wwPDB EM Validation Summary Report (i)

Mar 20, 2026 – 03:18 AM UTC

PDB ID	:	7L6A / pdb_0000716a
EMDB ID	:	EMD-23200
Title	:	The genome-containing AAV12 capsid
Authors	:	Mietzsch, M.; Agbandje-McKenna, M.
Deposited on	:	2020-12-23
Resolution	:	2.67 Å(reported)

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

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

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

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

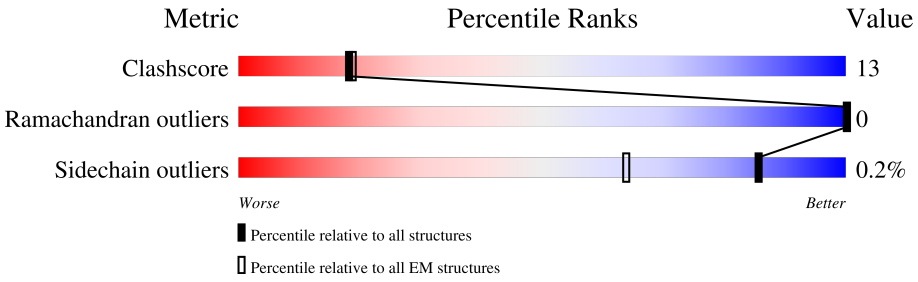
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	NOT EXECUTED
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.67 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	1	521	72% 28%
1	2	521	71% 29%
1	3	521	72% 28%
1	4	521	72% 28%
1	5	521	72% 27%
1	6	521	71% 28%
1	7	521	72% 28%
1	8	521	72% 27%
1	A	521	72% 28%

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Mol	Chain	Length	Quality of chain
1	B	521	72% 28%
1	C	521	71% 29%
1	D	521	72% 28%
1	E	521	73% 27%
1	F	521	72% 28%
1	G	521	72% 28%
1	H	521	72% 28%
1	I	521	72% 28%
1	J	521	71% 29%
1	K	521	72% 28%
1	L	521	72% 28%
1	M	521	72% 28%
1	N	521	71% 28%
1	O	521	73% 27%
1	P	521	72% 28%
1	Q	521	72% 28%
1	R	521	72% 28%
1	S	521	72% 27%
1	T	521	72% 27%
1	U	521	72% 28%
1	V	521	72% 28%
1	W	521	71% 29%
1	X	521	72% 28%
1	Y	521	72% 27%
1	Z	521	72% 28%

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Mol	Chain	Length	Quality of chain
1	a	521	71% 29%
1	b	521	71% 28%
1	c	521	72% 28%
1	d	521	72% 28%
1	e	521	72% 28%
1	f	521	72% 28%
1	g	521	72% 28%
1	h	521	72% 28%
1	i	521	71% 28%
1	j	521	72% 28%
1	k	521	71% 28%
1	l	521	72% 28%
1	m	521	72% 27%
1	n	521	72% 28%
1	o	521	72% 28%
1	p	521	71% 28%
1	q	521	72% 28%
1	r	521	73% 27%
1	s	521	72% 28%
1	t	521	72% 28%
1	u	521	72% 28%
1	v	521	71% 28%
1	w	521	73% 27%
1	x	521	72% 28%
1	y	521	72% 28%

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Mol	Chain	Length	Quality of chain
1	z	521	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 250440 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	B	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	C	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	D	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	E	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	F	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	G	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	H	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	I	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	J	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	K	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	L	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	M	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	N	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	O	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	P	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	Q	521	Total 4152	C 2616	N 726	O 791	S 19	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	S	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	T	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	U	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	V	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	W	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	X	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	Y	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	Z	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	a	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	b	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	c	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	d	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	e	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	f	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	g	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	h	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	i	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	j	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	k	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		
1	l	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	n	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	o	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	p	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	q	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	r	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	s	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	t	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	u	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	v	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	w	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	x	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	y	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	z	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	1	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	2	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	3	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	4	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	5	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	6	521	Total 4152	C 2616	N 726	O 791	S 19	2	0
1	7	521	Total 4152	C 2616	N 726	O 791	S 19	2	0

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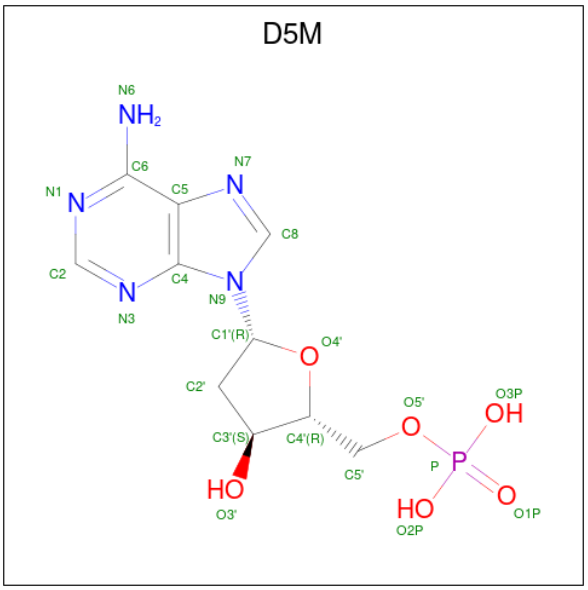
Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	521	Total	C	N	O	S	2	0
			4152	2616	726	791	19		

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (CCD ID: D5M) (formula: $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	B	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	C	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	D	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	E	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	F	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	G	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	H	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	I	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	J	1	Total	C	N	O	P	0
			22	10	5	6	1	

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Mol	Chain	Residues	Atoms					AltConf
2	K	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	L	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	M	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	N	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	O	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	P	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	Q	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	R	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	S	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	T	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	U	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	V	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	W	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	X	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	Y	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	Z	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	a	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	b	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	c	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	d	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	e	1	Total	C	N	O	P	0
			22	10	5	6	1	

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Mol	Chain	Residues	Atoms					AltConf
2	f	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	g	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	h	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	i	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	j	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	k	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	l	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	m	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	n	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	o	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	p	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	q	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	r	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	s	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	t	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	u	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	v	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	w	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	x	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	y	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	z	1	Total	C	N	O	P	0
			22	10	5	6	1	

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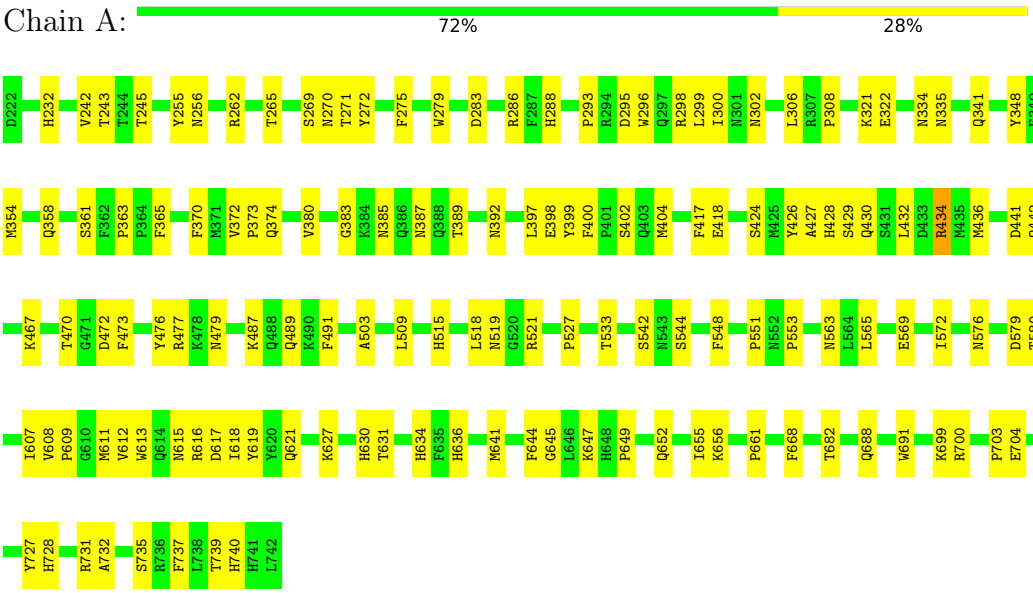
Mol	Chain	Residues	Atoms					AltConf
2	1	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	2	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	3	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	4	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	5	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	6	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	7	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	8	1	Total	C	N	O	P	0
			22	10	5	6	1	

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

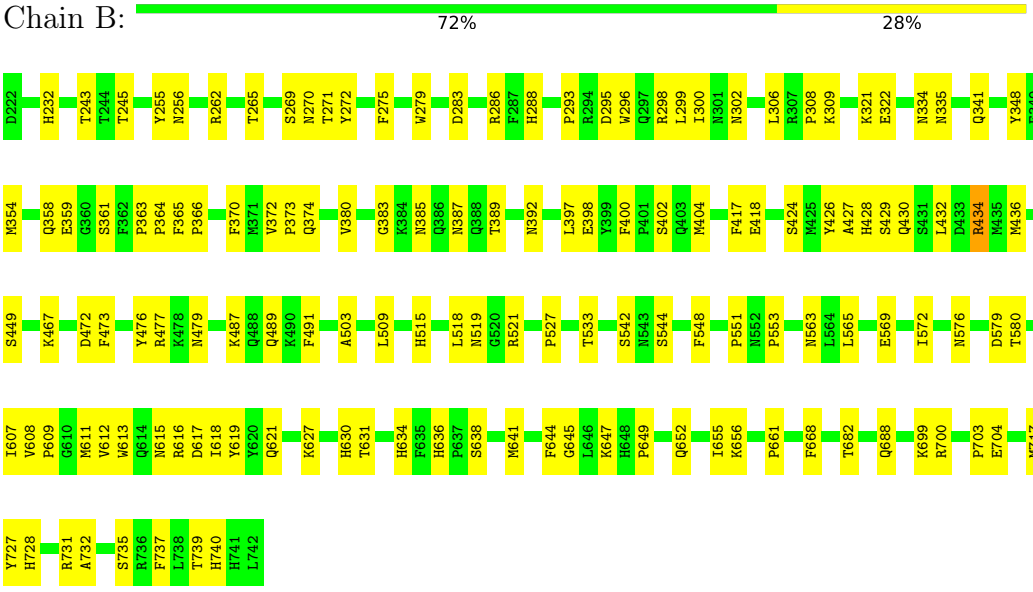
- Molecule 1: VP1

Chain A:



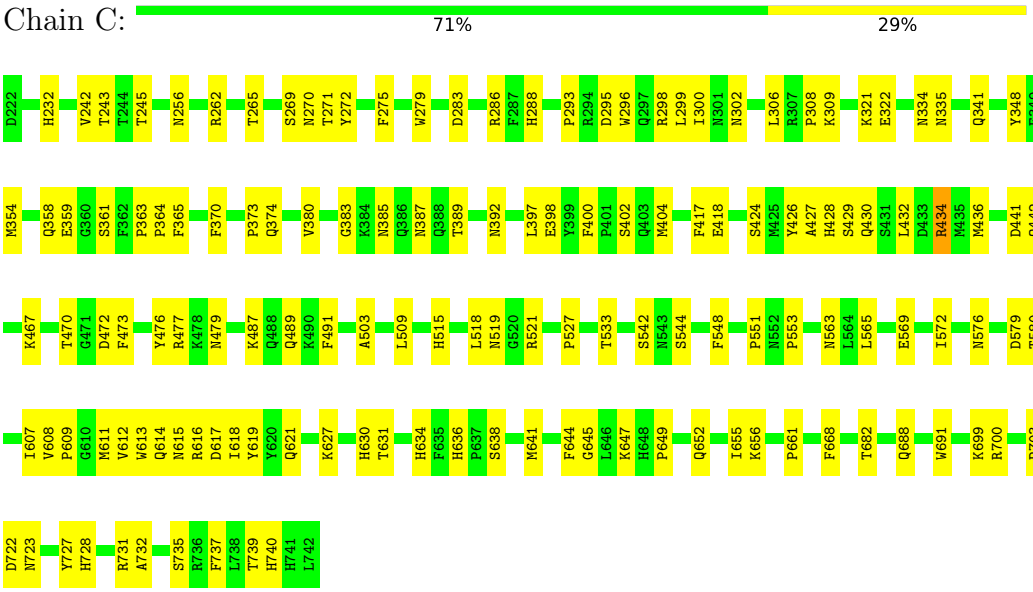
- Molecule 1: VP1

Chain B:



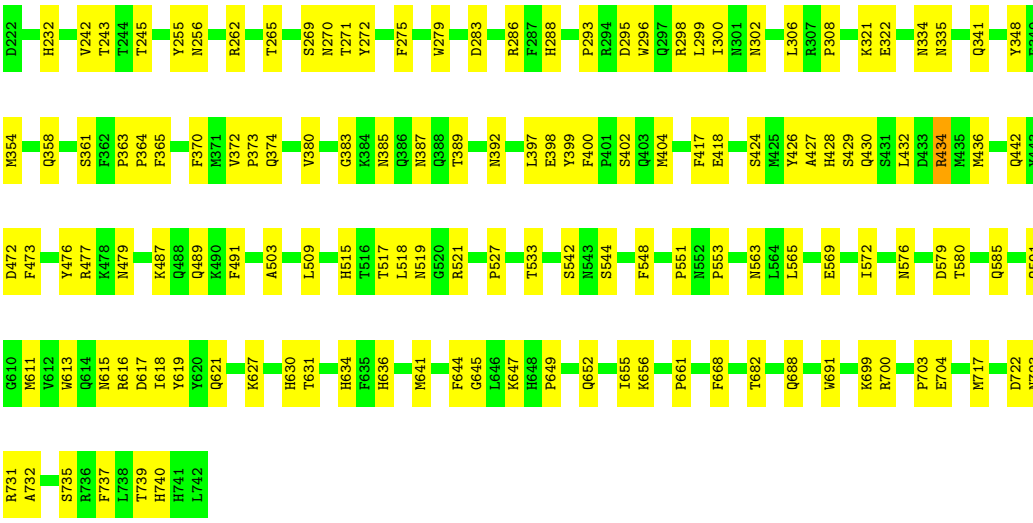
- Molecule 1: VP1

Chain C:



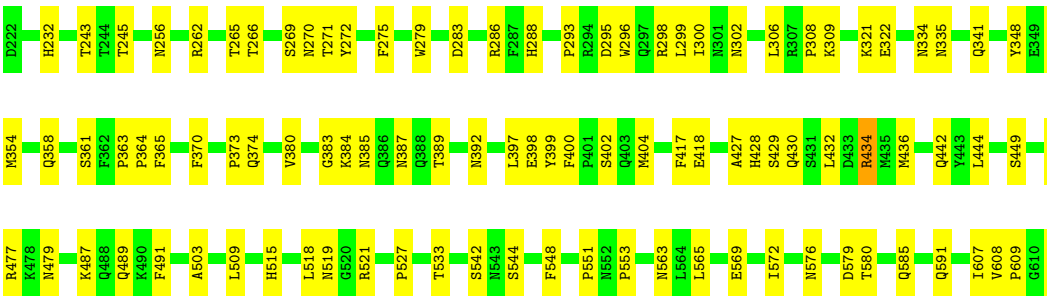
• Molecule 1: VP1

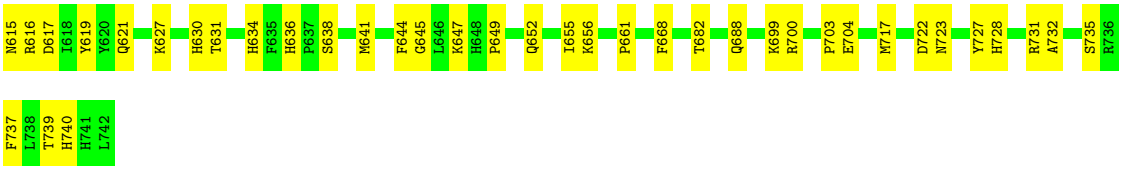
Chain D:



• Molecule 1: VP1

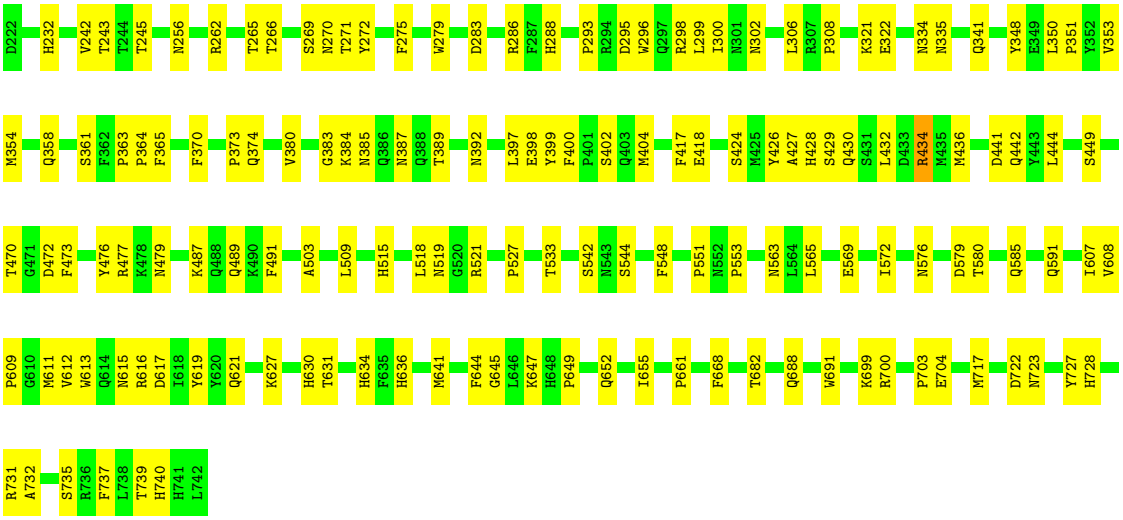
Chain E:





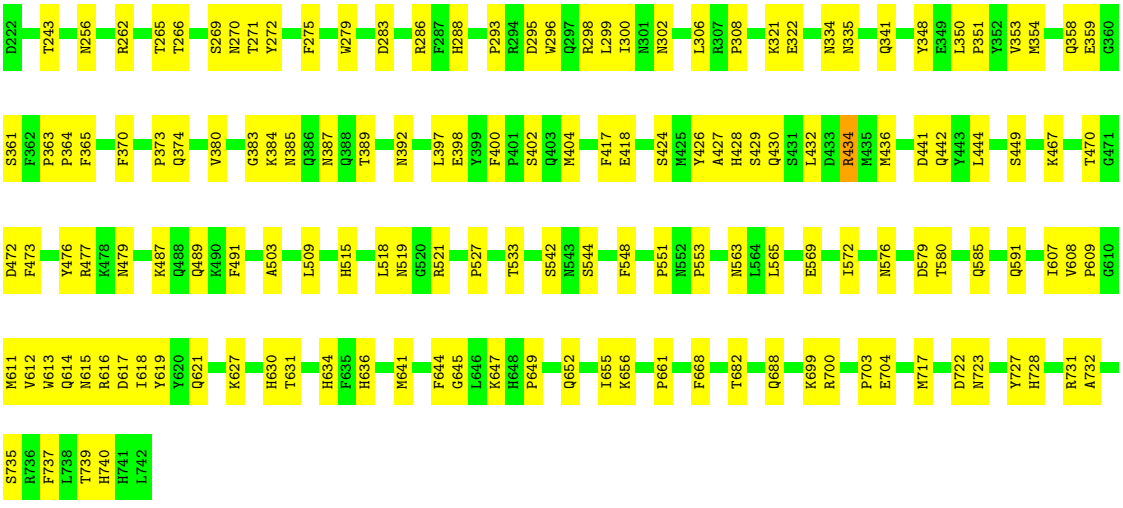
• Molecule 1: VP1

Chain F:



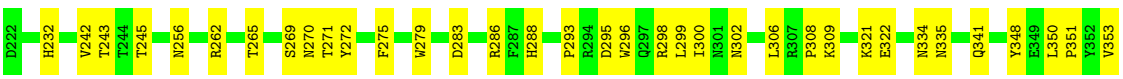
• Molecule 1: VP1

Chain G:



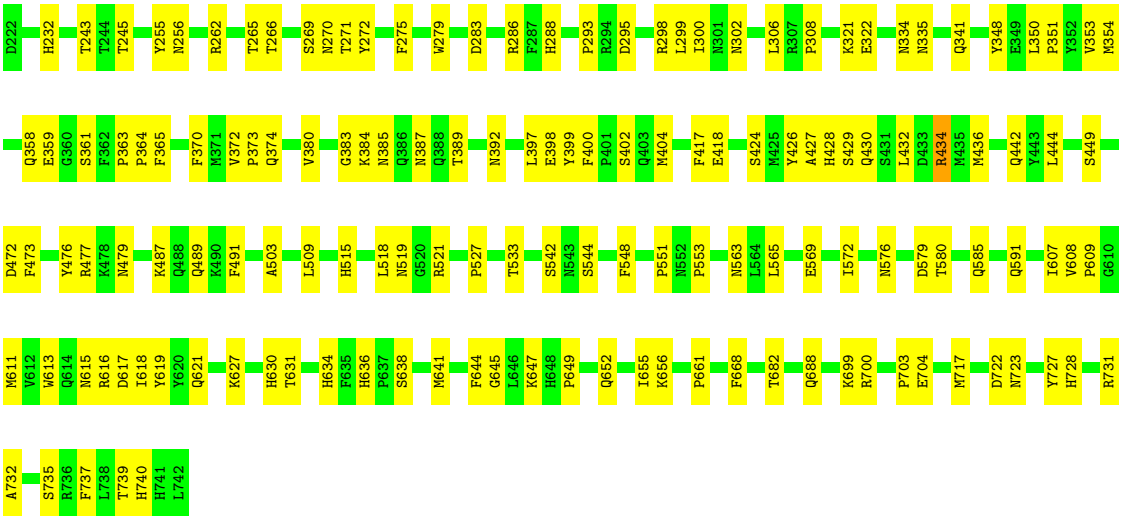
• Molecule 1: VP1

Chain H:



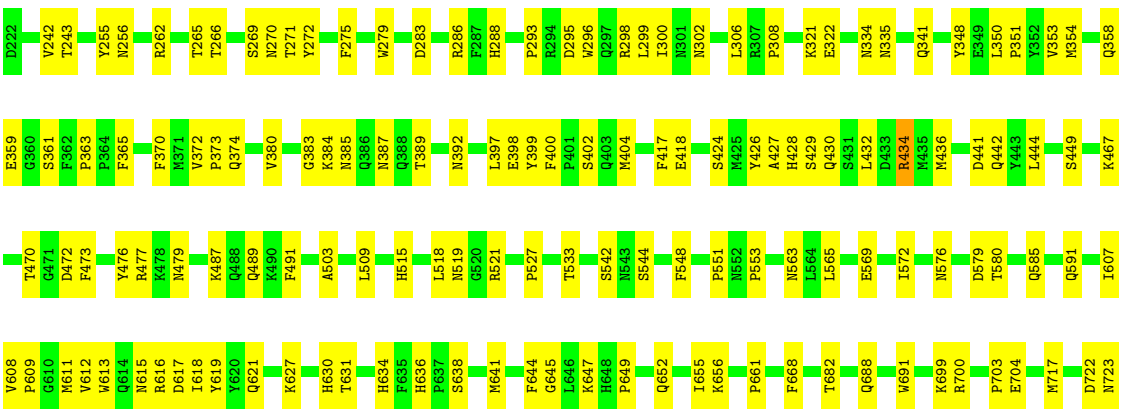
• Molecule 1: VP1

Chain I:



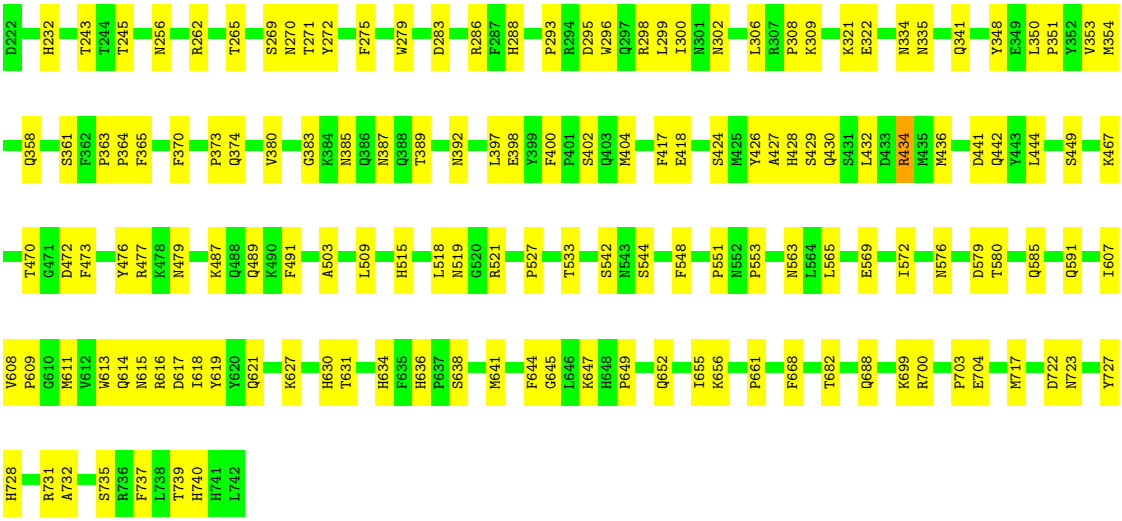
• Molecule 1: VP1

Chain J:



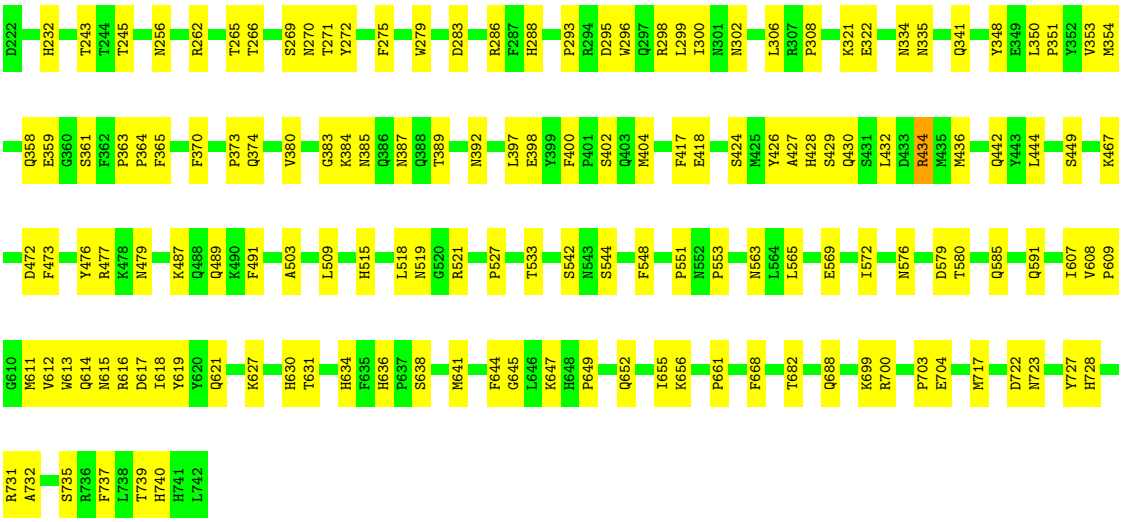
• Molecule 1: VP1

Chain K:



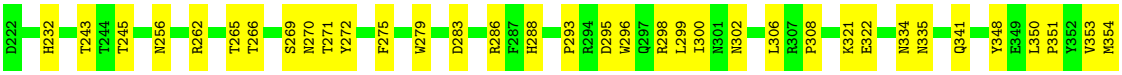
• Molecule 1: VP1

Chain L:



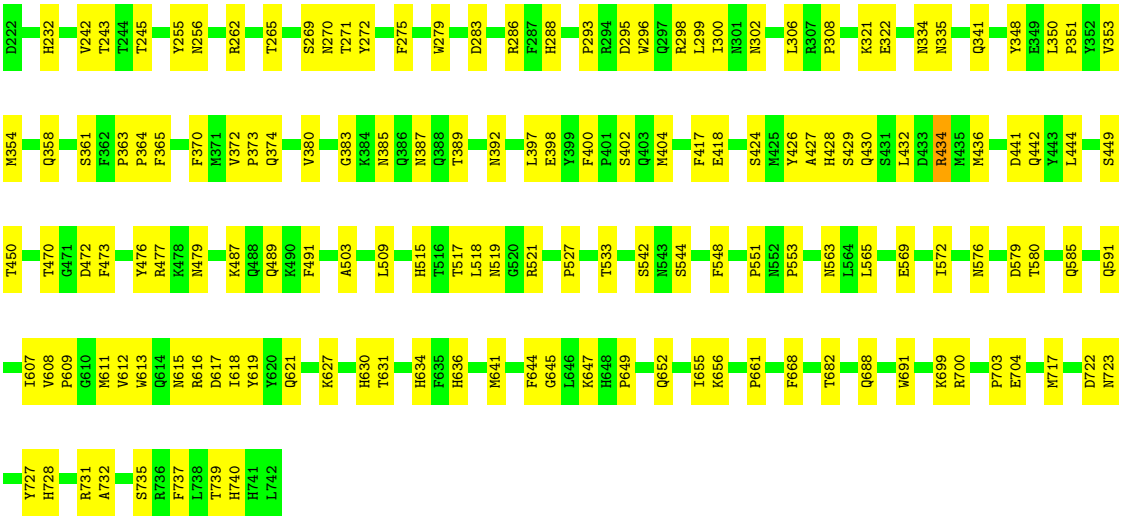
• Molecule 1: VP1

Chain M:



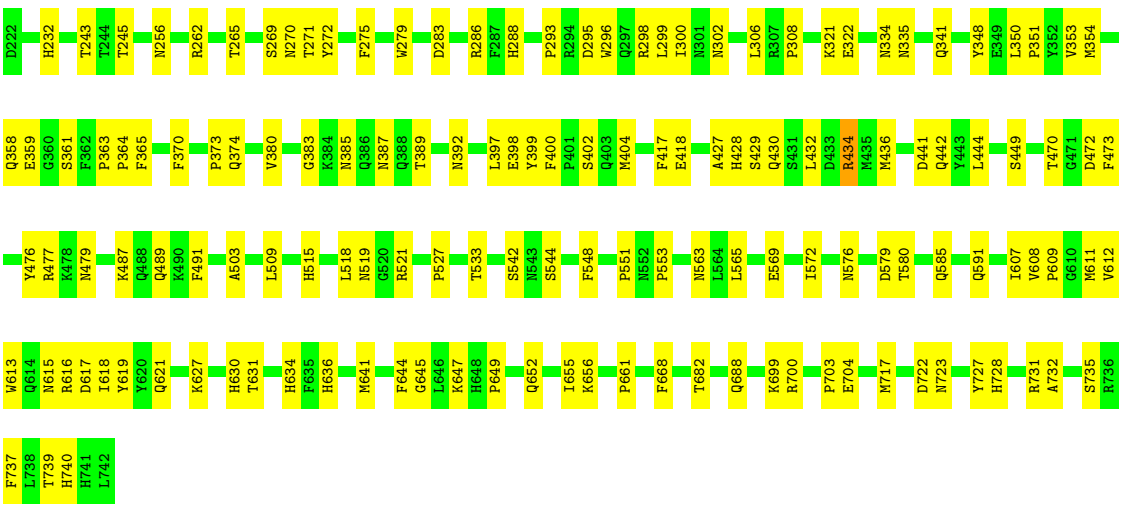
• Molecule 1: VP1

Chain N:



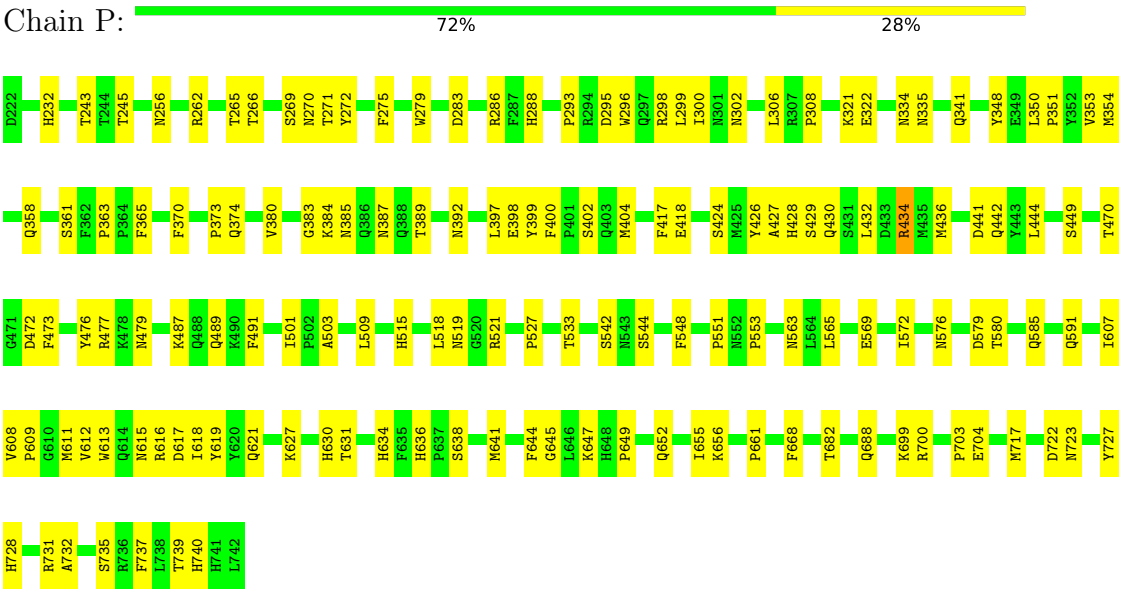
• Molecule 1: VP1

Chain O:



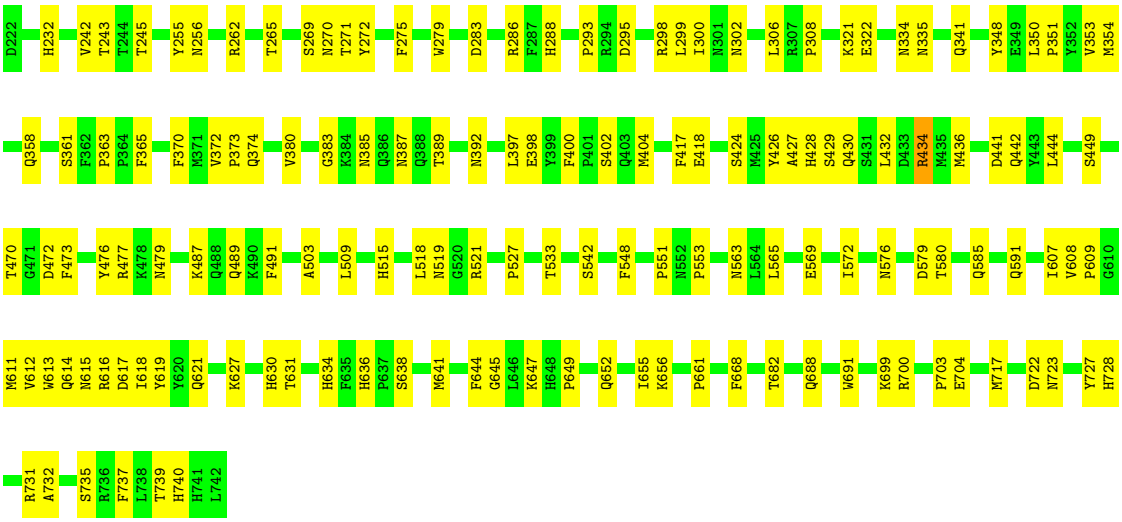
• Molecule 1: VP1

Chain P:



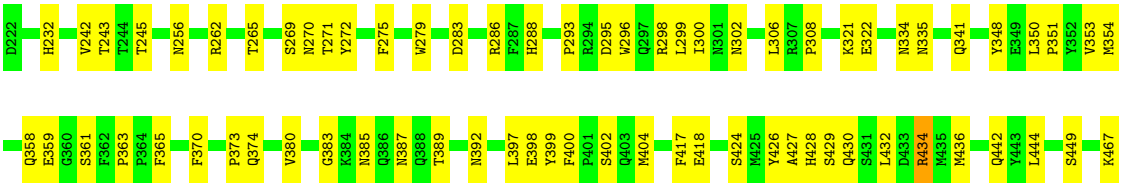
• Molecule 1: VP1

Chain Q:



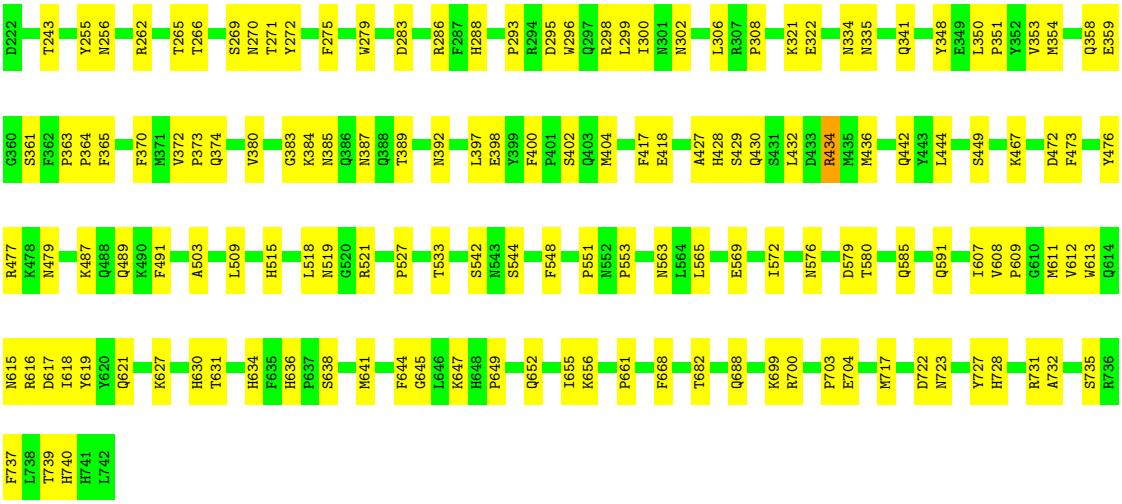
• Molecule 1: VP1

Chain R:



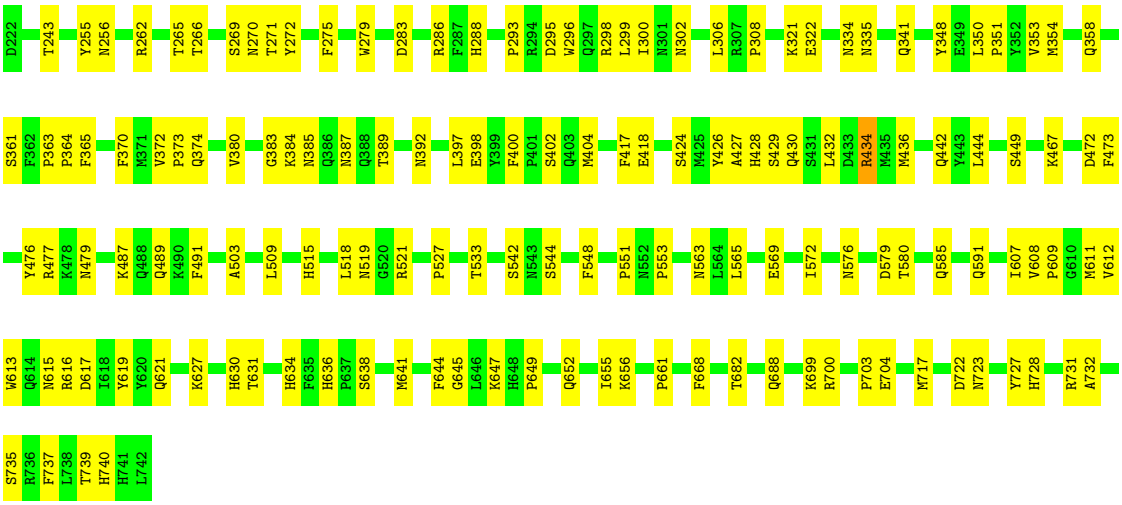
• Molecule 1: VP1

Chain S:



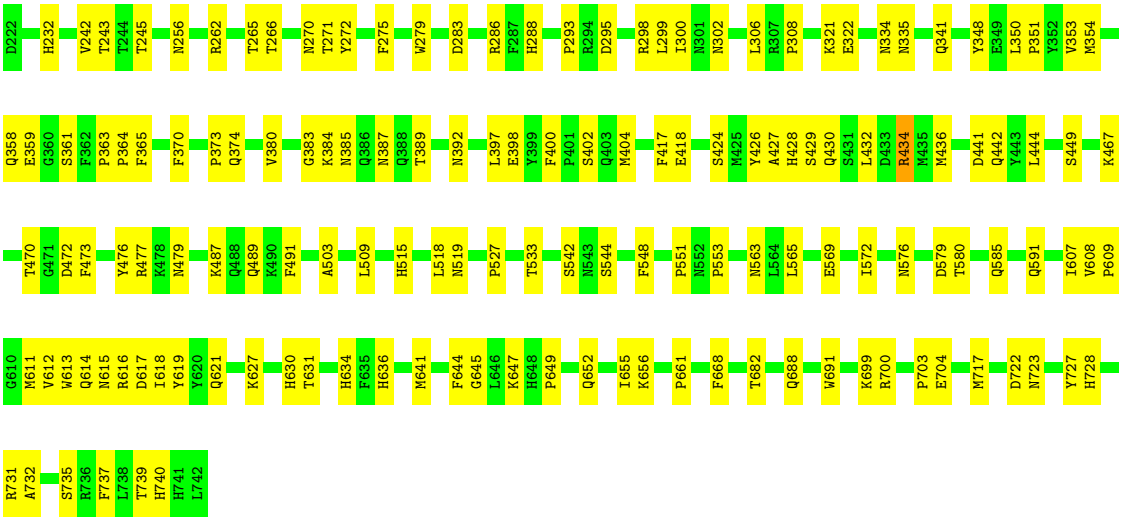
• Molecule 1: VP1

Chain T:



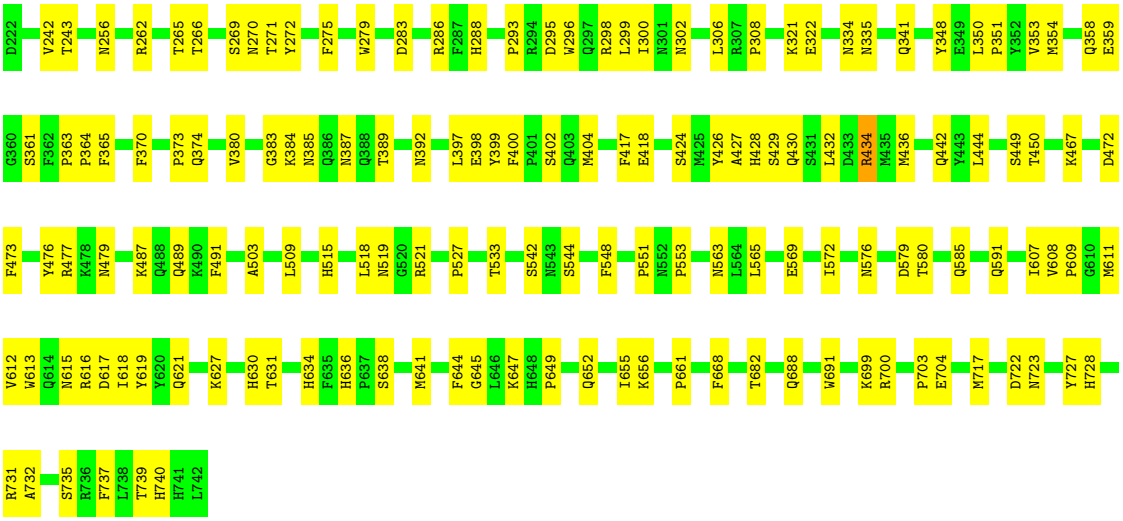
• Molecule 1: VP1

Chain U:



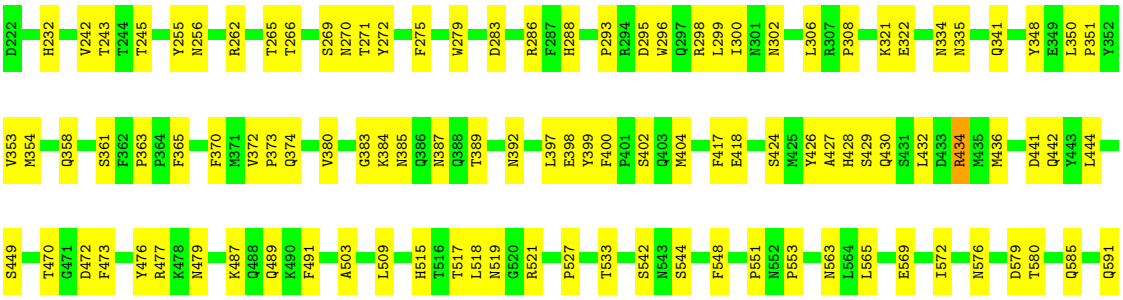
- Molecule 1: VP1

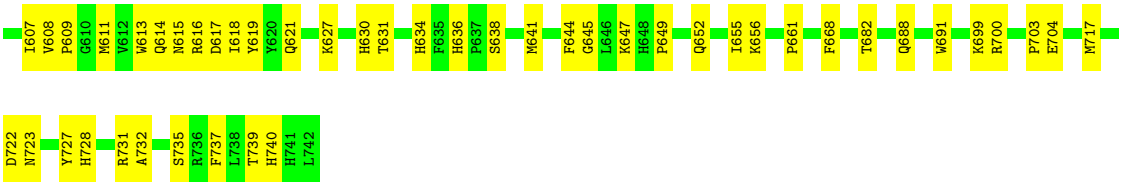
Chain V:



- Molecule 1: VP1

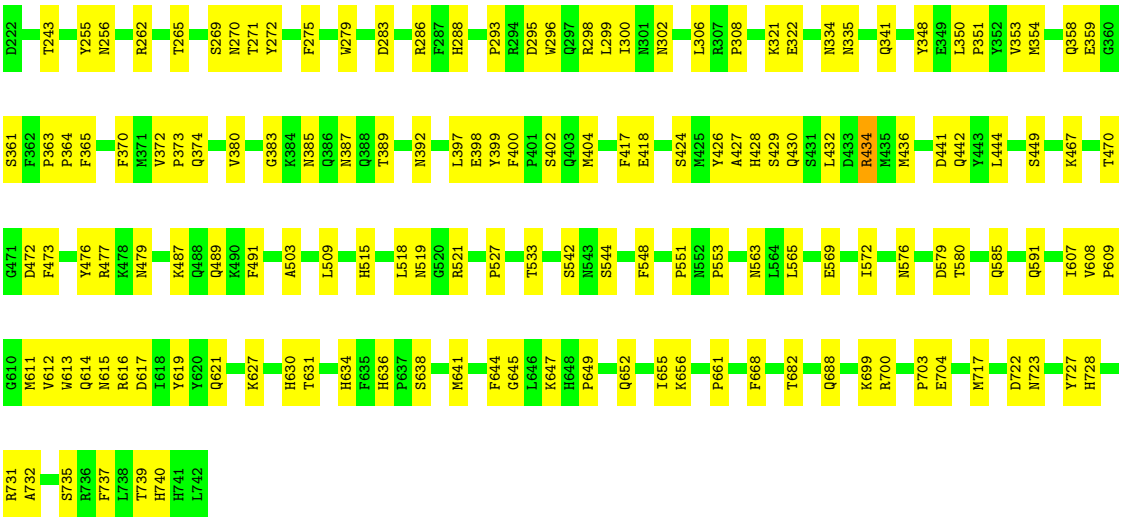
Chain W:





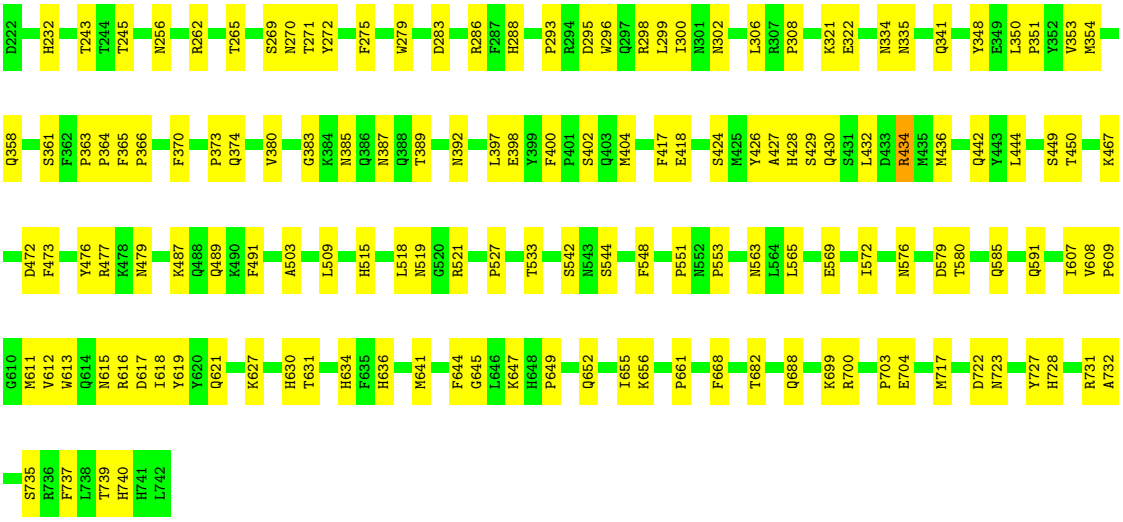
• Molecule 1: VP1

Chain X:



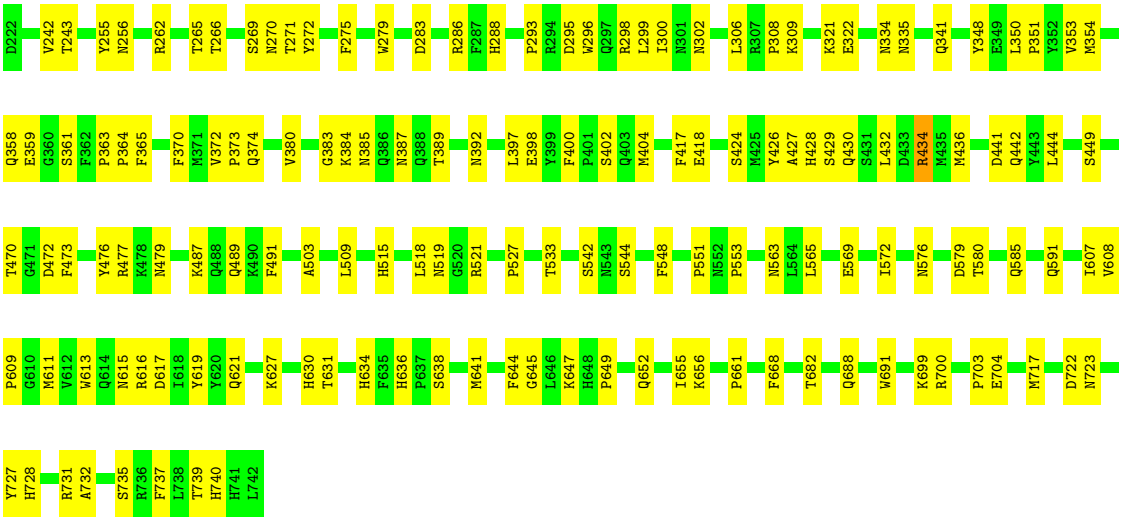
• Molecule 1: VP1

Chain Y:



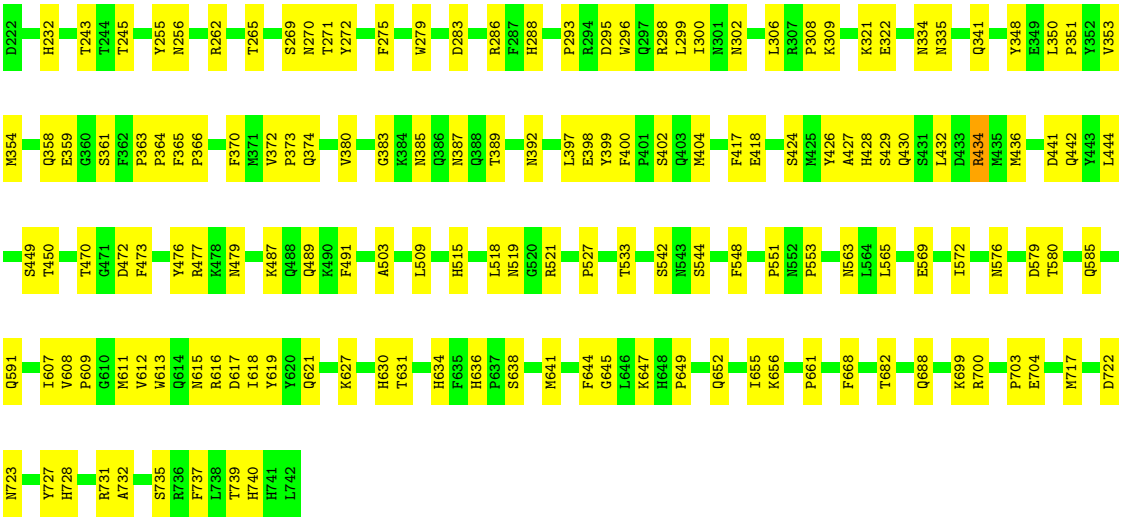
• Molecule 1: VP1

Chain Z:



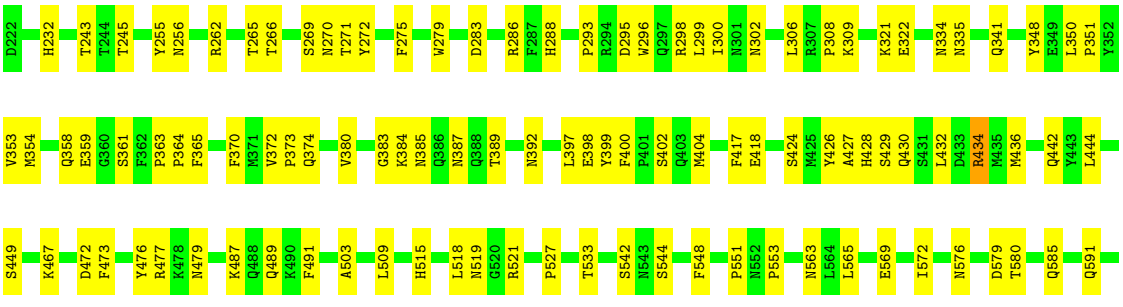
• Molecule 1: VP1

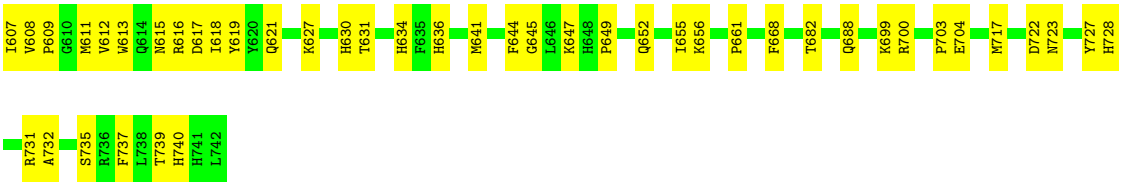
Chain a:



• Molecule 1: VP1

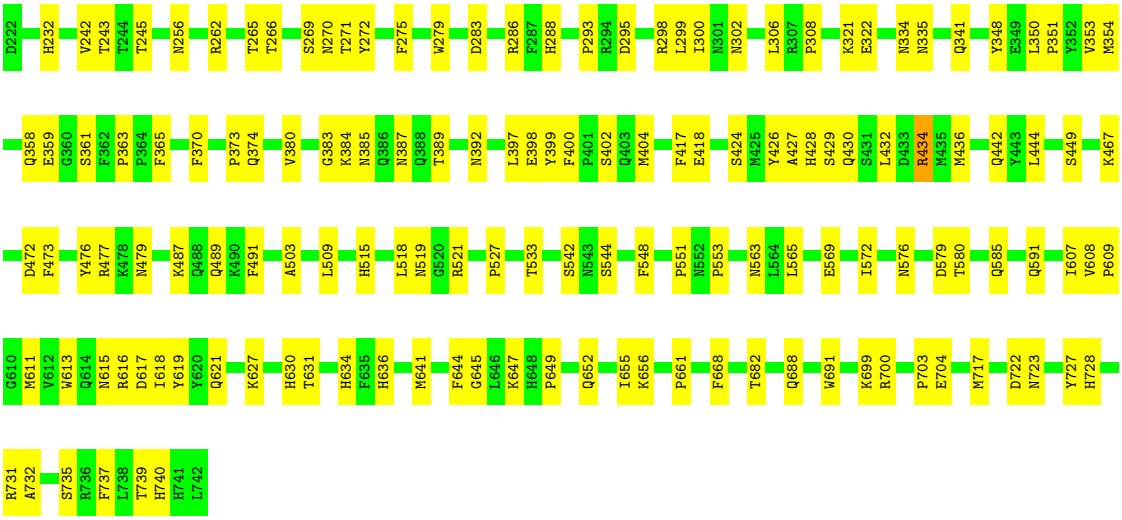
Chain b:





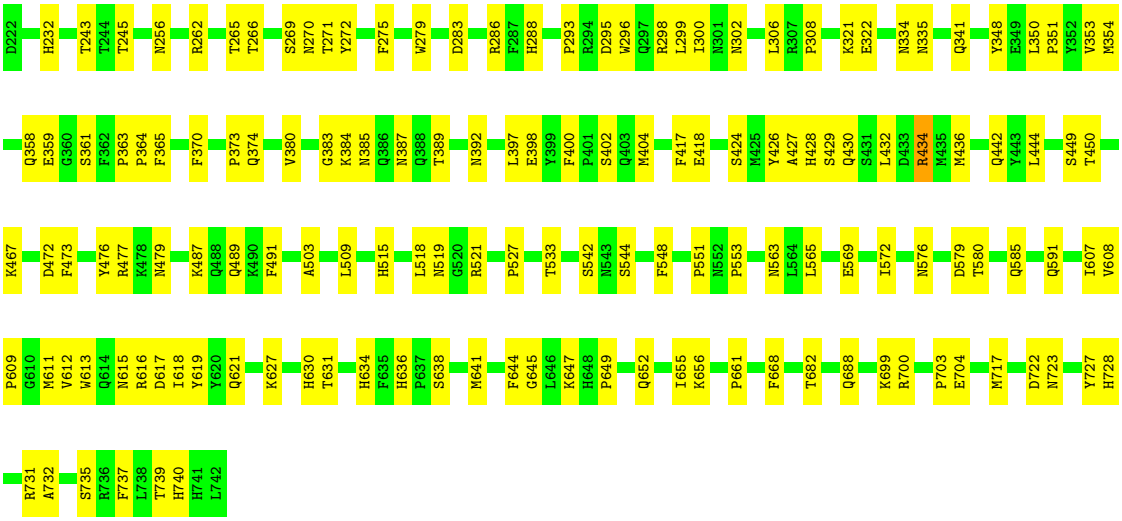
• Molecule 1: VP1

Chain c:



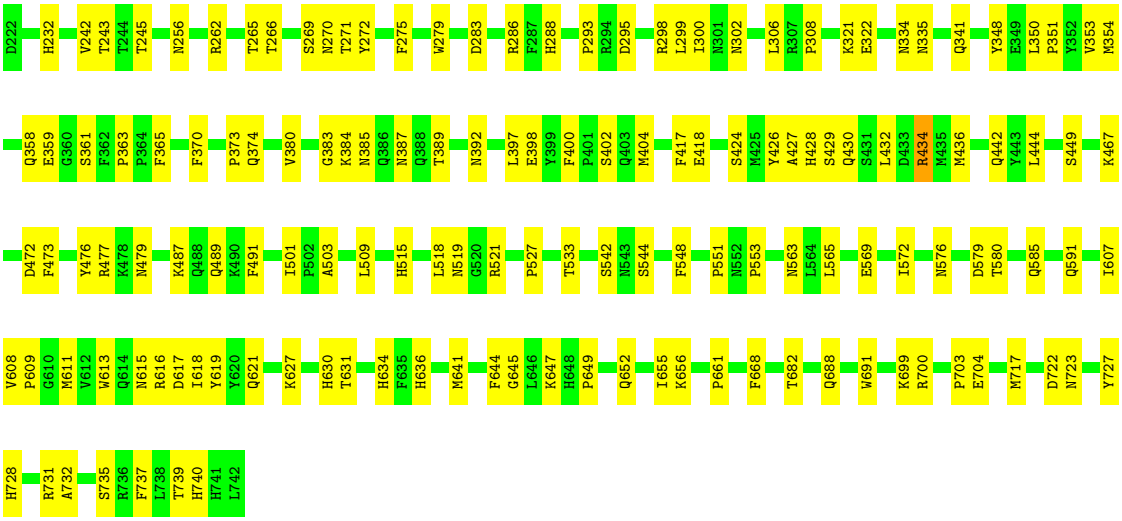
• Molecule 1: VP1

Chain d:



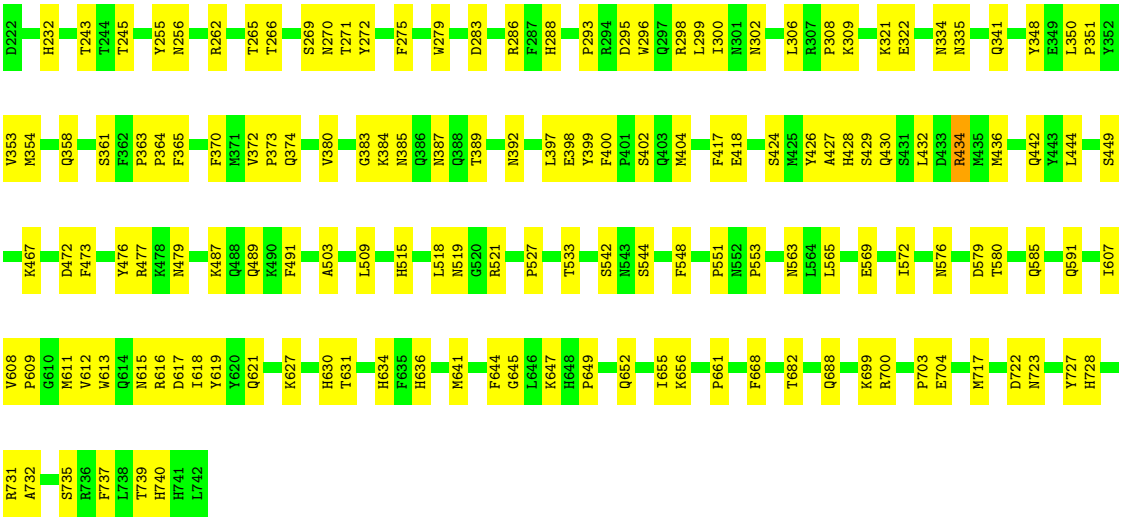
• Molecule 1: VP1

Chain e:



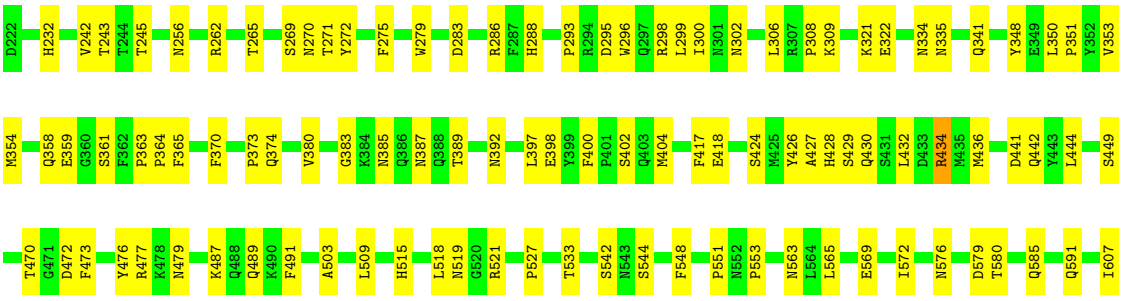
• Molecule 1: VP1

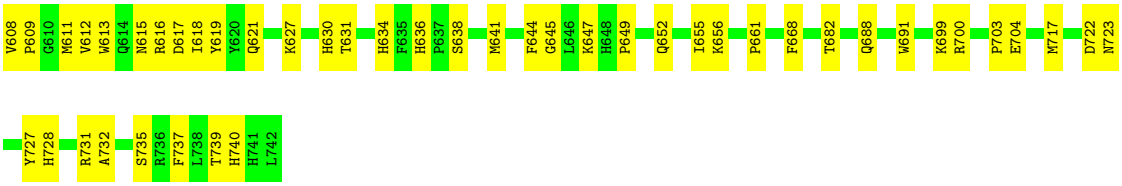
Chain f:



• Molecule 1: VP1

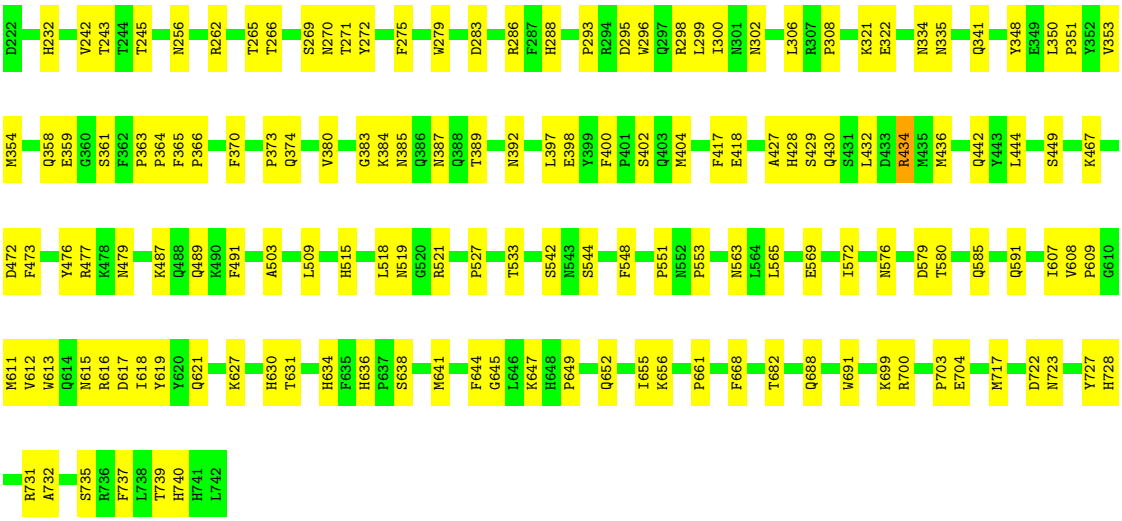
Chain g:





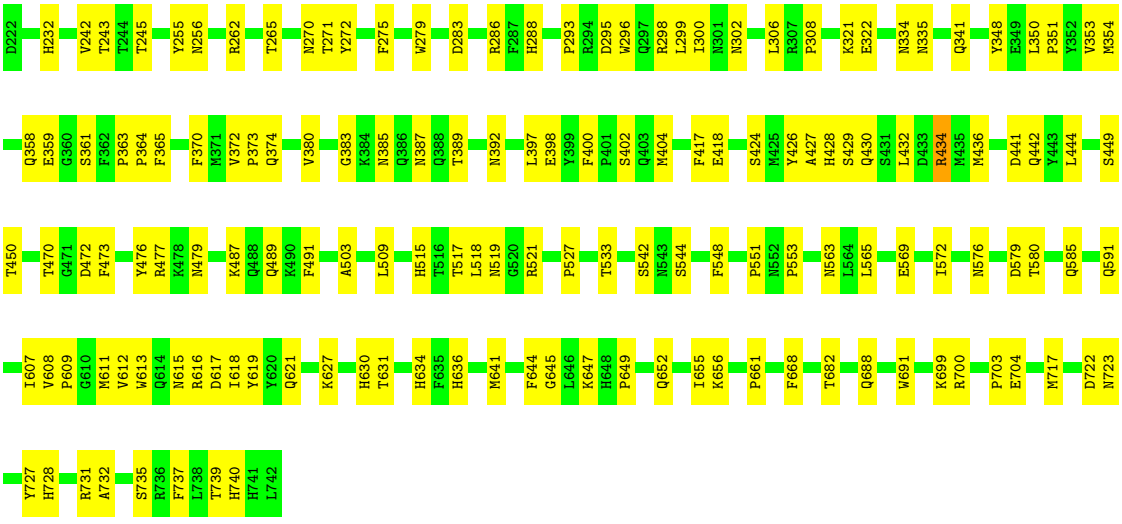
• Molecule 1: VP1

Chain h:



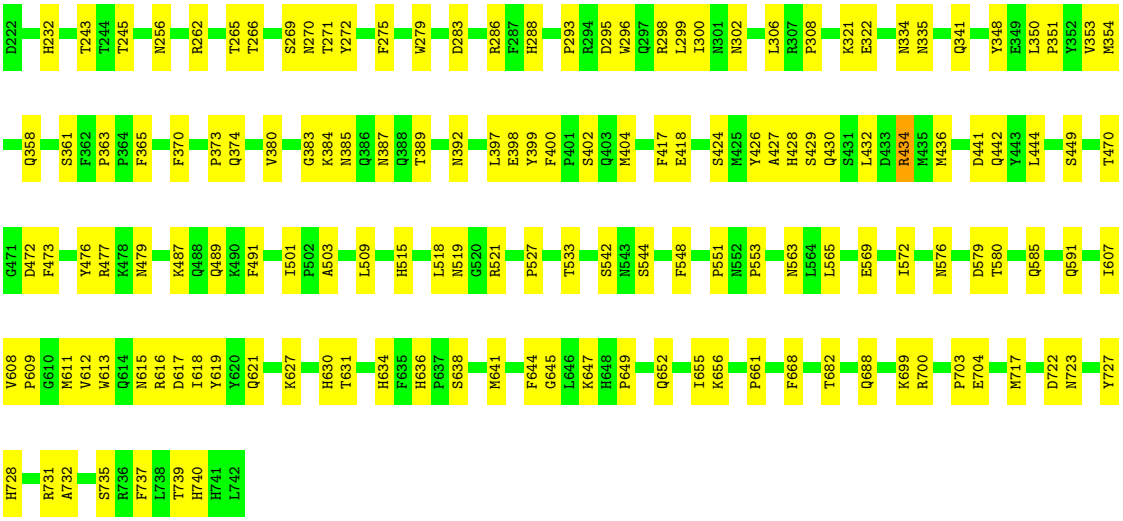
• Molecule 1: VP1

Chain i:



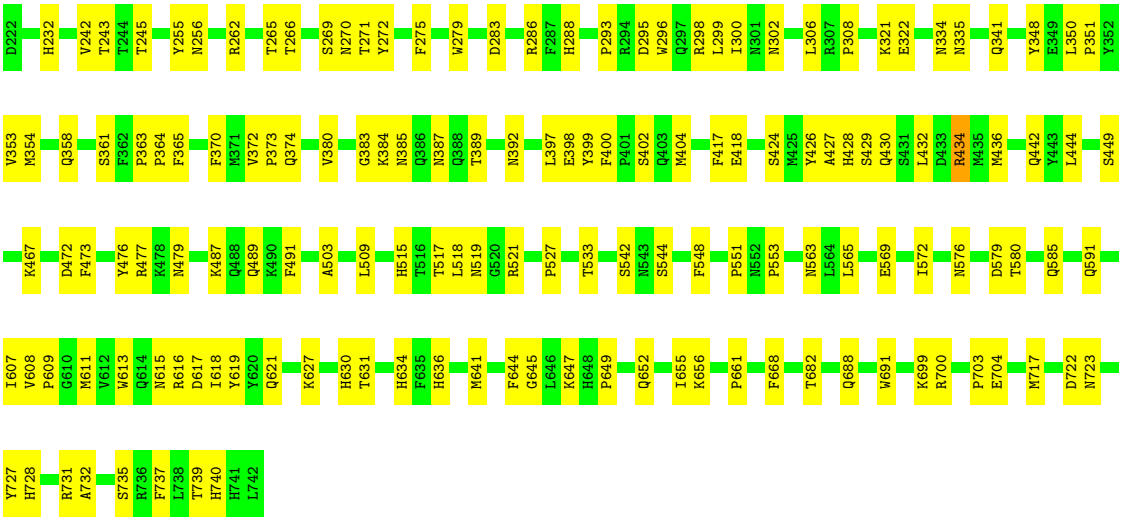
• Molecule 1: VP1

Chain j:



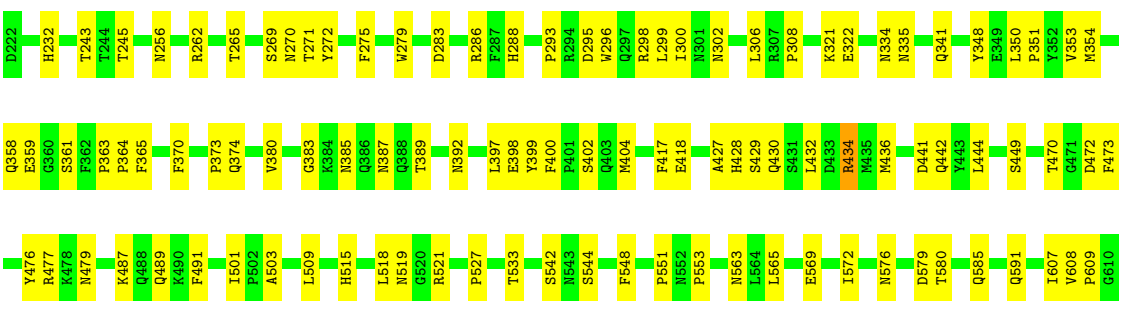
• Molecule 1: VP1

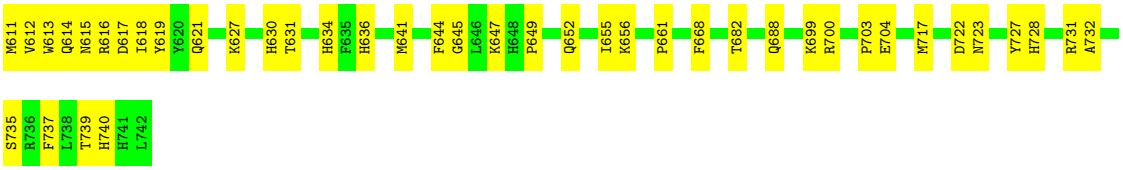
Chain k:



• Molecule 1: VP1

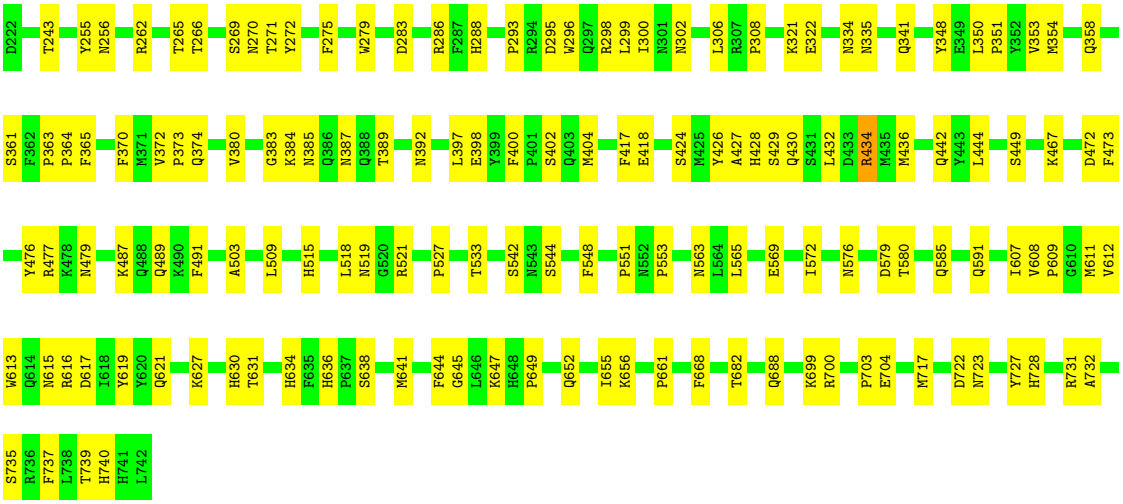
Chain l:





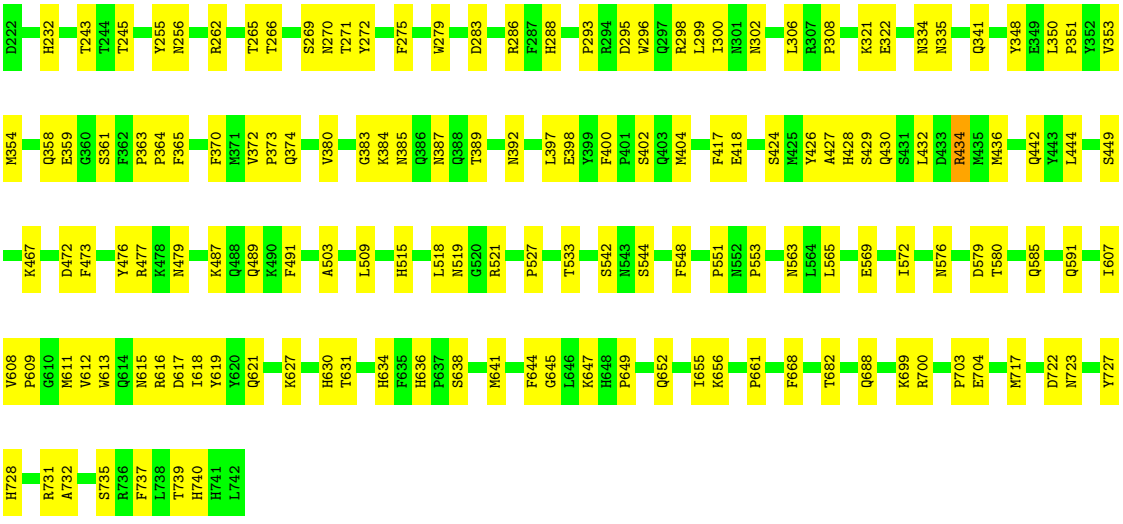
• Molecule 1: VP1

Chain m:



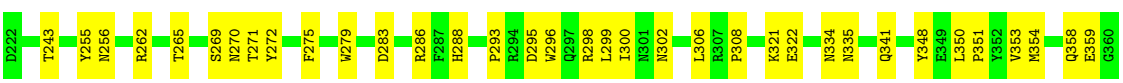
• Molecule 1: VP1

Chain n:



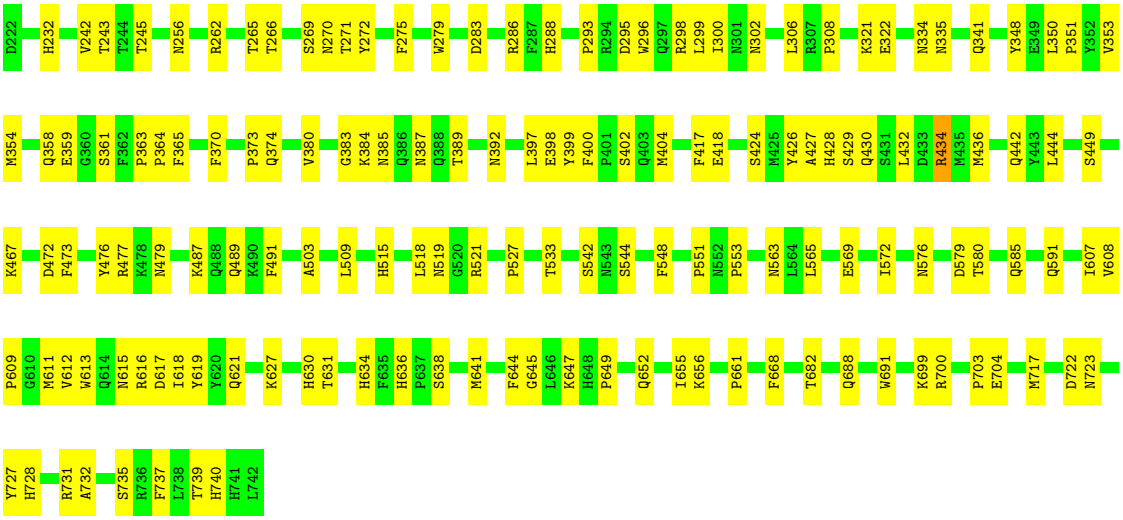
• Molecule 1: VP1

Chain o:



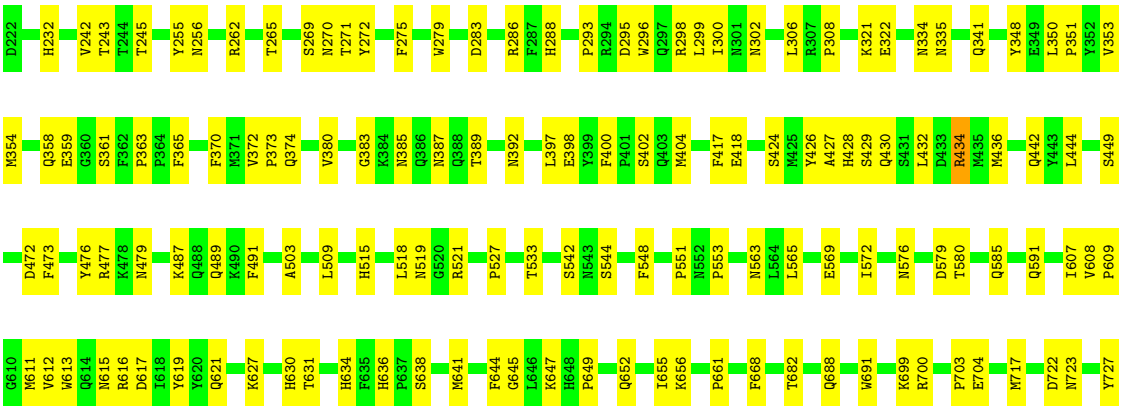
• Molecule 1: VP1

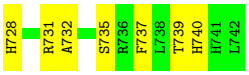
Chain p:



• Molecule 1: VP1

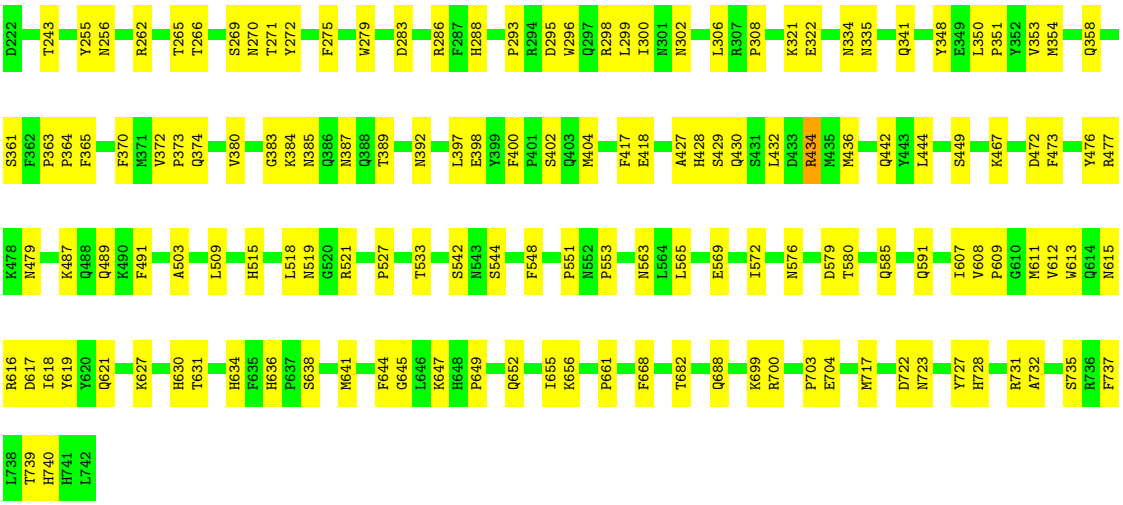
Chain q:





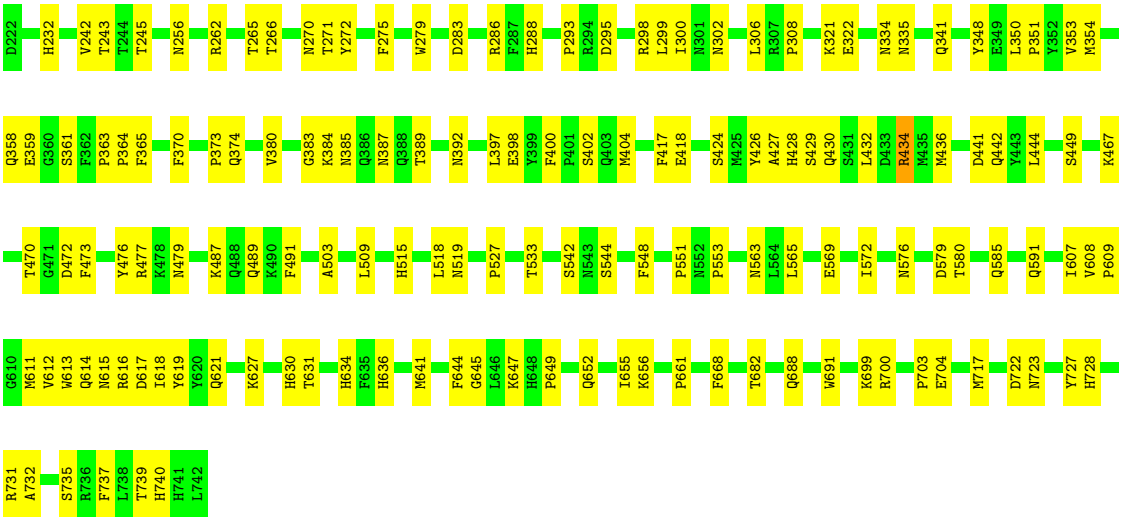
• Molecule 1: VP1

Chain r:



• Molecule 1: VP1

Chain s:

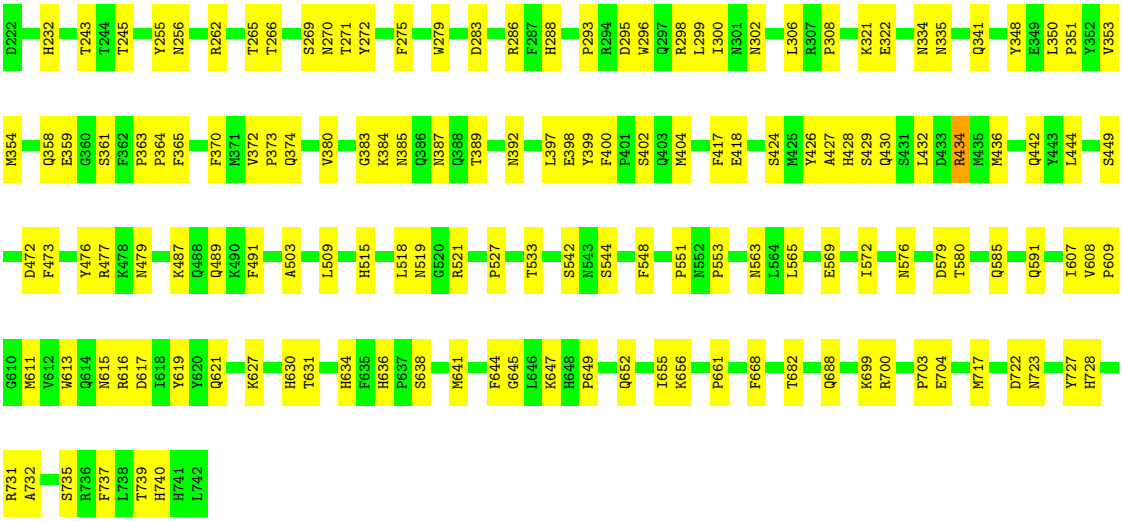


• Molecule 1: VP1

Chain t:

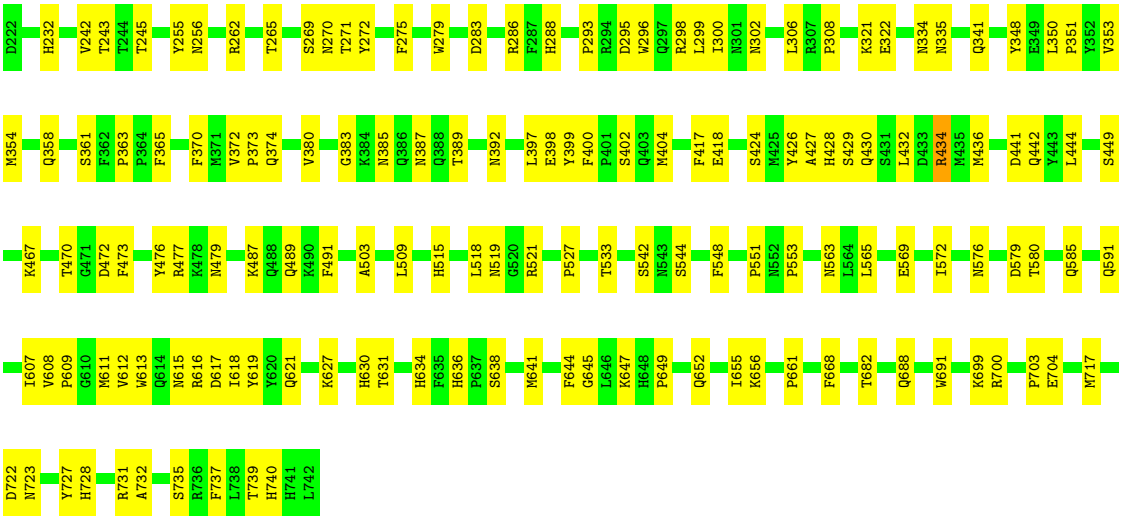
• Molecule 1: VP1

Chain u:



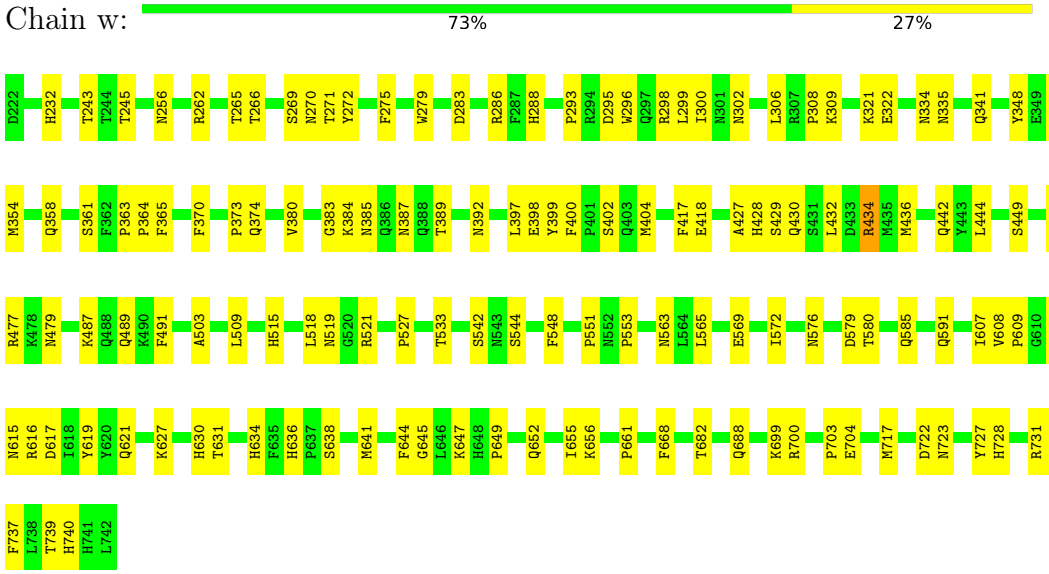
• Molecule 1: VP1

Chain v:



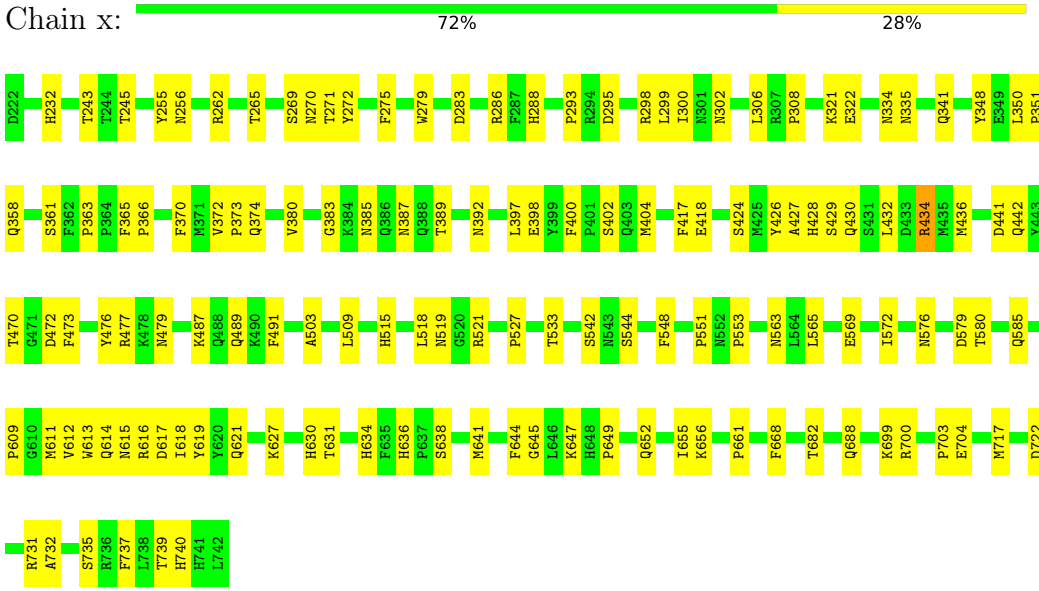
• Molecule 1: VP1

Chain w:



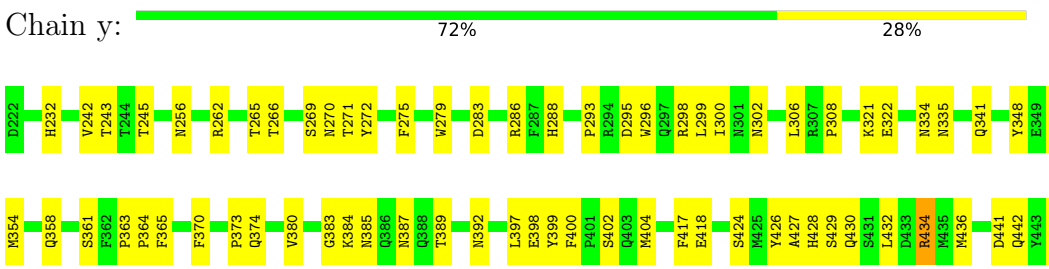
• Molecule 1: VP1

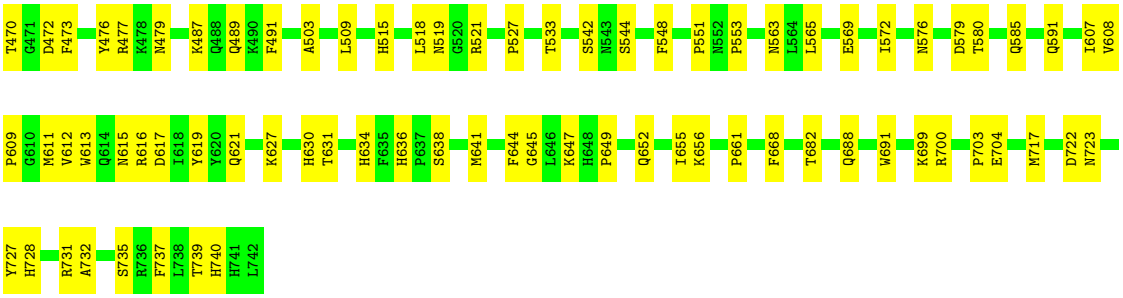
Chain x:



• Molecule 1: VP1

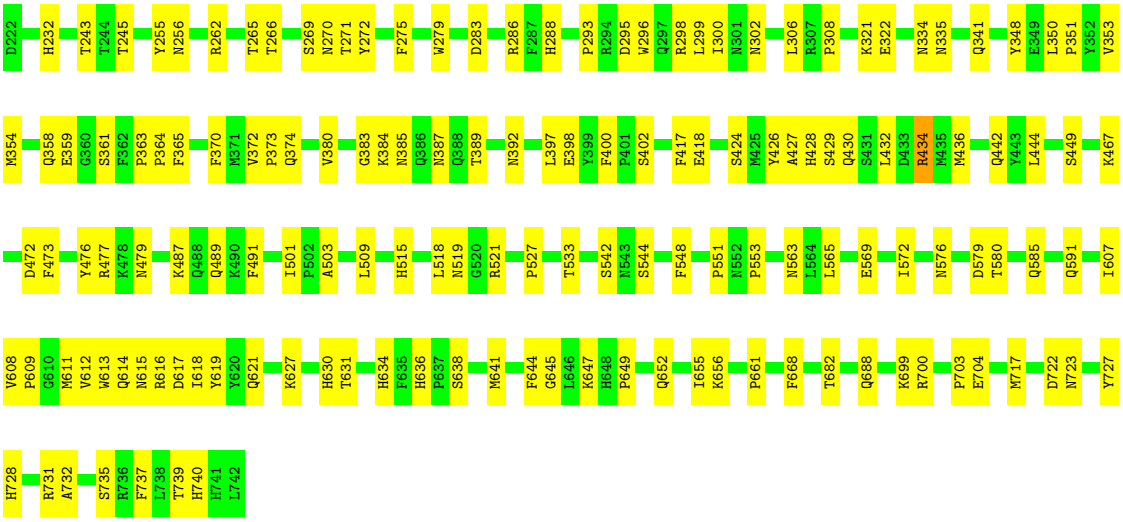
Chain y:





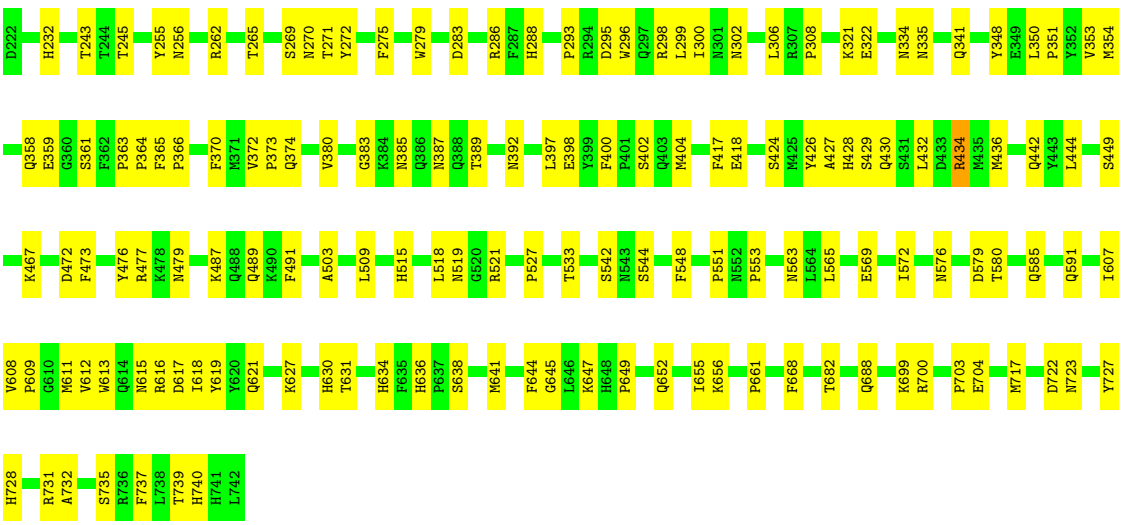
• Molecule 1: VP1

Chain z:



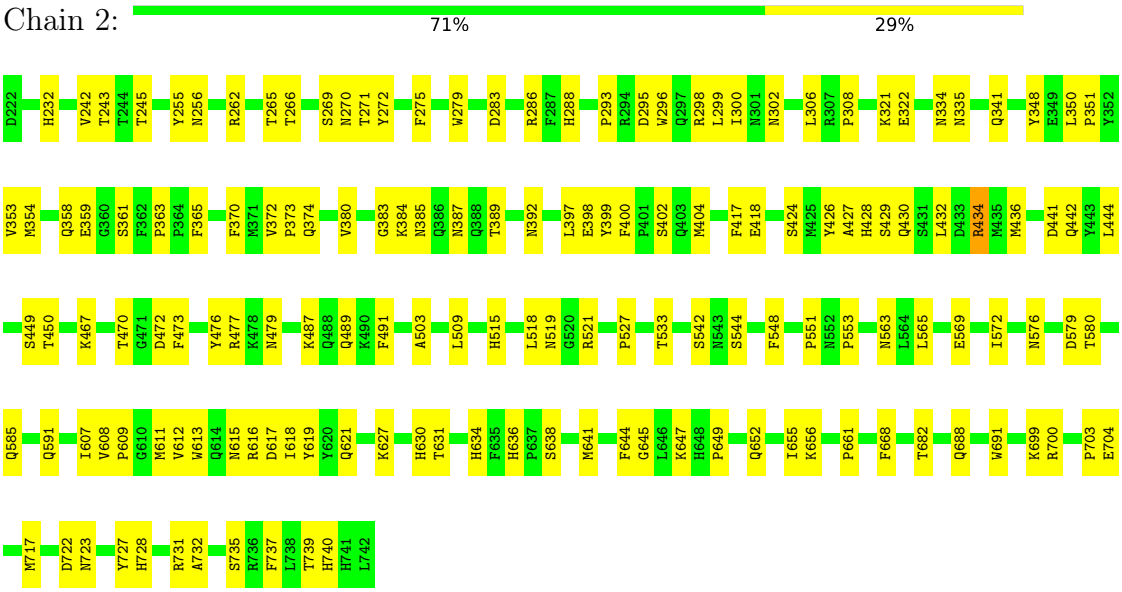
• Molecule 1: VP1

Chain 1:



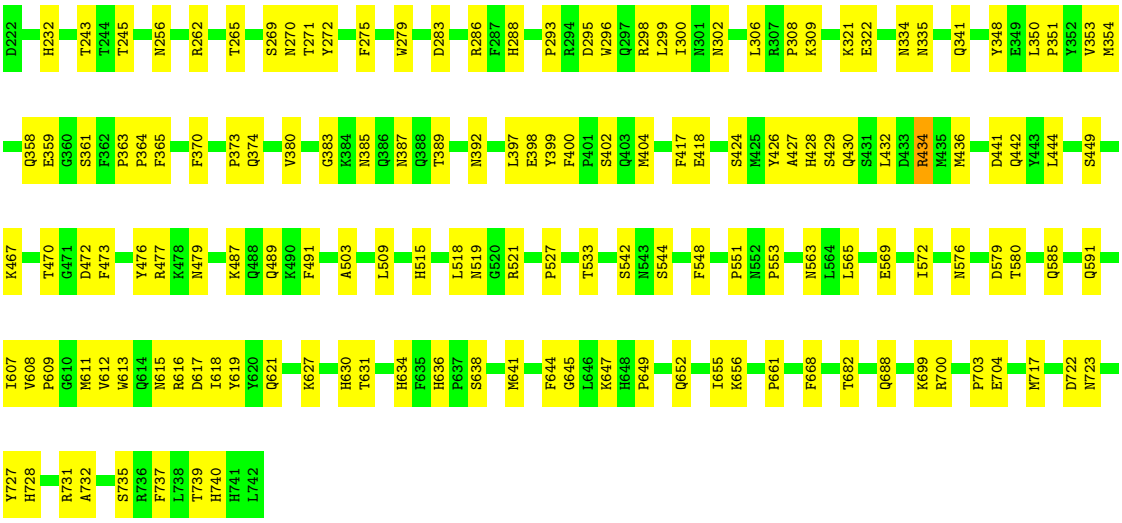
• Molecule 1: VP1

Chain 2:



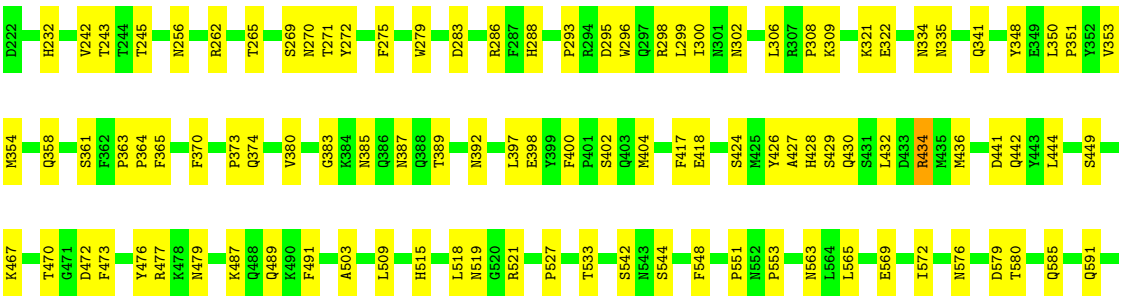
• Molecule 1: VP1

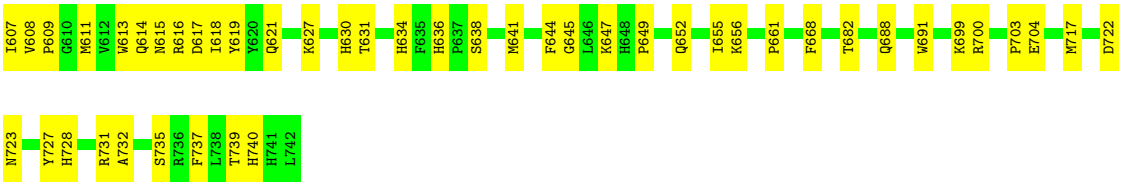
Chain 3:



• Molecule 1: VP1

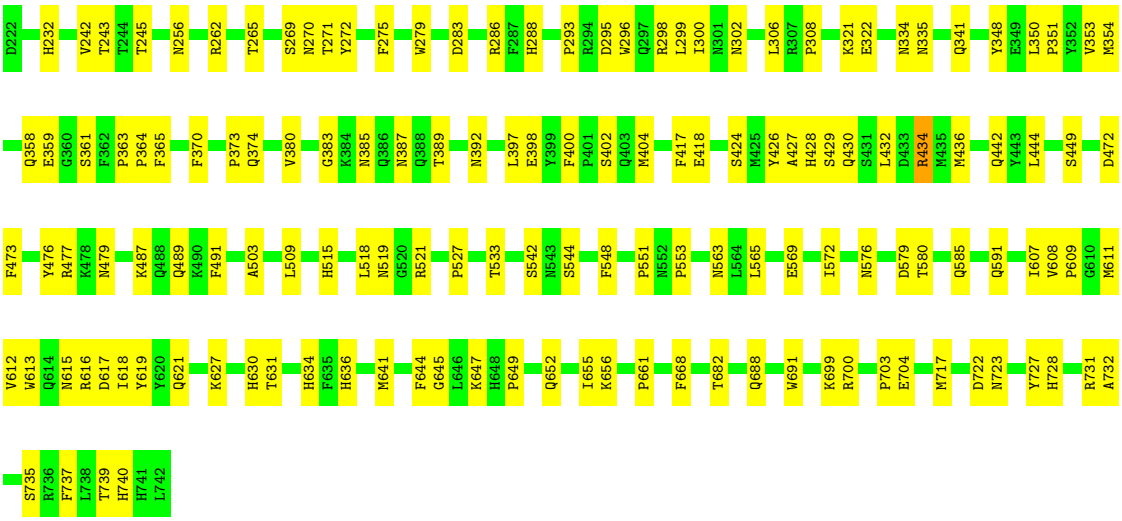
Chain 4:





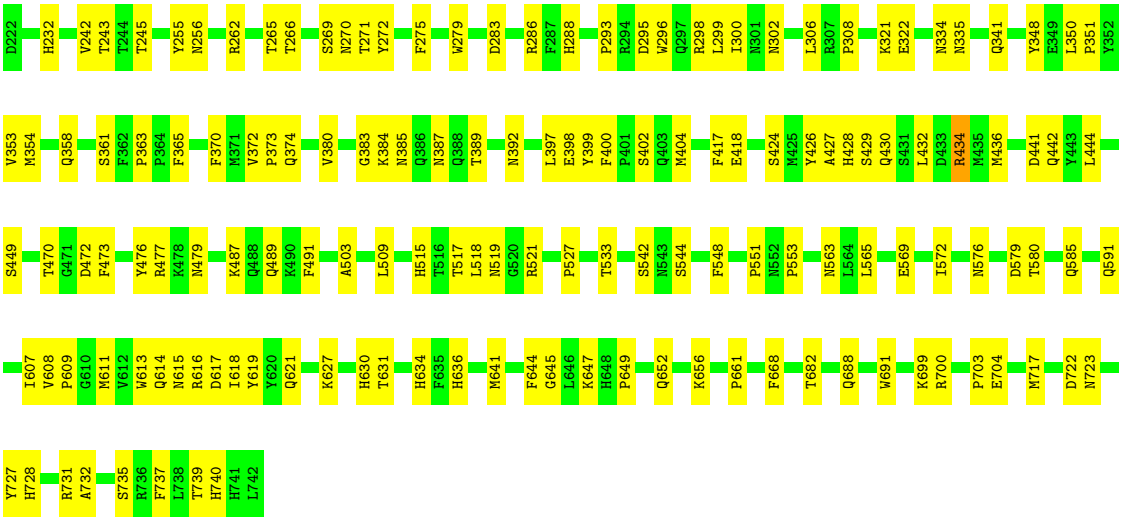
• Molecule 1: VP1

Chain 5:



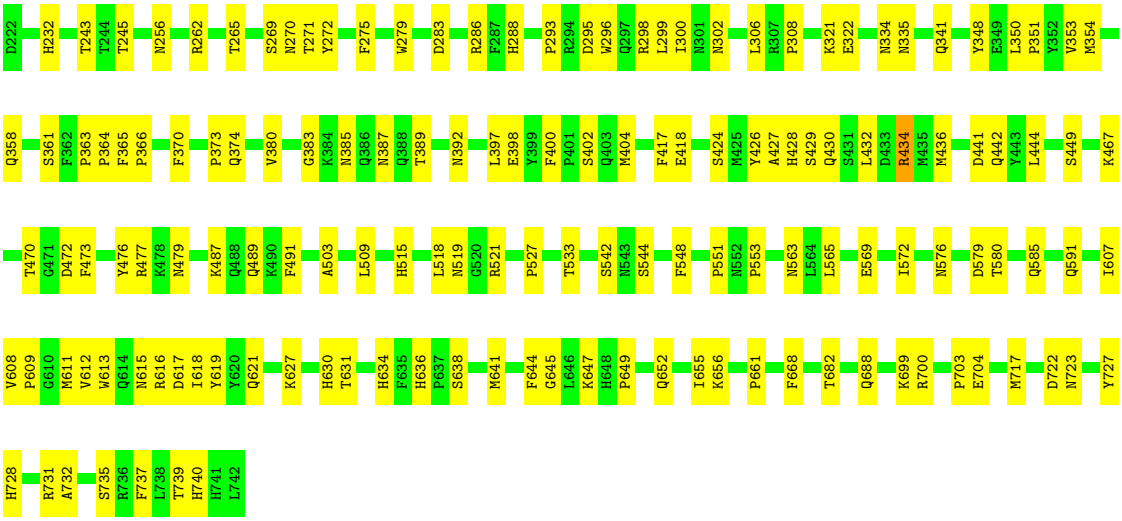
• Molecule 1: VP1

Chain 6:



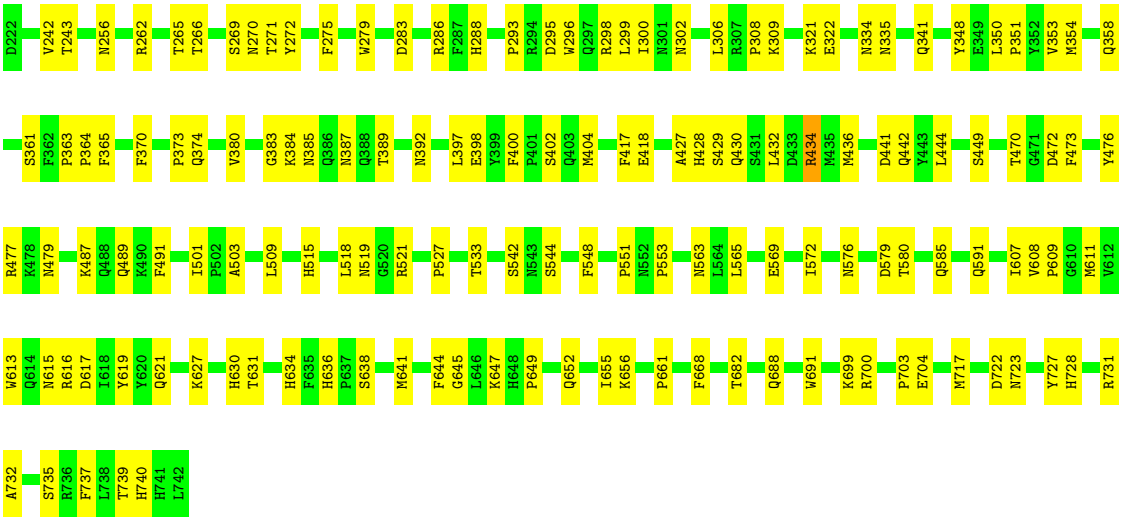
• Molecule 1: VP1

Chain 7:



- Molecule 1: VP1

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40764	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: D5M

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	1	0.45	0/4283	0.58	1/5847 (0.0%)
1	2	0.45	0/4283	0.58	1/5847 (0.0%)
1	3	0.45	0/4283	0.58	1/5847 (0.0%)
1	4	0.45	0/4283	0.58	1/5847 (0.0%)
1	5	0.45	0/4283	0.58	1/5847 (0.0%)
1	6	0.45	0/4283	0.58	1/5847 (0.0%)
1	7	0.45	0/4283	0.58	1/5847 (0.0%)
1	8	0.45	0/4283	0.58	1/5847 (0.0%)
1	A	0.45	0/4283	0.58	1/5847 (0.0%)
1	B	0.45	0/4283	0.58	1/5847 (0.0%)
1	C	0.45	0/4283	0.58	1/5847 (0.0%)
1	D	0.45	0/4283	0.58	1/5847 (0.0%)
1	E	0.45	0/4283	0.58	1/5847 (0.0%)
1	F	0.45	0/4283	0.58	1/5847 (0.0%)
1	G	0.45	0/4283	0.58	1/5847 (0.0%)
1	H	0.45	0/4283	0.58	1/5847 (0.0%)
1	I	0.45	0/4283	0.58	1/5847 (0.0%)
1	J	0.45	0/4283	0.58	1/5847 (0.0%)
1	K	0.45	0/4283	0.58	1/5847 (0.0%)
1	L	0.45	0/4283	0.58	1/5847 (0.0%)
1	M	0.45	0/4283	0.58	1/5847 (0.0%)
1	N	0.45	0/4283	0.58	1/5847 (0.0%)
1	O	0.45	0/4283	0.58	1/5847 (0.0%)
1	P	0.45	0/4283	0.58	1/5847 (0.0%)
1	Q	0.45	0/4283	0.58	1/5847 (0.0%)
1	R	0.45	0/4283	0.58	1/5847 (0.0%)
1	S	0.45	0/4283	0.58	1/5847 (0.0%)
1	T	0.45	0/4283	0.58	1/5847 (0.0%)
1	U	0.45	0/4283	0.58	1/5847 (0.0%)
1	V	0.45	0/4283	0.58	1/5847 (0.0%)
1	W	0.45	0/4283	0.58	1/5847 (0.0%)
1	X	0.45	0/4283	0.58	1/5847 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Y	0.45	0/4283	0.58	1/5847 (0.0%)
1	Z	0.45	0/4283	0.58	1/5847 (0.0%)
1	a	0.45	0/4283	0.58	1/5847 (0.0%)
1	b	0.45	0/4283	0.58	1/5847 (0.0%)
1	c	0.45	0/4283	0.58	1/5847 (0.0%)
1	d	0.45	0/4283	0.58	1/5847 (0.0%)
1	e	0.45	0/4283	0.58	1/5847 (0.0%)
1	f	0.45	0/4283	0.58	1/5847 (0.0%)
1	g	0.45	0/4283	0.58	1/5847 (0.0%)
1	h	0.45	0/4283	0.58	1/5847 (0.0%)
1	i	0.45	0/4283	0.58	1/5847 (0.0%)
1	j	0.45	0/4283	0.58	1/5847 (0.0%)
1	k	0.45	0/4283	0.58	1/5847 (0.0%)
1	l	0.45	0/4283	0.58	1/5847 (0.0%)
1	m	0.45	0/4283	0.58	1/5847 (0.0%)
1	n	0.45	0/4283	0.58	1/5847 (0.0%)
1	o	0.45	0/4283	0.58	1/5847 (0.0%)
1	p	0.45	0/4283	0.58	1/5847 (0.0%)
1	q	0.45	0/4283	0.58	1/5847 (0.0%)
1	r	0.45	0/4283	0.58	1/5847 (0.0%)
1	s	0.45	0/4283	0.58	1/5847 (0.0%)
1	t	0.45	0/4283	0.58	1/5847 (0.0%)
1	u	0.45	0/4283	0.58	1/5847 (0.0%)
1	v	0.45	0/4283	0.58	1/5847 (0.0%)
1	w	0.45	0/4283	0.58	1/5847 (0.0%)
1	x	0.45	0/4283	0.58	1/5847 (0.0%)
1	y	0.45	0/4283	0.58	1/5847 (0.0%)
1	z	0.45	0/4283	0.58	1/5847 (0.0%)
All	All	0.45	0/256980	0.58	60/350820 (0.0%)

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	434	ARG	CA-CB-CG	-5.57	102.96	114.10
1	U	434	ARG	CA-CB-CG	-5.57	102.96	114.10
1	q	434	ARG	CA-CB-CG	-5.57	102.96	114.10
1	s	434	ARG	CA-CB-CG	-5.57	102.96	114.10
1	2	434	ARG	CA-CB-CG	-5.57	102.96	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4152	0	3878	135	0
1	2	4152	0	3878	140	0
1	3	4152	0	3878	139	0
1	4	4152	0	3878	138	0
1	5	4152	0	3878	137	0
1	6	4152	0	3878	137	0
1	7	4152	0	3878	137	0
1	8	4152	0	3878	133	0
1	A	4152	0	3878	131	0
1	B	4152	0	3878	136	0
1	C	4152	0	3878	140	0
1	D	4152	0	3878	136	0
1	E	4152	0	3878	132	0
1	F	4152	0	3878	134	0
1	G	4152	0	3878	138	0
1	H	4152	0	3878	140	0
1	I	4152	0	3878	134	0
1	J	4152	0	3878	138	0
1	K	4152	0	3878	137	0
1	L	4152	0	3878	137	0
1	M	4152	0	3878	137	0
1	N	4152	0	3878	135	0
1	O	4152	0	3878	138	0
1	P	4152	0	3878	138	0
1	Q	4152	0	3878	132	0
1	R	4152	0	3878	136	0
1	S	4152	0	3878	137	0
1	T	4152	0	3878	136	0
1	U	4152	0	3878	136	0
1	V	4152	0	3878	137	0
1	W	4152	0	3878	138	0
1	X	4152	0	3878	140	0
1	Y	4152	0	3878	136	0
1	Z	4152	0	3878	134	0
1	a	4152	0	3878	141	0
1	b	4152	0	3878	140	0
1	c	4152	0	3878	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	4152	0	3878	138	0
1	e	4152	0	3878	134	0
1	f	4152	0	3878	139	0
1	g	4152	0	3878	138	0
1	h	4152	0	3878	136	0
1	i	4152	0	3878	135	0
1	j	4152	0	3878	137	0
1	k	4152	0	3878	137	0
1	l	4152	0	3878	141	0
1	m	4152	0	3878	135	0
1	n	4152	0	3878	138	0
1	o	4152	0	3878	140	0
1	p	4152	0	3878	137	0
1	q	4152	0	3878	136	0
1	r	4152	0	3878	138	0
1	s	4152	0	3878	136	0
1	t	4152	0	3878	138	0
1	u	4152	0	3878	135	0
1	v	4152	0	3878	135	0
1	w	4152	0	3878	132	0
1	x	4152	0	3878	132	0
1	y	4152	0	3878	134	0
1	z	4152	0	3878	139	0
2	1	22	0	12	1	0
2	2	22	0	12	1	0
2	3	22	0	12	1	0
2	4	22	0	12	1	0
2	5	22	0	12	1	0
2	6	22	0	12	1	0
2	7	22	0	12	1	0
2	8	22	0	12	1	0
2	A	22	0	12	1	0
2	B	22	0	12	1	0
2	C	22	0	12	1	0
2	D	22	0	12	1	0
2	E	22	0	12	1	0
2	F	22	0	12	1	0
2	G	22	0	12	1	0
2	H	22	0	12	1	0
2	I	22	0	12	1	0
2	J	22	0	12	1	0
2	K	22	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	22	0	12	1	0
2	M	22	0	12	1	0
2	N	22	0	12	1	0
2	O	22	0	12	1	0
2	P	22	0	12	1	0
2	Q	22	0	12	1	0
2	R	22	0	12	1	0
2	S	22	0	12	1	0
2	T	22	0	12	1	0
2	U	22	0	12	1	0
2	V	22	0	12	1	0
2	W	22	0	12	1	0
2	X	22	0	12	1	0
2	Y	22	0	12	1	0
2	Z	22	0	12	1	0
2	a	22	0	12	1	0
2	b	22	0	12	1	0
2	c	22	0	12	1	0
2	d	22	0	12	1	0
2	e	22	0	12	1	0
2	f	22	0	12	1	0
2	g	22	0	12	1	0
2	h	22	0	12	1	0
2	i	22	0	12	1	0
2	j	22	0	12	1	0
2	k	22	0	12	1	0
2	l	22	0	12	1	0
2	m	22	0	12	1	0
2	n	22	0	12	1	0
2	o	22	0	12	1	0
2	p	22	0	12	1	0
2	q	22	0	12	1	0
2	r	22	0	12	1	0
2	s	22	0	12	1	0
2	t	22	0	12	1	0
2	u	22	0	12	1	0
2	v	22	0	12	1	0
2	w	22	0	12	1	0
2	x	22	0	12	1	0
2	y	22	0	12	1	0
2	z	22	0	12	1	0
All	All	250440	0	233400	6368	0

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

The worst 5 of 6368 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:THR:O	1:M:434:ARG:NH1	2.01	0.94
1:X:271:THR:O	1:e:434:ARG:NH1	2.01	0.94
1:c:434:ARG:NH1	1:o:271:THR:O	2.01	0.94
1:g:271:THR:O	1:h:434:ARG:NH1	2.01	0.94
1:o:434:ARG:NH1	1:p:271:THR:O	2.01	0.94

There are no symmetry-related clashes.

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	1	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	2	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	3	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	4	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	5	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	6	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	7	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	8	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	A	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	B	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	C	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	D	521/521 (100%)	513 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	F	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	G	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	H	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	I	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	J	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	K	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	L	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	M	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	N	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	O	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	P	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	Q	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	R	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	S	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	T	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	U	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	V	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	W	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	X	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	Y	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	Z	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	a	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	b	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	c	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	d	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	e	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	f	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	g	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	h	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	i	521/521 (100%)	513 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	k	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	l	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	m	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	n	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	o	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	p	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	q	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	r	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	s	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	t	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	u	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	v	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	w	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	x	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	y	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
1	z	521/521 (100%)	513 (98%)	8 (2%)	0	100	100
All	All	31260/31260 (100%)	30780 (98%)	480 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	2	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	3	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	4	451/449 (100%)	450 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	6	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	7	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	8	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	A	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	B	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	C	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	D	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	E	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	F	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	G	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	H	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	I	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	J	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	K	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	L	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	M	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	N	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	O	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	P	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	Q	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	R	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	S	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	T	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	U	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	V	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	W	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	X	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	Y	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	Z	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	a	451/449 (100%)	450 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	c	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	d	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	e	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	f	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	g	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	h	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	i	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	j	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	k	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	l	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	m	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	n	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	o	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	p	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	q	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	r	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	s	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	t	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	u	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	v	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	w	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	x	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	y	451/449 (100%)	450 (100%)	1 (0%)	87	95
1	z	451/449 (100%)	450 (100%)	1 (0%)	87	95
All	All	27060/26940 (100%)	27000 (100%)	60 (0%)	85	95

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	402	SER
1	4	402	SER
1	j	402	SER

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Mol	Chain	Res	Type
1	3	402	SER
1	8	402	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 836 such sidechains are listed below:

Mol	Chain	Res	Type
1	g	740	HIS
1	p	367	ASN
1	6	479	ASN
1	h	652	GLN
1	g	688	GLN

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)

60 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	D5M	J	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	D5M	x	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	q	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	V	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	u	801	-	24,24,24	0.62	0	35,36,36	0.45	1 (2%)
2	D5M	3	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	m	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	i	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	R	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	g	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	A	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	P	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	I	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	K	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	5	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	f	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	E	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	Y	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	B	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	j	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	D	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	M	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	y	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	Z	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	o	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	7	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	H	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	b	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	F	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	6	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	Q	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	c	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	p	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	s	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	T	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	2	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	D5M	e	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	L	801	-	24,24,24	0.60	0	35,36,36	0.45	1 (2%)
2	D5M	r	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	t	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	G	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	O	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	d	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	1	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	X	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	l	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	C	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	S	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	k	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	w	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	v	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	W	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	N	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	8	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	h	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	z	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	n	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	4	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	U	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)
2	D5M	a	801	-	24,24,24	0.61	0	35,36,36	0.45	1 (2%)

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
2	D5M	J	801	-	-	3/10/22/22	0/3/3/3
2	D5M	x	801	-	-	3/10/22/22	0/3/3/3
2	D5M	q	801	-	-	3/10/22/22	0/3/3/3
2	D5M	V	801	-	-	3/10/22/22	0/3/3/3
2	D5M	u	801	-	-	3/10/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	3	801	-	-	3/10/22/22	0/3/3/3
2	D5M	m	801	-	-	3/10/22/22	0/3/3/3
2	D5M	i	801	-	-	3/10/22/22	0/3/3/3
2	D5M	R	801	-	-	3/10/22/22	0/3/3/3
2	D5M	g	801	-	-	3/10/22/22	0/3/3/3
2	D5M	A	801	-	-	3/10/22/22	0/3/3/3
2	D5M	P	801	-	-	3/10/22/22	0/3/3/3
2	D5M	I	801	-	-	3/10/22/22	0/3/3/3
2	D5M	K	801	-	-	3/10/22/22	0/3/3/3
2	D5M	5	801	-	-	3/10/22/22	0/3/3/3
2	D5M	f	801	-	-	3/10/22/22	0/3/3/3
2	D5M	E	801	-	-	3/10/22/22	0/3/3/3
2	D5M	Y	801	-	-	3/10/22/22	0/3/3/3
2	D5M	B	801	-	-	3/10/22/22	0/3/3/3
2	D5M	j	801	-	-	3/10/22/22	0/3/3/3
2	D5M	D	801	-	-	3/10/22/22	0/3/3/3
2	D5M	M	801	-	-	3/10/22/22	0/3/3/3
2	D5M	y	801	-	-	3/10/22/22	0/3/3/3
2	D5M	Z	801	-	-	3/10/22/22	0/3/3/3
2	D5M	o	801	-	-	3/10/22/22	0/3/3/3
2	D5M	7	801	-	-	3/10/22/22	0/3/3/3
2	D5M	H	801	-	-	3/10/22/22	0/3/3/3
2	D5M	b	801	-	-	3/10/22/22	0/3/3/3
2	D5M	F	801	-	-	3/10/22/22	0/3/3/3
2	D5M	6	801	-	-	3/10/22/22	0/3/3/3
2	D5M	Q	801	-	-	3/10/22/22	0/3/3/3
2	D5M	c	801	-	-	3/10/22/22	0/3/3/3
2	D5M	p	801	-	-	3/10/22/22	0/3/3/3
2	D5M	s	801	-	-	3/10/22/22	0/3/3/3
2	D5M	T	801	-	-	3/10/22/22	0/3/3/3
2	D5M	2	801	-	-	3/10/22/22	0/3/3/3
2	D5M	e	801	-	-	3/10/22/22	0/3/3/3
2	D5M	L	801	-	-	3/10/22/22	0/3/3/3
2	D5M	r	801	-	-	3/10/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	t	801	-	-	3/10/22/22	0/3/3/3
2	D5M	G	801	-	-	3/10/22/22	0/3/3/3
2	D5M	O	801	-	-	3/10/22/22	0/3/3/3
2	D5M	d	801	-	-	3/10/22/22	0/3/3/3
2	D5M	1	801	-	-	3/10/22/22	0/3/3/3
2	D5M	X	801	-	-	3/10/22/22	0/3/3/3
2	D5M	l	801	-	-	3/10/22/22	0/3/3/3
2	D5M	C	801	-	-	3/10/22/22	0/3/3/3
2	D5M	S	801	-	-	3/10/22/22	0/3/3/3
2	D5M	k	801	-	-	3/10/22/22	0/3/3/3
2	D5M	w	801	-	-	3/10/22/22	0/3/3/3
2	D5M	v	801	-	-	3/10/22/22	0/3/3/3
2	D5M	W	801	-	-	3/10/22/22	0/3/3/3
2	D5M	N	801	-	-	3/10/22/22	0/3/3/3
2	D5M	8	801	-	-	3/10/22/22	0/3/3/3
2	D5M	h	801	-	-	3/10/22/22	0/3/3/3
2	D5M	z	801	-	-	3/10/22/22	0/3/3/3
2	D5M	n	801	-	-	3/10/22/22	0/3/3/3
2	D5M	4	801	-	-	3/10/22/22	0/3/3/3
2	D5M	U	801	-	-	3/10/22/22	0/3/3/3
2	D5M	a	801	-	-	3/10/22/22	0/3/3/3

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	q	801	D5M	O2P-P-O1P	2.02	118.71	110.83
2	s	801	D5M	O2P-P-O1P	2.02	118.71	110.83
2	2	801	D5M	O2P-P-O1P	2.02	118.71	110.83
2	E	801	D5M	O2P-P-O1P	2.02	118.70	110.83
2	G	801	D5M	O2P-P-O1P	2.02	118.70	110.83

There are no chirality outliers.

5 of 180 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	D5M	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	A	801	D5M	C5'-O5'-P-O3P
2	A	801	D5M	C5'-O5'-P-O2P
2	B	801	D5M	C5'-O5'-P-O1P
2	B	801	D5M	C5'-O5'-P-O3P

There are no ring outliers.

60 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	801	D5M	1	0
2	x	801	D5M	1	0
2	q	801	D5M	1	0
2	V	801	D5M	1	0
2	u	801	D5M	1	0
2	3	801	D5M	1	0
2	m	801	D5M	1	0
2	i	801	D5M	1	0
2	R	801	D5M	1	0
2	g	801	D5M	1	0
2	A	801	D5M	1	0
2	P	801	D5M	1	0
2	I	801	D5M	1	0
2	K	801	D5M	1	0
2	5	801	D5M	1	0
2	f	801	D5M	1	0
2	E	801	D5M	1	0
2	Y	801	D5M	1	0
2	B	801	D5M	1	0
2	j	801	D5M	1	0
2	D	801	D5M	1	0
2	M	801	D5M	1	0
2	y	801	D5M	1	0
2	Z	801	D5M	1	0
2	o	801	D5M	1	0
2	7	801	D5M	1	0
2	H	801	D5M	1	0
2	b	801	D5M	1	0
2	F	801	D5M	1	0
2	6	801	D5M	1	0
2	Q	801	D5M	1	0
2	c	801	D5M	1	0
2	p	801	D5M	1	0

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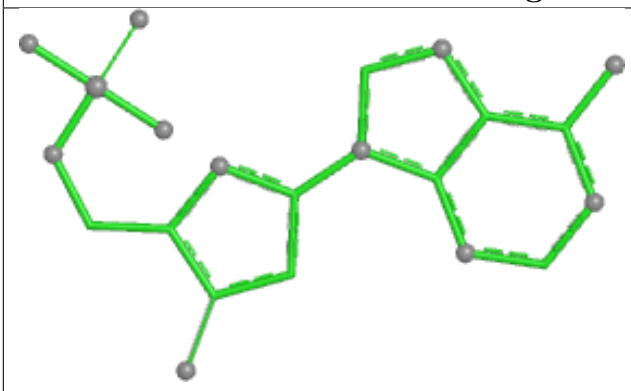
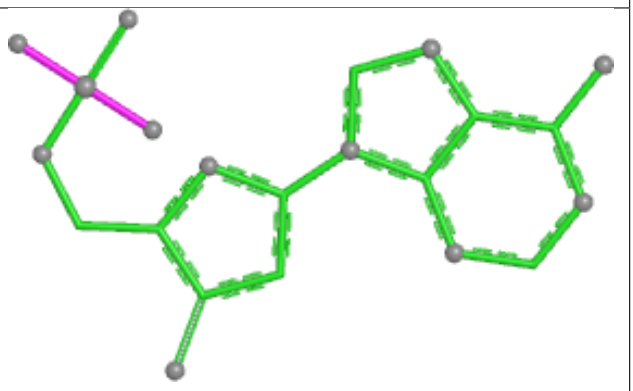
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	s	801	D5M	1	0
2	T	801	D5M	1	0
2	2	801	D5M	1	0
2	e	801	D5M	1	0
2	L	801	D5M	1	0
2	r	801	D5M	1	0
2	t	801	D5M	1	0
2	G	801	D5M	1	0
2	O	801	D5M	1	0
2	d	801	D5M	1	0
2	1	801	D5M	1	0
2	X	801	D5M	1	0
2	l	801	D5M	1	0
2	C	801	D5M	1	0
2	S	801	D5M	1	0
2	k	801	D5M	1	0
2	w	801	D5M	1	0
2	v	801	D5M	1	0
2	W	801	D5M	1	0
2	N	801	D5M	1	0
2	8	801	D5M	1	0
2	h	801	D5M	1	0
2	z	801	D5M	1	0
2	n	801	D5M	1	0
2	4	801	D5M	1	0
2	U	801	D5M	1	0
2	a	801	D5M	1	0

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

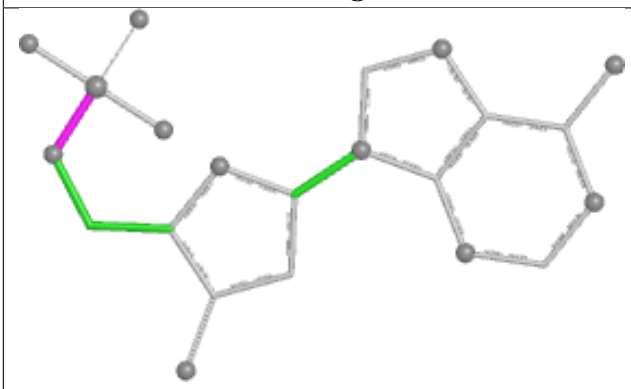
Ligand D5M J 801



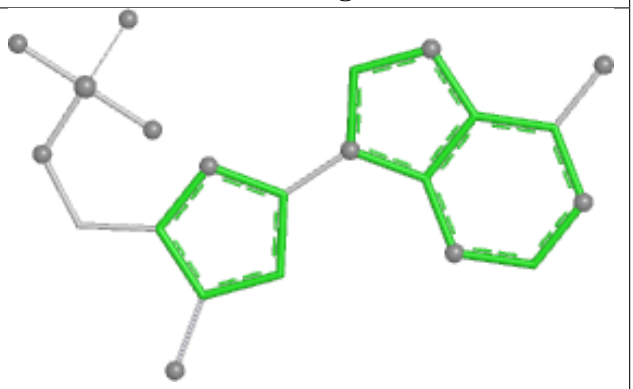
Bond lengths



Bond angles

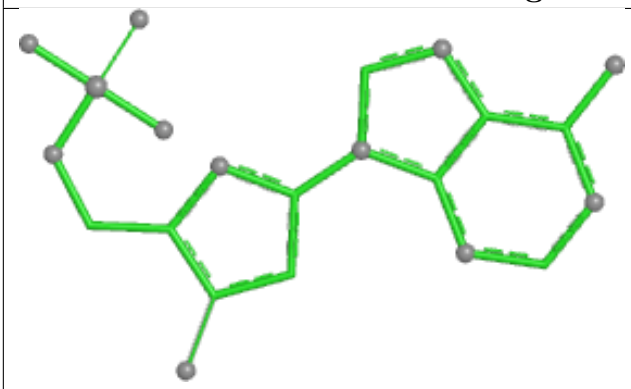


Torsions

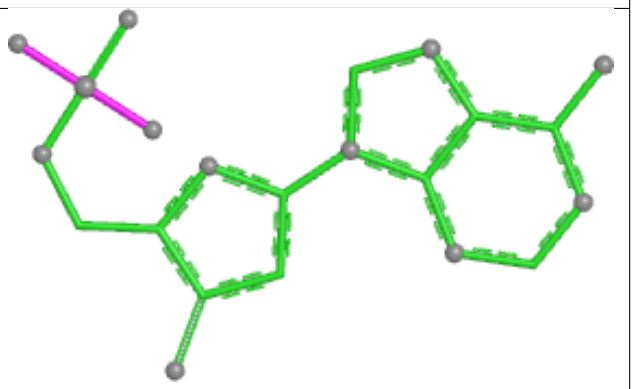


Rings

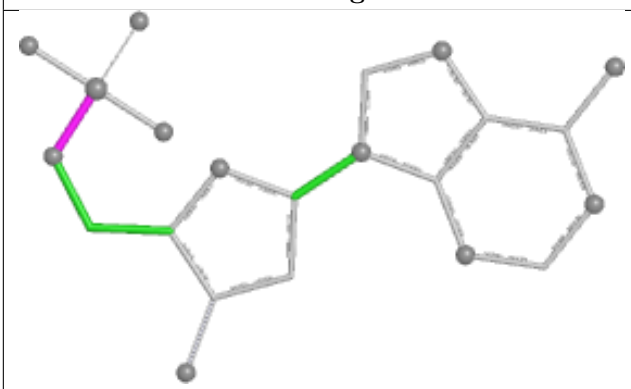
Ligand D5M x 801



Bond lengths



Bond angles



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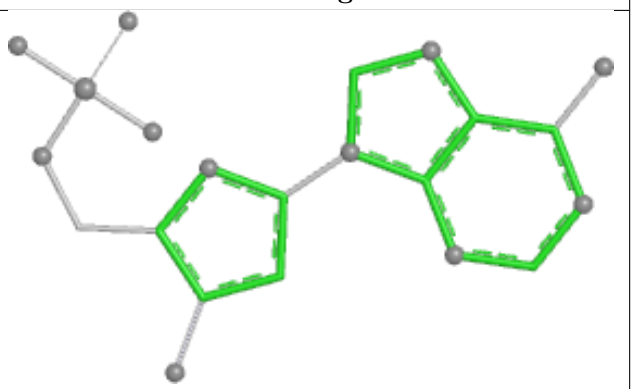
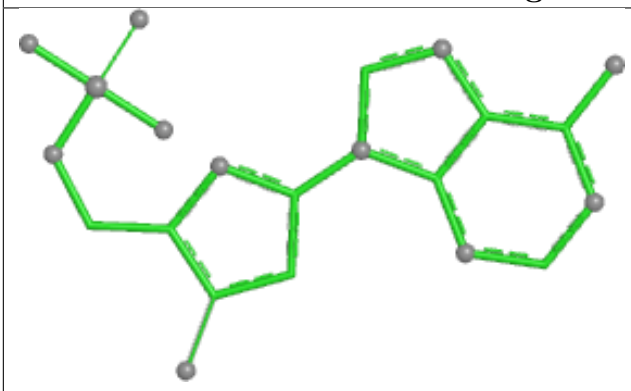


Rings

Ligand D5M q 801



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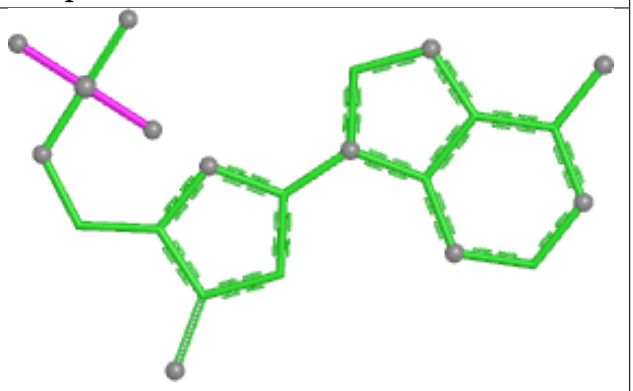

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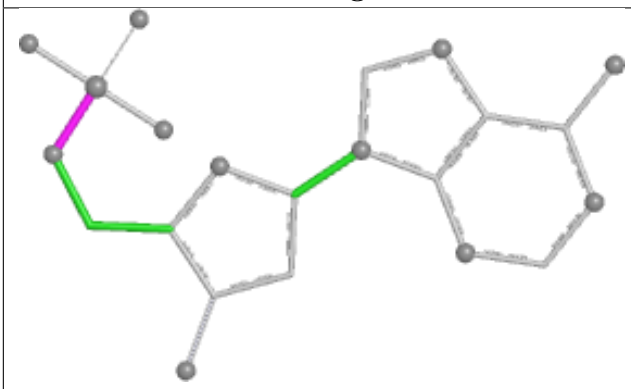

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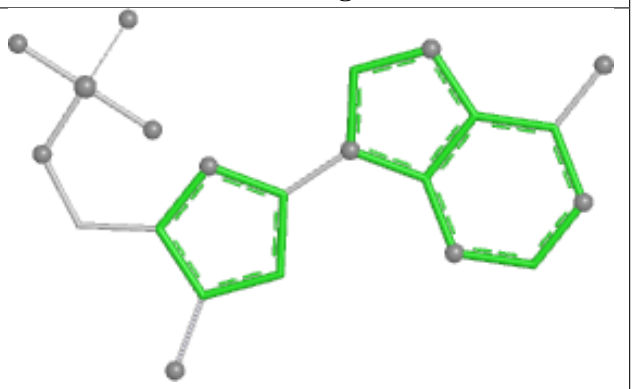

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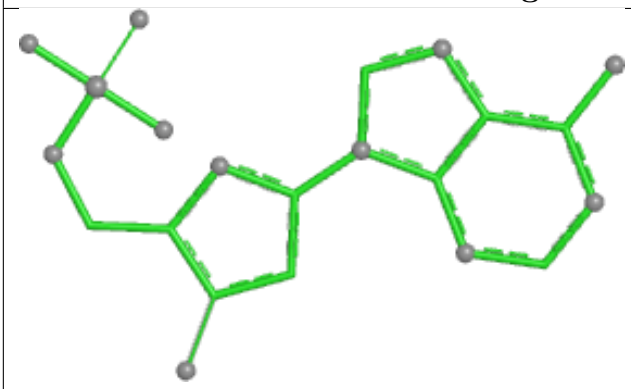

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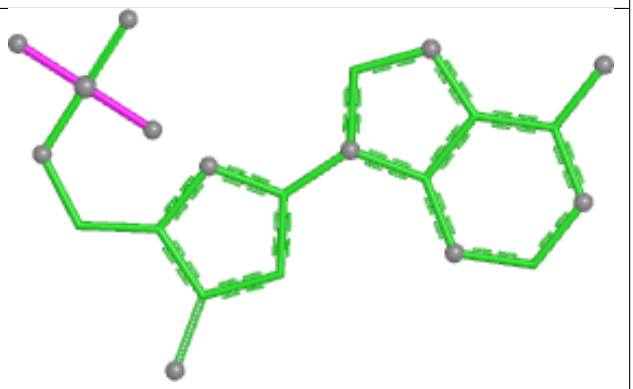

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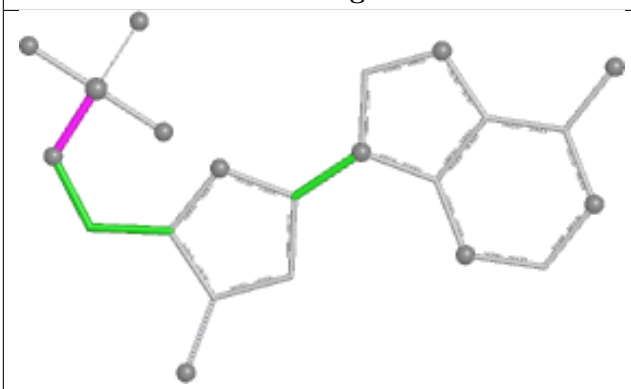

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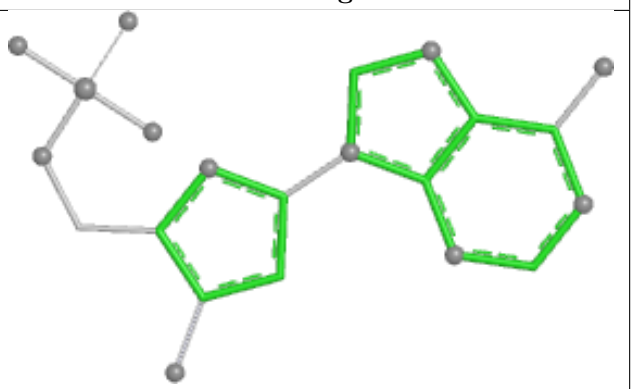

Rings

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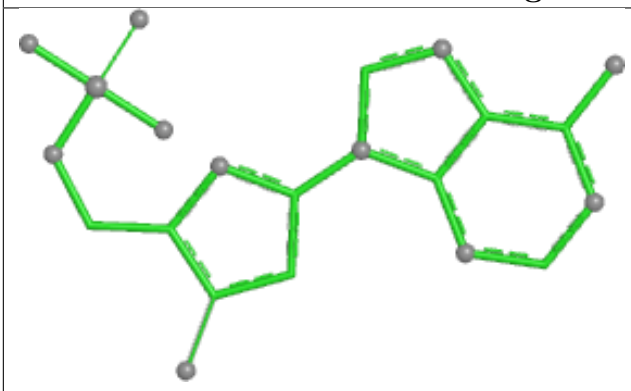

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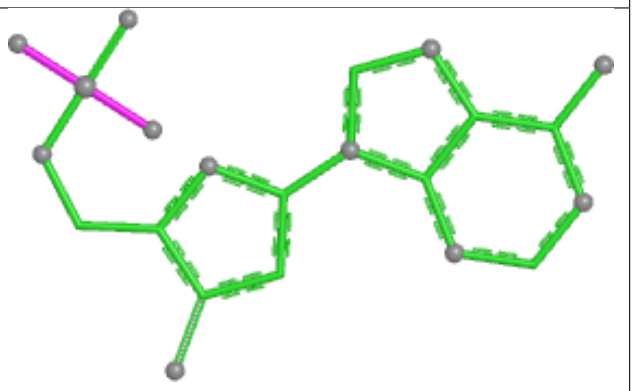

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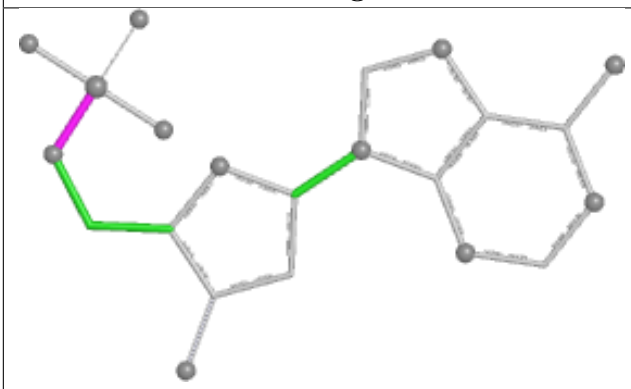

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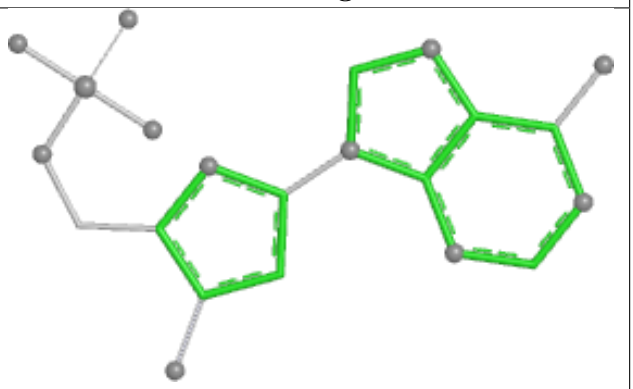

Rings

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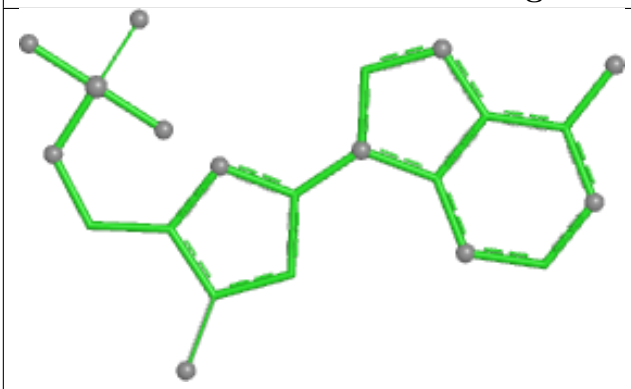

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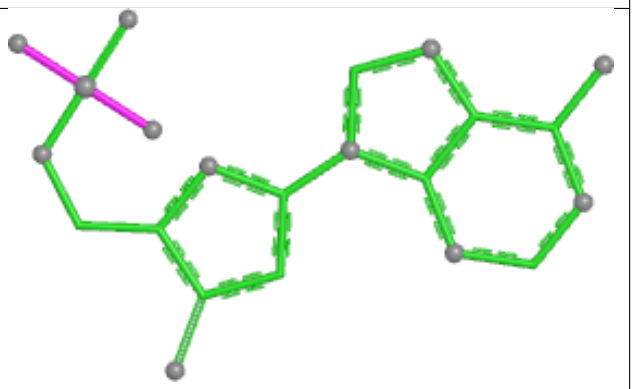

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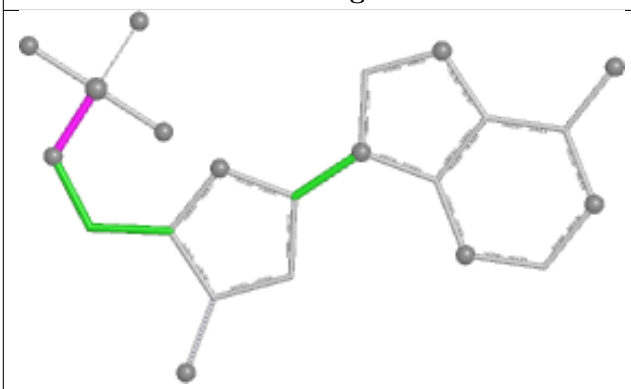

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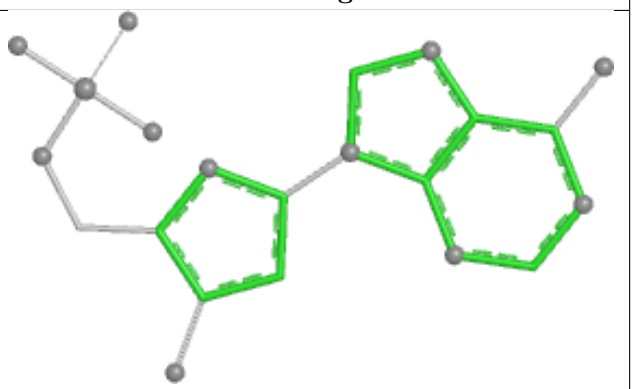

Rings

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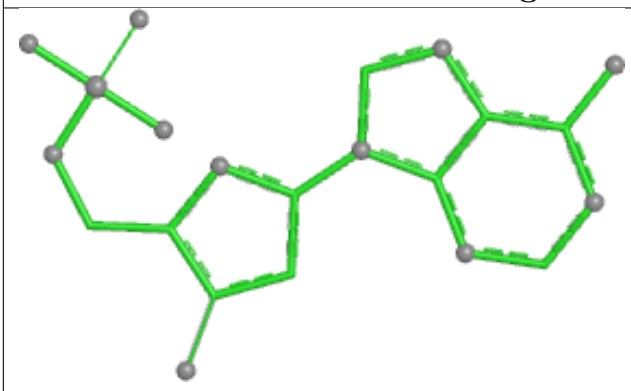

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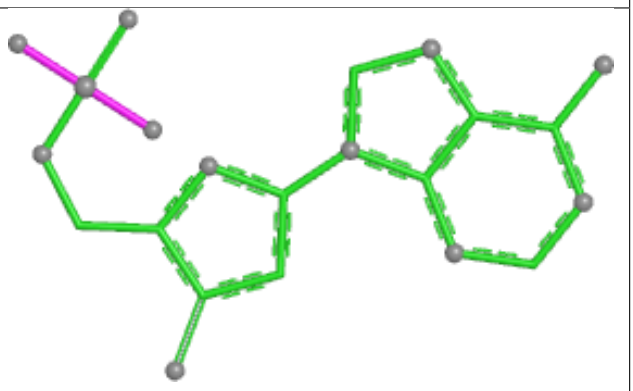

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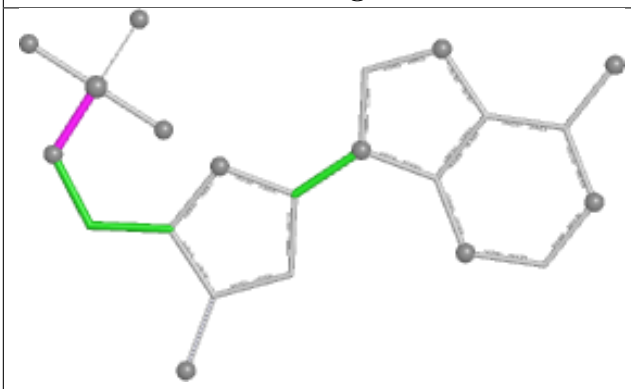

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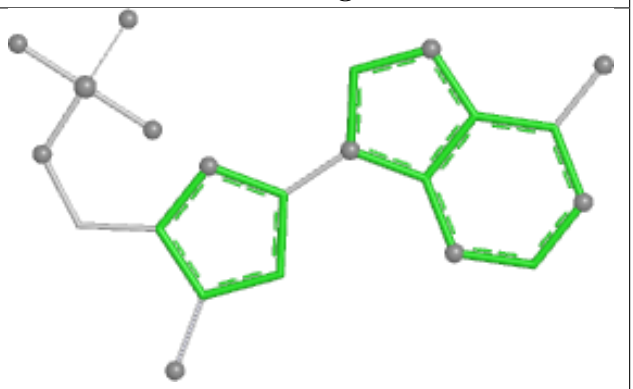

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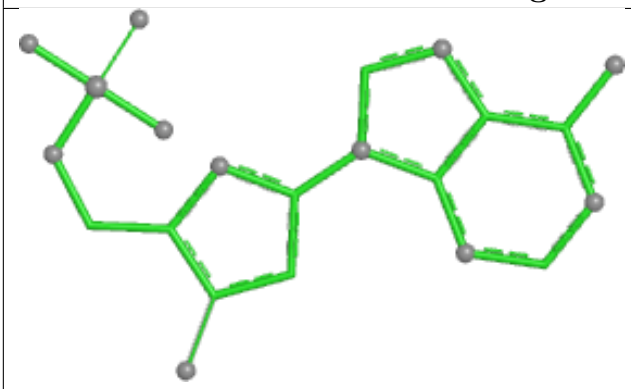

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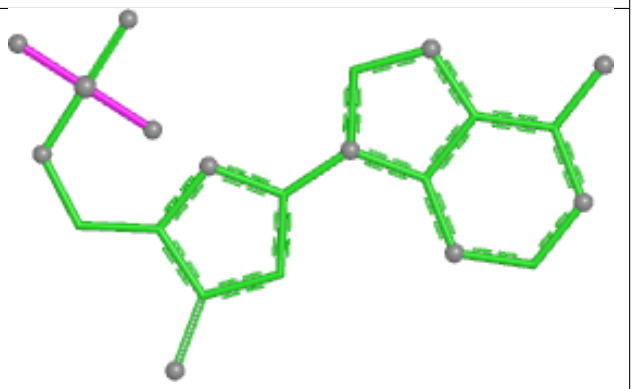

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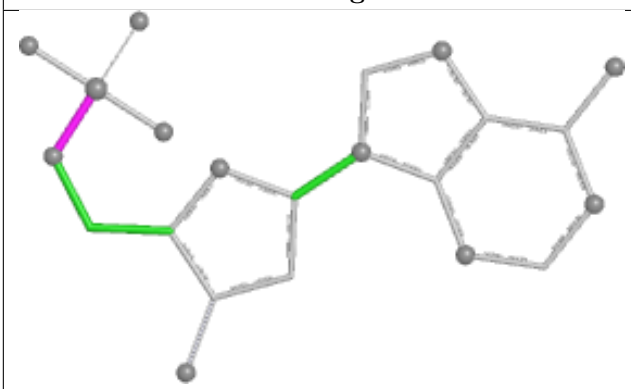

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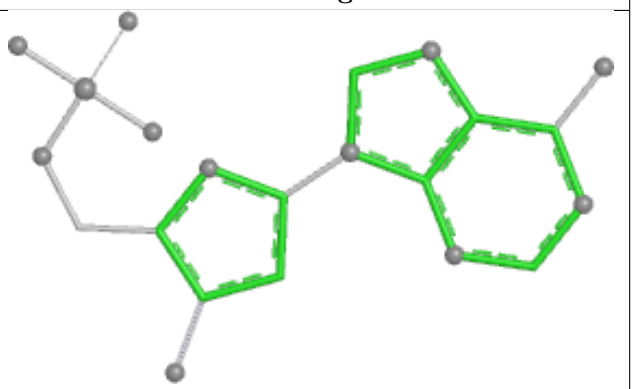

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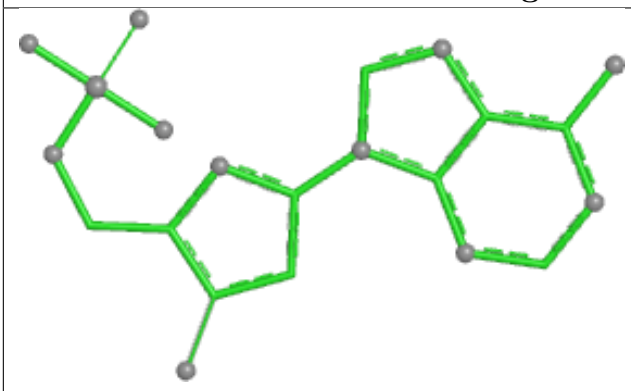

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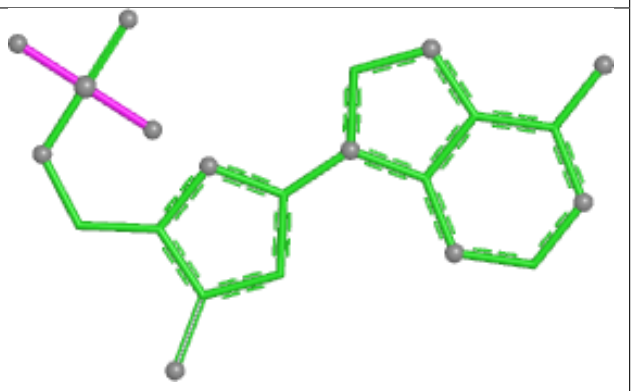

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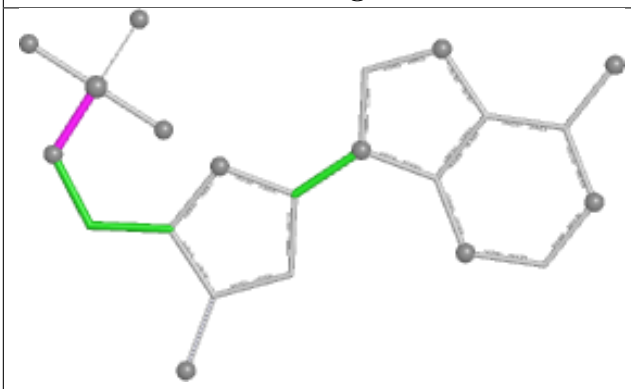

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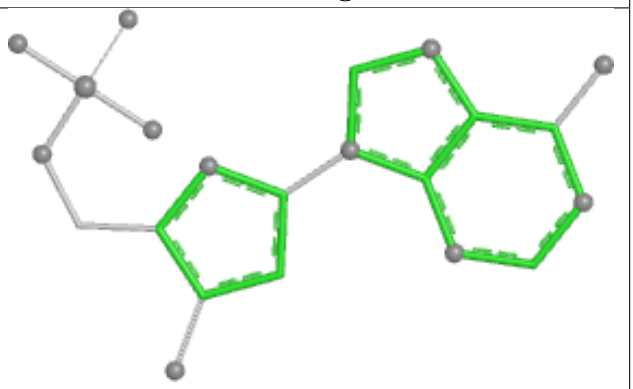

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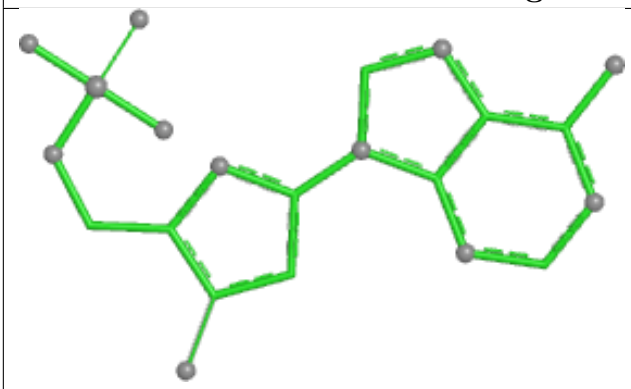

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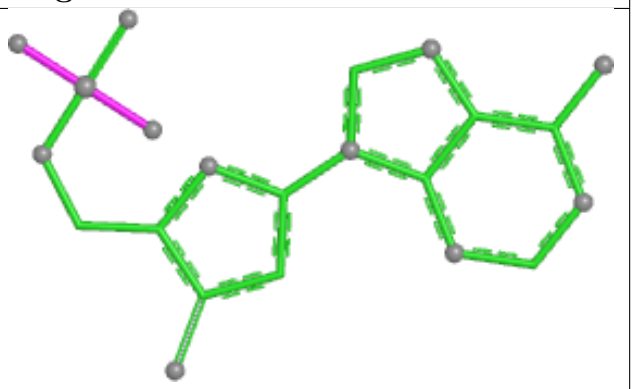

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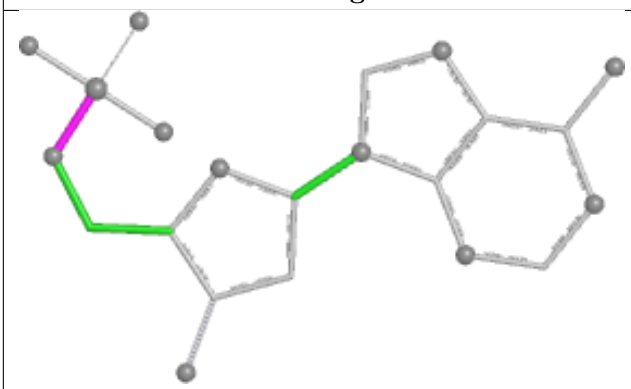

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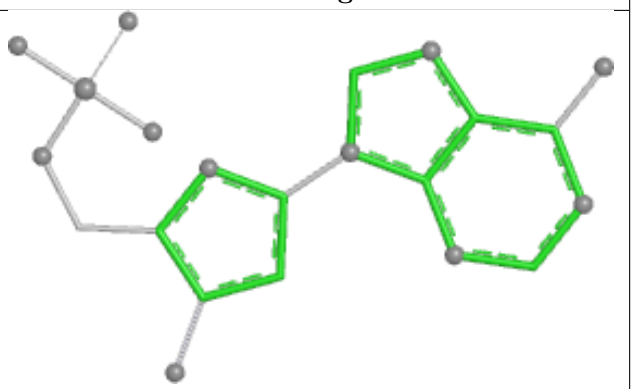

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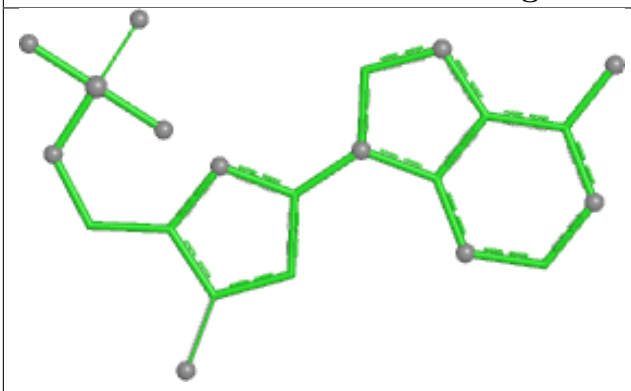

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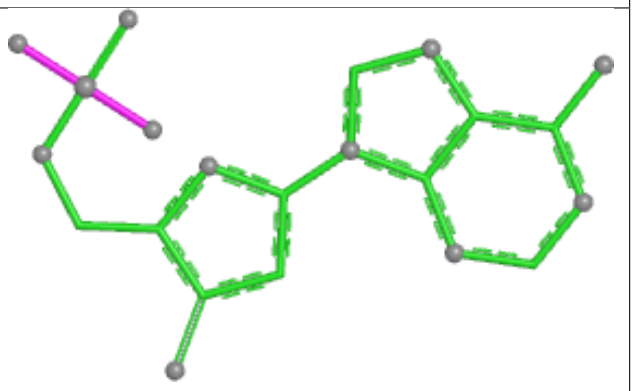

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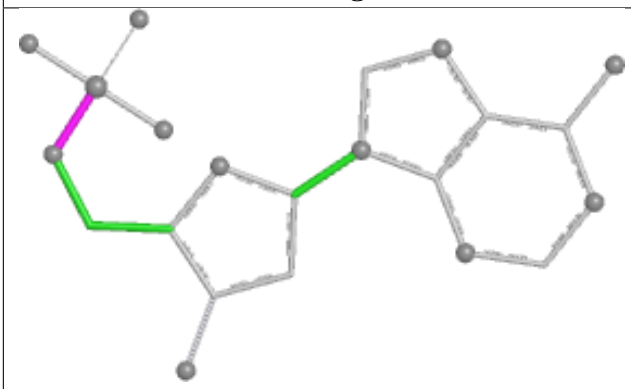

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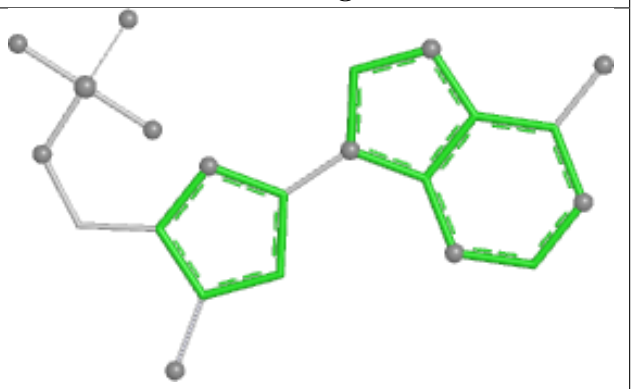

Rings

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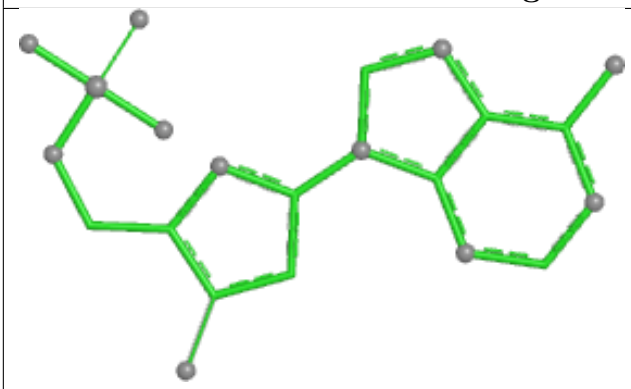

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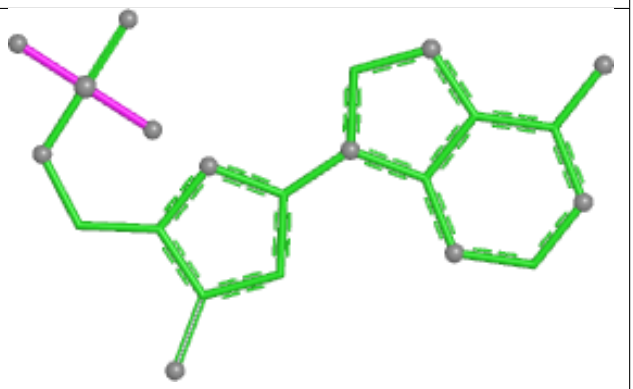

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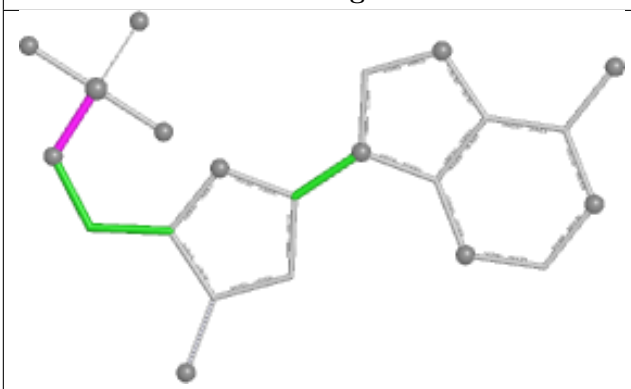

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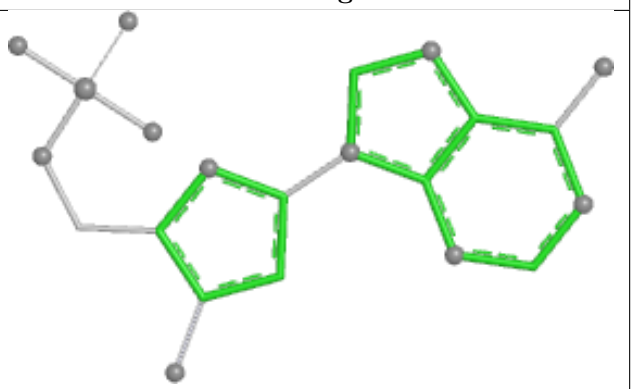

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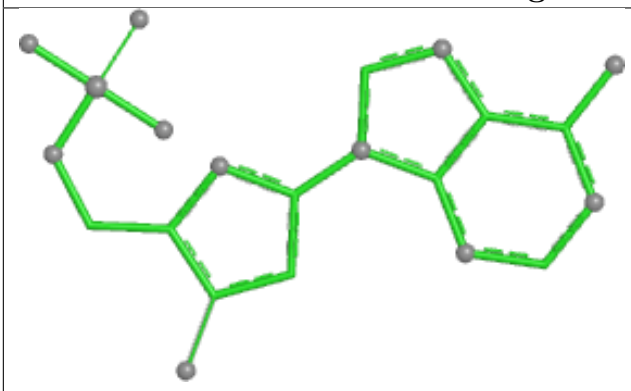

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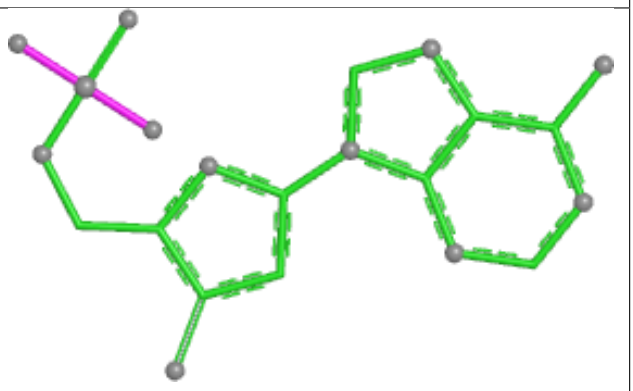

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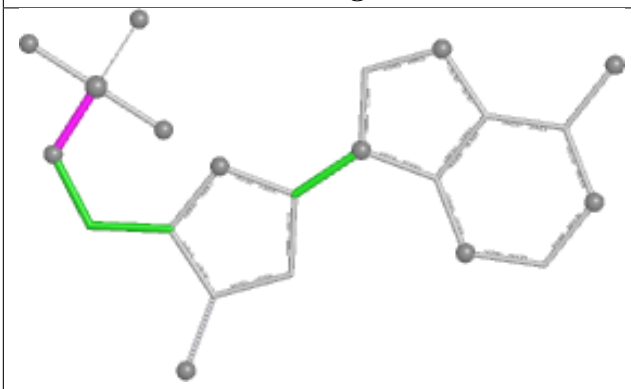

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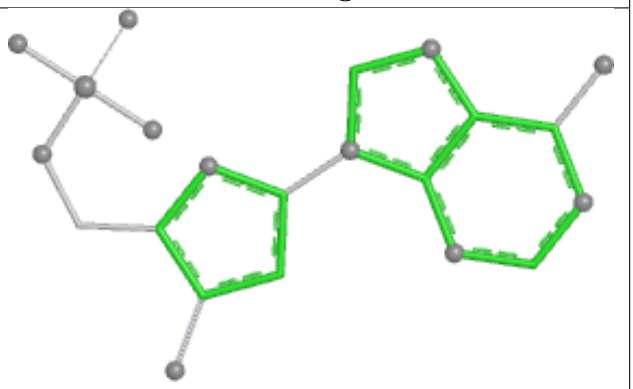
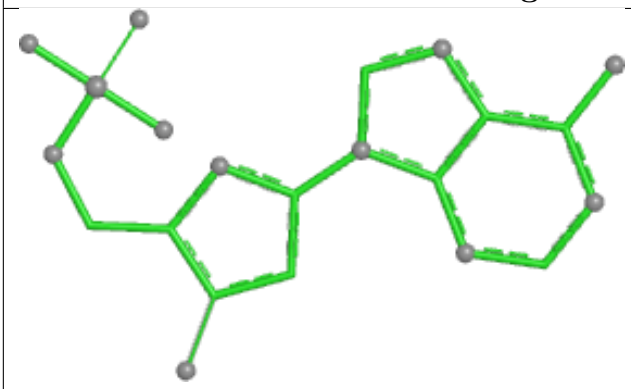


Rings

Ligand D5M K 801



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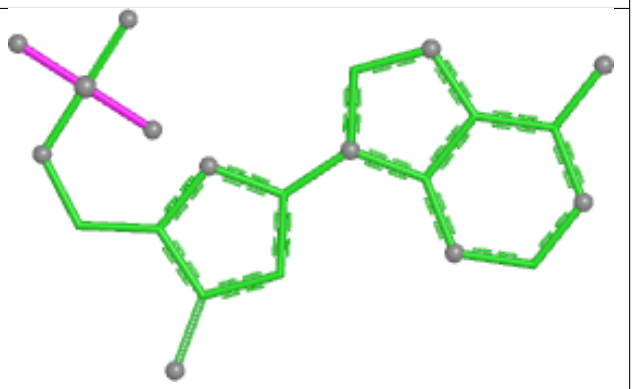

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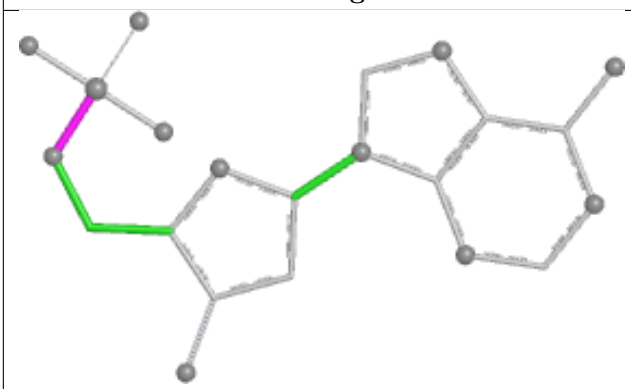

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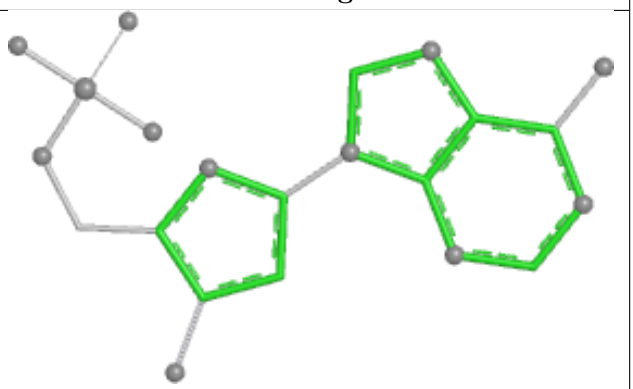
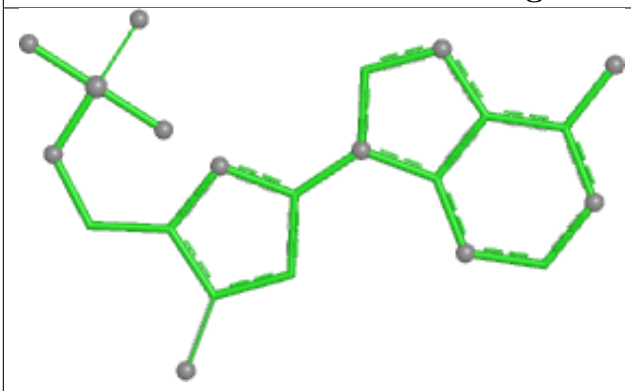


Rings

Ligand D5M 5 801



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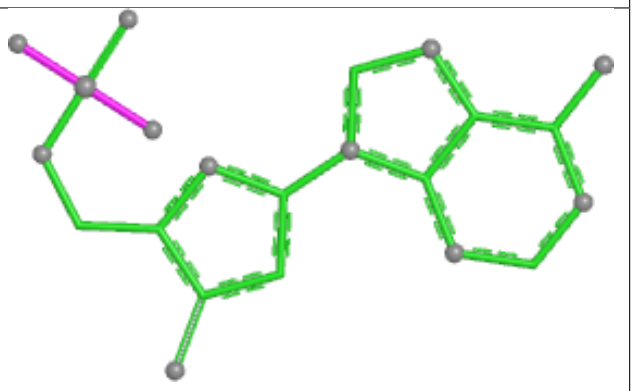

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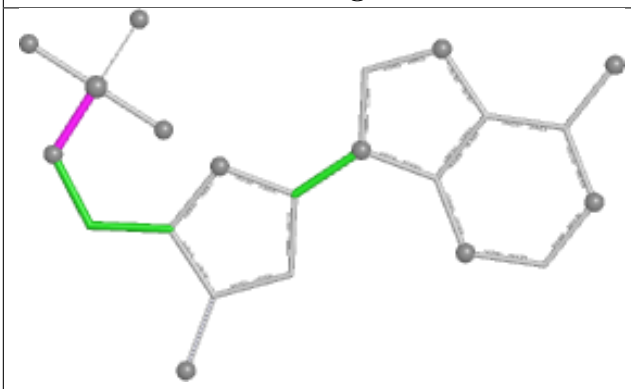

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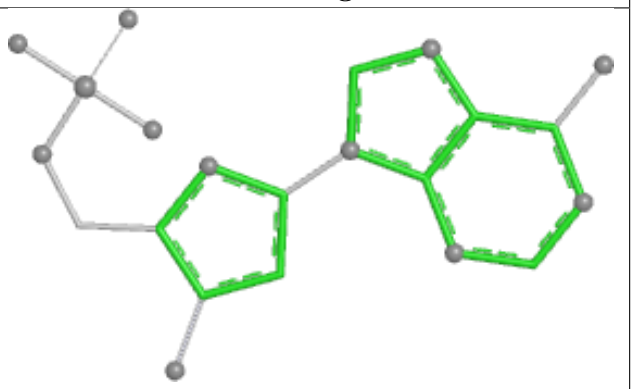
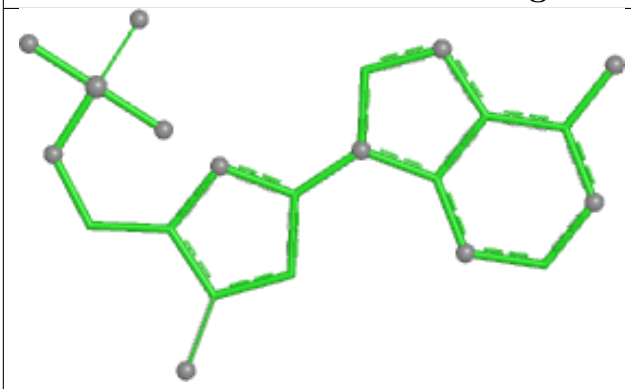


Rings

Ligand D5M f 801



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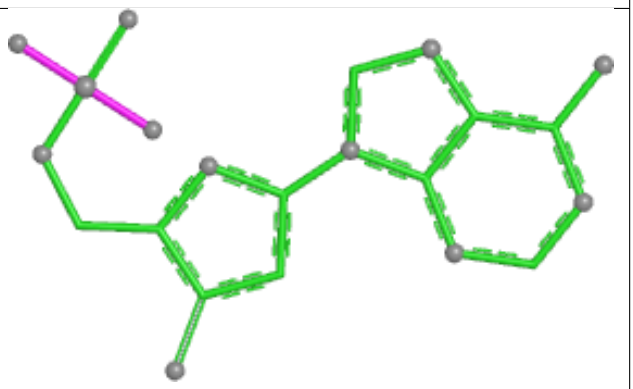

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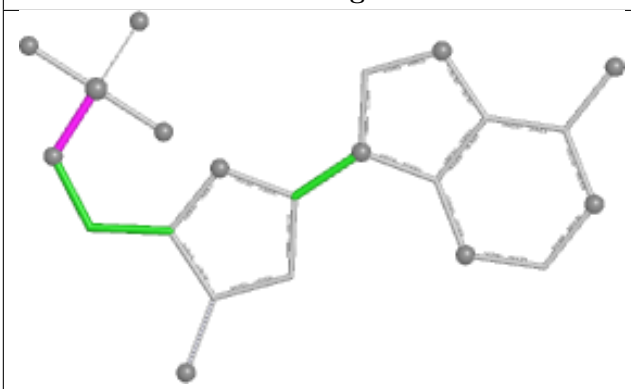

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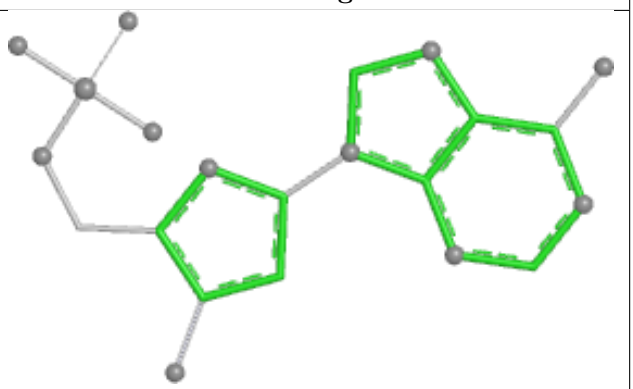
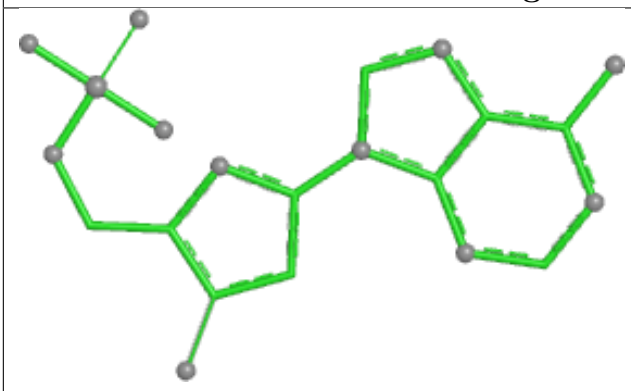


Rings

Ligand D5M E 801



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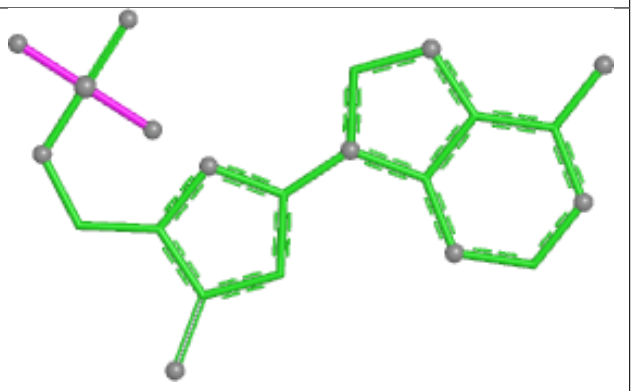

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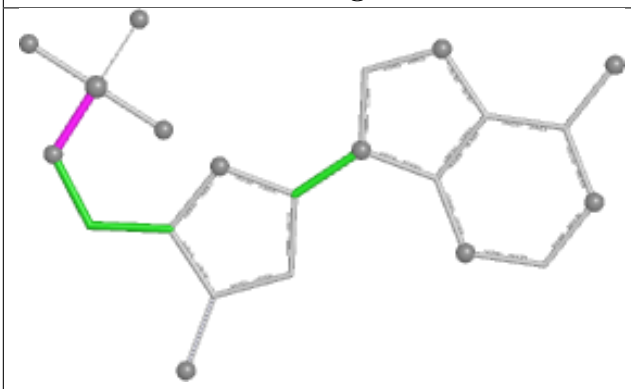

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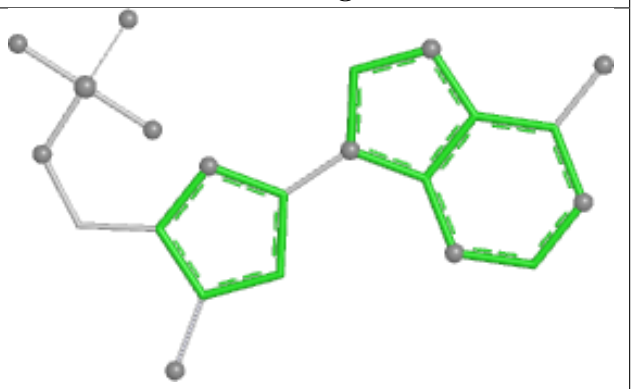

Rings

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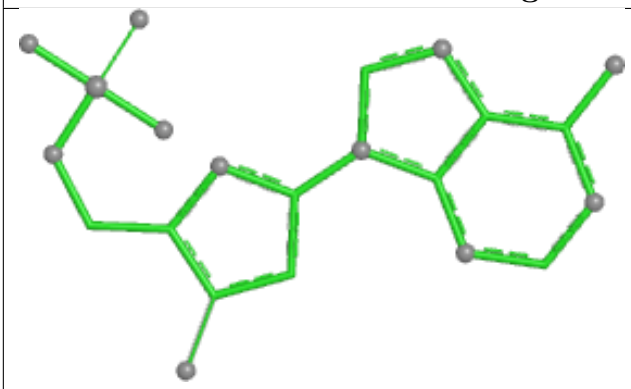

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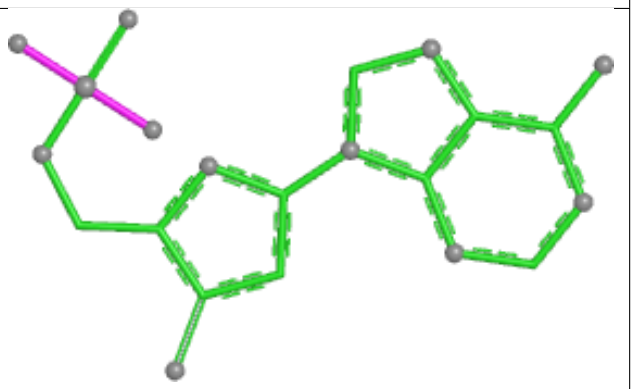

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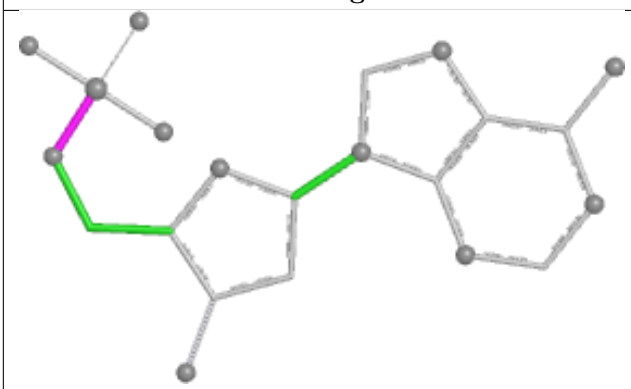

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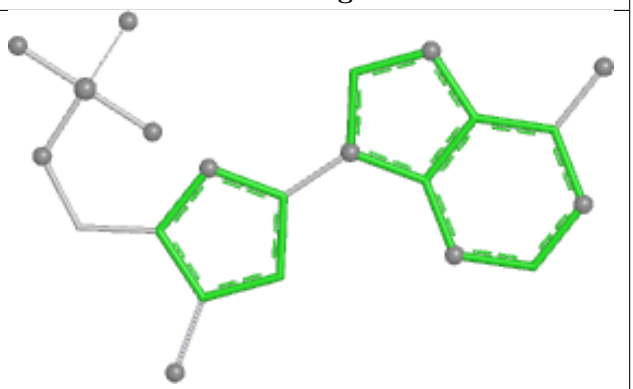

Rings

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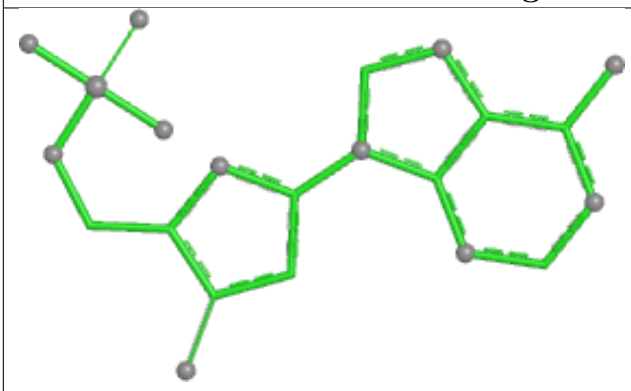

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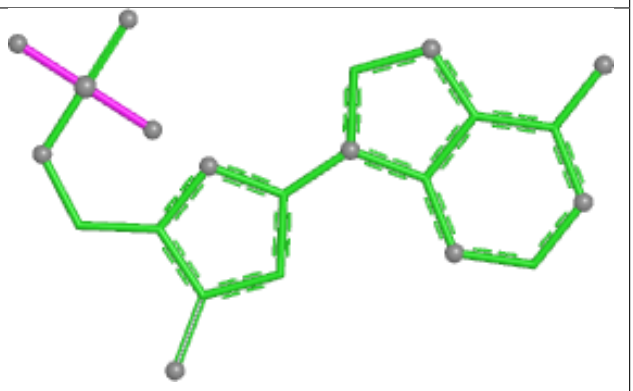

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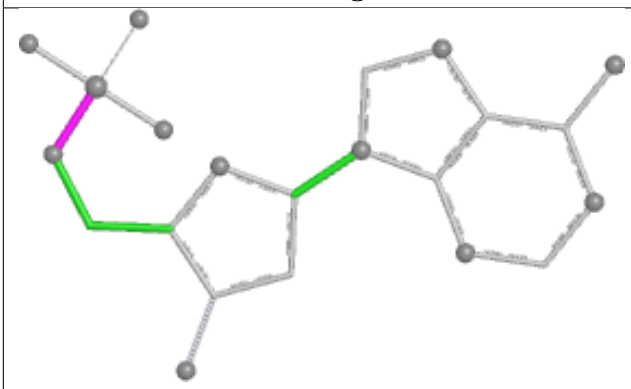

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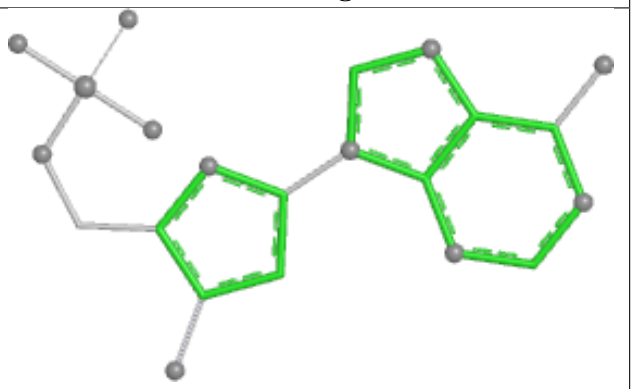
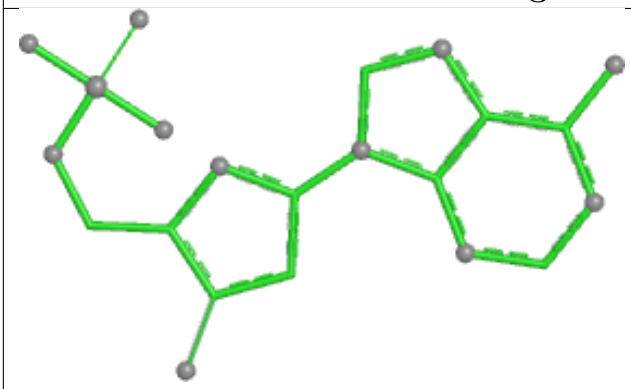


Rings

Ligand D5M j 801



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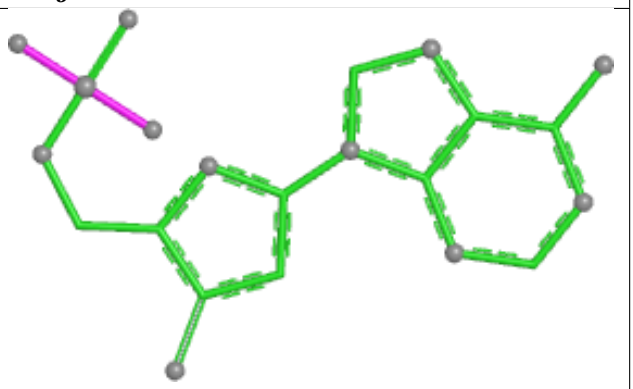

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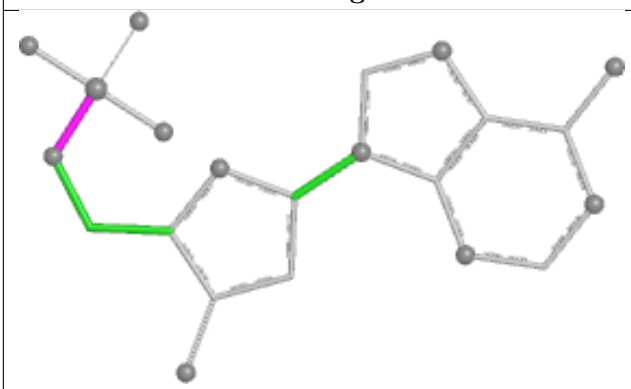

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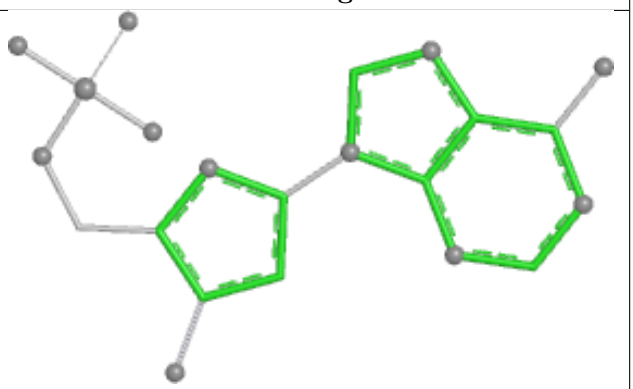

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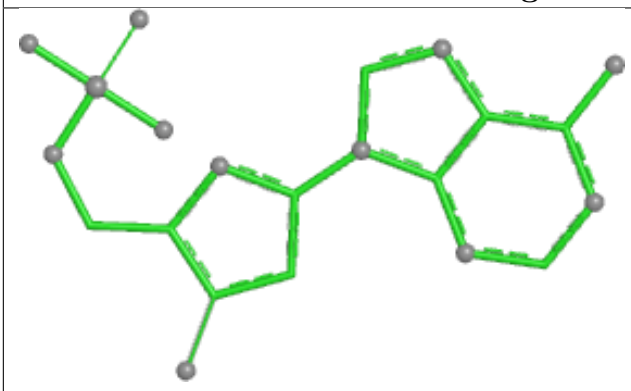

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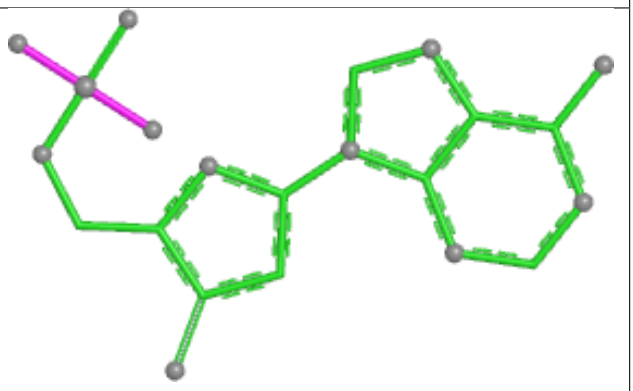

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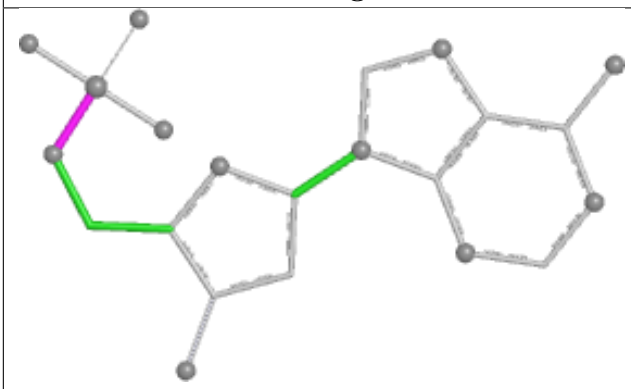

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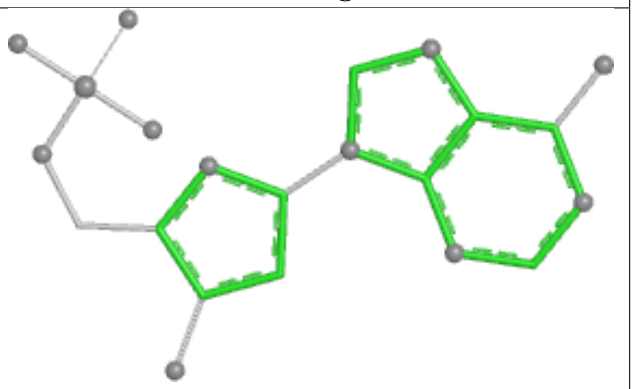

Rings

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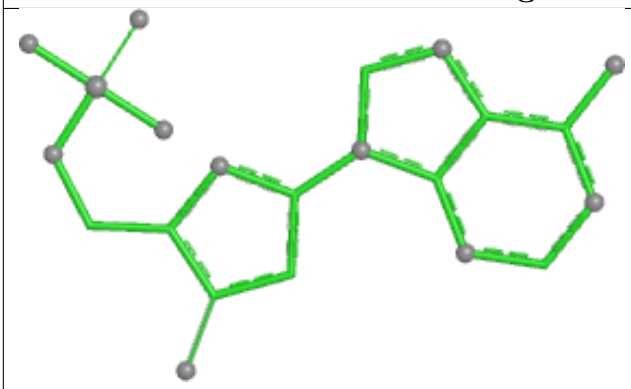

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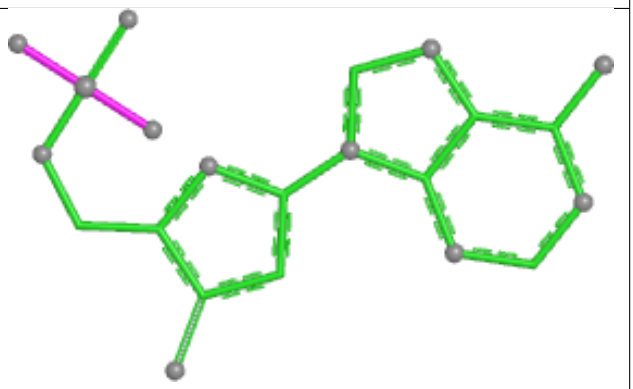

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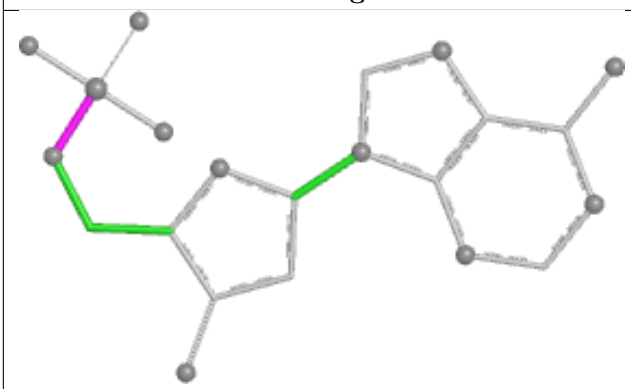

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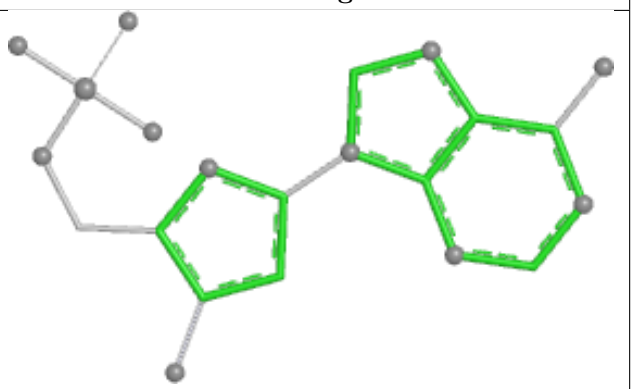

Rings

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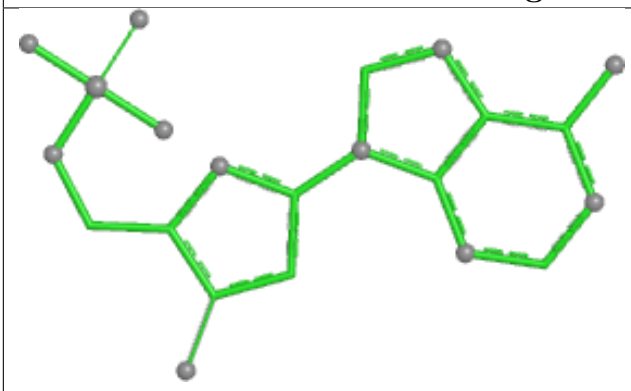

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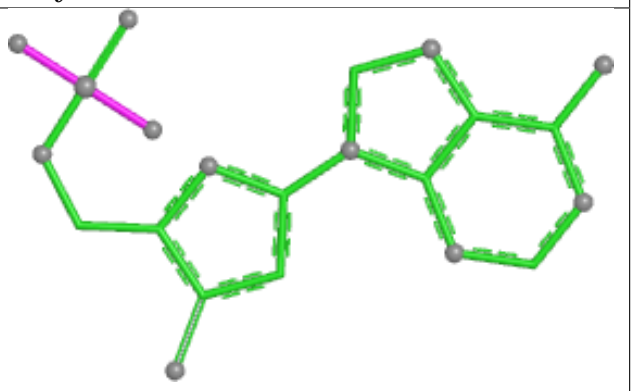

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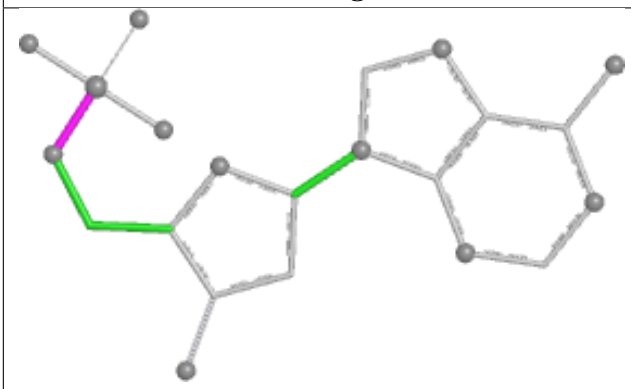

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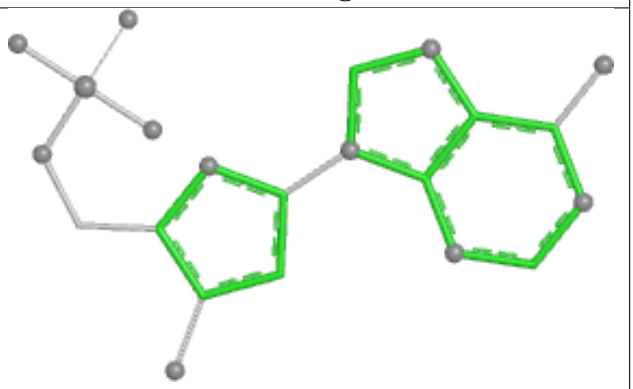

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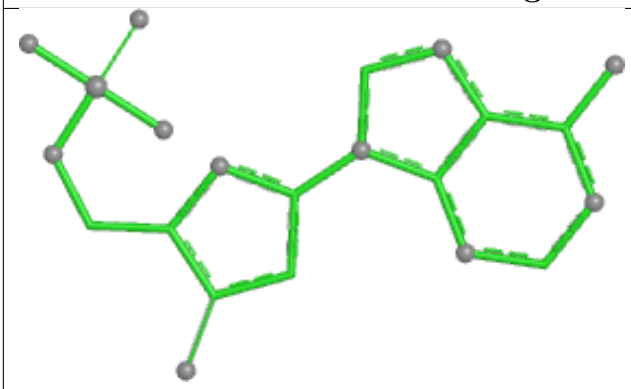

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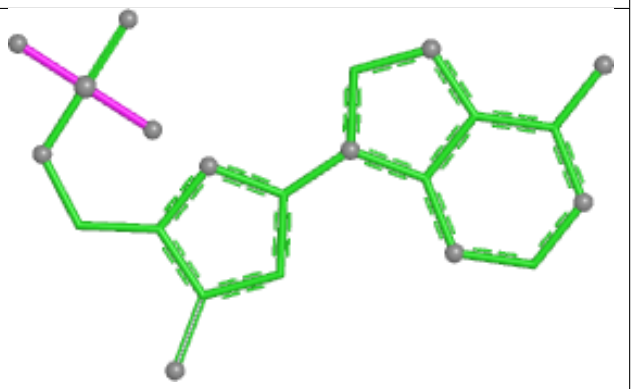

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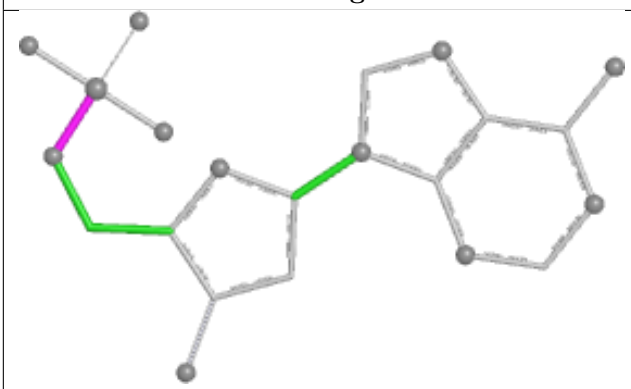

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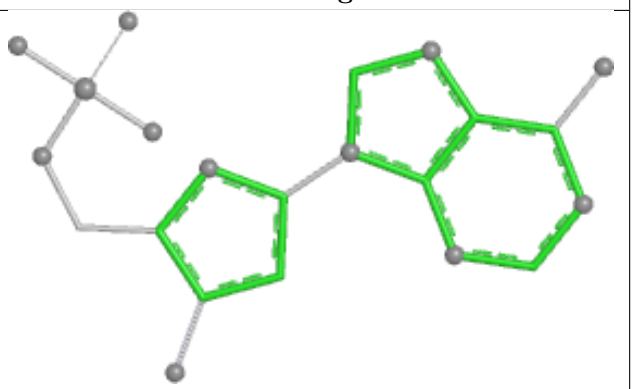

Rings

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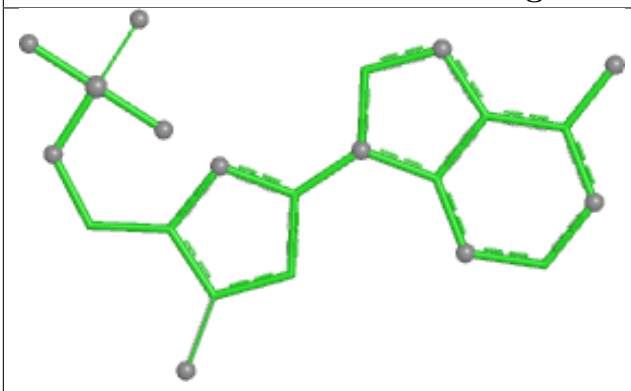

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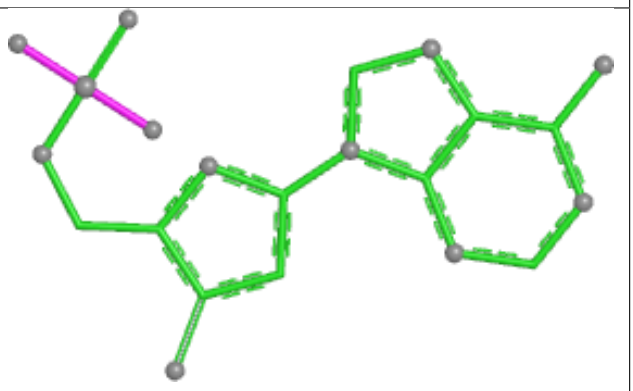

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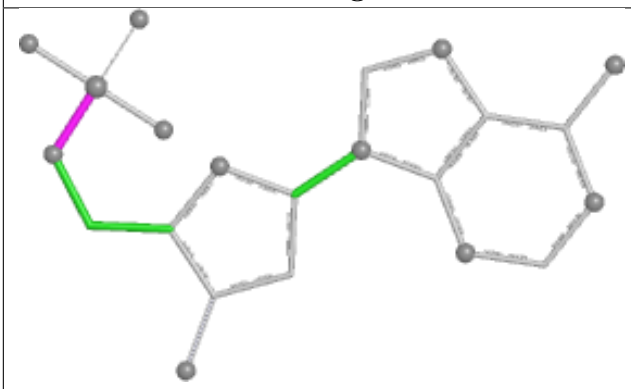

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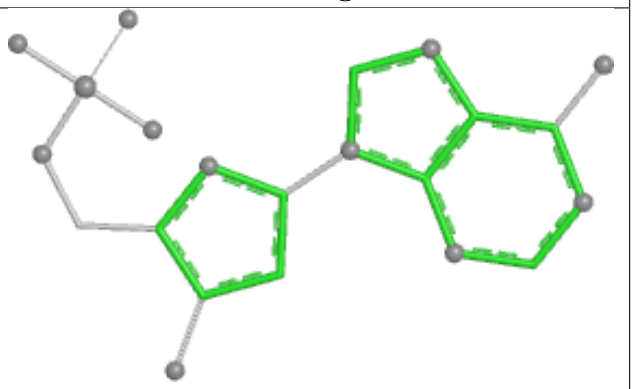
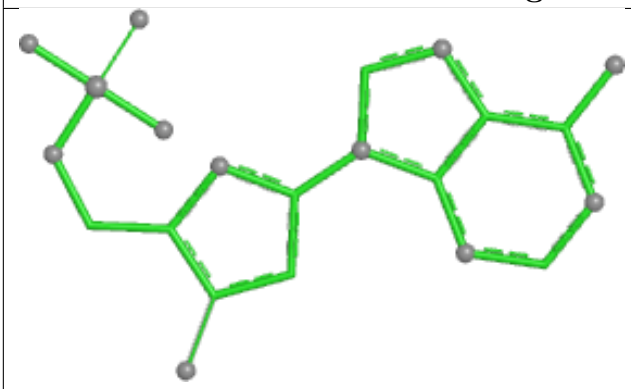


Rings

Ligand D5M 7 801



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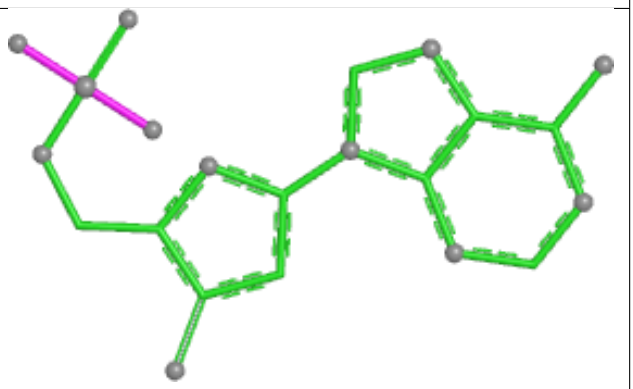

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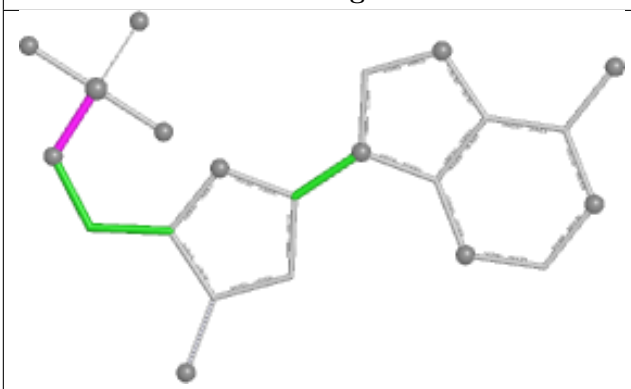

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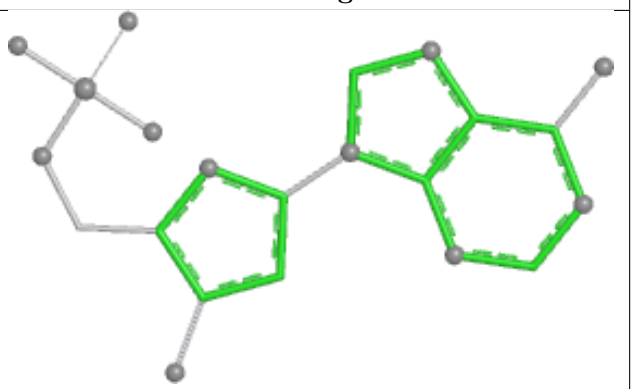
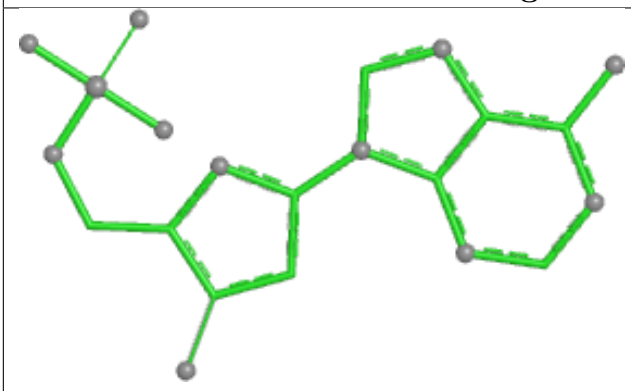


Rings

Ligand D5M H 801



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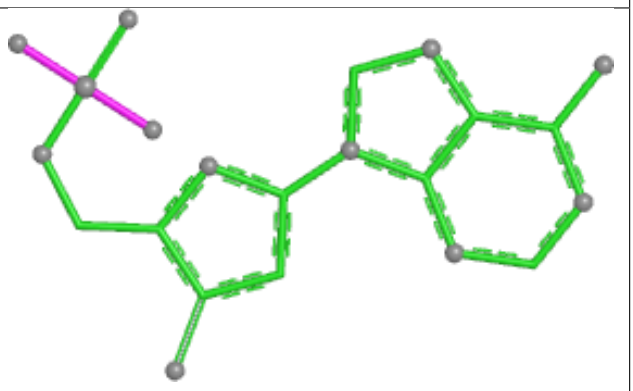

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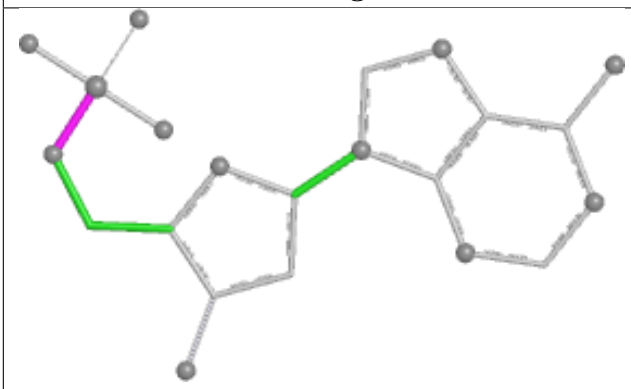

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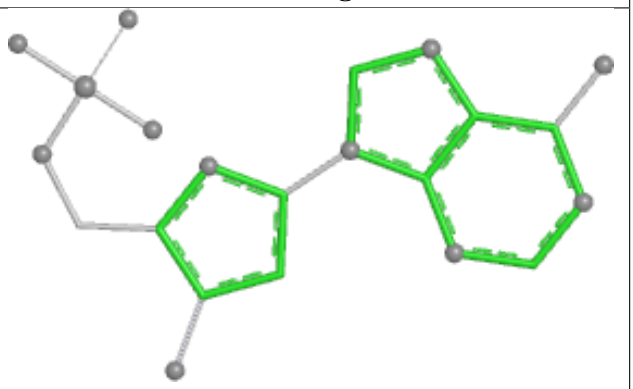
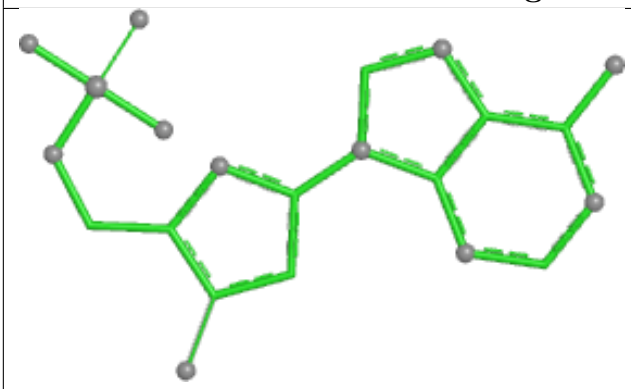


Rings

Ligand D5M b 801



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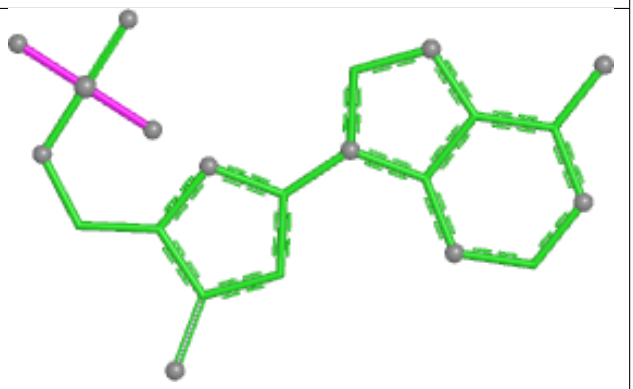
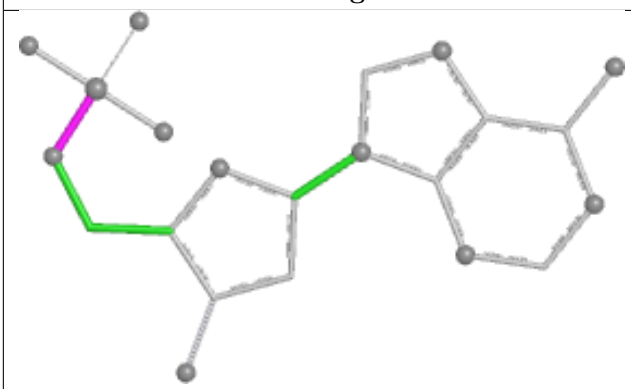


Bond angles



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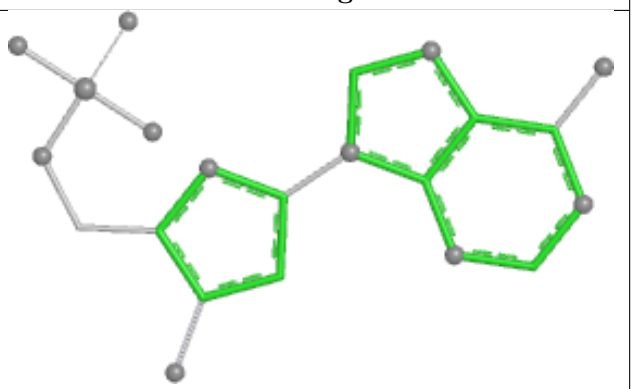
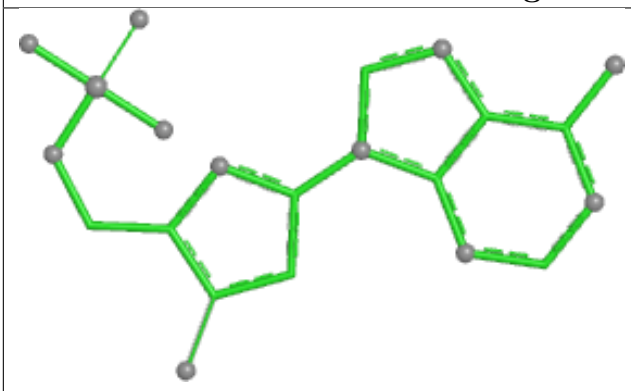


Rings

Ligand D5M F 801



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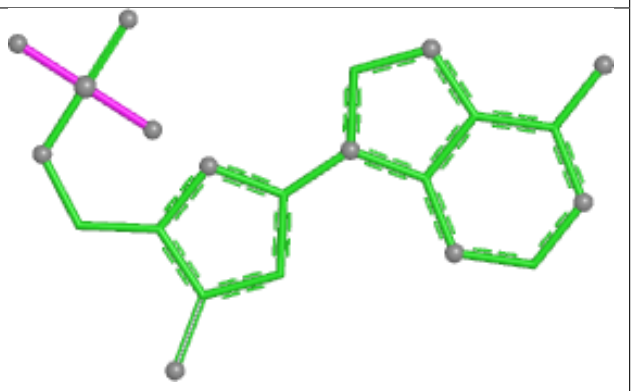
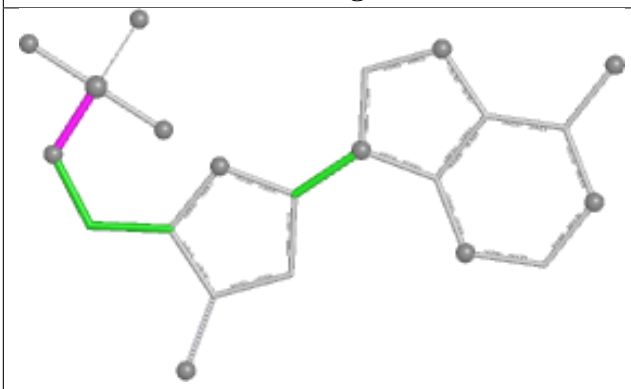


Bond angles



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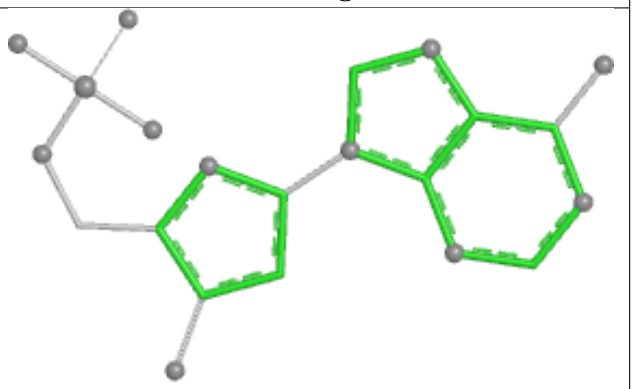

Rings

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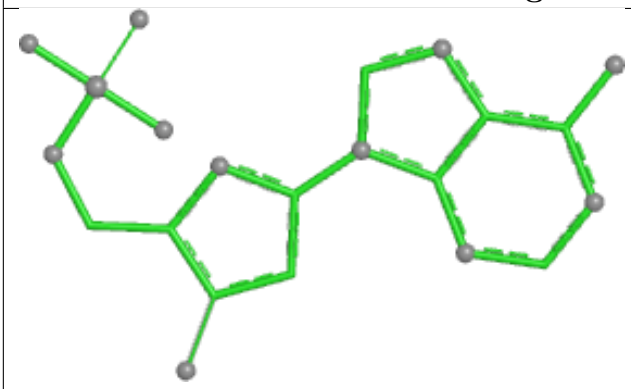

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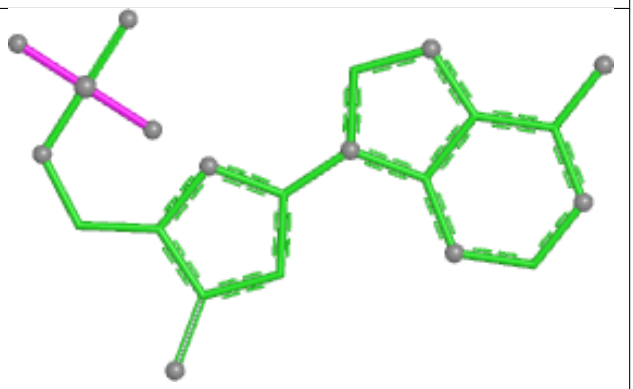

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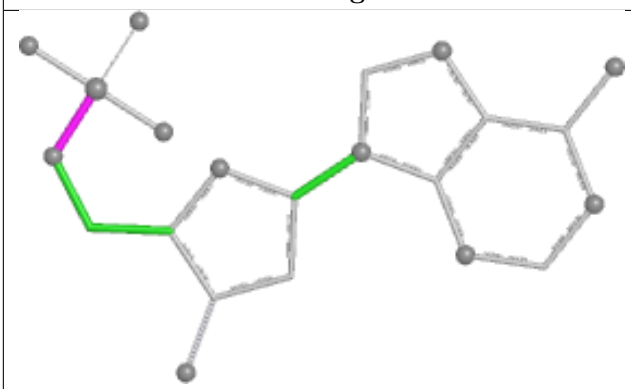

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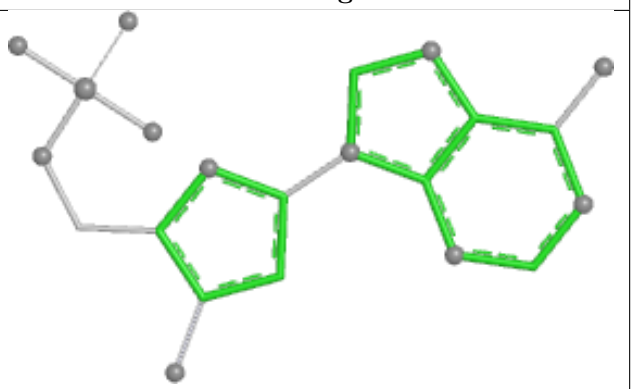

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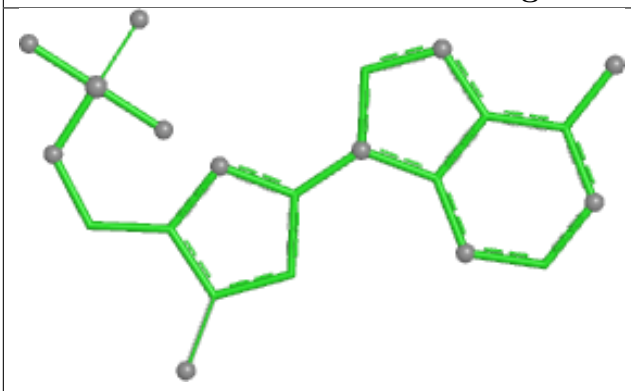

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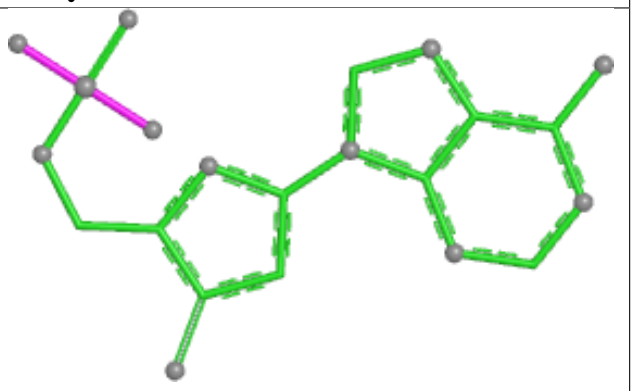

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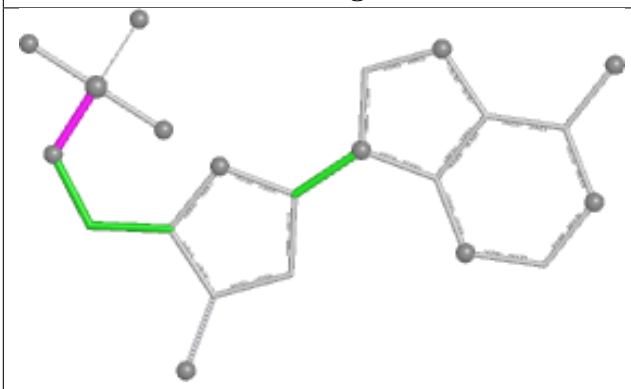

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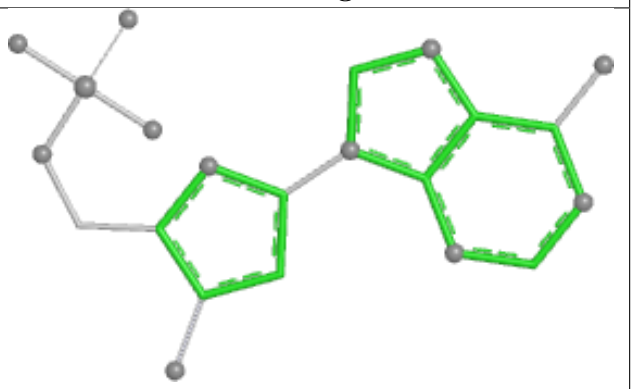

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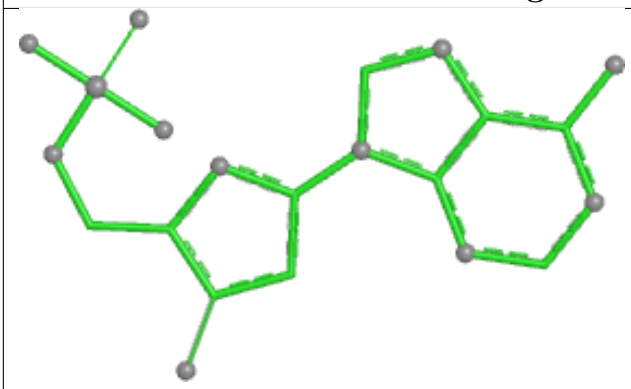

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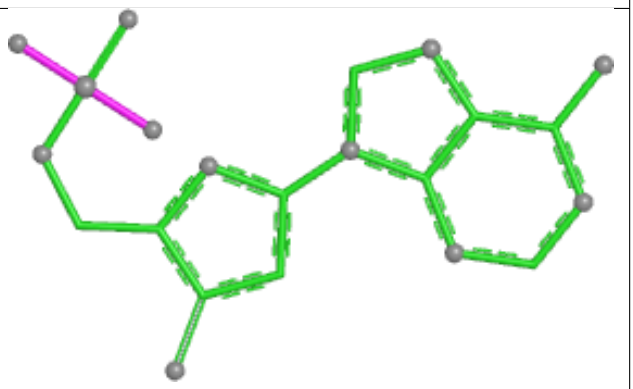

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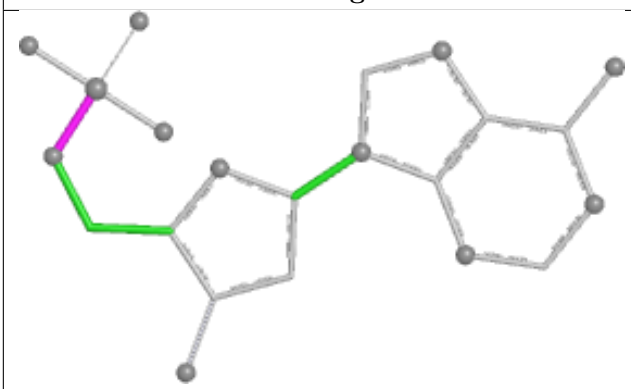

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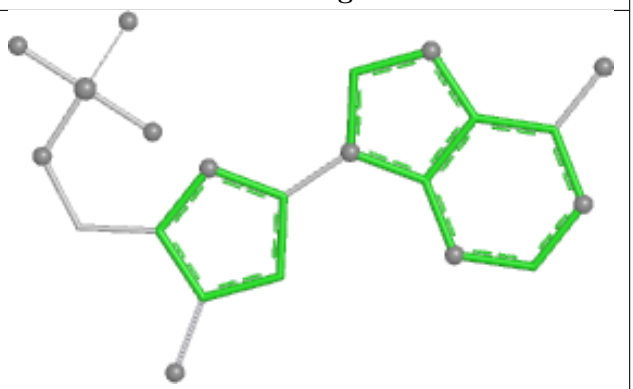

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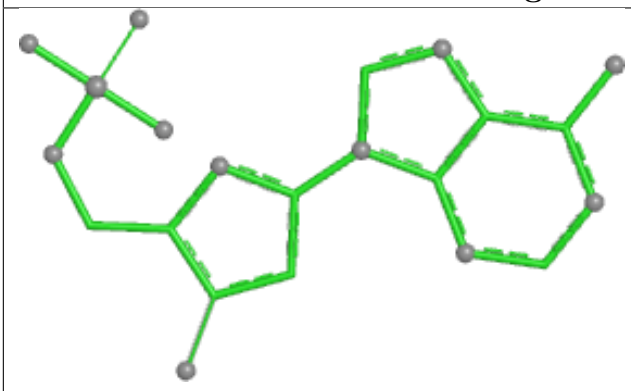

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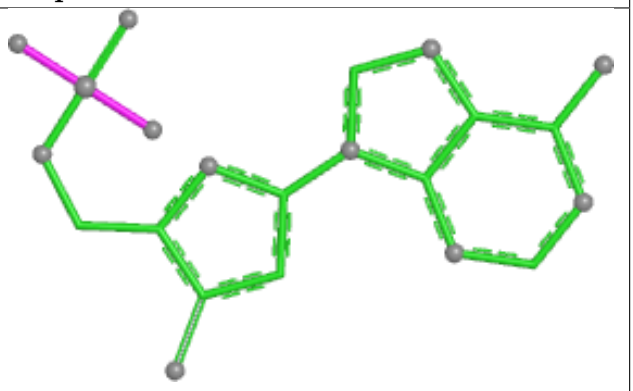

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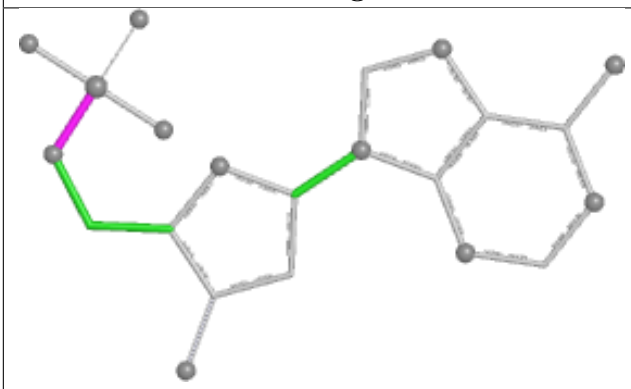

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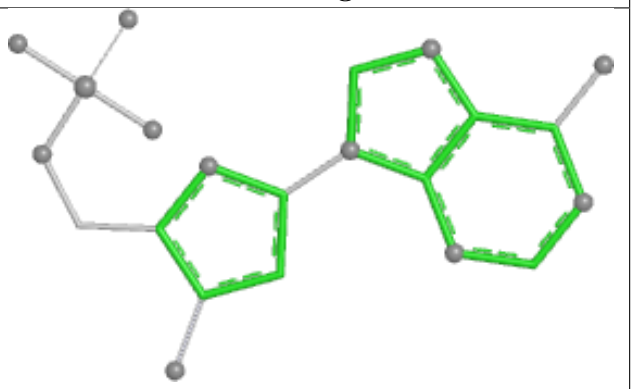

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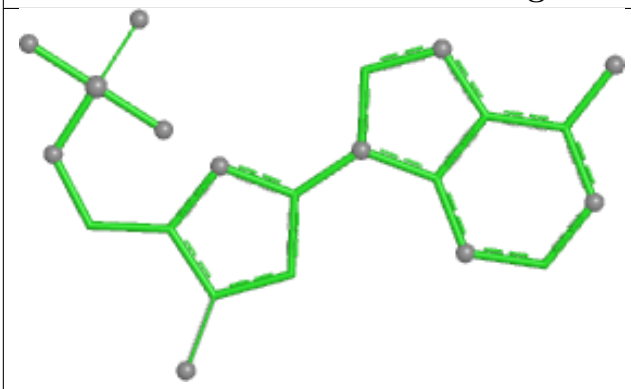

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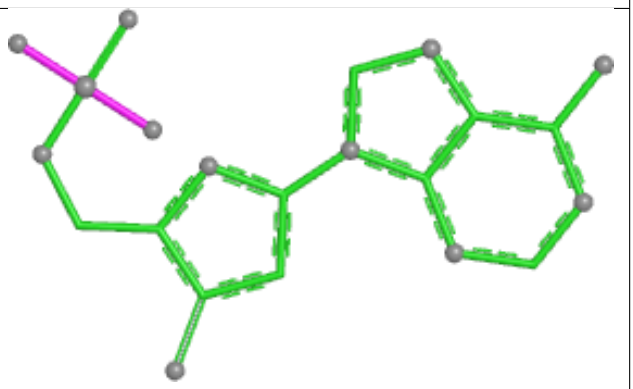

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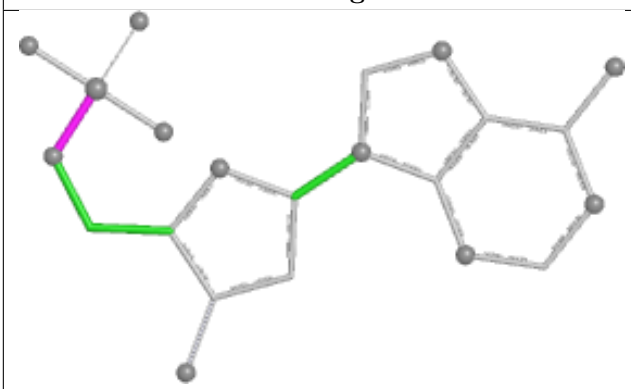

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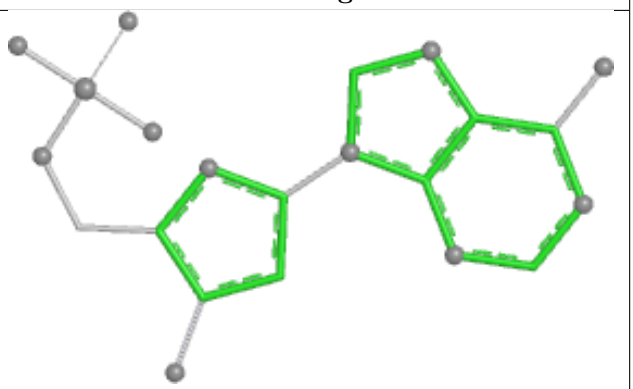

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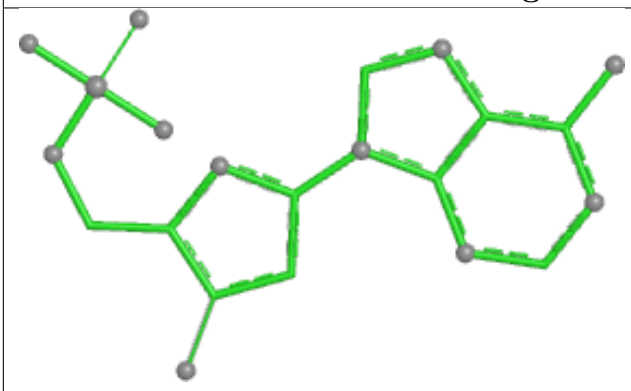

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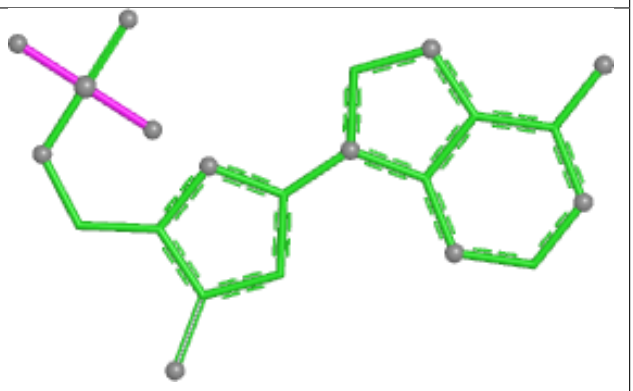

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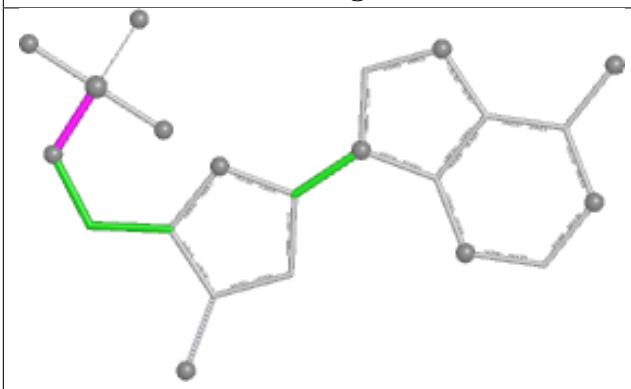

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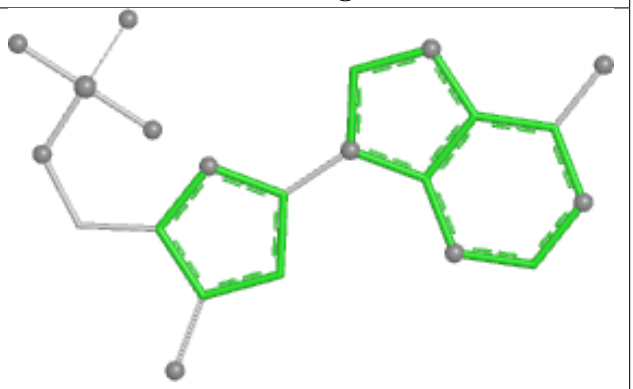

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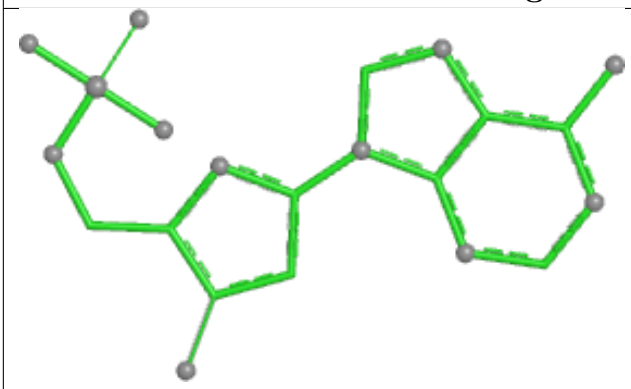

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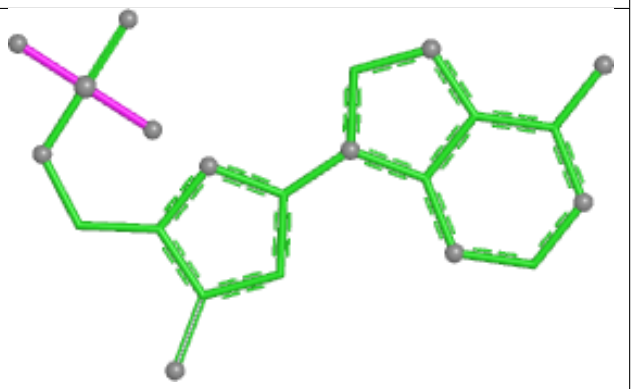

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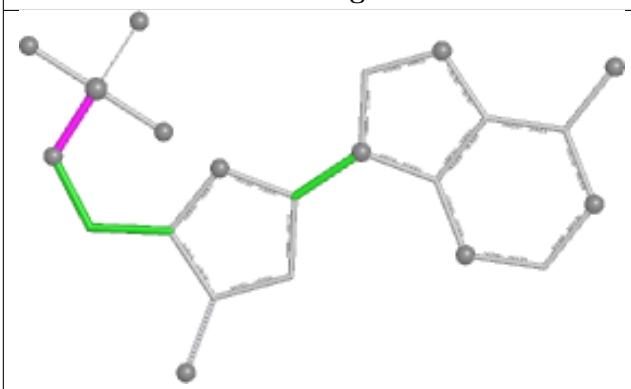

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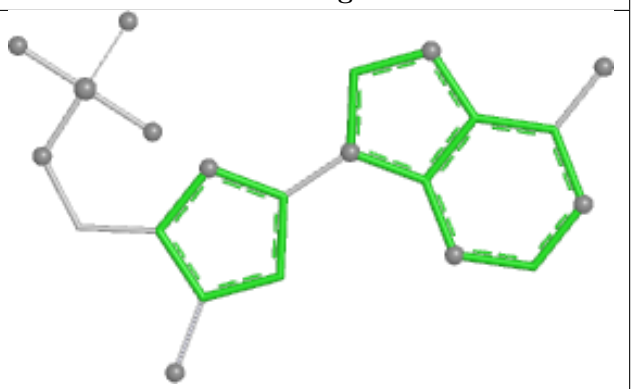

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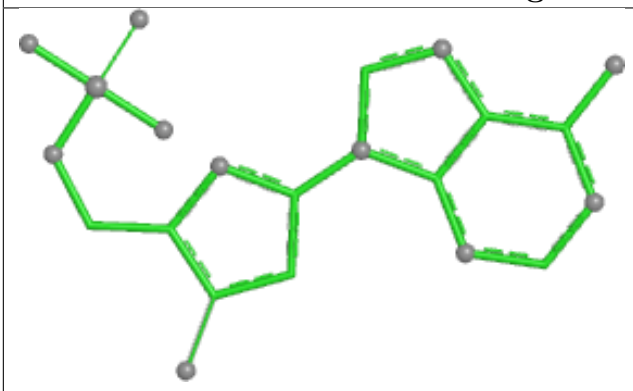

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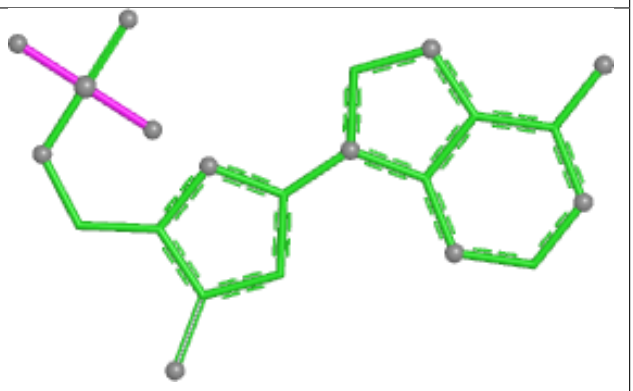

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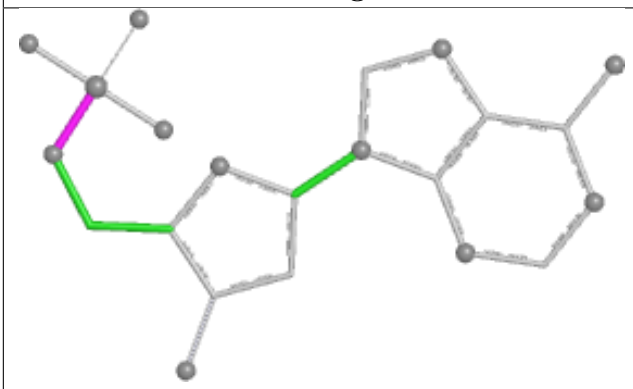

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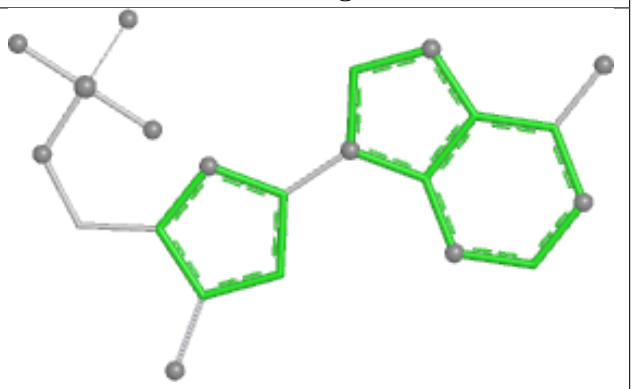

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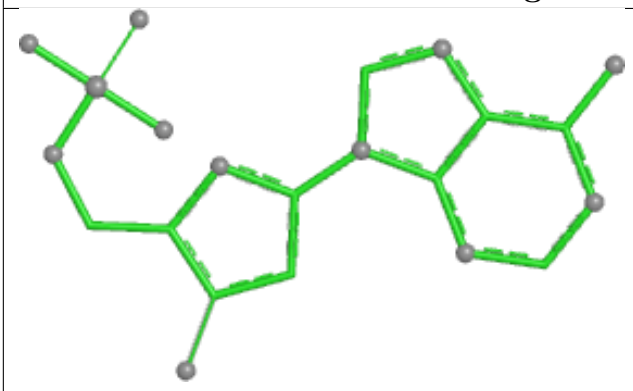

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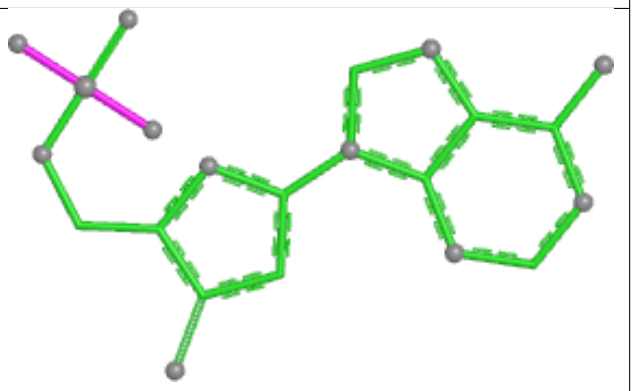

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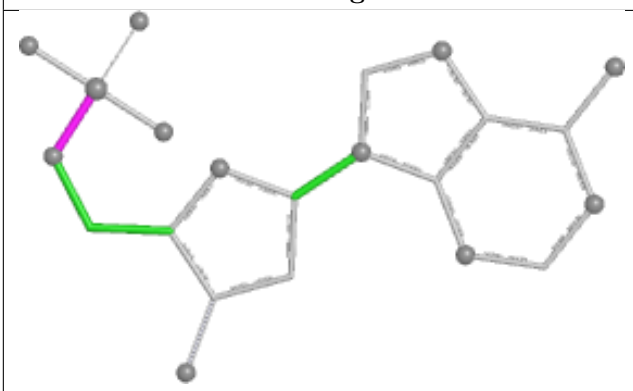

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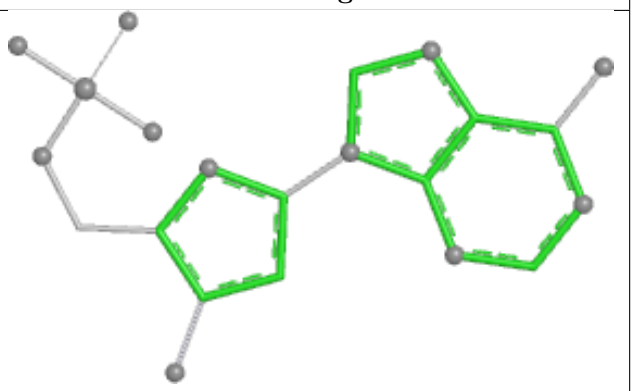

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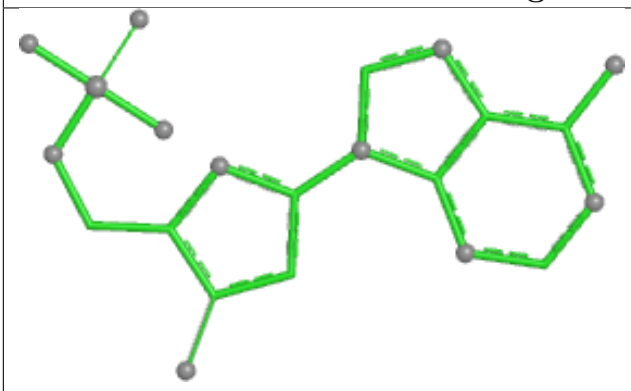

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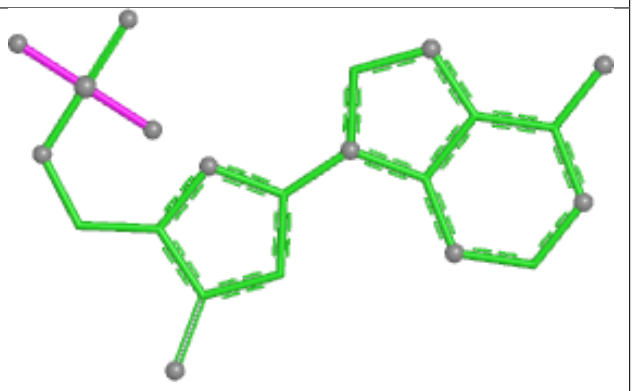

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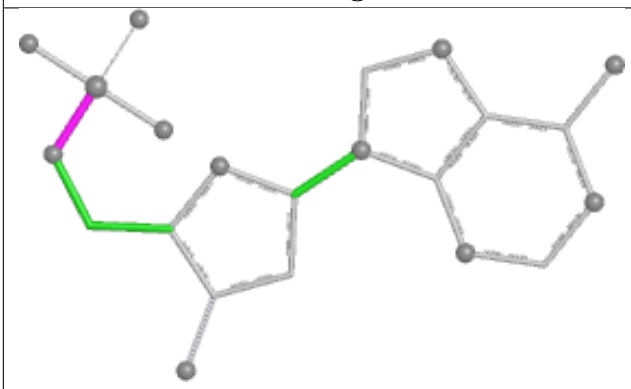

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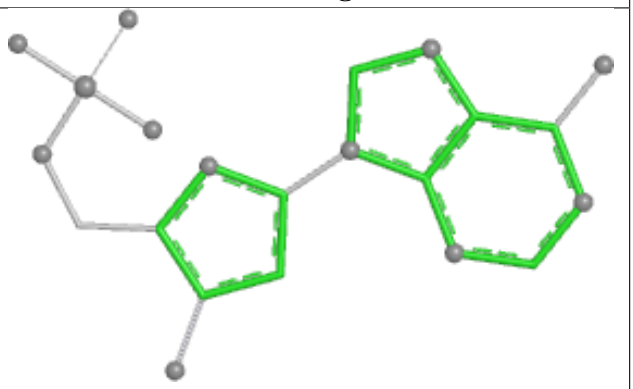

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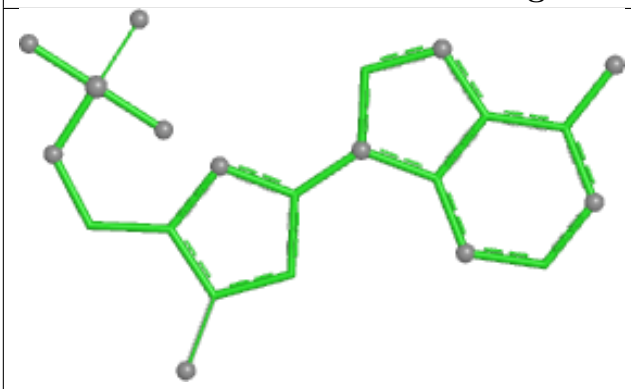

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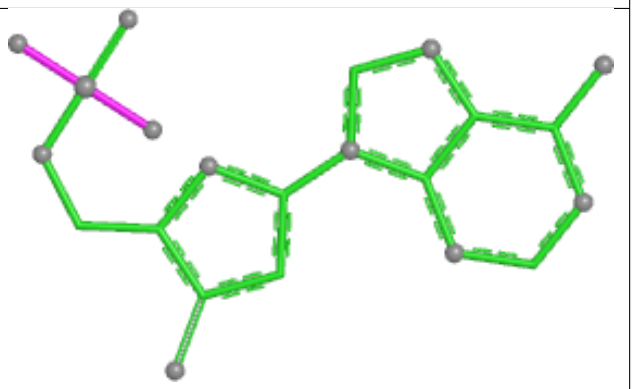

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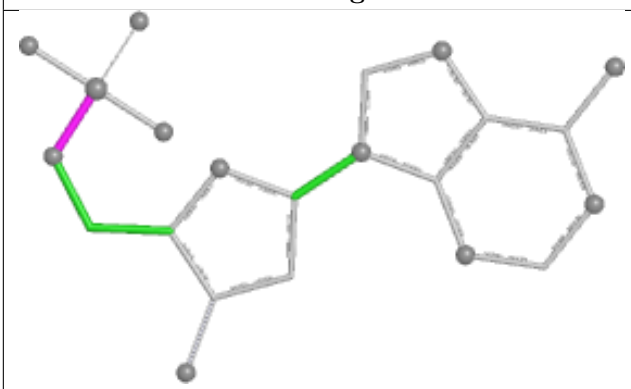

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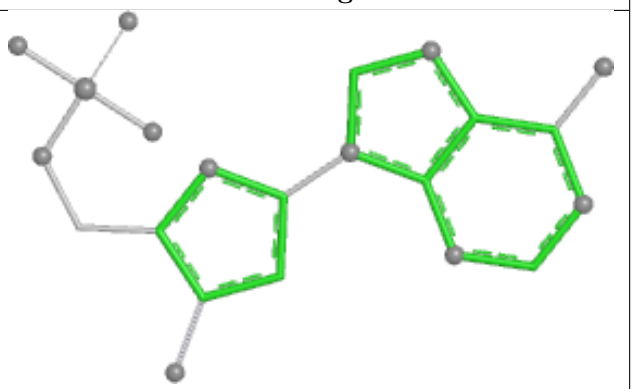

Rings

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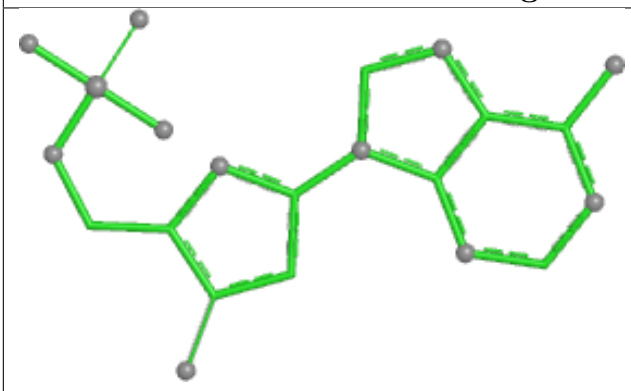

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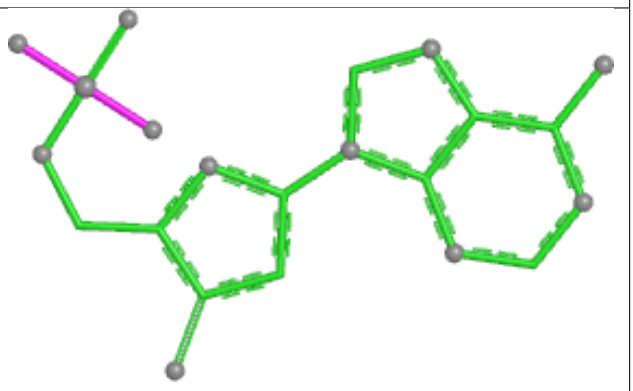

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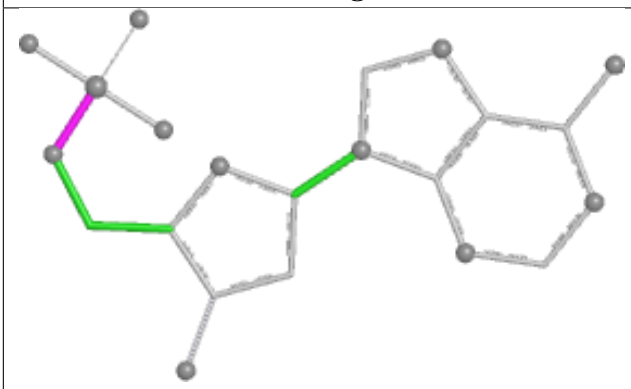

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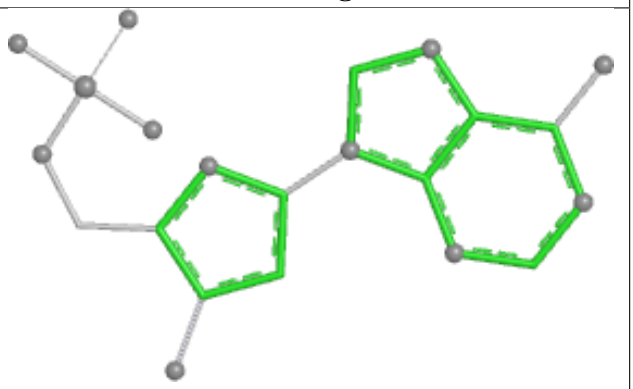

Rings

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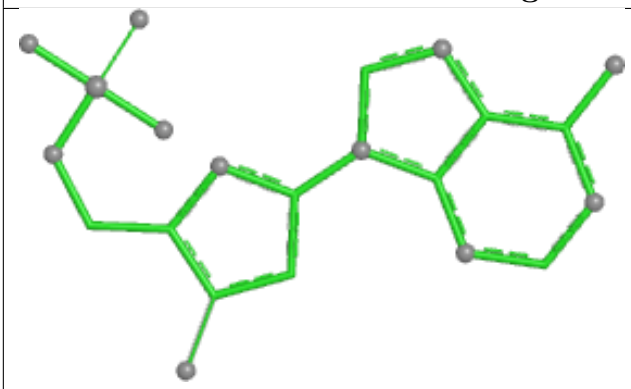

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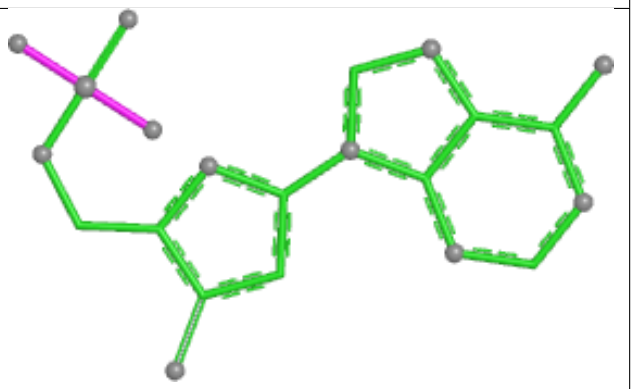

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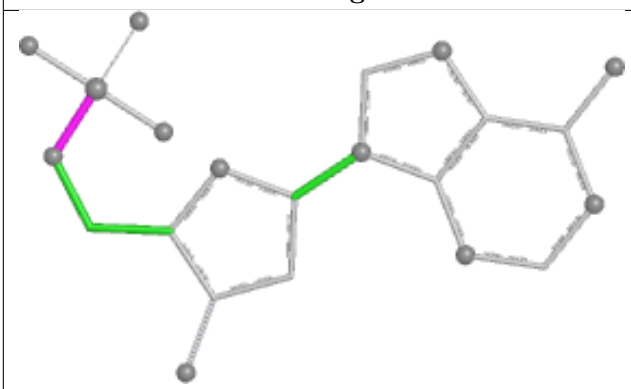

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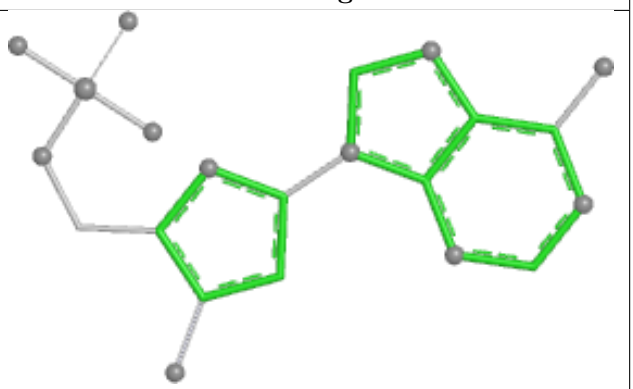
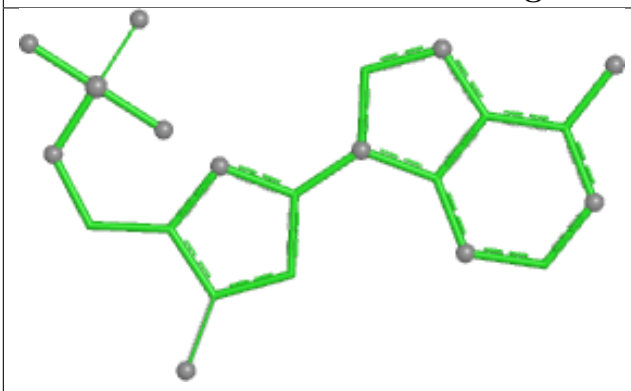


Rings

Ligand D5M d 801



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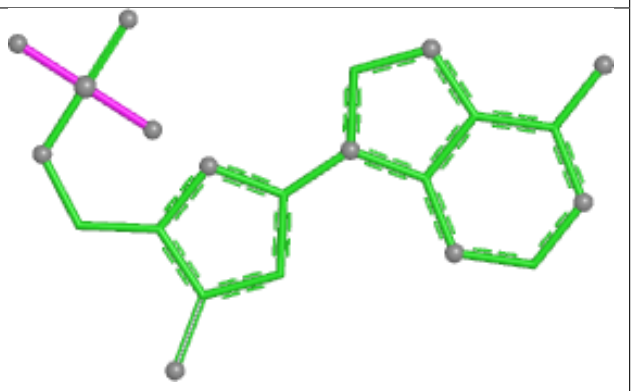

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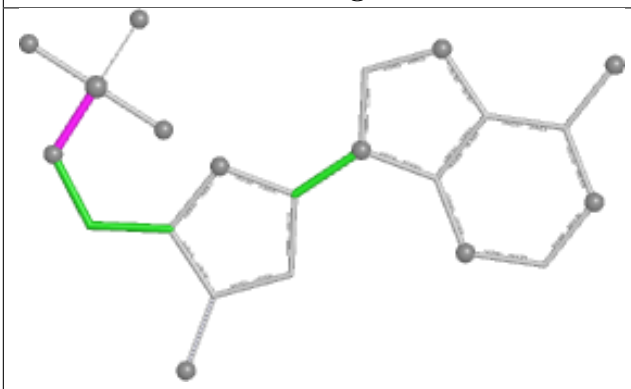
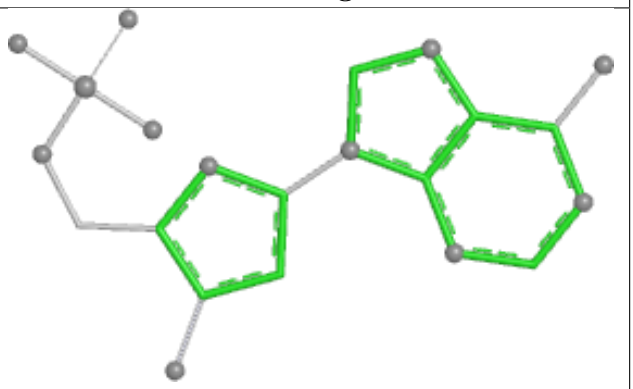


Torsions



Rings

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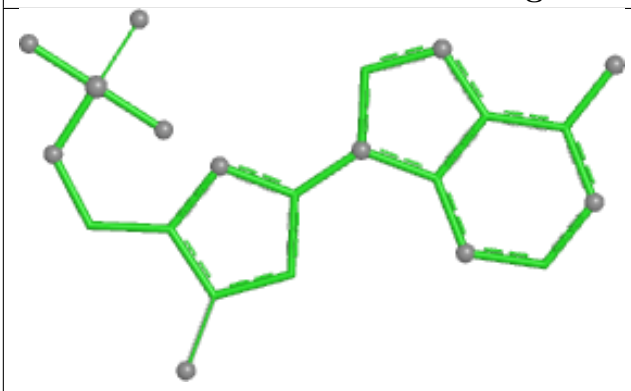

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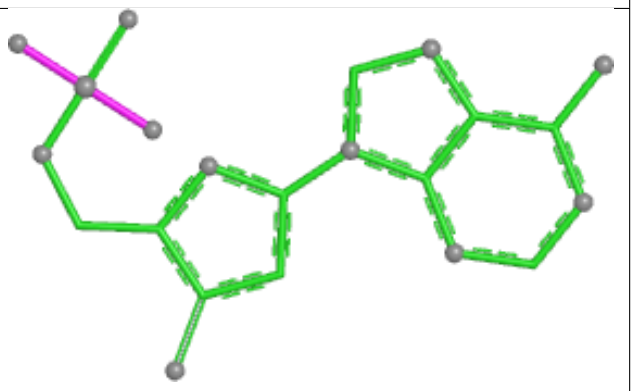

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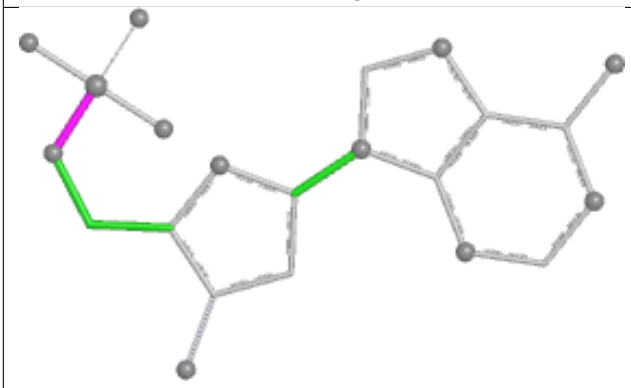

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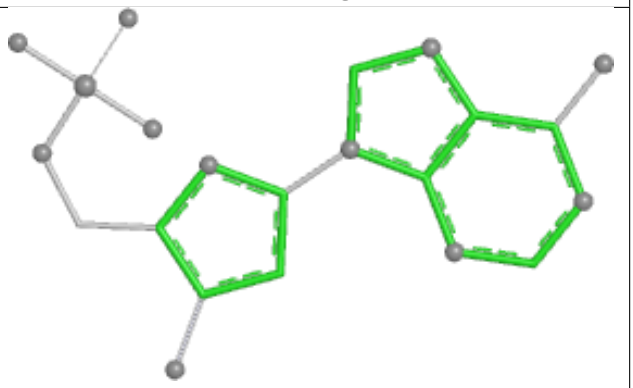

Rings

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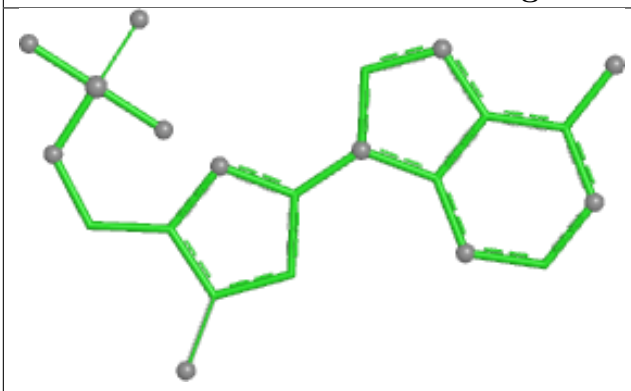

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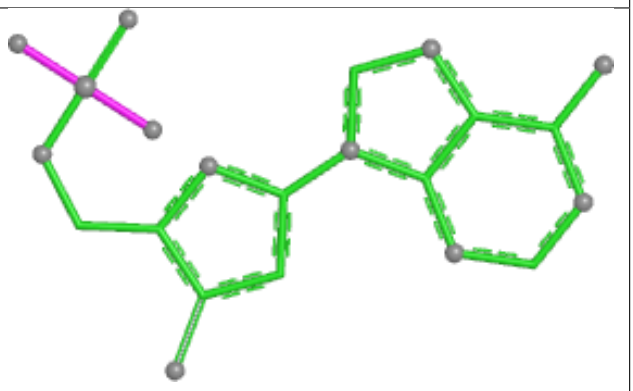

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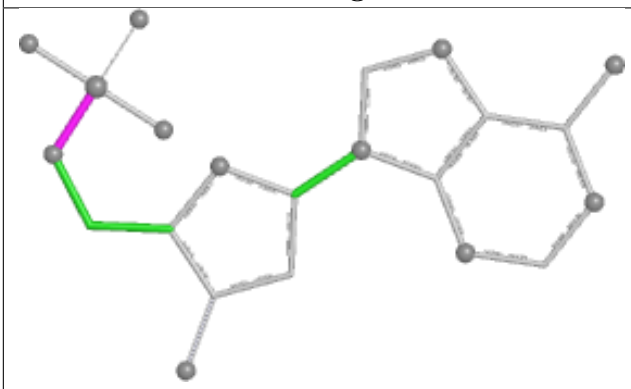

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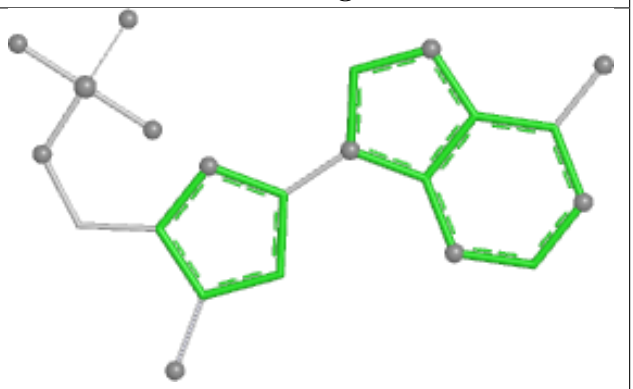

Rings

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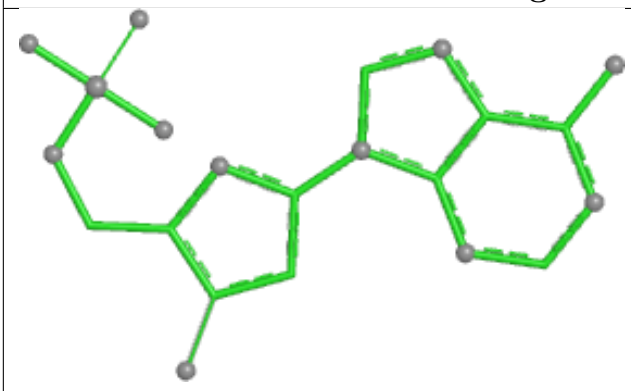

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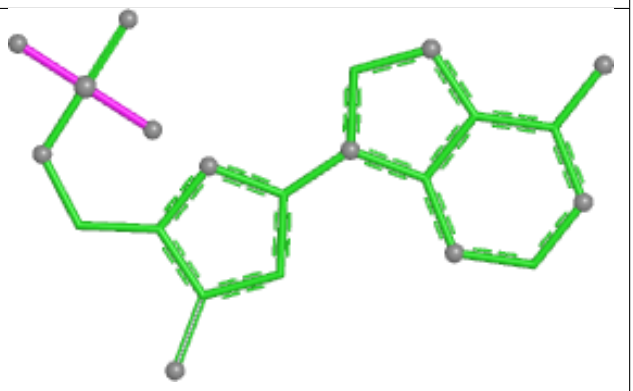

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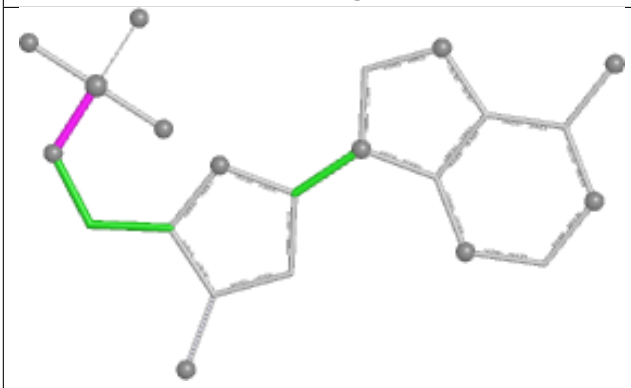

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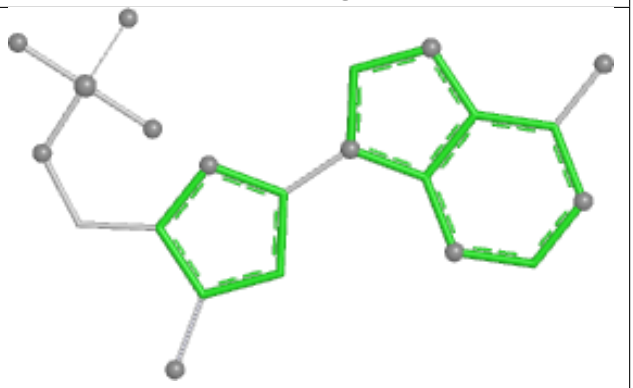

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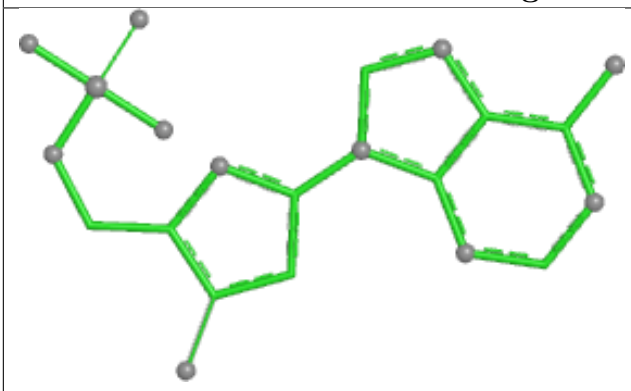

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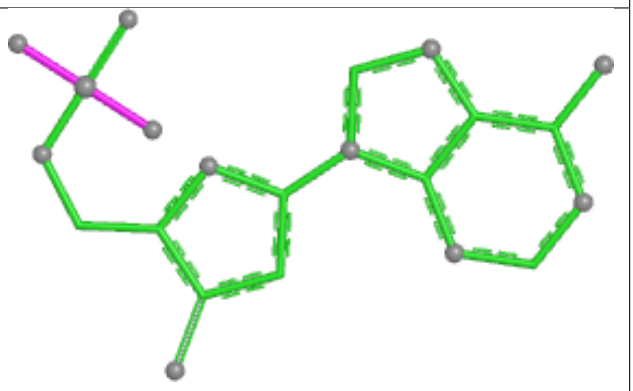

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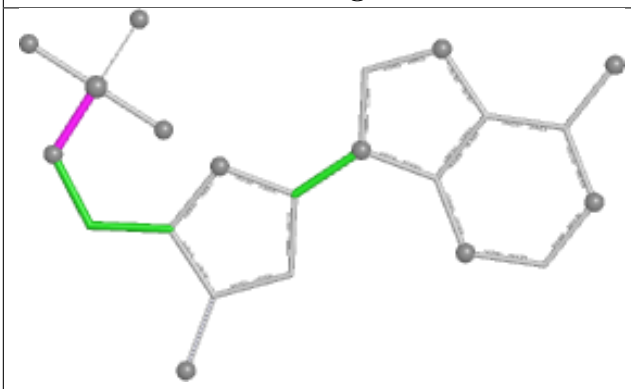

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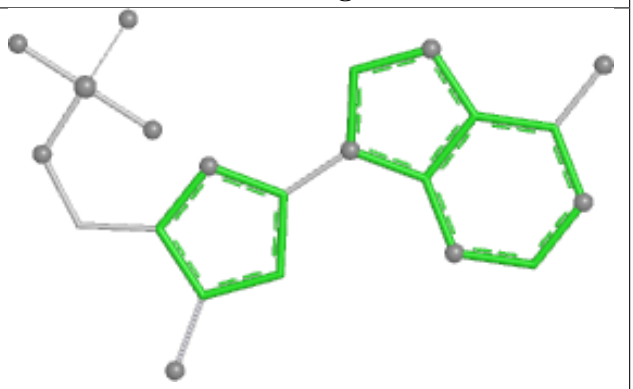

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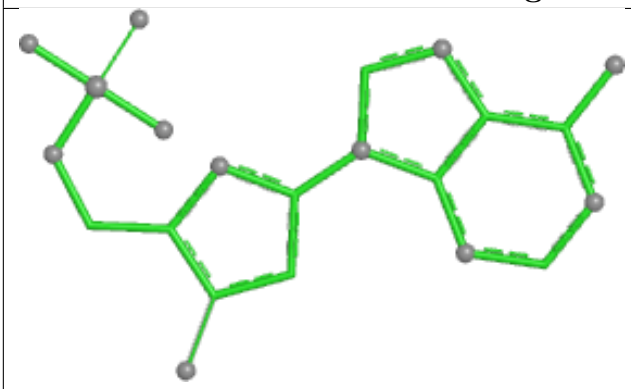

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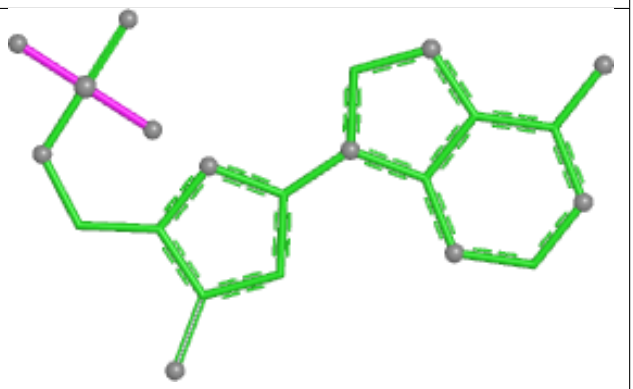

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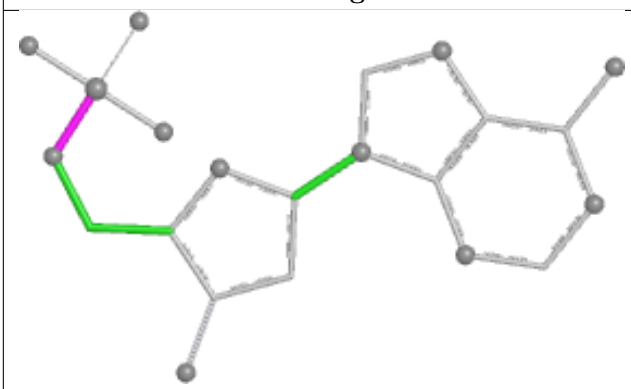

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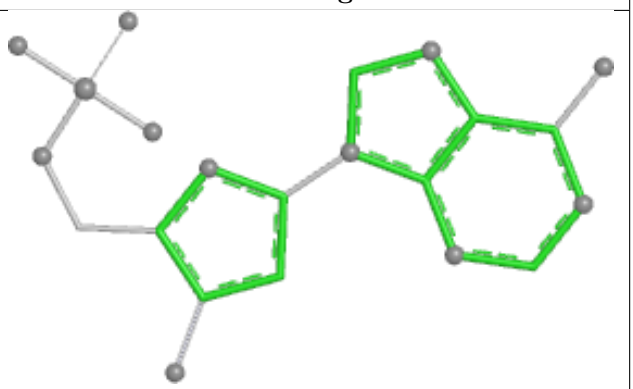

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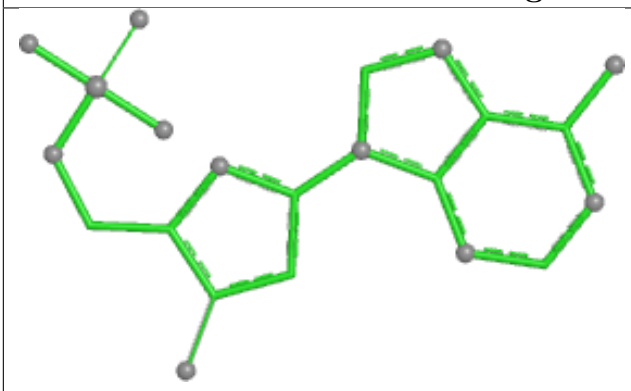

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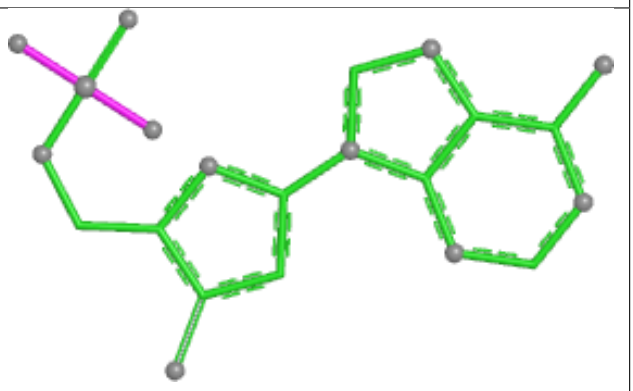

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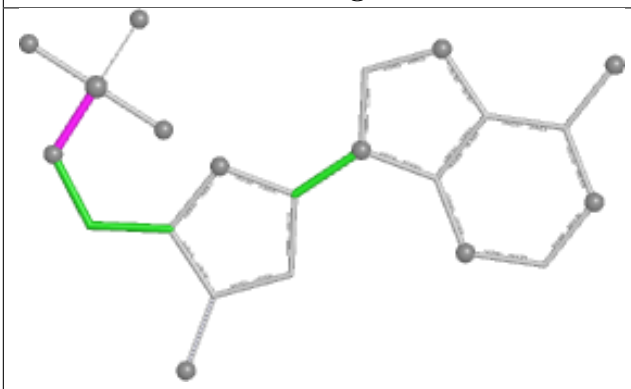

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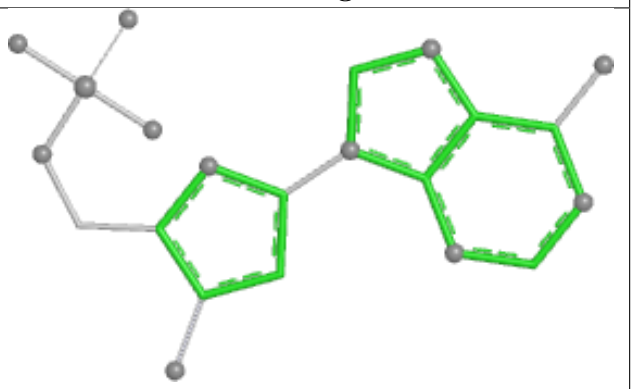

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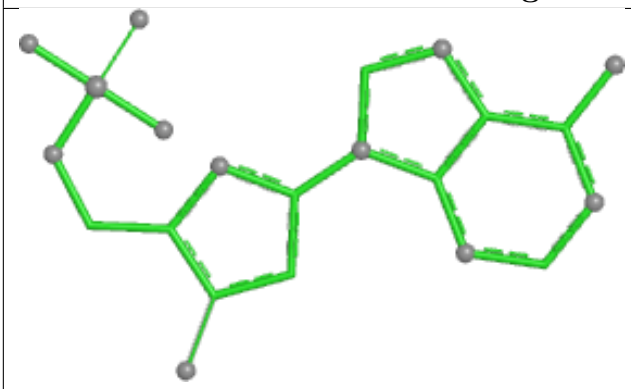

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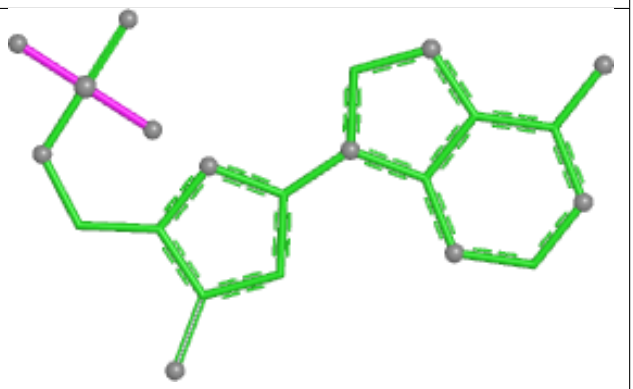

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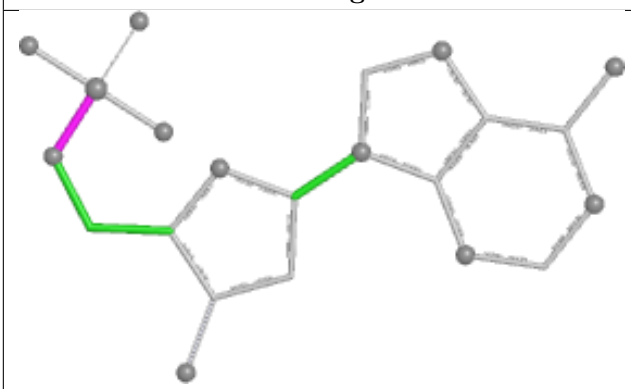

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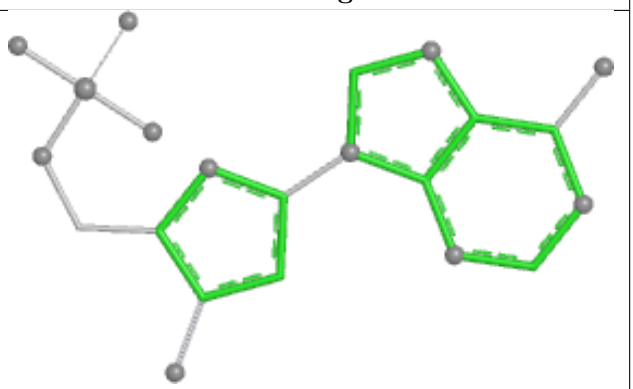

Rings

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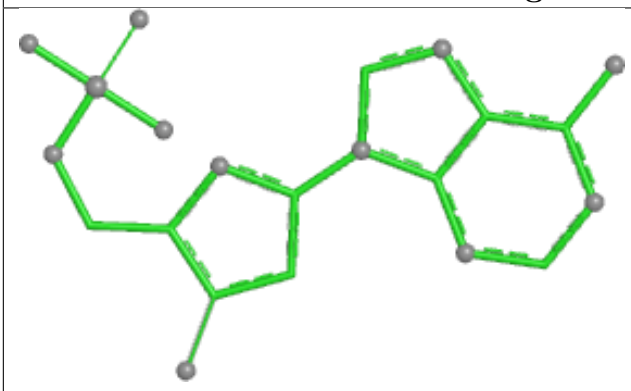

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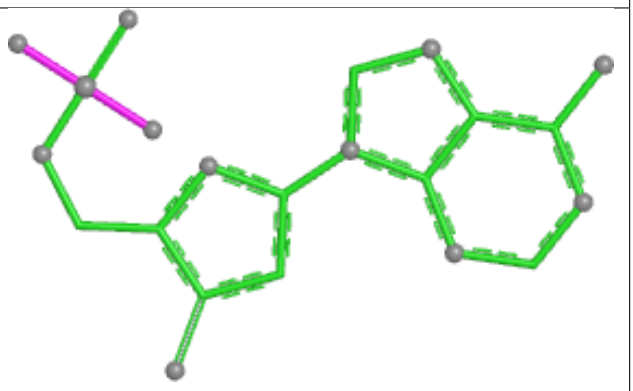

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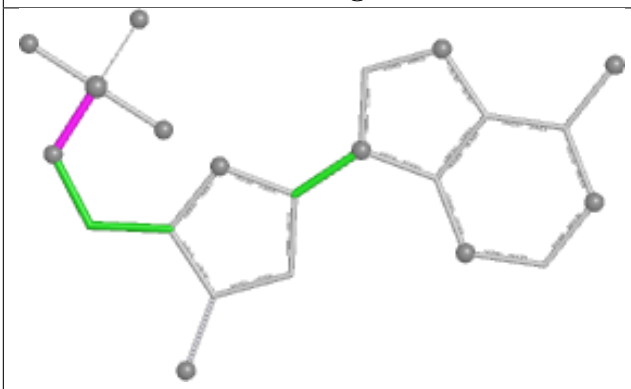

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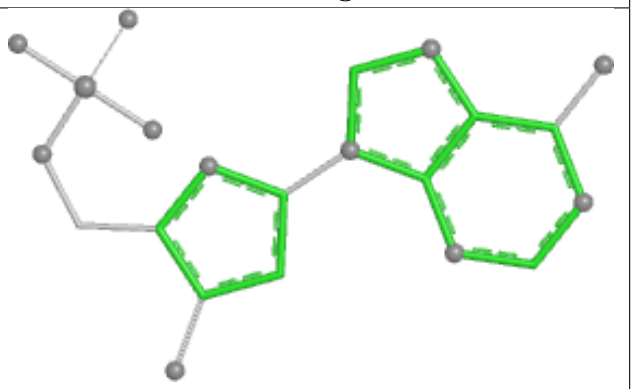

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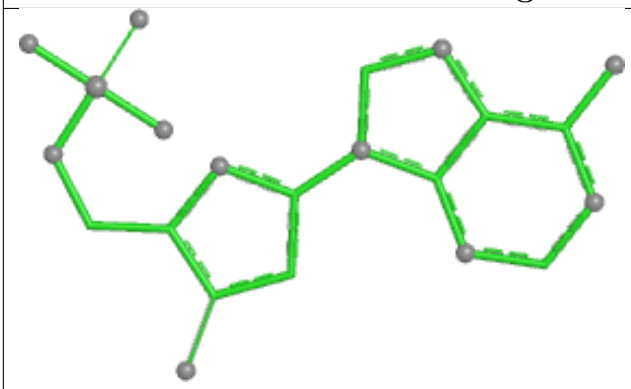

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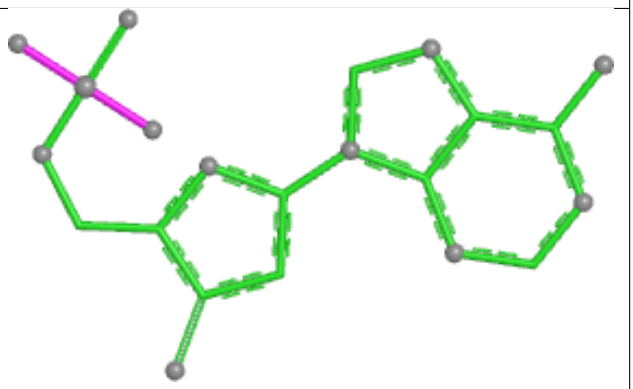

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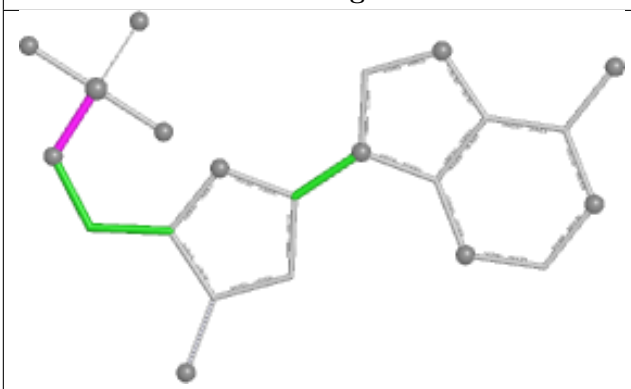

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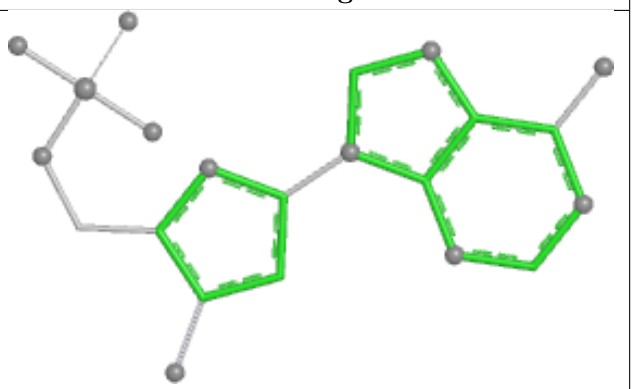

Rings

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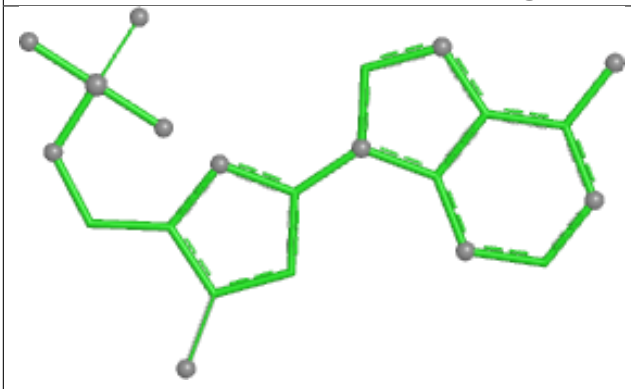

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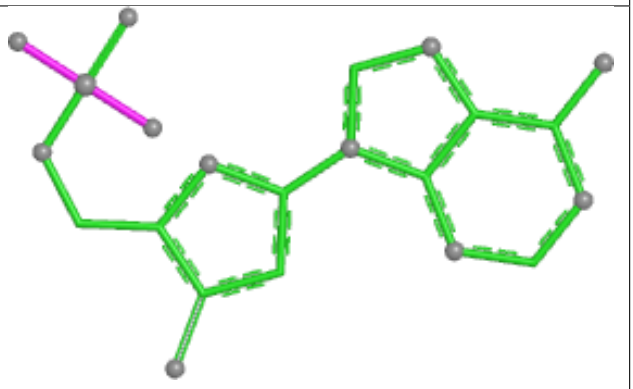

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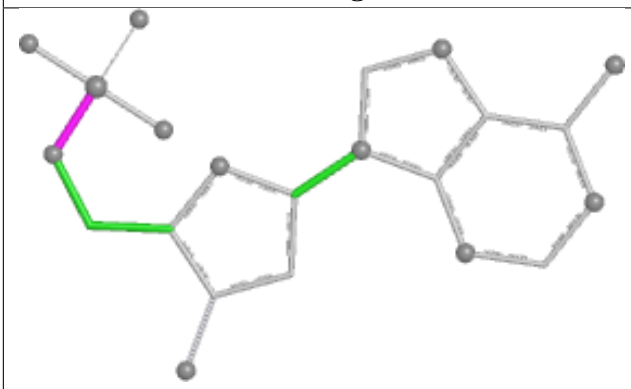

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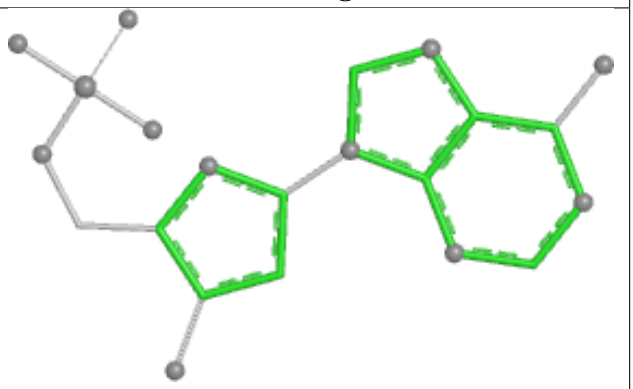

Rings

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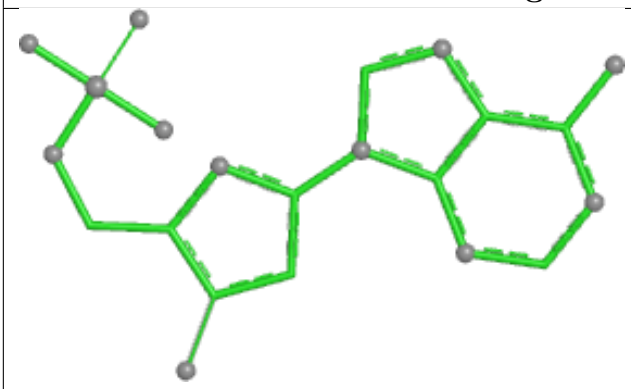

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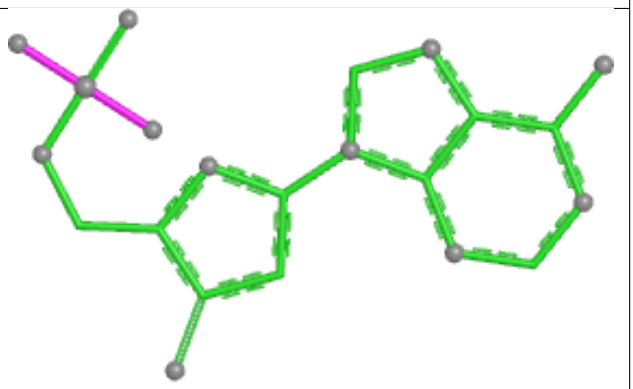

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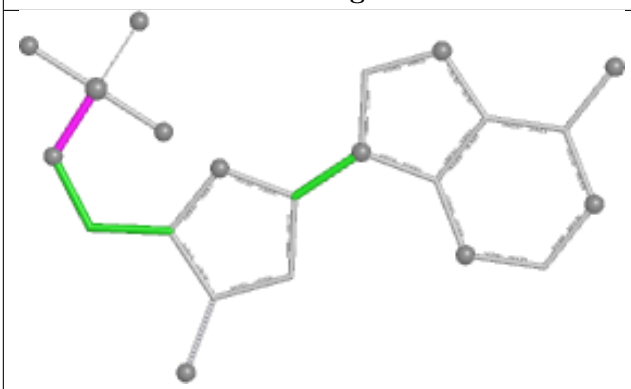

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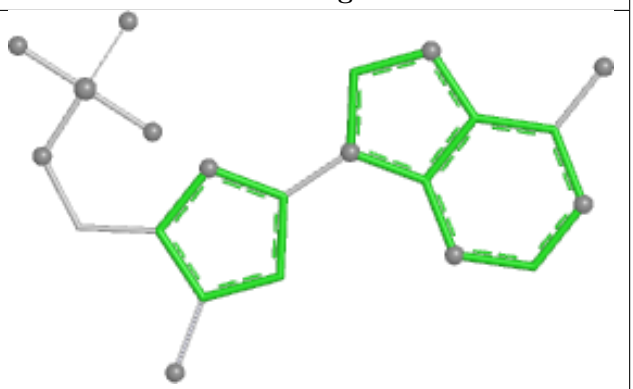
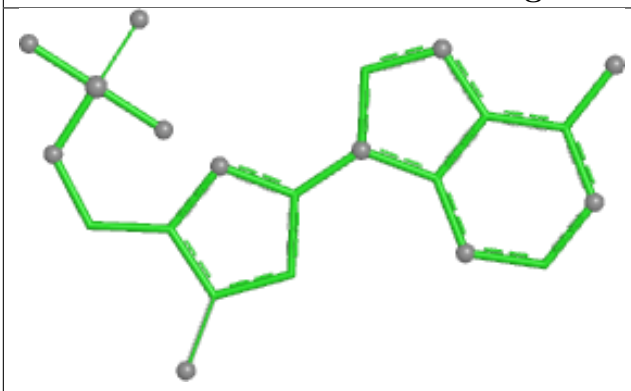


Rings

Ligand D5M h 801



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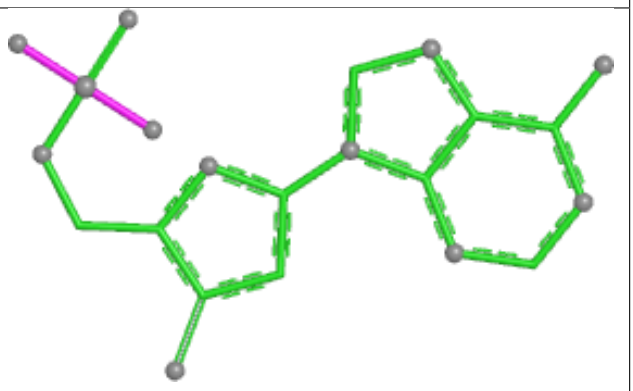

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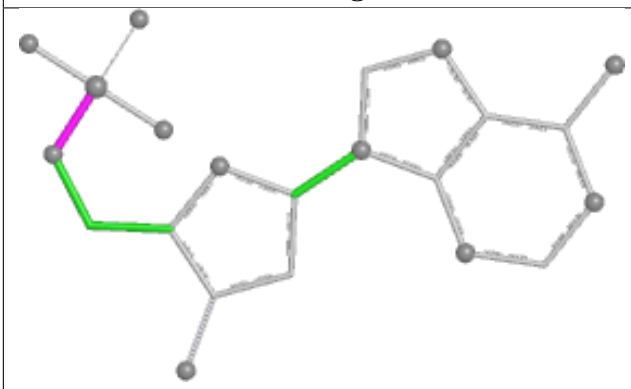

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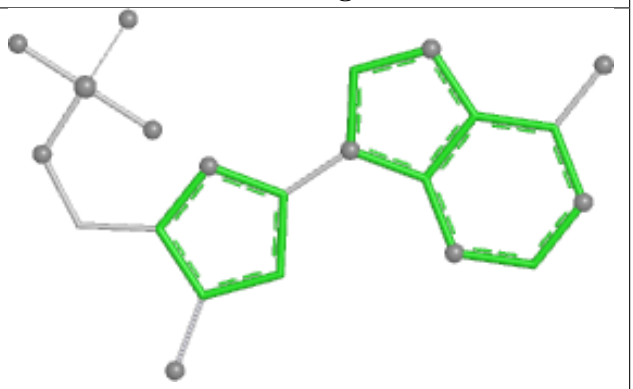

Rings

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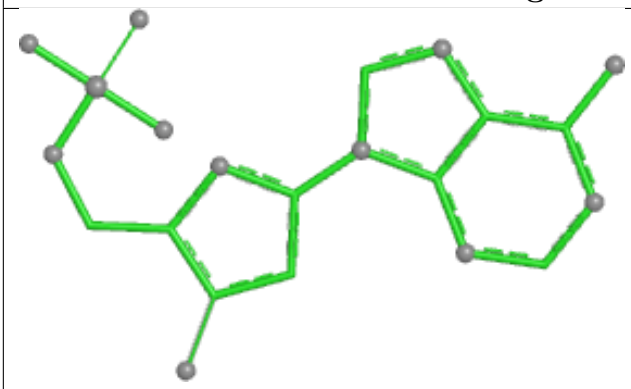

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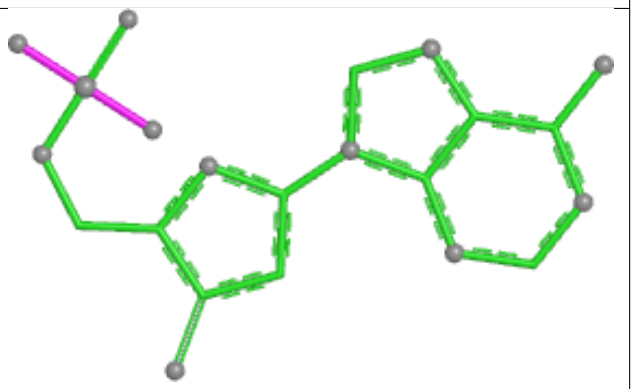
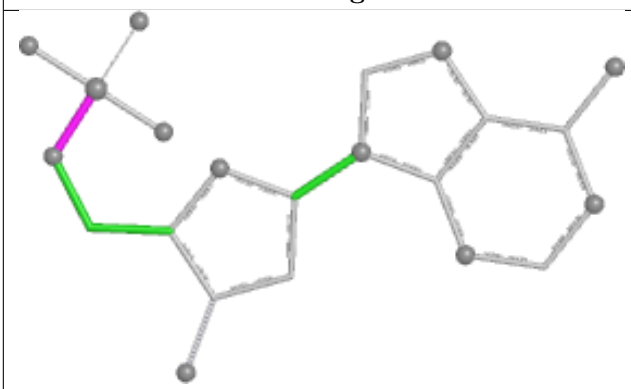
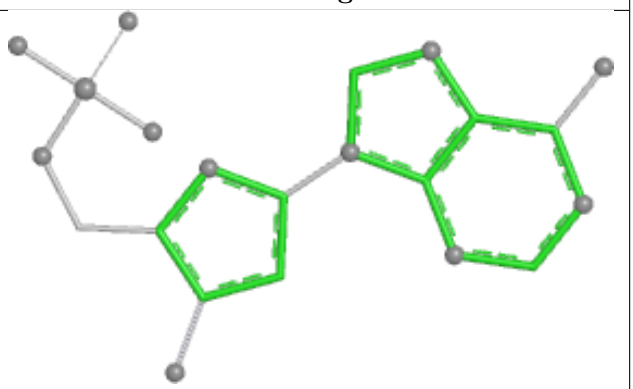


Bond angles

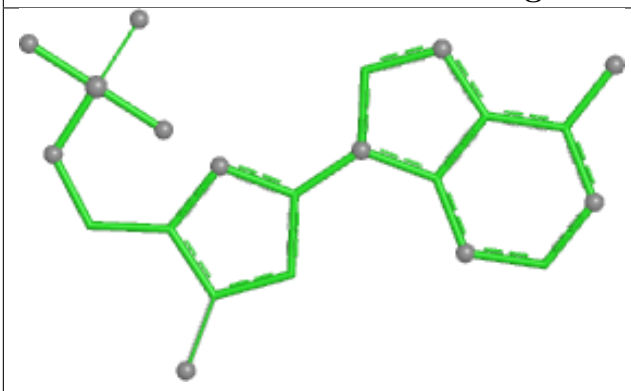


Torsions

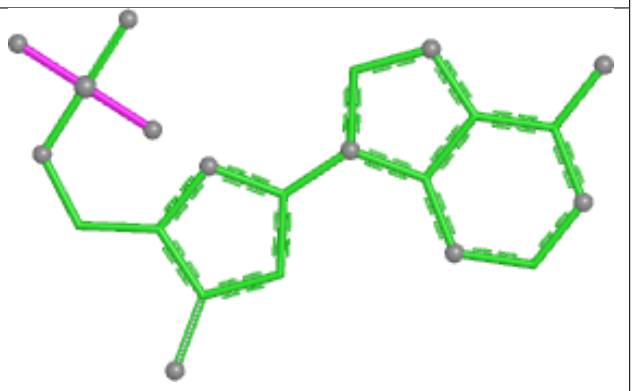


Rings

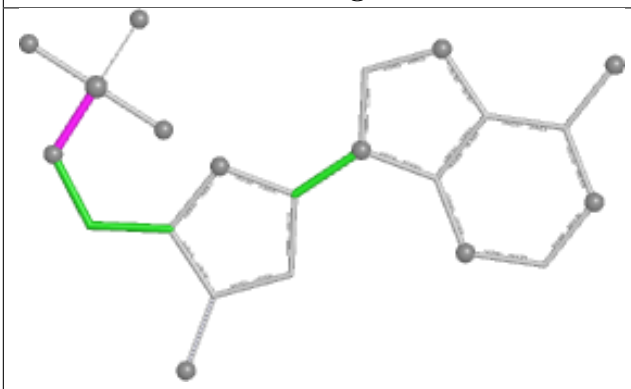
Ligand D5M n 801



Bond lengths



Bond angles



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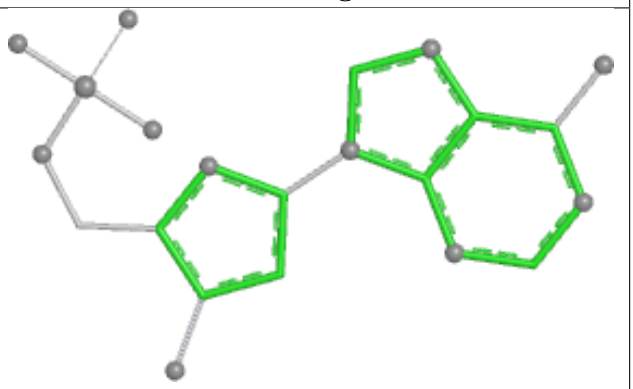
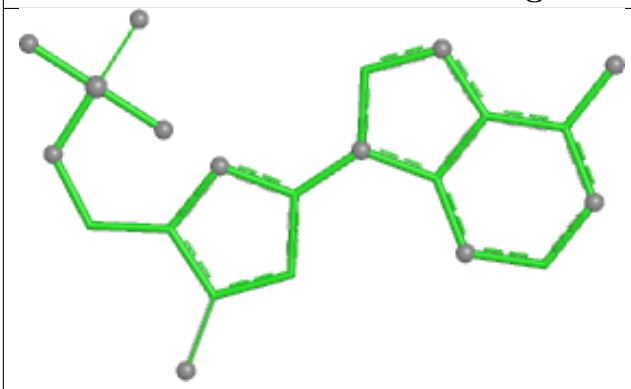


Rings

Ligand D5M 4 801



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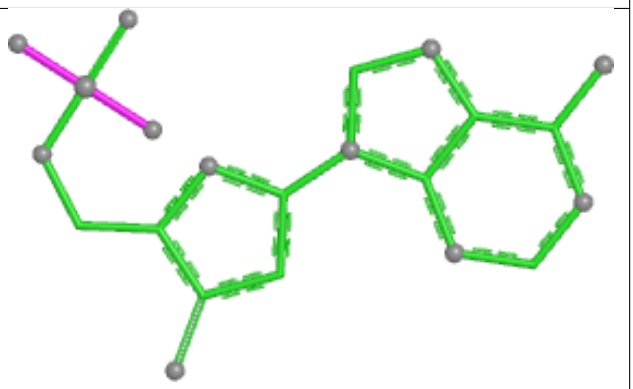
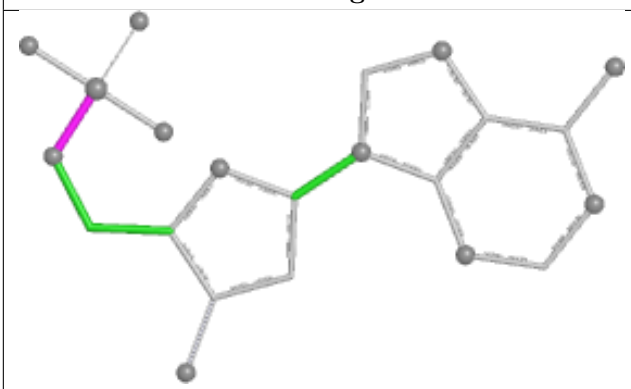
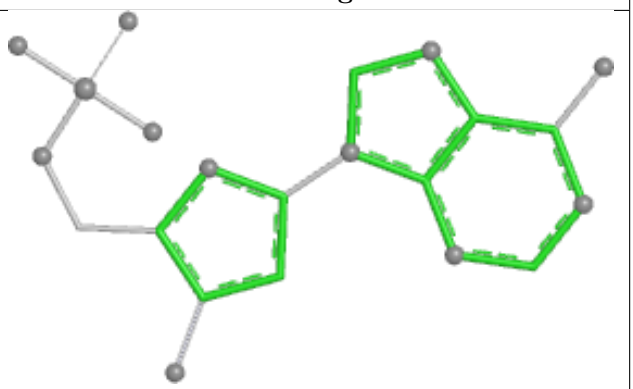


Bond angles

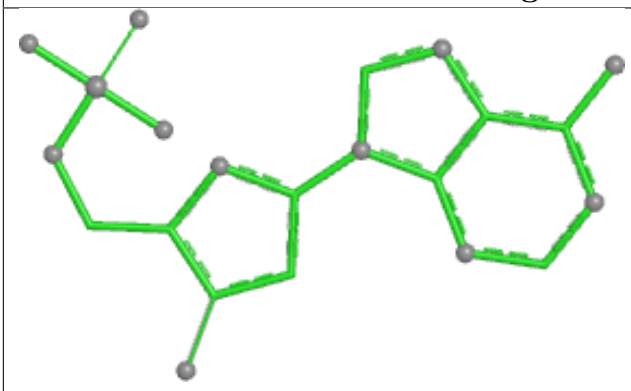


Torsions



Rings

Ligand D5M U 801



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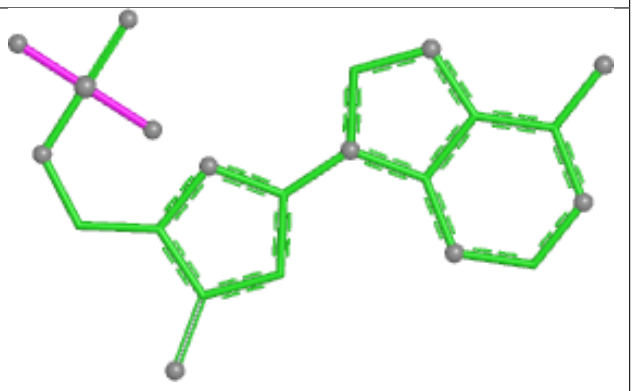
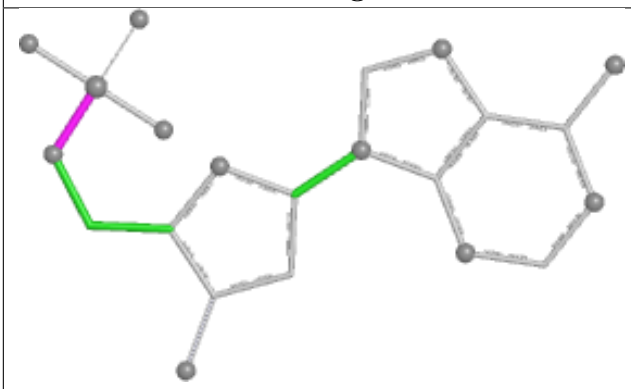
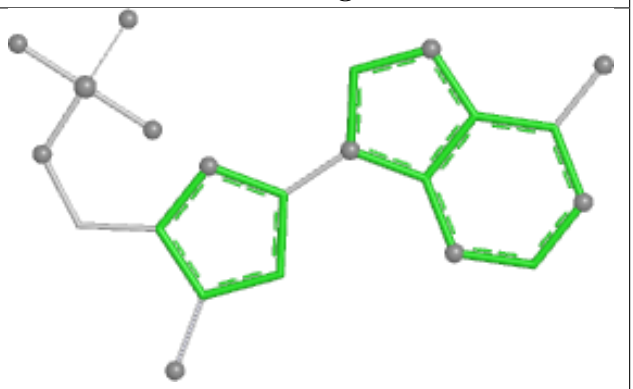


Bond angles

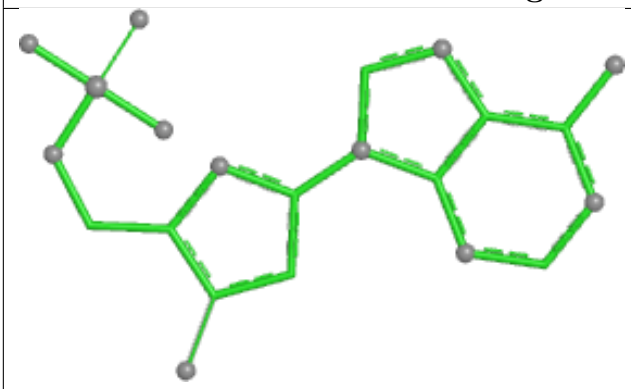


Torsions



Rings

Ligand D5M a 801



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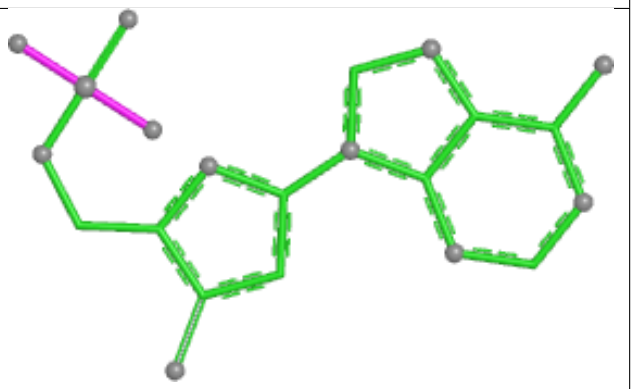
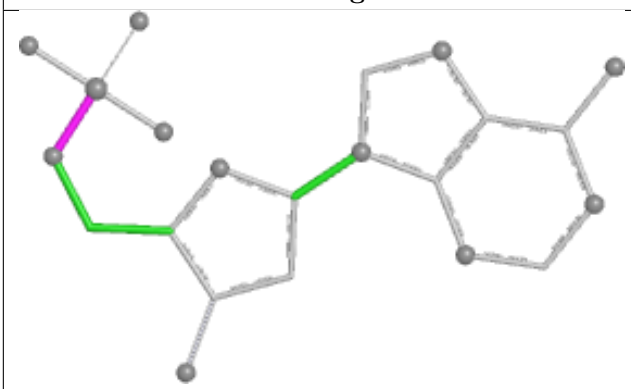
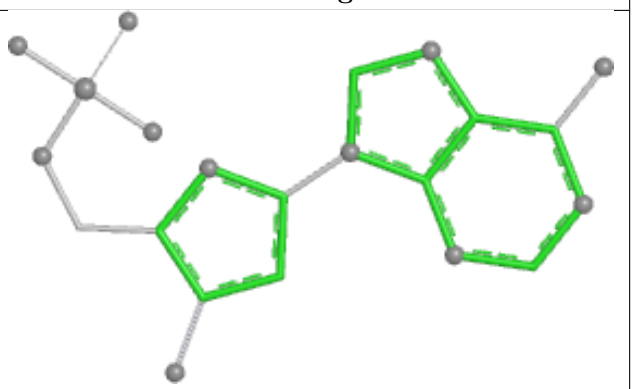


Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23200. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.