



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:49 PM UTC

PDB ID : 6U9D / pdb_00006u9d
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

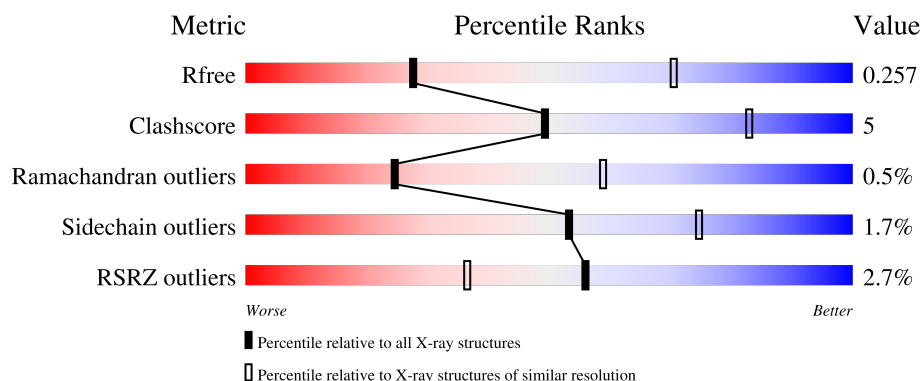
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	644	
1	B	644	
1	E	644	
1	F	644	
1	I	644	

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Mol	Chain	Length	Quality of chain
1	J	644	
1	M	644	
1	N	644	
1	Q	644	
1	R	644	
1	U	644	
1	V	644	
2	C	297	
2	D	297	
2	G	297	
2	H	297	
2	K	297	
2	L	297	
2	O	297	
2	P	297	
2	S	297	
2	T	297	
2	W	297	
2	X	297	

2 Entry composition

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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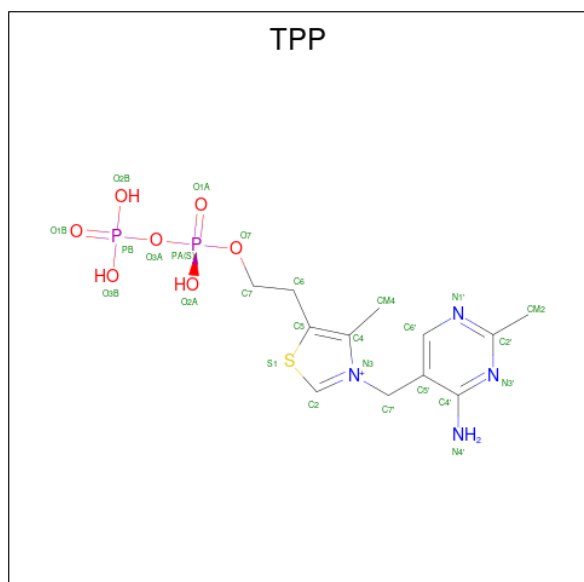
Chain	Residue	Modelled	Actual	Comment	Reference
T	30	GLY	-	expression tag	UNP B3LU66
T	31	SER	-	expression tag	UNP B3LU66
T	32	HIS	-	expression tag	UNP B3LU66
T	33	MET	-	expression tag	UNP B3LU66
T	34	GLU	-	expression tag	UNP B3LU66
T	35	ASN	-	expression tag	UNP B3LU66
T	36	LEU	-	expression tag	UNP B3LU66
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 (CCD ID: 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 (CCD ID: 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 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	Q	1	Total 1	Mg 1	0	0
4	U	1	Total 1	Mg 1	0	0
4	V	1	Total 1	Mg 1	0	0
4	W	1	Total 1	Mg 1	0	0

- # FAD

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

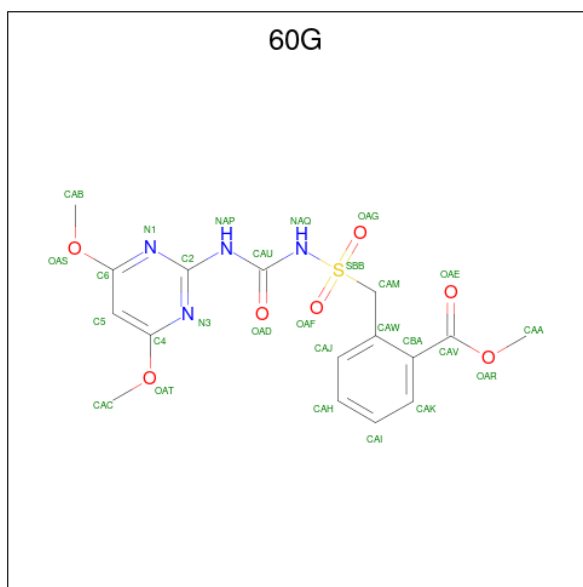


WORLD WIDE
PDB
PROTEIN DATA BANK

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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 (CCD ID: 60G) (formula: C₁₆H₁₈N₄O₇S) (labeled as "Ligand of Interest" by depositor).



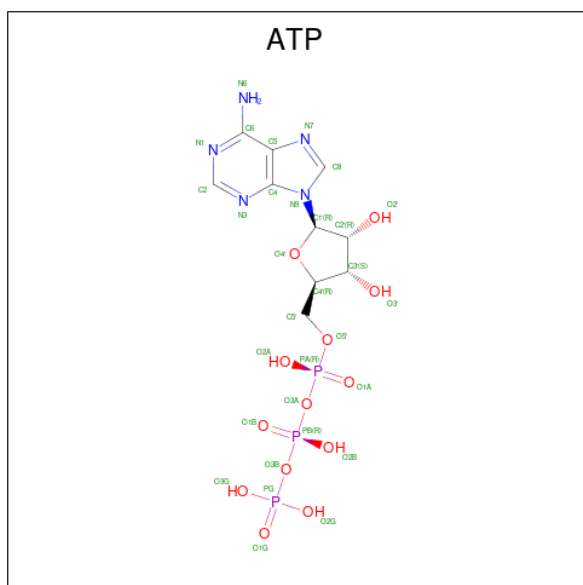
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	B	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	E	1	Total	C	N	O	S	0	0
			28	16	4	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: 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		
7	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

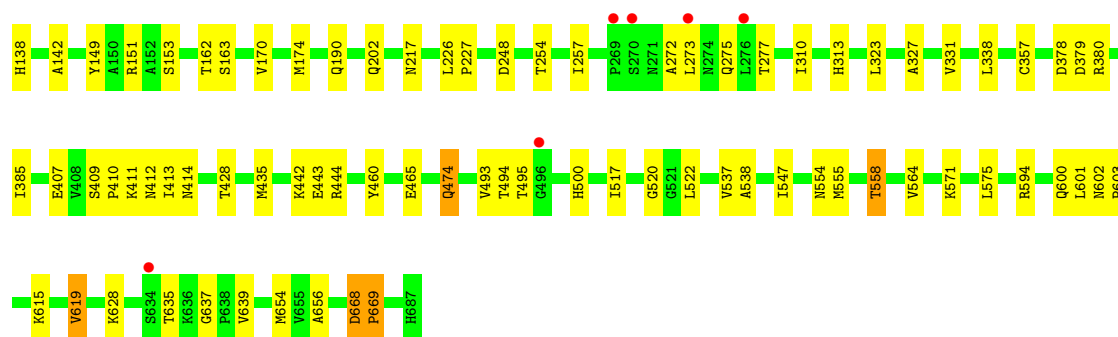
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total 6	O 6	0	0
8	B	9	Total 9	O 9	0	0
8	D	1	Total 1	O 1	0	0
8	E	3	Total 3	O 3	0	0
8	F	3	Total 3	O 3	0	0
8	I	2	Total 2	O 2	0	0
8	J	1	Total 1	O 1	0	0
8	M	3	Total 3	O 3	0	0
8	N	4	Total 4	O 4	0	0

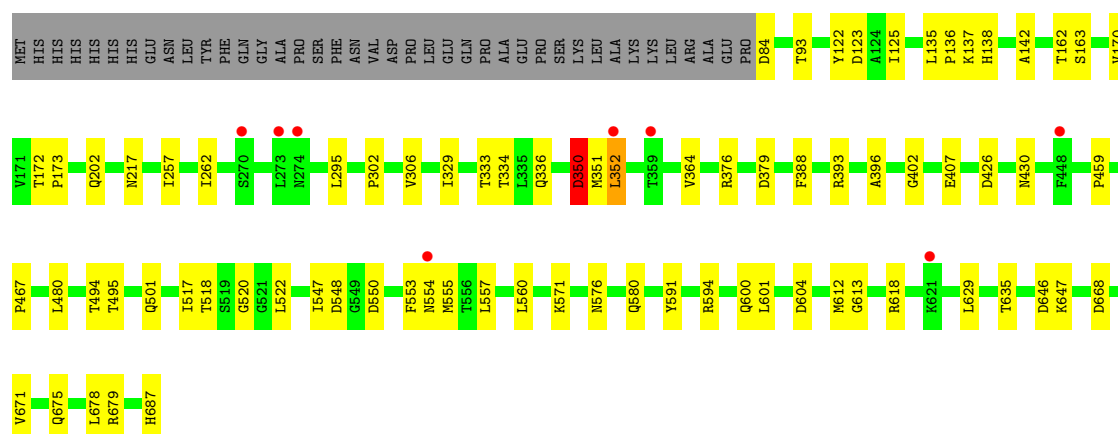
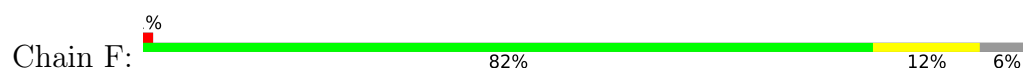
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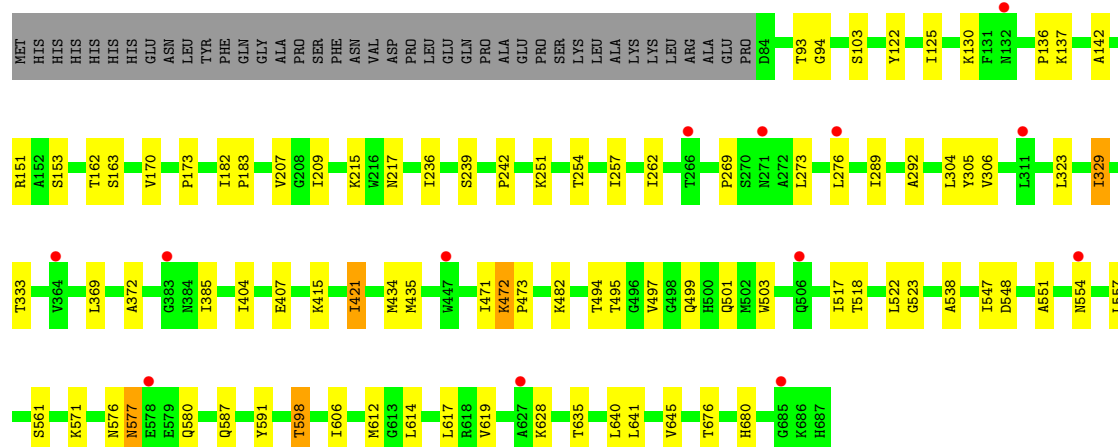
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	Q	1	Total 1	O 1	0	0
8	R	1	Total 1	O 1	0	0
8	S	1	Total 1	O 1	0	0
8	U	4	Total 4	O 4	0	0
8	V	5	Total 5	O 5	0	0



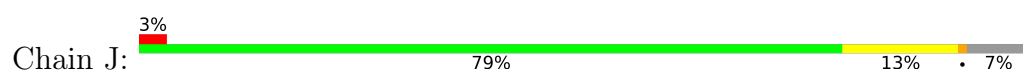
• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

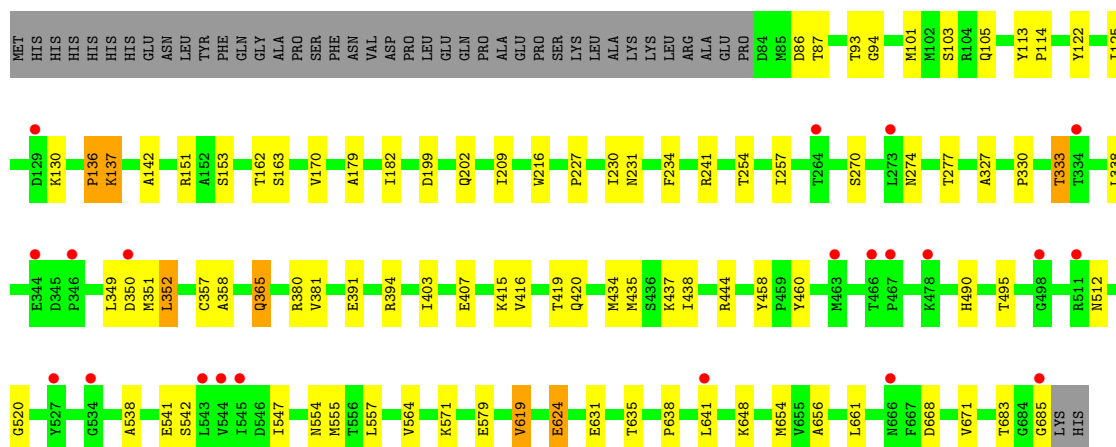


• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial



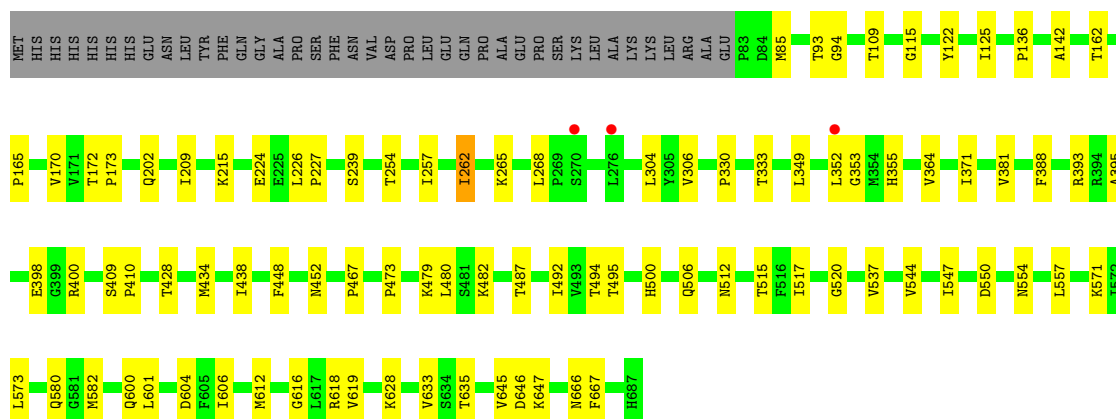
• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





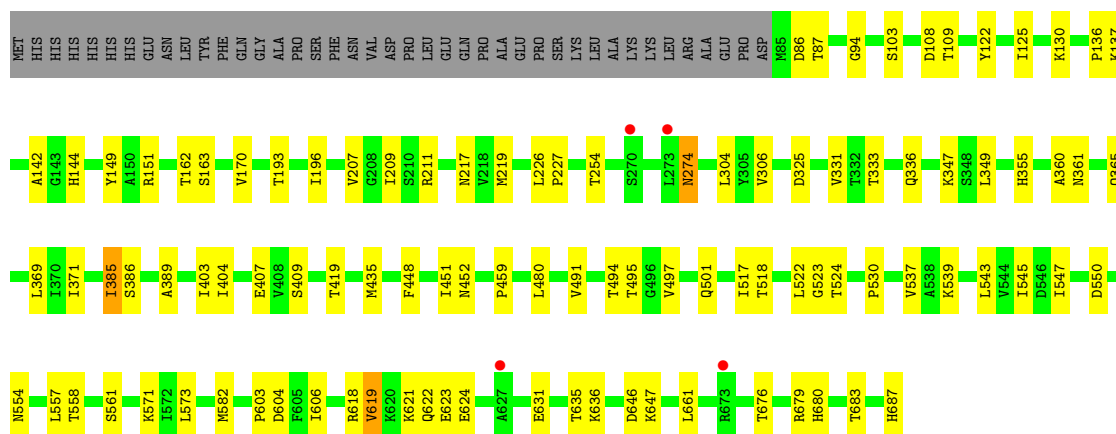
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain M: 80% 14% 6%

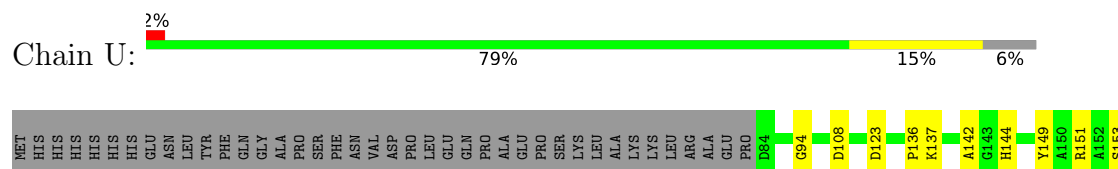
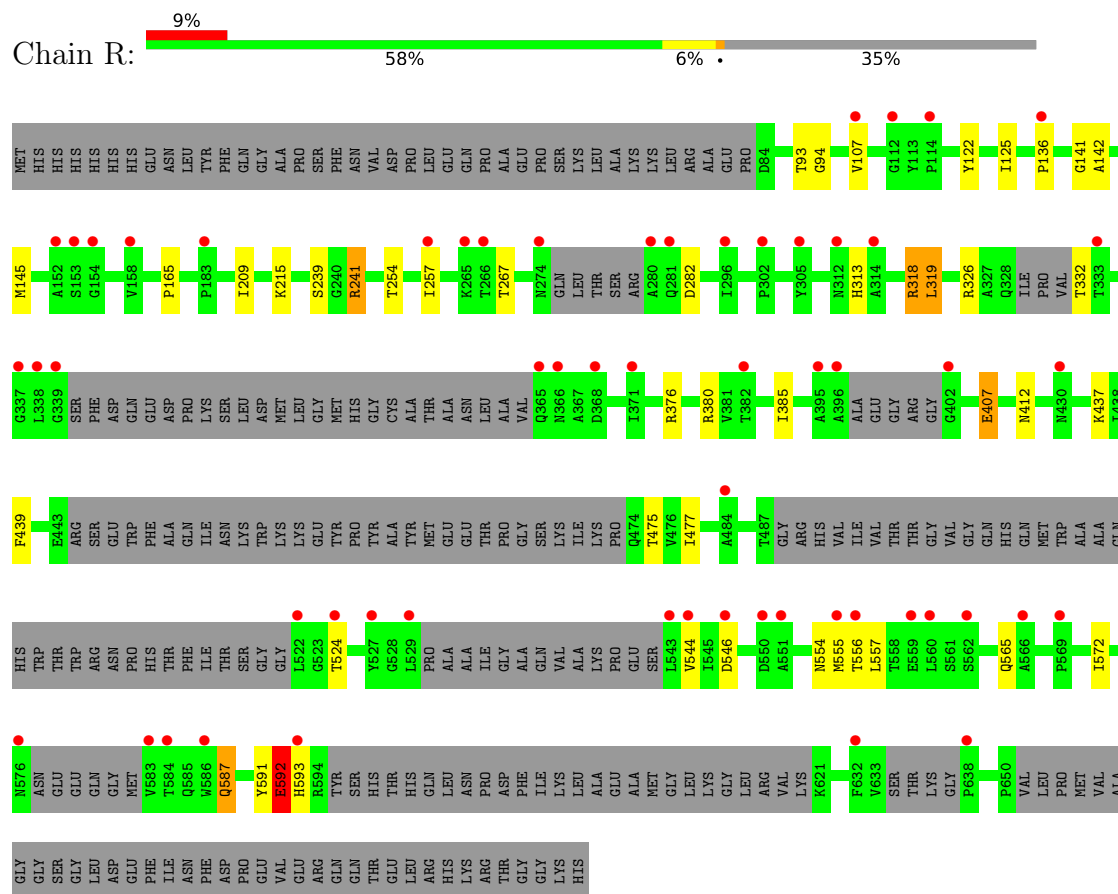


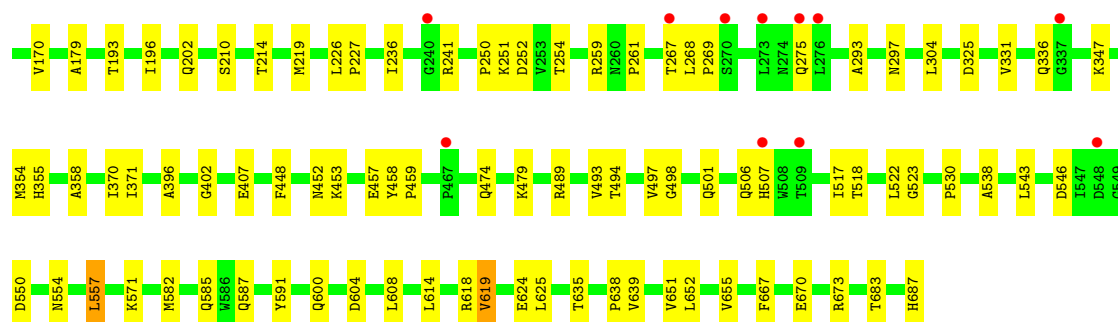
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain N: 78% 15% 6%



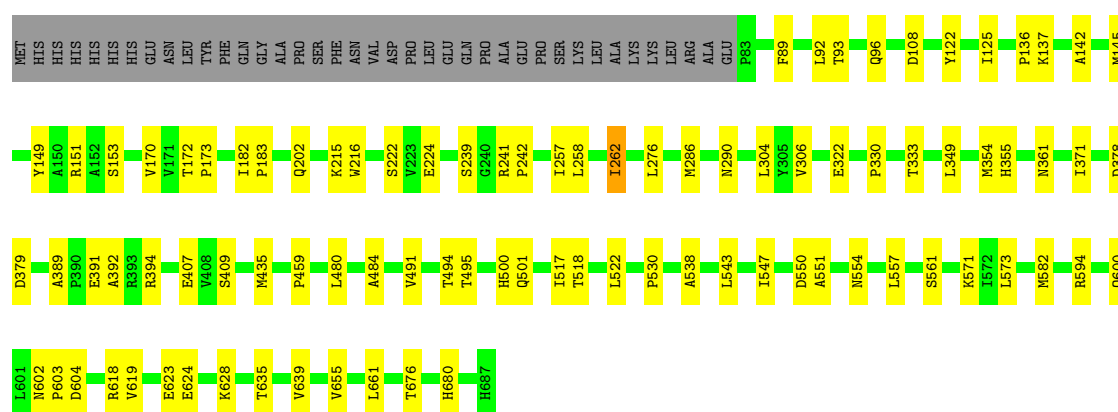
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





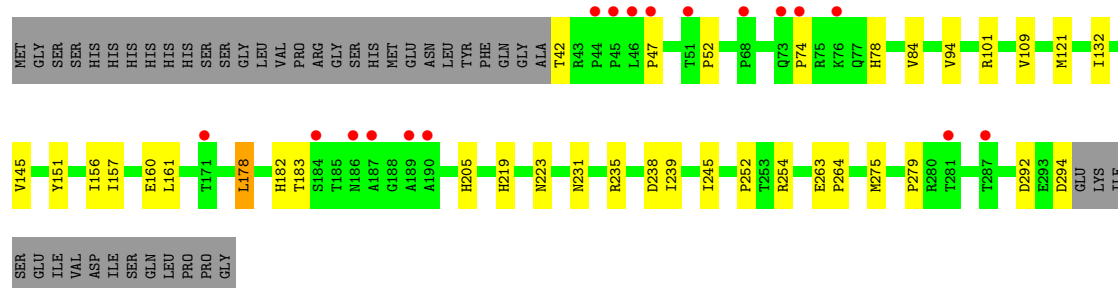
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain V: 80% 14% 6%



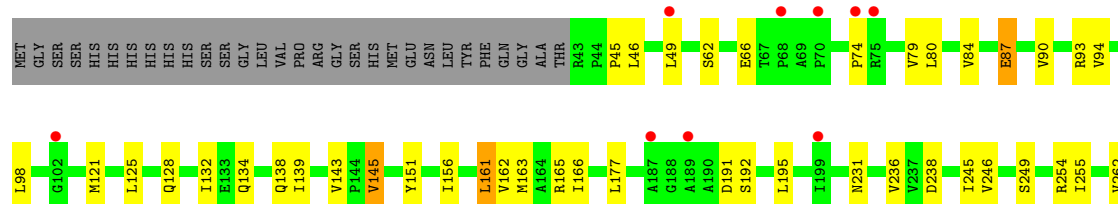
- Molecule 2: Acetolactate synthase small subunit, mitochondrial

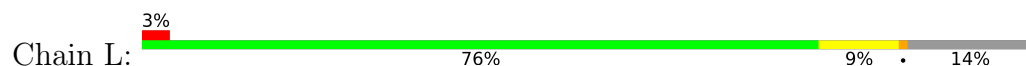
Chain C: 6% 73% 12% 15%

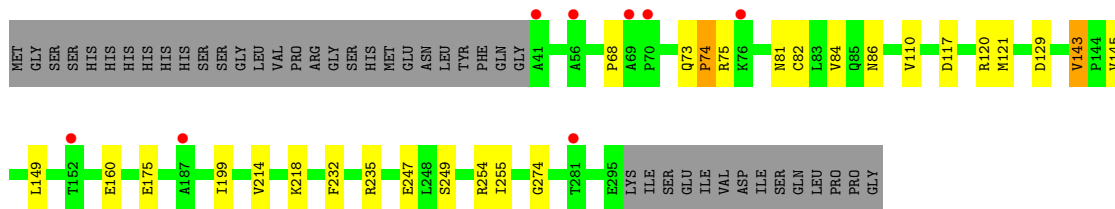


- Molecule 2: Acetolactate synthase small subunit, mitochondrial

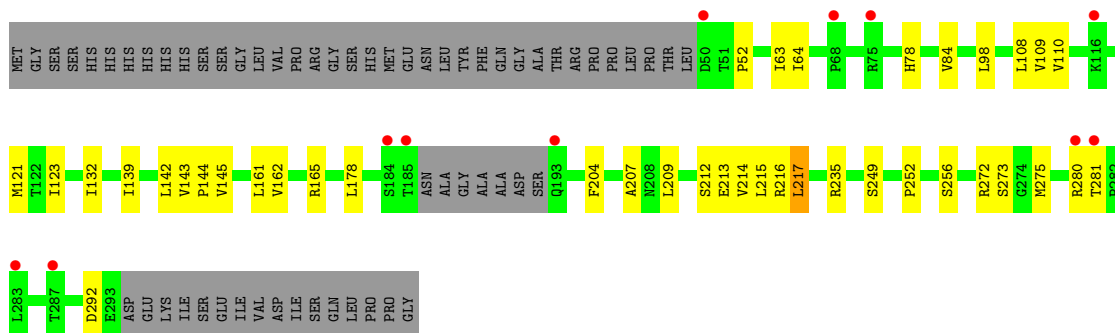
Chain D: 4% 68% 15% 16%



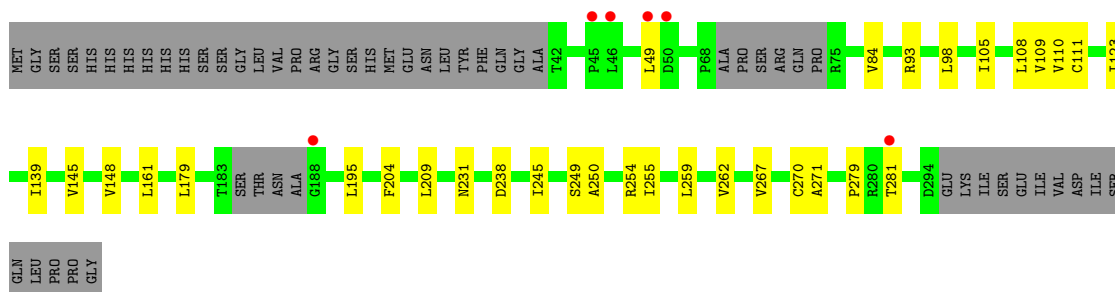




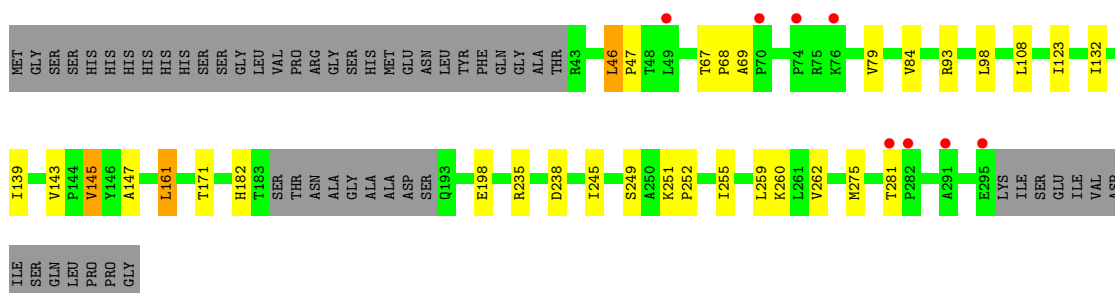
• Molecule 2: Acetolactate synthase small subunit, mitochondrial



• Molecule 2: Acetolactate synthase small subunit, mitochondrial



• Molecule 2: Acetolactate synthase small subunit, mitochondrial



• Molecule 2: Acetolactate synthase small subunit, mitochondrial

4 Data and refinement statistics

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 49.11 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.11-3.19) 99.5 (49.11-3.19)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.252 0.212 , 0.257	Depositor DCC
R_{free} test set	1998 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, ATP, MG, 60G, TPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/4701	0.72	2/6378 (0.0%)
1	B	0.27	0/4717	0.73	2/6402 (0.0%)
1	E	0.27	0/4675	0.72	3/6346 (0.0%)
1	F	0.27	0/4667	0.72	0/6339
1	I	0.27	0/4635	0.73	2/6300 (0.0%)
1	J	0.27	0/4626	0.72	0/6289
1	M	0.27	0/4709	0.72	3/6389 (0.0%)
1	N	0.27	0/4682	0.72	3/6351 (0.0%)
1	Q	0.29	0/4602	0.75	3/6255 (0.0%)
1	R	0.28	0/3058	0.72	0/4152
1	U	0.27	0/4649	0.73	1/6319 (0.0%)
1	V	0.27	0/4697	0.72	0/6375
2	C	0.27	0/1971	0.72	0/2686
2	D	0.27	0/1948	0.75	2/2654 (0.1%)
2	G	0.28	0/1971	0.70	0/2686
2	H	0.28	0/1977	0.75	2/2692 (0.1%)
2	K	0.29	0/1921	0.74	4/2617 (0.2%)
2	L	0.27	0/1990	0.70	2/2711 (0.1%)
2	O	0.28	0/1847	0.74	2/2513 (0.1%)
2	P	0.28	0/1910	0.70	0/2596
2	S	0.28	0/1904	0.75	0/2596
2	T	0.28	0/1820	0.72	2/2474 (0.1%)
2	W	0.28	0/1926	0.74	0/2621
2	X	0.44	0/1873	0.78	1/2544 (0.0%)
All	All	0.28	0/77476	0.73	34/105285 (0.0%)

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	143	VAL	CA-C-N	-7.97	111.75	121.00
2	O	143	VAL	C-N-CA	-7.97	111.75	121.00
2	H	143	VAL	CA-C-N	-7.75	111.84	120.45
2	H	143	VAL	C-N-CA	-7.75	111.84	120.45
2	D	143	VAL	CA-C-N	-7.48	112.15	120.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4606	0	4614	61	0
1	B	4621	0	4621	48	0
1	E	4580	0	4578	63	0
1	F	4572	0	4540	48	0
1	I	4540	0	4503	47	0
1	J	4533	0	4486	48	0
1	M	4613	0	4622	53	0
1	N	4589	0	4602	62	0
1	Q	4508	0	4439	48	0
1	R	3014	0	2909	29	0
1	U	4554	0	4503	59	0
1	V	4601	0	4601	57	0
2	C	1938	0	1925	27	0
2	D	1915	0	1917	32	0
2	G	1938	0	1928	18	0
2	H	1944	0	1951	29	0
2	K	1889	0	1883	21	0
2	L	1957	0	1952	16	0
2	O	1818	0	1811	28	0
2	P	1881	0	1885	18	0
2	S	1872	0	1854	20	0
2	T	1792	0	1805	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	1894	0	1901	24	0
2	X	1846	0	1823	28	0
3	A	26	0	16	1	0
3	B	26	0	16	2	0
3	E	26	0	16	3	0
3	F	26	0	16	2	0
3	I	26	0	16	2	0
3	J	26	0	16	1	0
3	M	26	0	16	3	0
3	N	26	0	16	1	0
3	Q	26	0	16	2	0
3	U	26	0	16	1	0
3	V	26	0	16	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	Q	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
5	A	53	0	30	3	0
5	B	53	0	30	1	0
5	E	53	0	30	3	0
5	F	53	0	30	4	0
5	I	53	0	30	1	0
5	J	53	0	31	4	0
5	M	53	0	30	2	0
5	N	53	0	30	2	0
5	Q	53	0	30	3	0
5	R	53	0	30	7	0
5	U	53	0	30	2	0
5	V	53	0	30	1	0
6	A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	0	2	0
6	E	28	0	0	1	0
6	F	28	0	0	0	0
6	I	28	0	0	0	0
6	J	28	0	0	2	0
6	N	56	0	0	0	0
6	Q	28	0	0	0	0
6	R	28	0	0	1	0
6	U	28	0	0	0	0
6	V	28	0	0	1	0
7	C	31	0	12	2	0
7	D	31	0	10	2	0
7	G	31	0	10	3	0
7	H	31	0	11	1	0
7	K	31	0	11	1	0
7	L	31	0	12	4	0
7	O	31	0	12	0	0
7	P	31	0	11	2	0
7	S	31	0	12	2	0
7	T	31	0	11	1	0
7	W	62	0	23	3	0
8	A	6	0	0	0	0
8	B	9	0	0	0	0
8	D	1	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
8	I	2	0	0	0	0
8	J	1	0	0	0	0
8	M	3	0	0	0	0
8	N	4	0	0	1	0
8	Q	1	0	0	0	0
8	R	1	0	0	0	0
8	S	1	0	0	0	0
8	U	4	0	0	0	0
8	V	5	0	0	0	0
All	All	77705	0	76325	824	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 824 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:635:THR:HG21	1:E:639:VAL:HG11	1.27	1.08
1:R:241:ARG:HD3	5:R:701:FAD:H2B	1.57	0.85
1:E:635:THR:CG2	1:E:639:VAL:HG11	2.08	0.81
1:Q:273:LEU:O	1:Q:273:LEU:HD22	1.85	0.76
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.71	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	602/644 (94%)	581 (96%)	21 (4%)	0	100	100
1	B	605/644 (94%)	578 (96%)	27 (4%)	0	100	100
1	E	601/644 (93%)	571 (95%)	28 (5%)	2 (0%)	36	68
1	F	602/644 (94%)	572 (95%)	26 (4%)	4 (1%)	18	52
1	I	602/644 (94%)	582 (97%)	20 (3%)	0	100	100
1	J	600/644 (93%)	569 (95%)	28 (5%)	3 (0%)	24	59
1	M	603/644 (94%)	566 (94%)	36 (6%)	1 (0%)	43	73
1	N	601/644 (93%)	569 (95%)	31 (5%)	1 (0%)	43	73
1	Q	594/644 (92%)	570 (96%)	22 (4%)	2 (0%)	36	68
1	R	394/644 (61%)	369 (94%)	21 (5%)	4 (1%)	12	45
1	U	602/644 (94%)	569 (94%)	31 (5%)	2 (0%)	36	68
1	V	603/644 (94%)	574 (95%)	28 (5%)	1 (0%)	43	73
2	C	251/297 (84%)	243 (97%)	7 (3%)	1 (0%)	30	62
2	D	248/297 (84%)	235 (95%)	10 (4%)	3 (1%)	10	42
2	G	251/297 (84%)	237 (94%)	13 (5%)	1 (0%)	30	62
2	H	250/297 (84%)	235 (94%)	13 (5%)	2 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	241/297 (81%)	221 (92%)	15 (6%)	5 (2%)	5	31
2	L	253/297 (85%)	237 (94%)	13 (5%)	3 (1%)	10	42
2	O	233/297 (78%)	221 (95%)	11 (5%)	1 (0%)	30	62
2	P	237/297 (80%)	228 (96%)	9 (4%)	0	100	100
2	S	240/297 (81%)	227 (95%)	12 (5%)	1 (0%)	30	62
2	T	226/297 (76%)	214 (95%)	11 (5%)	1 (0%)	30	62
2	W	241/297 (81%)	228 (95%)	10 (4%)	3 (1%)	10	42
2	X	234/297 (79%)	216 (92%)	14 (6%)	4 (2%)	7	35
All	All	9914/11292 (88%)	9412 (95%)	457 (5%)	45 (0%)	24	59

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	477	ILE
2	T	46	LEU
2	W	109	VAL
2	X	69	ALA
2	X	70	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/531 (93%)	488 (99%)	7 (1%)	59	77
1	B	496/531 (93%)	493 (99%)	3 (1%)	78	84
1	E	490/531 (92%)	482 (98%)	8 (2%)	55	75
1	F	487/531 (92%)	480 (99%)	7 (1%)	59	77
1	I	481/531 (91%)	468 (97%)	13 (3%)	39	68
1	J	481/531 (91%)	470 (98%)	11 (2%)	44	70
1	M	496/531 (93%)	493 (99%)	3 (1%)	78	84
1	N	493/531 (93%)	488 (99%)	5 (1%)	68	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	475/531 (90%)	468 (98%)	7 (2%)	57	76
1	R	307/531 (58%)	292 (95%)	15 (5%)	22	55
1	U	483/531 (91%)	477 (99%)	6 (1%)	63	79
1	V	493/531 (93%)	490 (99%)	3 (1%)	78	84
2	C	217/260 (84%)	211 (97%)	6 (3%)	38	68
2	D	215/260 (83%)	209 (97%)	6 (3%)	38	68
2	G	218/260 (84%)	213 (98%)	5 (2%)	44	70
2	H	220/260 (85%)	217 (99%)	3 (1%)	59	77
2	K	213/260 (82%)	208 (98%)	5 (2%)	44	70
2	L	219/260 (84%)	218 (100%)	1 (0%)	81	85
2	O	204/260 (78%)	203 (100%)	1 (0%)	81	85
2	P	213/260 (82%)	206 (97%)	7 (3%)	33	65
2	S	210/260 (81%)	201 (96%)	9 (4%)	26	59
2	T	203/260 (78%)	199 (98%)	4 (2%)	48	72
2	W	216/260 (83%)	214 (99%)	2 (1%)	70	81
2	X	207/260 (80%)	201 (97%)	6 (3%)	37	67
All	All	8232/9492 (87%)	8089 (98%)	143 (2%)	53	75

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	132	ILE
2	S	198	GLU
1	U	557	LEU
1	I	421	ILE
1	I	329	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	223	ASN
2	X	219	HIS
1	N	450	GLN
1	V	485	ASN
2	T	134	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 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	$\# Z > 2$
7	ATP	H	401	4	32,33,33	3.53	15 (46%)	48,52,52	1.69	9 (18%)
7	ATP	C	401	4	32,33,33	3.51	15 (46%)	48,52,52	1.69	9 (18%)
6	60G	V	704	-	28,29,29	1.44	3 (10%)	37,40,40	3.46	13 (35%)
5	FAD	A	703	-	58,58,58	1.63	14 (24%)	85,89,89	1.62	19 (22%)
5	FAD	R	701	-	58,58,58	1.63	14 (24%)	85,89,89	1.65	19 (22%)
7	ATP	L	401	4	32,33,33	3.53	15 (46%)	48,52,52	1.72	9 (18%)
6	60G	F	704	-	28,29,29	1.46	4 (14%)	37,40,40	3.55	13 (35%)
7	ATP	W	401	-	32,33,33	3.53	15 (46%)	48,52,52	1.70	9 (18%)
3	TPP	E	701	4	26,27,27	1.39	5 (19%)	38,40,40	1.56	9 (23%)
3	TPP	V	701	4	26,27,27	1.37	5 (19%)	38,40,40	1.53	9 (23%)
6	60G	I	704	-	28,29,29	1.45	3 (10%)	37,40,40	3.50	14 (37%)
5	FAD	E	703	-	58,58,58	1.64	14 (24%)	85,89,89	1.63	19 (22%)
6	60G	J	704	-	28,29,29	1.48	4 (14%)	37,40,40	3.51	13 (35%)
3	TPP	B	701	4	26,27,27	1.39	5 (19%)	38,40,40	1.61	10 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	B	703	-	58,58,58	1.63	15 (25%)	85,89,89	1.64	19 (22%)
3	TPP	A	701	4	26,27,27	1.37	5 (19%)	38,40,40	1.60	10 (26%)
7	ATP	T	401	4	32,33,33	3.51	15 (46%)	48,52,52	1.74	10 (20%)
7	ATP	S	401	-	32,33,33	3.52	15 (46%)	48,52,52	1.67	9 (18%)
5	FAD	V	703	-	58,58,58	1.65	15 (25%)	85,89,89	1.64	19 (22%)
3	TPP	I	701	4	26,27,27	1.39	5 (19%)	38,40,40	1.57	10 (26%)
5	FAD	Q	703	-	58,58,58	1.62	13 (22%)	85,89,89	1.63	19 (22%)
6	60G	R	702	-	28,29,29	1.48	3 (10%)	37,40,40	3.48	13 (35%)
3	TPP	M	701	4	26,27,27	1.40	5 (19%)	38,40,40	1.57	10 (26%)
3	TPP	F	701	4	26,27,27	1.41	5 (19%)	38,40,40	1.58	9 (23%)
3	TPP	N	701	4	26,27,27	1.40	5 (19%)	38,40,40	1.57	10 (26%)
6	60G	Q	704	-	28,29,29	1.49	3 (10%)	37,40,40	3.49	12 (32%)
3	TPP	U	701	4	26,27,27	1.36	5 (19%)	38,40,40	1.57	10 (26%)
6	60G	N	705	-	28,29,29	1.46	3 (10%)	37,40,40	3.49	12 (32%)
6	60G	A	704	-	28,29,29	1.47	3 (10%)	37,40,40	3.50	13 (35%)
6	60G	N	704	-	28,29,29	1.44	3 (10%)	37,40,40	3.49	12 (32%)
7	ATP	D	401	4	32,33,33	3.51	15 (46%)	48,52,52	1.79	11 (22%)
7	ATP	G	401	4	32,33,33	3.54	15 (46%)	48,52,52	1.73	10 (20%)
5	FAD	I	703	-	58,58,58	1.62	12 (20%)	85,89,89	1.63	20 (23%)
5	FAD	N	703	-	58,58,58	1.63	15 (25%)	85,89,89	1.63	20 (23%)
6	60G	E	704	-	28,29,29	1.46	5 (17%)	37,40,40	3.52	12 (32%)
7	ATP	W	402	4	32,33,33	3.53	15 (46%)	48,52,52	1.69	9 (18%)
7	ATP	K	401	4	32,33,33	3.52	15 (46%)	48,52,52	1.70	10 (20%)
5	FAD	F	703	-	58,58,58	1.68	14 (24%)	85,89,89	1.66	19 (22%)
3	TPP	Q	701	4	26,27,27	1.36	5 (19%)	38,40,40	1.57	10 (26%)
7	ATP	O	401	4	32,33,33	3.52	15 (46%)	48,52,52	1.69	9 (18%)
3	TPP	J	701	4	26,27,27	1.42	5 (19%)	38,40,40	1.57	7 (18%)
5	FAD	U	703	-	58,58,58	1.63	14 (24%)	85,89,89	1.64	19 (22%)
5	FAD	M	703	-	58,58,58	1.63	14 (24%)	85,89,89	1.63	19 (22%)
5	FAD	J	703	-	58,58,58	1.63	12 (20%)	85,89,89	1.72	23 (27%)
6	60G	B	704	-	28,29,29	1.46	4 (14%)	37,40,40	3.49	13 (35%)
7	ATP	P	401	4	32,33,33	3.52	15 (46%)	48,52,52	1.70	9 (18%)
6	60G	U	704	-	28,29,29	1.45	3 (10%)	37,40,40	3.50	14 (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
7	ATP	H	401	4	-	5/22/38/38	0/3/3/3
7	ATP	C	401	4	-	6/22/38/38	0/3/3/3
6	60G	V	704	-	-	7/24/24/24	0/2/2/2
5	FAD	A	703	-	-	3/34/50/50	0/6/6/6
5	FAD	R	701	-	-	13/34/50/50	0/6/6/6
7	ATP	L	401	4	-	4/22/38/38	0/3/3/3
6	60G	F	704	-	-	7/24/24/24	0/2/2/2
7	ATP	W	401	-	-	6/22/38/38	0/3/3/3
3	TPP	E	701	4	-	4/17/17/17	0/2/2/2
3	TPP	V	701	4	-	2/17/17/17	0/2/2/2
6	60G	I	704	-	-	10/24/24/24	0/2/2/2
5	FAD	E	703	-	-	2/34/50/50	0/6/6/6
6	60G	J	704	-	-	7/24/24/24	0/2/2/2
3	TPP	B	701	4	-	4/17/17/17	0/2/2/2
5	FAD	B	703	-	-	4/34/50/50	0/6/6/6
3	TPP	A	701	4	-	6/17/17/17	0/2/2/2
7	ATP	T	401	4	-	3/22/38/38	0/3/3/3
7	ATP	S	401	-	-	10/22/38/38	0/3/3/3
5	FAD	V	703	-	-	13/34/50/50	0/6/6/6
3	TPP	I	701	4	-	4/17/17/17	0/2/2/2
5	FAD	Q	703	-	-	4/34/50/50	0/6/6/6
6	60G	R	702	-	-	10/24/24/24	0/2/2/2
3	TPP	M	701	4	-	4/17/17/17	0/2/2/2
3	TPP	F	701	4	-	4/17/17/17	0/2/2/2
3	TPP	N	701	4	-	4/17/17/17	0/2/2/2
6	60G	Q	704	-	-	7/24/24/24	0/2/2/2
3	TPP	U	701	4	-	4/17/17/17	0/2/2/2
6	60G	N	705	-	-	8/24/24/24	0/2/2/2
6	60G	A	704	-	-	10/24/24/24	0/2/2/2
6	60G	N	704	-	-	8/24/24/24	0/2/2/2
7	ATP	D	401	4	-	4/22/38/38	0/3/3/3
7	ATP	G	401	4	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	I	703	-	-	7/34/50/50	0/6/6/6
5	FAD	N	703	-	-	3/34/50/50	0/6/6/6
6	60G	E	704	-	-	8/24/24/24	0/2/2/2
7	ATP	W	402	4	-	4/22/38/38	0/3/3/3
7	ATP	K	401	4	-	7/22/38/38	0/3/3/3
5	FAD	F	703	-	-	8/34/50/50	0/6/6/6
3	TPP	Q	701	4	-	5/17/17/17	0/2/2/2
7	ATP	O	401	4	-	8/22/38/38	0/3/3/3
3	TPP	J	701	4	-	4/17/17/17	0/2/2/2
5	FAD	U	703	-	-	16/34/50/50	0/6/6/6
5	FAD	M	703	-	-	3/34/50/50	0/6/6/6
5	FAD	J	703	-	-	11/34/50/50	0/6/6/6
6	60G	B	704	-	-	9/24/24/24	0/2/2/2
7	ATP	P	401	4	-	2/22/38/38	0/3/3/3
6	60G	U	704	-	-	7/24/24/24	0/2/2/2

The worst 5 of 442 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	401	ATP	C2'-C3'	-11.44	1.22	1.53
7	C	401	ATP	C2'-C3'	-11.37	1.22	1.53
7	W	402	ATP	C2'-C3'	-11.36	1.22	1.53
7	O	401	ATP	C2'-C3'	-11.36	1.22	1.53
7	S	401	ATP	C2'-C3'	-11.35	1.22	1.53

The worst 5 of 605 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	704	60G	OAG-SBB-OAF	-13.79	100.05	119.34
6	A	704	60G	OAG-SBB-OAF	-13.76	100.09	119.34
6	I	704	60G	OAG-SBB-OAF	-13.71	100.17	119.34
6	E	704	60G	OAG-SBB-OAF	-13.70	100.17	119.34
6	Q	704	60G	OAG-SBB-OAF	-13.66	100.23	119.34

There are no chirality outliers.

5 of 292 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	C7-O7-PA-O3A
3	A	701	TPP	PA-O3A-PB-O3B

There are no ring outliers.

38 monomers are involved in 82 short contacts:

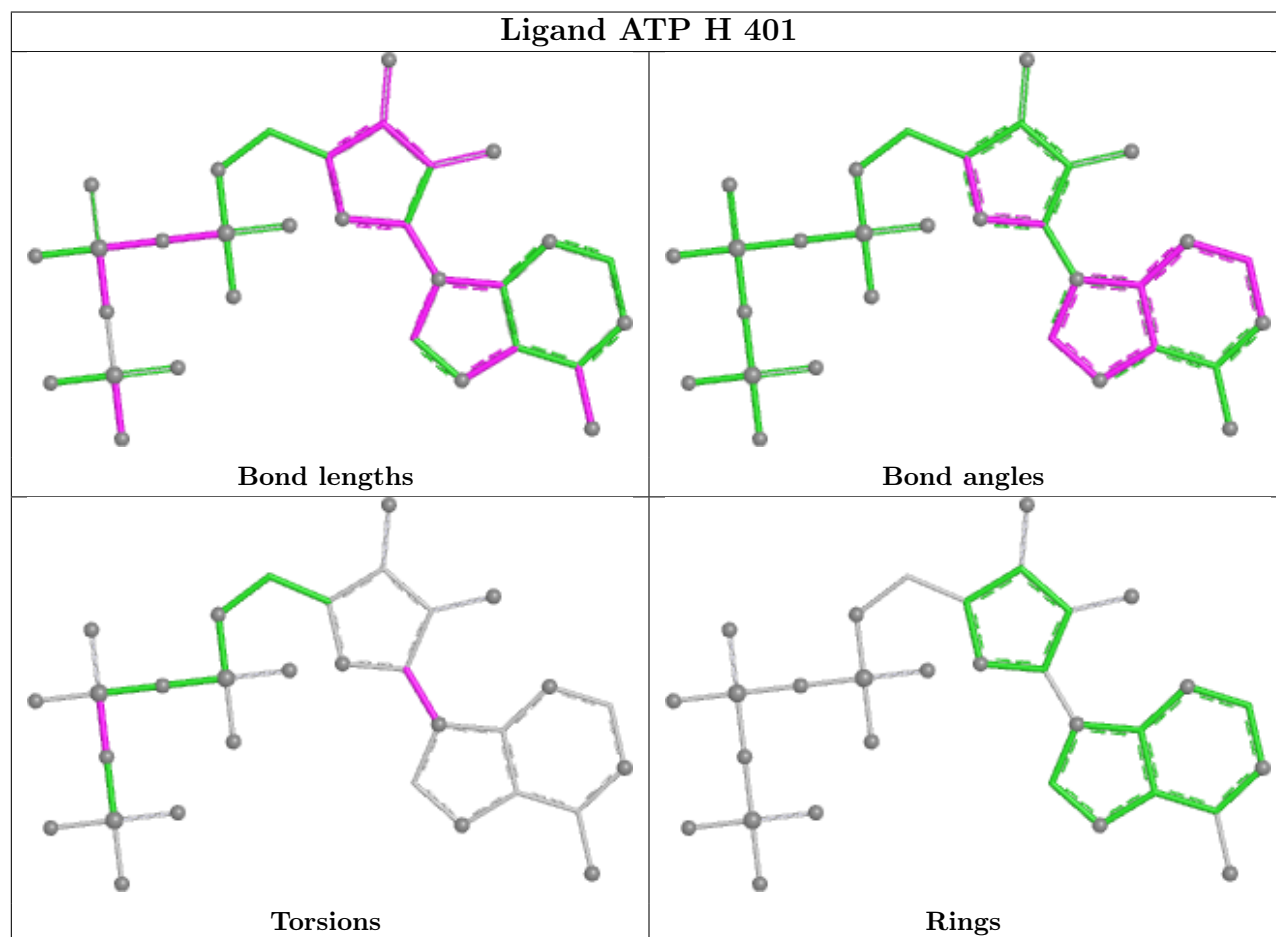
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	401	ATP	1	0
7	C	401	ATP	2	0
6	V	704	60G	1	0
5	A	703	FAD	3	0
5	R	701	FAD	7	0
7	L	401	ATP	4	0
3	E	701	TPP	3	0
3	V	701	TPP	3	0
5	E	703	FAD	3	0
6	J	704	60G	2	0
3	B	701	TPP	2	0
5	B	703	FAD	1	0
3	A	701	TPP	1	0
7	T	401	ATP	1	0
7	S	401	ATP	2	0
5	V	703	FAD	1	0
3	I	701	TPP	2	0
5	Q	703	FAD	3	0
6	R	702	60G	1	0
3	M	701	TPP	3	0
3	F	701	TPP	2	0
3	N	701	TPP	1	0
3	U	701	TPP	1	0
7	D	401	ATP	2	0
7	G	401	ATP	3	0
5	I	703	FAD	1	0
5	N	703	FAD	2	0
6	E	704	60G	1	0
7	W	402	ATP	3	0
7	K	401	ATP	1	0
5	F	703	FAD	4	0
3	Q	701	TPP	2	0
3	J	701	TPP	1	0

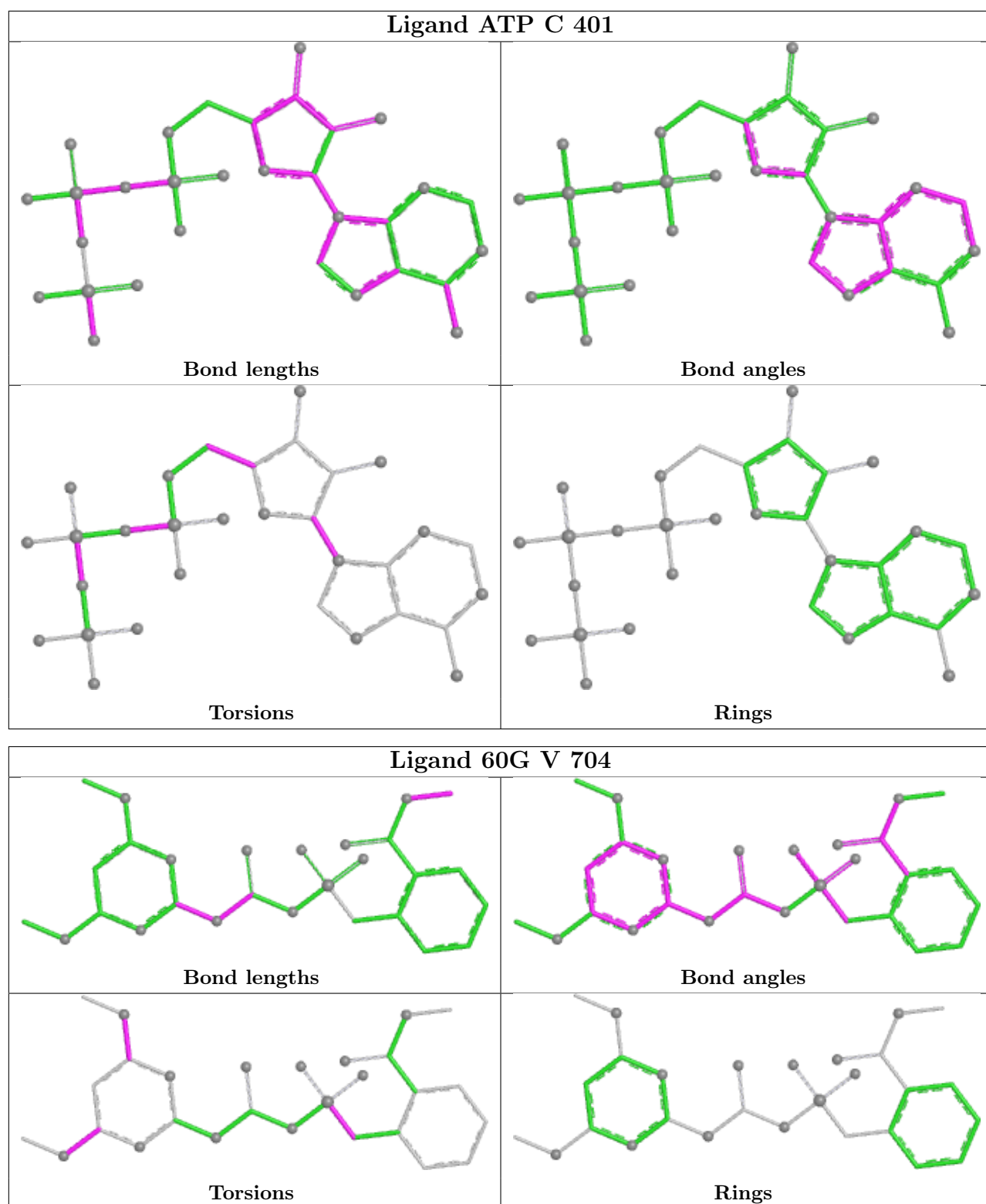
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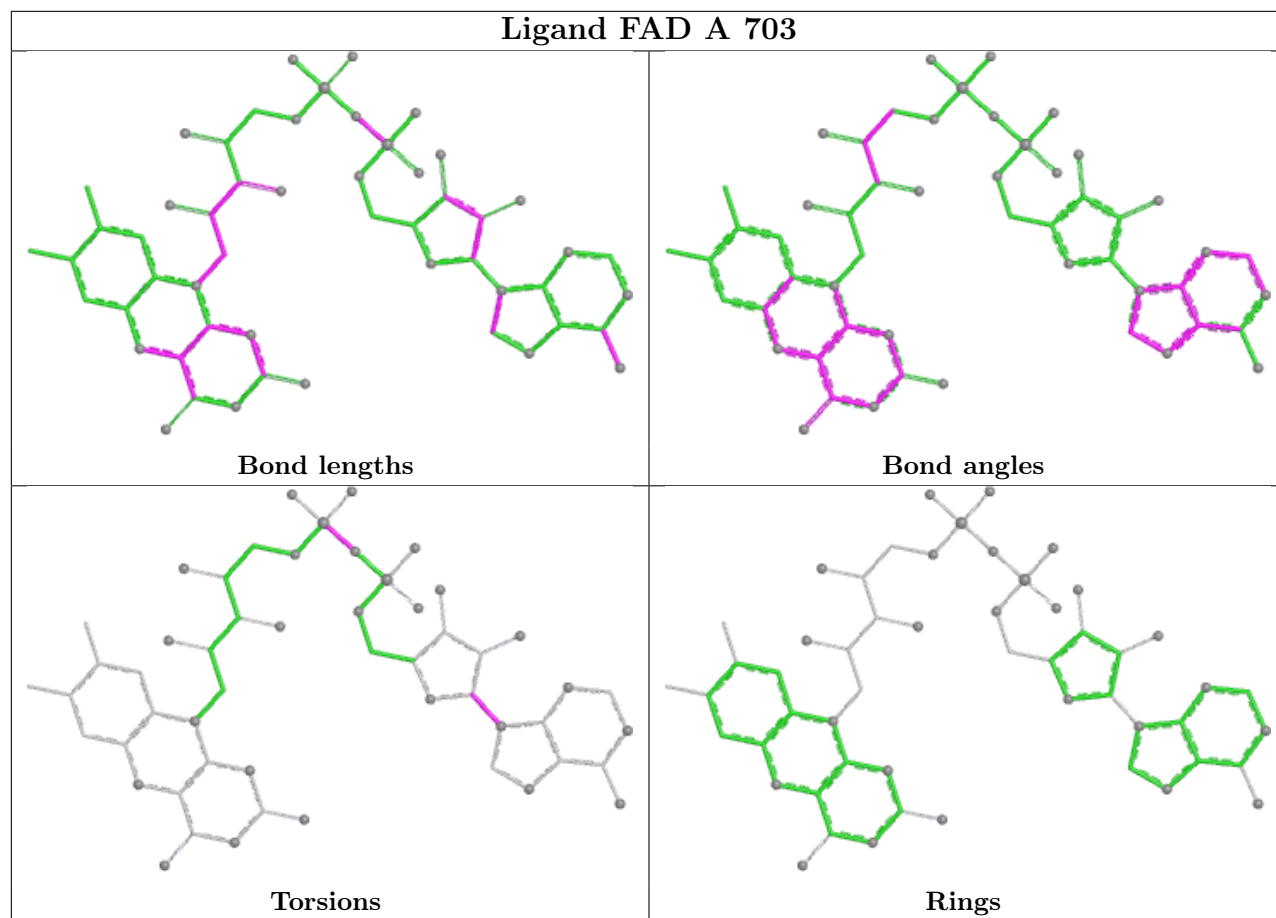
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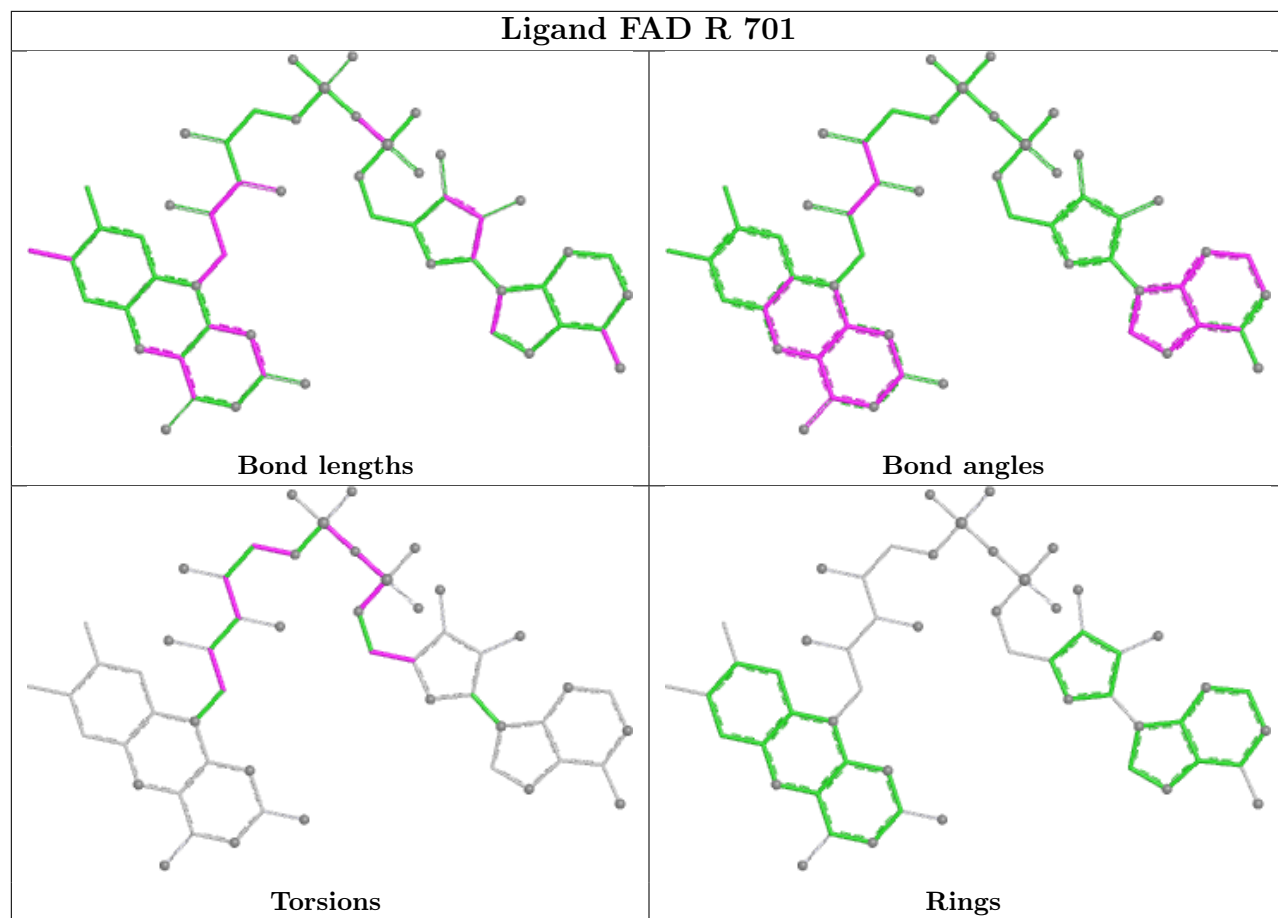
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	U	703	FAD	2	0
5	M	703	FAD	2	0
5	J	703	FAD	4	0
6	B	704	60G	2	0
7	P	401	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

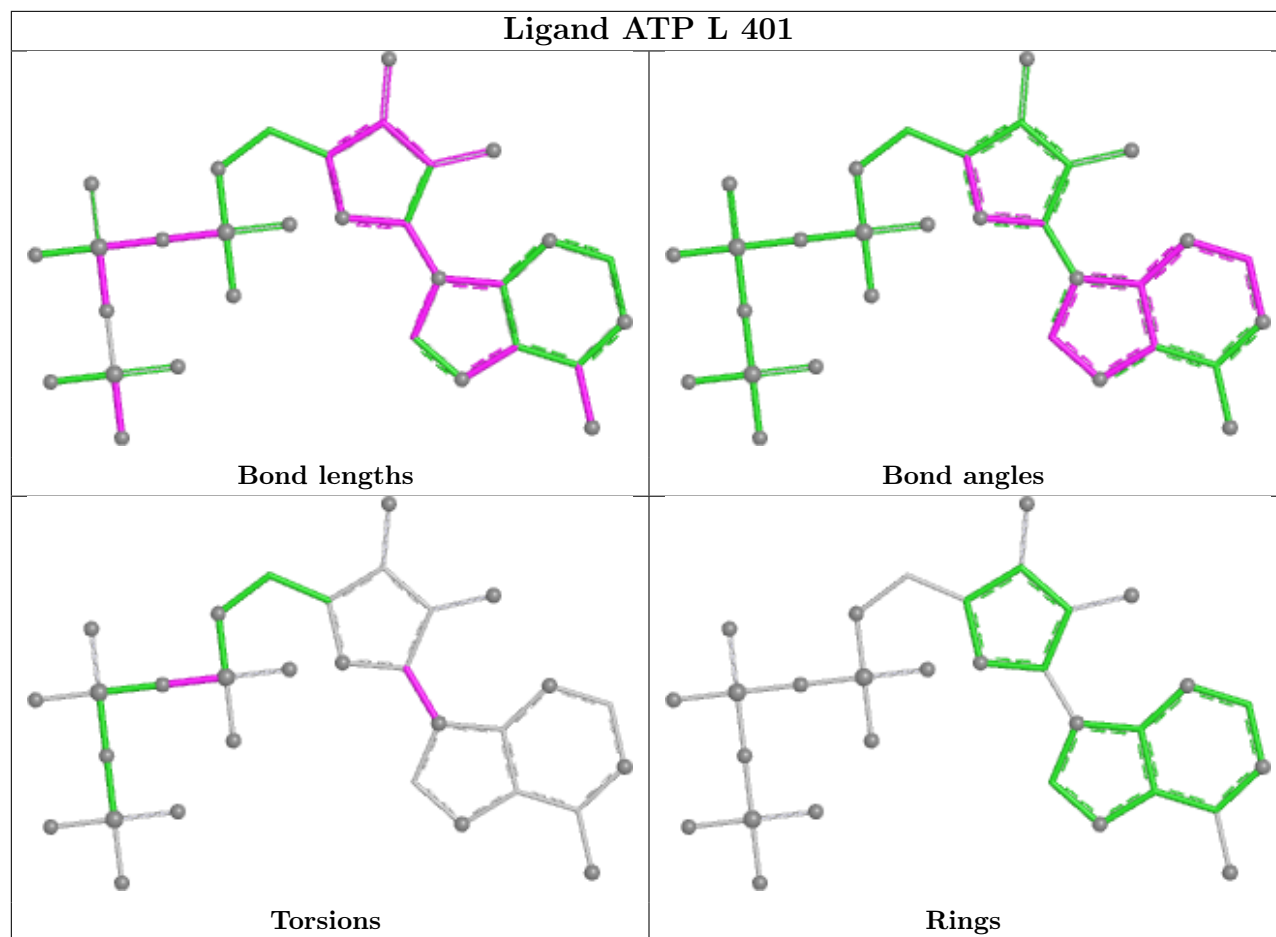




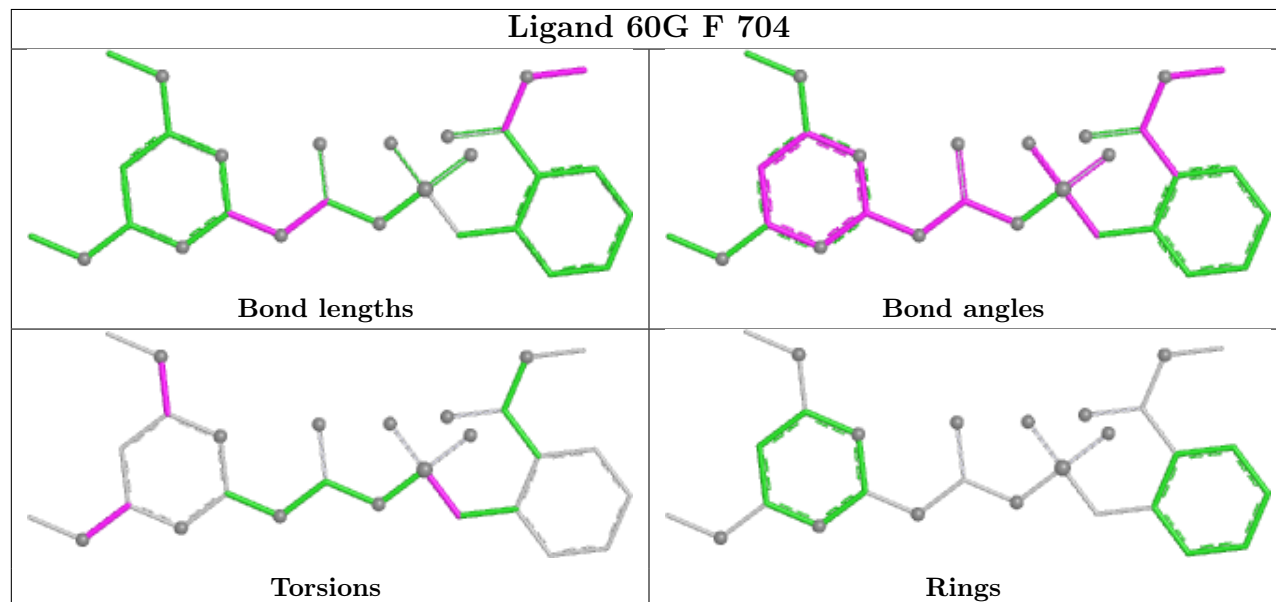


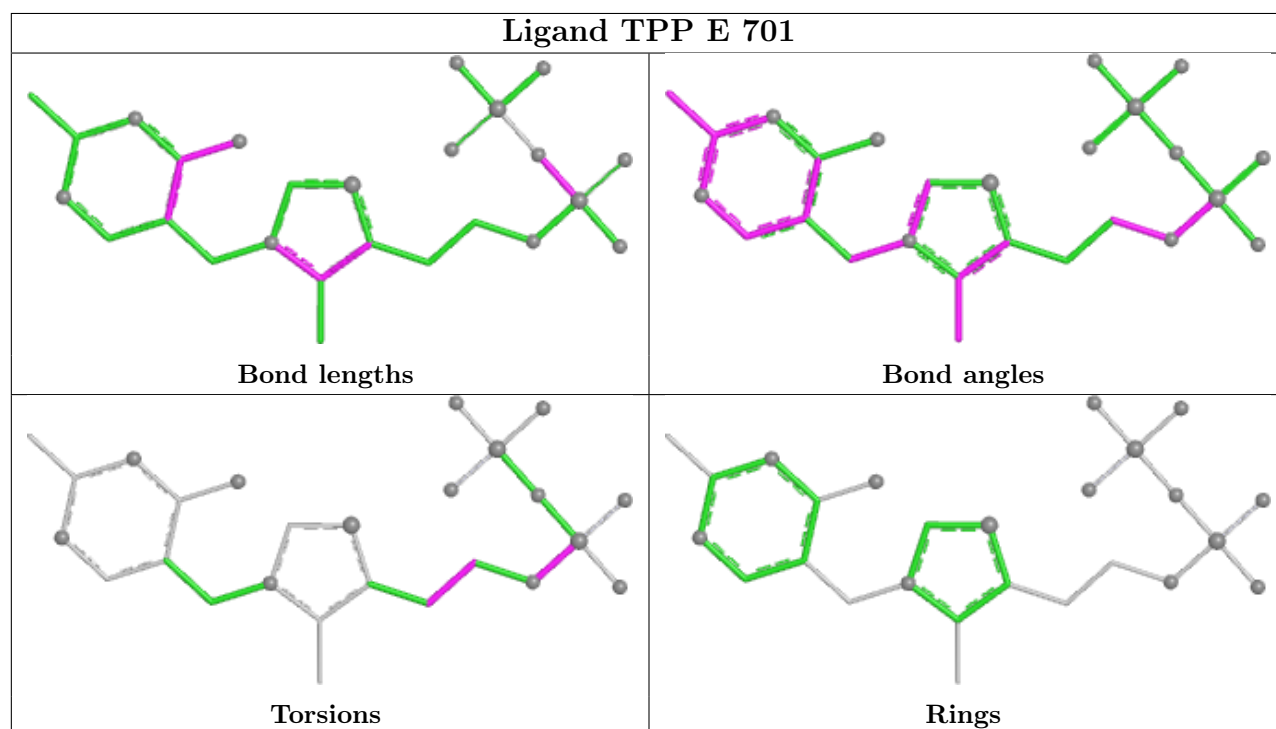
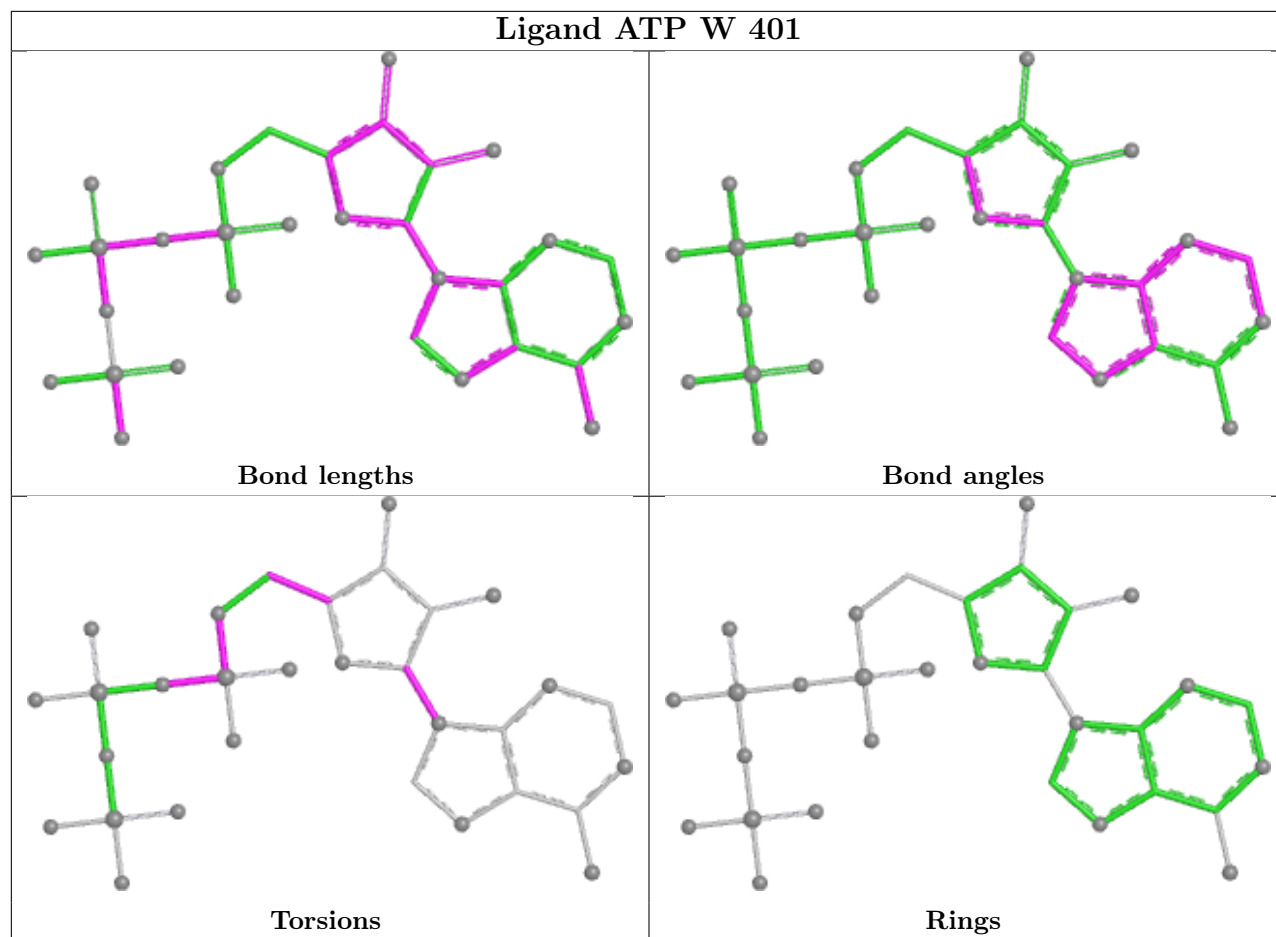


Ligand ATP L 401

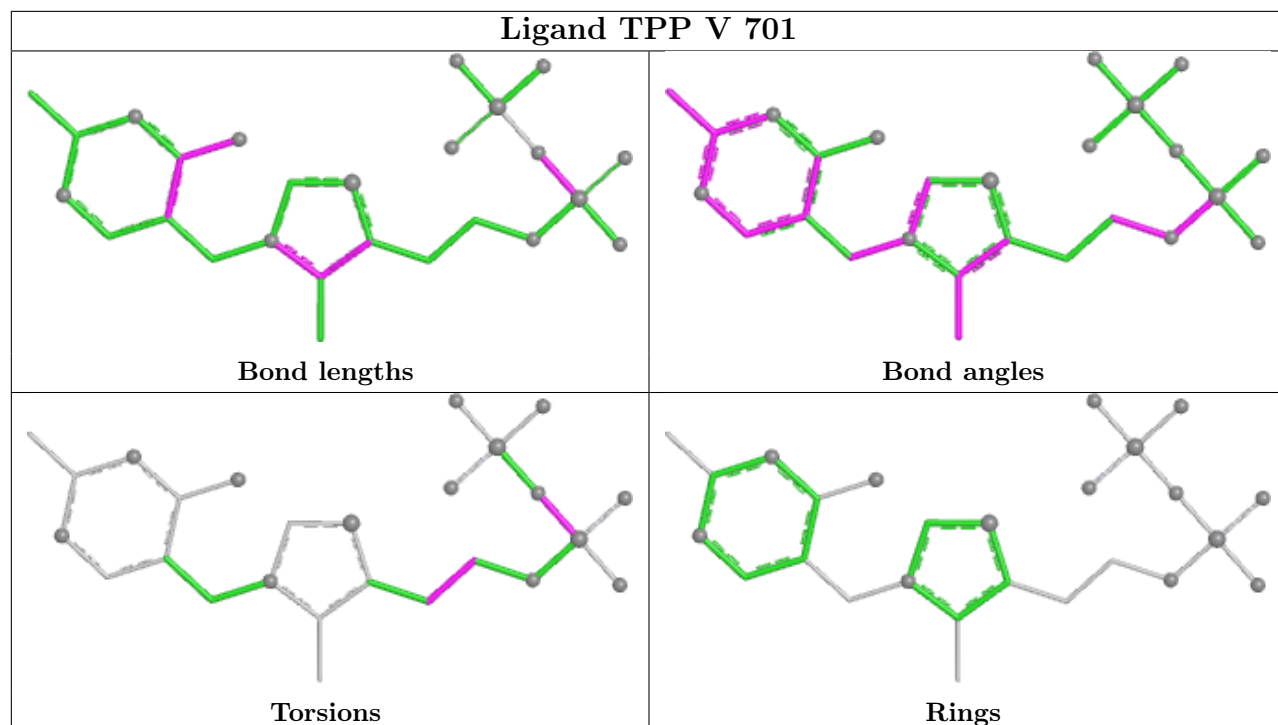


Ligand 60G F 704

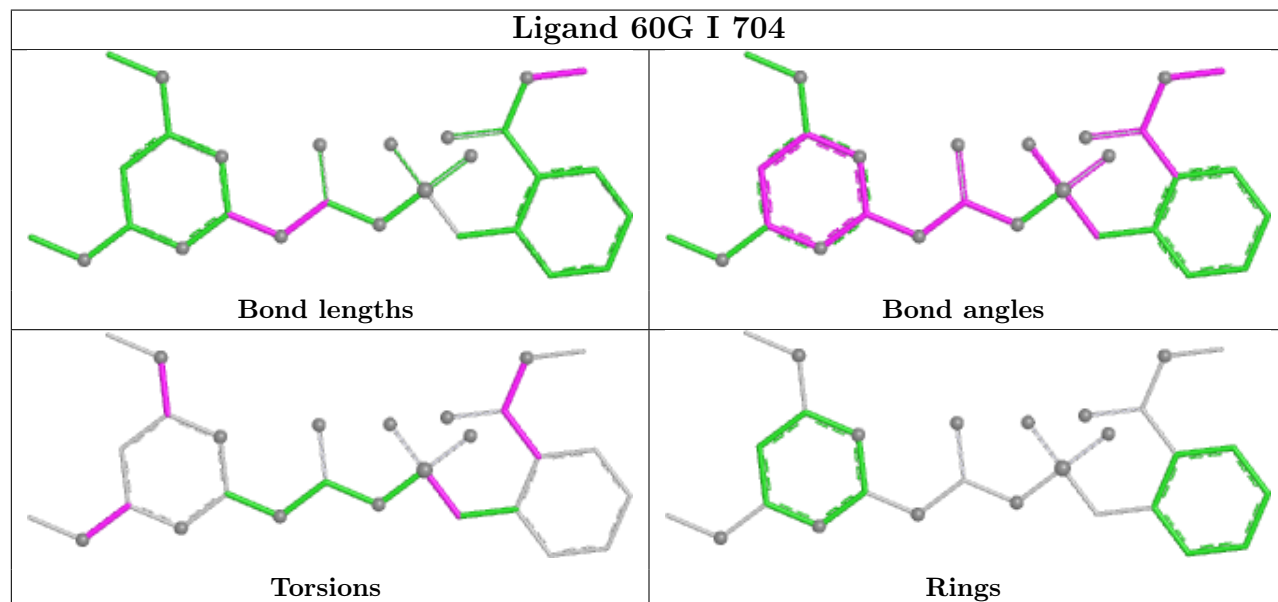




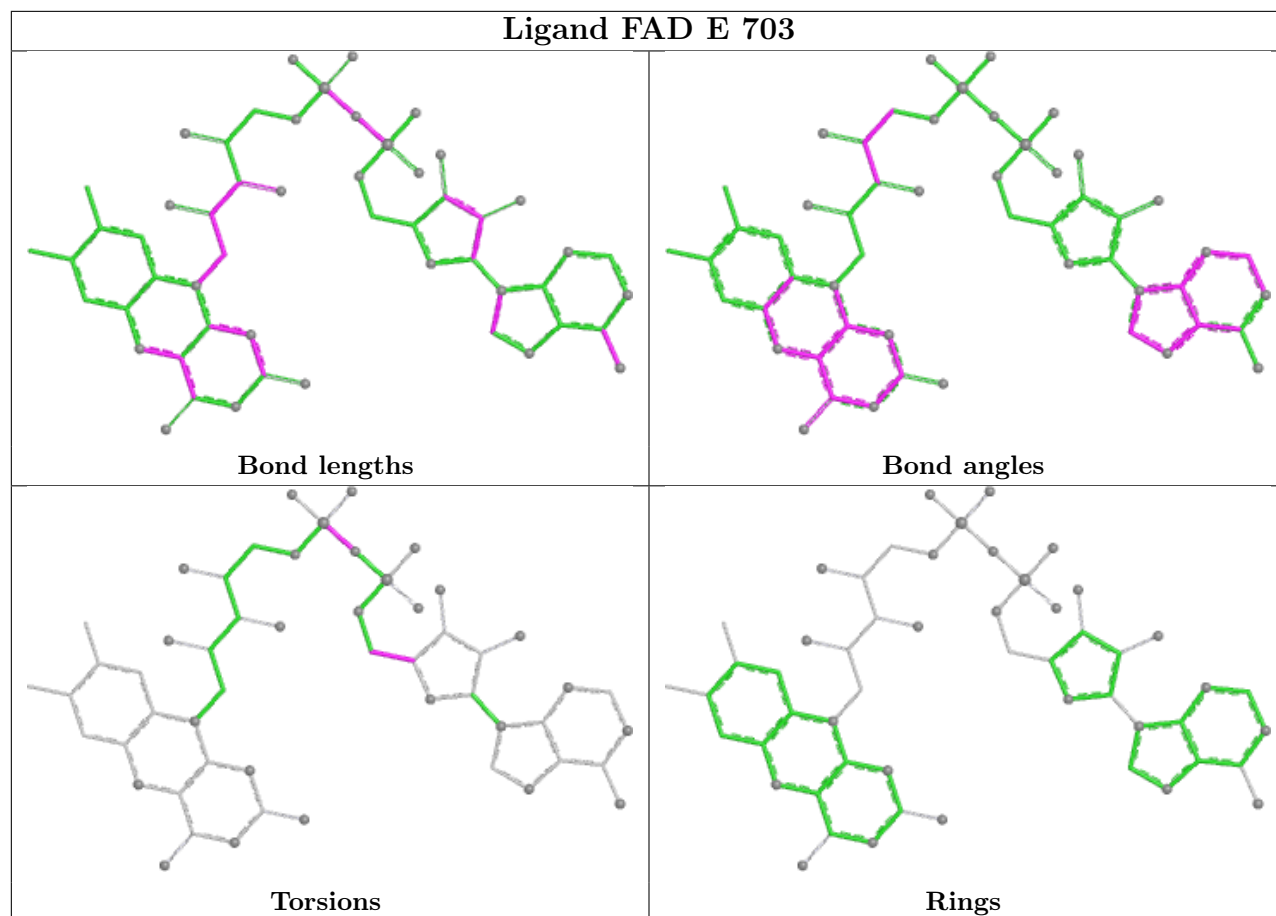
Ligand TPP V 701



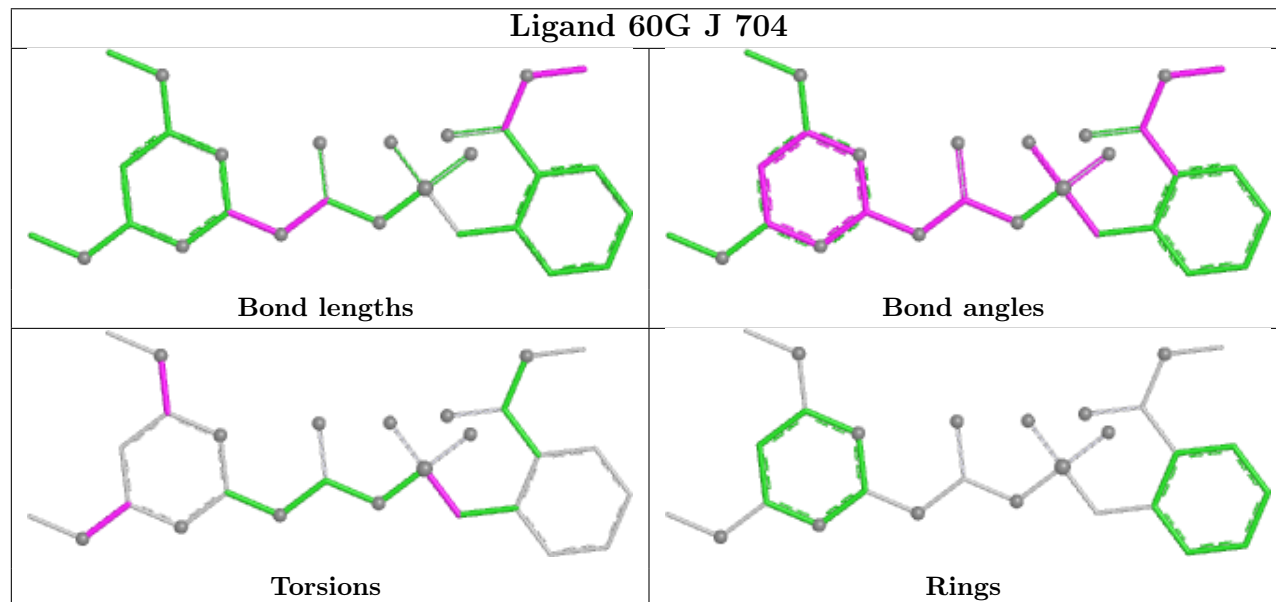
Ligand 60G I 704



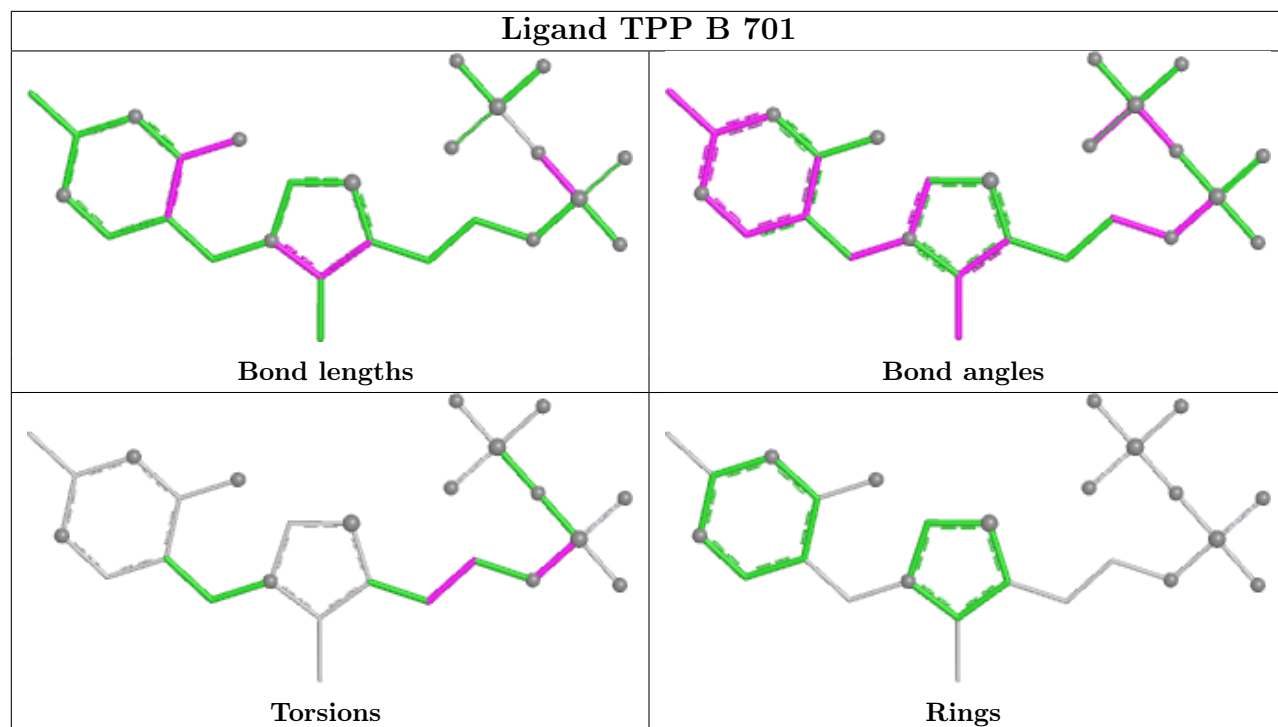
Ligand FAD E 703



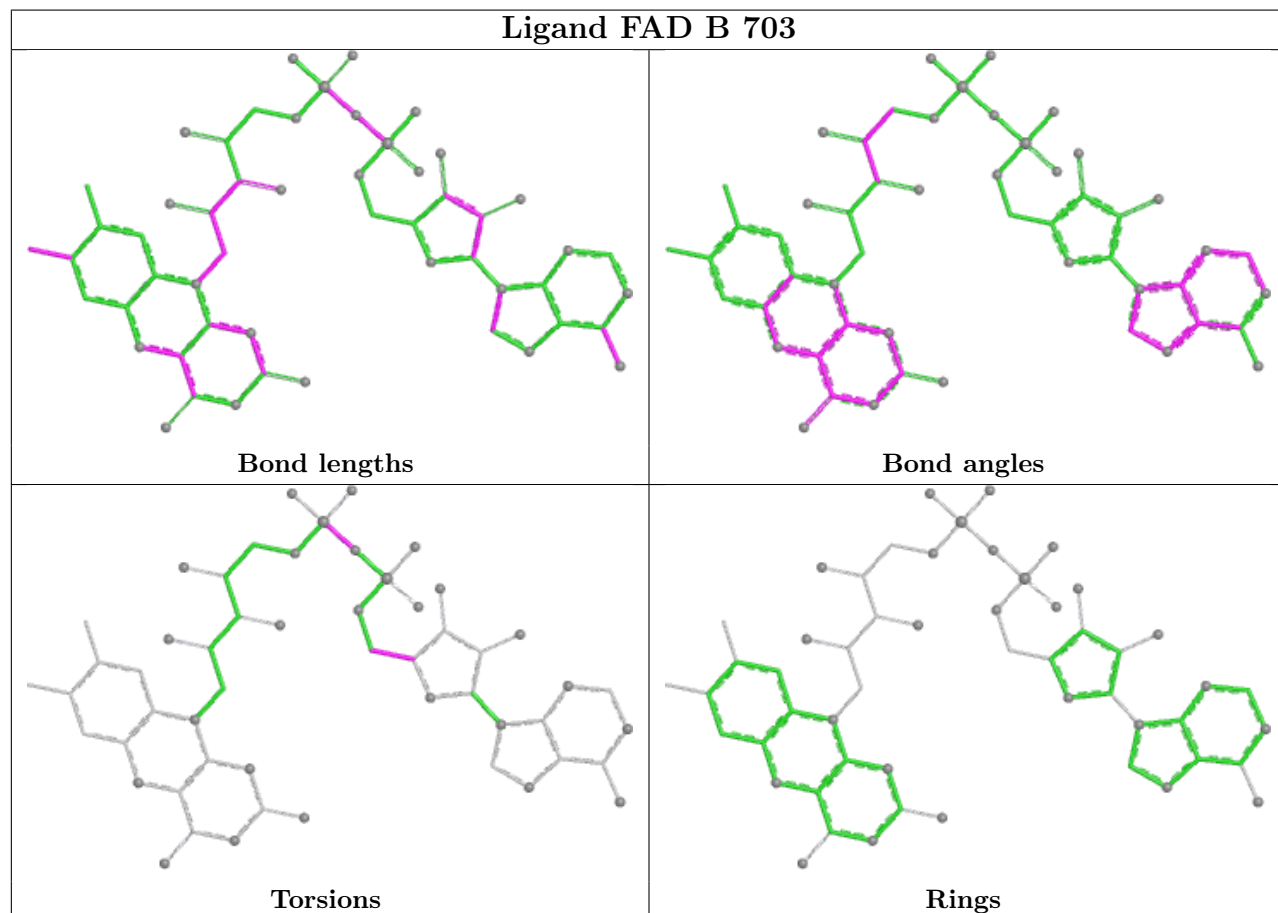
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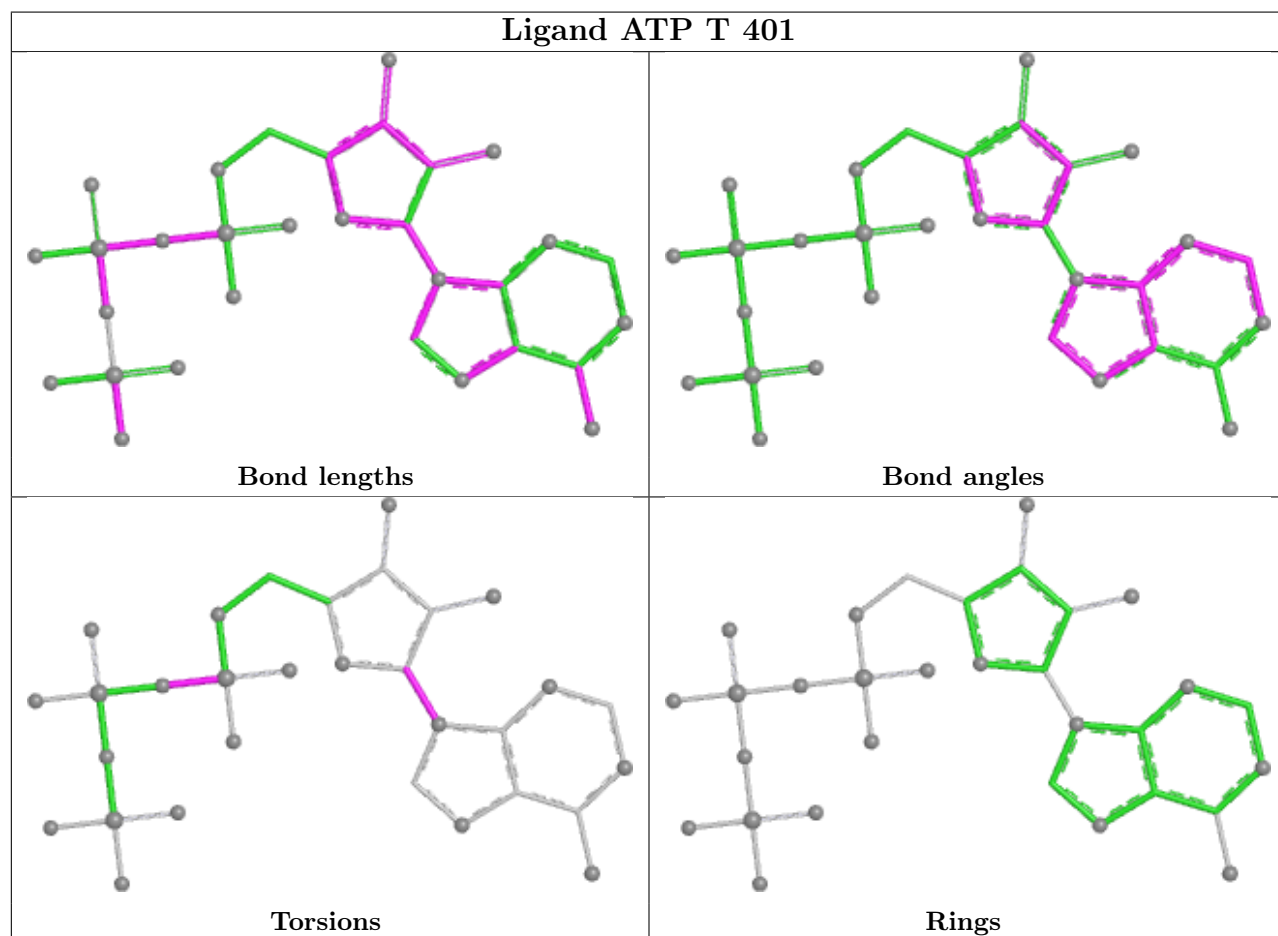
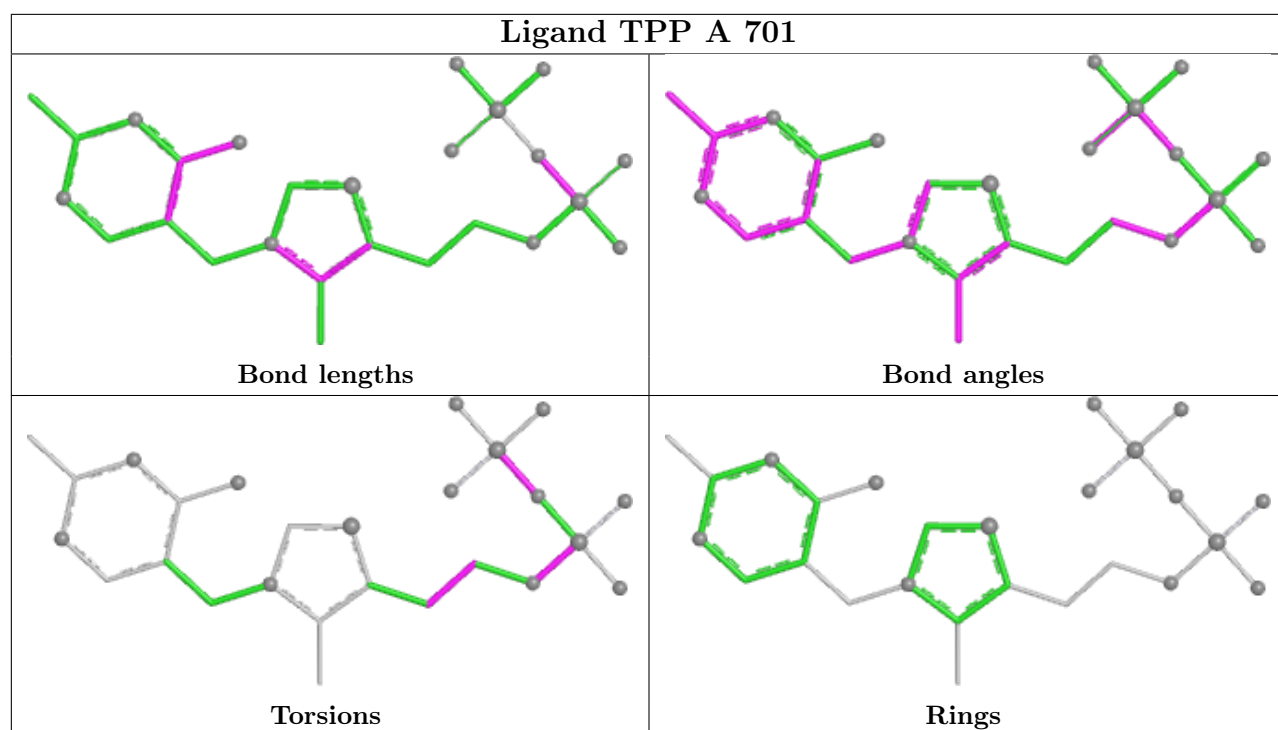


Ligand TPP B 701

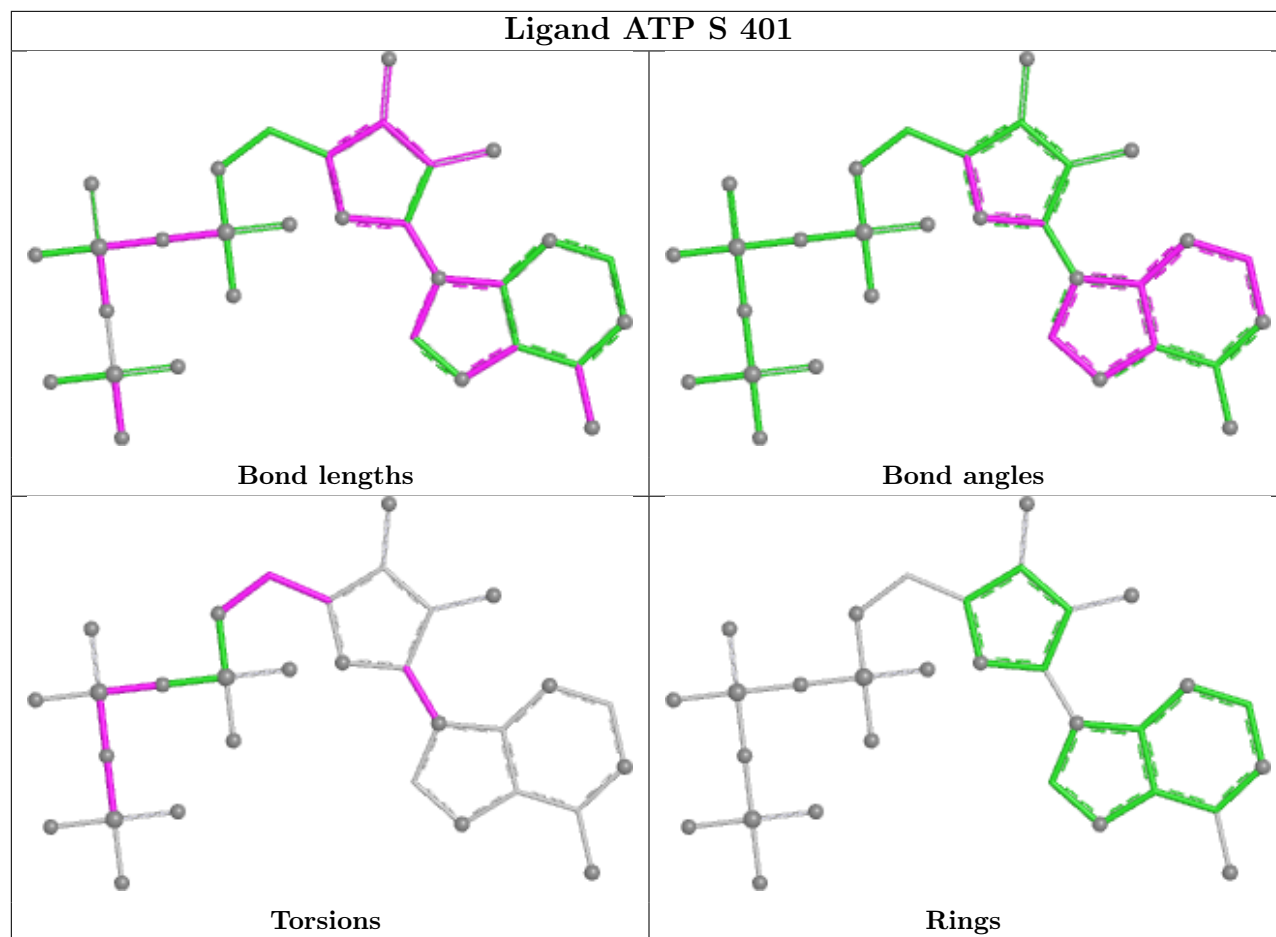


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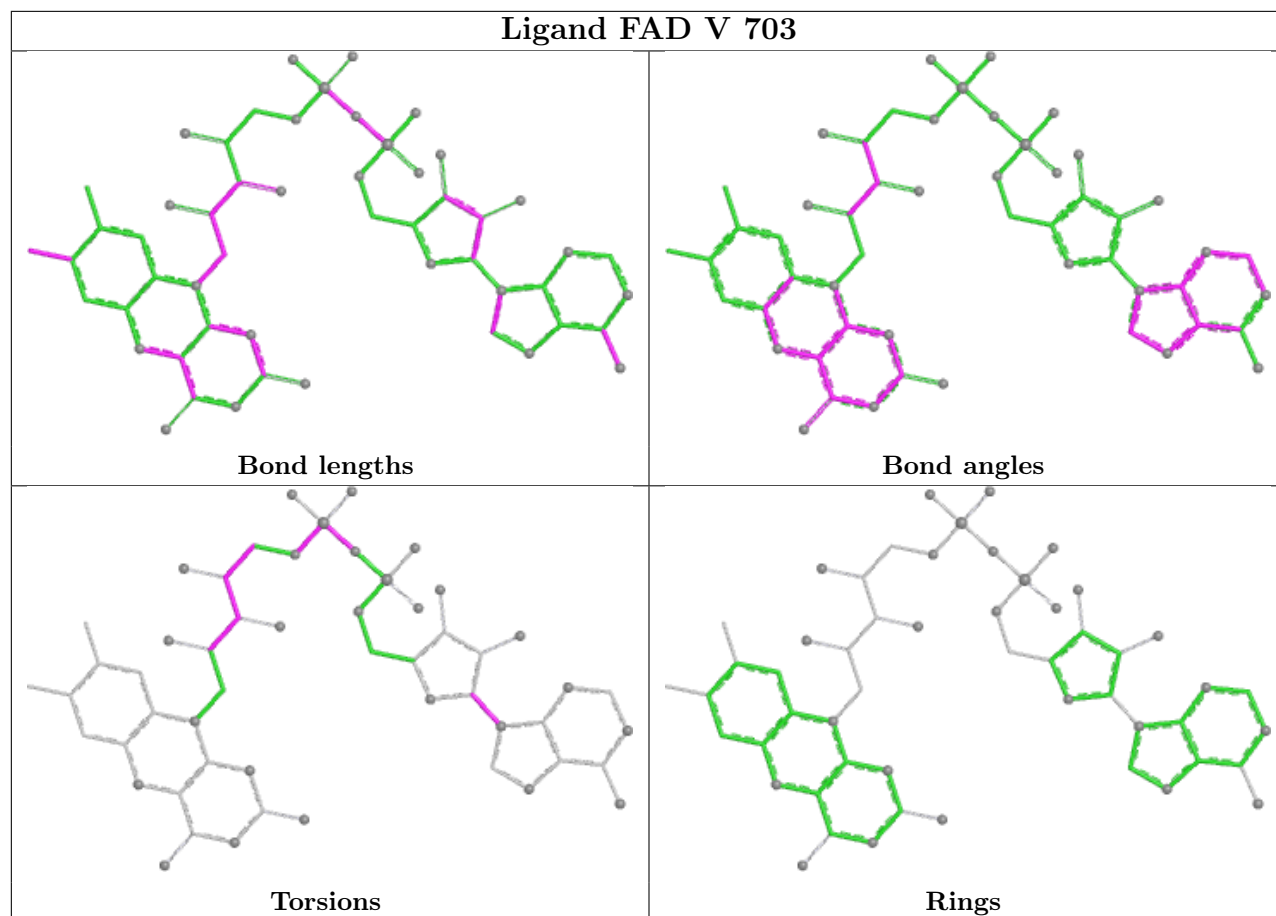




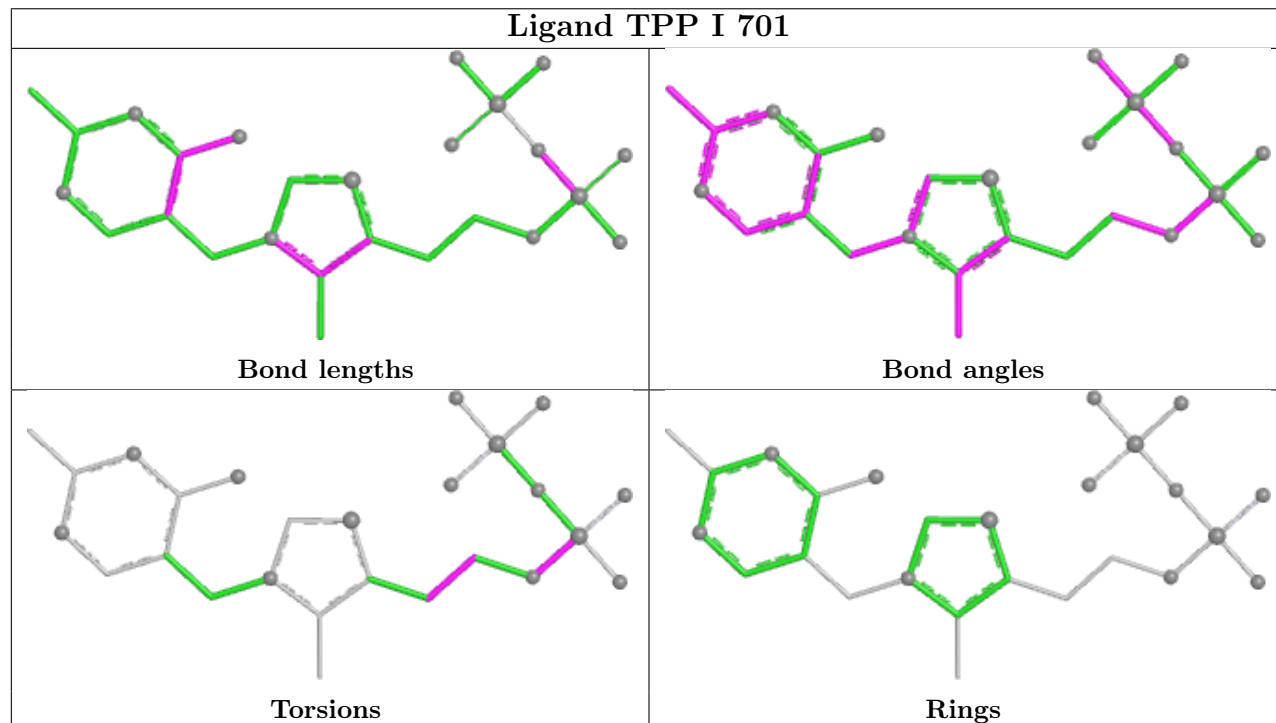
Ligand ATP S 401



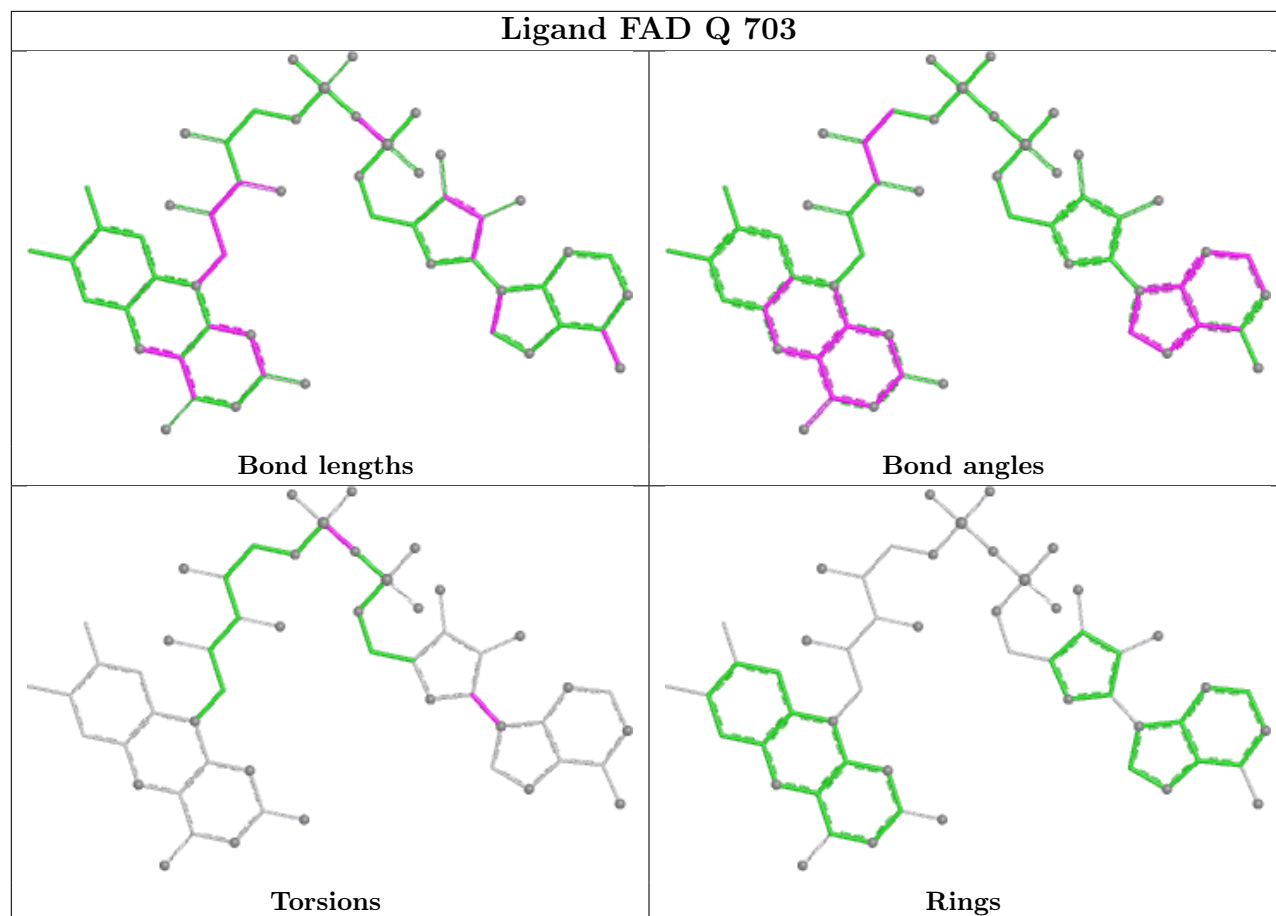
Ligand FAD V 703



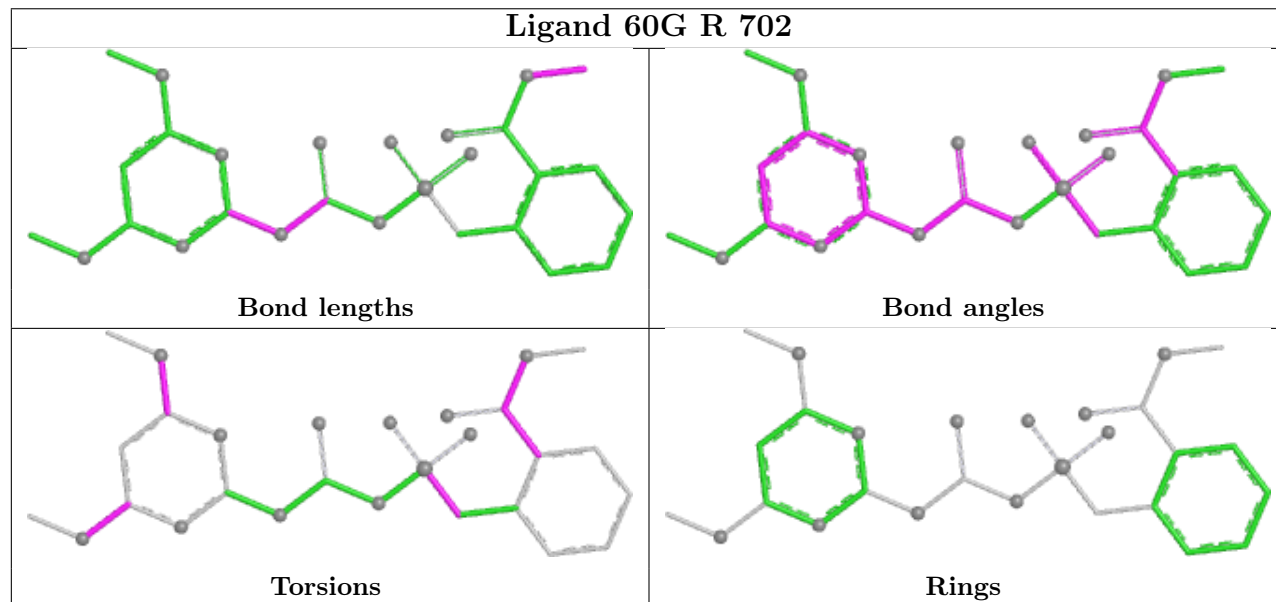
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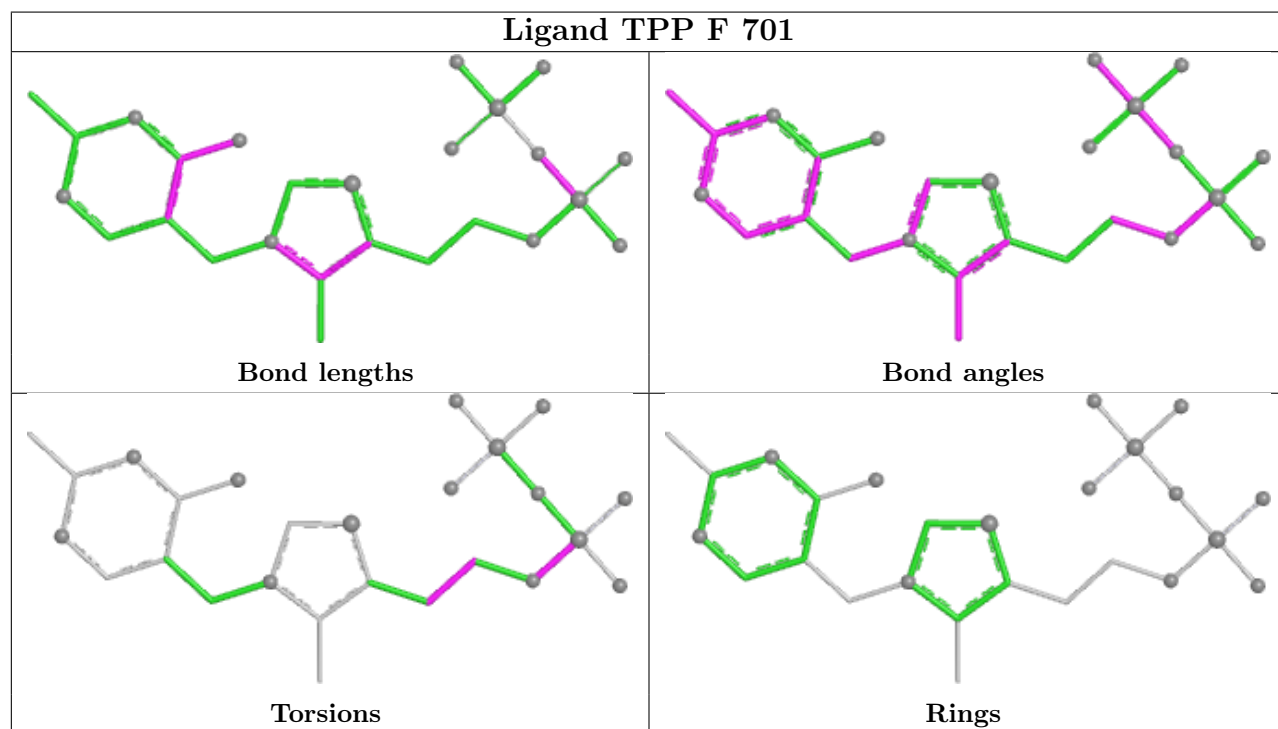
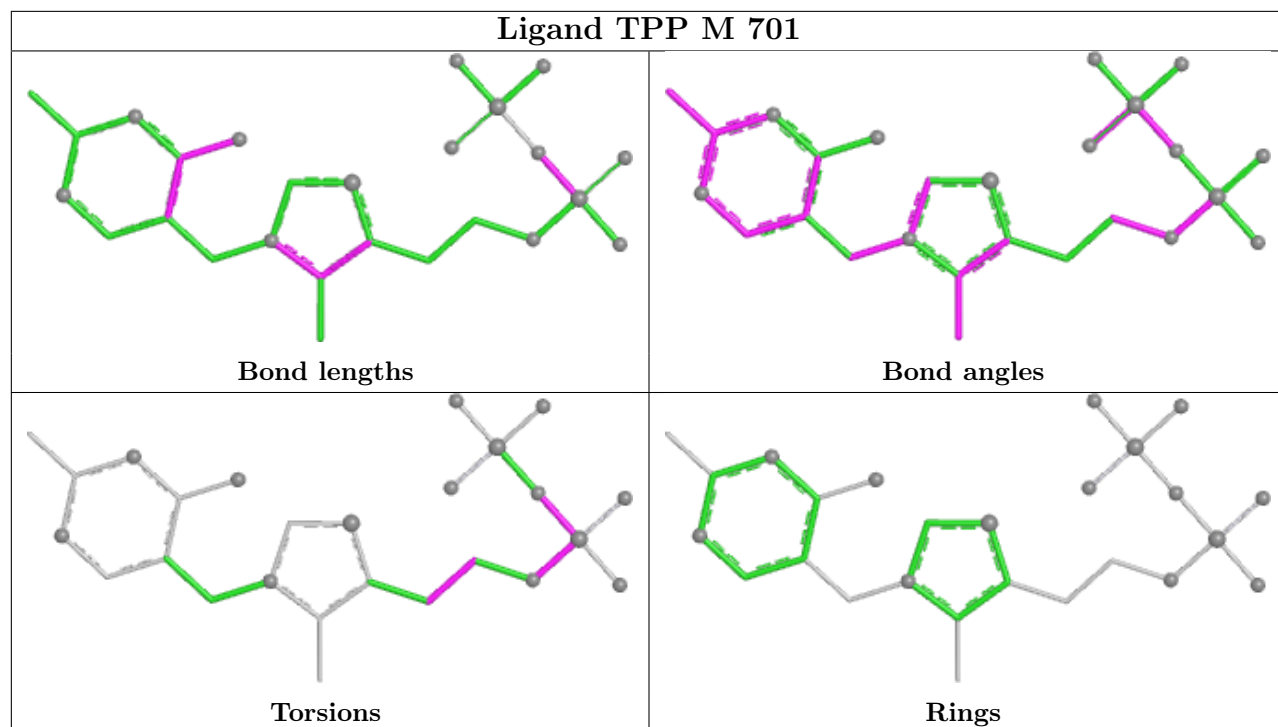


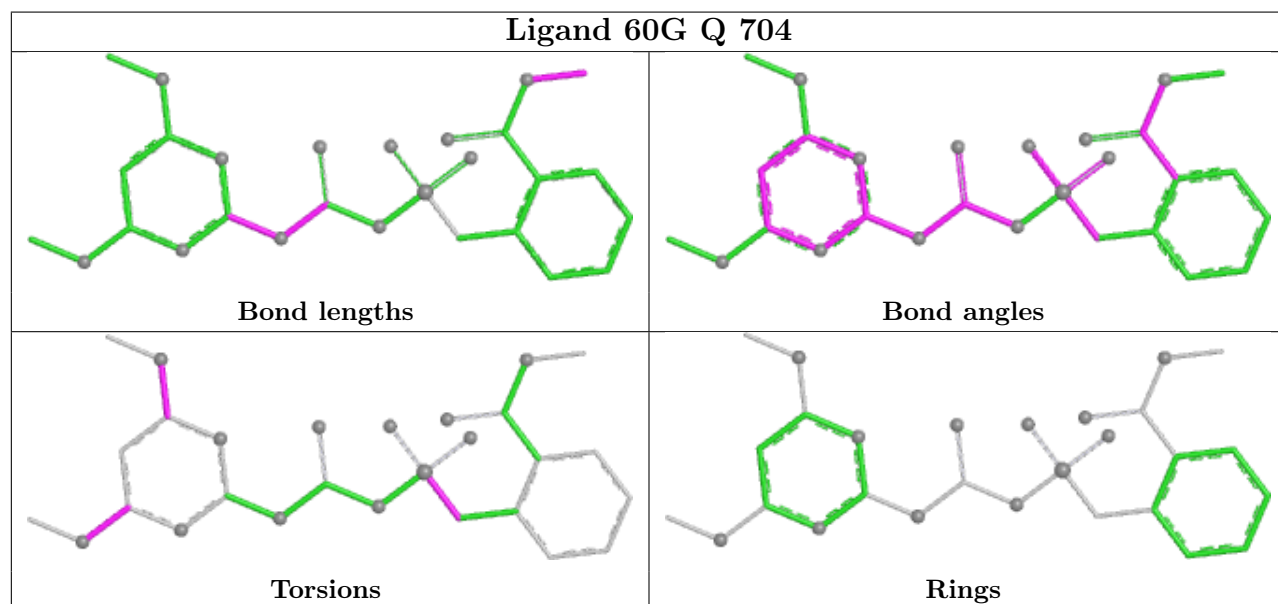
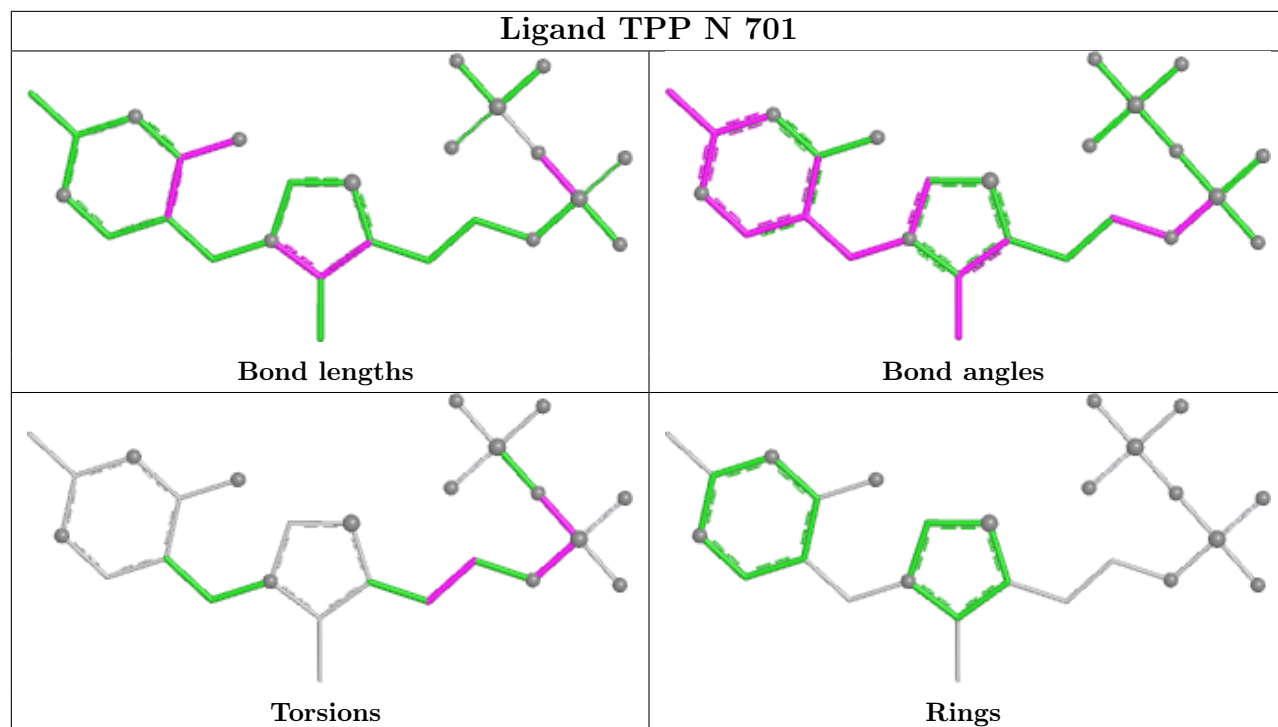
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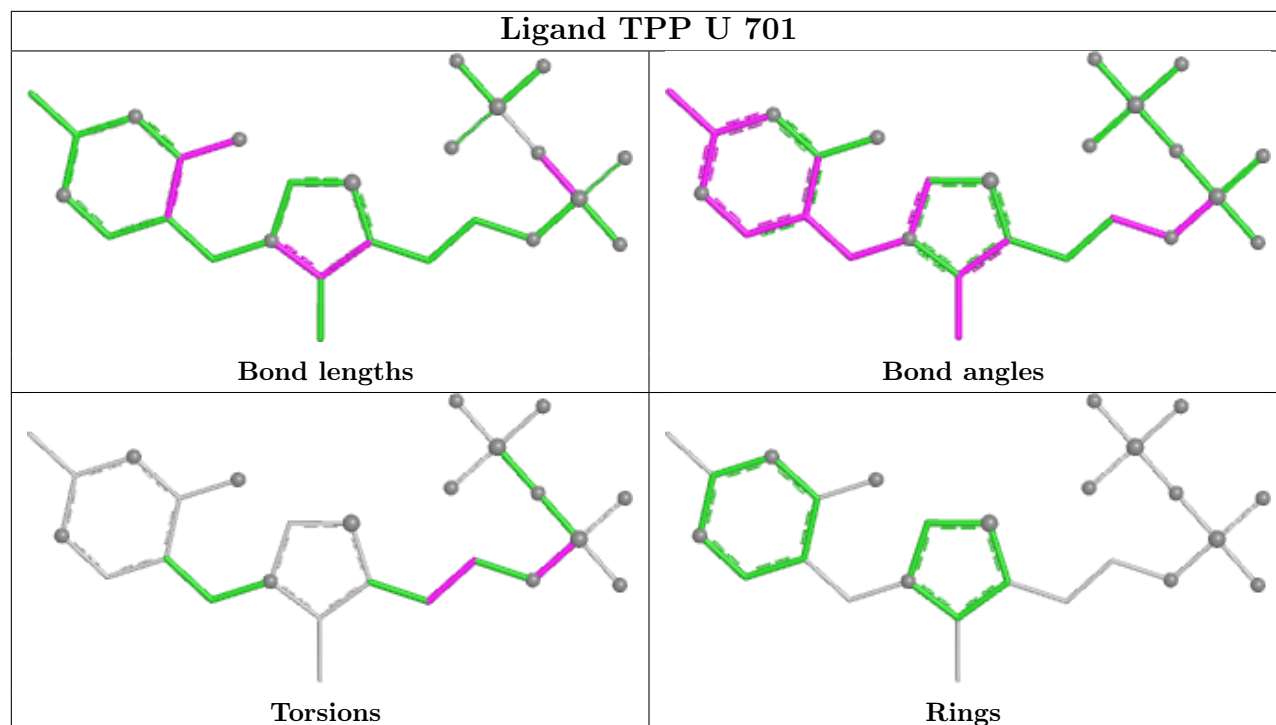
Ligand 60G R 702



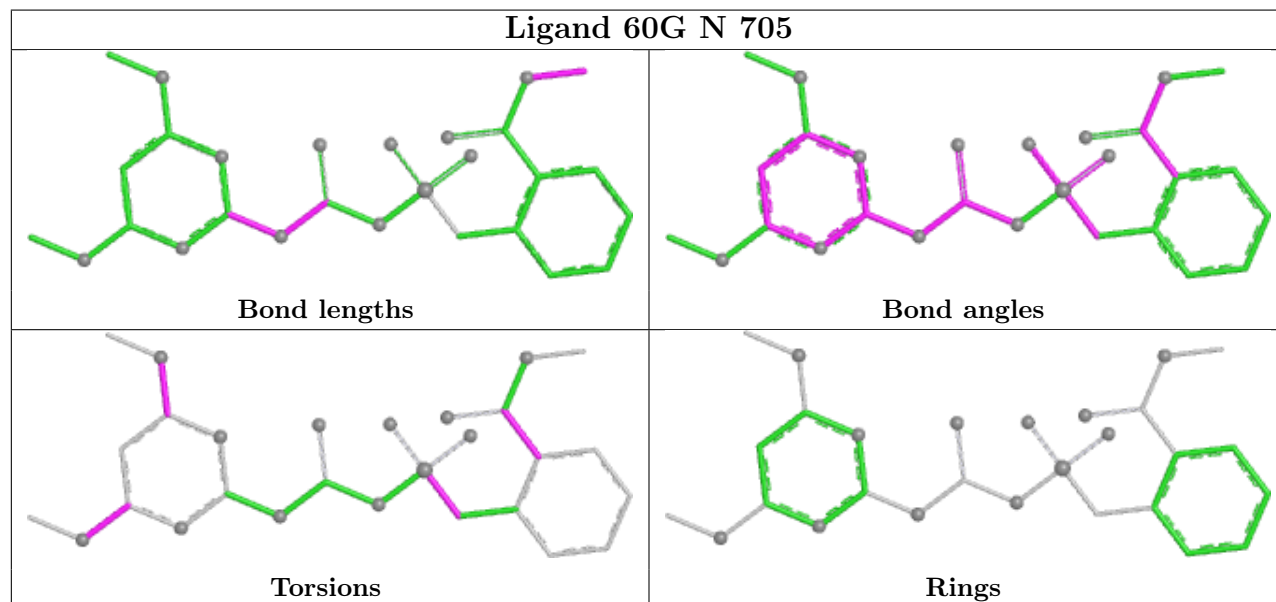


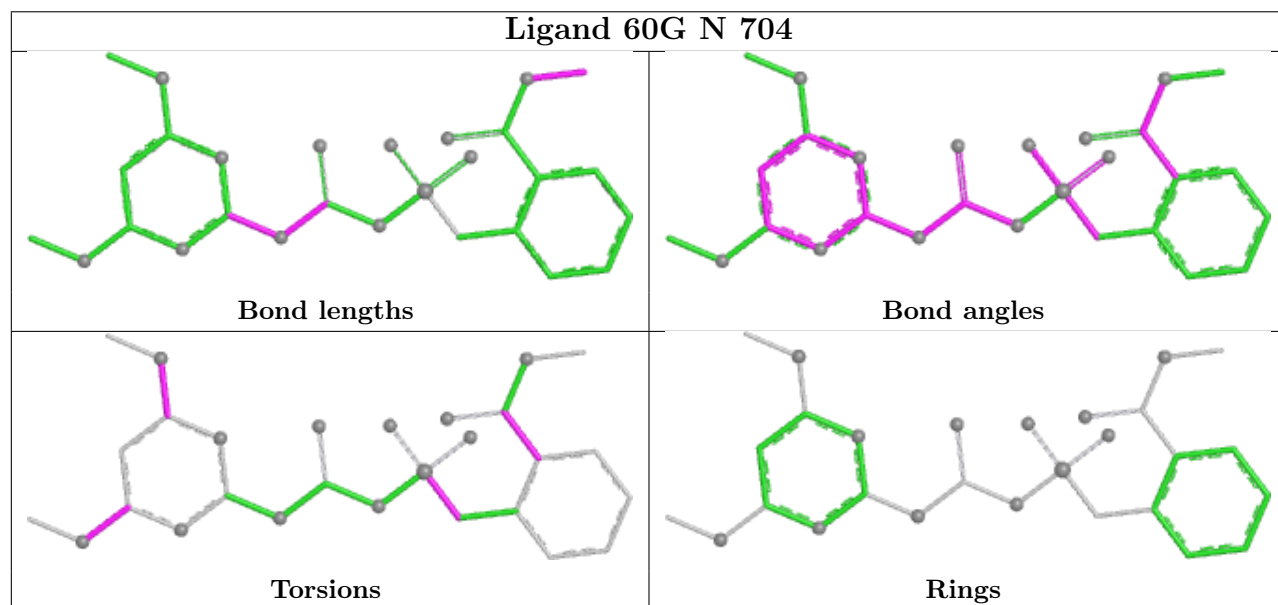
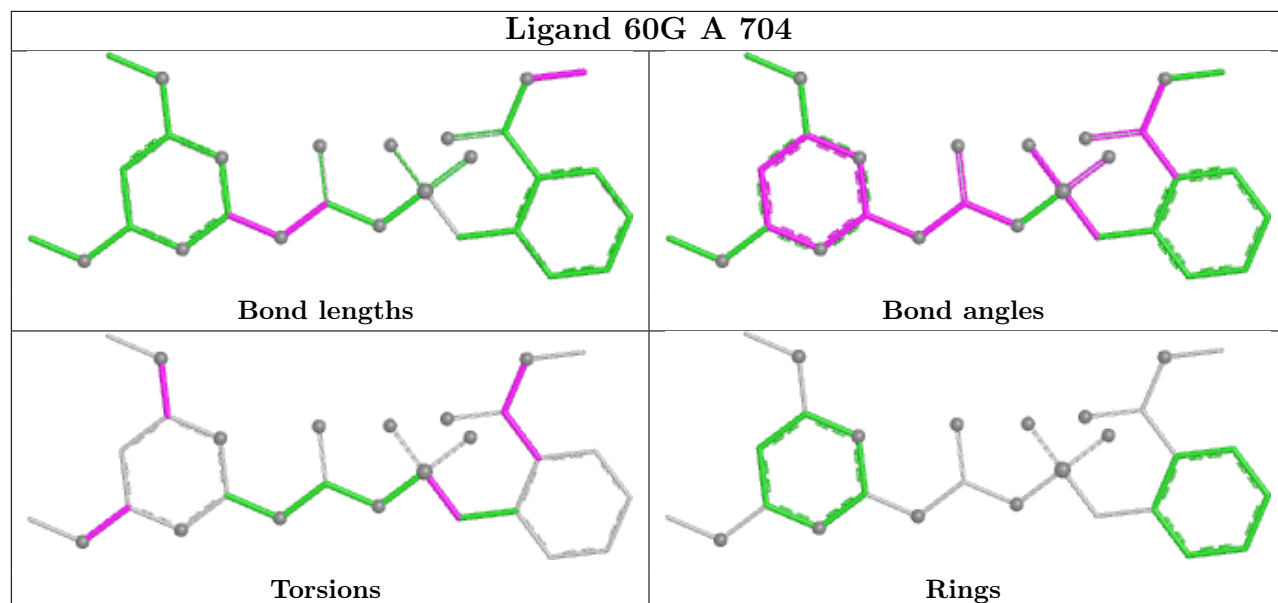


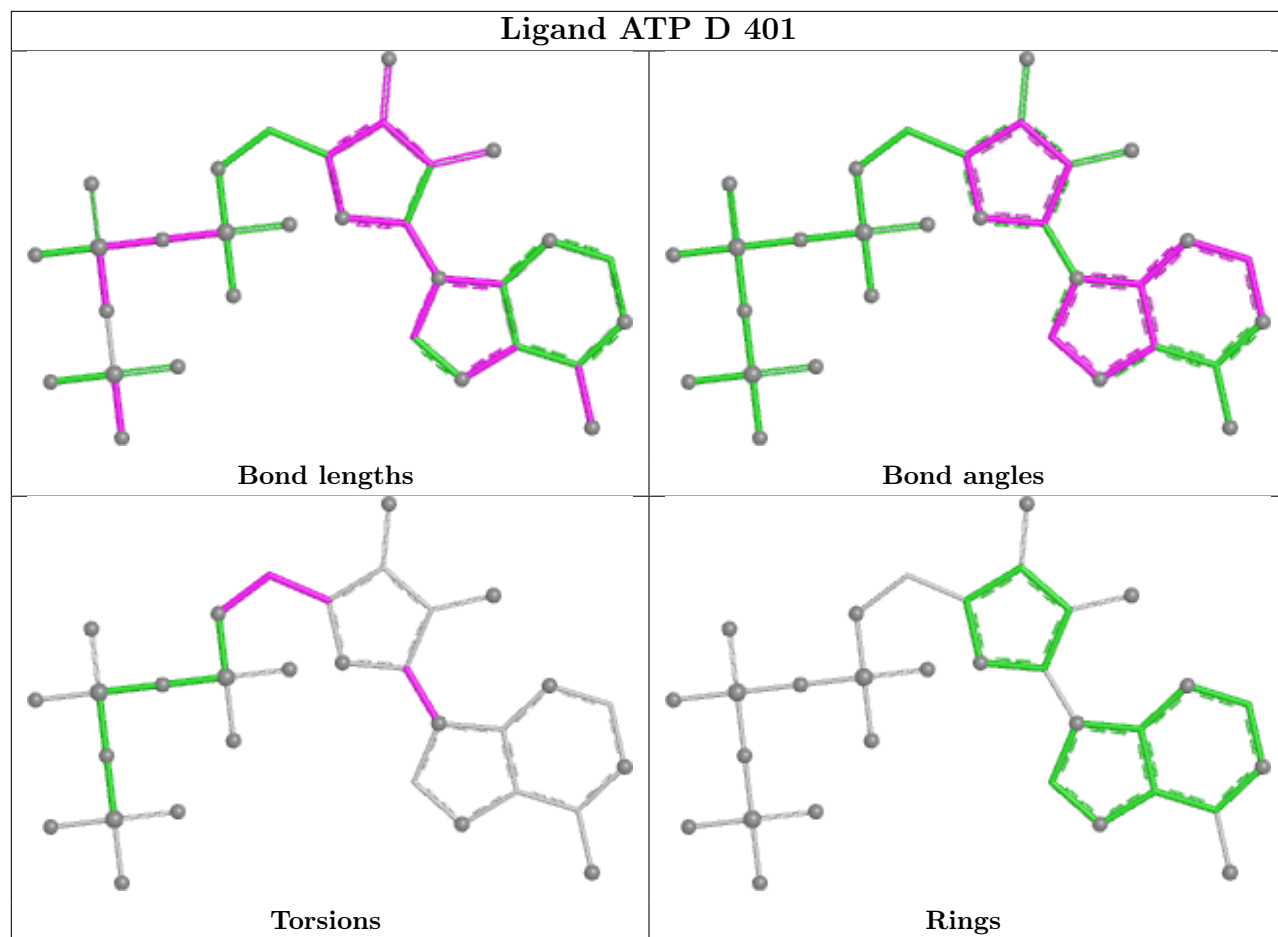
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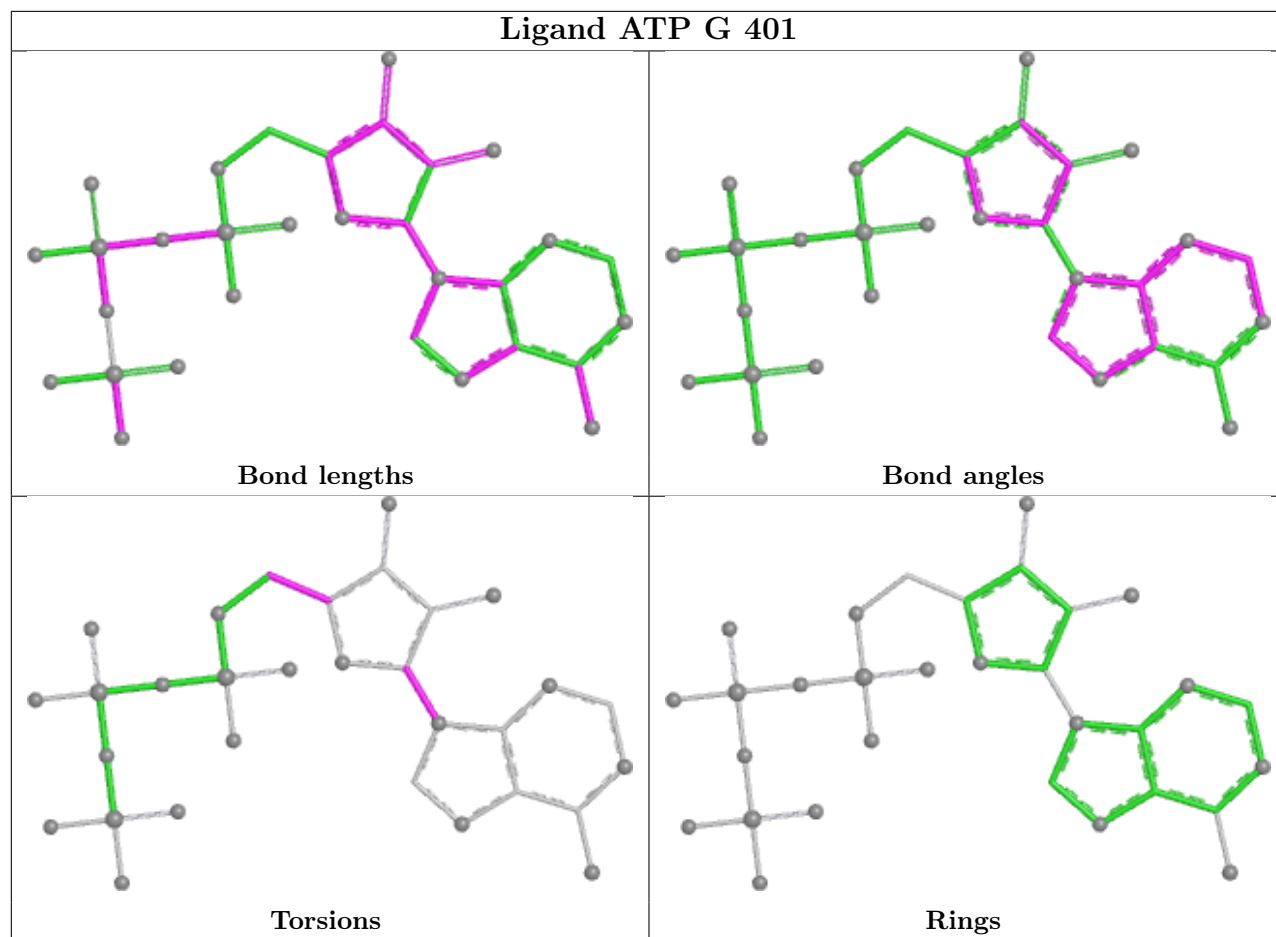


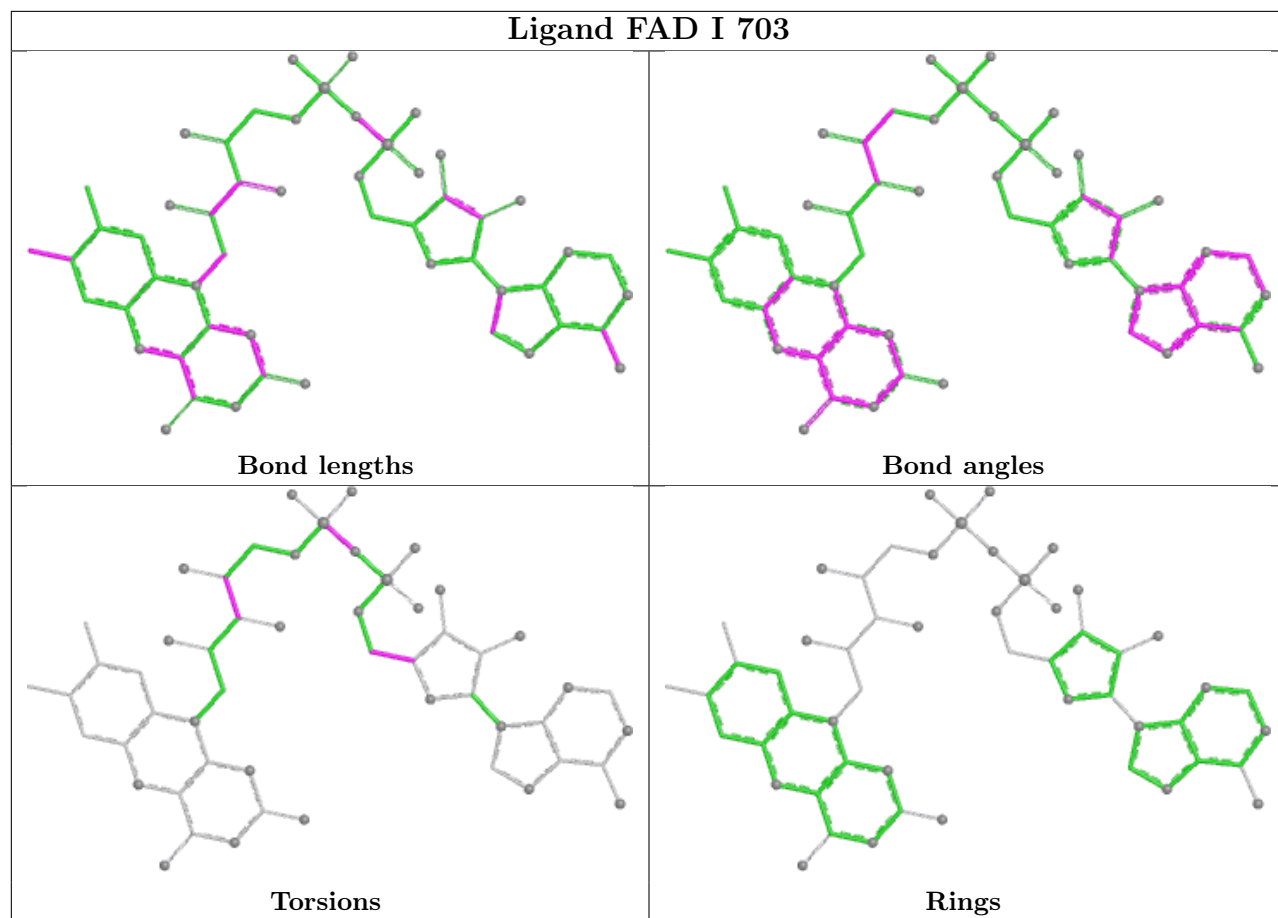
Ligand 60G N 705



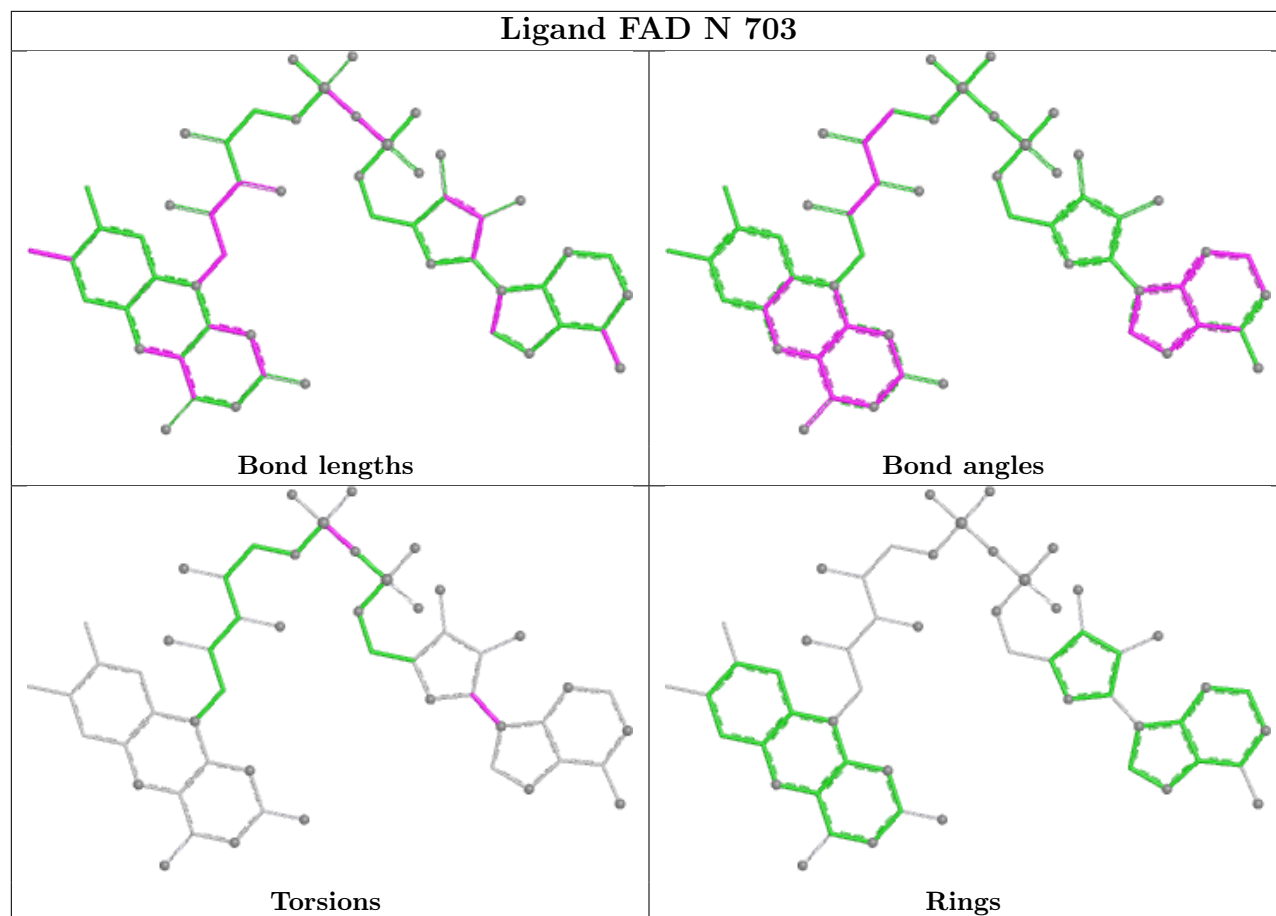




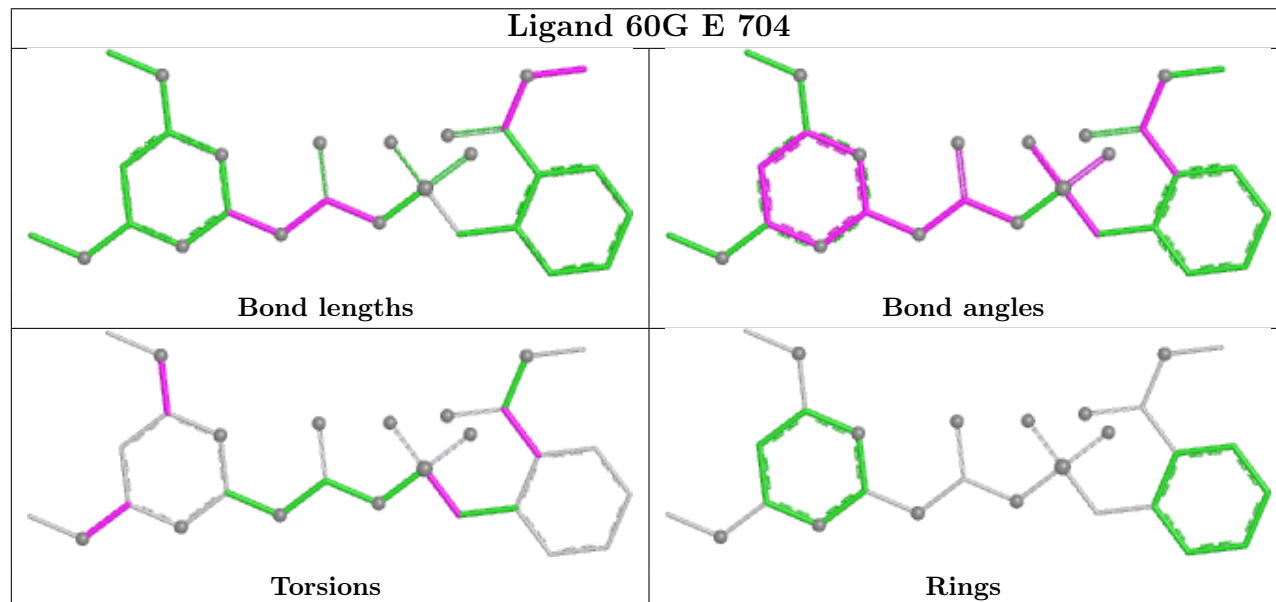


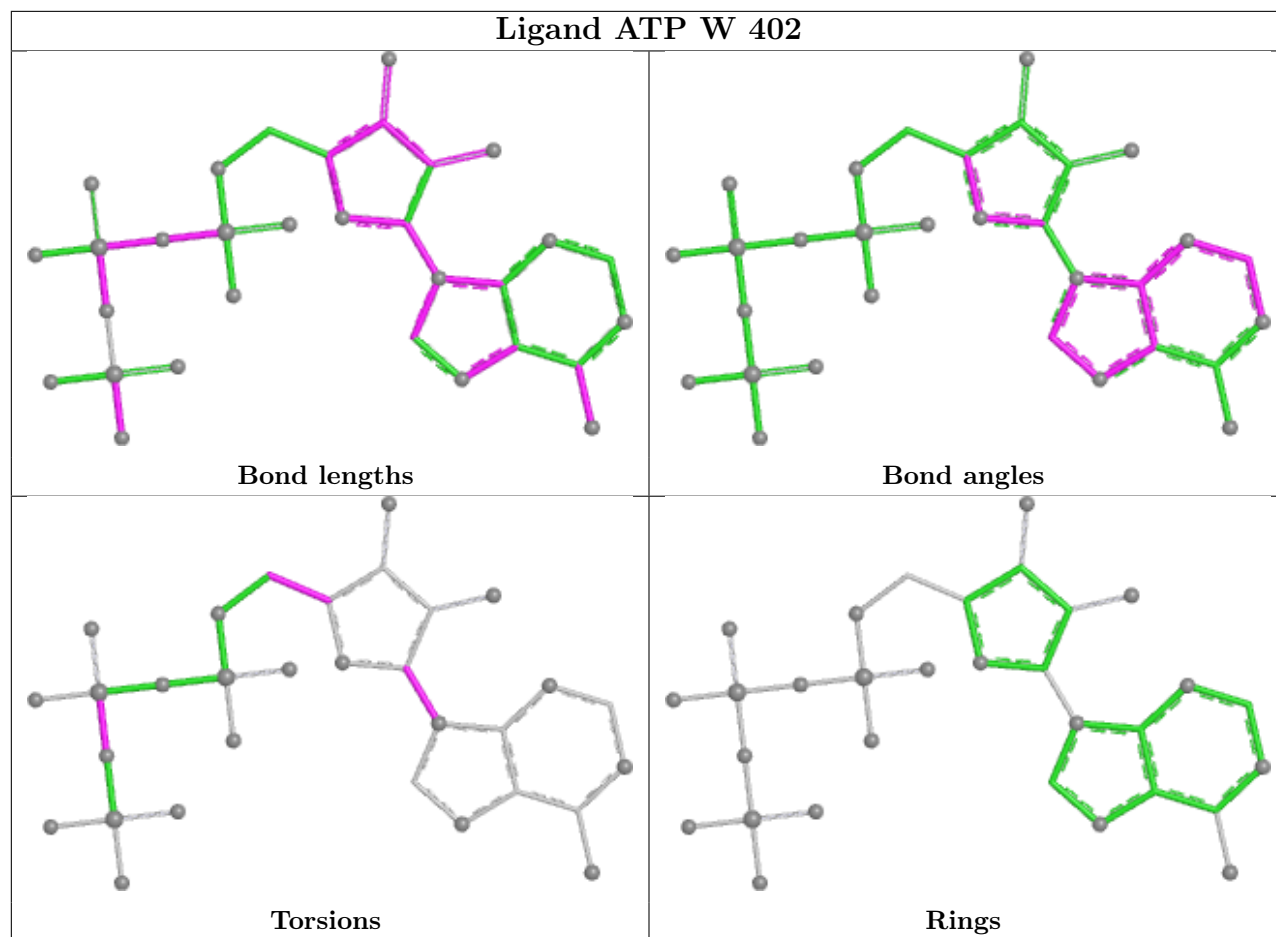


Ligand FAD N 703

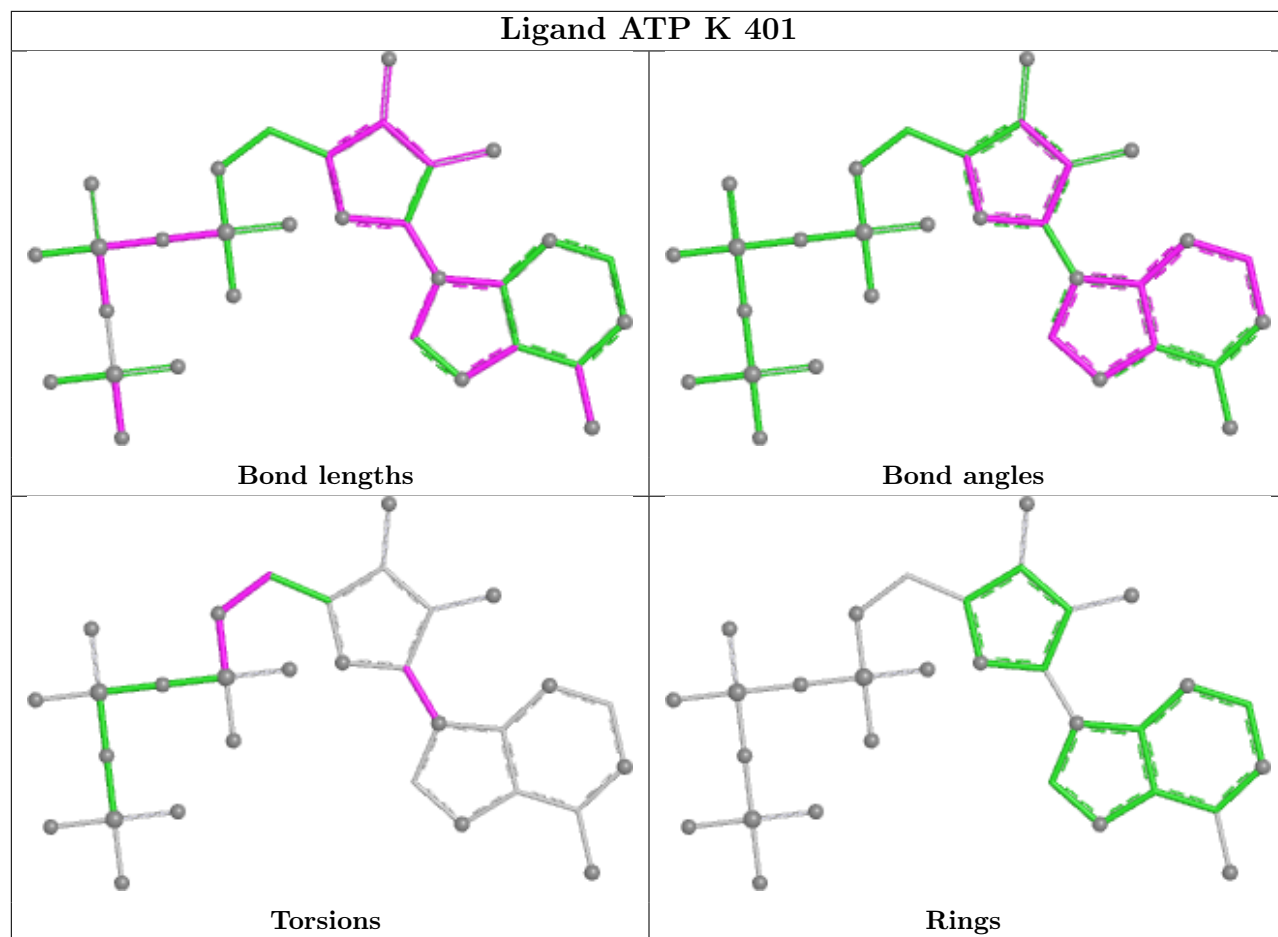


Ligand 60G E 704

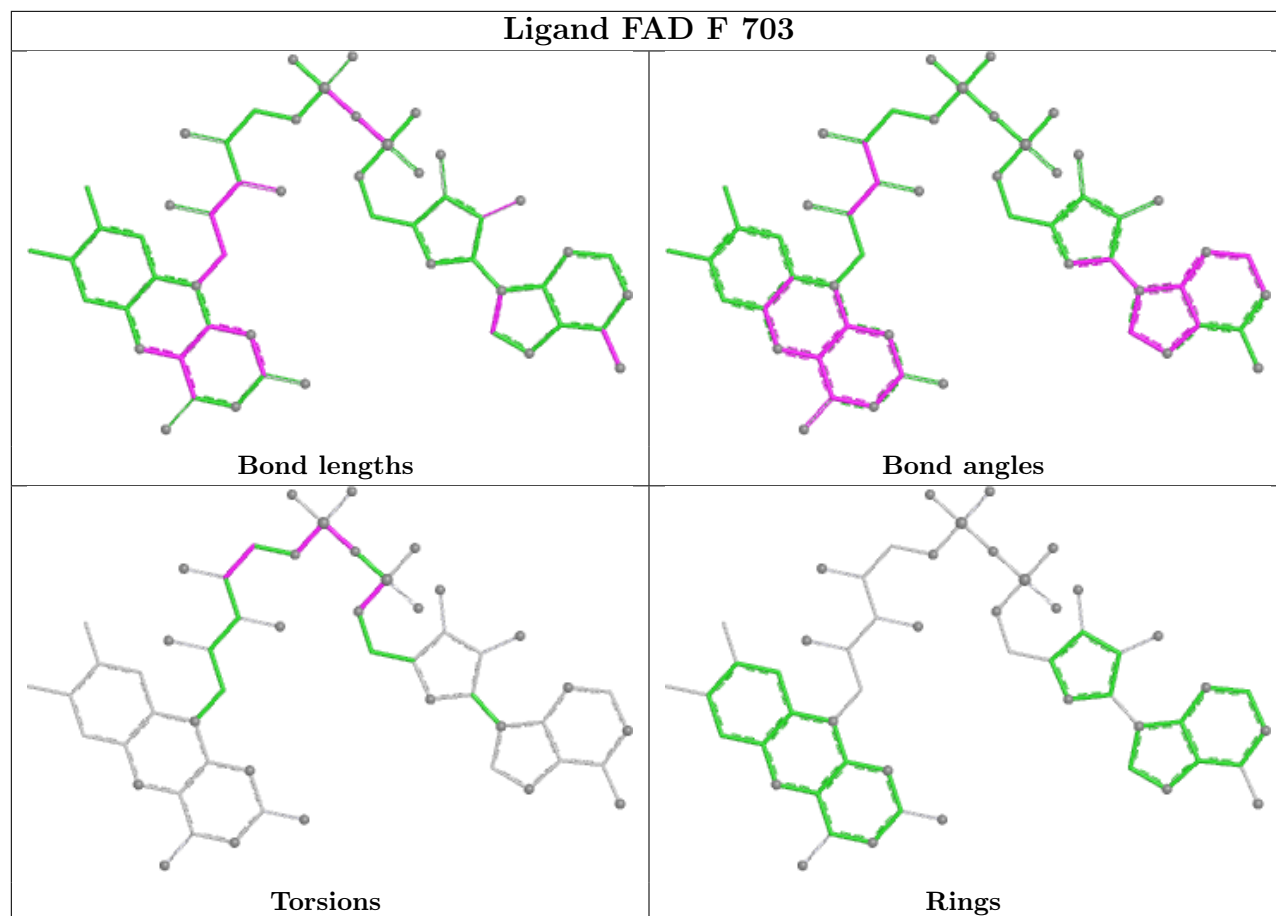




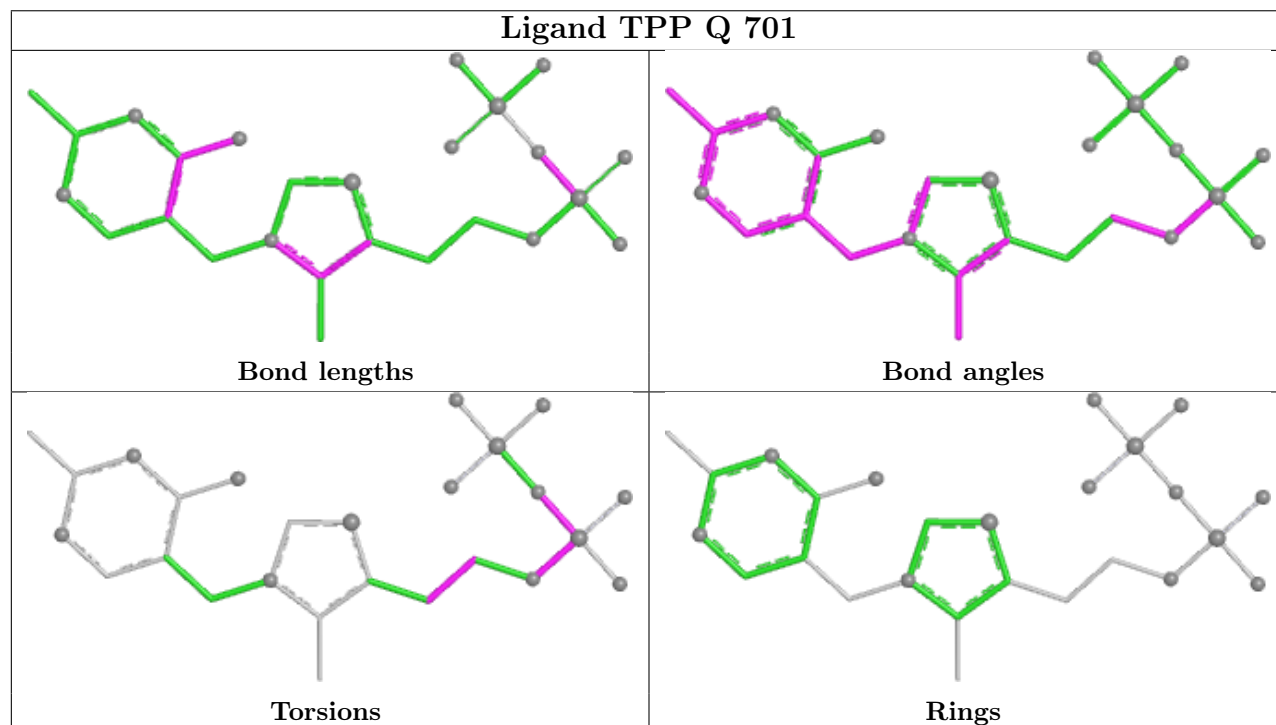
Ligand ATP K 401



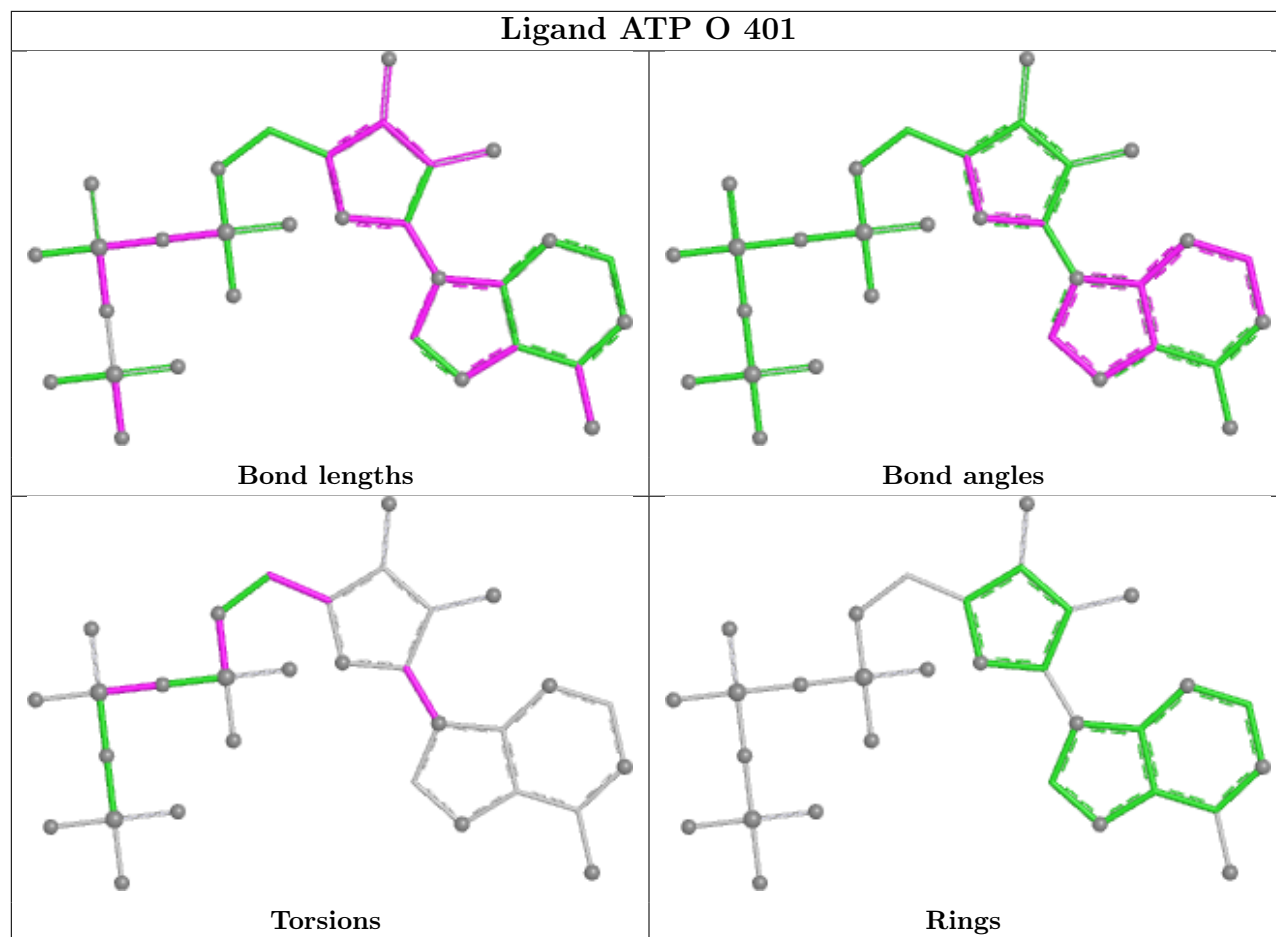
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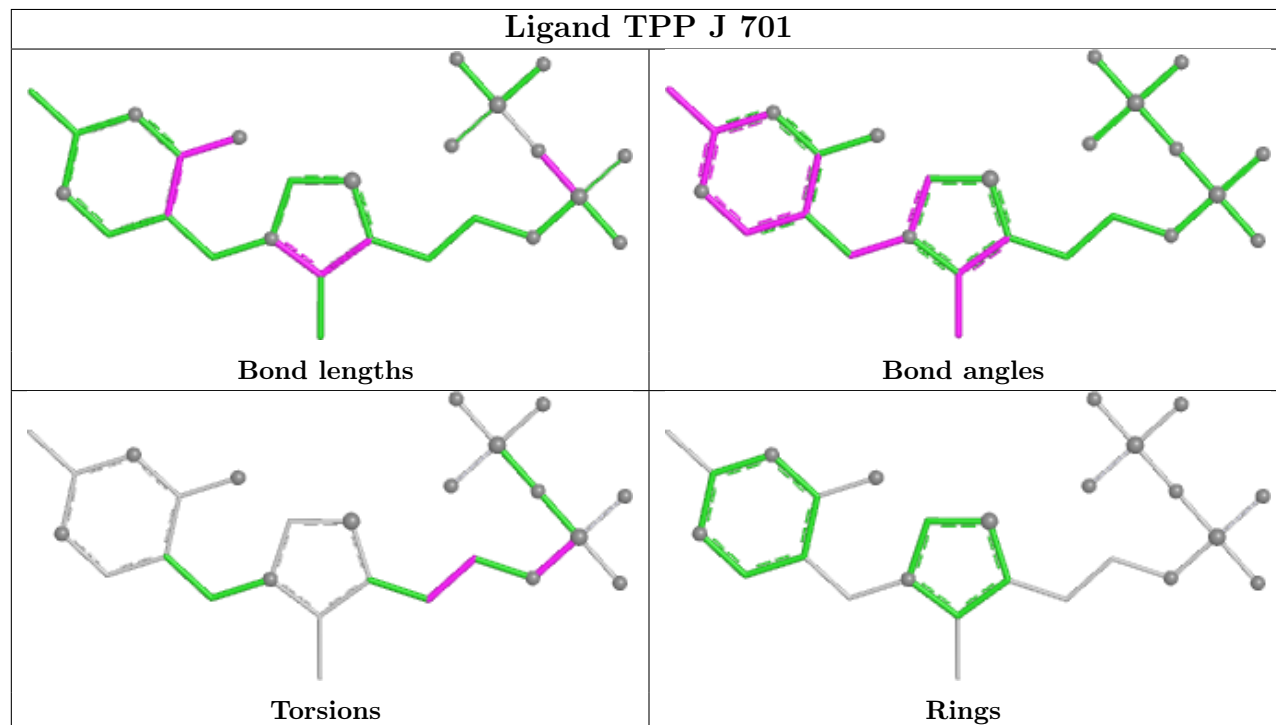
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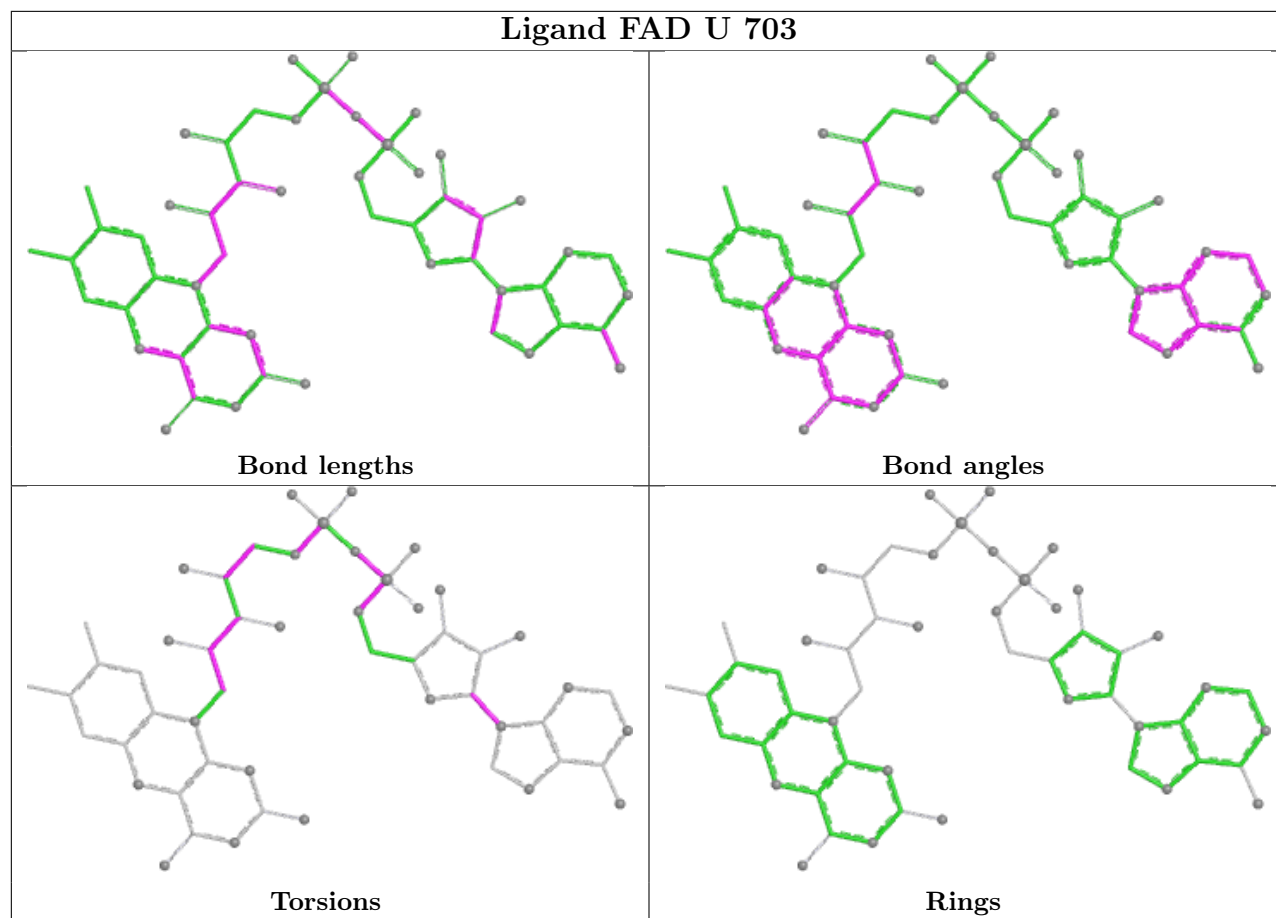


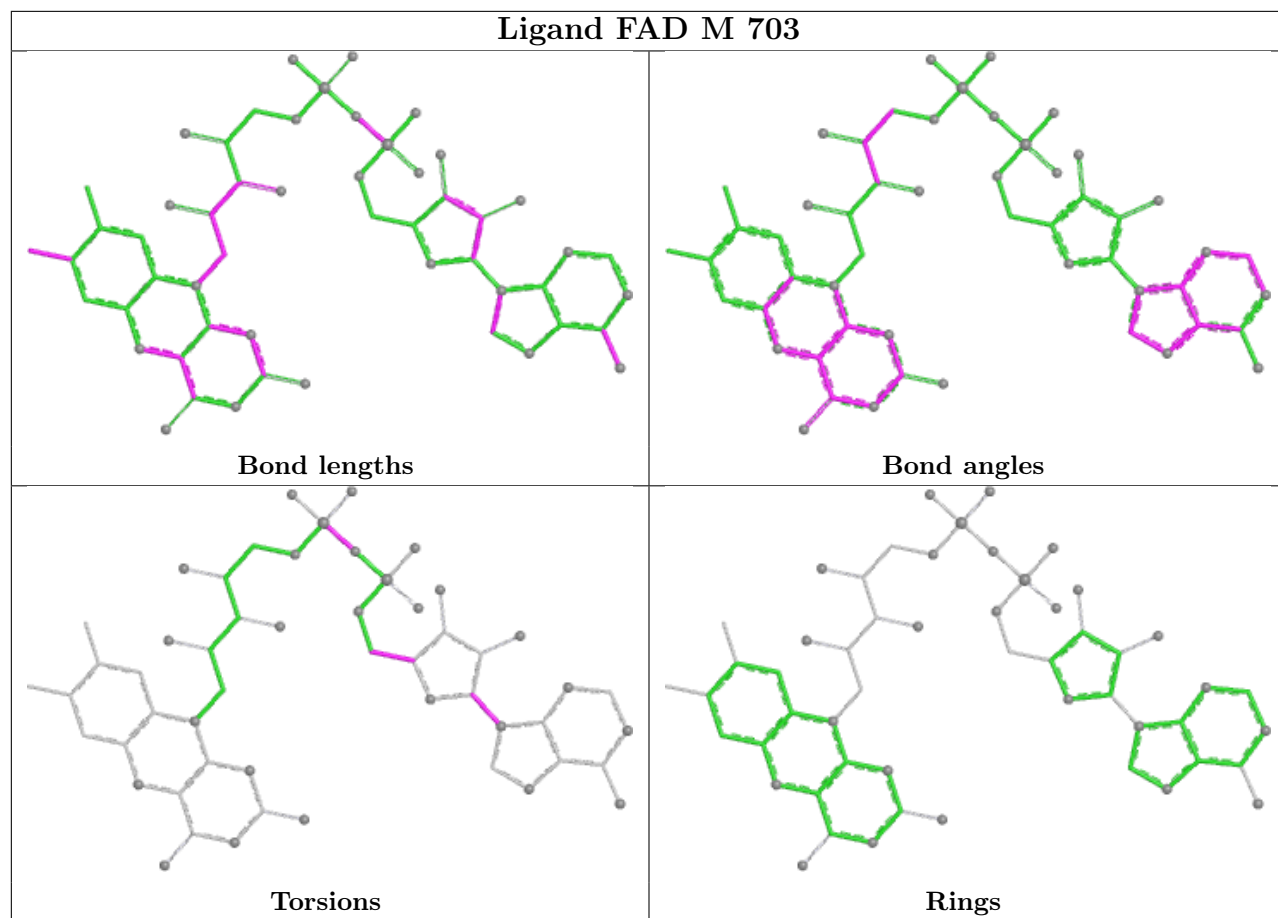
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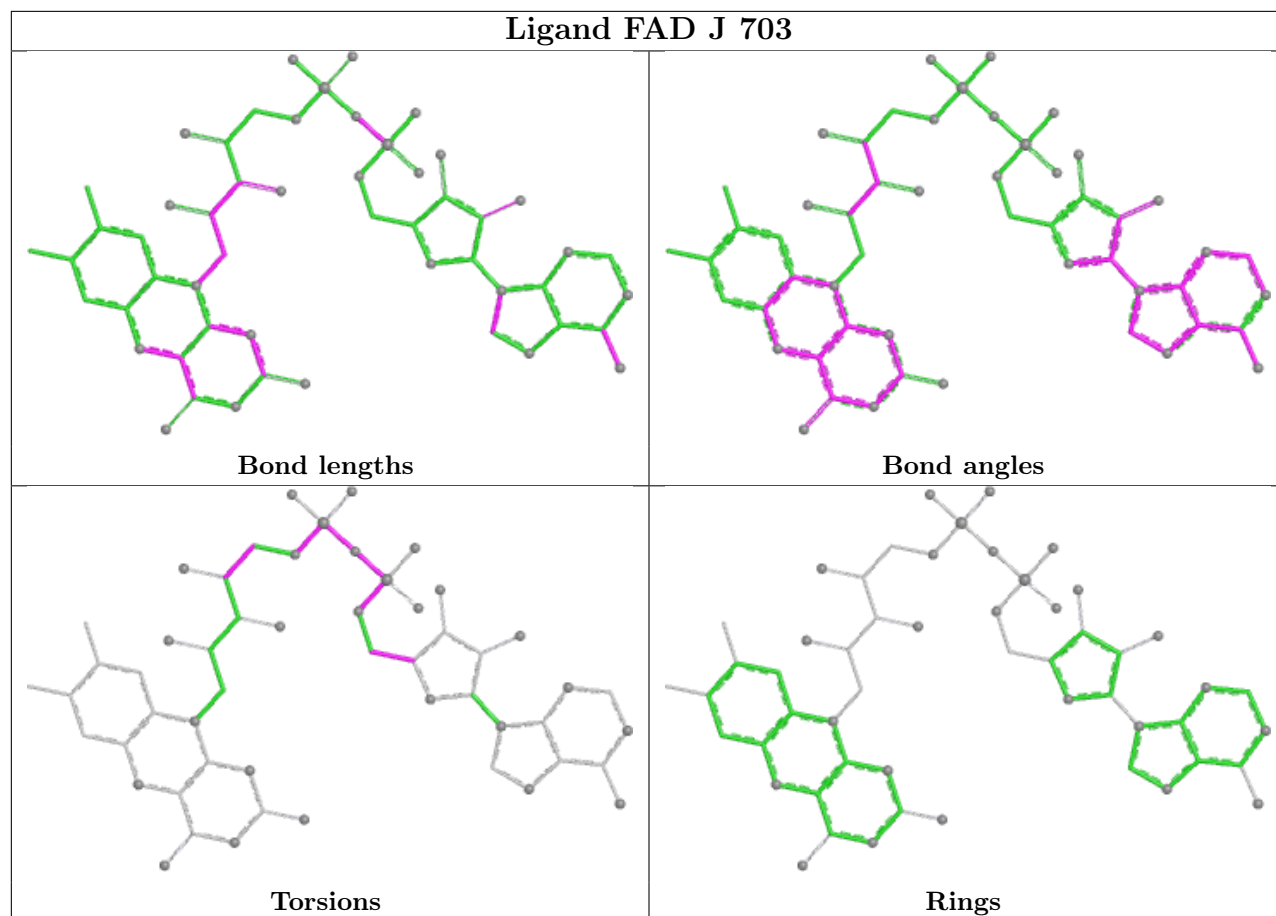
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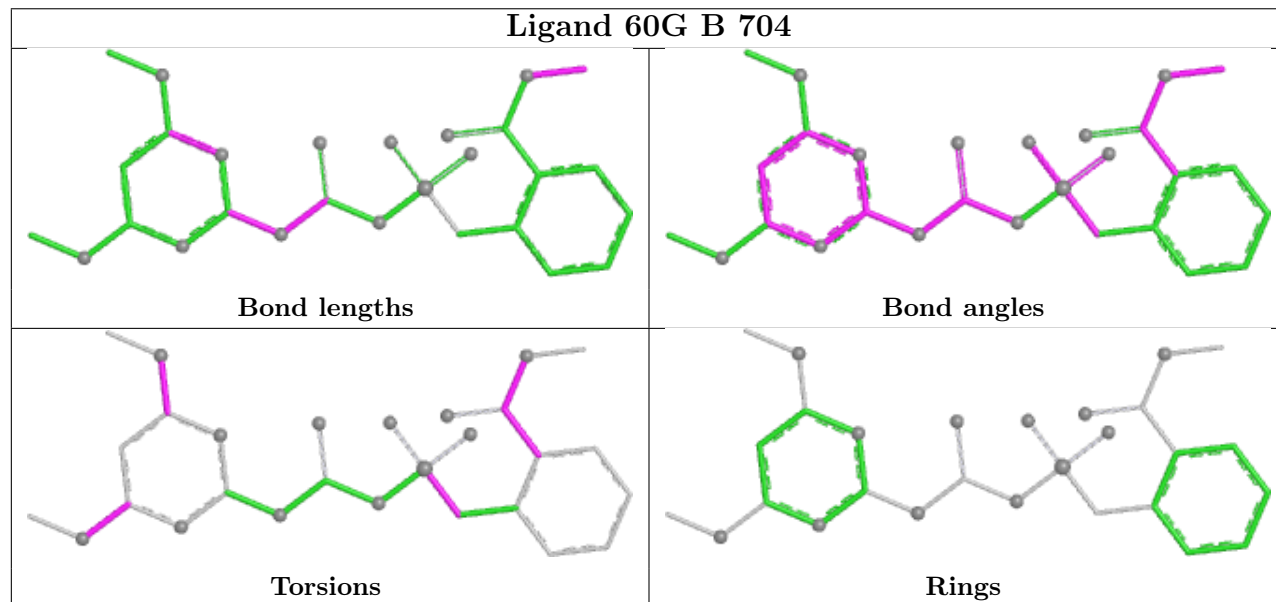


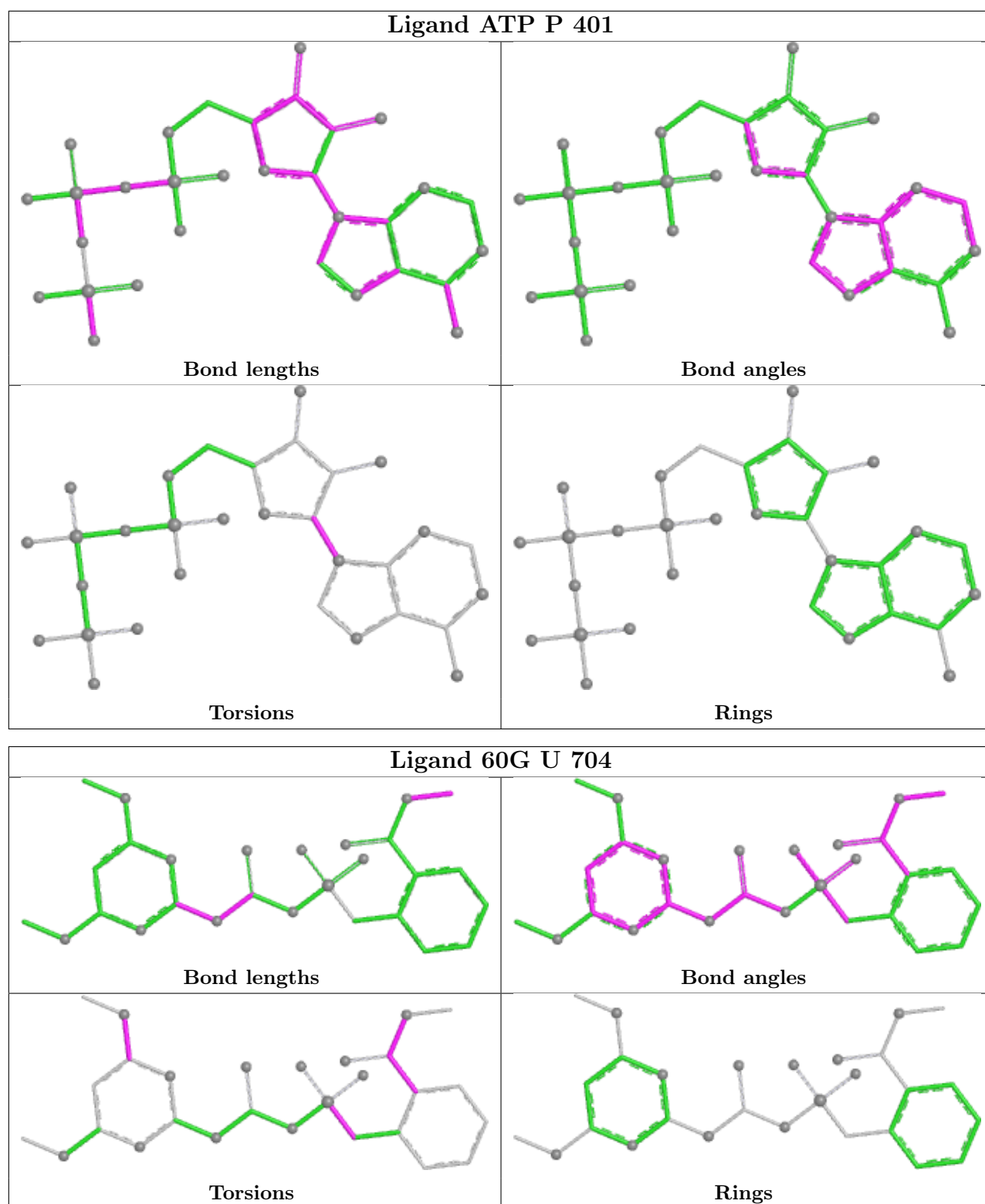


Ligand FAD J 703



Ligand 60G B 704





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	604/644 (93%)	-0.21	3 (0%) 87 76	25, 48, 86, 163	0
1	B	607/644 (94%)	-0.22	6 (0%) 79 63	26, 50, 90, 174	0
1	E	603/644 (93%)	0.11	6 (0%) 79 63	50, 74, 111, 191	0
1	F	604/644 (93%)	0.18	8 (1%) 75 55	50, 79, 121, 210	0
1	I	604/644 (93%)	0.36	13 (2%) 62 42	54, 93, 134, 205	0
1	J	602/644 (93%)	0.46	21 (3%) 47 29	56, 93, 135, 174	0
1	M	605/644 (93%)	-0.14	3 (0%) 87 76	29, 57, 101, 174	0
1	N	603/644 (93%)	0.16	4 (0%) 84 69	34, 73, 119, 197	0
1	Q	598/644 (92%)	0.40	22 (3%) 45 28	32, 82, 134, 168	0
1	R	416/644 (64%)	0.96	57 (13%) 6 5	46, 109, 161, 185	0
1	U	604/644 (93%)	-0.04	11 (1%) 67 48	27, 64, 105, 175	0
1	V	605/644 (93%)	-0.24	0 100 100	27, 50, 85, 149	0
2	C	253/297 (85%)	0.29	17 (6%) 24 15	36, 61, 164, 226	0
2	D	250/297 (84%)	0.22	13 (5%) 33 21	39, 60, 157, 222	0
2	G	253/297 (85%)	0.37	13 (5%) 33 21	48, 75, 151, 202	0
2	H	252/297 (84%)	0.30	7 (2%) 55 35	44, 76, 144, 187	0
2	K	245/297 (82%)	0.30	8 (3%) 49 30	48, 74, 150, 220	0
2	L	255/297 (85%)	0.27	8 (3%) 51 32	47, 72, 142, 183	0
2	O	237/297 (79%)	0.30	11 (4%) 37 23	40, 63, 154, 215	0
2	P	243/297 (81%)	0.12	6 (2%) 58 39	36, 61, 117, 156	0
2	S	244/297 (82%)	0.06	8 (3%) 49 30	34, 57, 133, 193	0
2	T	232/297 (78%)	0.20	7 (3%) 52 33	36, 61, 118, 159	0
2	W	245/297 (82%)	0.22	14 (5%) 29 19	31, 58, 140, 219	0
2	X	240/297 (80%)	-0.01	5 (2%) 63 43	29, 51, 114, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	10004/11292 (88%)	0.15	271 (2%) 56 36	25, 69, 131, 226	0

The worst 5 of 271 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	281	THR	5.3
1	J	685	GLY	4.9
1	R	402	GLY	4.8
1	R	559	GLU	4.7
2	C	281	THR	4.6

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	Q	702	1/1	0.76	0.12	137,137,137,137	0
6	60G	R	702	28/28	0.80	0.17	66,105,122,137	0
6	60G	I	704	28/28	0.84	0.16	53,75,91,104	0
5	FAD	R	701	53/53	0.84	0.14	79,105,131,145	0
3	TPP	Q	701	26/26	0.90	0.14	42,108,149,232	0
7	ATP	L	401	31/31	0.90	0.12	22,56,127,136	0
3	TPP	N	701	26/26	0.91	0.12	32,50,92,109	0
3	TPP	E	701	26/26	0.91	0.13	47,67,103,136	0
6	60G	J	704	28/28	0.91	0.12	51,75,90,104	0
3	TPP	I	701	26/26	0.91	0.13	46,91,106,154	0
4	MG	V	702	1/1	0.91	0.15	63,63,63,63	0
3	TPP	J	701	26/26	0.92	0.11	54,91,135,145	0
7	ATP	D	401	31/31	0.92	0.10	37,56,84,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	60G	E	704	28/28	0.92	0.12	60,70,88,99	0
7	ATP	W	401	31/31	0.92	0.10	10,42,76,83	0
3	TPP	U	701	26/26	0.93	0.13	26,64,105,143	0
5	FAD	I	703	53/53	0.93	0.11	32,74,100,132	0
6	60G	N	704	28/28	0.93	0.12	37,54,80,91	0
5	FAD	J	703	53/53	0.93	0.10	37,55,88,132	0
4	MG	E	702	1/1	0.93	0.06	77,77,77,77	0
7	ATP	H	401	31/31	0.93	0.10	8,58,82,105	0
7	ATP	K	401	31/31	0.93	0.09	36,65,75,82	0
3	TPP	F	701	26/26	0.93	0.12	36,68,92,132	0
7	ATP	S	401	31/31	0.93	0.09	25,51,71,75	0
6	60G	F	704	28/28	0.93	0.12	35,68,81,88	0
4	MG	W	403	1/1	0.94	0.15	29,29,29,29	0
7	ATP	G	401	31/31	0.94	0.09	27,55,82,116	0
5	FAD	E	703	53/53	0.94	0.09	39,60,85,134	0
5	FAD	F	703	53/53	0.94	0.09	43,69,84,102	0
6	60G	N	705	28/28	0.94	0.11	34,58,68,74	0
7	ATP	O	401	31/31	0.94	0.10	9,66,87,104	0
4	MG	F	702	1/1	0.94	0.07	50,50,50,50	0
6	60G	U	704	28/28	0.94	0.11	24,56,73,75	0
3	TPP	M	701	26/26	0.95	0.11	11,50,91,103	0
7	ATP	P	401	31/31	0.95	0.09	24,49,73,128	0
5	FAD	U	703	53/53	0.95	0.09	25,52,75,121	0
7	ATP	T	401	31/31	0.95	0.10	21,44,78,82	0
5	FAD	N	703	53/53	0.95	0.10	42,63,86,102	0
7	ATP	W	402	31/31	0.95	0.08	11,46,70,78	0
7	ATP	C	401	31/31	0.96	0.08	16,43,86,94	0
6	60G	B	704	28/28	0.96	0.09	11,40,62,69	0
5	FAD	B	703	53/53	0.96	0.08	10,42,56,61	0
5	FAD	M	703	53/53	0.96	0.08	25,41,59,63	0
3	TPP	B	701	26/26	0.96	0.09	15,41,63,74	0
5	FAD	Q	703	53/53	0.96	0.08	17,44,71,74	0
3	TPP	V	701	26/26	0.96	0.09	9,50,69,119	0
4	MG	H	402	1/1	0.96	0.10	53,53,53,53	0
6	60G	Q	704	28/28	0.96	0.11	45,63,75,82	0
5	FAD	V	703	53/53	0.96	0.08	22,37,50,57	0
6	60G	A	704	28/28	0.96	0.10	18,45,64,79	0
6	60G	V	704	28/28	0.96	0.10	17,48,64,82	0
5	FAD	A	703	53/53	0.97	0.07	19,37,51,65	0
4	MG	C	402	1/1	0.97	0.09	61,61,61,61	0
3	TPP	A	701	26/26	0.97	0.08	13,41,66,77	0
4	MG	N	702	1/1	0.97	0.04	84,84,84,84	0

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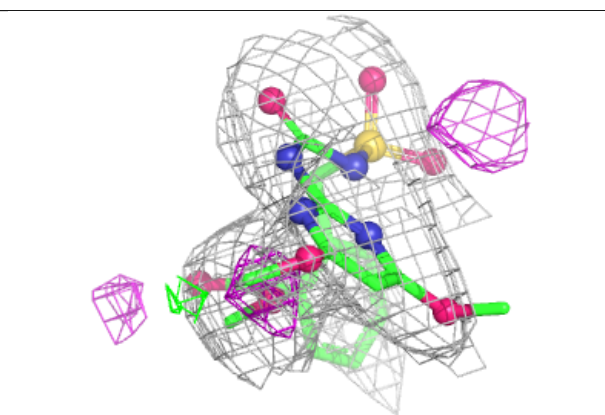
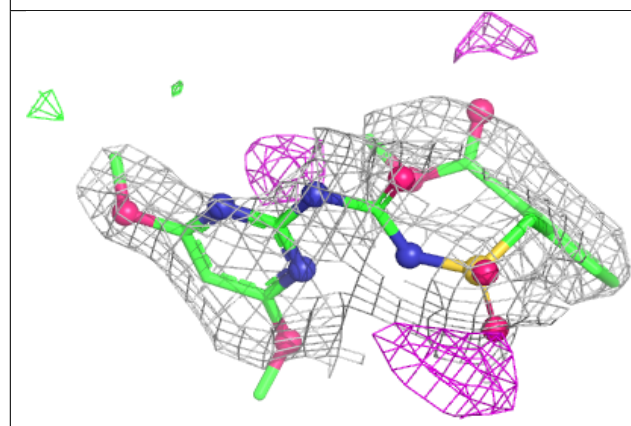
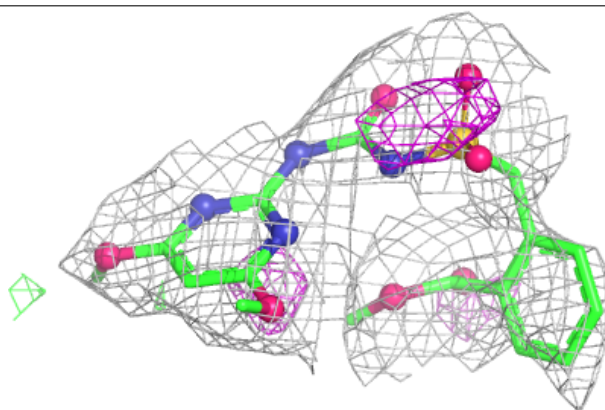
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	J	702	1/1	0.98	0.04	99,99,99,99	0
4	MG	L	402	1/1	0.98	0.07	74,74,74,74	0
4	MG	B	702	1/1	0.98	0.10	30,30,30,30	0
4	MG	A	702	1/1	0.98	0.06	19,19,19,19	0
4	MG	D	402	1/1	0.98	0.06	40,40,40,40	0
4	MG	I	702	1/1	0.98	0.04	49,49,49,49	0
4	MG	M	702	1/1	0.99	0.04	27,27,27,27	0
4	MG	U	702	1/1	0.99	0.02	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

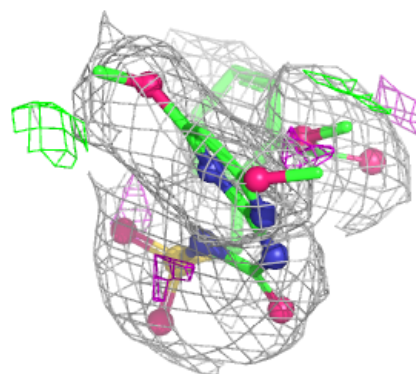
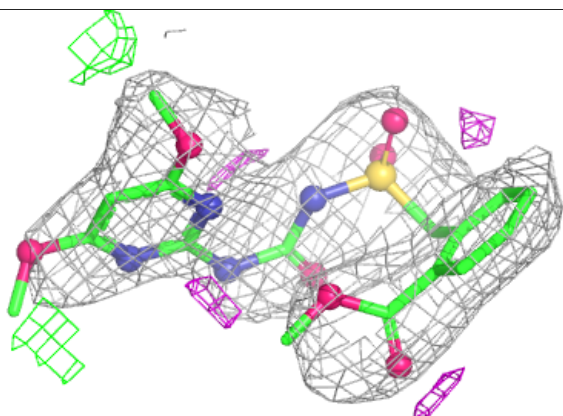
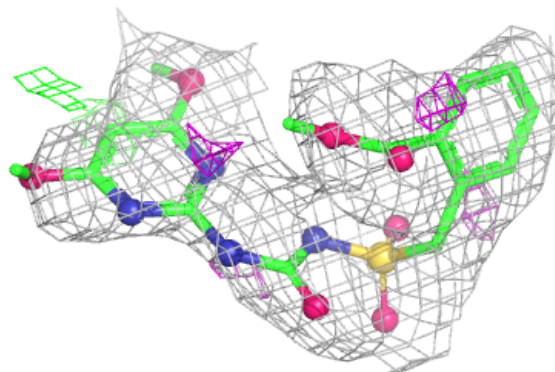
Electron density around 60G R 702:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

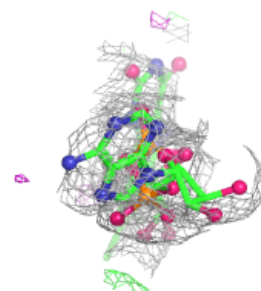
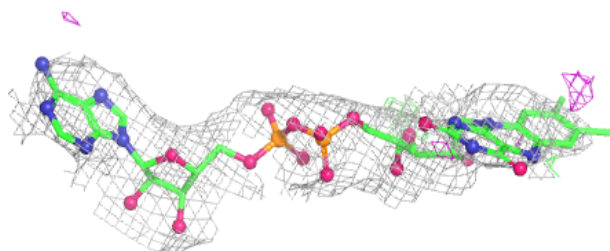
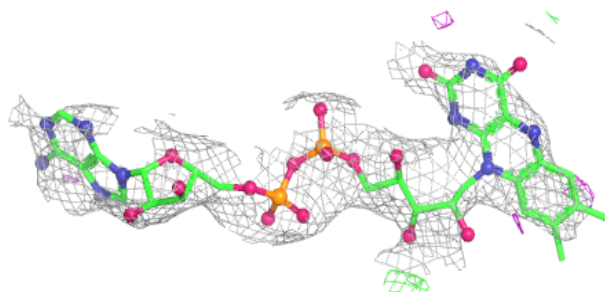


Electron density around 60G I 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

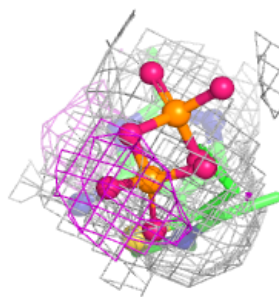
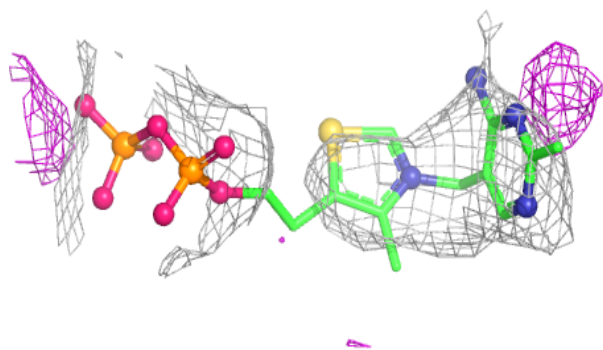
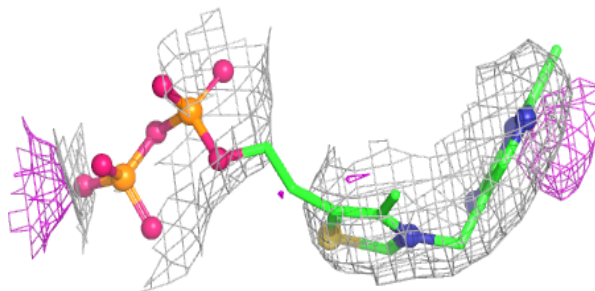
**Electron density around FAD R 701:**

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and green (positive)



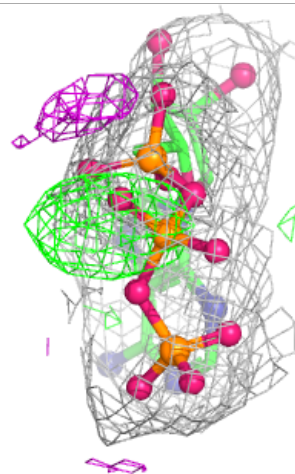
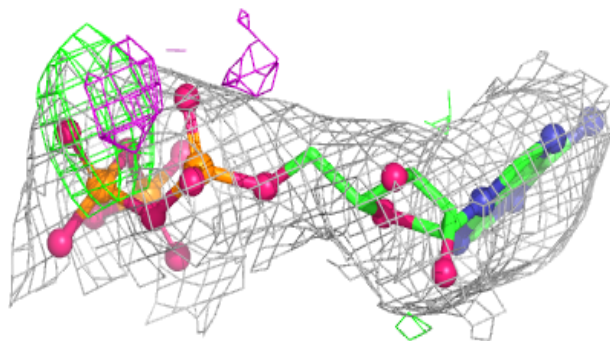
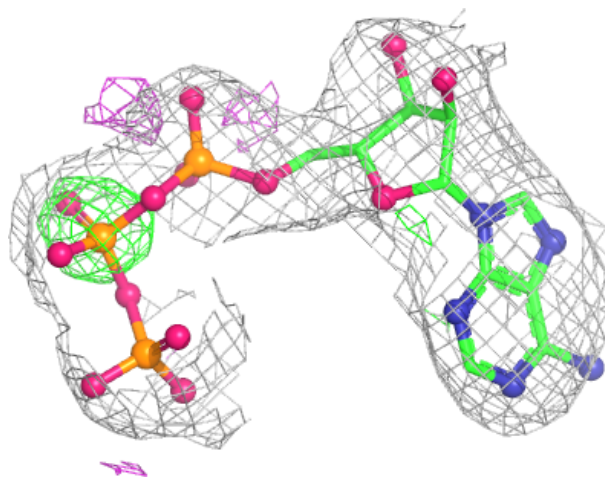
Electron density around TPP Q 701:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



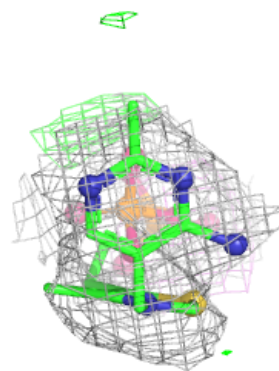
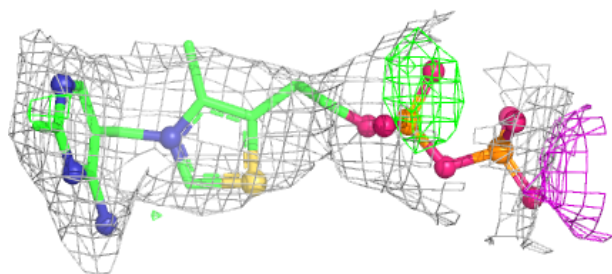
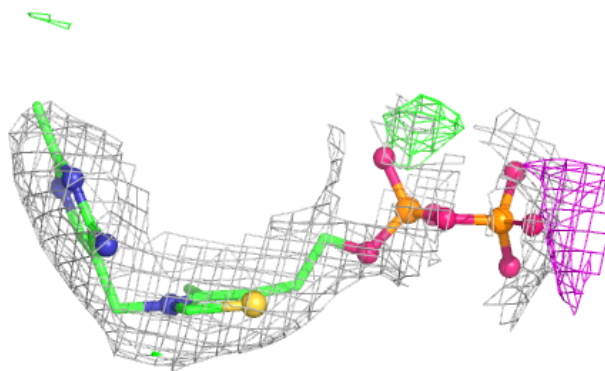
Electron density around ATP L 401:

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and green (positive)

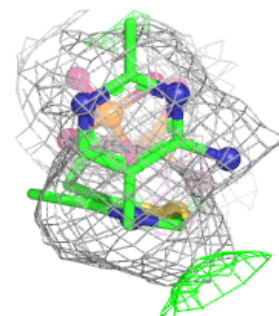
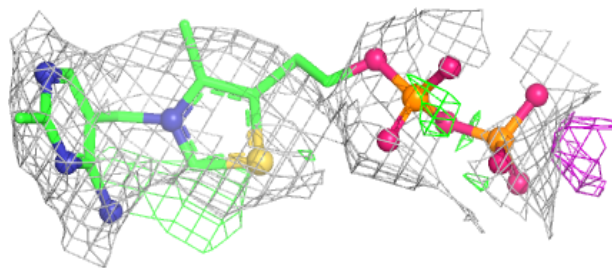
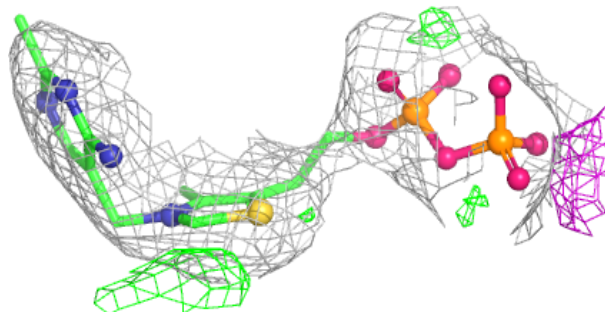


Electron density around TPP N 701:

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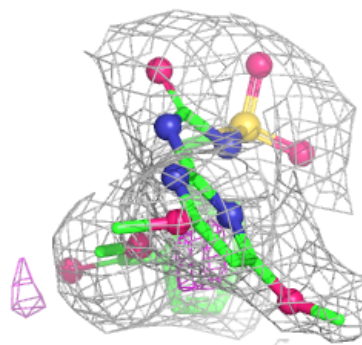
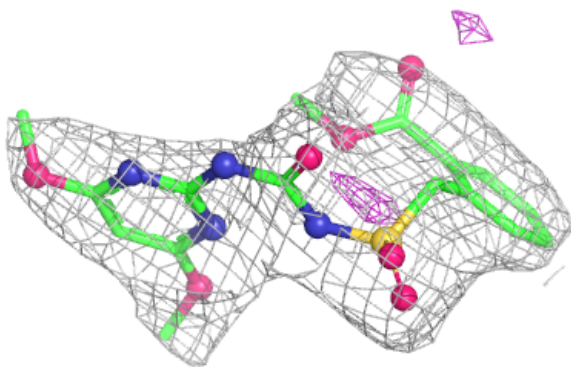
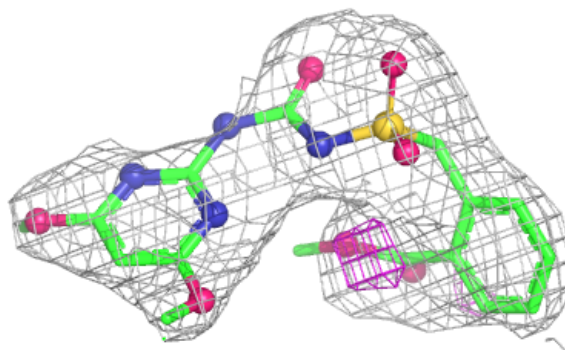
**Electron density around TPP E 701:**

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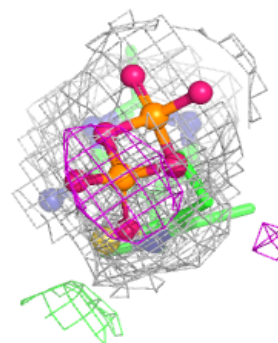
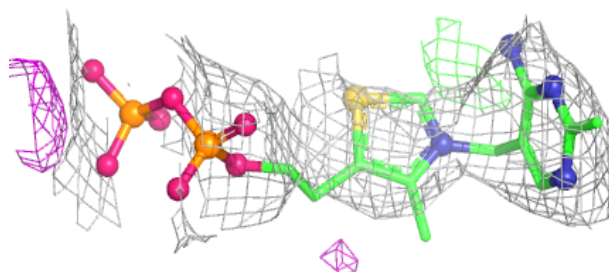
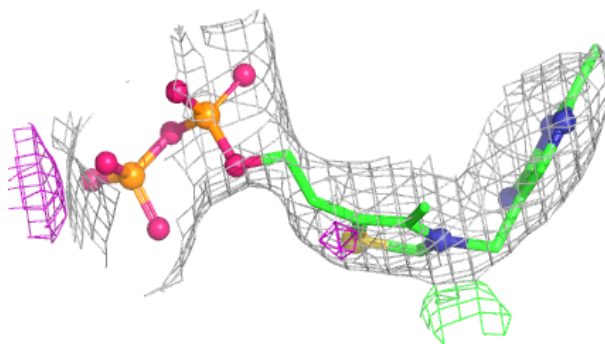


Electron density around 60G J 704:

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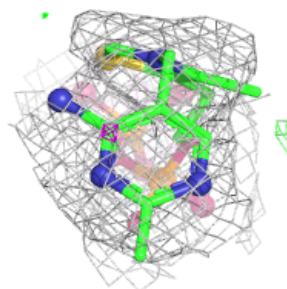
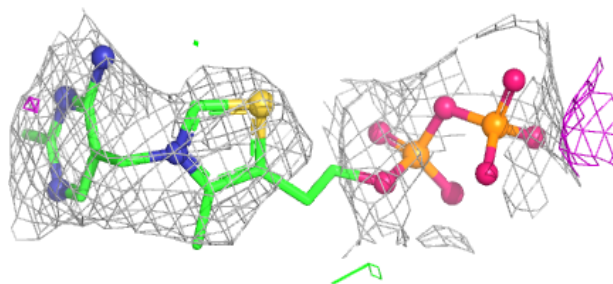
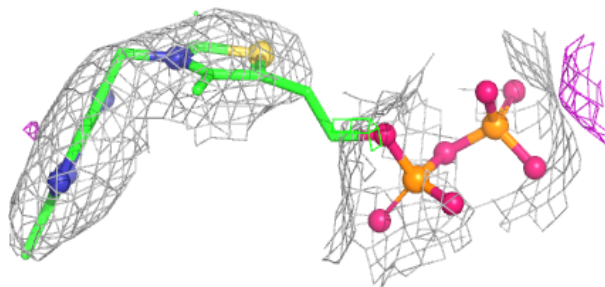
**Electron density around TPP I 701:**

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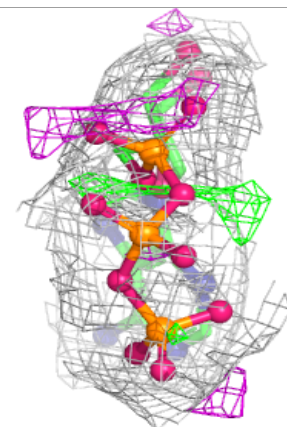
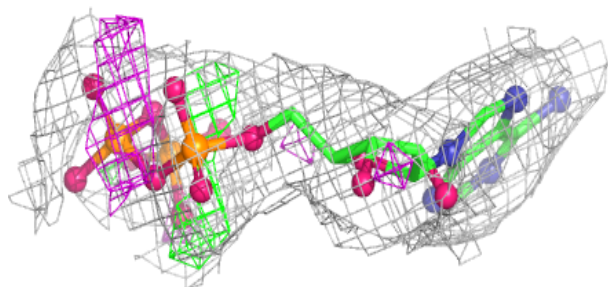
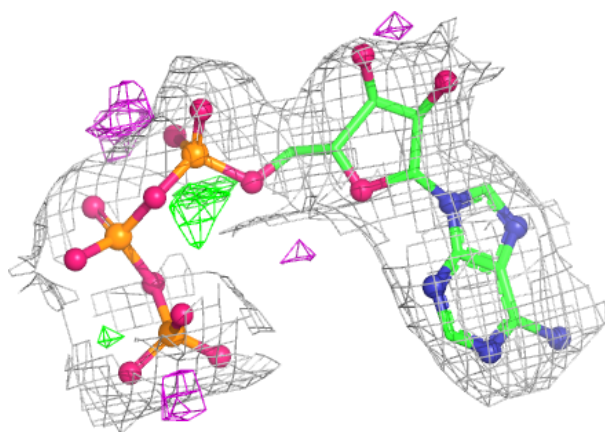


Electron density around TPP J 701:

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and green (positive)

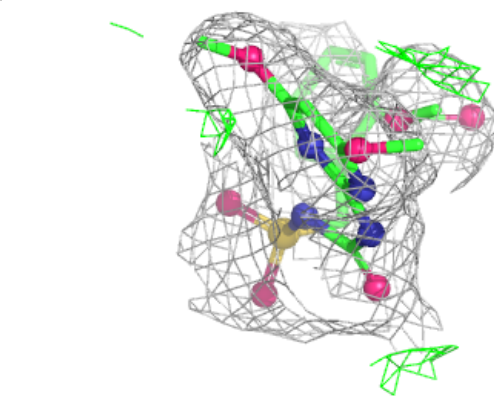
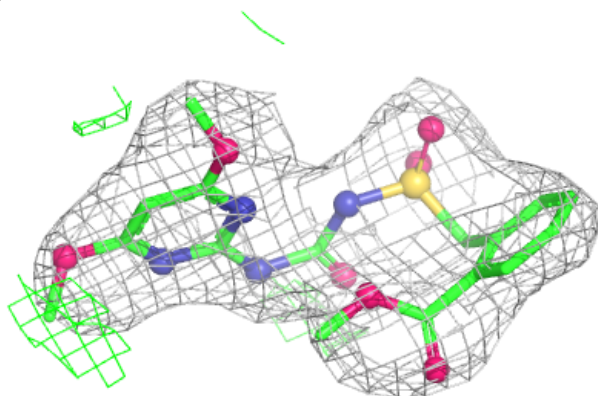
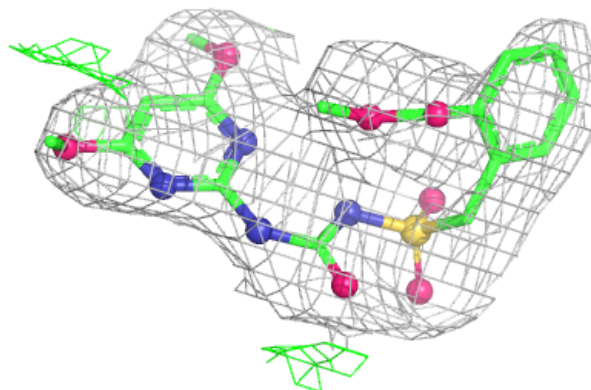
**Electron density around ATP D 401:**

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and green (positive)

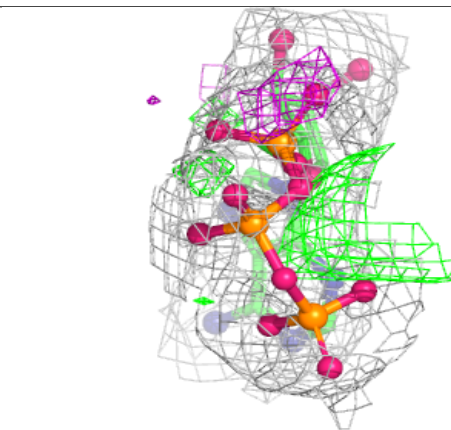
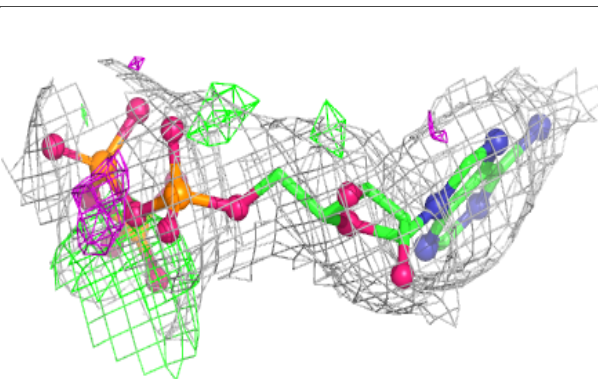
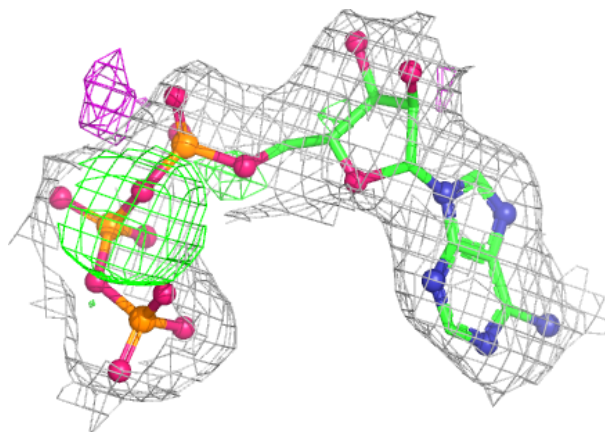


Electron density around 60G E 704:

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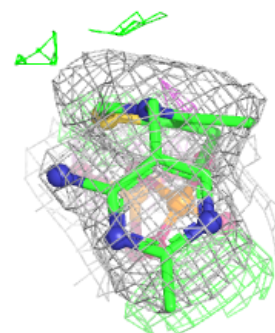
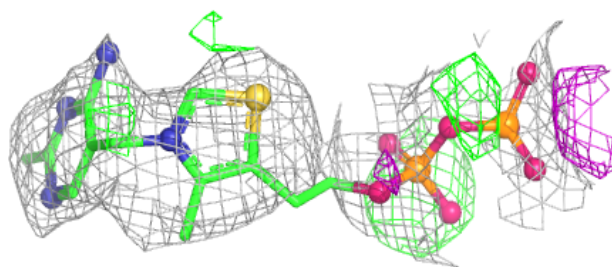
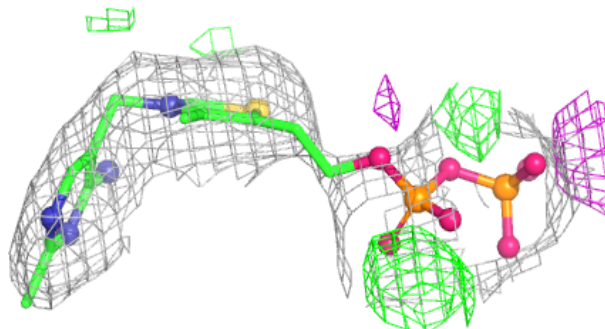
**Electron density around ATP W 401:**

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and green (positive)

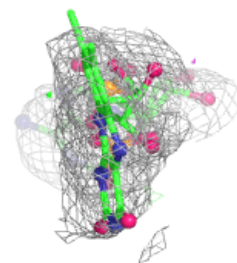
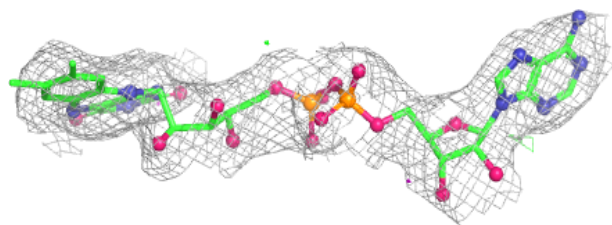
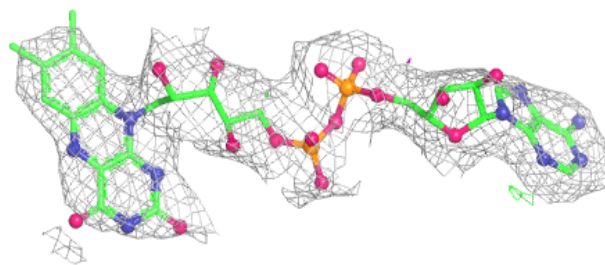


Electron density around TPP U 701:

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and green (positive)

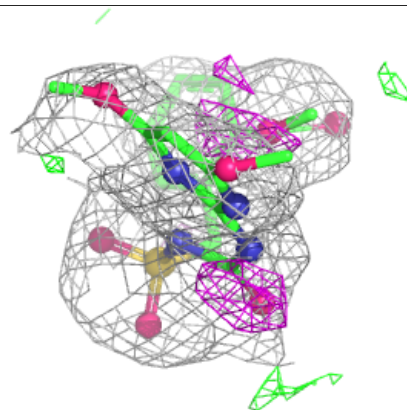
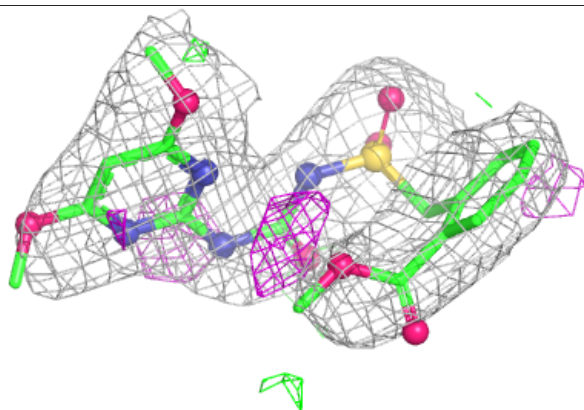
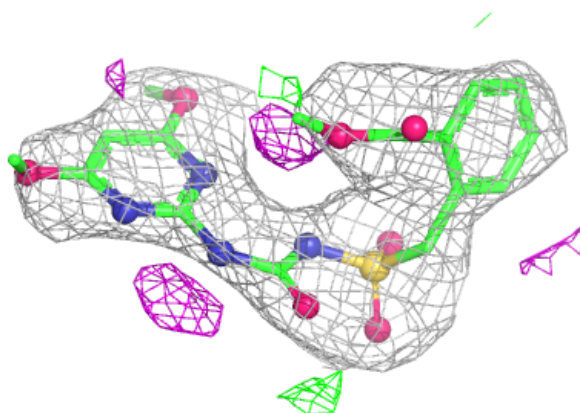
**Electron density around FAD I 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

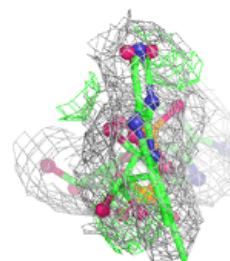
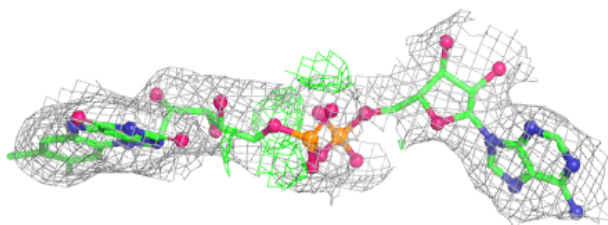
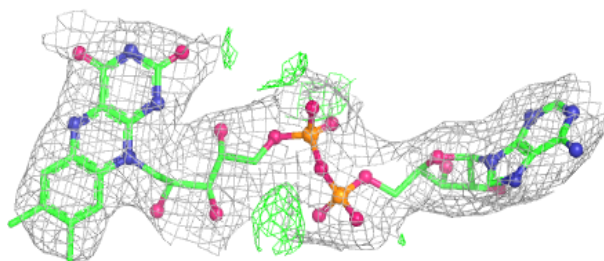


Electron density around 60G N 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

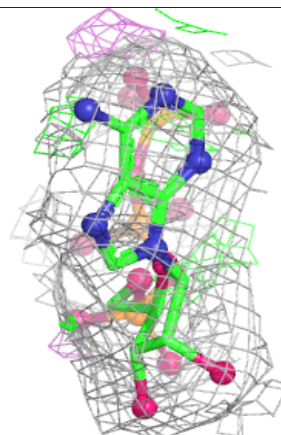
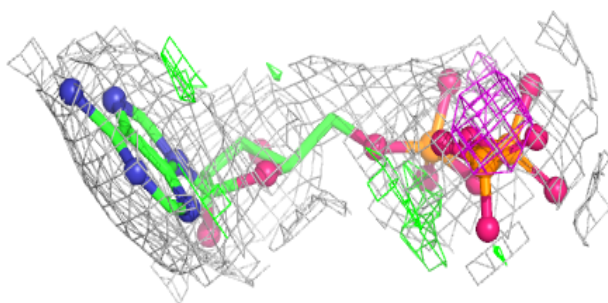
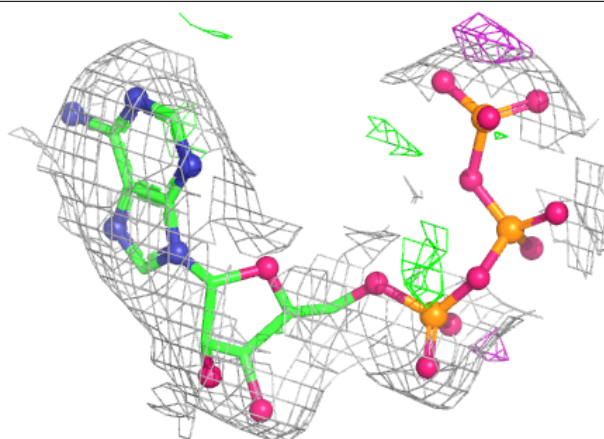
**Electron density around FAD J 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



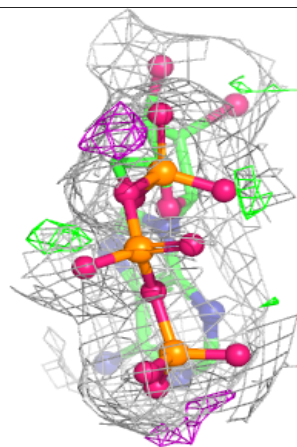
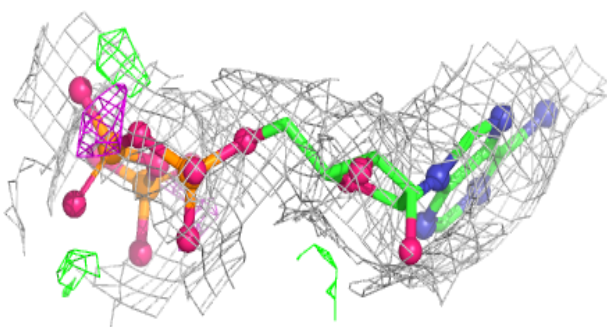
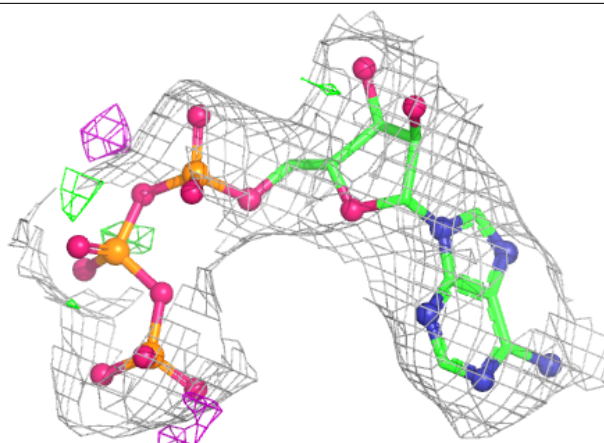
Electron density around ATP H 401:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

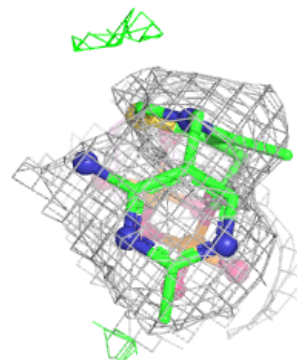
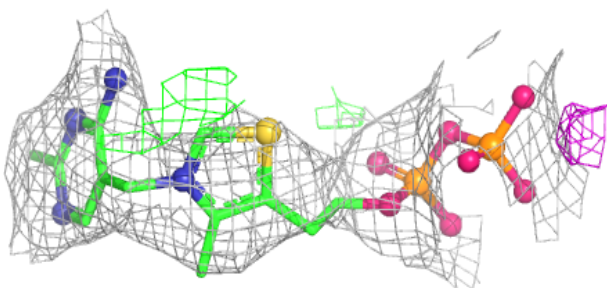
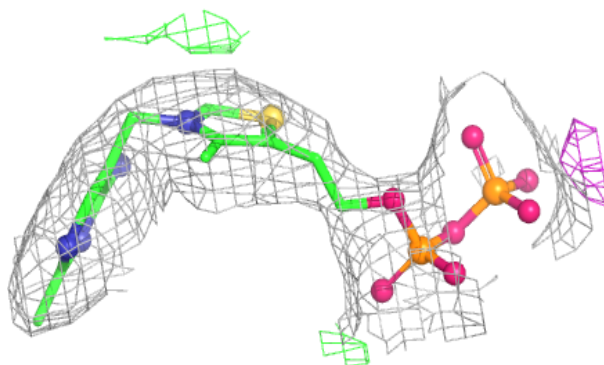


Electron density around ATP K 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

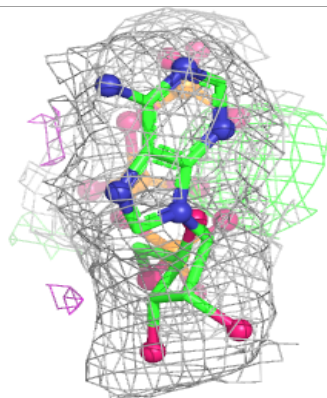
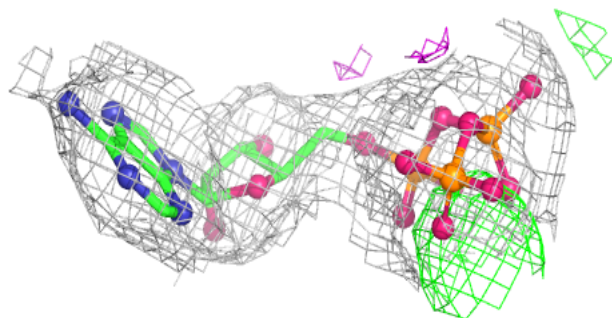
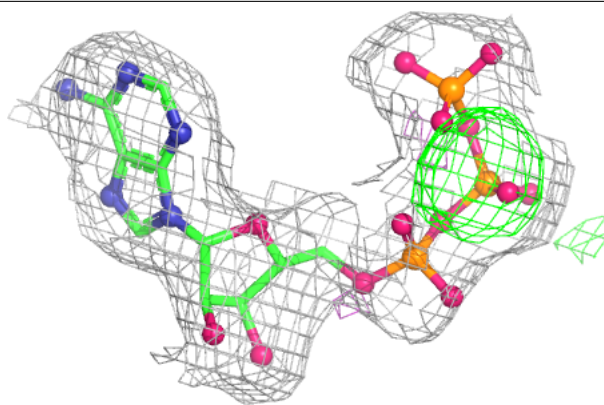
**Electron density around TPP F 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

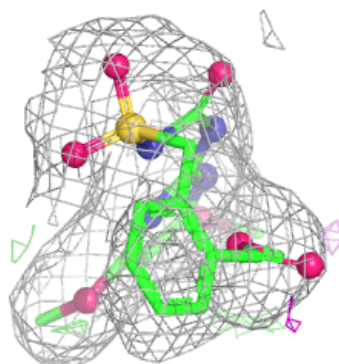
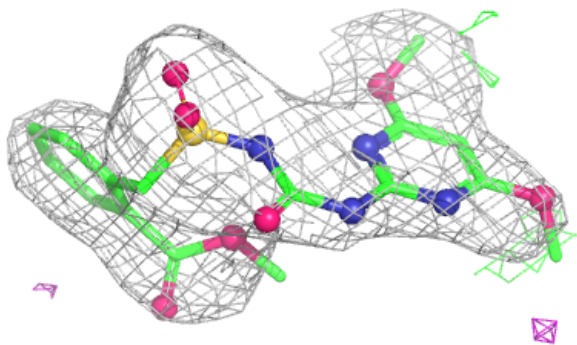
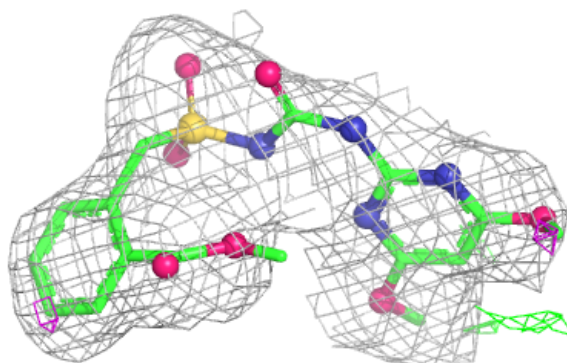


Electron density around ATP S 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

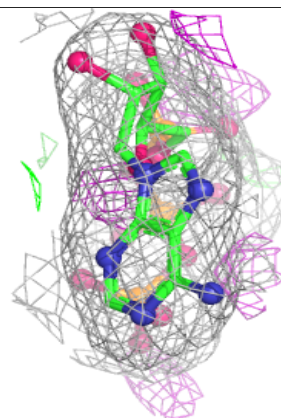
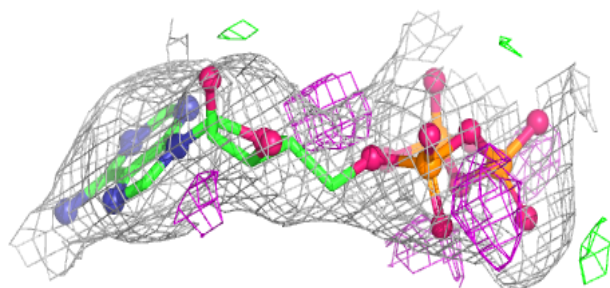
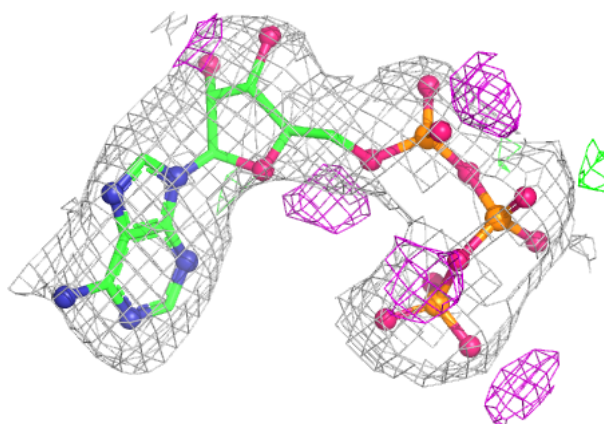
**Electron density around 60G F 704:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

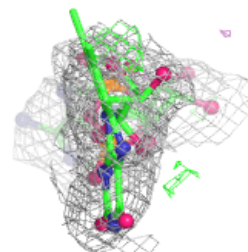
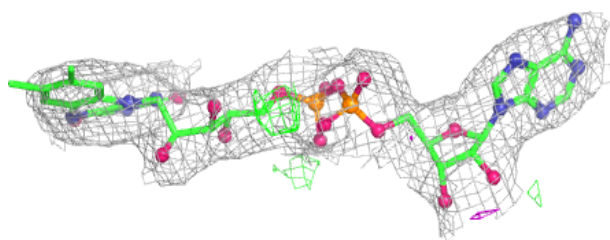


Electron density around ATP G 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

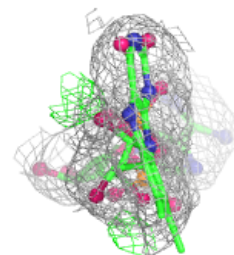
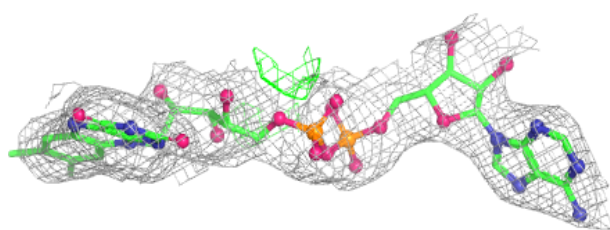
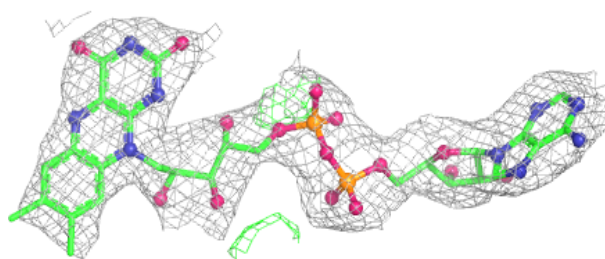
**Electron density around FAD E 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

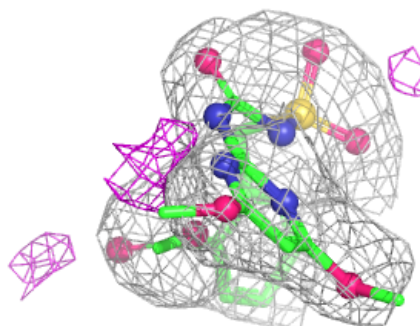
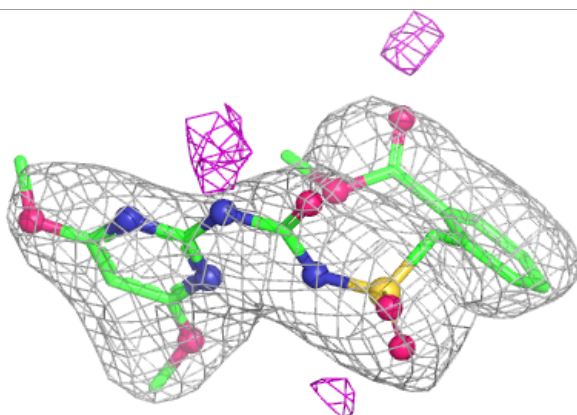
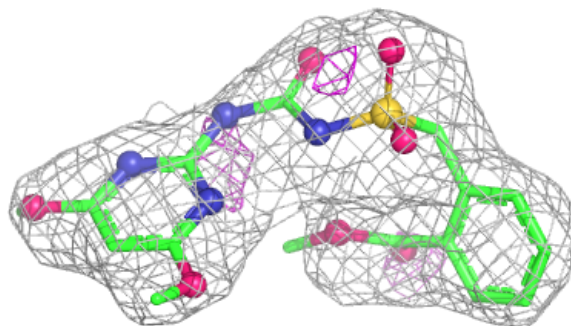


Electron density around FAD F 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

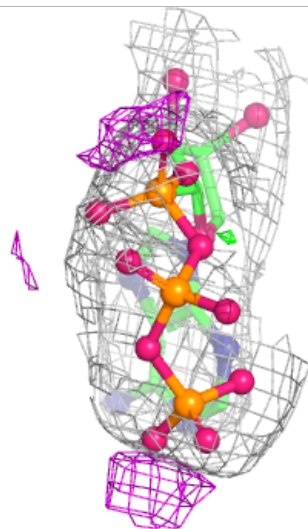
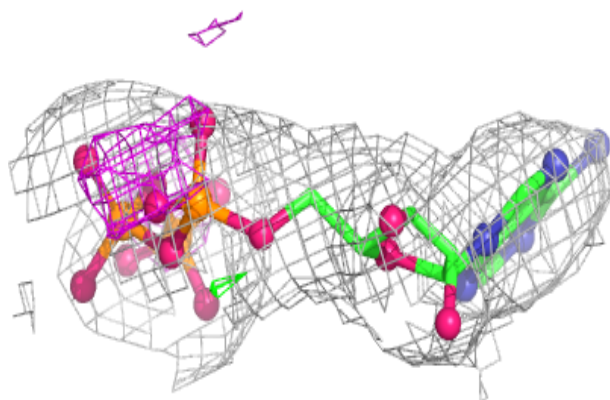
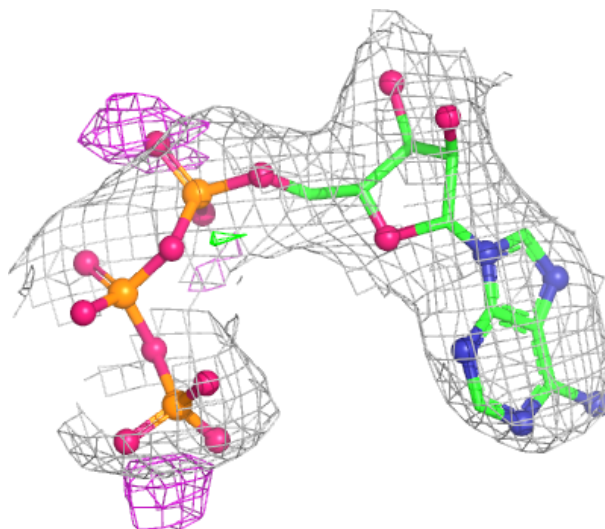
**Electron density around 60G N 705:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



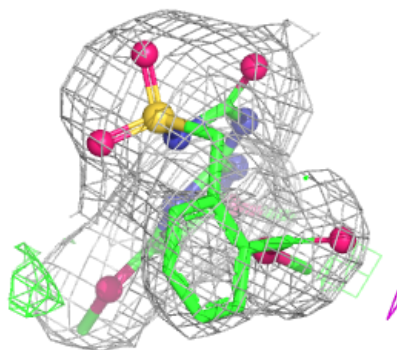
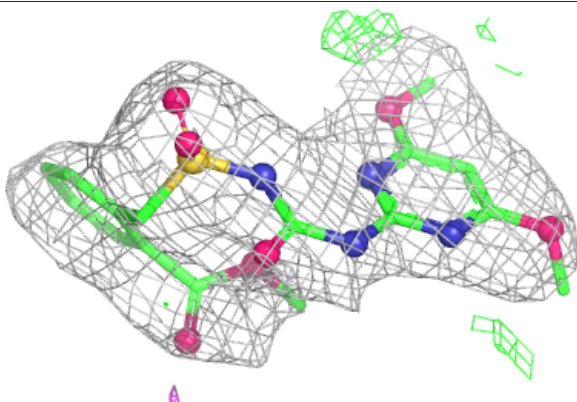
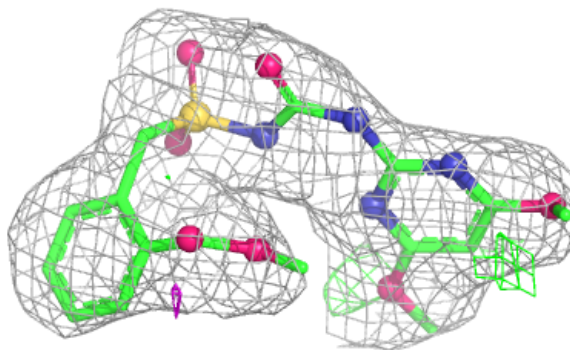
Electron density around ATP O 401:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

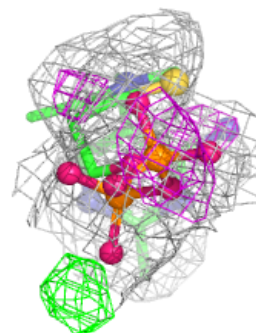
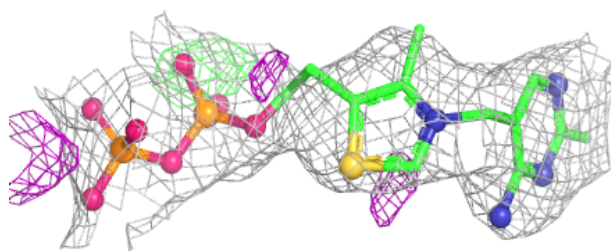
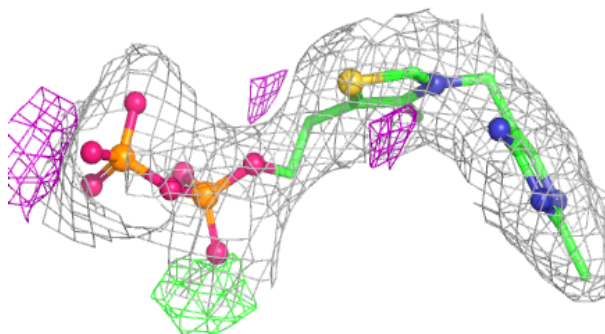


Electron density around 60G U 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

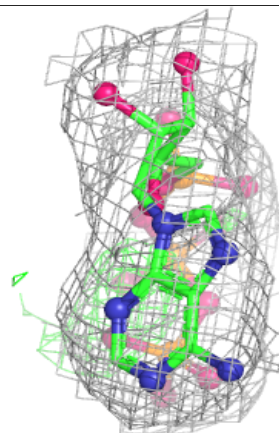
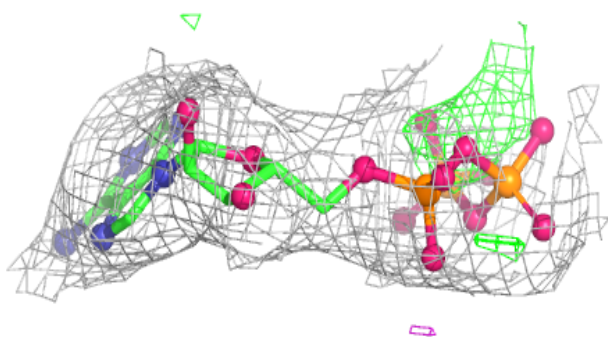
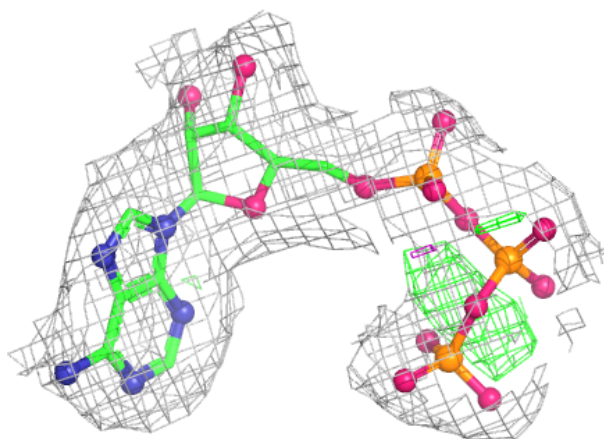
**Electron density around TPP M 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

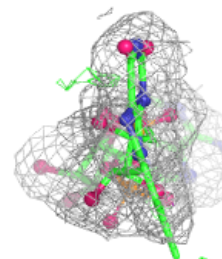
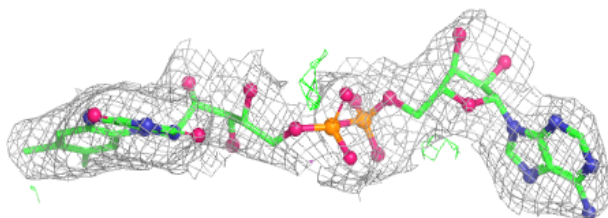
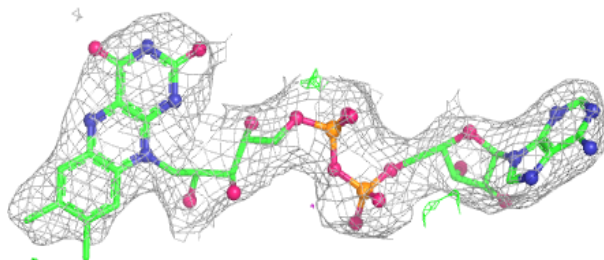


Electron density around ATP P 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

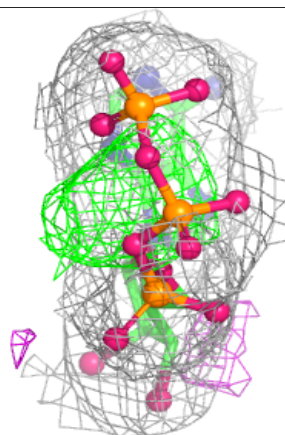
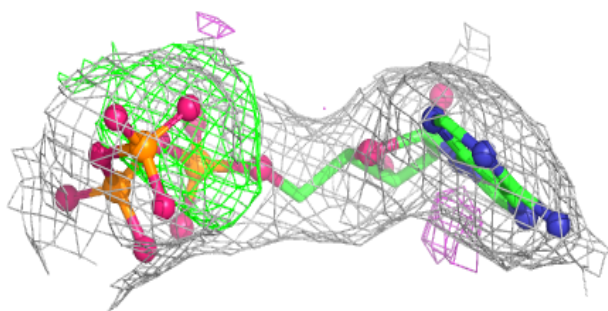
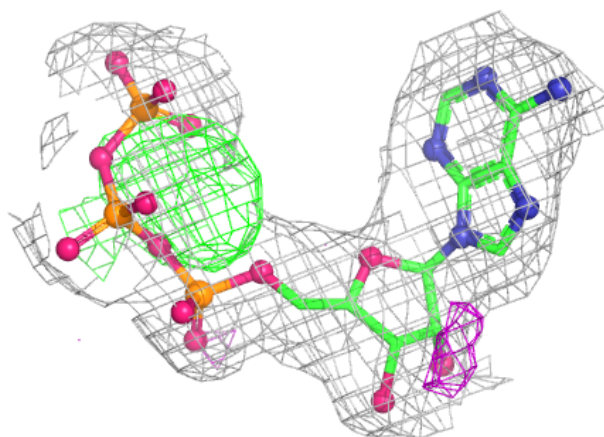
**Electron density around FAD U 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

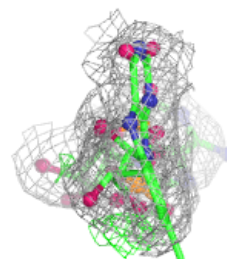
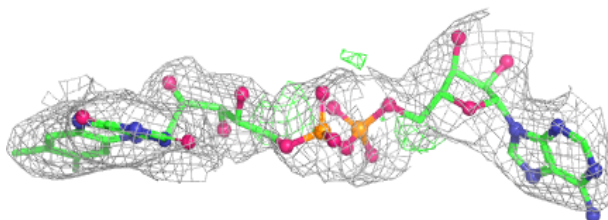
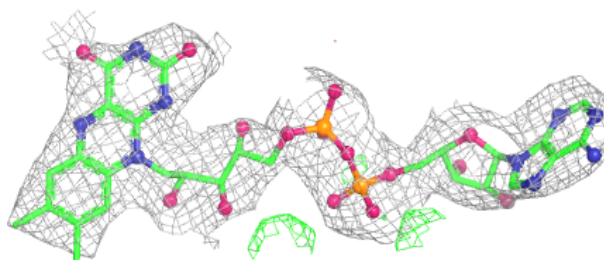


Electron density around ATP T 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

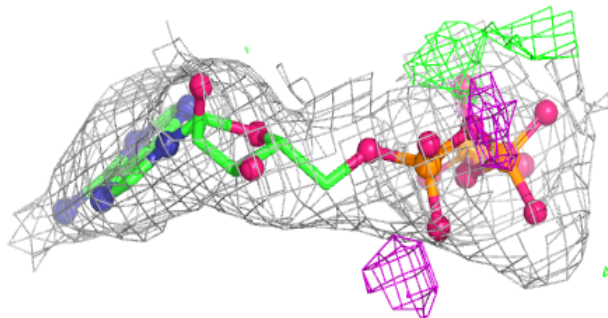
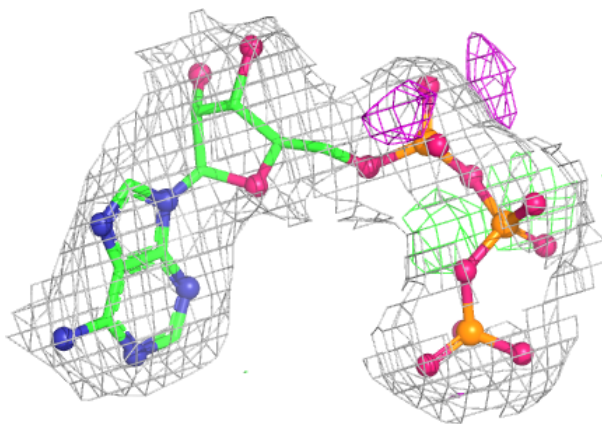
**Electron density around FAD N 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



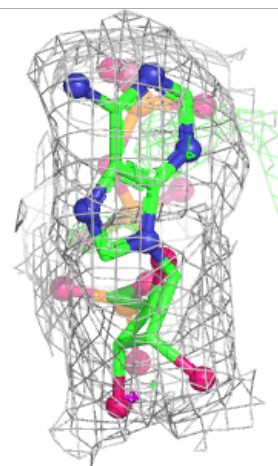
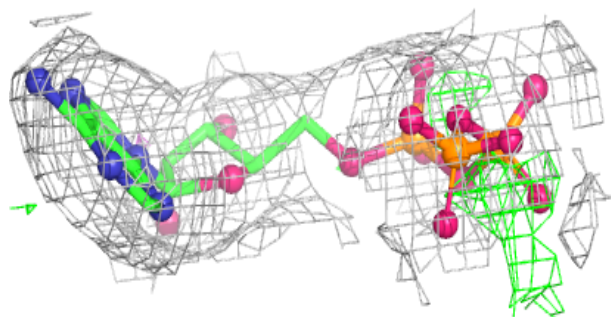
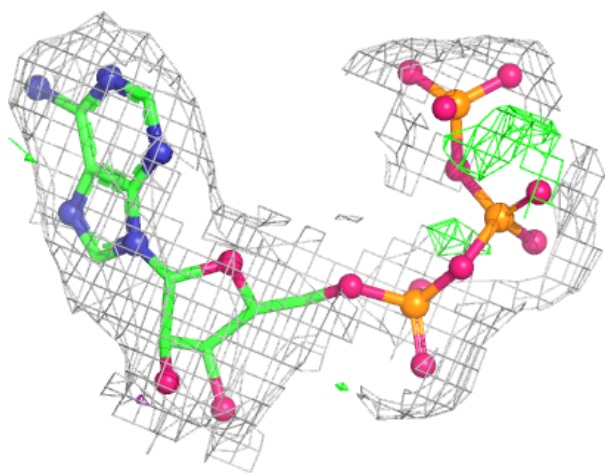
Electron density around ATP W 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



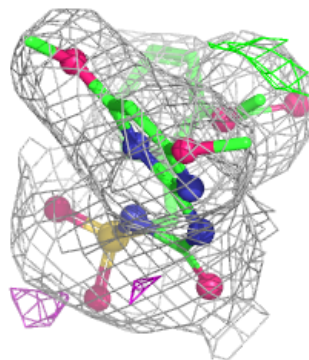
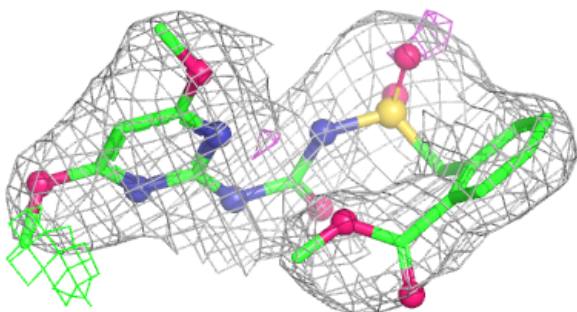
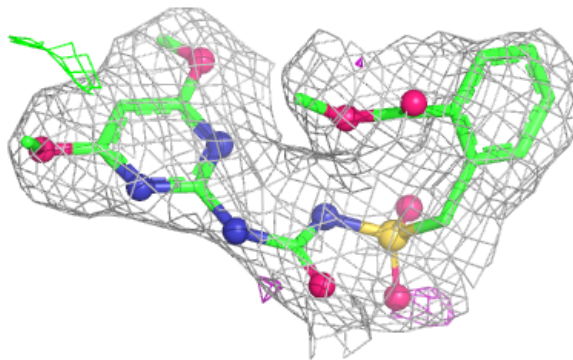
Electron density around ATP C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

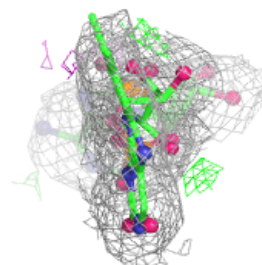
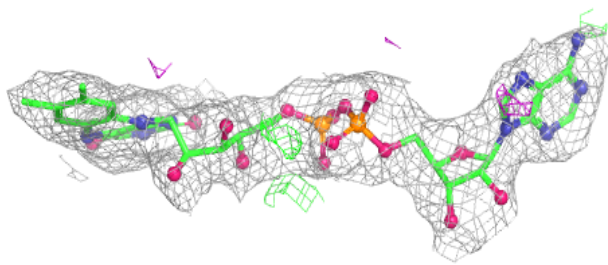
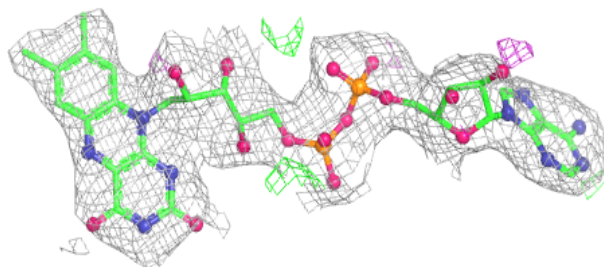


Electron density around 60G B 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

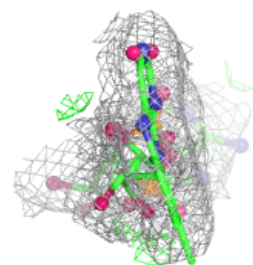
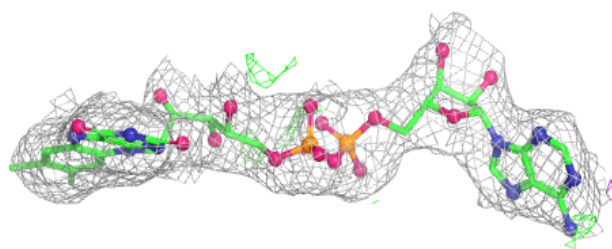
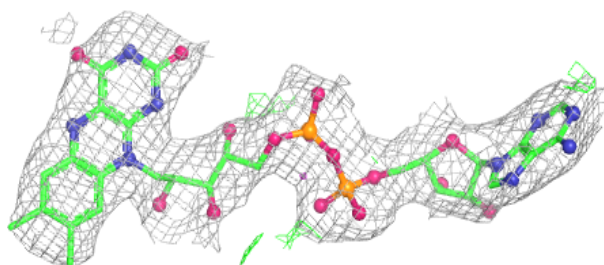
**Electron density around FAD B 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

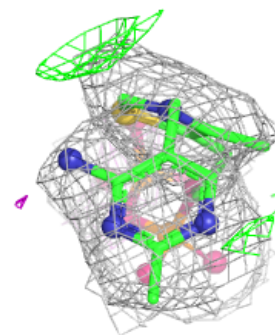
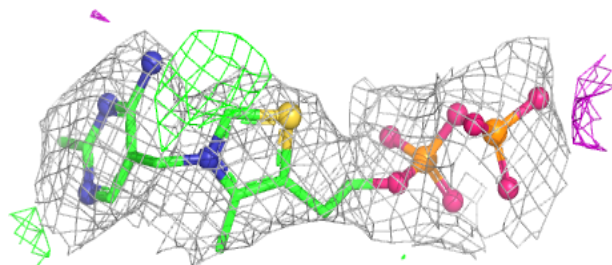
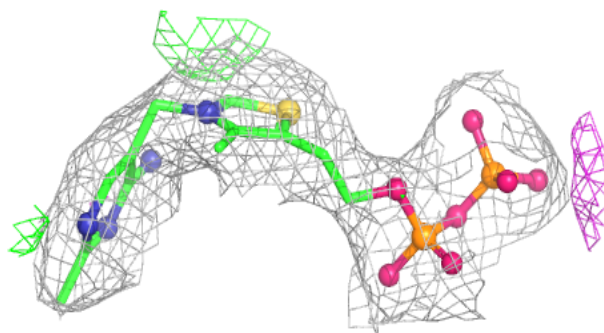


Electron density around FAD M 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

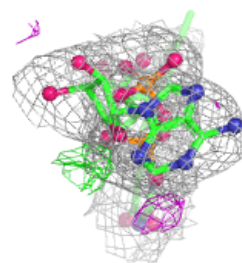
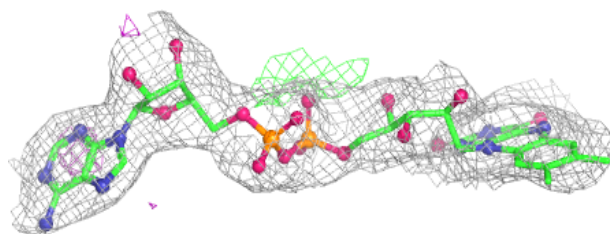
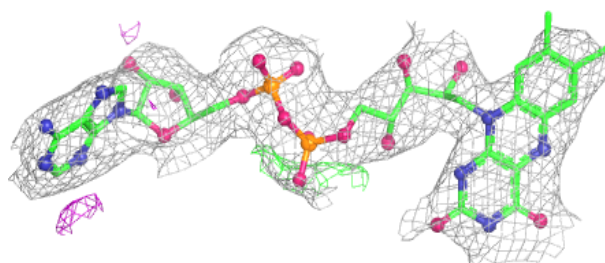
**Electron density around TPP B 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

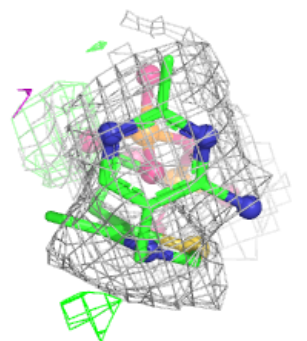
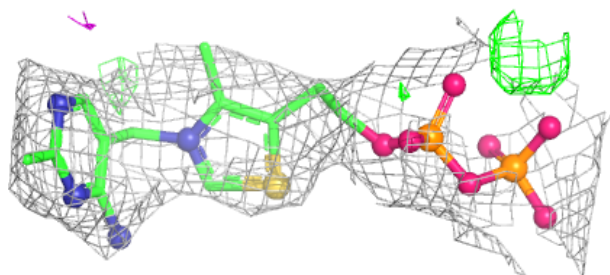
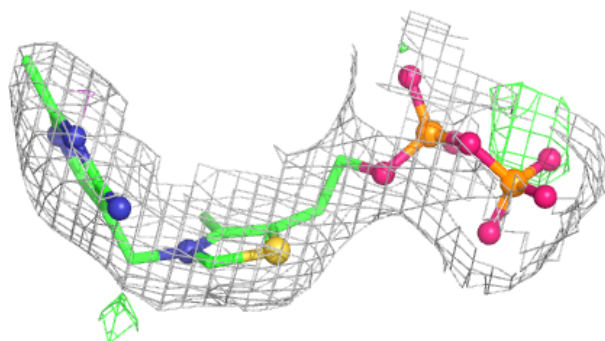


Electron density around FAD Q 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

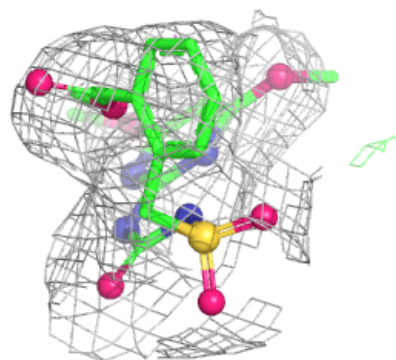
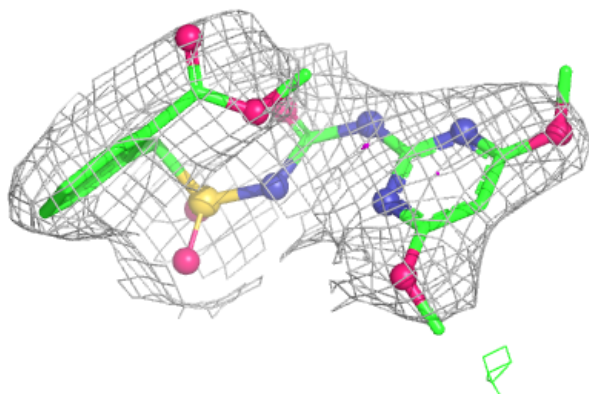
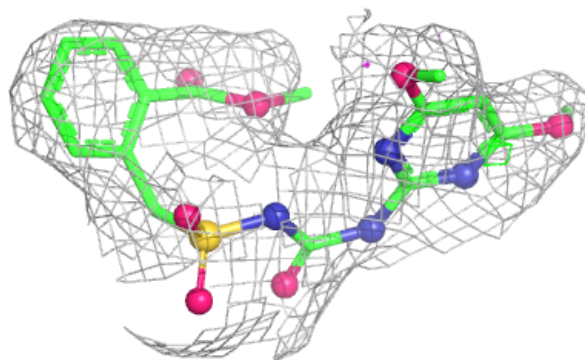
**Electron density around TPP V 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

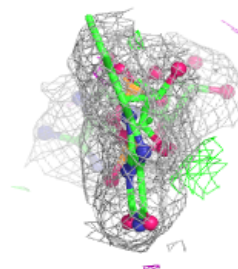
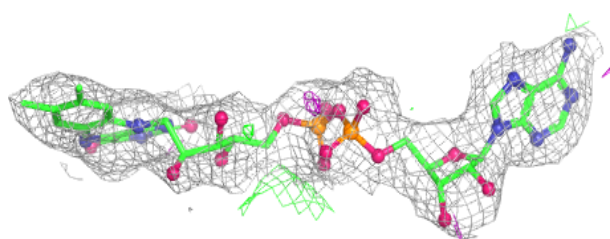
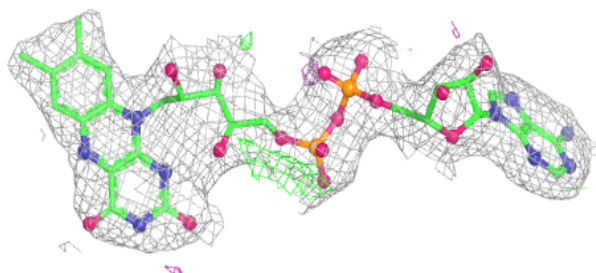


Electron density around 60G Q 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

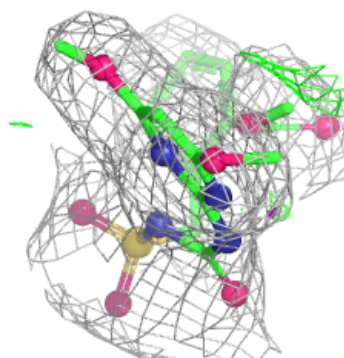
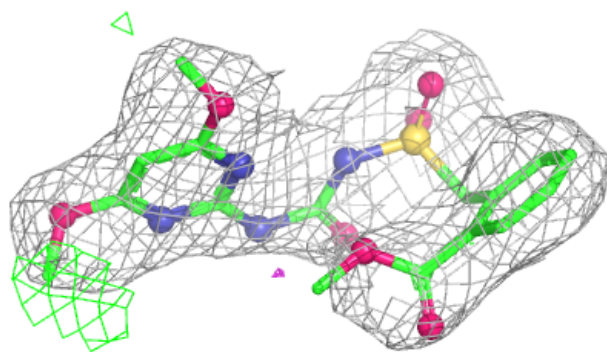
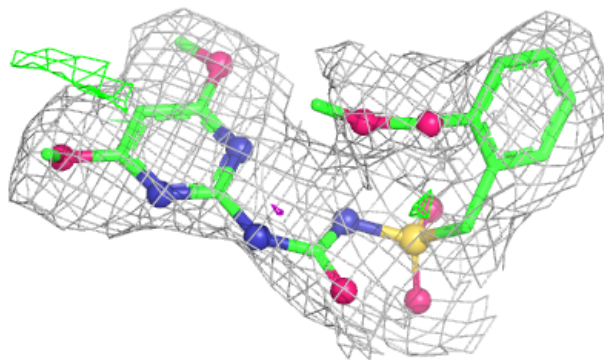
**Electron density around FAD V 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

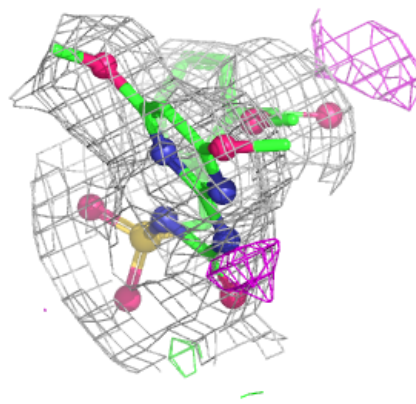
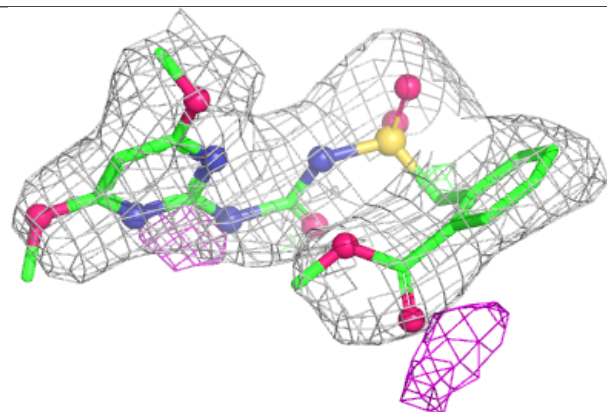
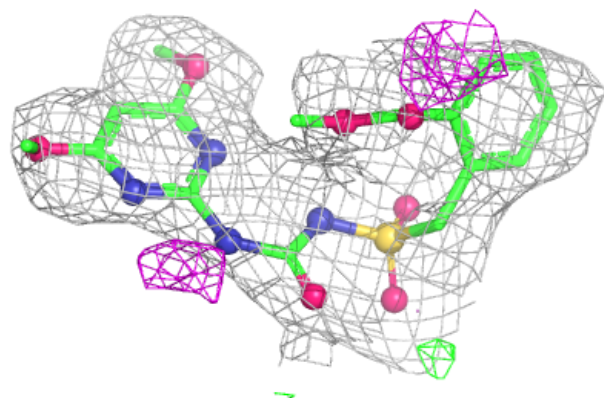


Electron density around 60G A 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

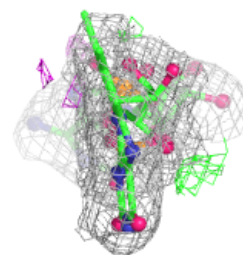
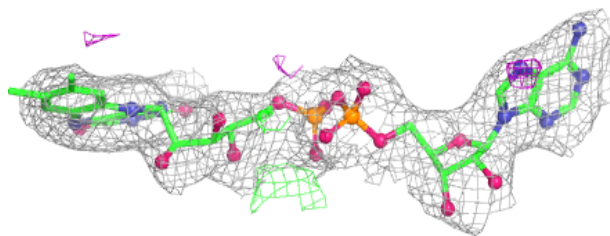
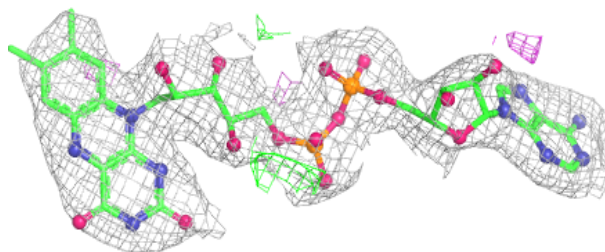
**Electron density around 60G V 704:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

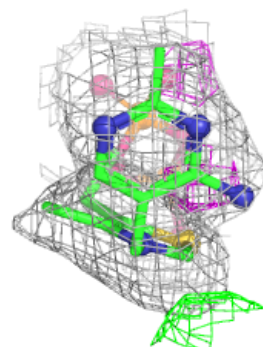
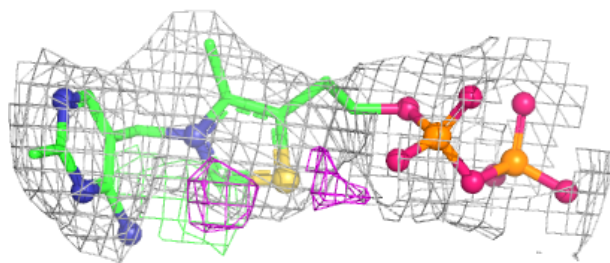
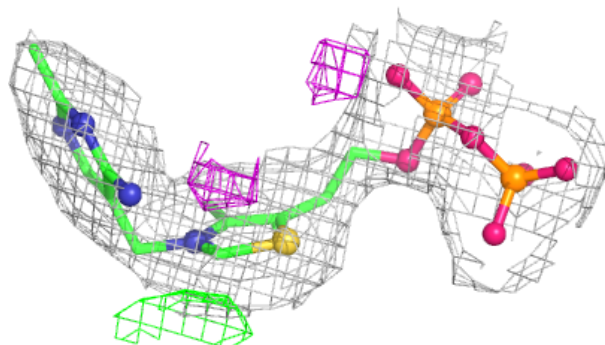


Electron density around FAD A 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TPP A 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.