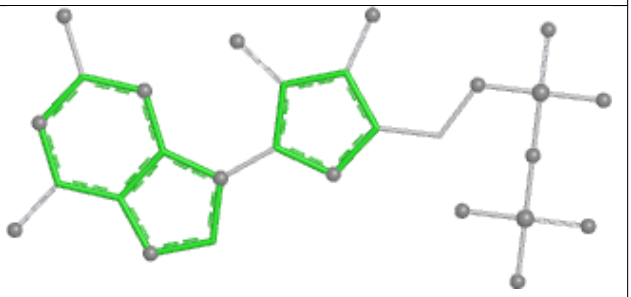
 Bond lengths	 Bond angles
 Torsions	 Rings

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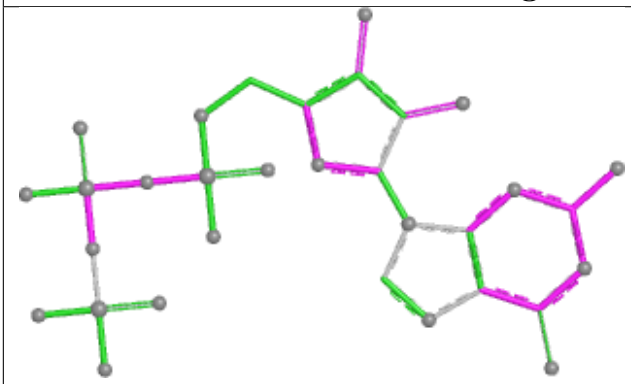
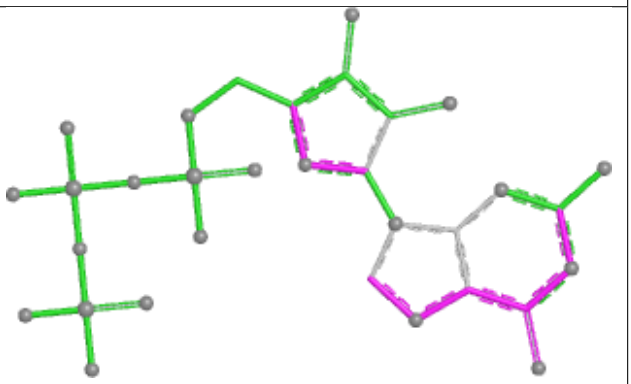
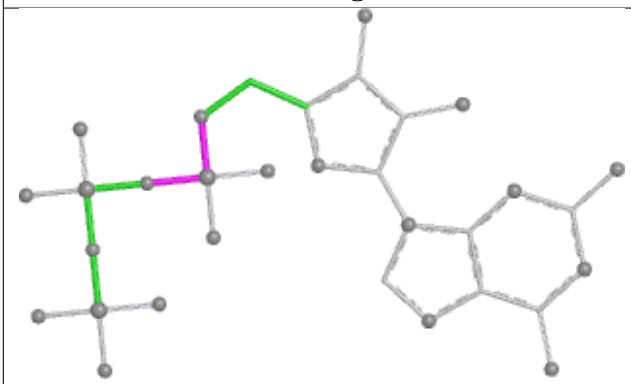
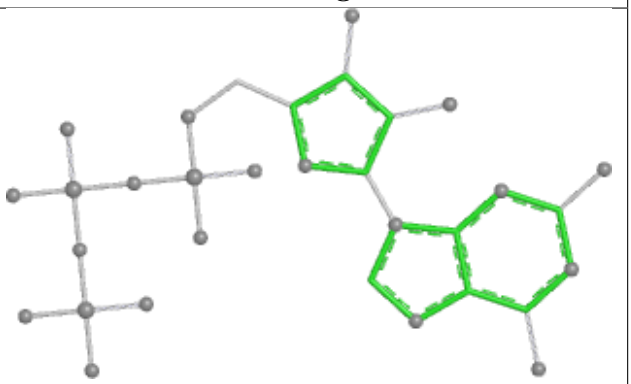
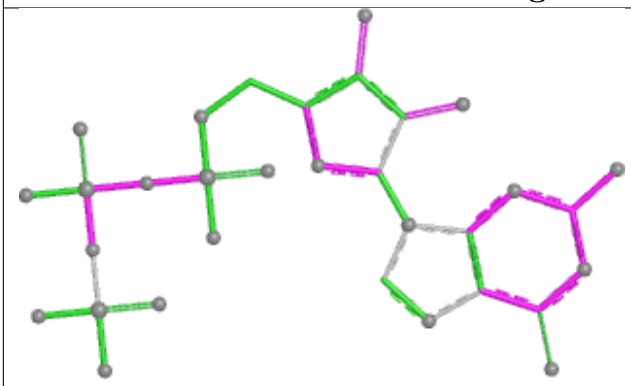
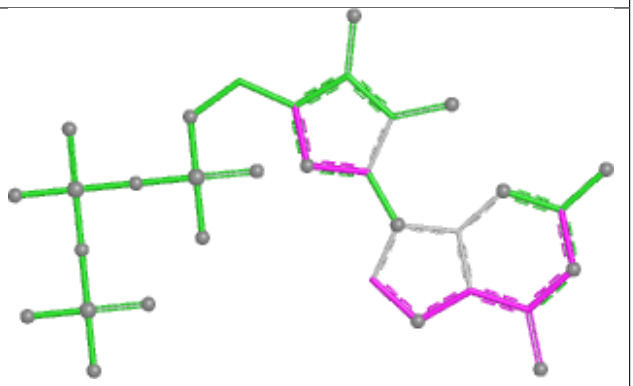
 Bond lengths	 Bond angles
 Torsions	 Rings

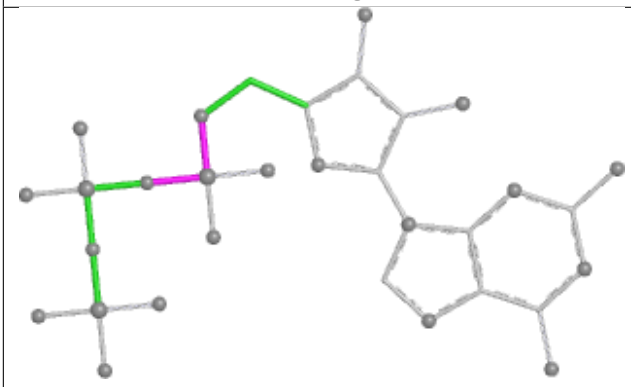
Ligand GTP s 501



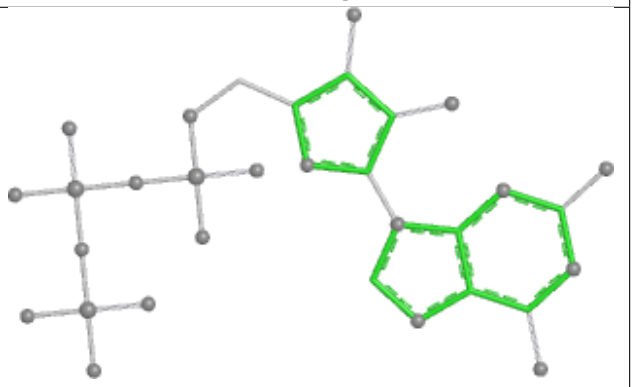
Bond lengths



Bond angles

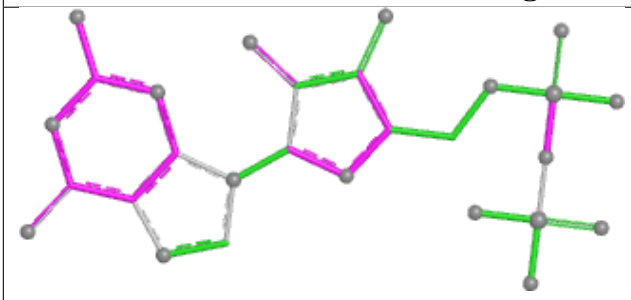


Torsions

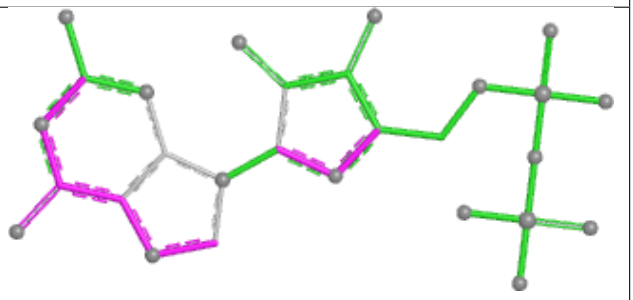


Rings

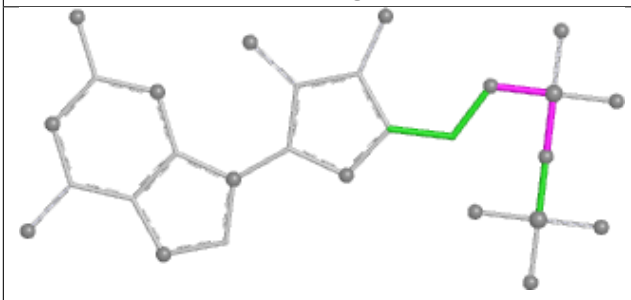
Ligand GDP w 501



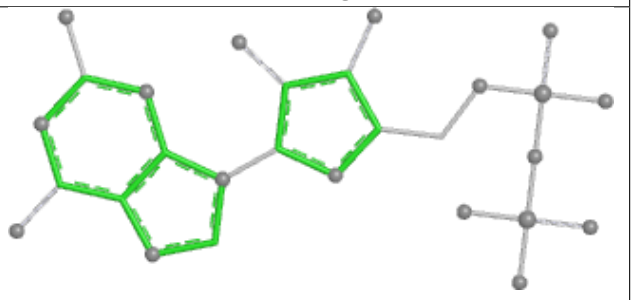
Bond lengths



Bond angles

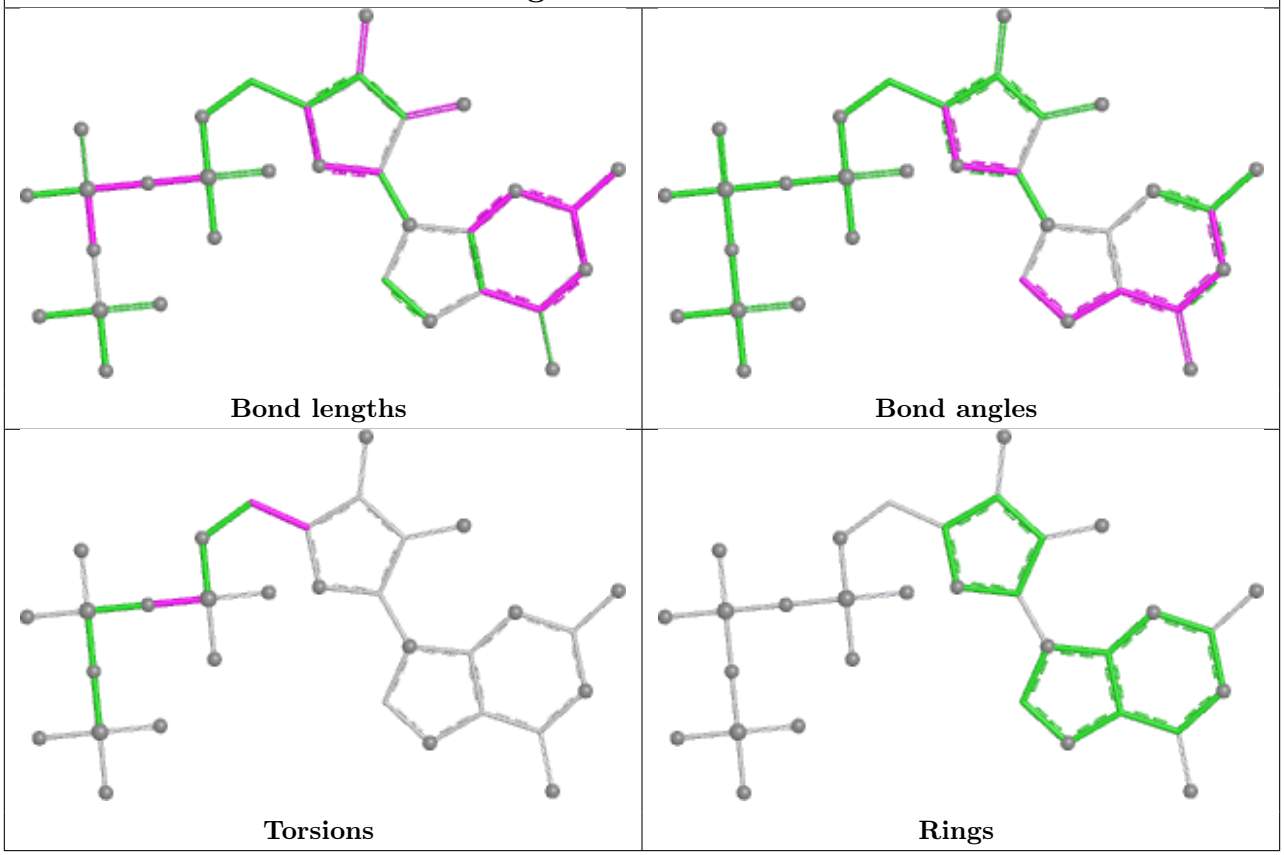


Torsions



Rings

Ligand GTP k 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

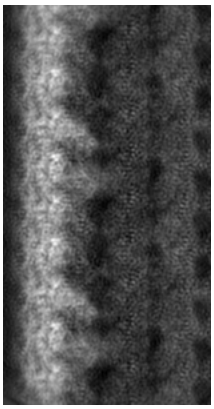
6 Map visualisation

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

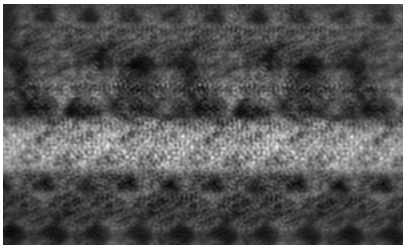
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

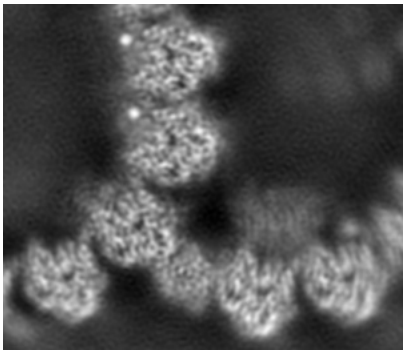
6.1.1 Primary map



X



Y

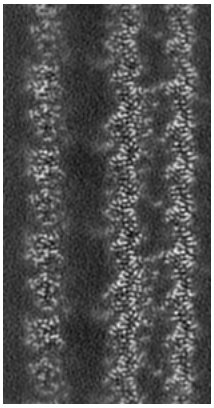


Z

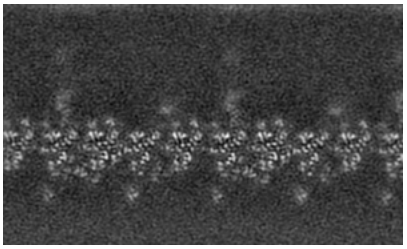
The images above show the map projected in three orthogonal directions.

6.2 Central slices

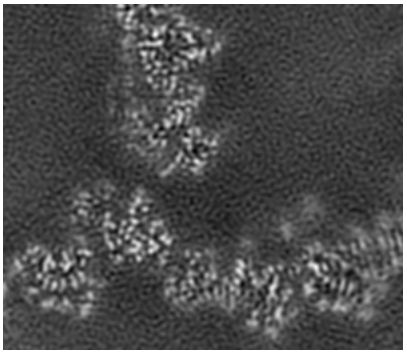
6.2.1 Primary map



X Index: 135



Y Index: 117

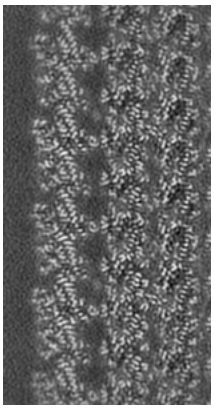


Z Index: 225

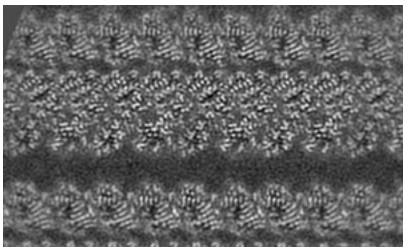
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

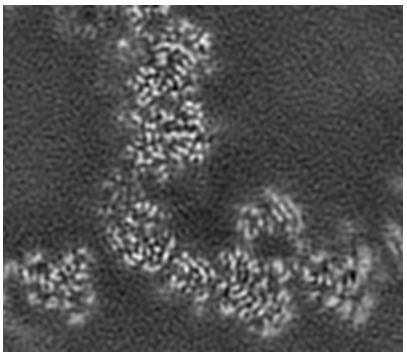
6.3.1 Primary map



X Index: 111



Y Index: 45

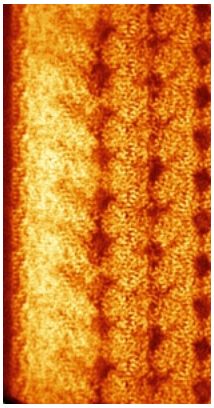


Z Index: 281

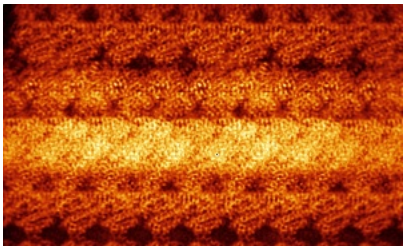
The images above show the largest variance slices of the map in three orthogonal directions.

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

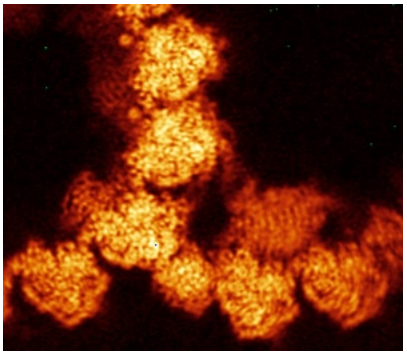
6.4.1 Primary map



X



Y

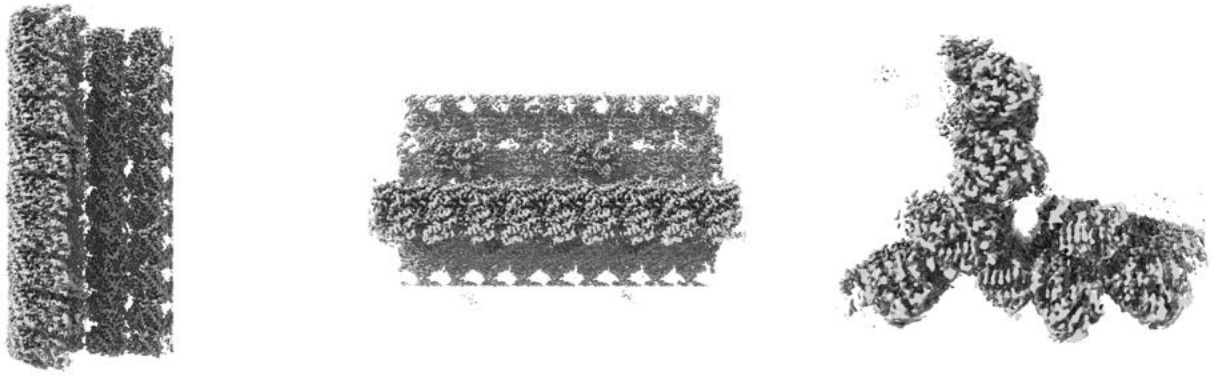


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 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.

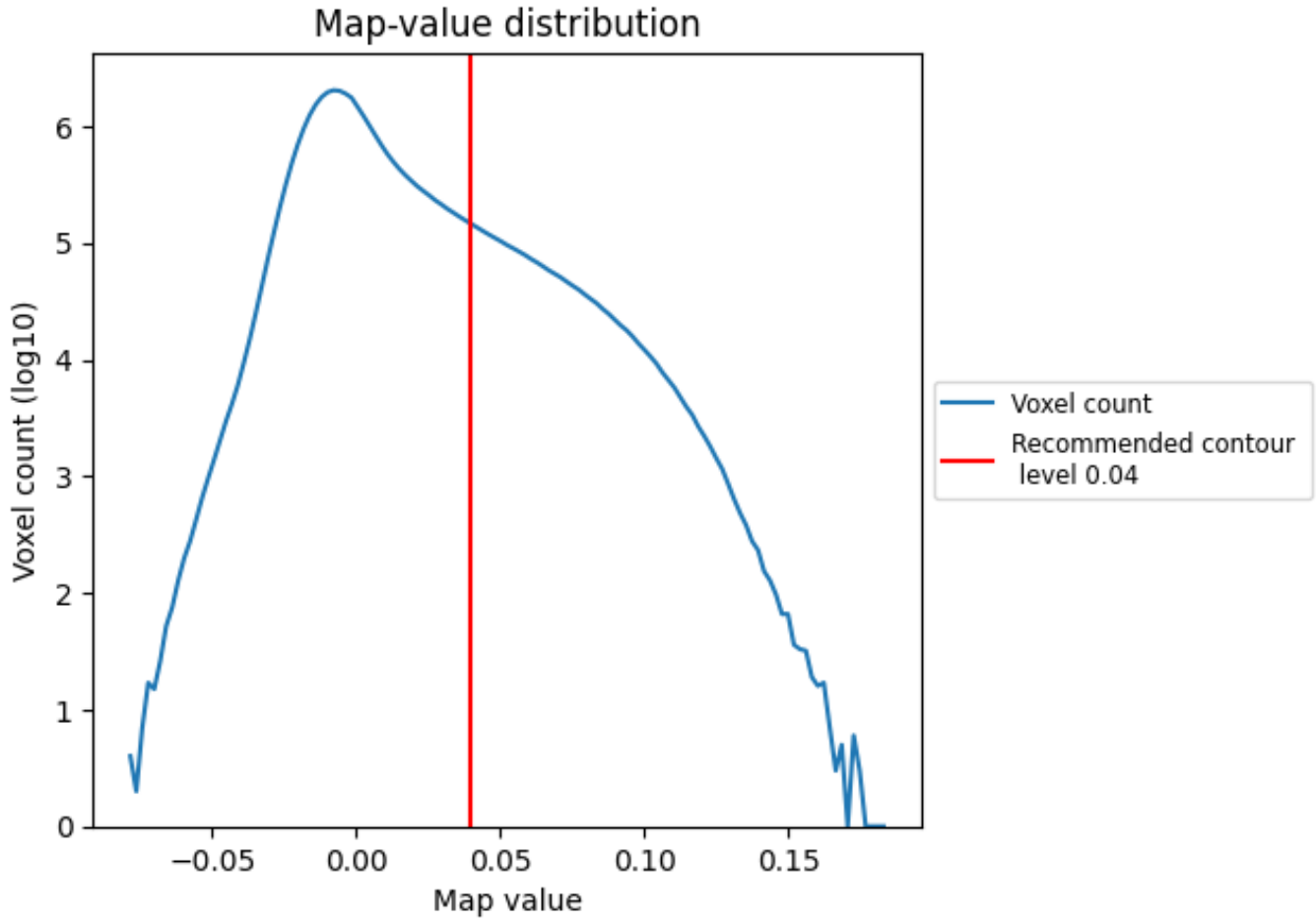
6.6 Mask visualisation (i)

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

7 Map analysis

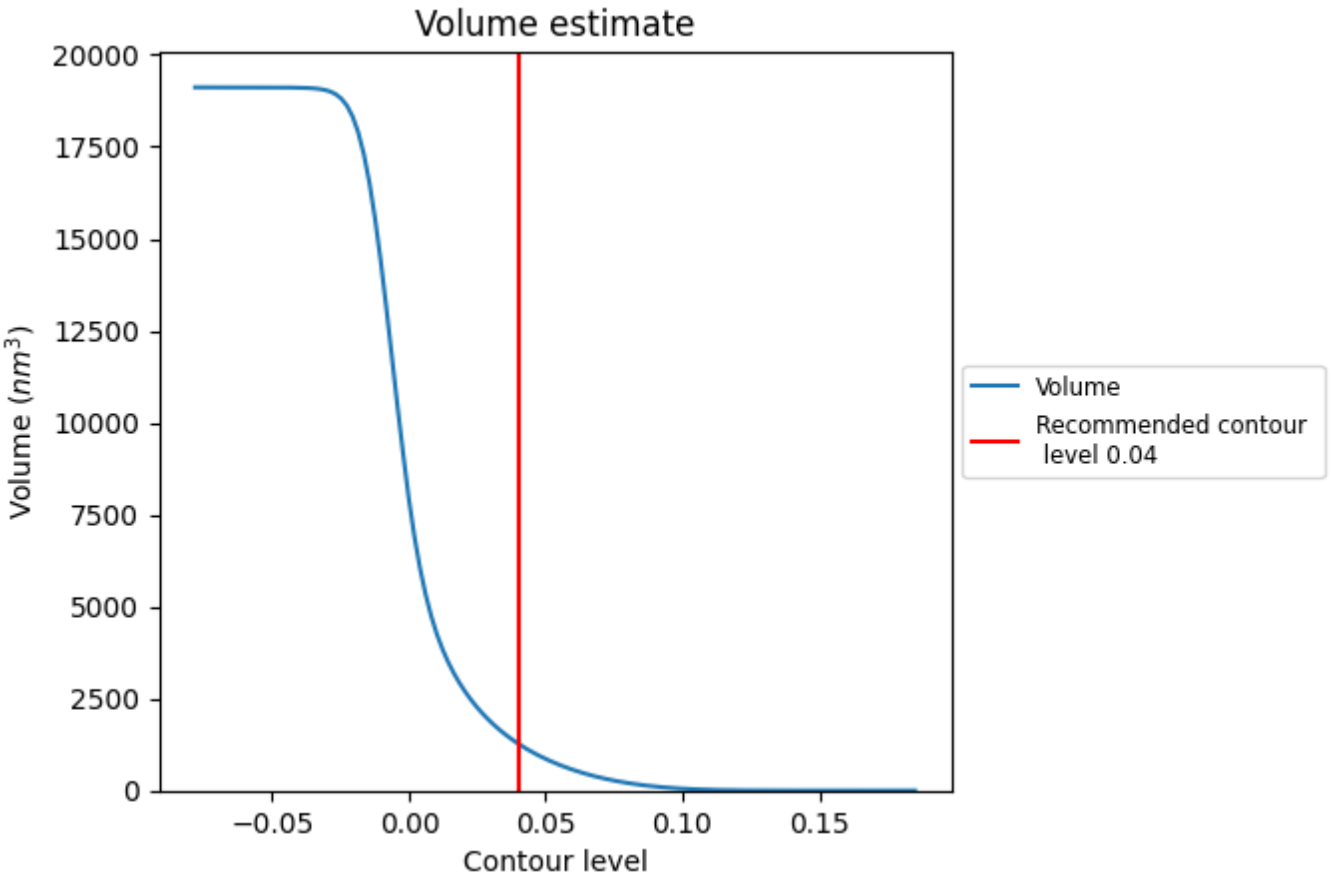
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 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

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

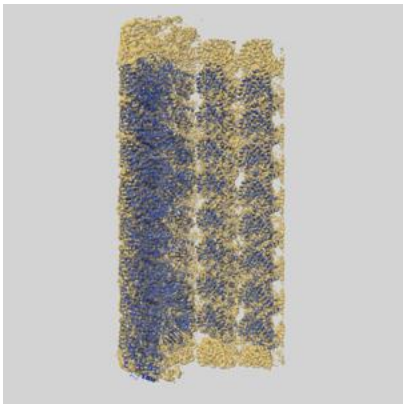
8 Fourier-Shell correlation (i)

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

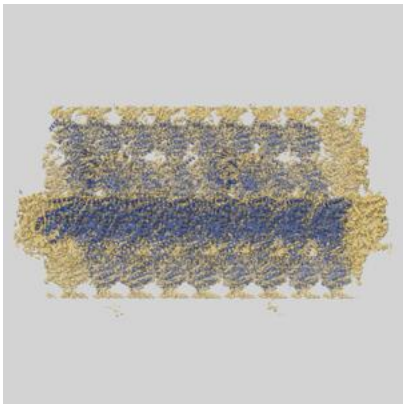
9 Map-model fit

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

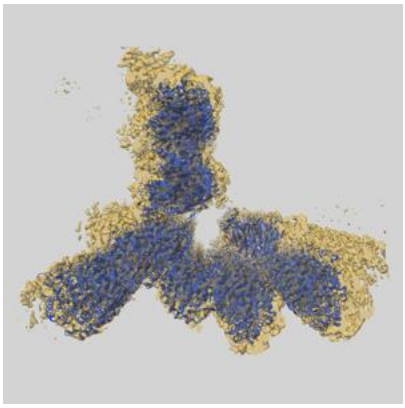
9.1 Map-model overlay



X



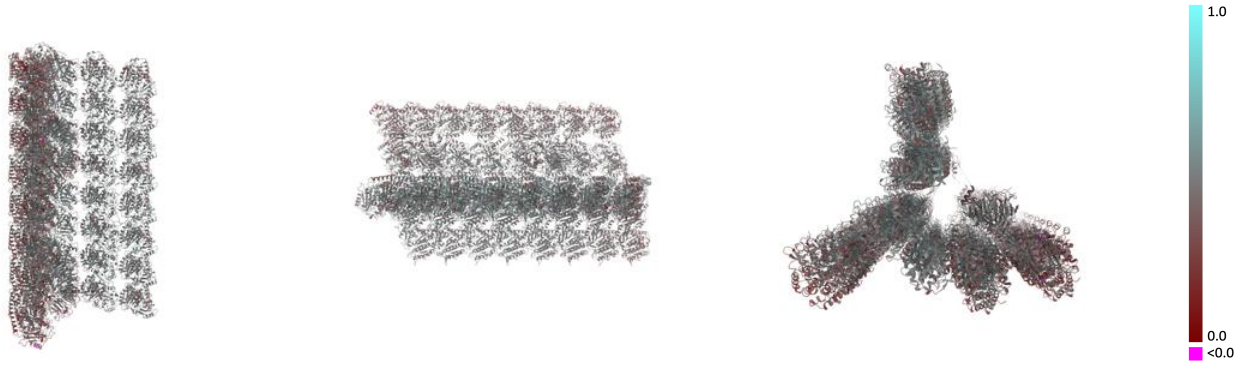
Y



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.

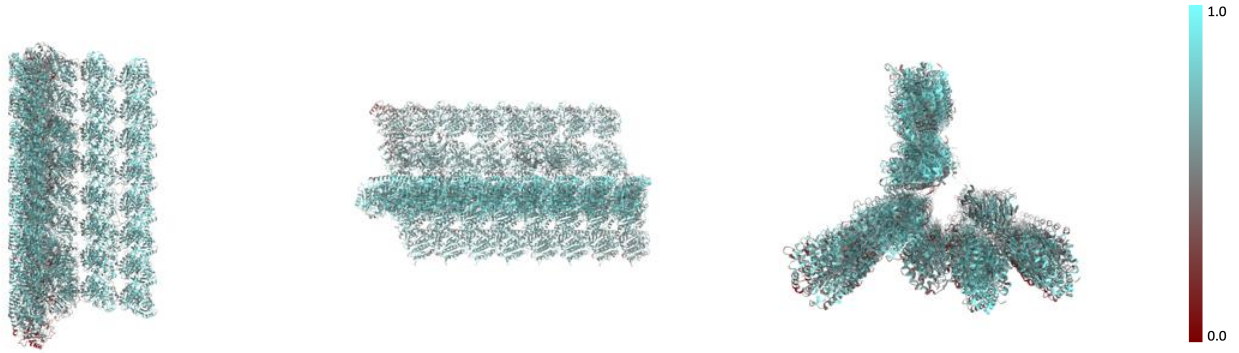
9.2 Q-score mapped to coordinate model



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.

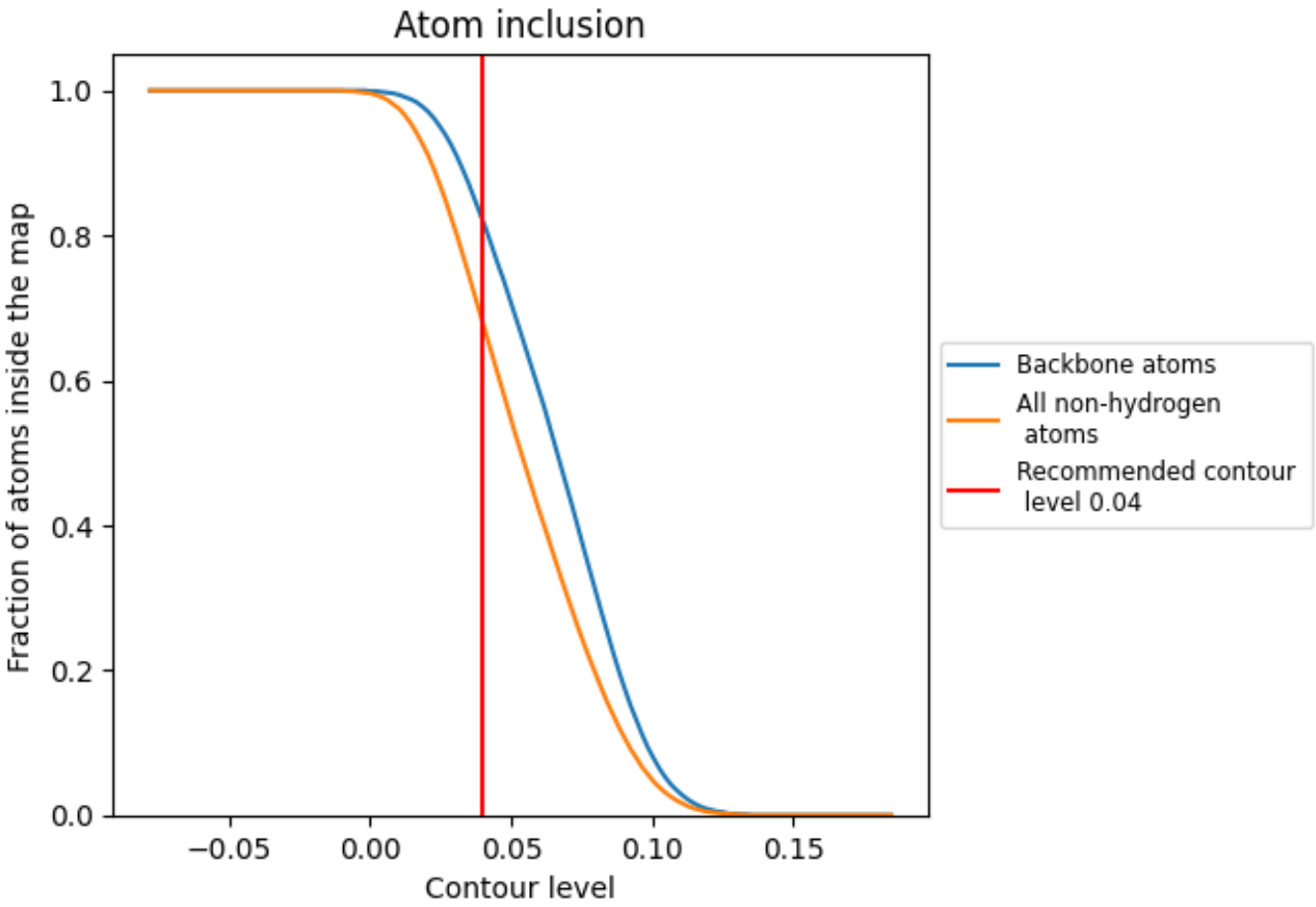
9.3 Atom inclusion mapped to coordinate model



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	0.6790	0.4550
0	0.6970	0.4940
1	0.6240	0.4110
2	0.5900	0.4670
3	0.7390	0.5060
4	0.5820	0.3770
5	0.7120	0.4520
6	0.4700	0.3470
7	0.6560	0.4360
8	0.6680	0.4440
9	0.6880	0.4460
A	0.5730	0.4350
B	0.5520	0.4100
C	0.5970	0.4340
D	0.7480	0.4970
E	0.6890	0.4540
F	0.6900	0.4590
G	0.6780	0.4530
H	0.7070	0.4720
I	0.7300	0.4820
J	0.7080	0.4600
K	0.7460	0.4880
L	0.7400	0.4840
M	0.7440	0.4870
N	0.7010	0.4680
O	0.7470	0.5000
P	0.7170	0.4820
Q	0.6910	0.4490
R	0.7540	0.5030
S	0.7210	0.4680
T	0.7510	0.4900
U	0.7520	0.5030
V	0.5930	0.3600
W	0.5100	0.4170
X	0.7300	0.4640

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Chain	Atom inclusion	Q-score
Y	0.6470	0.4090
Z	0.7060	0.4440
a	0.5720	0.3800
b	0.6460	0.3960
c	0.7220	0.4960
d	0.4850	0.4430
e	0.6250	0.3940
f	0.7330	0.4900
g	0.7430	0.4980
h	0.6420	0.4370
i	0.7330	0.4560
j	0.6930	0.4290
k	0.7460	0.4960
l	0.6890	0.4890
m	0.7310	0.5050
n	0.6760	0.4800
o	0.6850	0.4800
p	0.7260	0.5030
q	0.7180	0.4950
r	0.7080	0.4990
s	0.6130	0.4120
t	0.6470	0.4490
u	0.7340	0.4620
v	0.6420	0.3930
w	0.6990	0.4490
x	0.4650	0.3960
y	0.7270	0.5020
z	0.7100	0.4840