wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 11:56 PM EDT

PDB ID	:	6U9D
Title	:	Saccharomyces cerevisiae acetohydroxyacid synthase
Authors	:	Guddat, L.W.; Lonhienne, T.
Deposited on	:	2019-09-08
Resolution	:	3.19 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 77705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Acetolactate synthase catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	0	0
			4606	2912	800	873	21			
1	B	607	Total	C	N	O	S	0	0	0
			4621	2922	800	878	21			
1	E	603	Total	C	N	O	S	0	0	0
			4580	2898	794	867	21			
1	F	604	Total	C	N	O	S	0	0	0
			4572	2891	789	871	21			
1	I	604	Total	C	N	O	S	0	0	0
			4540	2877	780	862	21			
1	J	602	Total	C	N	O	S	0	0	0
			4533	2865	781	866	21			
1	M	605	Total	C	N	O	S	0	0	0
			4613	2917	801	874	21			
1	N	603	Total	C	N	O	S	0	0	0
			4589	2900	798	870	21			
1	Q	598	Total	C	N	O	S	0	0	0
			4508	2848	783	857	20			
1	R	416	Total	C	N	O	S	0	0	0
			3014	1901	518	582	13			
1	U	604	Total	C	N	O	S	0	0	0
			4554	2880	784	869	21			
1	V	605	Total	C	N	O	S	0	0	0
			4601	2910	799	871	21			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP P07342
A	45	HIS	-	expression tag	UNP P07342
A	46	HIS	-	expression tag	UNP P07342
A	47	HIS	-	expression tag	UNP P07342
A	48	HIS	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
A	49	HIS	-	expression tag	UNP P07342
A	50	HIS	-	expression tag	UNP P07342
A	51	GLU	-	expression tag	UNP P07342
A	52	ASN	-	expression tag	UNP P07342
A	53	LEU	-	expression tag	UNP P07342
A	54	TYR	-	expression tag	UNP P07342
A	55	PHE	-	expression tag	UNP P07342
A	56	GLN	-	expression tag	UNP P07342
A	57	GLY	-	expression tag	UNP P07342
B	44	MET	-	initiating methionine	UNP P07342
B	45	HIS	-	expression tag	UNP P07342
B	46	HIS	-	expression tag	UNP P07342
B	47	HIS	-	expression tag	UNP P07342
B	48	HIS	-	expression tag	UNP P07342
B	49	HIS	-	expression tag	UNP P07342
B	50	HIS	-	expression tag	UNP P07342
B	51	GLU	-	expression tag	UNP P07342
B	52	ASN	-	expression tag	UNP P07342
B	53	LEU	-	expression tag	UNP P07342
B	54	TYR	-	expression tag	UNP P07342
B	55	PHE	-	expression tag	UNP P07342
B	56	GLN	-	expression tag	UNP P07342
B	57	GLY	-	expression tag	UNP P07342
E	44	MET	-	initiating methionine	UNP P07342
E	45	HIS	-	expression tag	UNP P07342
E	46	HIS	-	expression tag	UNP P07342
E	47	HIS	-	expression tag	UNP P07342
E	48	HIS	-	expression tag	UNP P07342
E	49	HIS	-	expression tag	UNP P07342
E	50	HIS	-	expression tag	UNP P07342
E	51	GLU	-	expression tag	UNP P07342
E	52	ASN	-	expression tag	UNP P07342
E	53	LEU	-	expression tag	UNP P07342
E	54	TYR	-	expression tag	UNP P07342
E	55	PHE	-	expression tag	UNP P07342
E	56	GLN	-	expression tag	UNP P07342
E	57	GLY	-	expression tag	UNP P07342
F	44	MET	-	initiating methionine	UNP P07342
F	45	HIS	-	expression tag	UNP P07342
F	46	HIS	-	expression tag	UNP P07342
F	47	HIS	-	expression tag	UNP P07342
F	48	HIS	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
F	49	HIS	-	expression tag	UNP P07342
F	50	HIS	-	expression tag	UNP P07342
F	51	GLU	-	expression tag	UNP P07342
F	52	ASN	-	expression tag	UNP P07342
F	53	LEU	-	expression tag	UNP P07342
F	54	TYR	-	expression tag	UNP P07342
F	55	PHE	-	expression tag	UNP P07342
F	56	GLN	-	expression tag	UNP P07342
F	57	GLY	-	expression tag	UNP P07342
I	44	MET	-	initiating methionine	UNP P07342
I	45	HIS	-	expression tag	UNP P07342
I	46	HIS	-	expression tag	UNP P07342
I	47	HIS	-	expression tag	UNP P07342
I	48	HIS	-	expression tag	UNP P07342
I	49	HIS	-	expression tag	UNP P07342
I	50	HIS	-	expression tag	UNP P07342
I	51	GLU	-	expression tag	UNP P07342
I	52	ASN	-	expression tag	UNP P07342
I	53	LEU	-	expression tag	UNP P07342
I	54	TYR	-	expression tag	UNP P07342
I	55	PHE	-	expression tag	UNP P07342
I	56	GLN	-	expression tag	UNP P07342
I	57	GLY	-	expression tag	UNP P07342
J	44	MET	-	initiating methionine	UNP P07342
J	45	HIS	-	expression tag	UNP P07342
J	46	HIS	-	expression tag	UNP P07342
J	47	HIS	-	expression tag	UNP P07342
J	48	HIS	-	expression tag	UNP P07342
J	49	HIS	-	expression tag	UNP P07342
J	50	HIS	-	expression tag	UNP P07342
J	51	GLU	-	expression tag	UNP P07342
J	52	ASN	-	expression tag	UNP P07342
J	53	LEU	-	expression tag	UNP P07342
J	54	TYR	-	expression tag	UNP P07342
J	55	PHE	-	expression tag	UNP P07342
J	56	GLN	-	expression tag	UNP P07342
J	57	GLY	-	expression tag	UNP P07342
M	44	MET	-	initiating methionine	UNP P07342
M	45	HIS	-	expression tag	UNP P07342
M	46	HIS	-	expression tag	UNP P07342
M	47	HIS	-	expression tag	UNP P07342
M	48	HIS	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
M	49	HIS	-	expression tag	UNP P07342
M	50	HIS	-	expression tag	UNP P07342
M	51	GLU	-	expression tag	UNP P07342
M	52	ASN	-	expression tag	UNP P07342
M	53	LEU	-	expression tag	UNP P07342
M	54	TYR	-	expression tag	UNP P07342
M	55	PHE	-	expression tag	UNP P07342
M	56	GLN	-	expression tag	UNP P07342
M	57	GLY	-	expression tag	UNP P07342
N	44	MET	-	initiating methionine	UNP P07342
N	45	HIS	-	expression tag	UNP P07342
N	46	HIS	-	expression tag	UNP P07342
N	47	HIS	-	expression tag	UNP P07342
N	48	HIS	-	expression tag	UNP P07342
N	49	HIS	-	expression tag	UNP P07342
N	50	HIS	-	expression tag	UNP P07342
N	51	GLU	-	expression tag	UNP P07342
N	52	ASN	-	expression tag	UNP P07342
N	53	LEU	-	expression tag	UNP P07342
N	54	TYR	-	expression tag	UNP P07342
N	55	PHE	-	expression tag	UNP P07342
N	56	GLN	-	expression tag	UNP P07342
N	57	GLY	-	expression tag	UNP P07342
Q	44	MET	-	initiating methionine	UNP P07342
Q	45	HIS	-	expression tag	UNP P07342
Q	46	HIS	-	expression tag	UNP P07342
Q	47	HIS	-	expression tag	UNP P07342
Q	48	HIS	-	expression tag	UNP P07342
Q	49	HIS	-	expression tag	UNP P07342
Q	50	HIS	-	expression tag	UNP P07342
Q	51	GLU	-	expression tag	UNP P07342
Q	52	ASN	-	expression tag	UNP P07342
Q	53	LEU	-	expression tag	UNP P07342
Q	54	TYR	-	expression tag	UNP P07342
Q	55	PHE	-	expression tag	UNP P07342
Q	56	GLN	-	expression tag	UNP P07342
Q	57	GLY	-	expression tag	UNP P07342
R	44	MET	-	initiating methionine	UNP P07342
R	45	HIS	-	expression tag	UNP P07342
R	46	HIS	-	expression tag	UNP P07342
R	47	HIS	-	expression tag	UNP P07342
R	48	HIS	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
R	49	HIS	-	expression tag	UNP P07342
R	50	HIS	-	expression tag	UNP P07342
R	51	GLU	-	expression tag	UNP P07342
R	52	ASN	-	expression tag	UNP P07342
R	53	LEU	-	expression tag	UNP P07342
R	54	TYR	-	expression tag	UNP P07342
R	55	PHE	-	expression tag	UNP P07342
R	56	GLN	-	expression tag	UNP P07342
R	57	GLY	-	expression tag	UNP P07342
U	44	MET	-	initiating methionine	UNP P07342
U	45	HIS	-	expression tag	UNP P07342
U	46	HIS	-	expression tag	UNP P07342
U	47	HIS	-	expression tag	UNP P07342
U	48	HIS	-	expression tag	UNP P07342
U	49	HIS	-	expression tag	UNP P07342
U	50	HIS	-	expression tag	UNP P07342
U	51	GLU	-	expression tag	UNP P07342
U	52	ASN	-	expression tag	UNP P07342
U	53	LEU	-	expression tag	UNP P07342
U	54	TYR	-	expression tag	UNP P07342
U	55	PHE	-	expression tag	UNP P07342
U	56	GLN	-	expression tag	UNP P07342
U	57	GLY	-	expression tag	UNP P07342
V	44	MET	-	initiating methionine	UNP P07342
V	45	HIS	-	expression tag	UNP P07342
V	46	HIS	-	expression tag	UNP P07342
V	47	HIS	-	expression tag	UNP P07342
V	48	HIS	-	expression tag	UNP P07342
V	49	HIS	-	expression tag	UNP P07342
V	50	HIS	-	expression tag	UNP P07342
V	51	GLU	-	expression tag	UNP P07342
V	52	ASN	-	expression tag	UNP P07342
V	53	LEU	-	expression tag	UNP P07342
V	54	TYR	-	expression tag	UNP P07342
V	55	PHE	-	expression tag	UNP P07342
V	56	GLN	-	expression tag	UNP P07342
V	57	GLY	-	expression tag	UNP P07342

- Molecule 2 is a protein called Acetolactate synthase small subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	253	Total	C	N	O	S	0	0	0
			1938	1209	340	381	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	250	Total	C	N	O	S	0	0	0
			1915	1199	335	373	8			
2	G	253	Total	C	N	O	S	0	0	0
			1938	1211	337	382	8			
2	H	252	Total	C	N	O	S	0	0	0
			1944	1214	342	380	8			
2	K	245	Total	C	N	O	S	0	0	0
			1889	1184	329	368	8			
2	L	255	Total	C	N	O	S	0	0	0
			1957	1221	345	383	8			
2	O	237	Total	C	N	O	S	0	0	0
			1818	1140	315	355	8			
2	P	243	Total	C	N	O	S	0	0	0
			1881	1177	328	368	8			
2	S	244	Total	C	N	O	S	0	0	0
			1872	1174	324	366	8			
2	T	232	Total	C	N	O	S	0	0	0
			1792	1127	312	345	8			
2	W	245	Total	C	N	O	S	0	0	0
			1894	1186	331	369	8			
2	X	240	Total	C	N	O	S	0	0	0
			1846	1153	320	365	8			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	13	MET	-	initiating methionine	UNP B3LU66
C	14	GLY	-	expression tag	UNP B3LU66
C	15	SER	-	expression tag	UNP B3LU66
C	16	SER	-	expression tag	UNP B3LU66
C	17	HIS	-	expression tag	UNP B3LU66
C	18	HIS	-	expression tag	UNP B3LU66
C	19	HIS	-	expression tag	UNP B3LU66
C	20	HIS	-	expression tag	UNP B3LU66
C	21	HIS	-	expression tag	UNP B3LU66
C	22	HIS	-	expression tag	UNP B3LU66
C	23	SER	-	expression tag	UNP B3LU66
C	24	SER	-	expression tag	UNP B3LU66
C	25	GLY	-	expression tag	UNP B3LU66
C	26	LEU	-	expression tag	UNP B3LU66
C	27	VAL	-	expression tag	UNP B3LU66
C	28	PRO	-	expression tag	UNP B3LU66
C	29	ARG	-	expression tag	UNP B3LU66

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Chain	Residue	Modelled	Actual	Comment	Reference
C	30	GLY	-	expression tag	UNP B3LU66
C	31	SER	-	expression tag	UNP B3LU66
C	32	HIS	-	expression tag	UNP B3LU66
C	33	MET	-	expression tag	UNP B3LU66
C	34	GLU	-	expression tag	UNP B3LU66
C	35	ASN	-	expression tag	UNP B3LU66
C	36	LEU	-	expression tag	UNP B3LU66
C	37	TYR	-	expression tag	UNP B3LU66
C	38	PHE	-	expression tag	UNP B3LU66
C	39	GLN	-	expression tag	UNP B3LU66
C	40	GLY	-	expression tag	UNP B3LU66
D	13	MET	-	initiating methionine	UNP B3LU66
D	14	GLY	-	expression tag	UNP B3LU66
D	15	SER	-	expression tag	UNP B3LU66
D	16	SER	-	expression tag	UNP B3LU66
D	17	HIS	-	expression tag	UNP B3LU66
D	18	HIS	-	expression tag	UNP B3LU66
D	19	HIS	-	expression tag	UNP B3LU66
D	20	HIS	-	expression tag	UNP B3LU66
D	21	HIS	-	expression tag	UNP B3LU66
D	22	HIS	-	expression tag	UNP B3LU66
D	23	SER	-	expression tag	UNP B3LU66
D	24	SER	-	expression tag	UNP B3LU66
D	25	GLY	-	expression tag	UNP B3LU66
D	26	LEU	-	expression tag	UNP B3LU66
D	27	VAL	-	expression tag	UNP B3LU66
D	28	PRO	-	expression tag	UNP B3LU66
D	29	ARG	-	expression tag	UNP B3LU66
D	30	GLY	-	expression tag	UNP B3LU66
D	31	SER	-	expression tag	UNP B3LU66
D	32	HIS	-	expression tag	UNP B3LU66
D	33	MET	-	expression tag	UNP B3LU66
D	34	GLU	-	expression tag	UNP B3LU66
D	35	ASN	-	expression tag	UNP B3LU66
D	36	LEU	-	expression tag	UNP B3LU66
D	37	TYR	-	expression tag	UNP B3LU66
D	38	PHE	-	expression tag	UNP B3LU66
D	39	GLN	-	expression tag	UNP B3LU66
D	40	GLY	-	expression tag	UNP B3LU66
G	13	MET	-	initiating methionine	UNP B3LU66
G	14	GLY	-	expression tag	UNP B3LU66
G	15	SER	-	expression tag	UNP B3LU66

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Chain	Residue	Modelled	Actual	Comment	Reference
G	16	SER	-	expression tag	UNP B3LU66
G	17	HIS	-	expression tag	UNP B3LU66
G	18	HIS	-	expression tag	UNP B3LU66
G	19	HIS	-	expression tag	UNP B3LU66
G	20	HIS	-	expression tag	UNP B3LU66
G	21	HIS	-	expression tag	UNP B3LU66
G	22	HIS	-	expression tag	UNP B3LU66
G	23	SER	-	expression tag	UNP B3LU66
G	24	SER	-	expression tag	UNP B3LU66
G	25	GLY	-	expression tag	UNP B3LU66
G	26	LEU	-	expression tag	UNP B3LU66
G	27	VAL	-	expression tag	UNP B3LU66
G	28	PRO	-	expression tag	UNP B3LU66
G	29	ARG	-	expression tag	UNP B3LU66
G	30	GLY	-	expression tag	UNP B3LU66
G	31	SER	-	expression tag	UNP B3LU66
G	32	HIS	-	expression tag	UNP B3LU66
G	33	MET	-	expression tag	UNP B3LU66
G	34	GLU	-	expression tag	UNP B3LU66
G	35	ASN	-	expression tag	UNP B3LU66
G	36	LEU	-	expression tag	UNP B3LU66
G	37	TYR	-	expression tag	UNP B3LU66
G	38	PHE	-	expression tag	UNP B3LU66
G	39	GLN	-	expression tag	UNP B3LU66
G	40	GLY	-	expression tag	UNP B3LU66
H	13	MET	-	initiating methionine	UNP B3LU66
H	14	GLY	-	expression tag	UNP B3LU66
H	15	SER	-	expression tag	UNP B3LU66
H	16	SER	-	expression tag	UNP B3LU66
H	17	HIS	-	expression tag	UNP B3LU66
H	18	HIS	-	expression tag	UNP B3LU66
H	19	HIS	-	expression tag	UNP B3LU66
H	20	HIS	-	expression tag	UNP B3LU66
H	21	HIS	-	expression tag	UNP B3LU66
H	22	HIS	-	expression tag	UNP B3LU66
H	23	SER	-	expression tag	UNP B3LU66
H	24	SER	-	expression tag	UNP B3LU66
H	25	GLY	-	expression tag	UNP B3LU66
H	26	LEU	-	expression tag	UNP B3LU66
H	27	VAL	-	expression tag	UNP B3LU66
H	28	PRO	-	expression tag	UNP B3LU66
H	29	ARG	-	expression tag	UNP B3LU66

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Chain	Residue	Modelled	Actual	Comment	Reference
H	30	GLY	-	expression tag	UNP B3LU66
H	31	SER	-	expression tag	UNP B3LU66
H	32	HIS	-	expression tag	UNP B3LU66
H	33	MET	-	expression tag	UNP B3LU66
H	34	GLU	-	expression tag	UNP B3LU66
H	35	ASN	-	expression tag	UNP B3LU66
H	36	LEU	-	expression tag	UNP B3LU66
H	37	TYR	-	expression tag	UNP B3LU66
H	38	PHE	-	expression tag	UNP B3LU66
H	39	GLN	-	expression tag	UNP B3LU66
H	40	GLY	-	expression tag	UNP B3LU66
K	13	MET	-	initiating methionine	UNP B3LU66
K	14	GLY	-	expression tag	UNP B3LU66
K	15	SER	-	expression tag	UNP B3LU66
K	16	SER	-	expression tag	UNP B3LU66
K	17	HIS	-	expression tag	UNP B3LU66
K	18	HIS	-	expression tag	UNP B3LU66
K	19	HIS	-	expression tag	UNP B3LU66
K	20	HIS	-	expression tag	UNP B3LU66
K	21	HIS	-	expression tag	UNP B3LU66
K	22	HIS	-	expression tag	UNP B3LU66
K	23	SER	-	expression tag	UNP B3LU66
K	24	SER	-	expression tag	UNP B3LU66
K	25	GLY	-	expression tag	UNP B3LU66
K	26	LEU	-	expression tag	UNP B3LU66
K	27	VAL	-	expression tag	UNP B3LU66
K	28	PRO	-	expression tag	UNP B3LU66
K	29	ARG	-	expression tag	UNP B3LU66
K	30	GLY	-	expression tag	UNP B3LU66
K	31	SER	-	expression tag	UNP B3LU66
K	32	HIS	-	expression tag	UNP B3LU66
K	33	MET	-	expression tag	UNP B3LU66
K	34	GLU	-	expression tag	UNP B3LU66
K	35	ASN	-	expression tag	UNP B3LU66
K	36	LEU	-	expression tag	UNP B3LU66
K	37	TYR	-	expression tag	UNP B3LU66
K	38	PHE	-	expression tag	UNP B3LU66
K	39	GLN	-	expression tag	UNP B3LU66
K	40	GLY	-	expression tag	UNP B3LU66
L	13	MET	-	initiating methionine	UNP B3LU66
L	14	GLY	-	expression tag	UNP B3LU66
L	15	SER	-	expression tag	UNP B3LU66

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Chain	Residue	Modelled	Actual	Comment	Reference
L	16	SER	-	expression tag	UNP B3LU66
L	17	HIS	-	expression tag	UNP B3LU66
L	18	HIS	-	expression tag	UNP B3LU66
L	19	HIS	-	expression tag	UNP B3LU66
L	20	HIS	-	expression tag	UNP B3LU66
L	21	HIS	-	expression tag	UNP B3LU66
L	22	HIS	-	expression tag	UNP B3LU66
L	23	SER	-	expression tag	UNP B3LU66
L	24	SER	-	expression tag	UNP B3LU66
L	25	GLY	-	expression tag	UNP B3LU66
L	26	LEU	-	expression tag	UNP B3LU66
L	27	VAL	-	expression tag	UNP B3LU66
L	28	PRO	-	expression tag	UNP B3LU66
L	29	ARG	-	expression tag	UNP B3LU66
L	30	GLY	-	expression tag	UNP B3LU66
L	31	SER	-	expression tag	UNP B3LU66
L	32	HIS	-	expression tag	UNP B3LU66
L	33	MET	-	expression tag	UNP B3LU66
L	34	GLU	-	expression tag	UNP B3LU66
L	35	ASN	-	expression tag	UNP B3LU66
L	36	LEU	-	expression tag	UNP B3LU66
L	37	TYR	-	expression tag	UNP B3LU66
L	38	PHE	-	expression tag	UNP B3LU66
L	39	GLN	-	expression tag	UNP B3LU66
L	40	GLY	-	expression tag	UNP B3LU66
O	13	MET	-	initiating methionine	UNP B3LU66
O	14	GLY	-	expression tag	UNP B3LU66
O	15	SER	-	expression tag	UNP B3LU66
O	16	SER	-	expression tag	UNP B3LU66
O	17	HIS	-	expression tag	UNP B3LU66
O	18	HIS	-	expression tag	UNP B3LU66
O	19	HIS	-	expression tag	UNP B3LU66
O	20	HIS	-	expression tag	UNP B3LU66
O	21	HIS	-	expression tag	UNP B3LU66
O	22	HIS	-	expression tag	UNP B3LU66
O	23	SER	-	expression tag	UNP B3LU66
O	24	SER	-	expression tag	UNP B3LU66
O	25	GLY	-	expression tag	UNP B3LU66
O	26	LEU	-	expression tag	UNP B3LU66
O	27	VAL	-	expression tag	UNP B3LU66
O	28	PRO	-	expression tag	UNP B3LU66
O	29	ARG	-	expression tag	UNP B3LU66

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Chain	Residue	Modelled	Actual	Comment	Reference
O	30	GLY	-	expression tag	UNP B3LU66
O	31	SER	-	expression tag	UNP B3LU66
O	32	HIS	-	expression tag	UNP B3LU66
O	33	MET	-	expression tag	UNP B3LU66
O	34	GLU	-	expression tag	UNP B3LU66
O	35	ASN	-	expression tag	UNP B3LU66
O	36	LEU	-	expression tag	UNP B3LU66
O	37	TYR	-	expression tag	UNP B3LU66
O	38	PHE	-	expression tag	UNP B3LU66
O	39	GLN	-	expression tag	UNP B3LU66
O	40	GLY	-	expression tag	UNP B3LU66
P	13	MET	-	initiating methionine	UNP B3LU66
P	14	GLY	-	expression tag	UNP B3LU66
P	15	SER	-	expression tag	UNP B3LU66
P	16	SER	-	expression tag	UNP B3LU66
P	17	HIS	-	expression tag	UNP B3LU66
P	18	HIS	-	expression tag	UNP B3LU66
P	19	HIS	-	expression tag	UNP B3LU66
P	20	HIS	-	expression tag	UNP B3LU66
P	21	HIS	-	expression tag	UNP B3LU66
P	22	HIS	-	expression tag	UNP B3LU66
P	23	SER	-	expression tag	UNP B3LU66
P	24	SER	-	expression tag	UNP B3LU66
P	25	GLY	-	expression tag	UNP B3LU66
P	26	LEU	-	expression tag	UNP B3LU66
P	27	VAL	-	expression tag	UNP B3LU66
P	28	PRO	-	expression tag	UNP B3LU66
P	29	ARG	-	expression tag	UNP B3LU66
P	30	GLY	-	expression tag	UNP B3LU66
P	31	SER	-	expression tag	UNP B3LU66
P	32	HIS	-	expression tag	UNP B3LU66
P	33	MET	-	expression tag	UNP B3LU66
P	34	GLU	-	expression tag	UNP B3LU66
P	35	ASN	-	expression tag	UNP B3LU66
P	36	LEU	-	expression tag	UNP B3LU66
P	37	TYR	-	expression tag	UNP B3LU66
P	38	PHE	-	expression tag	UNP B3LU66
P	39	GLN	-	expression tag	UNP B3LU66
P	40	GLY	-	expression tag	UNP B3LU66
S	13	MET	-	initiating methionine	UNP B3LU66
S	14	GLY	-	expression tag	UNP B3LU66
S	15	SER	-	expression tag	UNP B3LU66

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Chain	Residue	Modelled	Actual	Comment	Reference
S	16	SER	-	expression tag	UNP B3LU66
S	17	HIS	-	expression tag	UNP B3LU66
S	18	HIS	-	expression tag	UNP B3LU66
S	19	HIS	-	expression tag	UNP B3LU66
S	20	HIS	-	expression tag	UNP B3LU66
S	21	HIS	-	expression tag	UNP B3LU66
S	22	HIS	-	expression tag	UNP B3LU66
S	23	SER	-	expression tag	UNP B3LU66
S	24	SER	-	expression tag	UNP B3LU66
S	25	GLY	-	expression tag	UNP B3LU66
S	26	LEU	-	expression tag	UNP B3LU66
S	27	VAL	-	expression tag	UNP B3LU66
S	28	PRO	-	expression tag	UNP B3LU66
S	29	ARG	-	expression tag	UNP B3LU66
S	30	GLY	-	expression tag	UNP B3LU66
S	31	SER	-	expression tag	UNP B3LU66
S	32	HIS	-	expression tag	UNP B3LU66
S	33	MET	-	expression tag	UNP B3LU66
S	34	GLU	-	expression tag	UNP B3LU66
S	35	ASN	-	expression tag	UNP B3LU66
S	36	LEU	-	expression tag	UNP B3LU66
S	37	TYR	-	expression tag	UNP B3LU66
S	38	PHE	-	expression tag	UNP B3LU66
S	39	GLN	-	expression tag	UNP B3LU66
S	40	GLY	-	expression tag	UNP B3LU66
T	13	MET	-	initiating methionine	UNP B3LU66
T	14	GLY	-	expression tag	UNP B3LU66
T	15	SER	-	expression tag	UNP B3LU66
T	16	SER	-	expression tag	UNP B3LU66
T	17	HIS	-	expression tag	UNP B3LU66
T	18	HIS	-	expression tag	UNP B3LU66
T	19	HIS	-	expression tag	UNP B3LU66
T	20	HIS	-	expression tag	UNP B3LU66
T	21	HIS	-	expression tag	UNP B3LU66
T	22	HIS	-	expression tag	UNP B3LU66
T	23	SER	-	expression tag	UNP B3LU66
T	24	SER	-	expression tag	UNP B3LU66
T	25	GLY	-	expression tag	UNP B3LU66
T	26	LEU	-	expression tag	UNP B3LU66
T	27	VAL	-	expression tag	UNP B3LU66
T	28	PRO	-	expression tag	UNP B3LU66
T	29	ARG	-	expression tag	UNP B3LU66

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Chain	Residue	Modelled	Actual	Comment	Reference
T	30	GLY	-	expression tag	UNP B3LU66
T	31	SER	-	expression tag	UNP B3LU66
T	32	HIS	-	expression tag	UNP B3LU66
T	33	MET	-	expression tag	UNP B3LU66
T	34	GLU	-	expression tag	UNP B3LU66
T	35	ASN	-	expression tag	UNP B3LU66
T	36	LEU	-	expression tag	UNP B3LU66
T	37	TYR	-	expression tag	UNP B3LU66
T	38	PHE	-	expression tag	UNP B3LU66
T	39	GLN	-	expression tag	UNP B3LU66
T	40	GLY	-	expression tag	UNP B3LU66
W	13	MET	-	initiating methionine	UNP B3LU66
W	14	GLY	-	expression tag	UNP B3LU66
W	15	SER	-	expression tag	UNP B3LU66
W	16	SER	-	expression tag	UNP B3LU66
W	17	HIS	-	expression tag	UNP B3LU66
W	18	HIS	-	expression tag	UNP B3LU66
W	19	HIS	-	expression tag	UNP B3LU66
W	20	HIS	-	expression tag	UNP B3LU66
W	21	HIS	-	expression tag	UNP B3LU66
W	22	HIS	-	expression tag	UNP B3LU66
W	23	SER	-	expression tag	UNP B3LU66
W	24	SER	-	expression tag	UNP B3LU66
W	25	GLY	-	expression tag	UNP B3LU66
W	26	LEU	-	expression tag	UNP B3LU66
W	27	VAL	-	expression tag	UNP B3LU66
W	28	PRO	-	expression tag	UNP B3LU66
W	29	ARG	-	expression tag	UNP B3LU66
W	30	GLY	-	expression tag	UNP B3LU66
W	31	SER	-	expression tag	UNP B3LU66
W	32	HIS	-	expression tag	UNP B3LU66
W	33	MET	-	expression tag	UNP B3LU66
W	34	GLU	-	expression tag	UNP B3LU66
W	35	ASN	-	expression tag	UNP B3LU66
W	36	LEU	-	expression tag	UNP B3LU66
W	37	TYR	-	expression tag	UNP B3LU66
W	38	PHE	-	expression tag	UNP B3LU66
W	39	GLN	-	expression tag	UNP B3LU66
W	40	GLY	-	expression tag	UNP B3LU66
X	13	MET	-	initiating methionine	UNP B3LU66
X	14	GLY	-	expression tag	UNP B3LU66
X	15	SER	-	expression tag	UNP B3LU66

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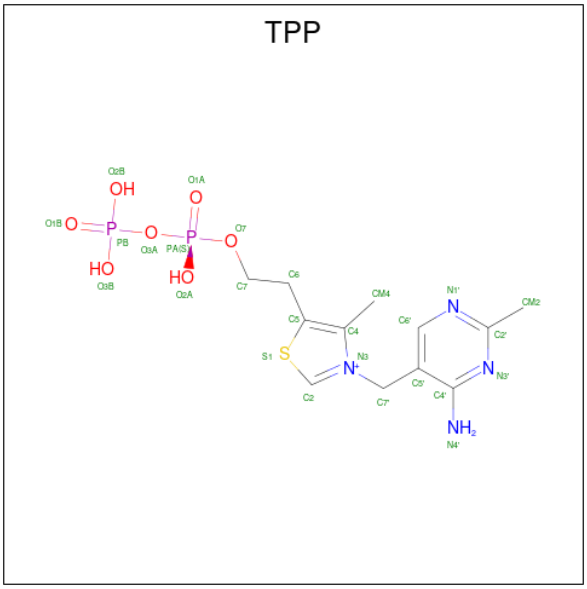
Chain	Residue	Modelled	Actual	Comment	Reference
X	16	SER	-	expression tag	UNP B3LU66
X	17	HIS	-	expression tag	UNP B3LU66
X	18	HIS	-	expression tag	UNP B3LU66
X	19	HIS	-	expression tag	UNP B3LU66
X	20	HIS	-	expression tag	UNP B3LU66
X	21	HIS	-	expression tag	UNP B3LU66
X	22	HIS	-	expression tag	UNP B3LU66
X	23	SER	-	expression tag	UNP B3LU66
X	24	SER	-	expression tag	UNP B3LU66
X	25	GLY	-	expression tag	UNP B3LU66
X	26	LEU	-	expression tag	UNP B3LU66
X	27	VAL	-	expression tag	UNP B3LU66
X	28	PRO	-	expression tag	UNP B3LU66
X	29	ARG	-	expression tag	UNP B3LU66
X	30	GLY	-	expression tag	UNP B3LU66
X	31	SER	-	expression tag	UNP B3LU66
X	32	HIS	-	expression tag	UNP B3LU66
X	33	MET	-	expression tag	UNP B3LU66
X	34	GLU	-	expression tag	UNP B3LU66
X	35	ASN	-	expression tag	UNP B3LU66
X	36	LEU	-	expression tag	UNP B3LU66
X	37	TYR	-	expression tag	UNP B3LU66
X	38	PHE	-	expression tag	UNP B3LU66
X	39	GLN	-	expression tag	UNP B3LU66
X	40	GLY	-	expression tag	UNP B3LU66

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	F	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	I	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	J	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	M	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	N	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	Q	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	U	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	V	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		

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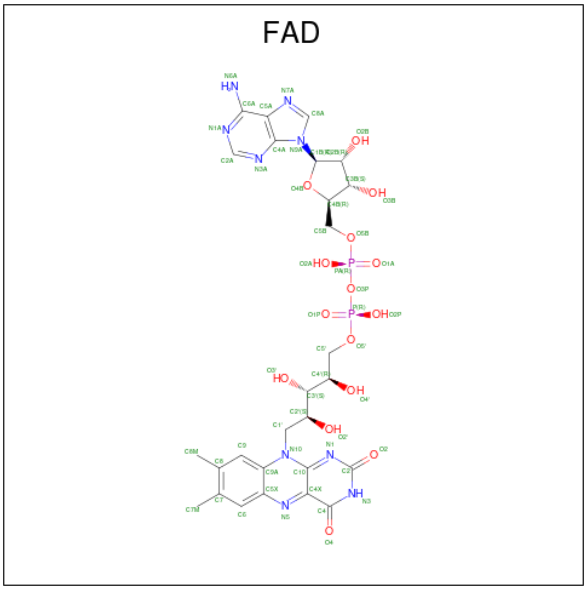
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0
4	N	1	Total Mg 1 1	0	0
4	Q	1	Total Mg 1 1	0	0
4	U	1	Total Mg 1 1	0	0
4	V	1	Total Mg 1 1	0	0
4	W	1	Total Mg 1 1	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 53 27 9 15 2	0	0
5	B	1	Total C N O P 53 27 9 15 2	0	0
5	E	1	Total C N O P 53 27 9 15 2	0	0
5	F	1	Total C N O P 53 27 9 15 2	0	0

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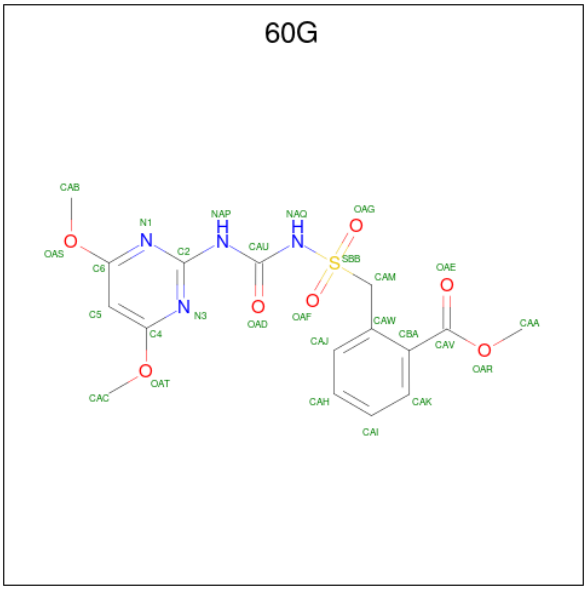
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	Q	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	R	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	U	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	V	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is methyl 2-[(4,6-dimethoxypyrimidin-2-yl)carbamoylsulfamoylmethyl]benzoate (three-letter code: 60G) (formula: $C_{16}H_{18}N_4O_7S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	B	1	Total	C	N	O	S	0	0
			28	16	4	7	1		

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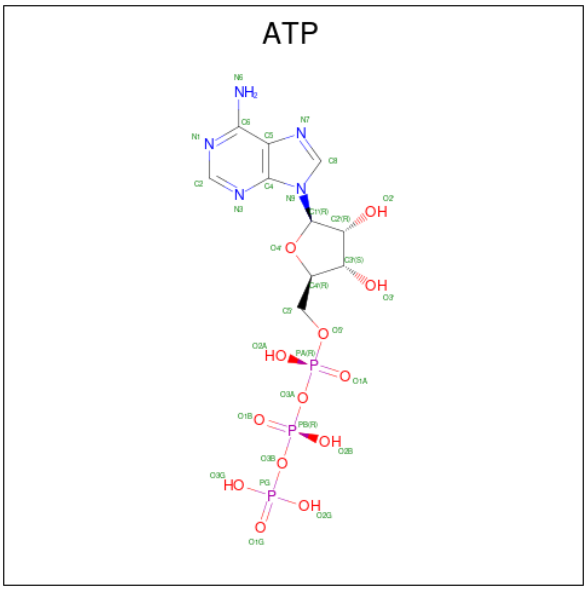
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	F	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	I	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	J	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	N	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	N	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	Q	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	R	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	U	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	V	1	Total	C	N	O	S	0	0
			28	16	4	7	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	S	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	T	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	W	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	W	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	O	0	0
			6	6		
8	B	9	Total	O	0	0
			9	9		
8	D	1	Total	O	0	0
			1	1		
8	E	3	Total	O	0	0
			3	3		
8	F	3	Total	O	0	0
			3	3		
8	I	2	Total	O	0	0
			2	2		
8	J	1	Total	O	0	0
			1	1		
8	M	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	N	4	Total O 4 4	0	0
8	Q	1	Total O 1 1	0	0
8	R	1	Total O 1 1	0	0
8	S	1	Total O 1 1	0	0
8	U	4	Total O 4 4	0	0
8	V	5	Total O 5 5	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	368.65Å 230.31Å 183.53Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	49.11 – 3.19	Depositor
% Data completeness (in resolution range)	99.5 (49.11-3.19)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.252	Depositor
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.207	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	77705	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 63 ligands modelled in this entry, 16 are monoatomic - leaving 47 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TPP	M	701	4	22,27,27	1.88	2 (9%)	29,40,40	2.11	11 (37%)
6	60G	A	704	-	28,29,29	1.46	4 (14%)	38,40,40	3.41	13 (34%)
3	TPP	U	701	4	22,27,27	1.85	3 (13%)	29,40,40	2.15	11 (37%)
7	ATP	L	401	4	26,33,33	3.54	9 (34%)	31,52,52	1.37	5 (16%)
5	FAD	B	703	-	53,58,58	1.70	10 (18%)	68,89,89	1.36	14 (20%)
7	ATP	G	401	4	26,33,33	3.53	9 (34%)	31,52,52	1.44	5 (16%)
5	FAD	U	703	-	53,58,58	1.70	11 (20%)	68,89,89	1.33	13 (19%)
5	FAD	V	703	-	53,58,58	1.70	11 (20%)	68,89,89	1.36	13 (19%)
7	ATP	W	401	-	26,33,33	3.54	9 (34%)	31,52,52	1.40	5 (16%)
5	FAD	A	703	-	53,58,58	1.70	11 (20%)	68,89,89	1.33	14 (20%)
5	FAD	R	701	-	53,58,58	1.71	11 (20%)	68,89,89	1.34	12 (17%)
7	ATP	C	401	4	26,33,33	3.53	9 (34%)	31,52,52	1.38	5 (16%)
6	60G	B	704	-	28,29,29	1.45	3 (10%)	38,40,40	3.40	13 (34%)
7	ATP	O	401	4	26,33,33	3.53	9 (34%)	31,52,52	1.39	5 (16%)
6	60G	V	704	-	28,29,29	1.43	3 (10%)	38,40,40	3.37	13 (34%)
5	FAD	M	703	-	53,58,58	1.70	11 (20%)	68,89,89	1.34	14 (20%)
6	60G	F	704	-	28,29,29	1.44	4 (14%)	38,40,40	3.46	13 (34%)
7	ATP	K	401	4	26,33,33	3.53	9 (34%)	31,52,52	1.40	5 (16%)
7	ATP	P	401	4	26,33,33	3.54	9 (34%)	31,52,52	1.38	5 (16%)
3	TPP	A	701	4	22,27,27	1.86	2 (9%)	29,40,40	2.15	13 (44%)
3	TPP	E	701	4	22,27,27	1.85	2 (9%)	29,40,40	2.15	11 (37%)
6	60G	J	704	-	28,29,29	1.47	4 (14%)	38,40,40	3.42	13 (34%)
7	ATP	W	402	4	26,33,33	3.53	9 (34%)	31,52,52	1.36	5 (16%)
3	TPP	I	701	4	22,27,27	1.85	3 (13%)	29,40,40	2.12	12 (41%)
6	60G	R	702	-	28,29,29	1.47	4 (14%)	38,40,40	3.38	13 (34%)
6	60G	N	704	-	28,29,29	1.43	3 (10%)	38,40,40	3.40	12 (31%)
5	FAD	F	703	-	53,58,58	1.69	11 (20%)	68,89,89	1.40	14 (20%)
3	TPP	B	701	4	22,27,27	1.86	2 (9%)	29,40,40	2.14	13 (44%)
6	60G	E	704	-	28,29,29	1.45	4 (14%)	38,40,40	3.43	13 (34%)
7	ATP	H	401	4	26,33,33	3.54	9 (34%)	31,52,52	1.38	5 (16%)
7	ATP	S	401	-	26,33,33	3.54	9 (34%)	31,52,52	1.36	5 (16%)
5	FAD	N	703	-	53,58,58	1.70	10 (18%)	68,89,89	1.34	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	60G	Q	704	-	28,29,29	1.48	4 (14%)	38,40,40	3.40	12 (31%)
3	TPP	N	701	4	22,27,27	1.88	3 (13%)	29,40,40	2.11	11 (37%)
3	TPP	V	701	4	22,27,27	1.83	2 (9%)	29,40,40	2.09	11 (37%)
3	TPP	F	701	4	22,27,27	1.83	3 (13%)	29,40,40	2.13	12 (41%)
7	ATP	T	401	4	26,33,33	3.52	9 (34%)	31,52,52	1.44	5 (16%)
5	FAD	Q	703	-	53,58,58	1.69	10 (18%)	68,89,89	1.33	13 (19%)
6	60G	N	705	-	28,29,29	1.45	3 (10%)	38,40,40	3.40	12 (31%)
5	FAD	E	703	-	53,58,58	1.70	11 (20%)	68,89,89	1.34	14 (20%)
7	ATP	D	401	4	26,33,33	3.48	9 (34%)	31,52,52	1.55	7 (22%)
5	FAD	J	703	-	53,58,58	1.65	10 (18%)	68,89,89	1.48	14 (20%)
6	60G	U	704	-	28,29,29	1.44	4 (14%)	38,40,40	3.41	14 (36%)
3	TPP	Q	701	4	22,27,27	1.83	3 (13%)	29,40,40	2.15	12 (41%)
6	60G	I	704	-	28,29,29	1.43	4 (14%)	38,40,40	3.41	15 (39%)
5	FAD	I	703	-	53,58,58	1.69	10 (18%)	68,89,89	1.35	13 (19%)
3	TPP	J	701	4	22,27,27	1.87	3 (13%)	29,40,40	2.13	11 (37%)

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
3	TPP	M	701	4	-	3/16/17/17	0/2/2/2
6	60G	A	704	-	-	7/24/24/24	0/2/2/2
3	TPP	U	701	4	-	5/16/17/17	0/2/2/2
7	ATP	L	401	4	-	1/18/38/38	0/3/3/3
5	FAD	B	703	-	-	4/30/50/50	0/6/6/6
7	ATP	G	401	4	-	1/18/38/38	0/3/3/3
5	FAD	U	703	-	-	15/30/50/50	0/6/6/6
5	FAD	V	703	-	-	14/30/50/50	0/6/6/6
7	ATP	W	401	-	-	4/18/38/38	0/3/3/3
5	FAD	A	703	-	-	3/30/50/50	0/6/6/6
5	FAD	R	701	-	-	13/30/50/50	0/6/6/6
7	ATP	C	401	4	-	4/18/38/38	0/3/3/3
6	60G	B	704	-	-	8/24/24/24	0/2/2/2
7	ATP	O	401	4	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	60G	V	704	-	-	7/24/24/24	0/2/2/2
5	FAD	M	703	-	-	3/30/50/50	0/6/6/6
6	60G	F	704	-	-	7/24/24/24	0/2/2/2
7	ATP	K	401	4	-	4/18/38/38	0/3/3/3
7	ATP	P	401	4	-	1/18/38/38	0/3/3/3
3	TPP	A	701	4	-	7/16/17/17	0/2/2/2
3	TPP	E	701	4	-	5/16/17/17	0/2/2/2
6	60G	J	704	-	-	7/24/24/24	0/2/2/2
7	ATP	W	402	4	-	2/18/38/38	0/3/3/3
3	TPP	I	701	4	-	5/16/17/17	0/2/2/2
6	60G	R	702	-	-	9/24/24/24	0/2/2/2
6	60G	N	704	-	-	8/24/24/24	0/2/2/2
5	FAD	F	703	-	-	8/30/50/50	0/6/6/6
3	TPP	B	701	4	-	5/16/17/17	0/2/2/2
6	60G	E	704	-	-	7/24/24/24	0/2/2/2
7	ATP	H	401	4	-	2/18/38/38	0/3/3/3
7	ATP	S	401	-	-	8/18/38/38	0/3/3/3
5	FAD	N	703	-	-	2/30/50/50	0/6/6/6
6	60G	Q	704	-	-	7/24/24/24	0/2/2/2
3	TPP	N	701	4	-	5/16/17/17	0/2/2/2
3	TPP	V	701	4	-	2/16/17/17	0/2/2/2
3	TPP	F	701	4	-	4/16/17/17	0/2/2/2
7	ATP	T	401	4	-	1/18/38/38	0/3/3/3
5	FAD	Q	703	-	-	2/30/50/50	0/6/6/6
6	60G	N	705	-	-	7/24/24/24	0/2/2/2
5	FAD	E	703	-	-	3/30/50/50	0/6/6/6
7	ATP	D	401	4	-	2/18/38/38	0/3/3/3
5	FAD	J	703	-	-	11/30/50/50	0/6/6/6
6	60G	U	704	-	-	6/24/24/24	0/2/2/2
3	TPP	Q	701	4	-	6/16/17/17	0/2/2/2
6	60G	I	704	-	-	8/24/24/24	0/2/2/2
5	FAD	I	703	-	-	7/30/50/50	0/6/6/6
3	TPP	J	701	4	-	5/16/17/17	0/2/2/2

The worst 5 of 307 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	401	ATP	C2'-C3'	-11.31	1.22	1.53
7	C	401	ATP	C2'-C3'	-11.25	1.22	1.53
7	W	402	ATP	C2'-C3'	-11.24	1.22	1.53
7	O	401	ATP	C2'-C3'	-11.24	1.22	1.53
7	S	401	ATP	C2'-C3'	-11.23	1.22	1.53

The worst 5 of 506 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	704	60G	OAG-SBB-OAF	-13.32	100.05	119.35
6	A	704	60G	OAG-SBB-OAF	-13.30	100.09	119.35
6	I	704	60G	OAG-SBB-OAF	-13.24	100.17	119.35
6	E	704	60G	OAG-SBB-OAF	-13.24	100.17	119.35
6	Q	704	60G	OAG-SBB-OAF	-13.20	100.23	119.35

There are no chirality outliers.

5 of 261 torsion outliers are listed below:

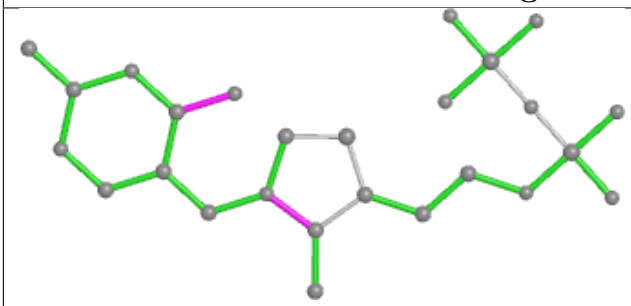
Mol	Chain	Res	Type	Atoms
3	A	701	TPP	C5-C6-C7-O7
3	A	701	TPP	C7-O7-PA-O1A
3	A	701	TPP	C7-O7-PA-O2A
3	A	701	TPP	PA-O3A-PB-O3B
3	B	701	TPP	C5-C6-C7-O7

There are no ring outliers.

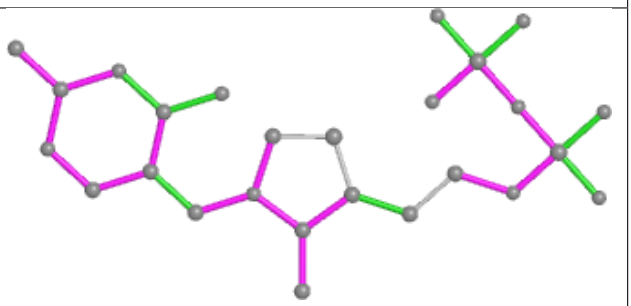
No monomer is involved in short contacts.

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

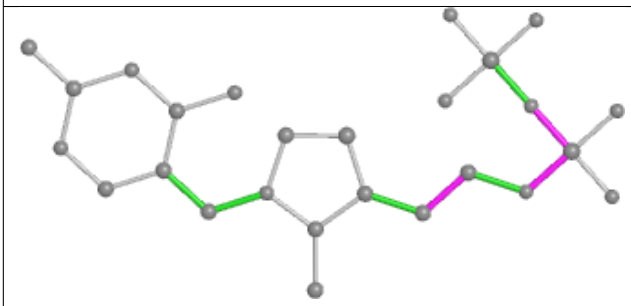
Ligand TPP M 701



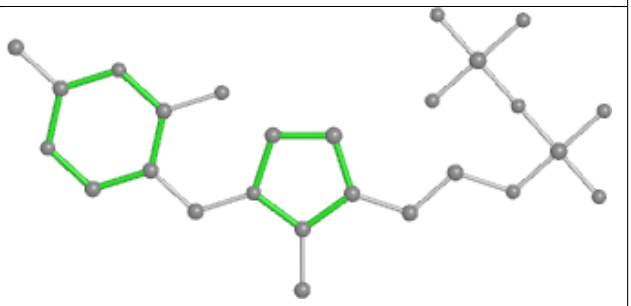
Bond lengths



Bond angles

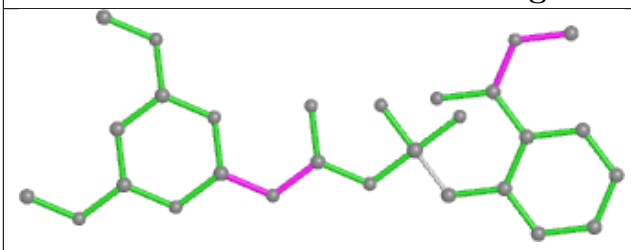


Torsions



Rings

Ligand 60G A 704



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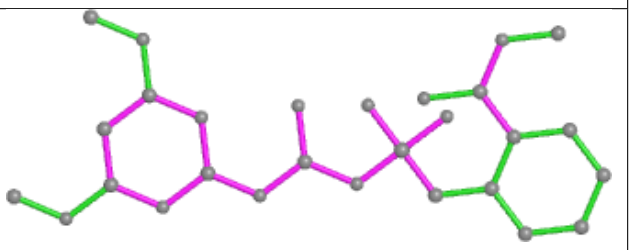

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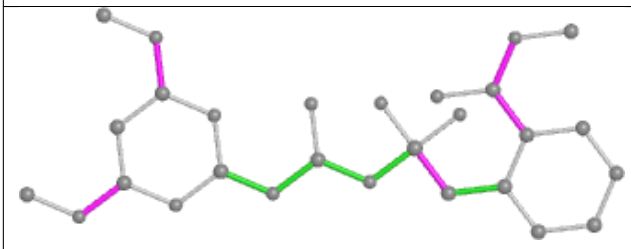

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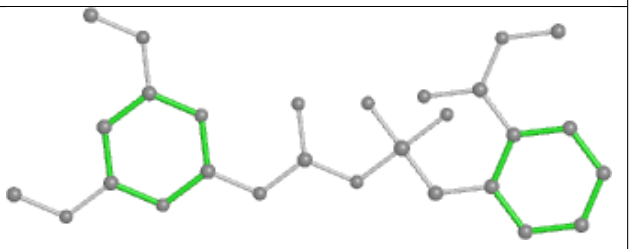
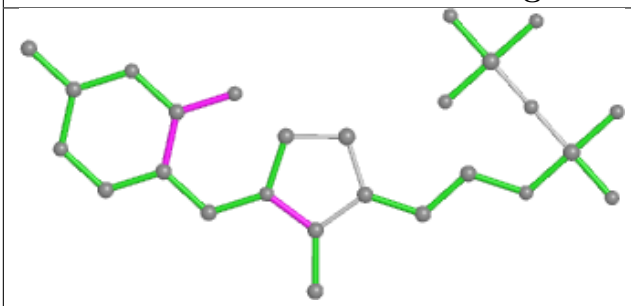


Rings

Ligand TPP U 701



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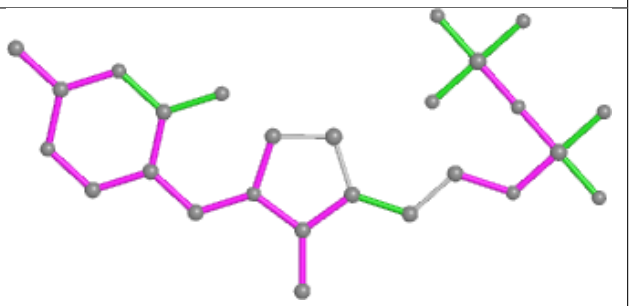

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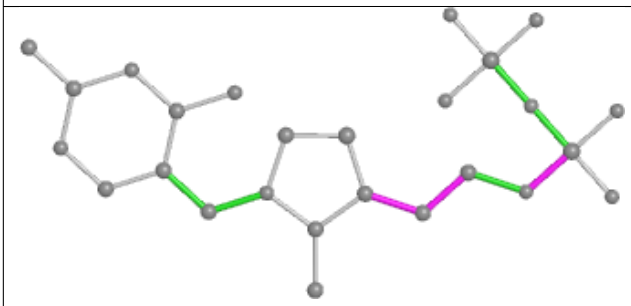

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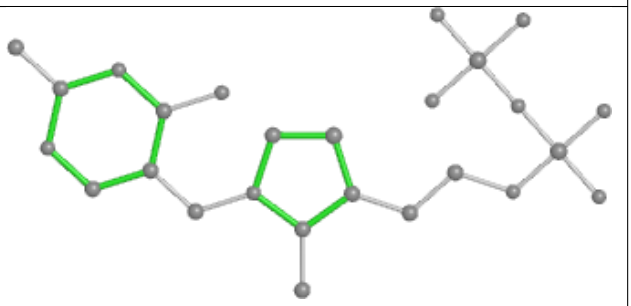
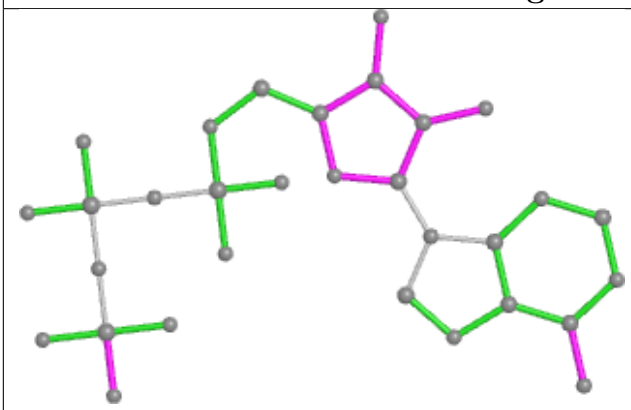


Rings

Ligand ATP L 401



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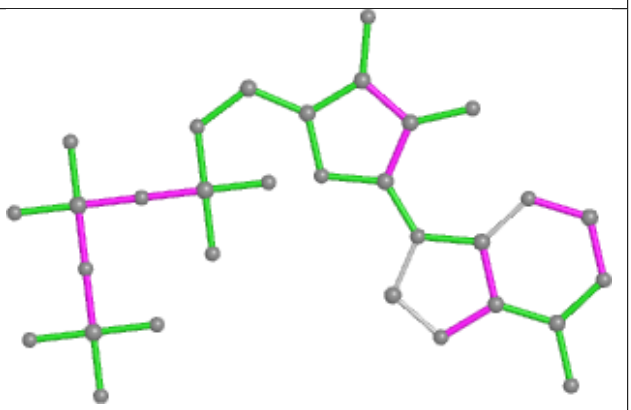
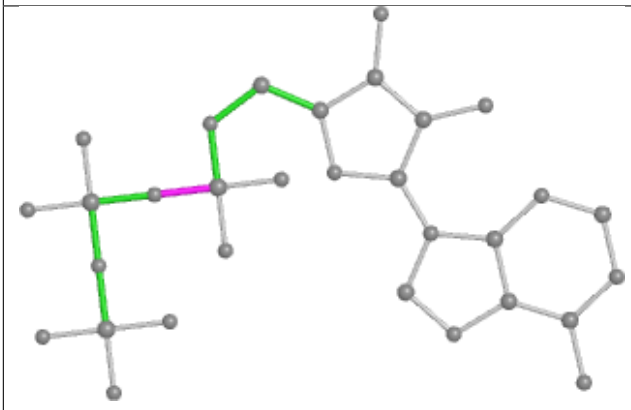


Bond angles



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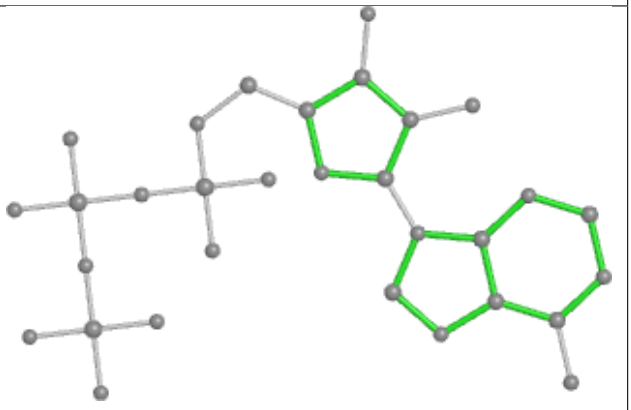
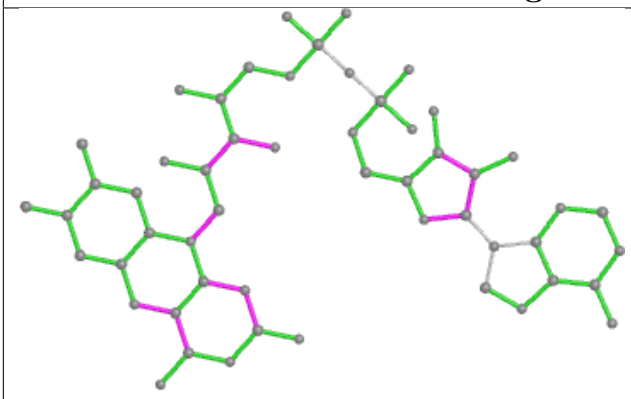


Rings

Ligand FAD B 703



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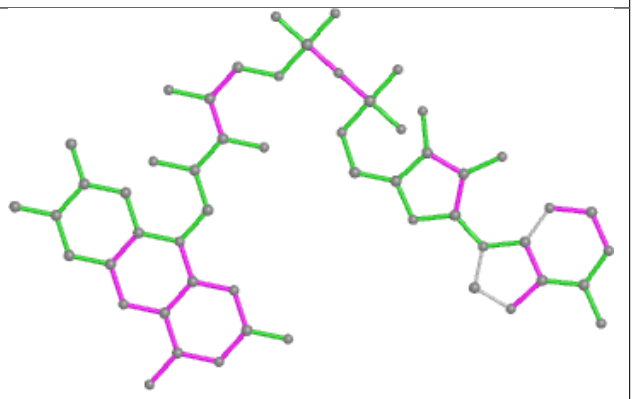

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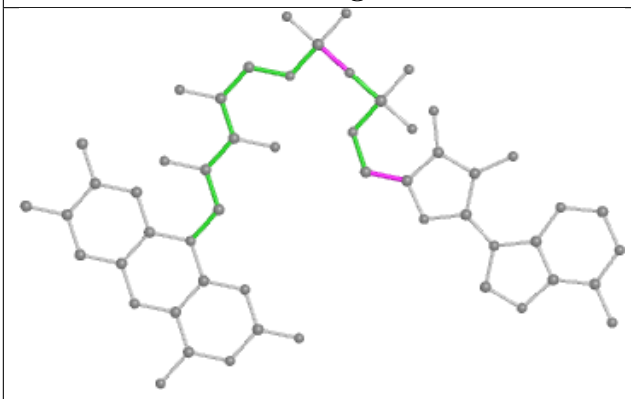

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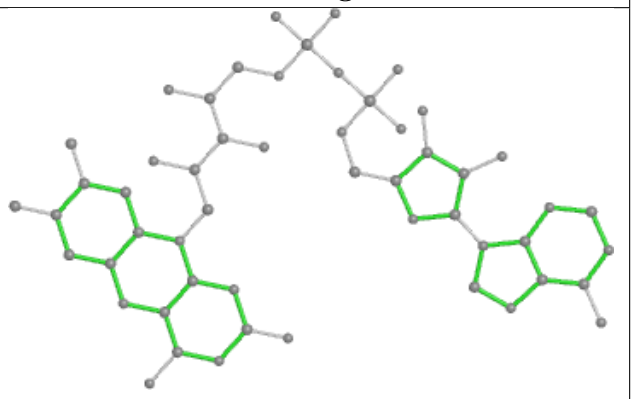
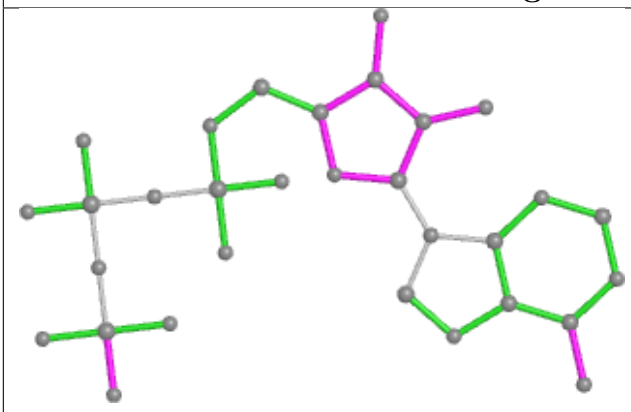


Rings

Ligand ATP G 401



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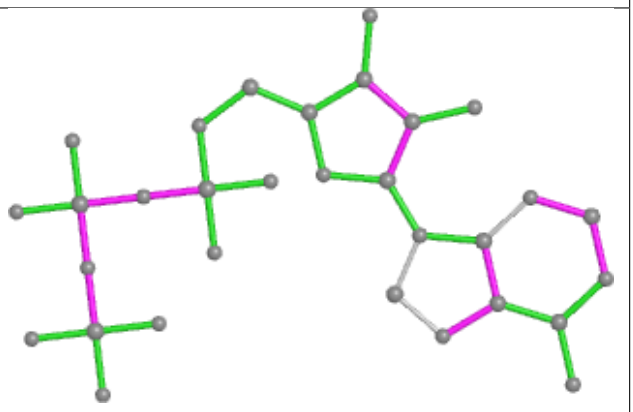
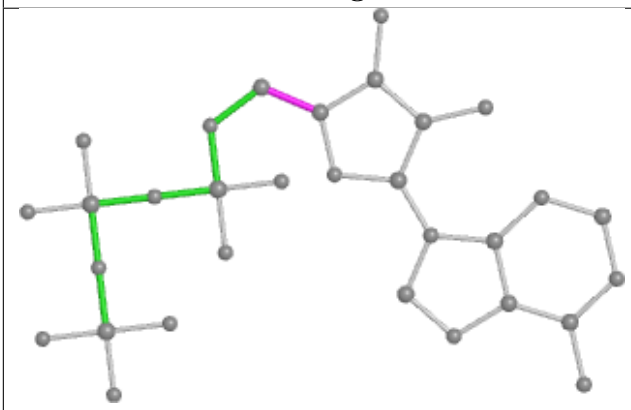


Bond angles



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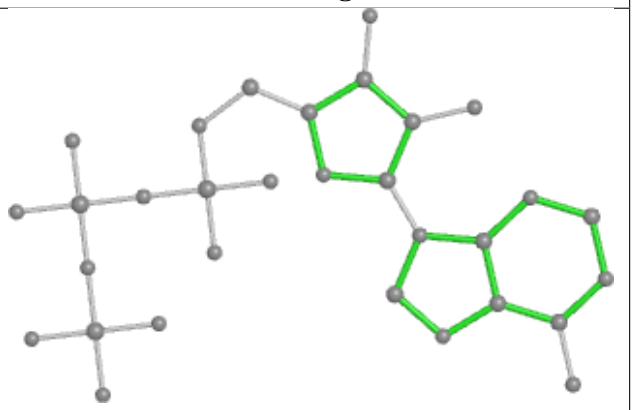
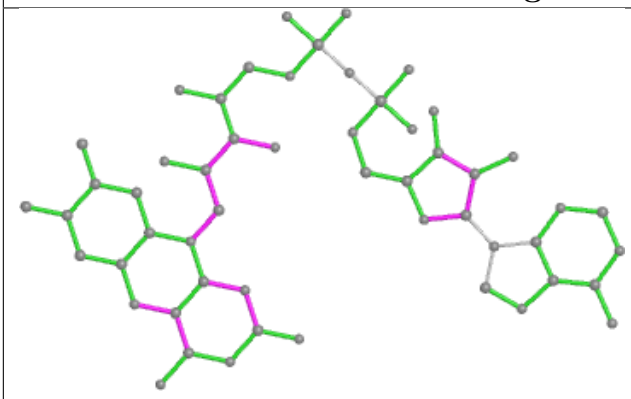
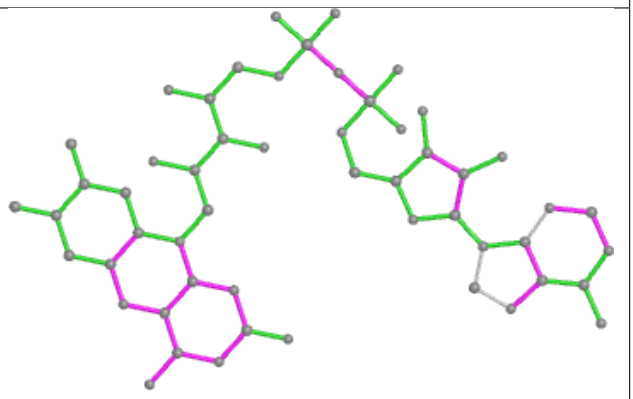


Rings

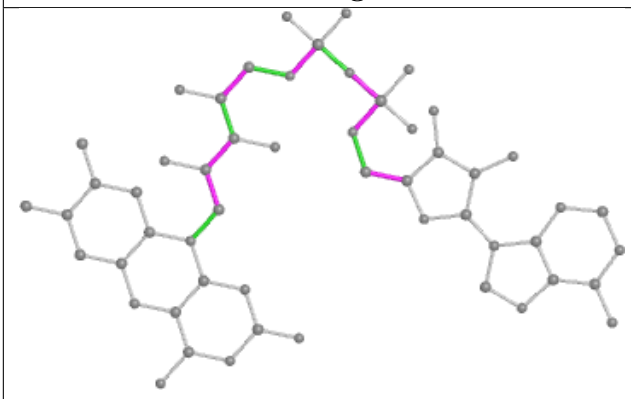
Ligand FAD U 703



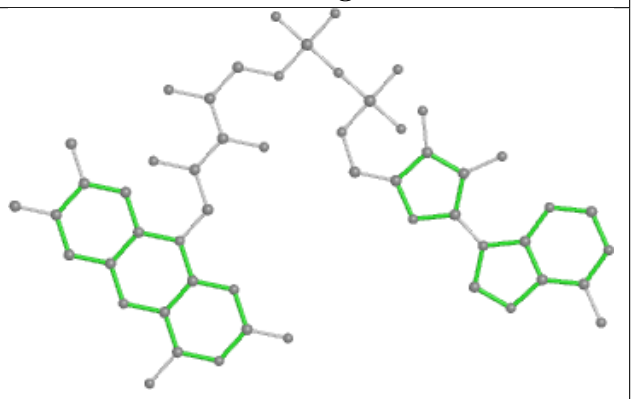
Bond lengths



Bond angles

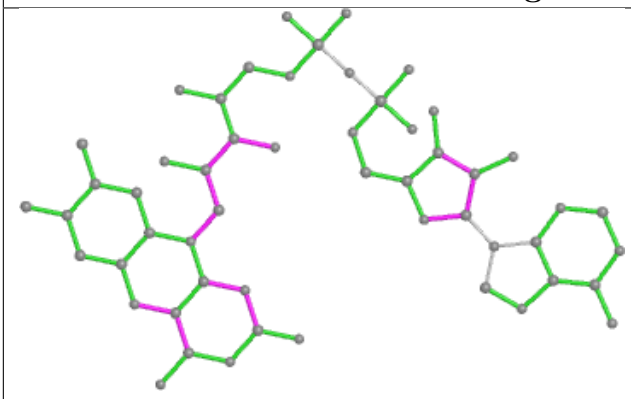


Torsions



Rings

Ligand FAD V 703



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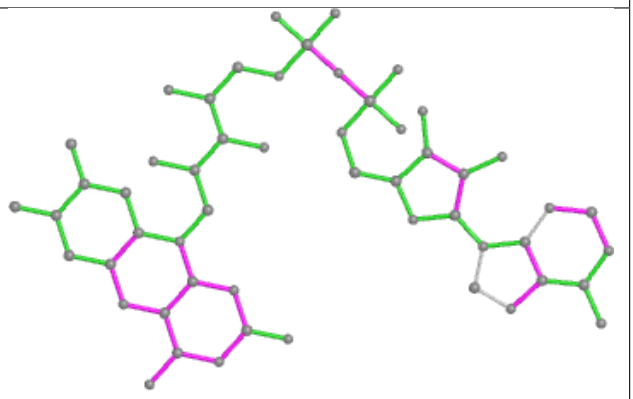

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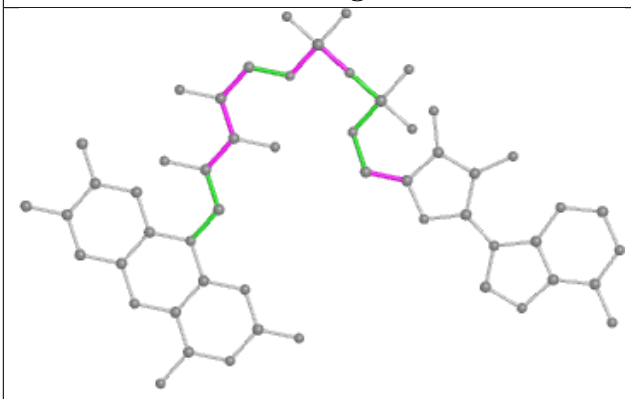

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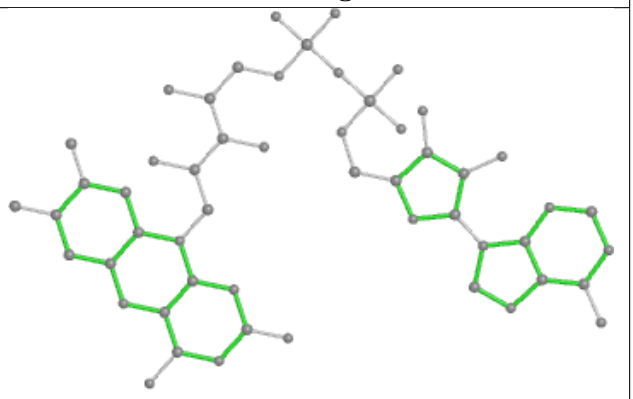
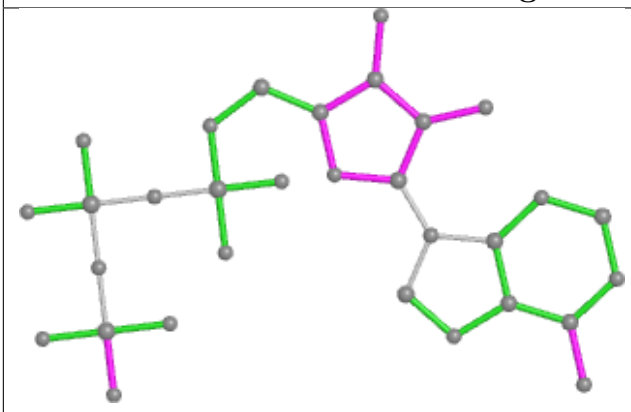


Rings

Ligand ATP W 401



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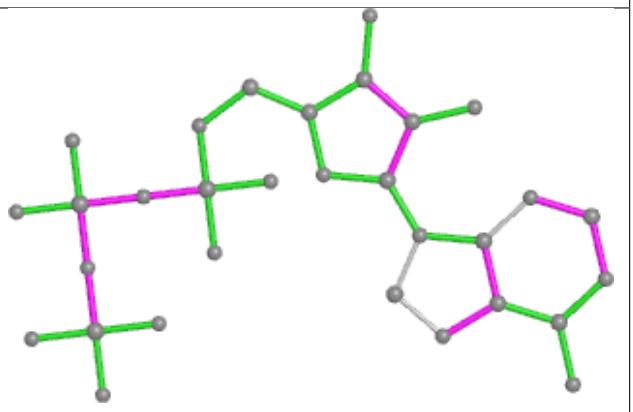

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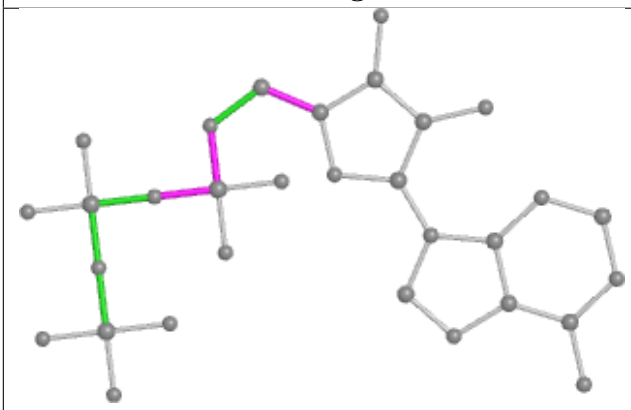

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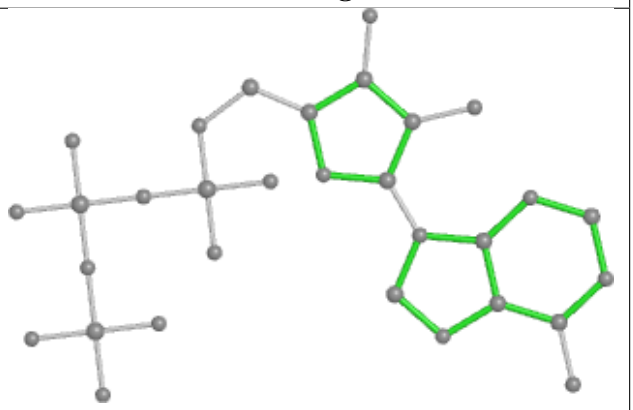
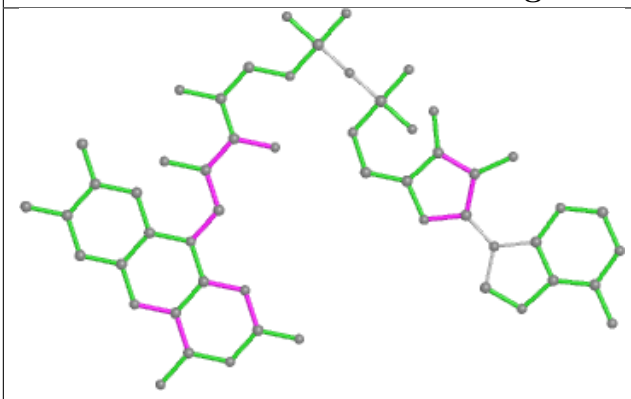


Rings

Ligand FAD A 703



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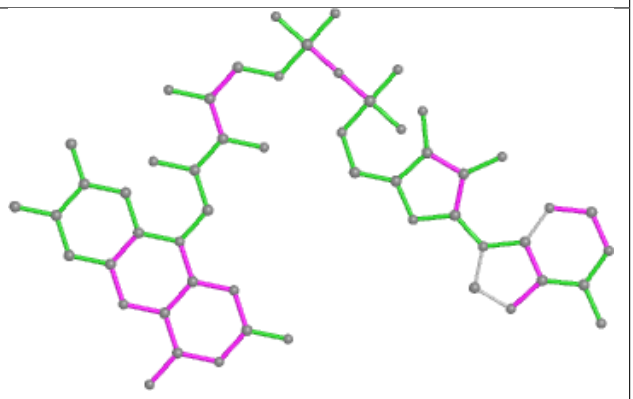

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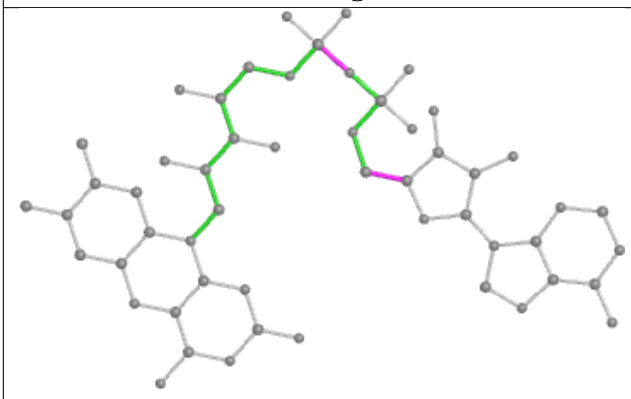

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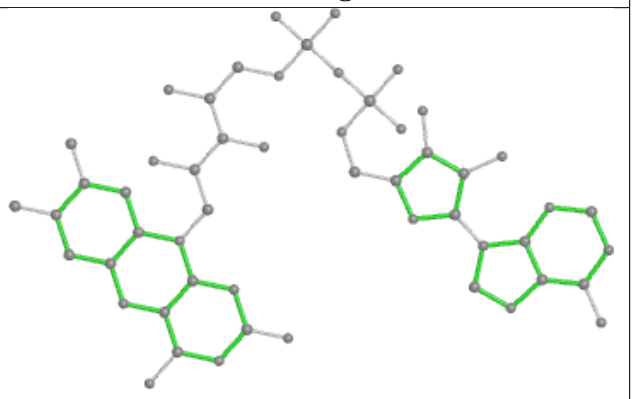
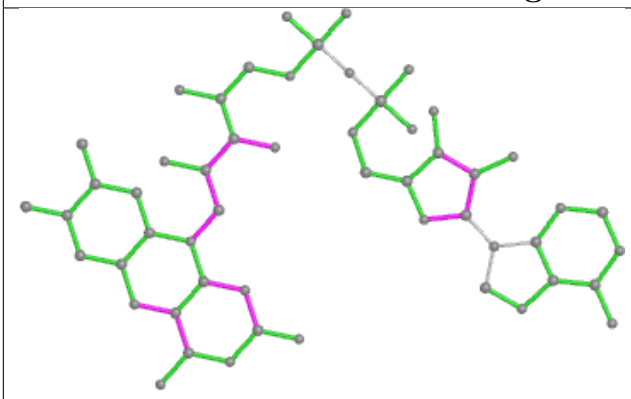


Rings

Ligand FAD R 701



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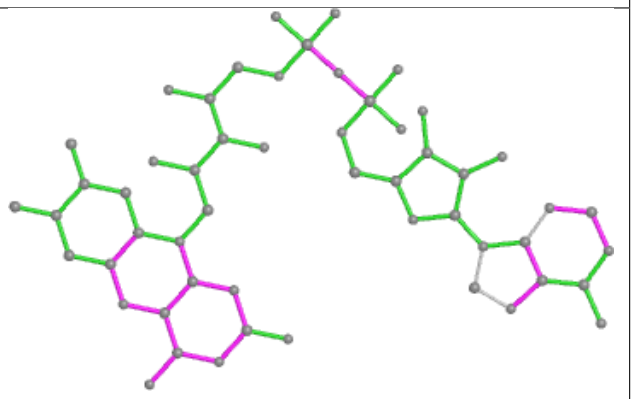

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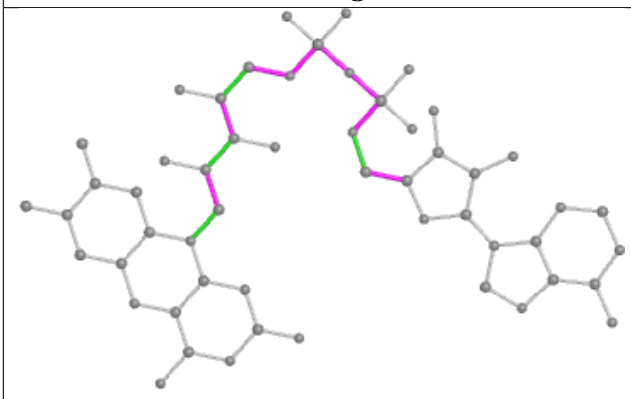

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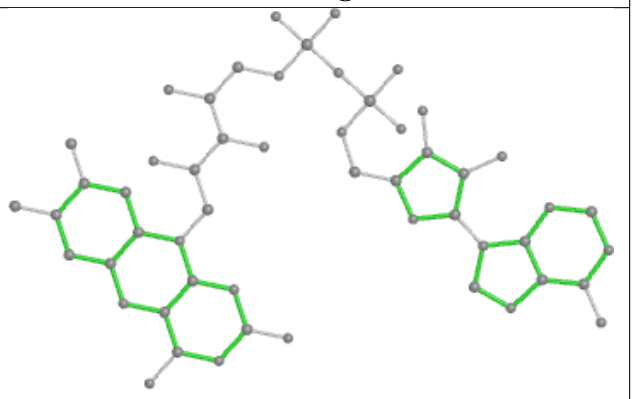
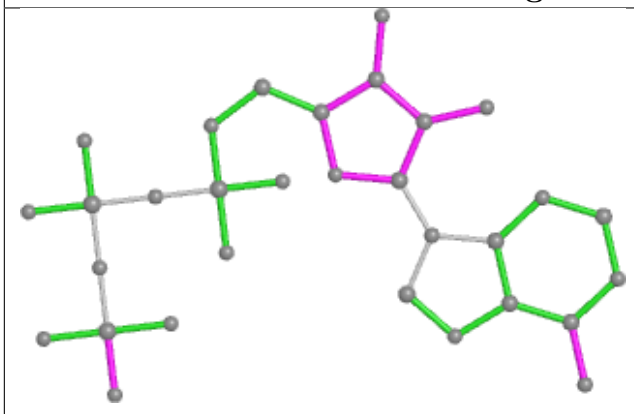


Rings

Ligand ATP C 401



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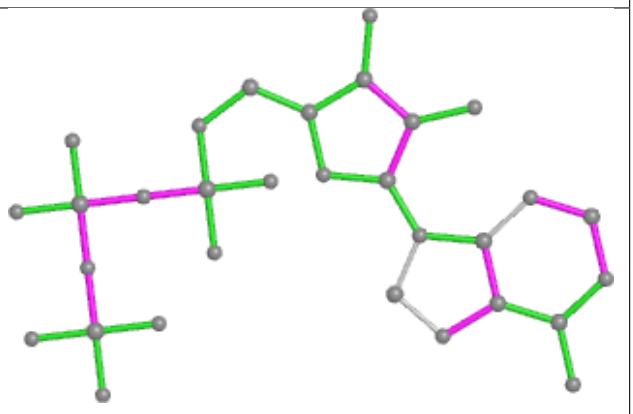

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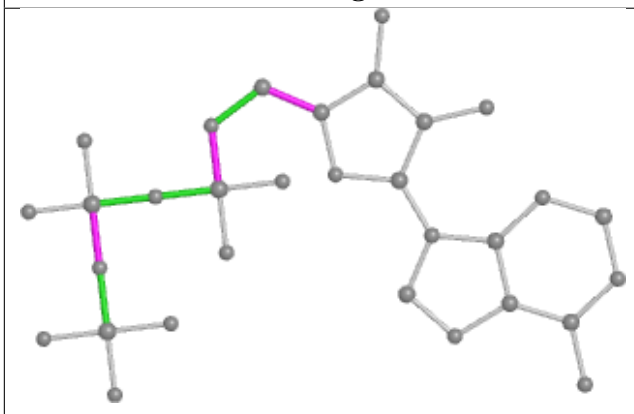

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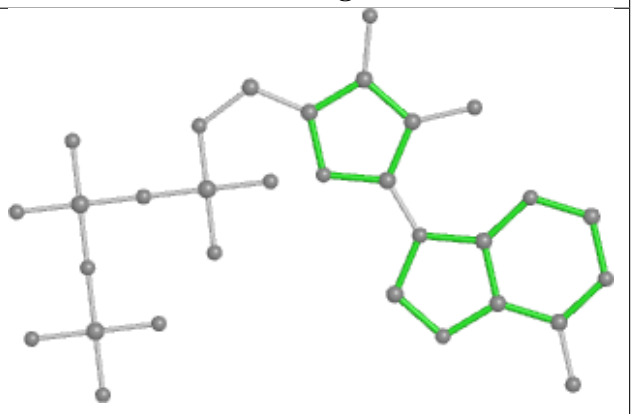
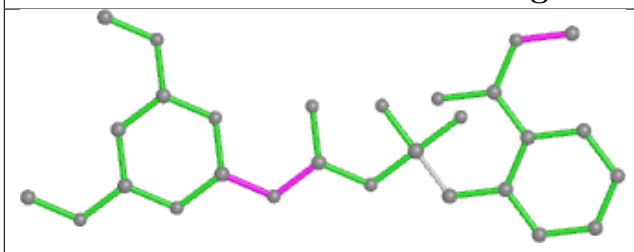


Rings

Ligand 60G B 704



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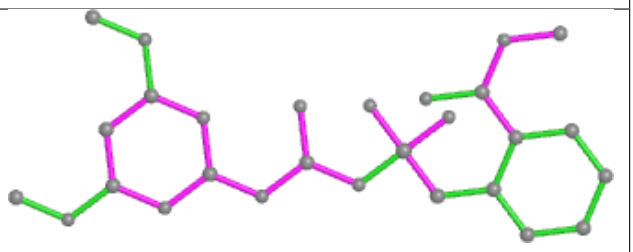

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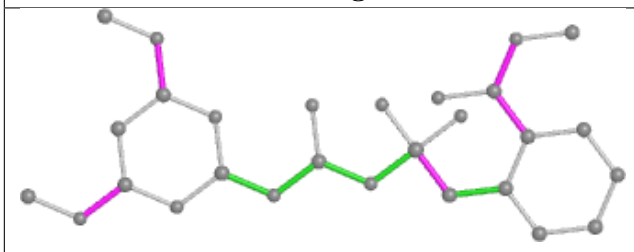

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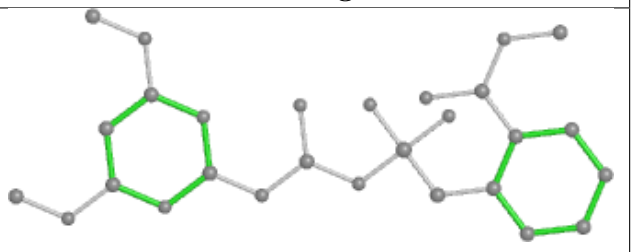
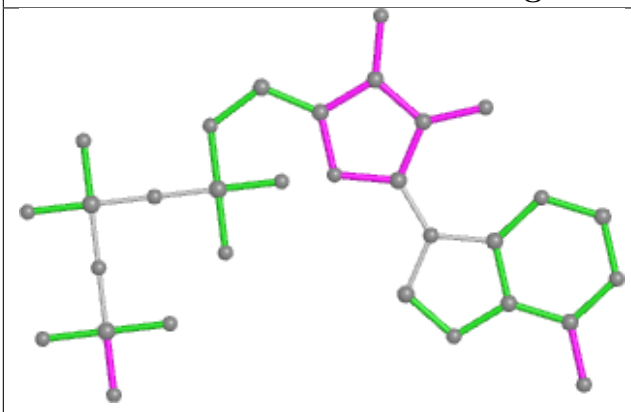


Rings

Ligand ATP O 401



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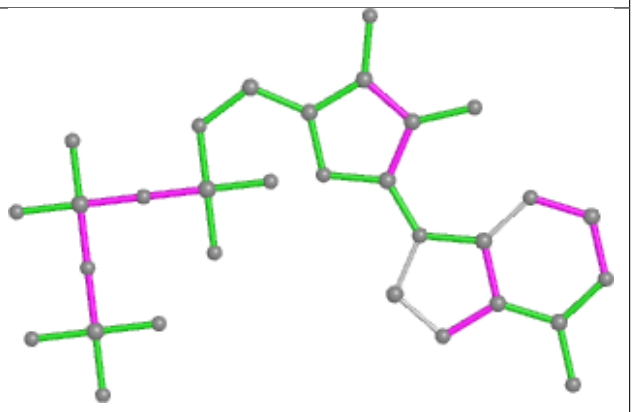

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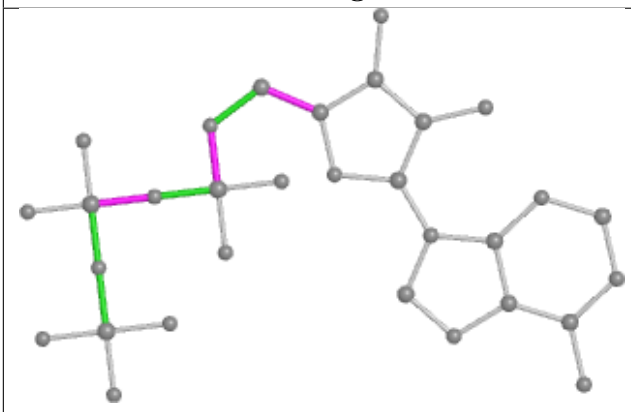

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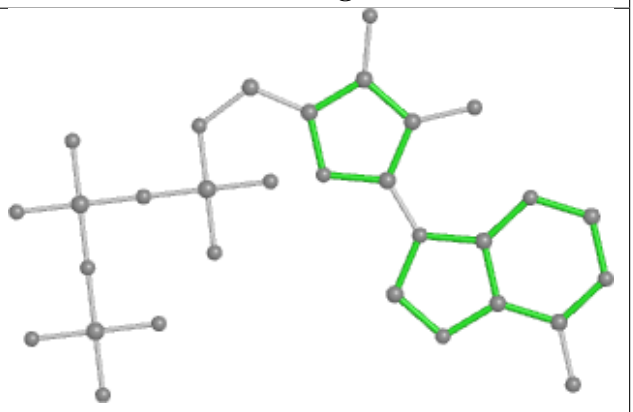
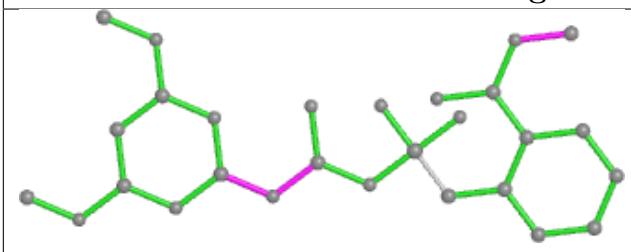


Rings

Ligand 60G V 704



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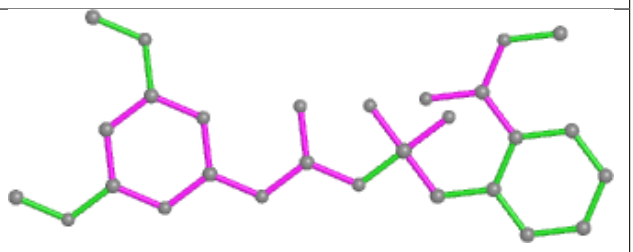

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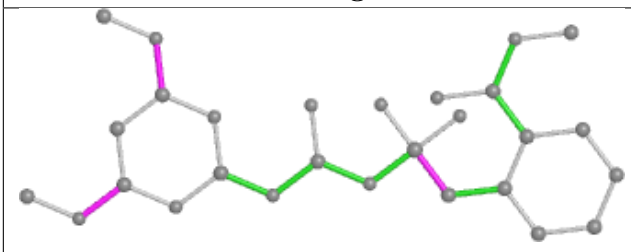

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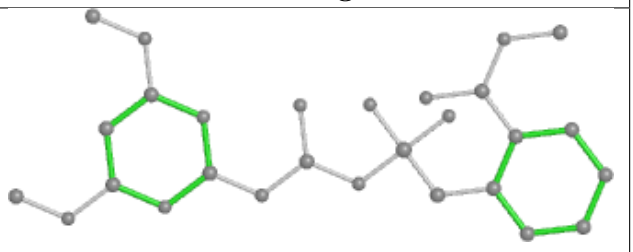
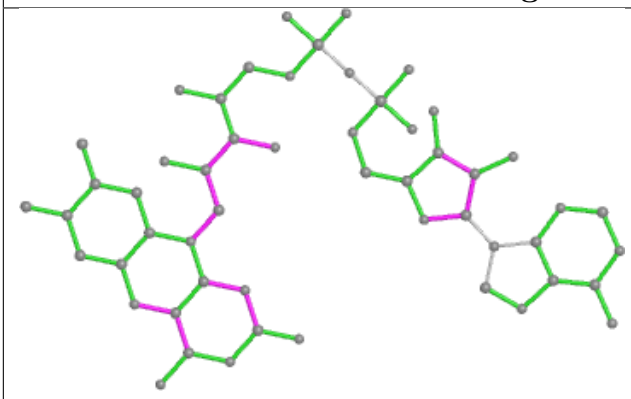


Rings

Ligand FAD M 703



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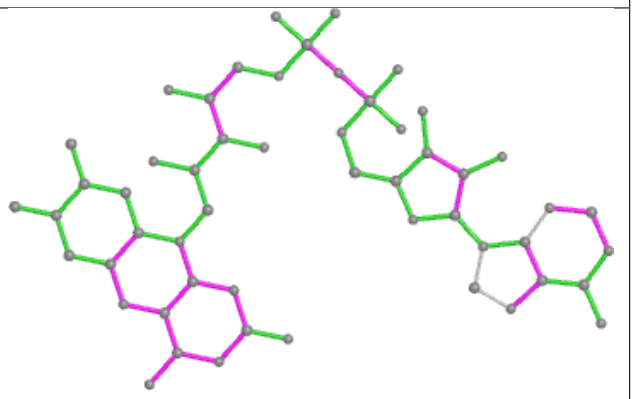

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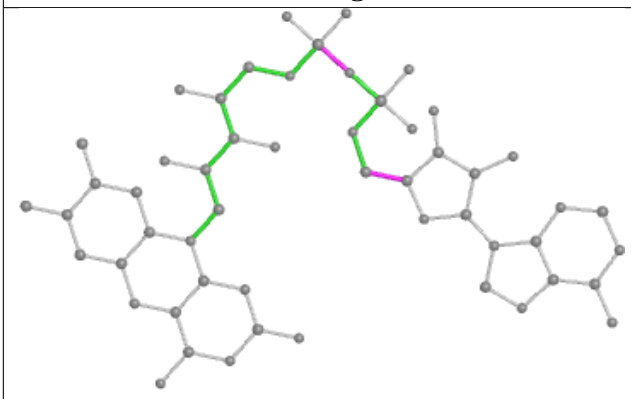

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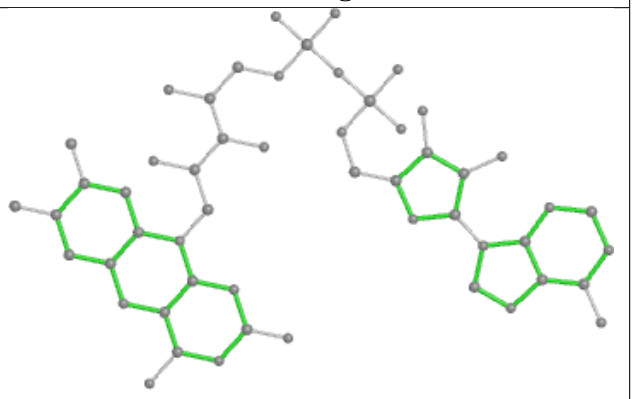
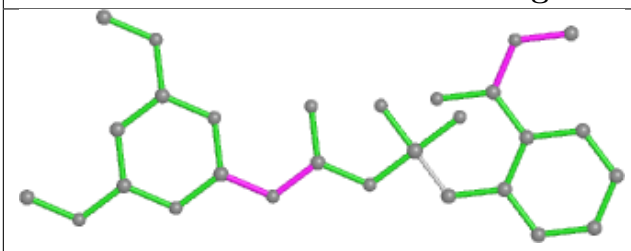


Rings

Ligand 60G F 704



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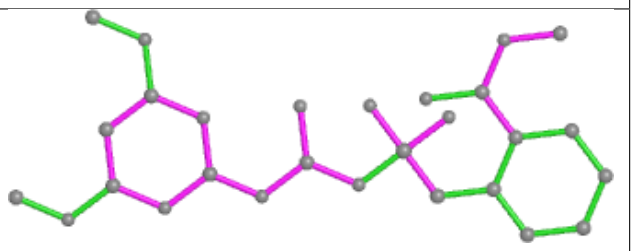

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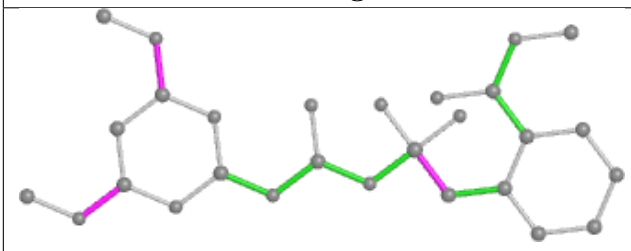

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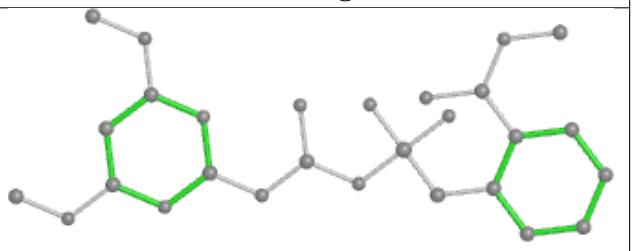
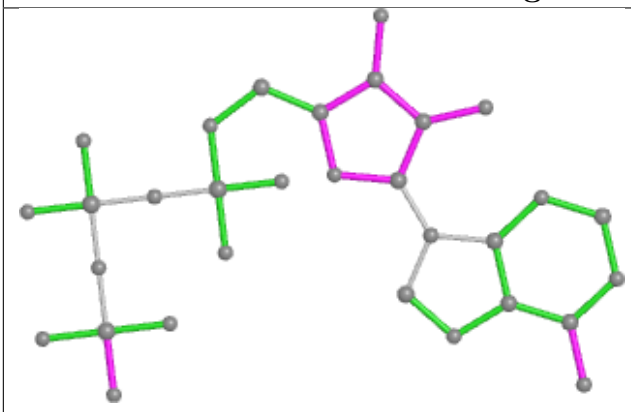


Rings

Ligand ATP K 401



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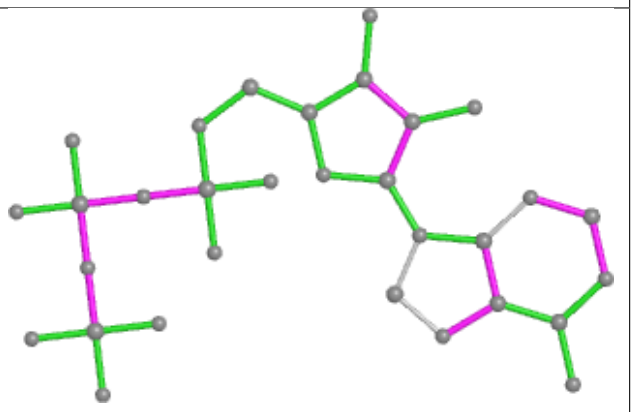
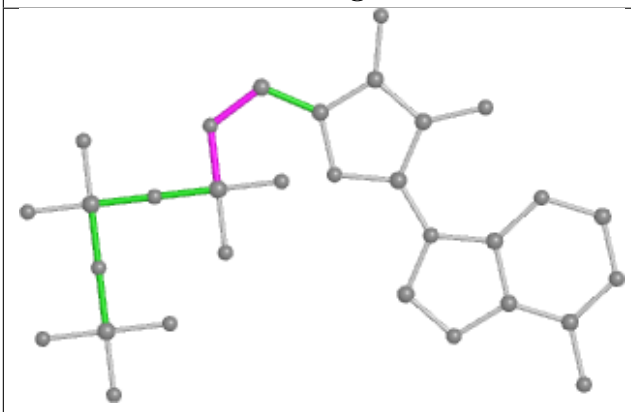


Bond angles



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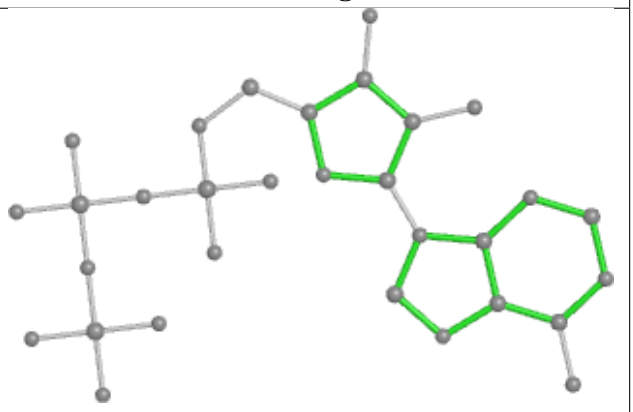
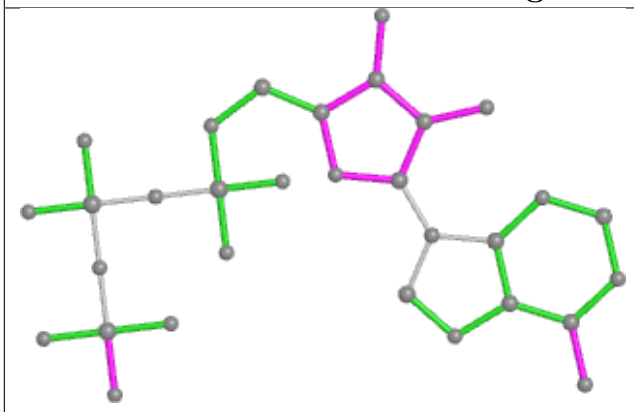


Rings

Ligand ATP P 401



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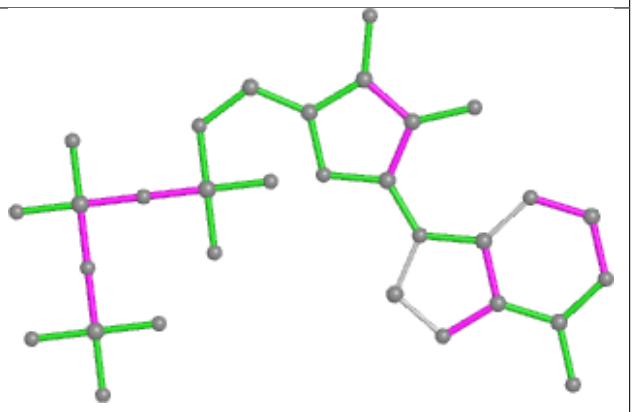
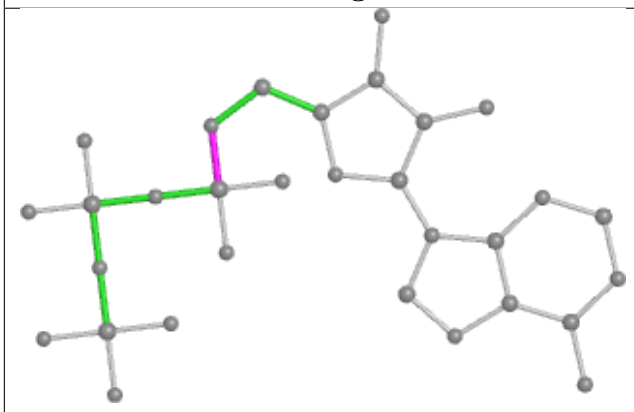


Bond angles



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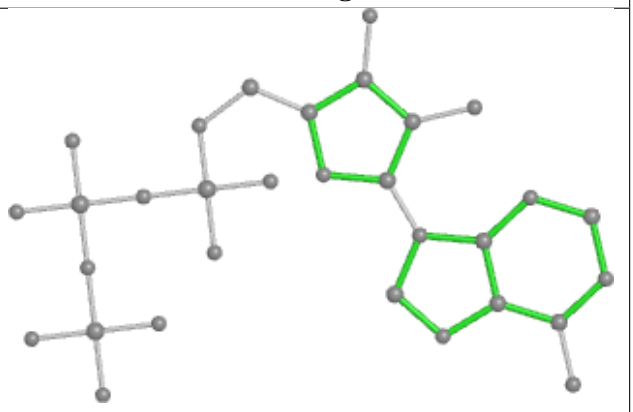
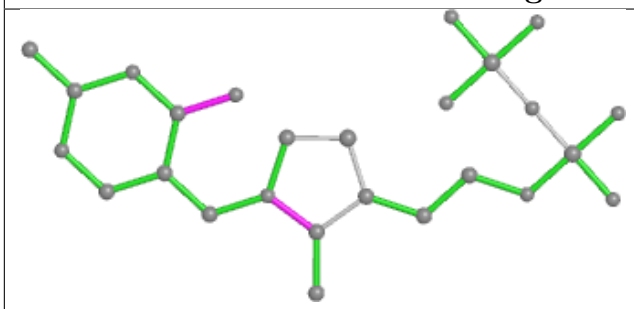


Rings

Ligand TPP A 701



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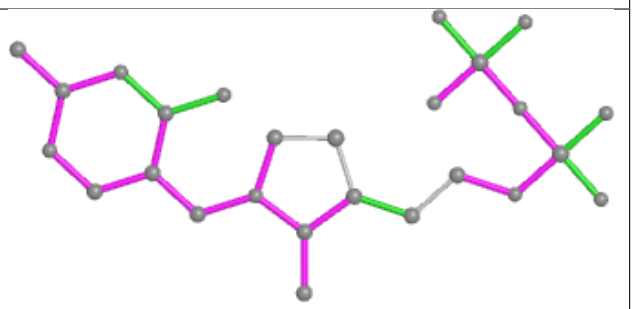
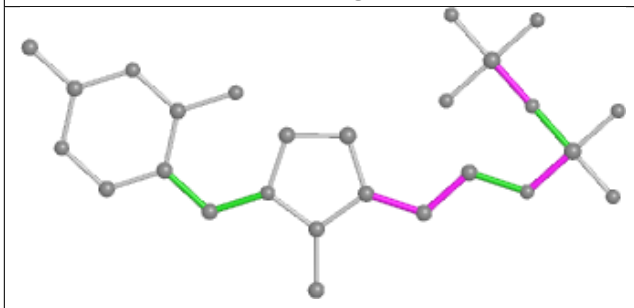
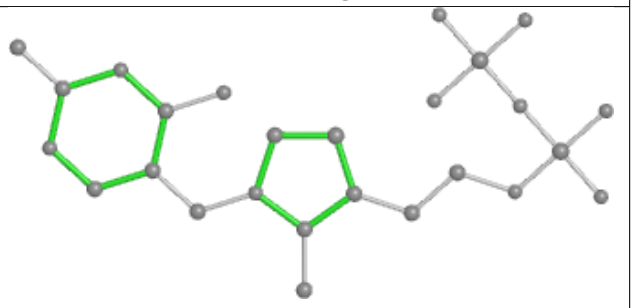


Bond angles

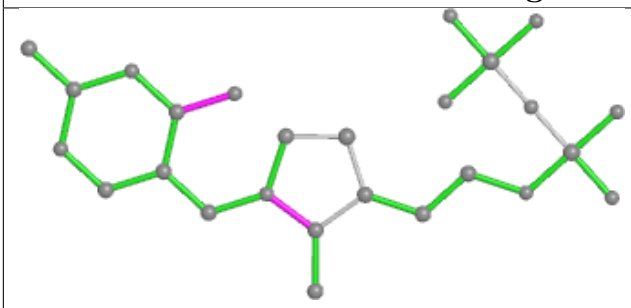


Torsions

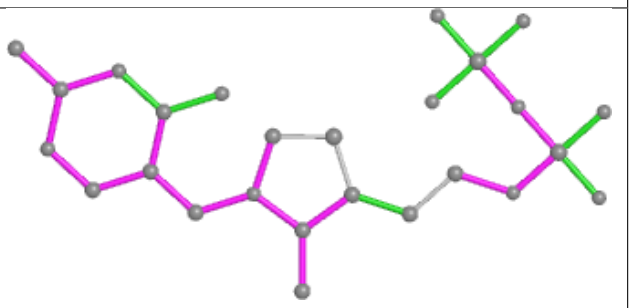


Rings

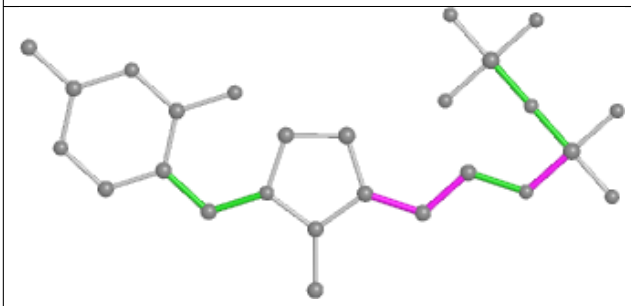
Ligand TPP E 701



Bond lengths



Bond angles



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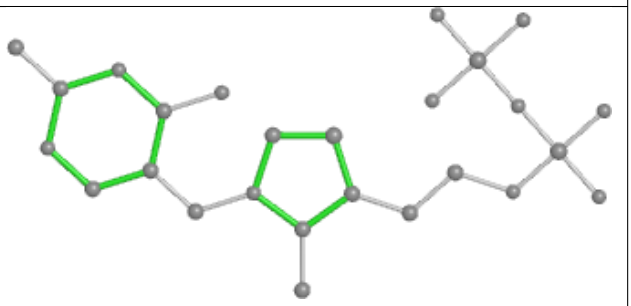
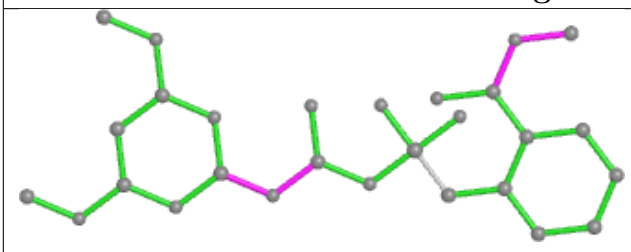


Rings

Ligand 60G J 704



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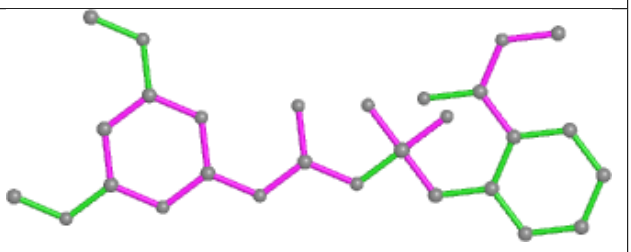

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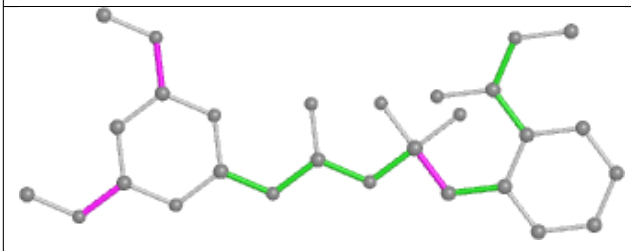

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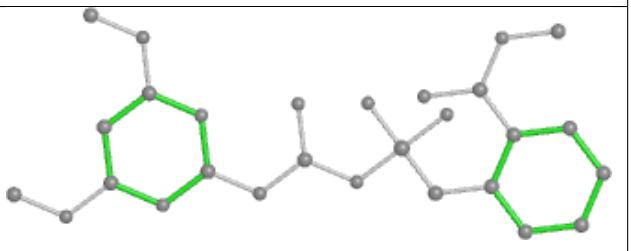
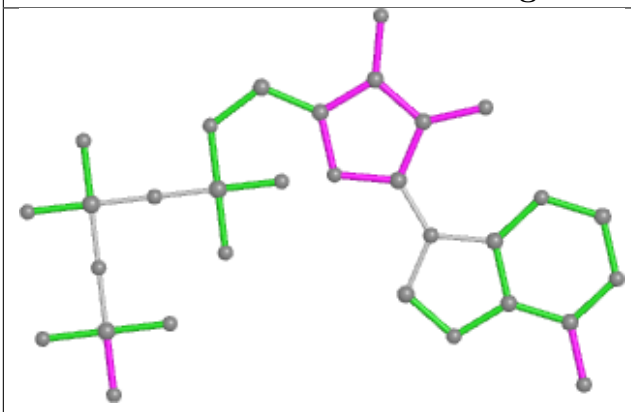


Rings

Ligand ATP W 402



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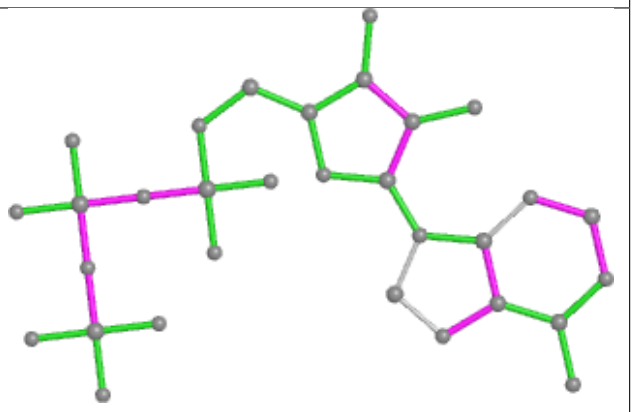

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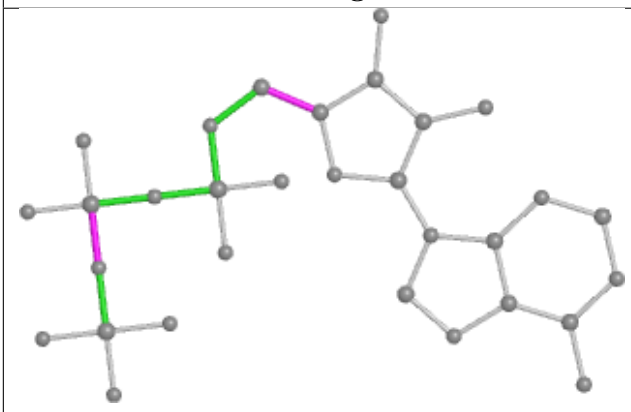

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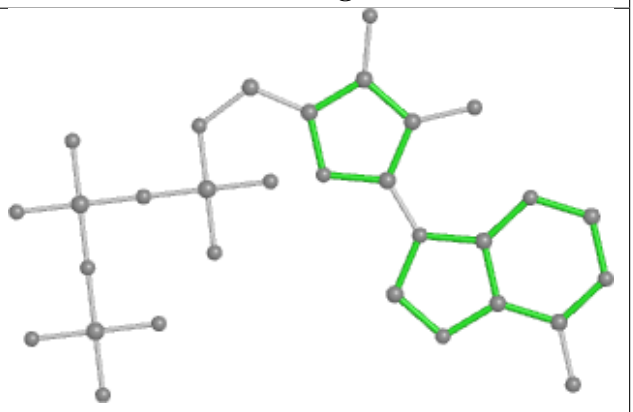
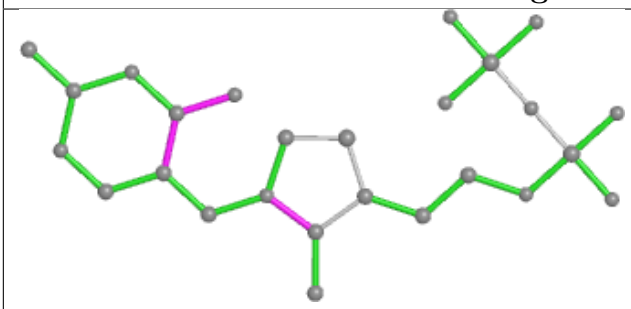


Rings

Ligand TPP I 701



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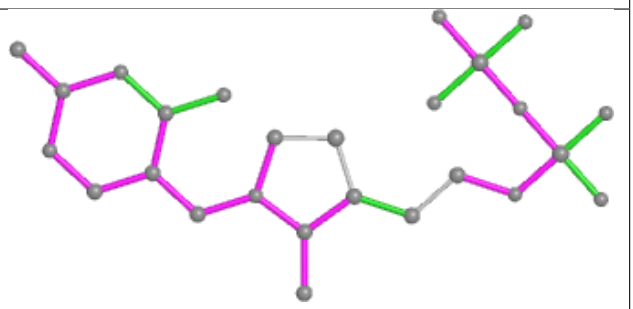

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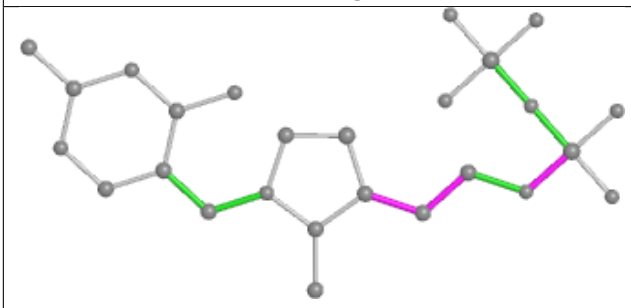

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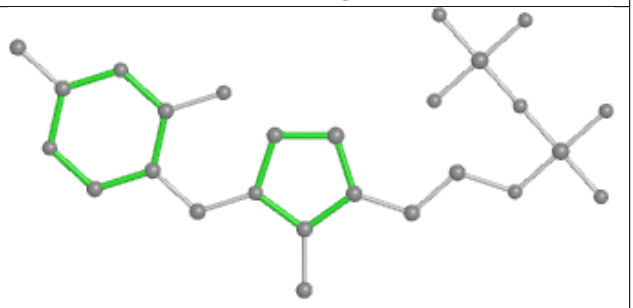
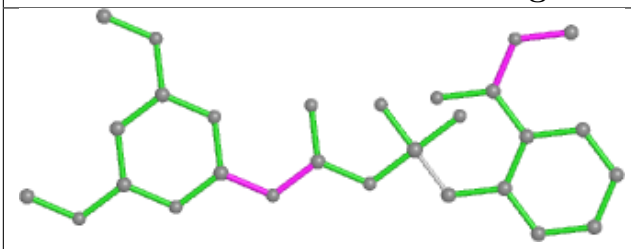


Rings

Ligand 60G R 702



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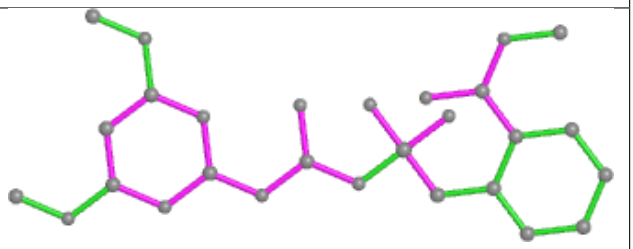

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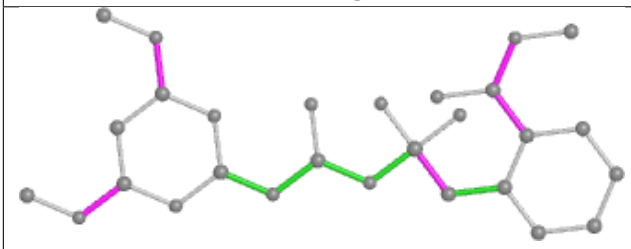

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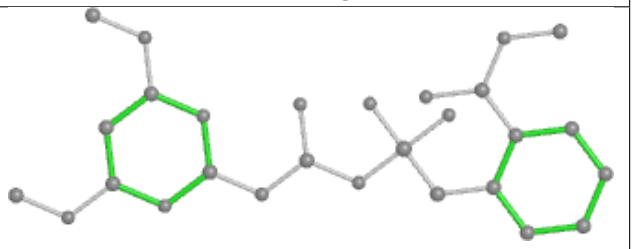
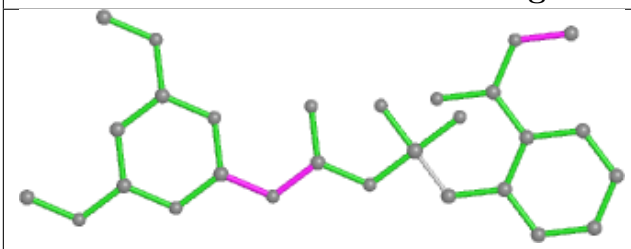


Rings

Ligand 60G N 704



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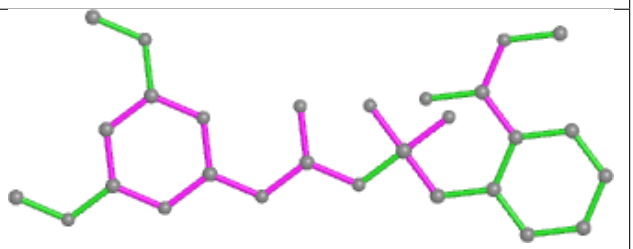

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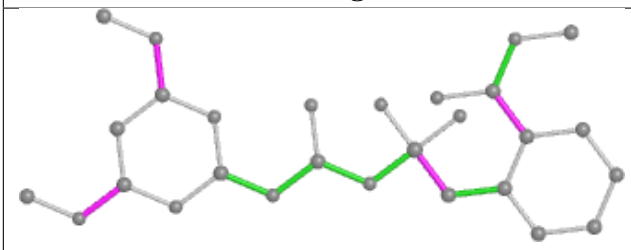

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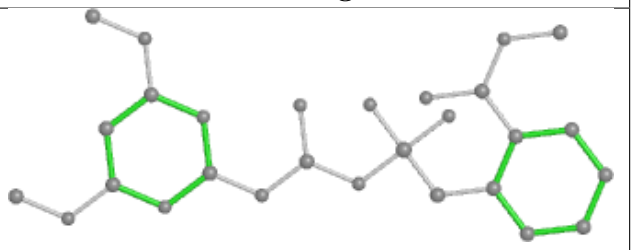
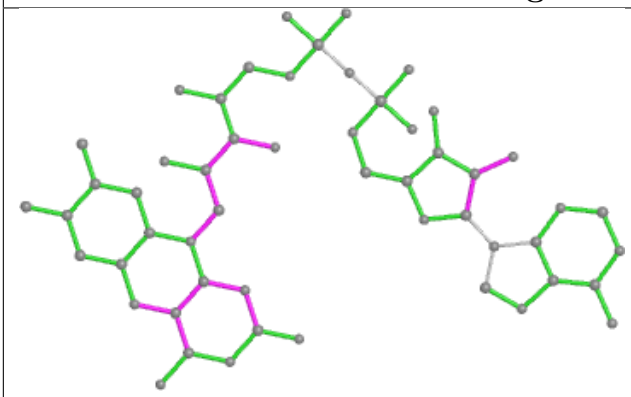


Rings

Ligand FAD F 703



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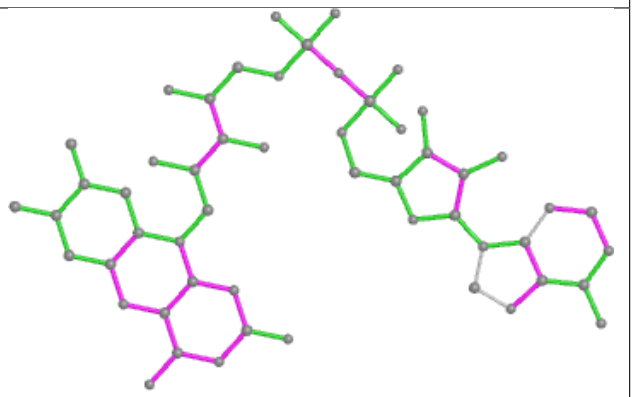

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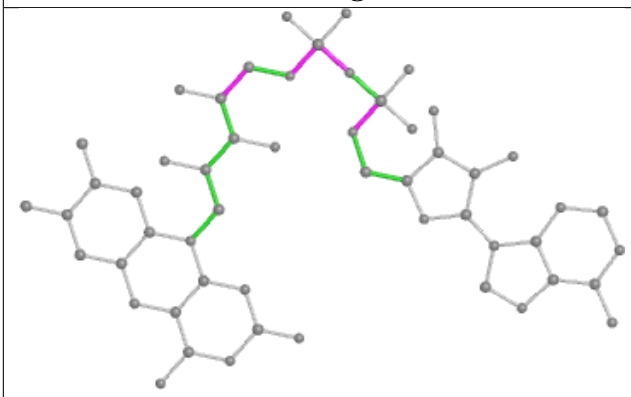

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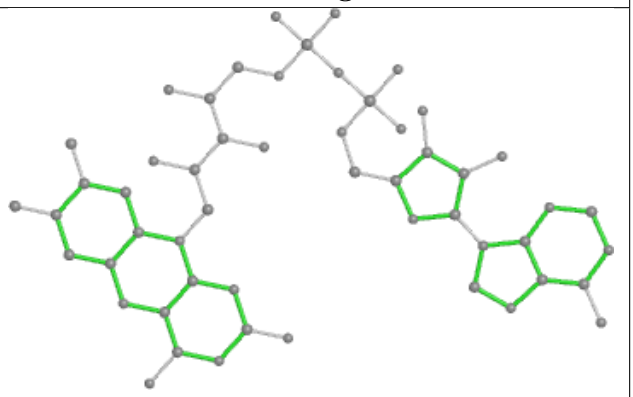
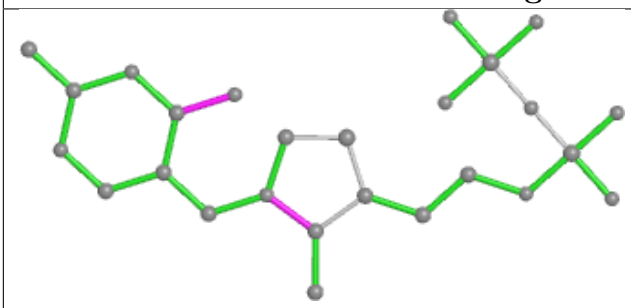


Rings

Ligand TPP B 701



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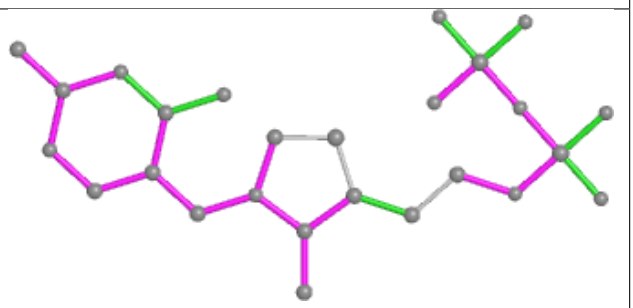

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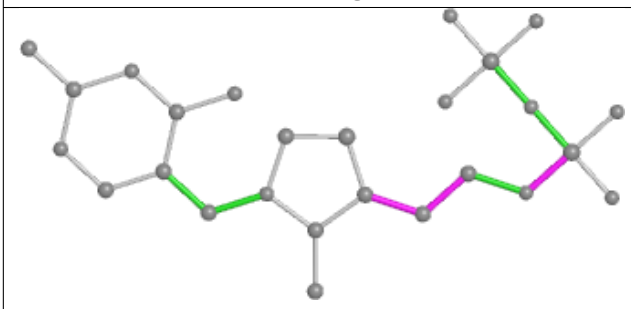

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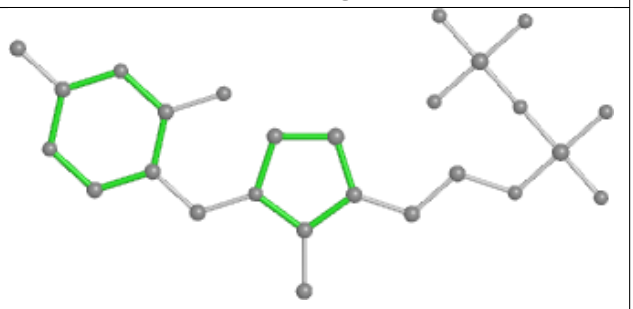
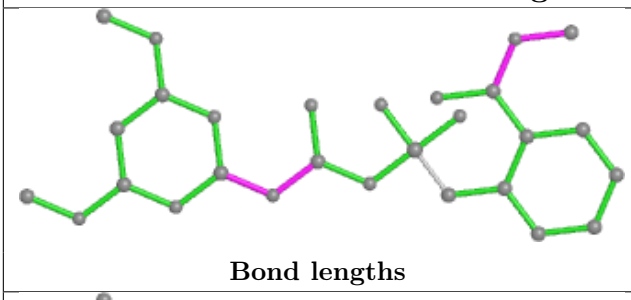


Rings

Ligand 60G E 704



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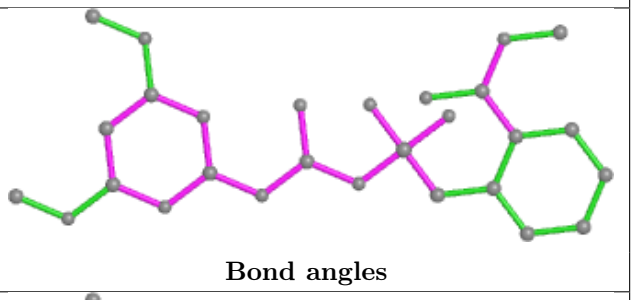

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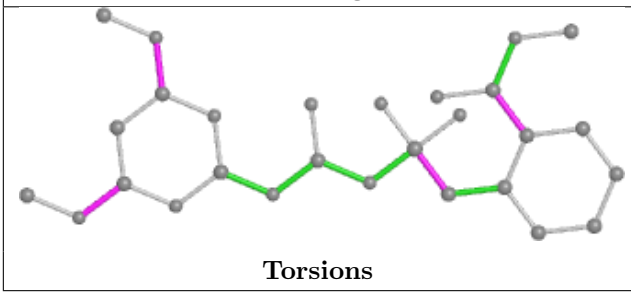

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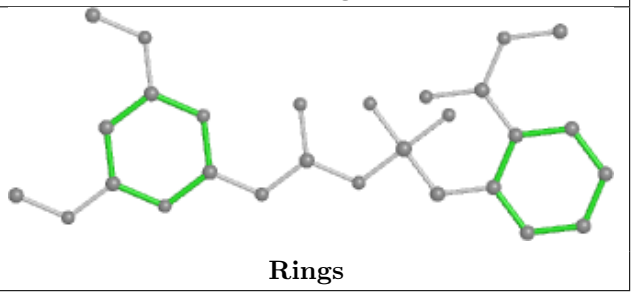
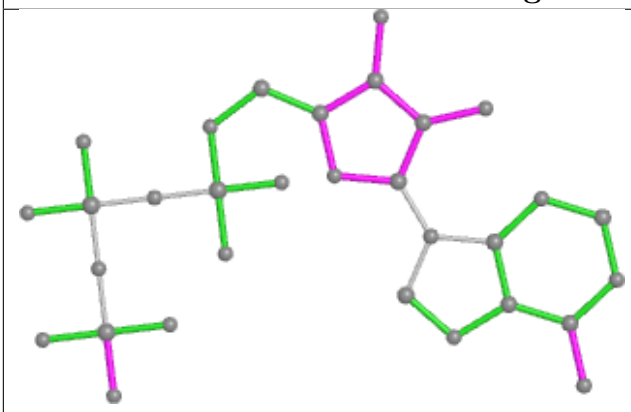


Rings

Ligand ATP H 401



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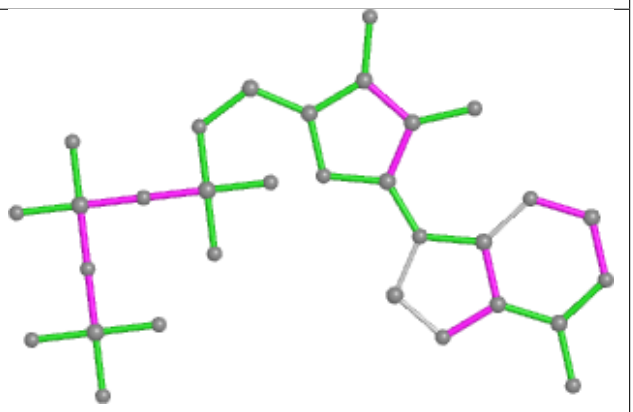

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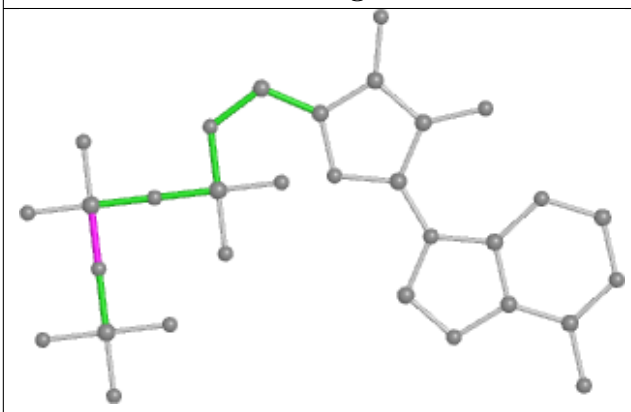

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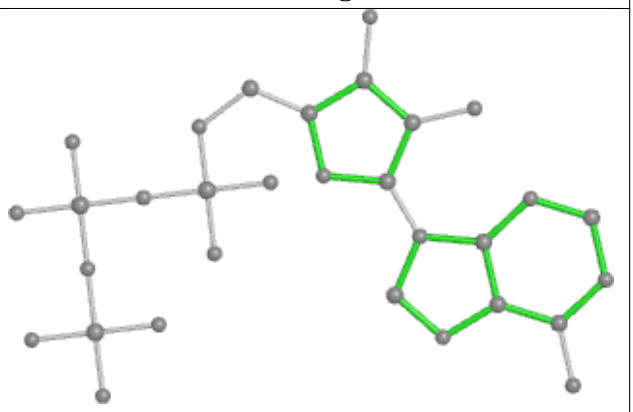
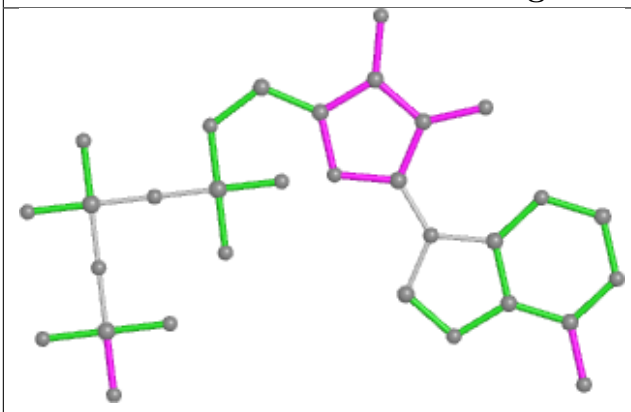


Rings

Ligand ATP S 401



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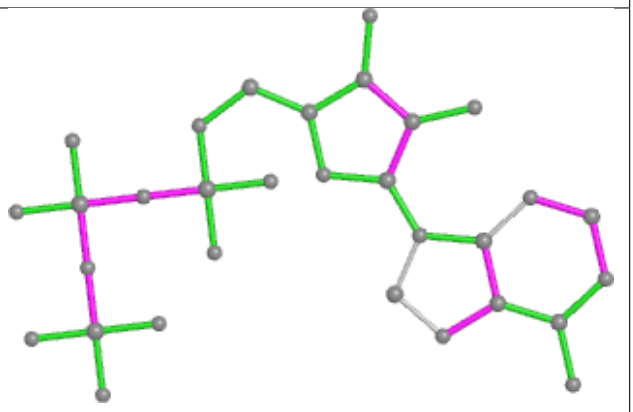

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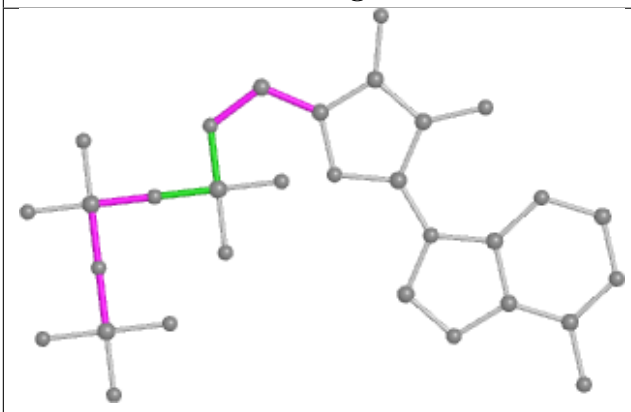

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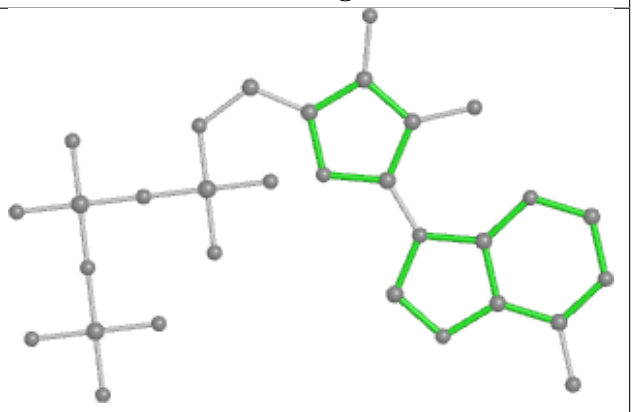
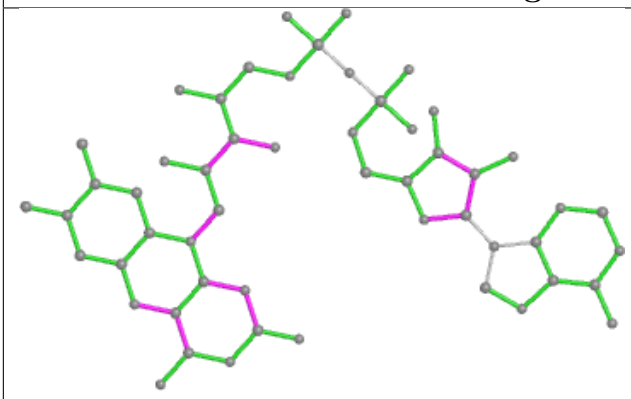


Rings

Ligand FAD N 703



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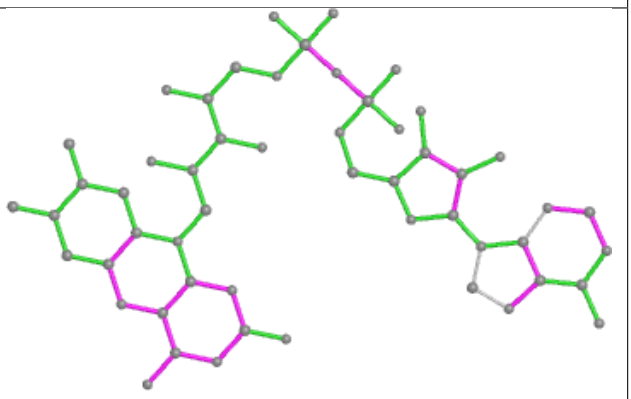
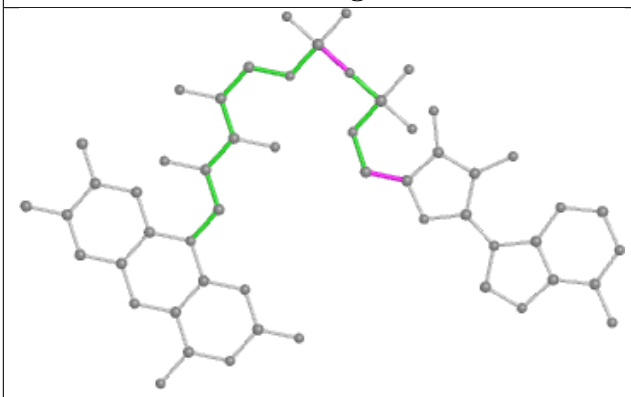


Bond angles



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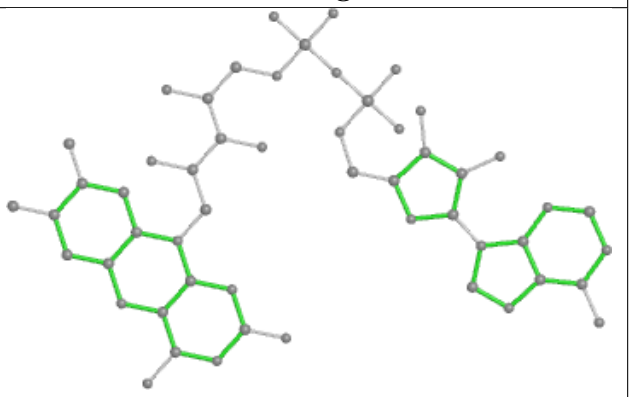
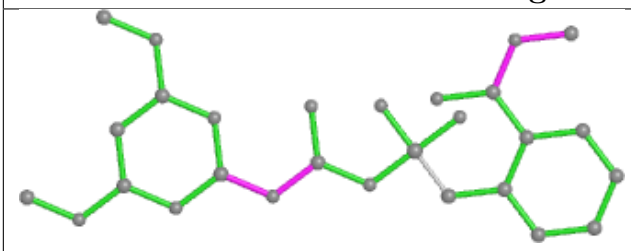


Rings

Ligand 60G Q 704



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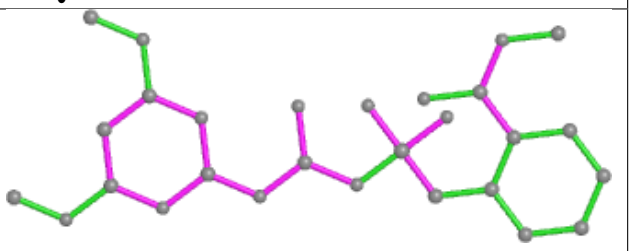
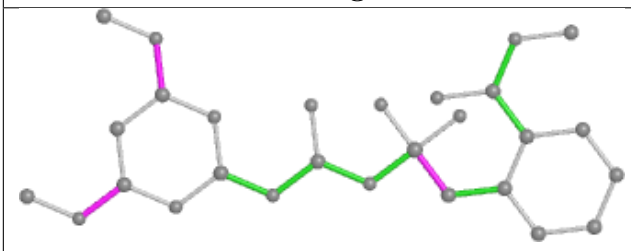


Bond angles



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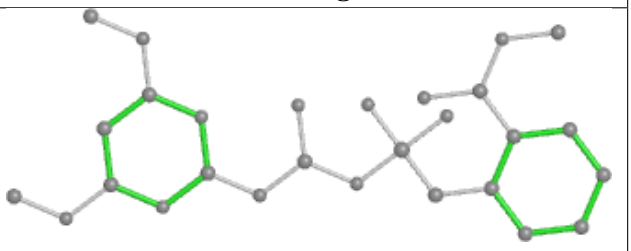
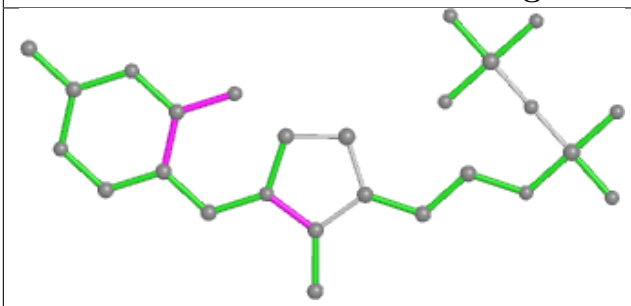
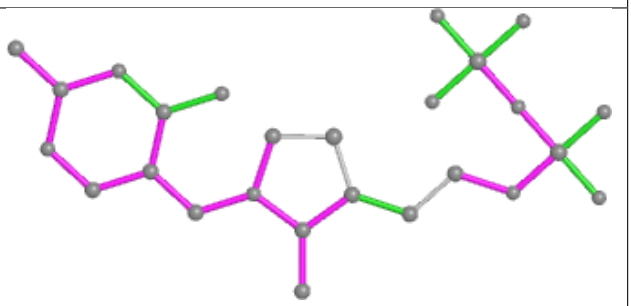


Rings

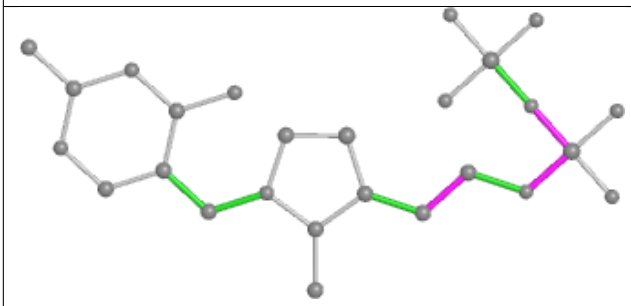
Ligand TPP N 701



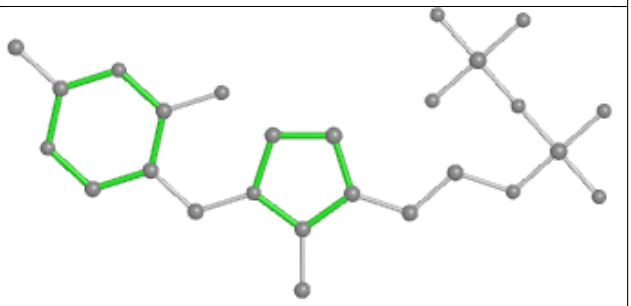
Bond lengths



Bond angles

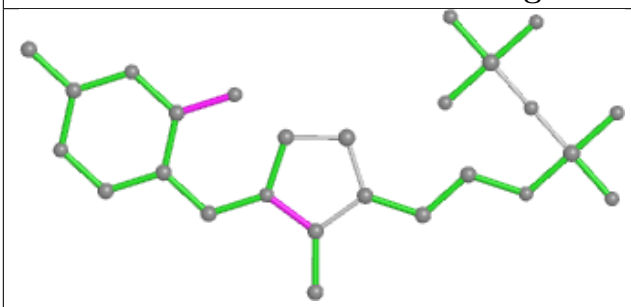


Torsions



Rings

Ligand TPP V 701



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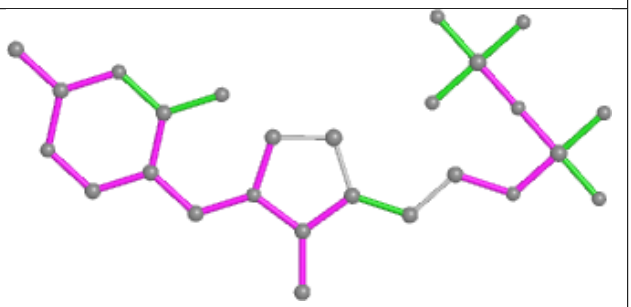

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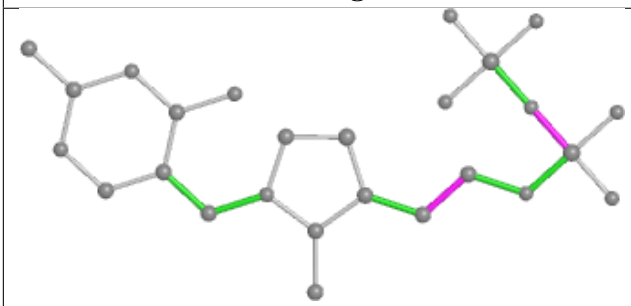

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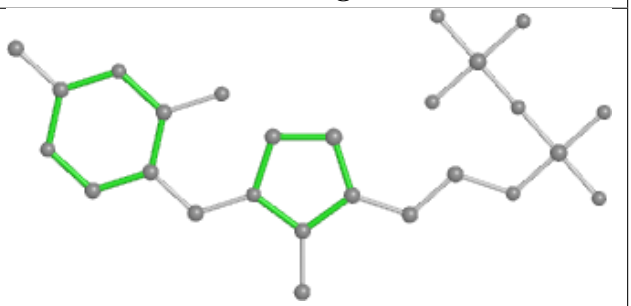
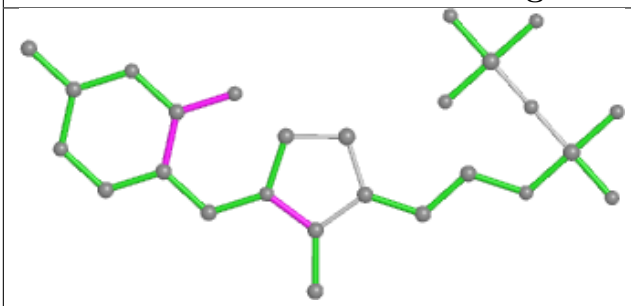


Rings

Ligand TPP F 701



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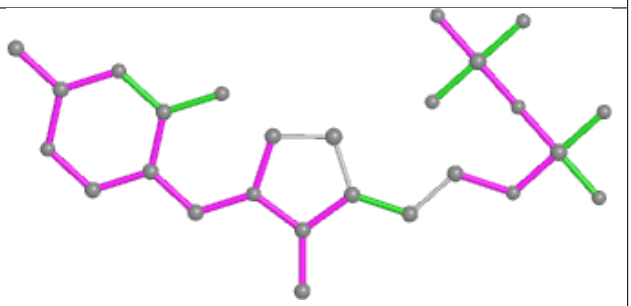

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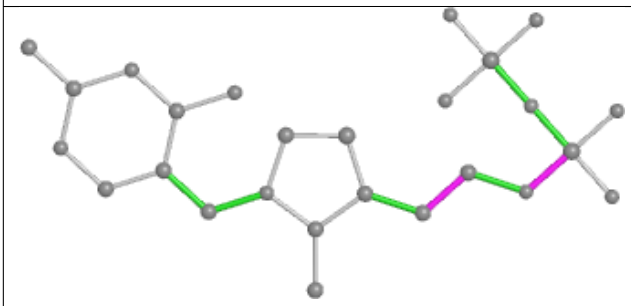

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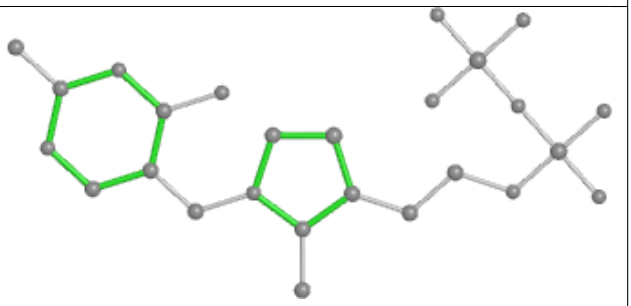
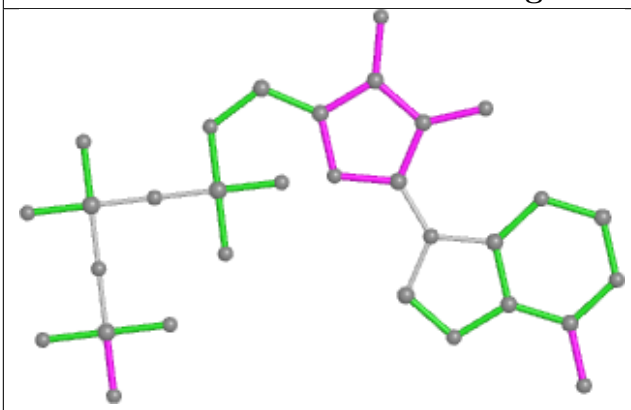


Rings

Ligand ATP T 401



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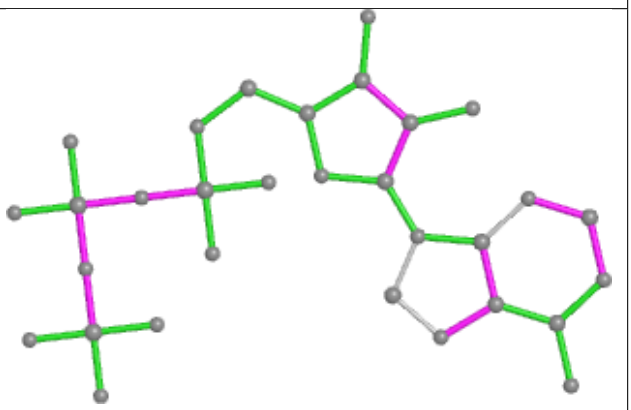

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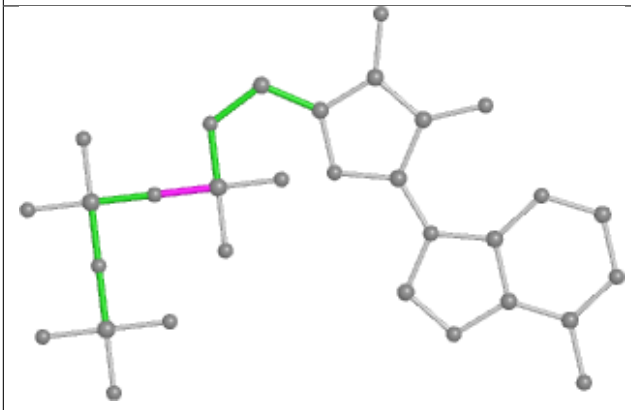

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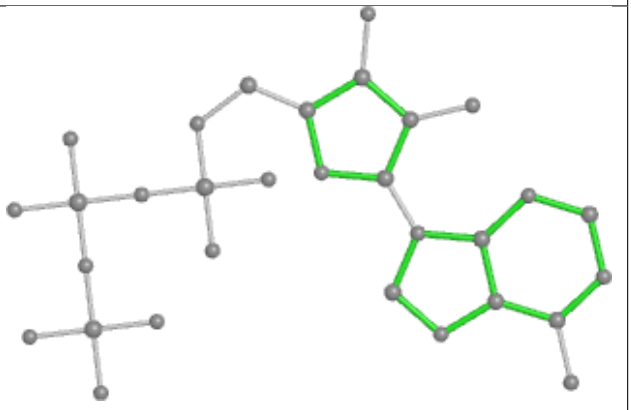
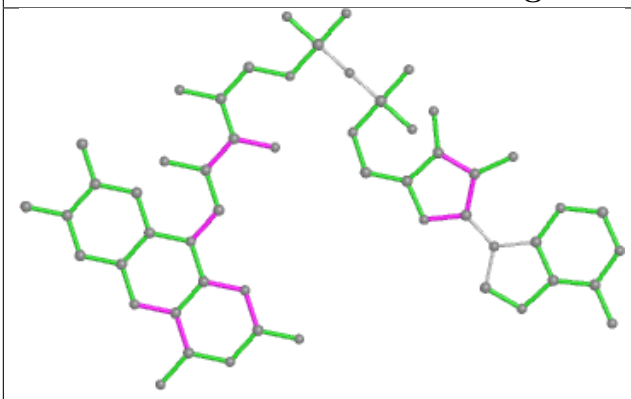


Rings

Ligand FAD Q 703



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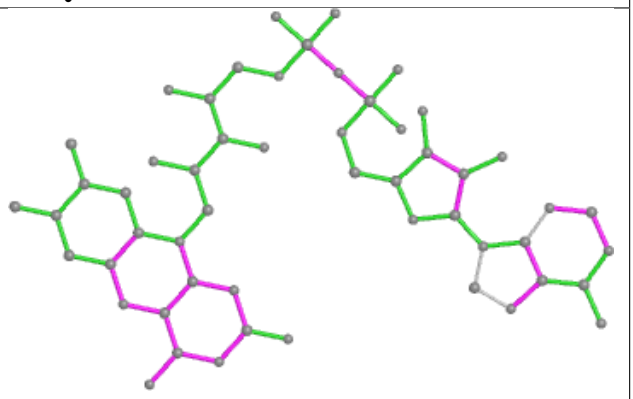

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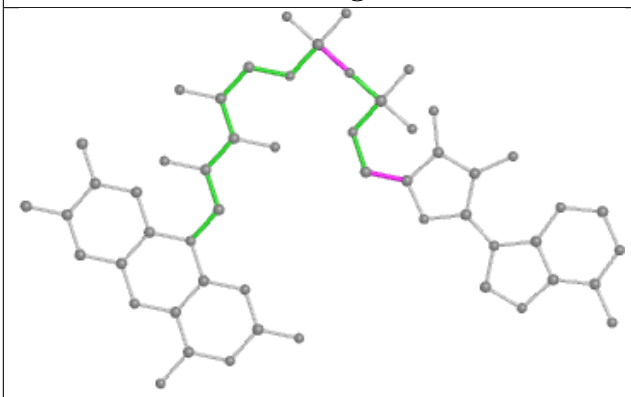

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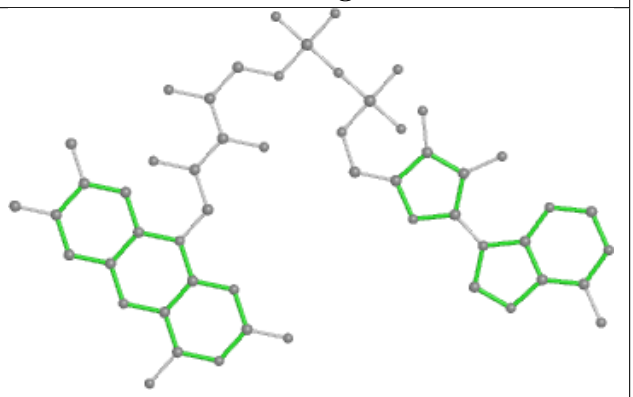
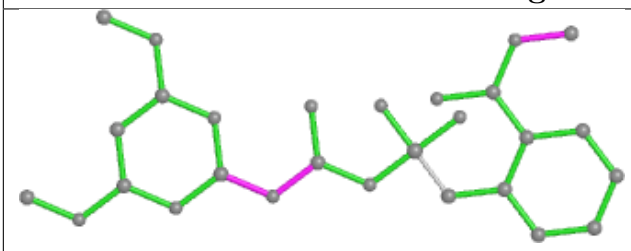


Rings

Ligand 60G N 705



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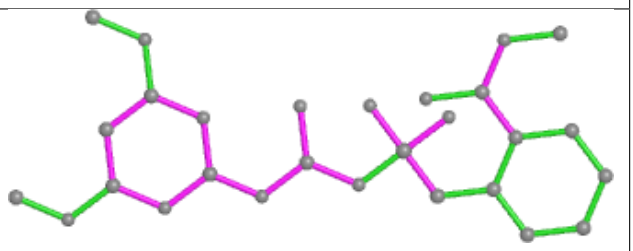

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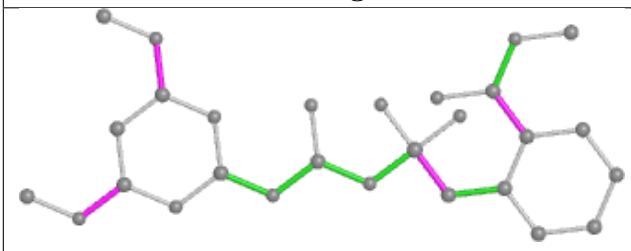

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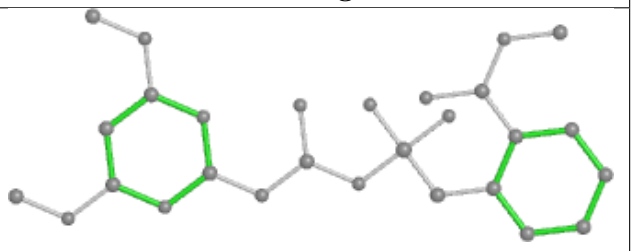
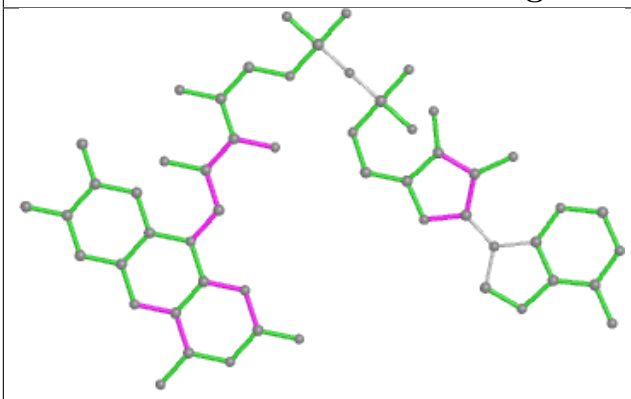


Rings

Ligand FAD E 703



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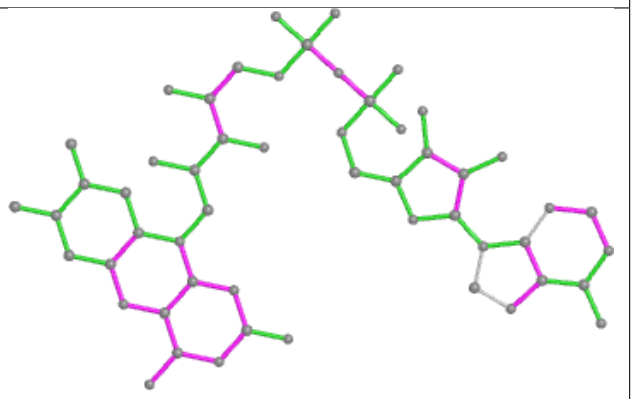

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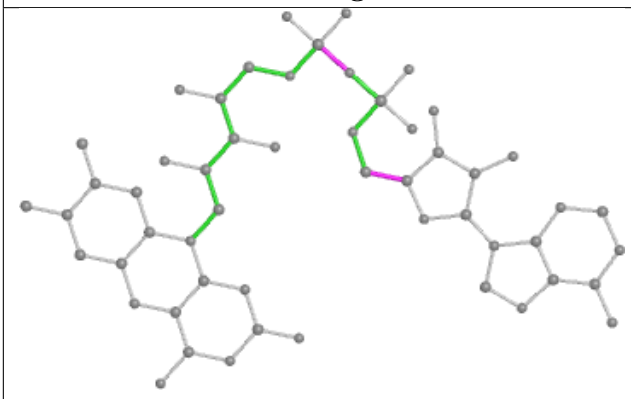

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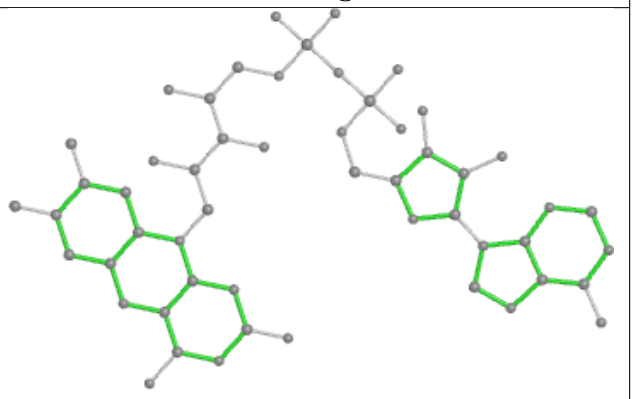
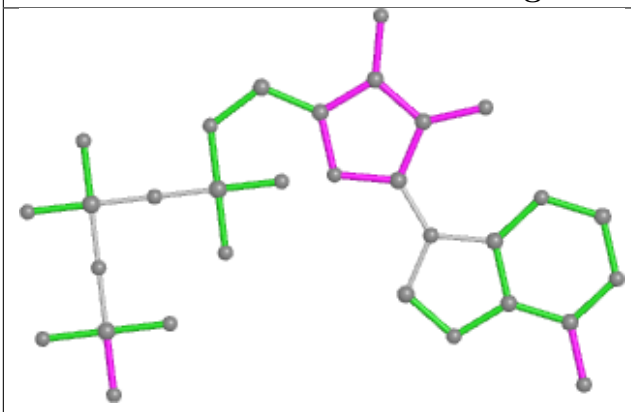


Rings

Ligand ATP D 401



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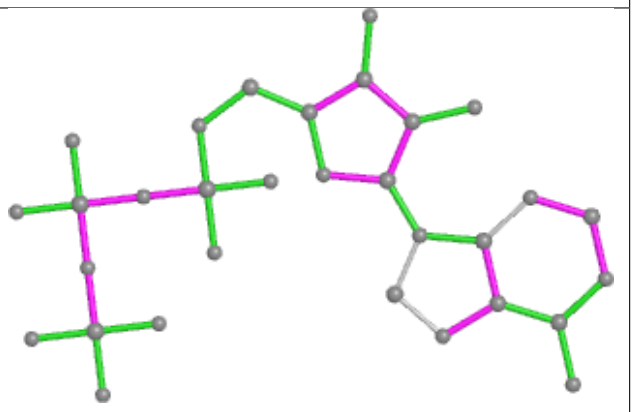

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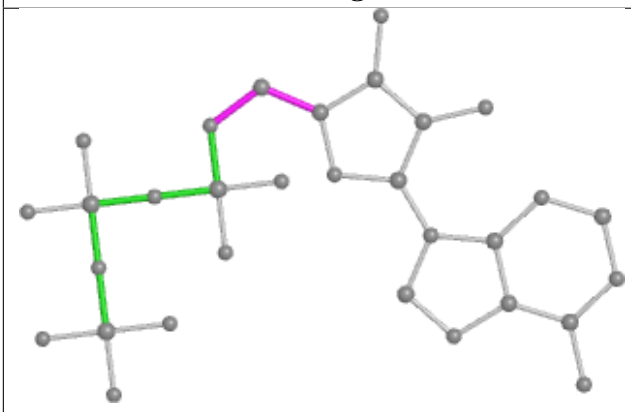

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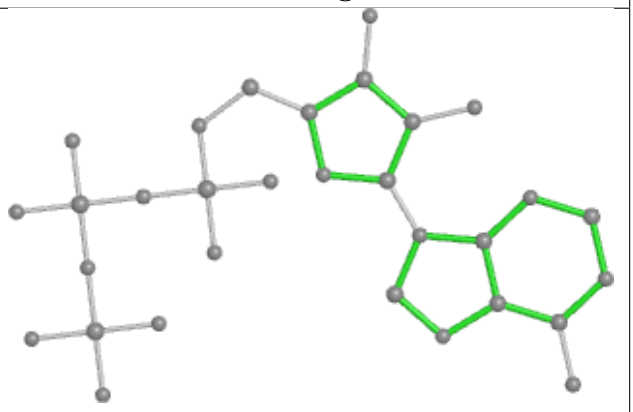
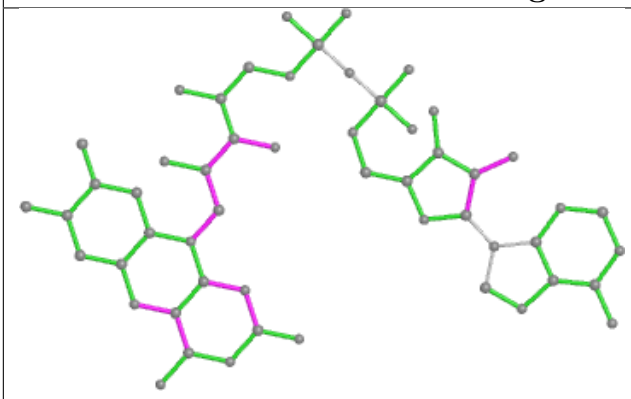


Rings

Ligand FAD J 703



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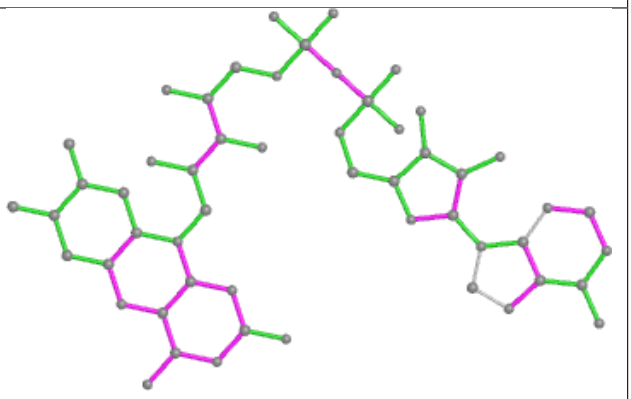

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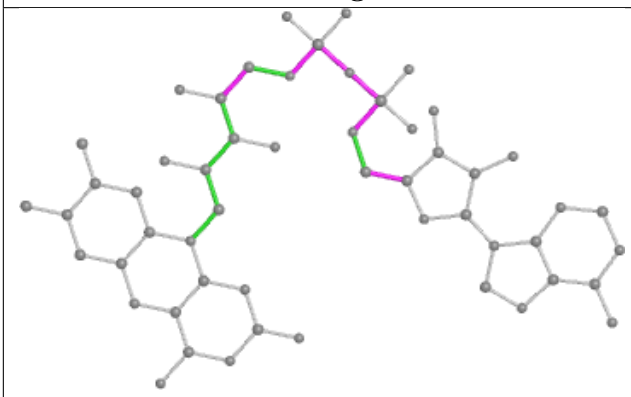

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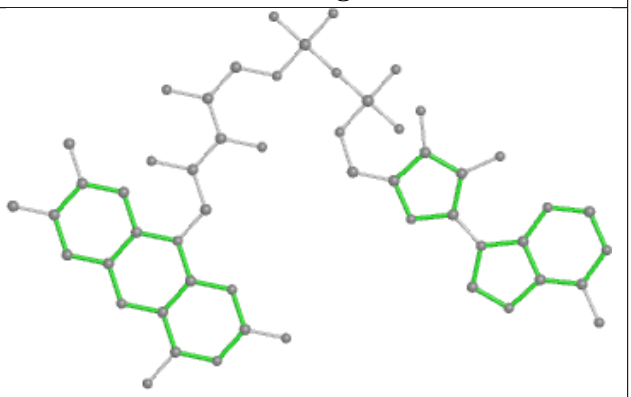
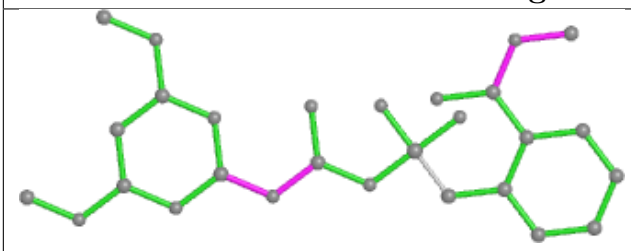


Rings

Ligand 60G U 704



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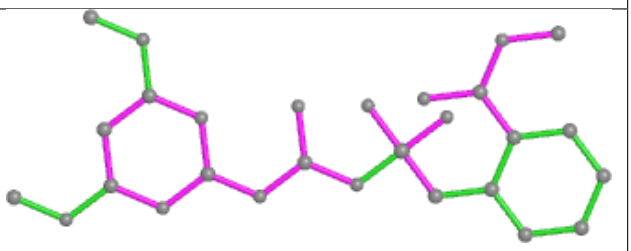

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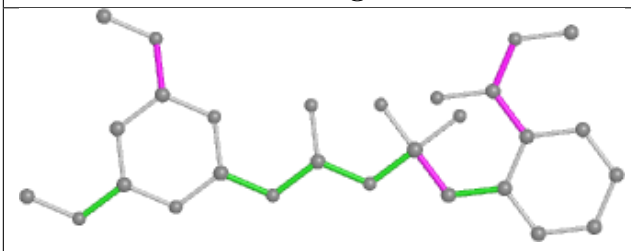

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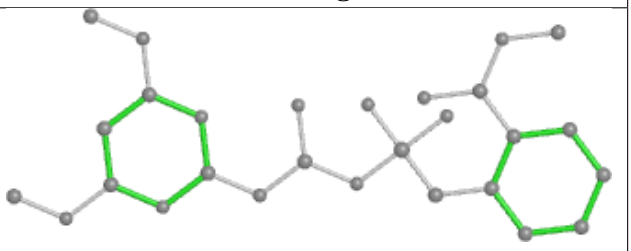
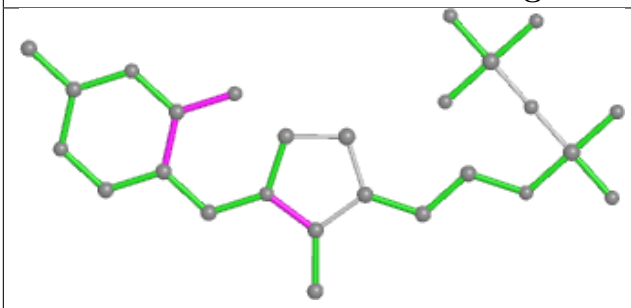
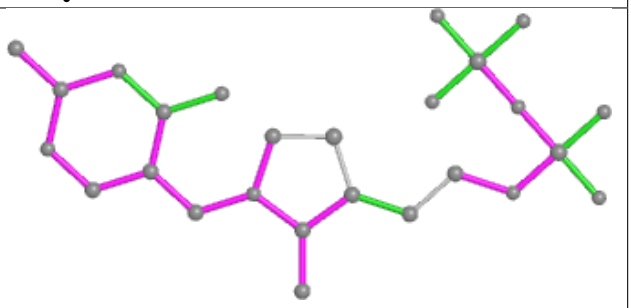
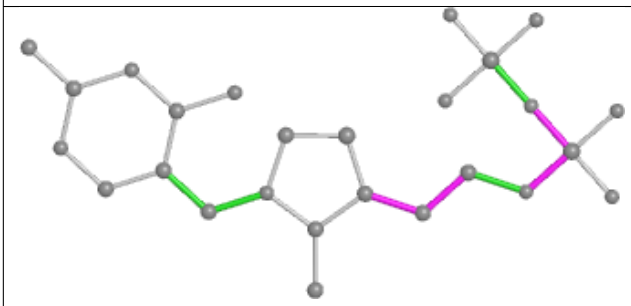
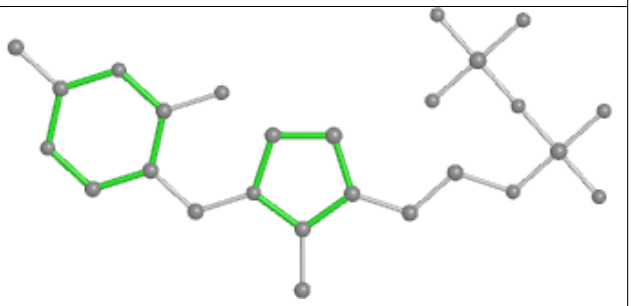


Rings

Ligand TPP Q 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

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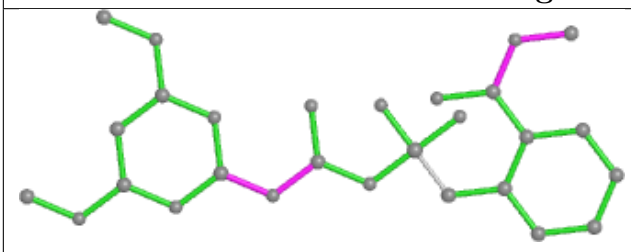
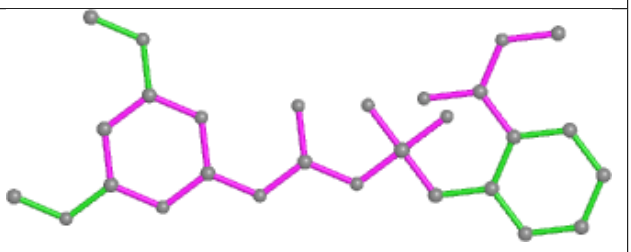
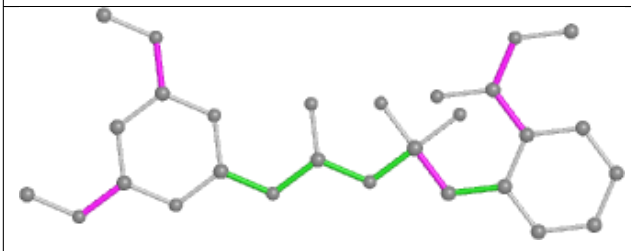
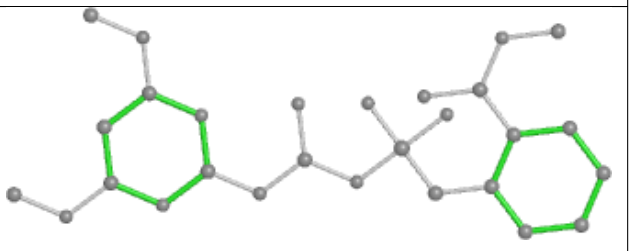
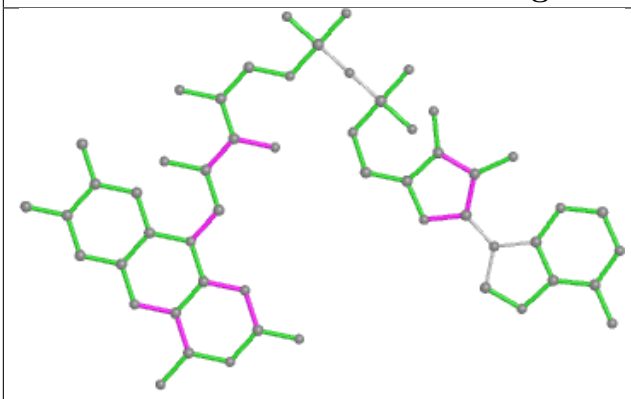
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD I 703



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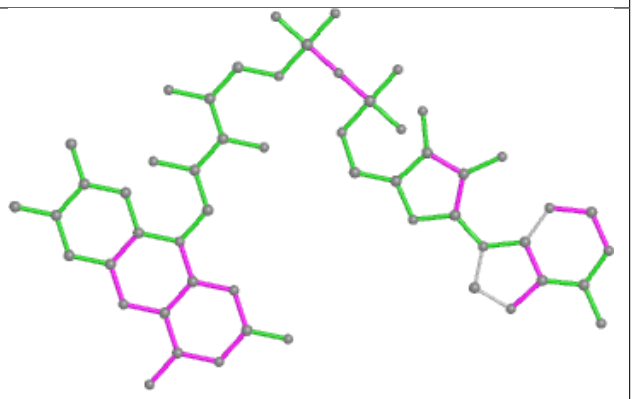
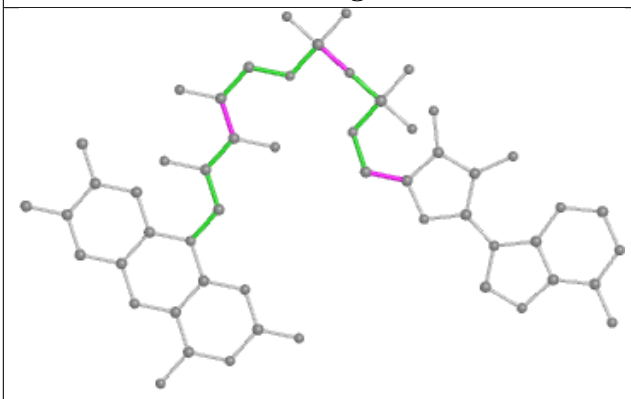
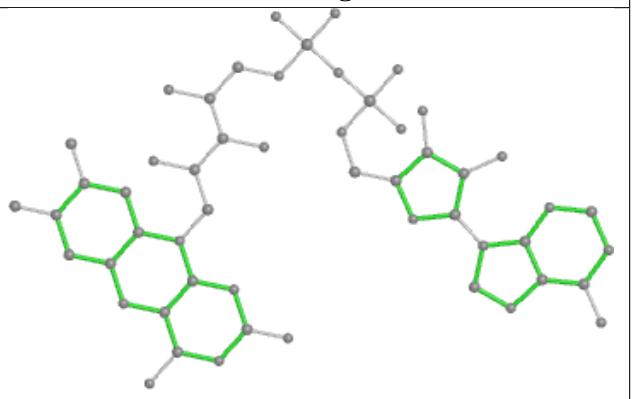


Bond angles

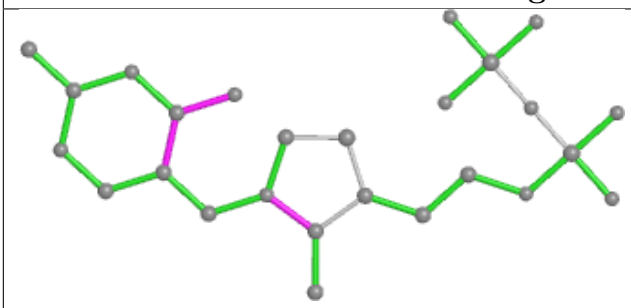


Torsions



Rings

Ligand TPP J 701



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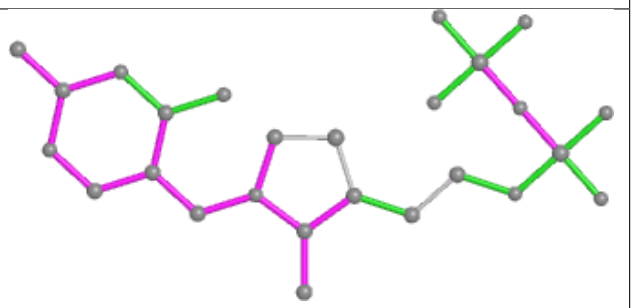
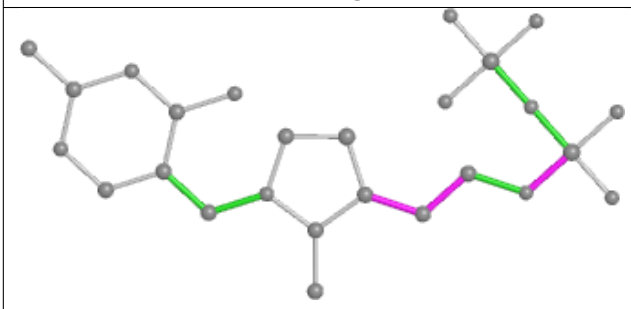
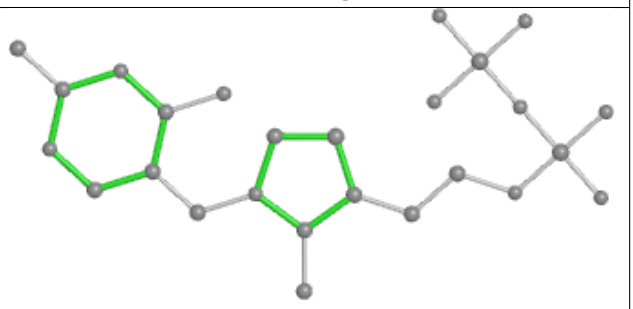


Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.