



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2020 – 12:33 PM EDT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

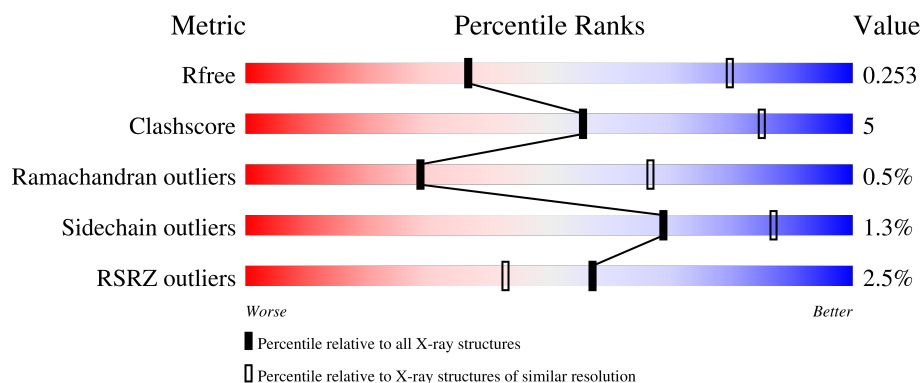
1 Overall quality at a glance

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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	 2% 80% 13% 7%
1	M	644	 1% 81% 13% 6%
1	N	644	 1% 79% 14% 6%
1	Q	644	 2% 82% 10% 7%
1	R	644	 8% 58% 6% 35%
1	U	644	 1% 80% 13% 6%
1	V	644	 80% 14% 6%
2	C	297	 5% 74% 10% 15%
2	D	297	 7% 69% 14% 16%
2	G	297	 3% 76% 9% 15%
2	H	297	 5% 69% 15% 15%
2	K	297	 3% 70% 11% 18%
2	L	297	 3% 76% 9% 14%
2	O	297	 4% 67% 13% 20%
2	P	297	 2% 72% 9% 18%
2	S	297	 2% 72% 9% 18%
2	T	297	 67% 10% 22%
2	W	297	 3% 71% 12% 18%
2	X	297	 1% 65% 14% 19%

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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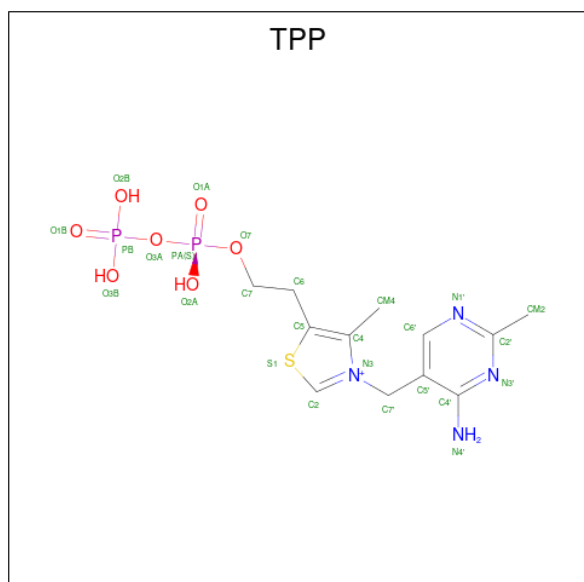
Chain	Residue	Modelled	Actual	Comment	Reference
T	30	GLY	-	expression tag	UNP B3LU66
T	31	SER	-	expression tag	UNP B3LU66
T	32	HIS	-	expression tag	UNP B3LU66
T	33	MET	-	expression tag	UNP B3LU66
T	34	GLU	-	expression tag	UNP B3LU66
T	35	ASN	-	expression tag	UNP B3LU66
T	36	LEU	-	expression tag	UNP B3LU66
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 (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

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

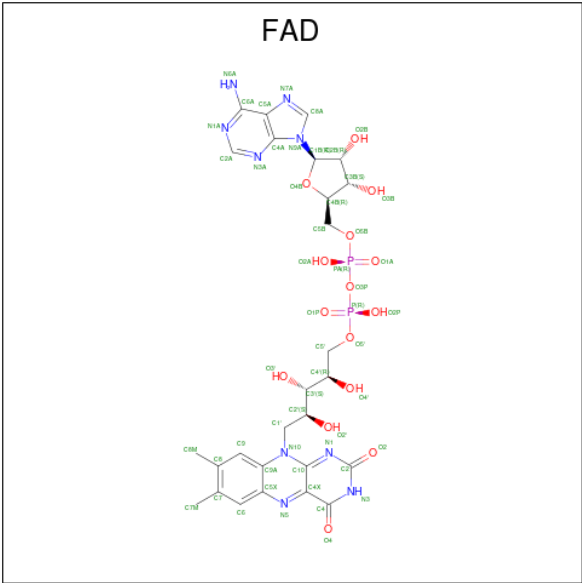
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Mg		
			1	1	0	0
4	Q	1	Total	Mg		
			1	1	0	0
4	D	1	Total	Mg		
			1	1	0	0
4	E	1	Total	Mg		
			1	1	0	0
4	H	1	Total	Mg		
			1	1	0	0
4	B	1	Total	Mg		
			1	1	0	0
4	I	1	Total	Mg		
			1	1	0	0
4	C	1	Total	Mg		
			1	1	0	0
4	V	1	Total	Mg		
			1	1	0	0

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

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by author).



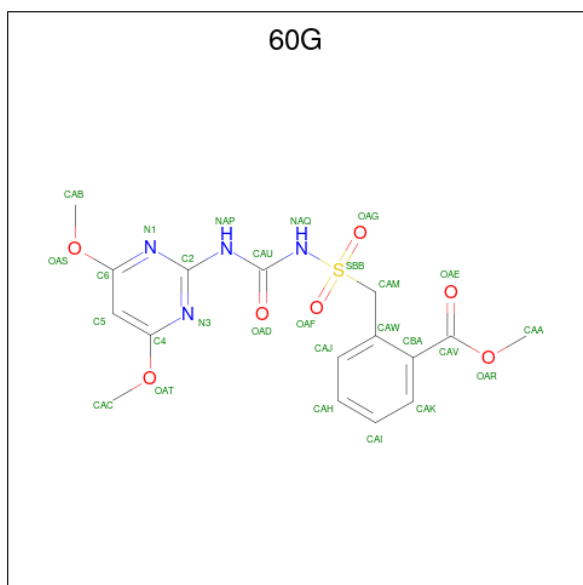
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 6 is methyl 2-[(4,6-dimethoxypyrimidin-2-yl)carbamoylsulfamoylmethyl]benzoate (three-letter code: 60G) (formula: C₁₆H₁₈N₄O₇S) (labeled as "Ligand of Interest" by author).



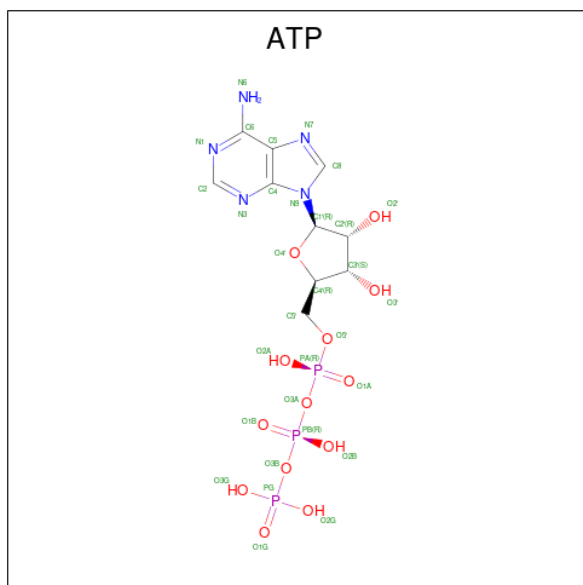
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	B	1	Total	C	N	O	S	0	0
			28	16	4	7	1		

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

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



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

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

- Molecule 8 is water.

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

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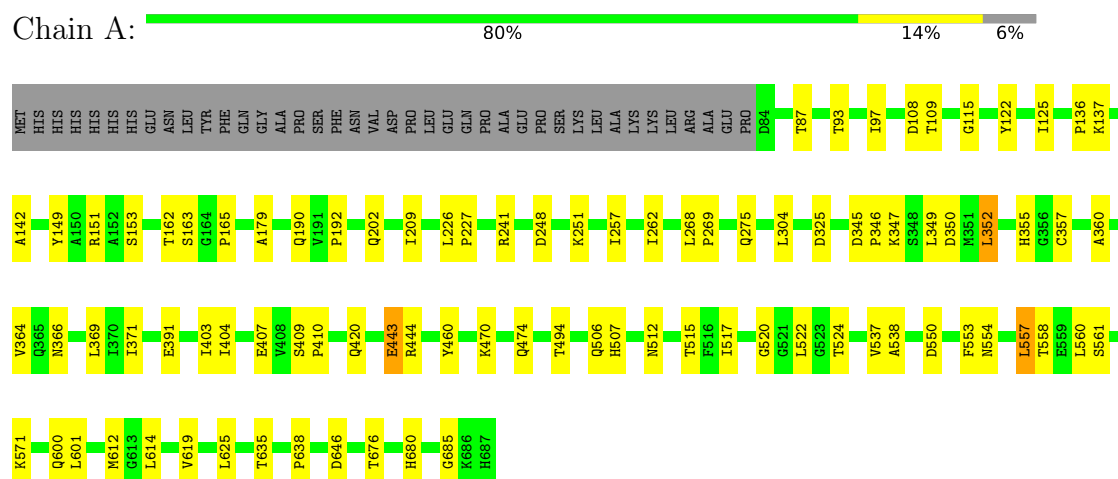
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	4	Total 4	O 4	0	0
8	Q	1	Total 1	O 1	0	0
8	R	1	Total 1	O 1	0	0
8	S	1	Total 1	O 1	0	0
8	U	4	Total 4	O 4	0	0
8	V	5	Total 5	O 5	0	0

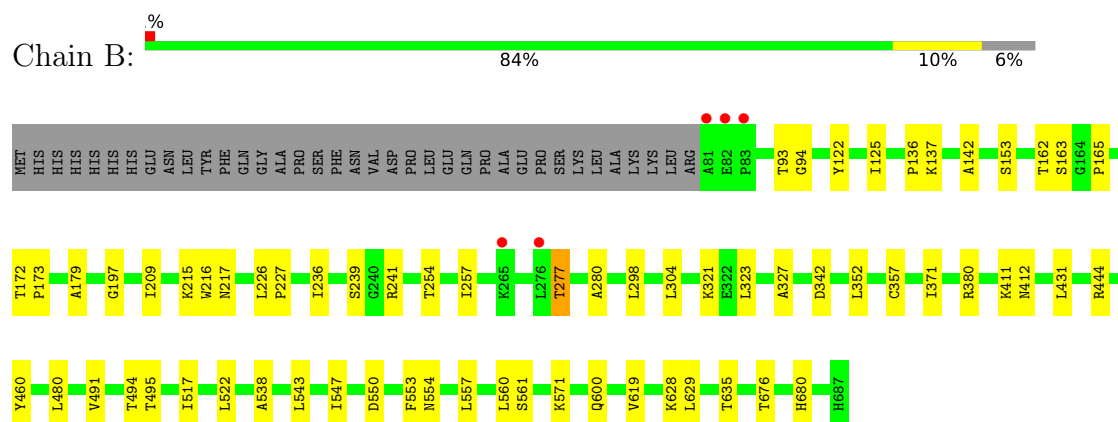
3 Residue-property plots

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

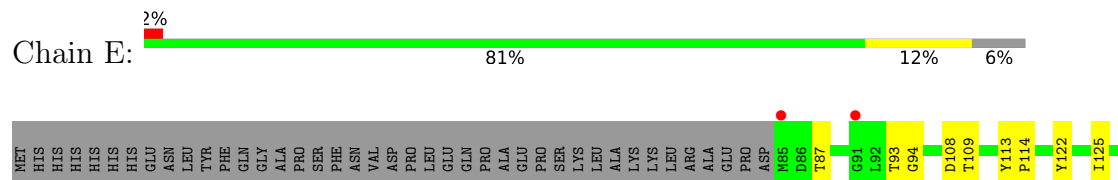
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

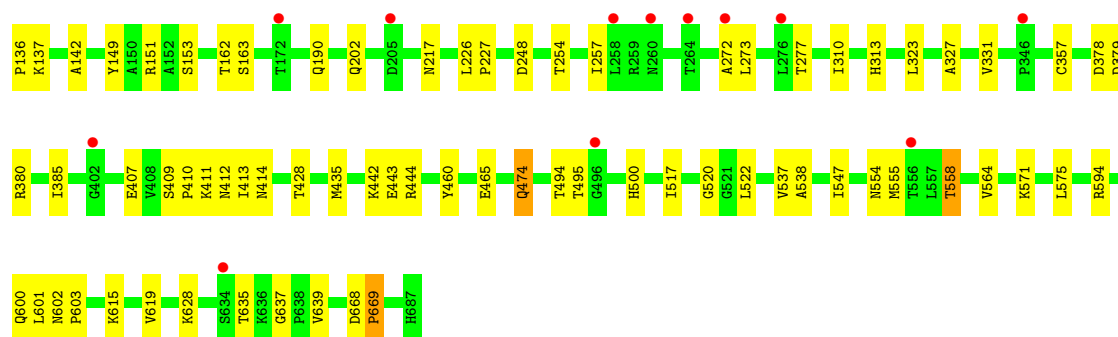


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

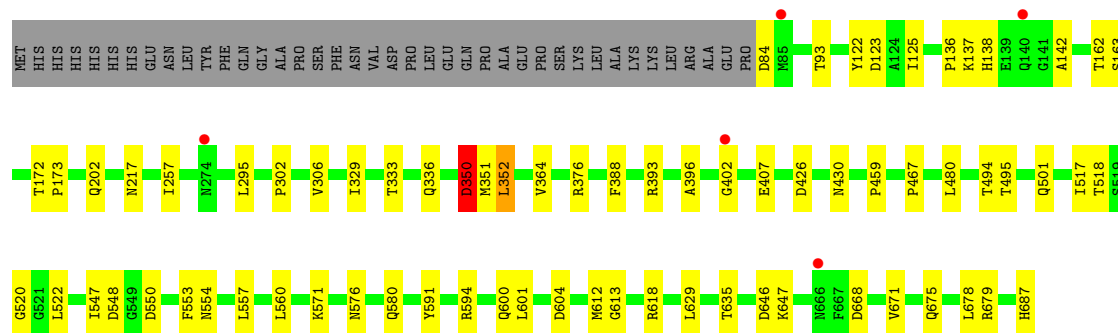
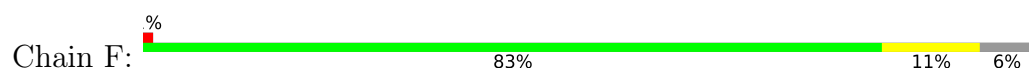


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

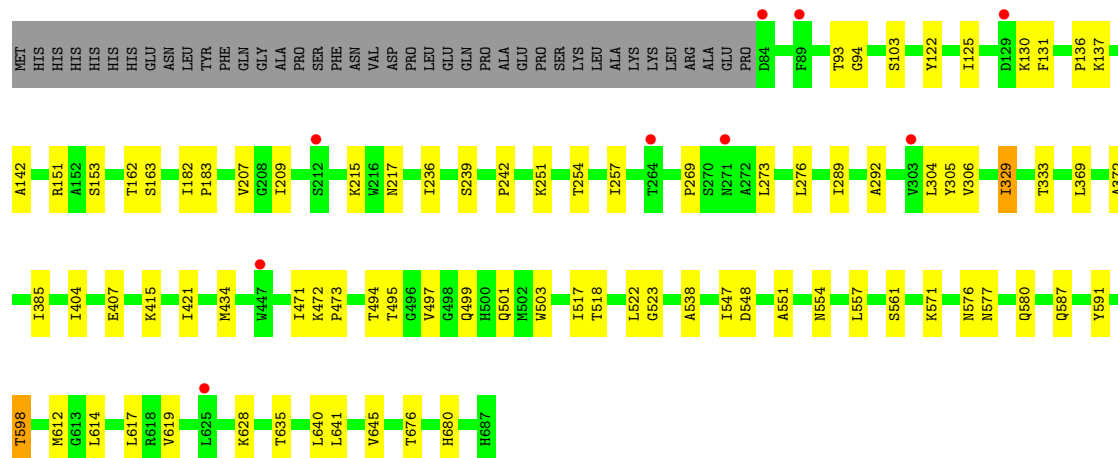
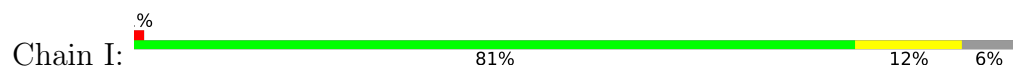




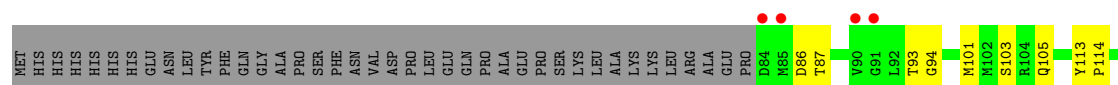
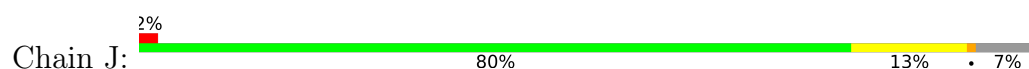
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

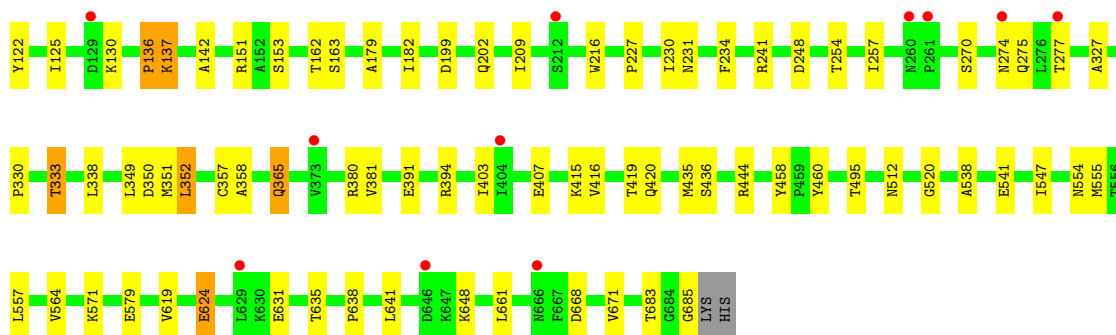


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

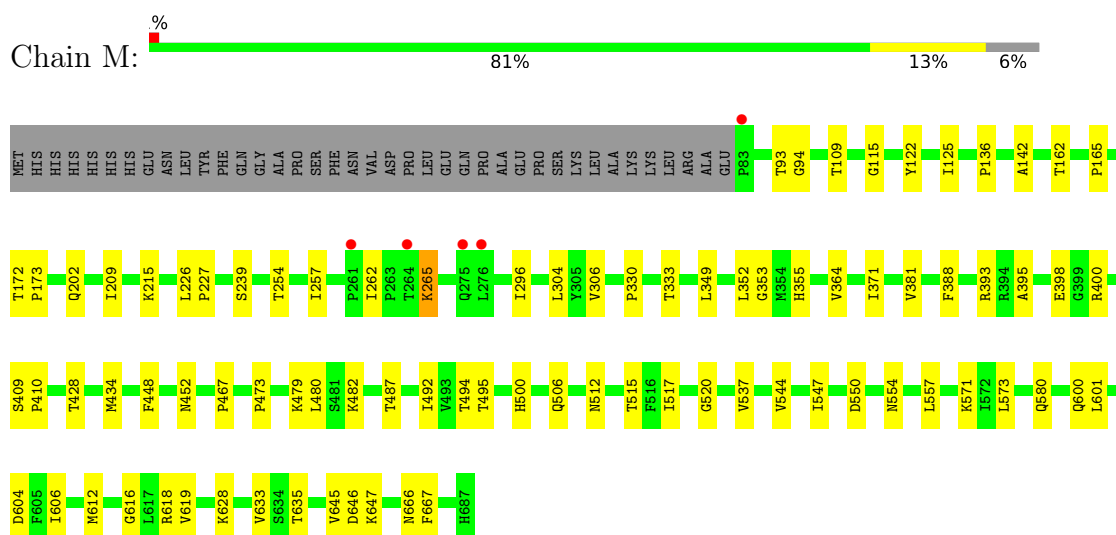


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

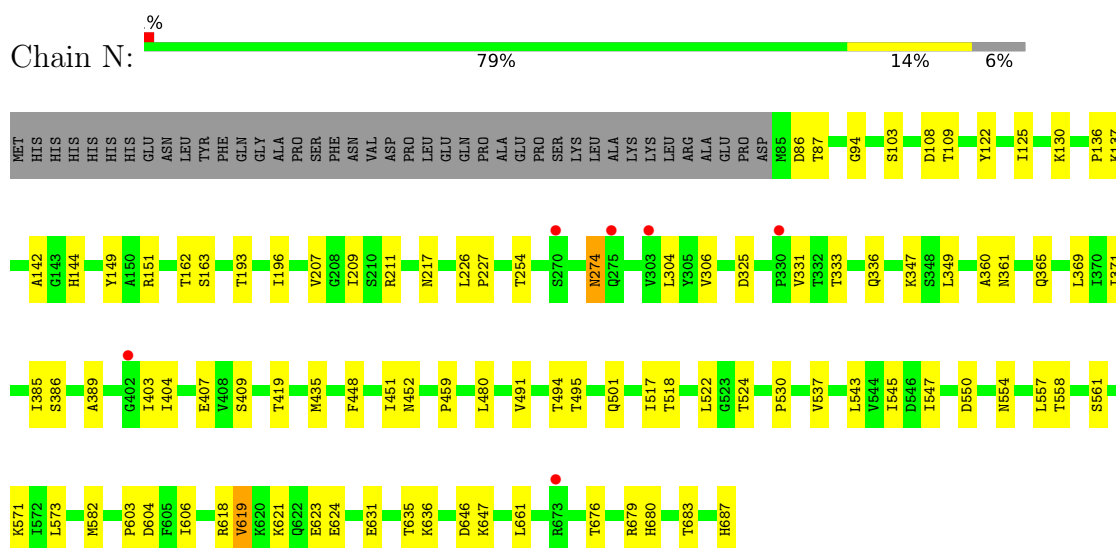




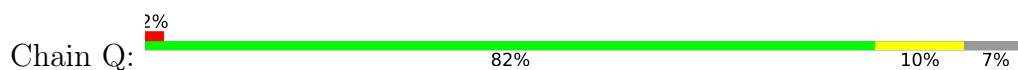
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial



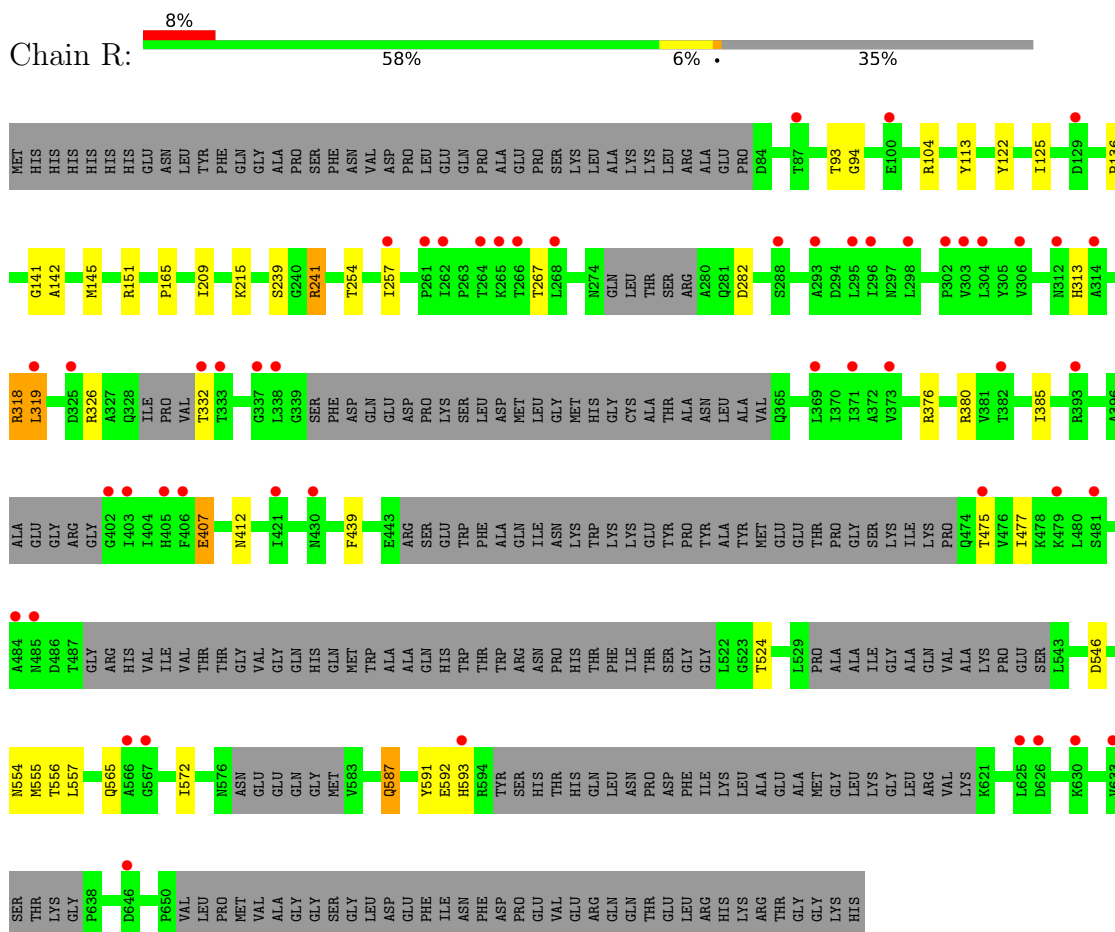
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial



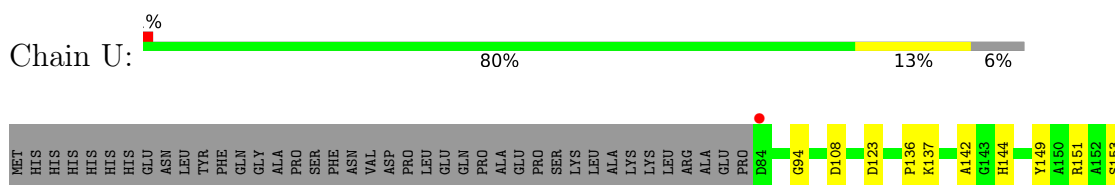
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

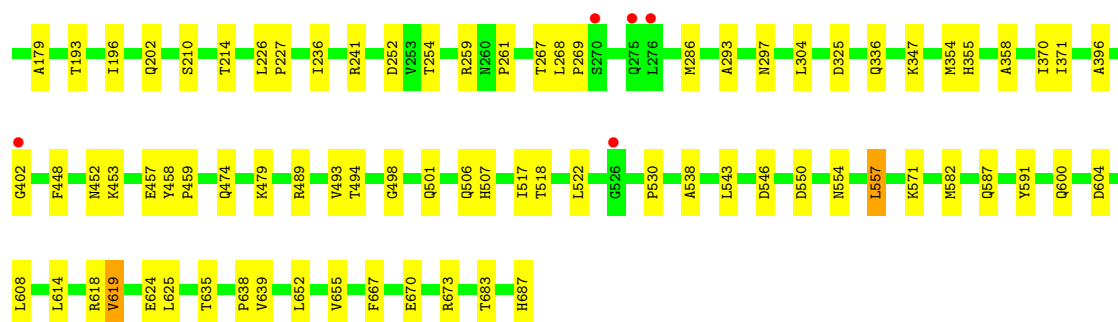


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial



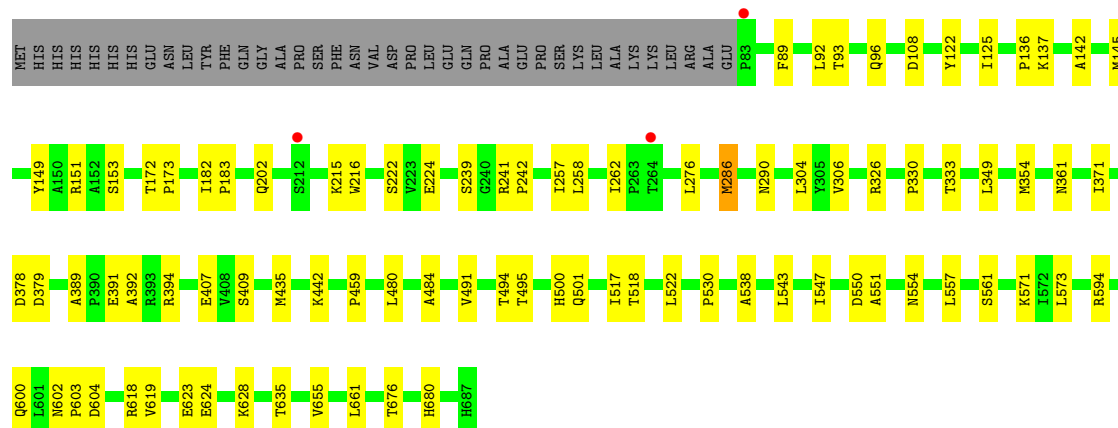
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





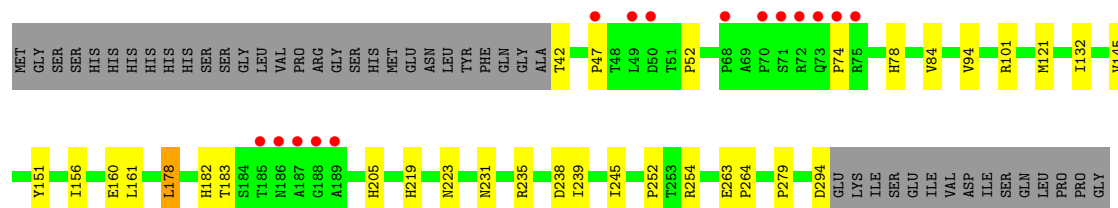
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain V: 80% 14% 6%



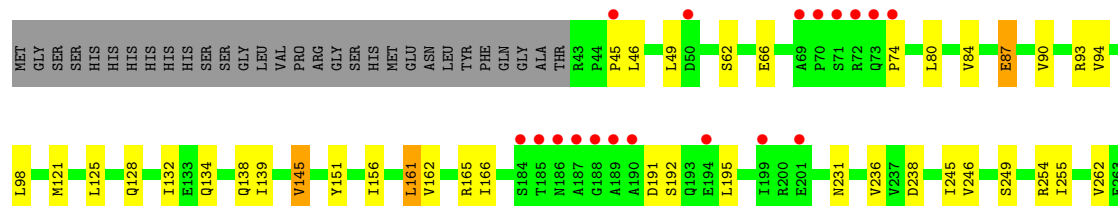
- Molecule 2: Acetolactate synthase small subunit, mitochondrial

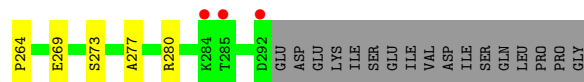
Chain C: 5% 74% 10% 15%



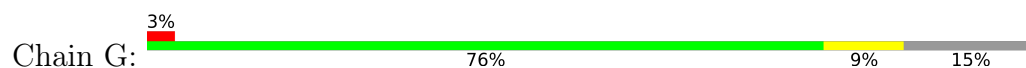
- Molecule 2: Acetolactate synthase small subunit, mitochondrial

Chain D: 7% 69% 14% 16%

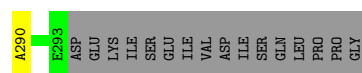
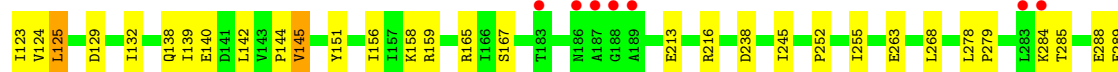
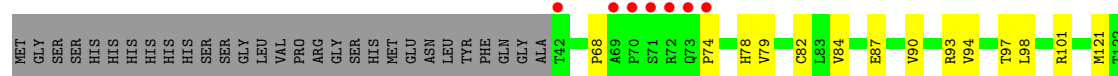




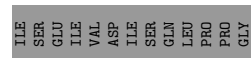
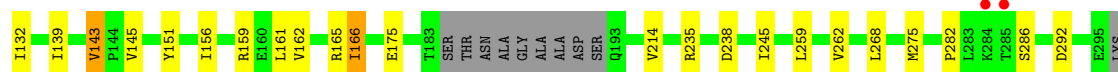
- Molecule 2: Acetolactate synthase small subunit, mitochondrial



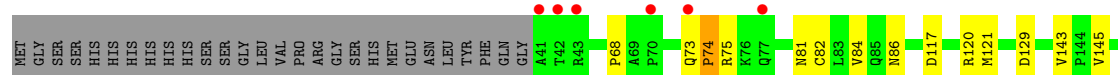
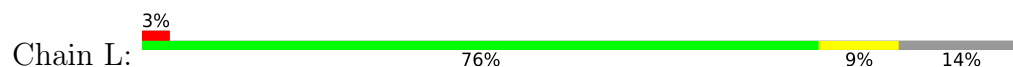
- Molecule 2: Acetolactate synthase small subunit, mitochondrial

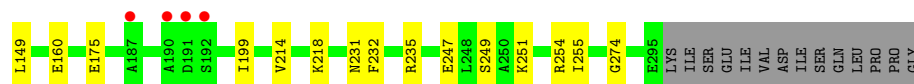


- Molecule 2: Acetolactate synthase small subunit, mitochondrial

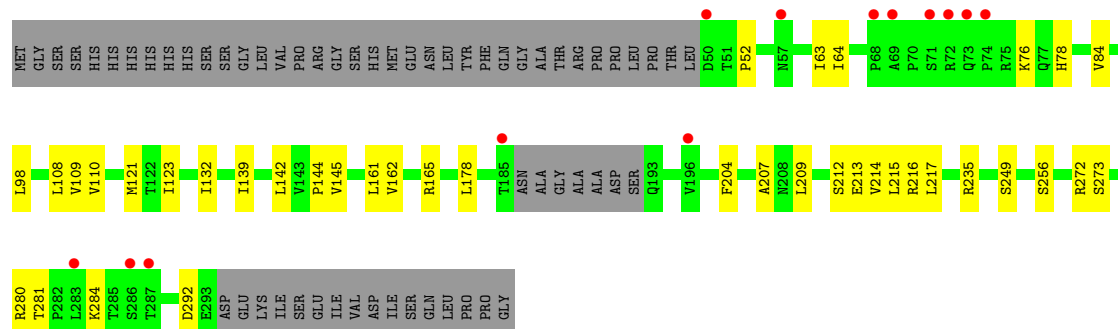


- Molecule 2: Acetolactate synthase small subunit, mitochondrial

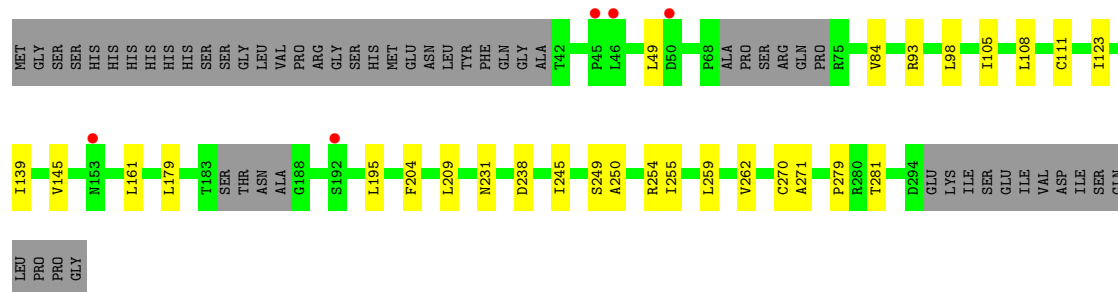
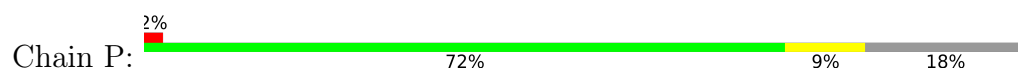




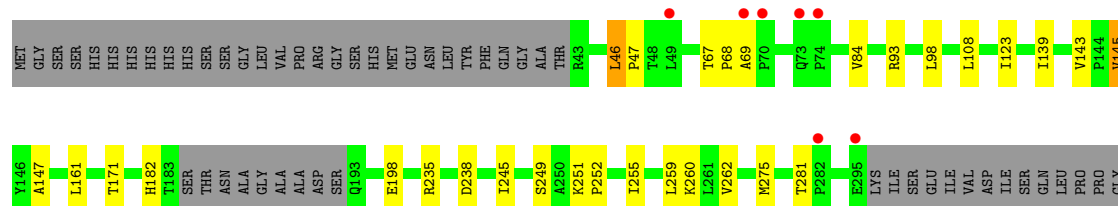
- Molecule 2: Acetolactate synthase small subunit, mitochondrial



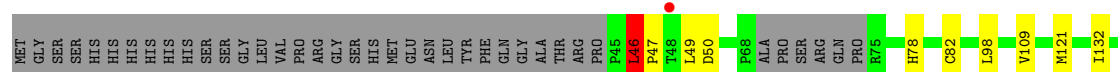
- Molecule 2: Acetolactate synthase small subunit, mitochondrial

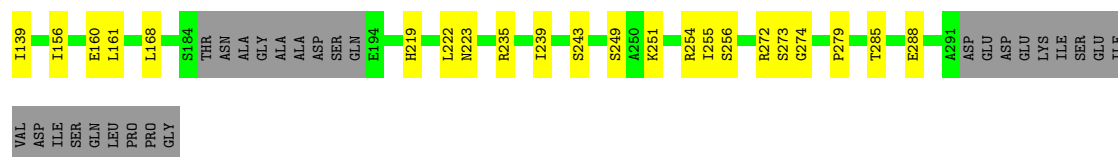


- Molecule 2: Acetolactate synthase small subunit, mitochondrial

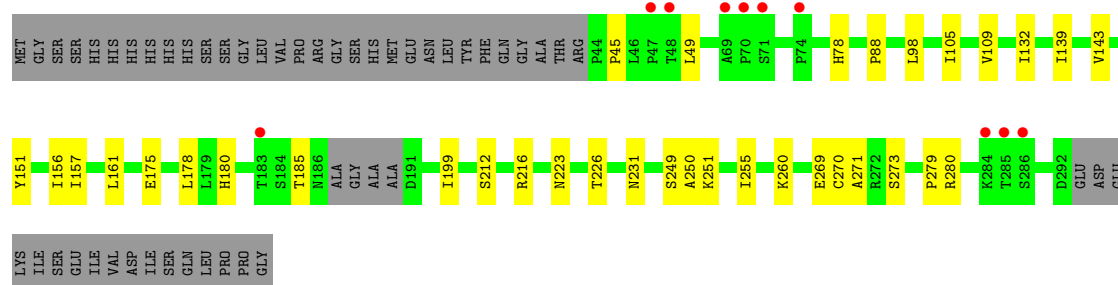


- Molecule 2: Acetolactate synthase small subunit, mitochondrial

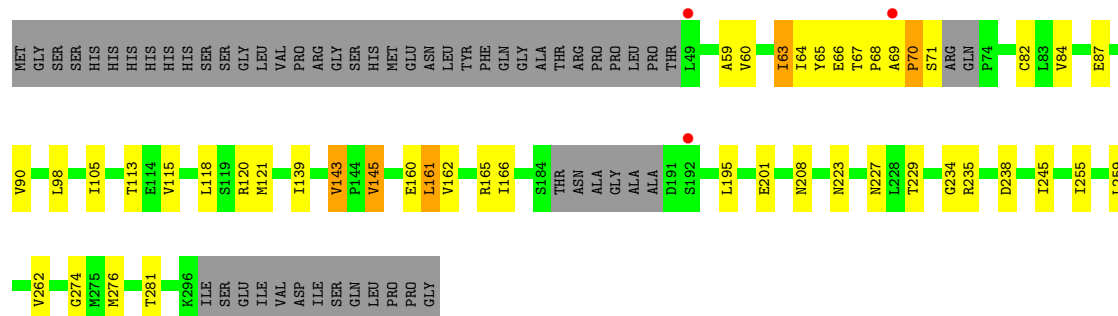




- Molecule 2: Acetolactate synthase small subunit, mitochondrial



- 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 0.210 , 0.253	Depositor DCC
R_{free} test set	1998 reflections (0.80%)	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)	0.29 , 68.0	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, MG, 60G, ATP, 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	0.21	0/4701	0.37	0/6378
1	B	0.20	0/4717	0.38	0/6402
1	E	0.20	0/4675	0.37	0/6346
1	F	0.20	0/4667	0.38	0/6339
1	I	0.20	0/4635	0.38	0/6300
1	J	0.20	0/4626	0.37	0/6289
1	M	0.20	0/4709	0.37	0/6389
1	N	0.20	0/4682	0.38	0/6351
1	Q	0.21	0/4602	0.39	0/6255
1	R	0.20	0/3058	0.39	0/4152
1	U	0.20	0/4649	0.38	0/6319
1	V	0.20	0/4697	0.37	0/6375
2	C	0.20	0/1971	0.38	0/2686
2	D	0.20	0/1948	0.40	0/2654
2	G	0.20	0/1971	0.38	0/2686
2	H	0.20	0/1977	0.40	0/2692
2	K	0.20	0/1921	0.39	0/2617
2	L	0.20	0/1990	0.38	0/2711
2	O	0.20	0/1847	0.39	0/2513
2	P	0.20	0/1910	0.38	0/2596
2	S	0.20	0/1904	0.39	0/2596
2	T	0.20	0/1820	0.39	0/2474
2	W	0.21	0/1926	0.40	0/2621
2	X	0.33	0/1873	0.45	0/2544
All	All	0.21	0/77476	0.38	0/105285

There are no bond length outliers.

There are no bond angle outliers.

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	59	0
1	B	4621	0	4621	45	0
1	E	4580	0	4578	60	0
1	F	4572	0	4540	44	0
1	I	4540	0	4503	45	0
1	J	4533	0	4486	45	0
1	M	4613	0	4622	51	0
1	N	4589	0	4602	58	0
1	Q	4508	0	4439	46	0
1	R	3014	0	2909	27	0
1	U	4554	0	4503	54	0
1	V	4601	0	4601	55	0
2	C	1938	0	1925	24	0
2	D	1915	0	1917	31	0
2	G	1938	0	1928	17	0
2	H	1944	0	1951	28	0
2	K	1889	0	1883	21	0
2	L	1957	0	1952	18	0
2	O	1818	0	1811	26	0
2	P	1881	0	1885	18	0
2	S	1872	0	1854	19	0
2	T	1792	0	1805	20	0
2	W	1894	0	1901	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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	6	0
5	U	53	0	30	1	0
5	V	53	0	30	1	0
6	A	28	0	0	0	0
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	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	31	0	12	5	0
7	O	31	0	12	1	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	784	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.

All (784) 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
2:D:94:VAL:HG21	2:D:121:MET:HE1	1.70	0.72
1:U:136:PRO:HG3	1:U:142:ALA:HB2	1.71	0.71
1:M:136:PRO:HG3	1:M:142:ALA:HB2	1.74	0.69
1:A:557:LEU:HD23	1:A:558:THR:N	2.07	0.69
2:C:279:PRO:O	2:D:165:ARG:NH1	2.25	0.69
1:F:93:THR:HG22	1:F:257:ILE:HG12	1.76	0.68
1:A:325:ASP:OD1	1:A:347:LYS:NZ	2.26	0.68
1:A:524:THR:HG22	1:B:165:PRO:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:O	1:B:444:ARG:NH1	2.27	0.68
1:N:136:PRO:HG3	1:N:142:ALA:HB2	1.75	0.68
1:Q:601:LEU:HD22	1:R:565:GLN:HB2	1.75	0.68
1:M:388:PHE:O	1:M:393:ARG:NH1	2.27	0.68
1:F:136:PRO:HG3	1:F:142:ALA:HB2	1.76	0.67
1:U:151:ARG:HD3	1:U:517:ILE:HG23	1.76	0.67
1:Q:524:THR:HG22	1:R:165:PRO:HB3	1.76	0.67
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.77	0.67
2:W:98:LEU:HD21	2:W:139:ILE:HD11	1.76	0.67
2:L:254:ARG:HD2	7:L:401:ATP:H1'	1.77	0.66
1:E:151:ARG:HD3	1:E:517:ILE:HG23	1.78	0.66
1:E:136:PRO:HG3	1:E:142:ALA:HB2	1.76	0.66
1:M:554:ASN:HA	1:M:557:LEU:HD23	1.77	0.66
2:T:98:LEU:HD21	2:T:139:ILE:HD11	1.78	0.66
2:C:47:PRO:HG3	2:K:214:VAL:HG21	1.78	0.65
2:X:64:ILE:O	2:X:67:THR:N	2.26	0.65
1:M:550:ASP:O	1:M:554:ASN:ND2	2.30	0.65
1:Q:165:PRO:HB3	1:R:524:THR:HG22	1.79	0.65
1:Q:325:ASP:OD1	1:Q:347:LYS:NZ	2.29	0.65
1:I:580:GLN:HB2	1:I:598:THR:HG22	1.79	0.65
1:Q:136:PRO:HG3	1:Q:142:ALA:HB2	1.79	0.65
1:U:494:THR:HG22	1:U:517:ILE:HB	1.78	0.64
1:N:494:THR:HG22	1:N:517:ILE:HB	1.79	0.64
1:B:571:LYS:NZ	1:B:635:THR:O	2.31	0.64
1:E:412:ASN:ND2	5:E:703:FAD:O3B	2.30	0.64
1:Q:151:ARG:HD3	1:Q:517:ILE:HG23	1.79	0.64
1:U:557:LEU:HD23	1:U:608:LEU:HD21	1.79	0.64
2:K:109:VAL:HG21	2:K:275:MET:H	1.63	0.64
1:M:215:LYS:NZ	1:M:239:SER:O	2.31	0.64
1:U:550:ASP:O	1:U:554:ASN:ND2	2.31	0.64
1:B:217:ASN:H	2:D:93:ARG:HH22	1.46	0.63
2:P:204:PHE:HA	2:P:209:LEU:HD11	1.79	0.63
1:A:557:LEU:C	1:A:557:LEU:HD23	2.18	0.63
1:E:217:ASN:H	2:G:93:ARG:HH22	1.47	0.63
1:B:494:THR:HG22	1:B:517:ILE:HB	1.80	0.63
1:B:411:LYS:HG3	2:D:138:GLN:HG2	1.79	0.63
1:B:217:ASN:OD1	2:D:93:ARG:NH2	2.32	0.63
1:E:442:LYS:HE3	1:E:443:GLU:HG2	1.80	0.63
1:E:494:THR:HG22	1:E:517:ILE:HB	1.81	0.63
1:V:286:MET:O	1:V:290:ASN:ND2	2.32	0.62
2:C:239:ILE:O	7:G:401:ATP:N6	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:571:LYS:NZ	1:M:635:THR:O	2.31	0.62
1:M:165:PRO:HB3	1:N:524:THR:HG22	1.79	0.62
1:U:293:ALA:O	1:U:297:ASN:ND2	2.32	0.62
2:D:80:LEU:HD13	2:D:125:LEU:HD23	1.80	0.62
2:O:161:LEU:HD23	2:O:249:SER:HB3	1.81	0.62
1:V:215:LYS:NZ	1:V:239:SER:O	2.33	0.62
2:O:98:LEU:HD21	2:O:139:ILE:HD11	1.81	0.61
2:G:134:GLN:HE22	2:G:138:GLN:HE21	1.49	0.61
2:G:226:THR:HG22	2:G:236:VAL:HG21	1.81	0.61
1:I:473:PRO:HD3	1:I:645:VAL:HB	1.82	0.61
1:J:227:PRO:O	1:J:231:ASN:ND2	2.33	0.61
1:F:571:LYS:NZ	1:F:635:THR:O	2.31	0.61
1:V:494:THR:HG22	1:V:517:ILE:HB	1.81	0.61
1:B:321:LYS:HE3	1:B:342:ASP:H	1.65	0.61
1:F:494:THR:HG22	1:F:517:ILE:HB	1.82	0.61
2:H:159:ARG:NH2	7:K:401:ATP:O1B	2.34	0.61
1:A:87:THR:HG21	1:U:261:PRO:HD3	1.83	0.61
1:A:151:ARG:HD3	1:A:517:ILE:HG23	1.81	0.61
1:N:676:THR:O	1:N:680:HIS:ND1	2.32	0.61
1:V:136:PRO:HG3	1:V:142:ALA:HB2	1.82	0.61
1:J:151:ARG:HD3	1:J:182:ILE:HD12	1.83	0.61
2:O:214:VAL:H	2:O:217:LEU:HD23	1.66	0.61
1:U:325:ASP:OD1	1:U:347:LYS:NZ	2.32	0.61
2:X:84:VAL:HG12	2:X:145:VAL:HB	1.82	0.61
1:F:388:PHE:O	1:F:393:ARG:NH1	2.34	0.60
7:L:401:ATP:O2G	2:O:280:ARG:NH2	2.34	0.60
2:G:279:PRO:O	2:H:165:ARG:NH1	2.33	0.60
1:V:501:GLN:NE2	1:V:518:THR:OG1	2.34	0.60
1:E:327:ALA:O	1:E:444:ARG:NH1	2.33	0.60
1:I:215:LYS:NZ	1:I:239:SER:O	2.34	0.60
2:D:84:VAL:HG12	2:D:145:VAL:HB	1.83	0.60
1:U:652:LEU:HD13	1:U:667:PHE:HA	1.84	0.60
1:I:251:LYS:NZ	6:J:704:60G:OAD	2.29	0.60
2:K:98:LEU:HD21	2:K:139:ILE:HD11	1.84	0.60
1:A:561:SER:OG	1:A:612:MET:SD	2.60	0.59
2:O:84:VAL:HG12	2:O:145:VAL:HG22	1.83	0.59
1:J:136:PRO:HG3	1:J:142:ALA:HB2	1.82	0.59
1:E:313:HIS:HB3	1:E:428:THR:HG21	1.84	0.59
1:M:227:PRO:HG2	1:M:262:ILE:HD12	1.85	0.59
1:R:122:TYR:HA	1:R:125:ILE:HG12	1.83	0.59
2:X:98:LEU:HD21	2:X:139:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:571:LYS:NZ	1:I:635:THR:O	2.35	0.59
1:N:103:SER:HB3	1:N:130:LYS:HD3	1.83	0.59
2:O:212:SER:HB2	2:O:216:ARG:HH22	1.67	0.59
1:Q:353:GLY:HA2	1:Q:381:VAL:HA	1.83	0.59
2:C:94:VAL:HG21	2:C:121:MET:HE1	1.84	0.58
1:N:369:LEU:HD11	1:N:404:ILE:HG13	1.85	0.58
2:W:251:LYS:NZ	7:W:402:ATP:O2G	2.37	0.58
1:E:635:THR:HG21	1:E:639:VAL:CG1	2.18	0.58
2:O:213:GLU:OE2	2:O:216:ARG:NH1	2.36	0.58
1:Q:207:VAL:O	1:Q:217:ASN:ND2	2.36	0.58
1:Q:138:HIS:CD2	1:R:555:MET:HB2	2.38	0.58
1:U:123:ASP:OD1	1:V:594:ARG:NH2	2.37	0.58
2:W:269:GLU:OE1	2:X:120:ARG:NH1	2.37	0.58
1:N:619:VAL:HG23	1:N:624:GLU:HB3	1.86	0.58
1:U:448:PHE:O	1:U:452:ASN:ND2	2.33	0.58
1:M:448:PHE:O	1:M:452:ASN:ND2	2.33	0.58
1:J:668:ASP:HB3	1:J:671:VAL:HG22	1.86	0.57
1:R:412:ASN:ND2	5:R:701:FAD:O3B	2.37	0.57
1:V:222:SER:OG	1:V:224:GLU:OE1	2.21	0.57
1:F:604:ASP:OD1	1:F:618:ARG:NH2	2.37	0.57
1:F:679:ARG:NH1	1:F:687:HIS:O	2.38	0.57
1:M:398:GLU:OE1	1:M:400:ARG:NH2	2.37	0.57
1:A:494:THR:HG22	1:A:517:ILE:HB	1.85	0.57
1:J:571:LYS:NZ	1:J:635:THR:O	2.32	0.57
1:N:621:LYS:NZ	1:N:623:GLU:OE1	2.32	0.57
1:N:151:ARG:NH2	1:N:336:GLN:OE1	2.36	0.57
1:A:251:LYS:NZ	6:B:704:60G:OAD	2.33	0.57
2:X:87:GLU:HG2	2:X:90:VAL:HG23	1.85	0.57
1:E:500:HIS:ND1	3:E:701:TPP:O1B	2.37	0.57
1:Q:273:LEU:HG	2:S:147:ALA:HB2	1.87	0.57
2:P:98:LEU:HD13	2:P:105:ILE:HG21	1.86	0.57
1:A:352:LEU:HD11	1:A:364:VAL:HG21	1.86	0.56
1:N:193:THR:HA	1:N:196:ILE:HD13	1.87	0.56
1:I:495:THR:HG22	1:I:547:ILE:HB	1.88	0.56
1:U:600:GLN:HB2	1:V:137:LYS:HE2	1.87	0.56
1:A:601:LEU:O	1:B:137:LYS:NZ	2.36	0.56
1:A:571:LYS:NZ	1:A:635:THR:O	2.39	0.56
2:T:46:LEU:H	2:T:47:PRO:HD2	1.71	0.56
1:N:407:GLU:OE2	5:N:703:FAD:O2B	2.21	0.56
2:W:279:PRO:O	2:X:165:ARG:NH1	2.29	0.56
1:A:550:ASP:O	1:A:554:ASN:ND2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:219:HIS:O	2:C:223:ASN:ND2	2.38	0.56
1:E:571:LYS:NZ	1:E:635:THR:O	2.37	0.56
1:I:619:VAL:HG23	1:I:641:LEU:HD11	1.88	0.56
1:R:241:ARG:HD3	5:R:701:FAD:C2B	2.34	0.56
2:T:82:CYS:HB2	2:T:121:MET:HB2	1.87	0.56
1:V:378:ASP:OD1	1:V:379:ASP:N	2.39	0.56
1:B:93:THR:HG22	1:B:257:ILE:HG12	1.88	0.55
1:N:448:PHE:O	1:N:452:ASN:ND2	2.33	0.55
2:T:46:LEU:HD12	2:T:47:PRO:HD3	1.87	0.55
1:V:216:TRP:HB2	2:X:143:VAL:HG11	1.87	0.55
2:H:213:GLU:OE1	2:H:216:ARG:NH1	2.37	0.55
1:I:407:GLU:OE2	5:I:703:FAD:O3B	2.20	0.55
1:U:179:ALA:O	1:U:241:ARG:NH2	2.39	0.55
1:V:571:LYS:NZ	1:V:635:THR:O	2.34	0.55
1:J:86:ASP:OD1	1:J:87:THR:N	2.38	0.55
1:U:304:LEU:HD23	1:U:371:ILE:HB	1.87	0.55
2:X:82:CYS:HB2	2:X:121:MET:HB2	1.87	0.55
1:J:122:TYR:HA	1:J:125:ILE:HG12	1.87	0.55
1:A:108:ASP:OD1	1:A:149:TYR:OH	2.25	0.55
2:K:89:GLY:O	2:K:91:LEU:N	2.40	0.55
2:X:59:ALA:O	2:X:63:ILE:HG13	2.07	0.55
1:F:407:GLU:OE2	5:F:703:FAD:O2B	2.25	0.55
2:P:98:LEU:HD21	2:P:139:ILE:HD11	1.89	0.54
2:D:231:ASN:O	7:D:401:ATP:O2'	2.25	0.54
2:K:238:ASP:HB3	2:K:245:ILE:HB	1.88	0.54
2:T:273:SER:OG	2:T:274:GLY:N	2.37	0.54
1:I:577:ASN:OD1	1:I:577:ASN:N	2.41	0.54
1:J:327:ALA:O	1:J:444:ARG:NH1	2.38	0.54
1:R:380:ARG:NH1	6:R:702:60G:OAT	2.41	0.54
2:H:278:LEU:HD12	2:H:279:PRO:HD2	1.90	0.54
1:M:494:THR:HG22	1:M:517:ILE:HB	1.89	0.54
1:E:495:THR:HG22	1:E:547:ILE:HB	1.90	0.54
2:X:66:GLU:O	2:X:68:PRO:HD3	2.08	0.54
1:U:604:ASP:OD1	1:U:618:ARG:NH2	2.40	0.54
1:U:554:ASN:HB3	1:V:137:LYS:HB3	1.90	0.53
1:V:391:GLU:OE2	1:V:394:ARG:NH2	2.41	0.53
1:Q:403:ILE:H	1:Q:420:GLN:HG2	1.73	0.53
1:J:358:ALA:HB3	1:J:458:TYR:HB3	1.90	0.53
2:L:84:VAL:HG22	2:L:145:VAL:HG12	1.90	0.53
1:R:407:GLU:OE1	5:R:701:FAD:O3B	2.23	0.53
1:U:193:THR:HA	1:U:196:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:600:GLN:HB2	1:N:137:LYS:HE2	1.89	0.53
1:Q:353:GLY:HA3	5:Q:703:FAD:HN3	1.74	0.53
1:Q:550:ASP:O	1:Q:554:ASN:ND2	2.39	0.53
1:Q:479:LYS:NZ	1:Q:626:ASP:OD1	2.36	0.53
2:S:108:LEU:HD13	2:S:123:ILE:HG12	1.90	0.53
1:U:108:ASP:OD1	1:U:149:TYR:OH	2.26	0.53
1:U:355:HIS:O	1:U:506:GLN:NE2	2.40	0.53
1:I:136:PRO:HG3	1:I:142:ALA:HB2	1.89	0.53
1:V:480:LEU:HD22	1:V:573:LEU:HD22	1.90	0.53
1:E:603:PRO:HB3	1:F:612:MET:HA	1.89	0.53
2:C:264:PRO:HB3	2:G:49:LEU:HD11	1.91	0.53
2:C:235:ARG:NH1	2:D:249:SER:O	2.42	0.53
2:D:125:LEU:HB3	2:D:132:ILE:HD12	1.90	0.53
1:E:411:LYS:HE3	2:G:141:ASP:HB3	1.90	0.53
1:Q:551:ALA:HB3	3:Q:701:TPP:H72	1.91	0.53
1:A:179:ALA:O	1:A:241:ARG:NH2	2.42	0.53
1:B:554:ASN:HA	1:B:557:LEU:HD23	1.90	0.53
2:C:205:HIS:HE1	2:K:45:PRO:HG2	1.74	0.53
2:K:84:VAL:HG12	2:K:145:VAL:HG22	1.91	0.53
1:N:144:HIS:HB2	1:N:530:PRO:HB2	1.91	0.53
2:W:250:ALA:H	2:W:255:ILE:HD11	1.71	0.53
1:I:94:GLY:HA3	1:I:254:THR:HA	1.90	0.53
1:M:93:THR:HG22	1:M:257:ILE:HG12	1.91	0.53
2:H:82:CYS:HB2	2:H:121:MET:HB2	1.91	0.52
1:J:93:THR:HG22	1:J:257:ILE:HG12	1.90	0.52
1:N:554:ASN:HA	1:N:557:LEU:HD11	1.91	0.52
1:M:666:ASN:OD1	1:M:667:PHE:N	2.40	0.52
1:N:86:ASP:OD1	1:N:87:THR:N	2.42	0.52
2:S:84:VAL:HG12	2:S:145:VAL:HB	1.91	0.52
1:B:380:ARG:NH2	6:B:704:60G:OAG	2.33	0.52
2:D:166:ILE:HD13	2:D:262:VAL:HG21	1.91	0.52
2:D:165:ARG:NH2	2:D:269:GLU:OE2	2.29	0.52
1:F:495:THR:HG22	1:F:547:ILE:HB	1.90	0.52
2:X:160:GLU:HB3	2:X:255:ILE:HD12	1.92	0.52
1:A:355:HIS:O	1:A:506:GLN:NE2	2.38	0.52
1:V:306:VAL:HB	1:V:333:THR:HG22	1.92	0.52
2:D:236:VAL:HG22	2:D:246:VAL:HG12	1.91	0.52
2:D:98:LEU:HD21	2:D:139:ILE:HD11	1.90	0.52
1:N:407:GLU:HG3	1:N:409:SER:H	1.75	0.52
2:P:254:ARG:NH2	7:P:401:ATP:O4'	2.42	0.52
1:U:137:LYS:HB3	1:V:554:ASN:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:161:LEU:HB2	2:X:161:LEU:HD12	1.91	0.52
1:B:215:LYS:NZ	1:B:239:SER:O	2.43	0.52
2:O:108:LEU:HD12	2:O:123:ILE:HG12	1.91	0.52
2:W:178:LEU:O	2:W:180:HIS:N	2.38	0.52
2:C:231:ASN:O	7:C:401:ATP:O2'	2.22	0.52
2:D:151:TYR:HB3	2:D:156:ILE:HG21	1.91	0.52
1:N:151:ARG:HD3	1:N:517:ILE:HG23	1.92	0.52
2:D:280:ARG:NH2	7:G:401:ATP:O3G	2.43	0.52
1:I:153:SER:HB3	1:I:538:ALA:HB1	1.92	0.52
1:J:179:ALA:O	1:J:241:ARG:NH2	2.43	0.52
1:N:122:TYR:HA	1:N:125:ILE:HG12	1.92	0.51
1:A:87:THR:OG1	1:U:259:ARG:O	2.26	0.51
1:E:108:ASP:OD1	1:E:149:TYR:OH	2.23	0.51
2:H:84:VAL:HA	2:H:145:VAL:HA	1.92	0.51
1:N:550:ASP:O	1:N:554:ASN:ND2	2.36	0.51
2:S:46:LEU:HD22	2:S:47:PRO:HD2	1.91	0.51
2:L:149:LEU:HD21	2:O:64:ILE:HG22	1.92	0.51
2:T:285:THR:HG23	2:T:288:GLU:H	1.75	0.51
1:V:604:ASP:OD1	1:V:618:ARG:NH2	2.44	0.51
2:X:60:VAL:O	2:X:64:ILE:HG13	2.09	0.51
1:A:162:THR:OG1	1:A:163:SER:N	2.43	0.51
1:M:601:LEU:O	1:N:561:SER:OG	2.28	0.51
1:N:480:LEU:HD22	1:N:573:LEU:HD22	1.93	0.51
2:X:98:LEU:HD13	2:X:105:ILE:HG21	1.92	0.51
1:J:216:TRP:HB2	2:L:143:VAL:HG21	1.92	0.51
1:Q:304:LEU:HD23	1:Q:371:ILE:HB	1.92	0.51
2:S:235:ARG:NH1	2:T:249:SER:O	2.43	0.51
1:E:137:LYS:HE2	1:F:600:GLN:HB2	1.92	0.51
1:I:676:THR:O	1:I:680:HIS:ND1	2.43	0.51
2:T:168:LEU:HD13	2:T:243:SER:HA	1.93	0.51
1:E:601:LEU:O	1:F:137:LYS:NZ	2.35	0.51
1:F:306:VAL:HB	1:F:333:THR:HG22	1.93	0.51
2:H:284:LYS:NZ	2:H:288:GLU:OE1	2.37	0.51
2:K:42:THR:OG1	2:K:43:ARG:N	2.44	0.51
1:B:550:ASP:O	1:B:554:ASN:ND2	2.34	0.51
1:M:395:ALA:HB1	1:M:400:ARG:HB3	1.93	0.51
1:R:591:TYR:O	1:R:593:HIS:N	2.44	0.51
2:T:46:LEU:H	2:T:47:PRO:CD	2.23	0.51
1:B:304:LEU:HD23	1:B:371:ILE:HB	1.93	0.51
1:E:378:ASP:OD1	1:E:379:ASP:N	2.44	0.51
2:G:49:LEU:HD23	2:G:49:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:165:ARG:HB3	2:K:268:LEU:HB2	1.92	0.51
1:M:304:LEU:HD23	1:M:371:ILE:HB	1.93	0.51
2:T:219:HIS:O	2:T:223:ASN:ND2	2.37	0.51
1:A:470:LYS:HD3	1:A:646:ASP:HA	1.91	0.51
2:C:254:ARG:NH2	7:C:401:ATP:O4'	2.43	0.51
2:H:252:PRO:HA	2:H:255:ILE:HG22	1.93	0.50
1:U:137:LYS:HE2	1:V:600:GLN:HB2	1.92	0.50
3:F:701:TPP:H2	3:F:701:TPP:HN42	1.77	0.50
1:M:495:THR:HG22	1:M:547:ILE:HB	1.92	0.50
2:S:249:SER:O	2:T:235:ARG:NH1	2.44	0.50
2:T:222:LEU:HD21	2:T:239:ILE:HD13	1.92	0.50
1:E:380:ARG:NH2	6:E:704:60G:OAG	2.40	0.50
1:B:153:SER:HB2	1:B:538:ALA:HB1	1.93	0.50
2:W:249:SER:O	2:X:235:ARG:NH2	2.45	0.50
1:Q:352:LEU:HD11	1:Q:364:VAL:HG21	1.93	0.50
1:V:551:ALA:HB3	3:V:701:TPP:H72	1.92	0.50
2:T:285:THR:HA	2:W:260:LYS:HG2	1.92	0.50
1:I:122:TYR:HA	1:I:125:ILE:HG12	1.94	0.50
1:M:122:TYR:HA	1:M:125:ILE:HG12	1.93	0.50
1:N:211:ARG:HD3	2:P:93:ARG:HA	1.93	0.50
1:U:151:ARG:NH2	1:U:336:GLN:OE1	2.35	0.50
1:V:619:VAL:HG13	1:V:624:GLU:HG3	1.92	0.50
1:M:619:VAL:HG22	1:M:628:LYS:HG3	1.92	0.50
1:B:411:LYS:O	2:D:134:GLN:NE2	2.45	0.50
1:E:217:ASN:H	2:G:93:ARG:NH2	2.10	0.50
7:H:401:ATP:O1A	2:K:159:ARG:NH1	2.45	0.50
1:N:365:GLN:HA	1:N:389:ALA:HA	1.93	0.50
2:O:213:GLU:O	2:O:215:LEU:N	2.44	0.50
2:W:175:GLU:HB3	2:W:199:ILE:HD13	1.94	0.50
1:I:236:ILE:HD13	2:K:143:VAL:HG11	1.94	0.49
2:K:235:ARG:NH2	2:L:249:SER:O	2.44	0.49
1:N:679:ARG:O	1:N:683:THR:OG1	2.26	0.49
1:A:227:PRO:HG2	1:A:262:ILE:HD12	1.94	0.49
2:H:142:LEU:HB3	2:H:144:PRO:HD2	1.94	0.49
1:M:479:LYS:HA	1:M:482:LYS:HE3	1.93	0.49
1:N:108:ASP:OD1	1:N:149:TYR:OH	2.30	0.49
1:N:207:VAL:O	1:N:217:ASN:ND2	2.45	0.49
2:X:223:ASN:O	2:X:227:ASN:ND2	2.28	0.49
1:E:273:LEU:HB2	1:E:277:THR:HG21	1.94	0.49
2:H:98:LEU:HD21	2:H:139:ILE:HD11	1.94	0.49
1:I:93:THR:HG22	1:I:257:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:614:LEU:HG	1:U:638:PRO:HB2	1.94	0.49
1:M:492:ILE:HB	1:M:544:VAL:HG22	1.95	0.49
2:L:251:LYS:NZ	7:O:401:ATP:O1B	2.44	0.49
2:D:191:ASP:OD1	2:D:192:SER:N	2.41	0.49
2:D:87:GLU:HG2	2:D:90:VAL:HG23	1.94	0.49
1:E:310:ILE:HD12	1:E:428:THR:HG22	1.95	0.49
2:H:79:VAL:HG12	2:H:124:VAL:HG22	1.94	0.49
1:J:403:ILE:O	1:J:419:THR:OG1	2.31	0.49
1:N:403:ILE:O	1:N:419:THR:OG1	2.29	0.49
1:F:122:TYR:HA	1:F:125:ILE:HG12	1.95	0.49
1:F:668:ASP:HB3	1:F:671:VAL:HG22	1.94	0.49
2:S:84:VAL:HA	2:S:145:VAL:HA	1.93	0.49
1:U:635:THR:HB	1:U:639:VAL:HG21	1.95	0.49
2:X:160:GLU:HG3	2:X:274:GLY:H	1.78	0.49
1:B:179:ALA:O	1:B:241:ARG:NH2	2.43	0.49
1:I:103:SER:HB3	1:I:130:LYS:HD3	1.95	0.49
1:I:494:THR:HG22	1:I:517:ILE:HB	1.95	0.49
1:J:631:GLU:O	1:J:635:THR:OG1	2.25	0.49
1:N:495:THR:HG22	1:N:547:ILE:HB	1.93	0.49
1:N:631:GLU:O	1:N:635:THR:OG1	2.23	0.49
2:O:162:VAL:HG12	2:O:272:ARG:HA	1.95	0.49
1:R:94:GLY:HA3	1:R:254:THR:HA	1.95	0.49
1:I:162:THR:OG1	1:I:163:SER:N	2.46	0.49
1:Q:274:ASN:O	1:Q:276:LEU:N	2.46	0.49
2:S:252:PRO:HG3	2:S:275:MET:HB3	1.95	0.49
1:R:554:ASN:HA	1:R:557:LEU:HD23	1.95	0.48
1:U:153:SER:HB3	1:U:538:ALA:HB1	1.95	0.48
1:N:304:LEU:HD12	1:N:371:ILE:HB	1.95	0.48
1:Q:153:SER:HB3	1:Q:538:ALA:HB1	1.95	0.48
1:Q:94:GLY:HA3	1:Q:254:THR:HA	1.95	0.48
1:J:352:LEU:HD13	1:J:381:VAL:HG13	1.95	0.48
1:Q:122:TYR:HA	1:Q:125:ILE:HG12	1.95	0.48
1:R:215:LYS:NZ	1:R:239:SER:O	2.46	0.48
2:H:87:GLU:HG2	2:H:90:VAL:HB	1.95	0.48
1:V:92:LEU:HB3	1:V:96:GLN:HG3	1.95	0.48
2:W:231:ASN:O	7:W:402:ATP:O2'	2.22	0.48
1:B:94:GLY:HA3	1:B:254:THR:HA	1.96	0.48
2:H:151:TYR:HB3	2:H:156:ILE:HG21	1.94	0.48
1:I:207:VAL:O	1:I:217:ASN:ND2	2.47	0.48
3:I:701:TPP:H2	3:I:701:TPP:HN42	1.78	0.48
5:R:701:FAD:H1'2	5:R:701:FAD:H4'	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:THR:HG22	1:E:257:ILE:HG12	1.96	0.48
1:J:270:SER:O	1:J:274:ASN:ND2	2.33	0.48
3:J:701:TPP:H2	3:J:701:TPP:HN42	1.79	0.48
1:Q:108:ASP:OD1	1:Q:149:TYR:OH	2.25	0.48
1:R:136:PRO:HG3	1:R:142:ALA:HB2	1.95	0.48
2:G:84:VAL:HG22	2:G:145:VAL:HG12	1.96	0.48
2:S:98:LEU:HD21	2:S:139:ILE:HD11	1.96	0.48
1:U:94:GLY:HA3	1:U:254:THR:HA	1.96	0.48
1:V:361:ASN:HB3	1:V:661:LEU:HB3	1.94	0.48
1:V:389:ALA:HB1	1:V:392:ALA:HB3	1.95	0.48
2:X:113:THR:HG23	2:X:115:VAL:HG22	1.96	0.48
1:E:619:VAL:HG12	1:E:628:LYS:HD2	1.95	0.48
1:E:555:MET:HB3	1:F:138:HIS:HD2	1.79	0.48
2:H:289:GLU:HG2	2:H:290:ALA:H	1.79	0.48
2:K:175:GLU:HG2	2:O:52:PRO:HG3	1.96	0.48
2:P:238:ASP:HB3	2:P:245:ILE:HB	1.96	0.48
2:W:212:SER:OG	2:W:216:ARG:NH2	2.44	0.48
1:A:520:GLY:HA2	5:A:703:FAD:H9	1.95	0.47
1:I:415:LYS:NZ	1:J:199:ASP:OD2	2.47	0.47
1:J:683:THR:HG22	1:J:685:GLY:H	1.78	0.47
2:L:75:ARG:NH2	2:L:129:ASP:OD2	2.46	0.47
1:M:352:LEU:HD22	1:M:381:VAL:HG13	1.95	0.47
3:V:701:TPP:HN42	3:V:701:TPP:H2	1.79	0.47
2:C:151:TYR:HB3	2:C:156:ILE:HD13	1.96	0.47
2:D:128:GLN:O	2:D:132:ILE:HG12	2.14	0.47
2:D:162:VAL:HB	2:D:255:ILE:HD11	1.96	0.47
2:D:84:VAL:HA	2:D:145:VAL:HA	1.96	0.47
1:E:615:LYS:HB2	1:E:639:VAL:HG12	1.96	0.47
2:H:138:GLN:O	2:H:140:GLU:N	2.38	0.47
1:M:94:GLY:HA3	1:M:254:THR:HA	1.96	0.47
1:V:326:ARG:HD3	1:V:435:MET:HE3	1.95	0.47
1:V:484:ALA:HB1	1:V:491:VAL:HG21	1.96	0.47
1:N:162:THR:OG1	1:N:163:SER:N	2.47	0.47
1:N:491:VAL:HG22	1:N:543:LEU:HD23	1.95	0.47
1:A:676:THR:O	1:A:680:HIS:ND1	2.46	0.47
1:A:165:PRO:HD3	1:B:522:LEU:HG	1.97	0.47
1:R:141:GLY:O	1:R:145:MET:HG2	2.14	0.47
2:W:223:ASN:HA	2:W:226:THR:HG22	1.96	0.47
1:M:209:ILE:HG23	1:N:209:ILE:HG23	1.96	0.47
1:N:679:ARG:NH1	1:N:687:HIS:O	2.46	0.47
2:P:250:ALA:H	2:P:255:ILE:HD11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:254:ARG:NH2	7:T:401:ATP:O4'	2.48	0.47
1:N:325:ASP:OD1	1:N:347:LYS:NZ	2.40	0.47
1:N:582:MET:N	8:N:802:HOH:O	2.44	0.47
1:E:442:LYS:HD2	1:V:618:ARG:NH1	2.30	0.47
1:J:619:VAL:HG23	1:J:624:GLU:HB3	1.96	0.47
1:A:403:ILE:H	1:A:420:GLN:HG2	1.79	0.47
1:A:600:GLN:HB2	1:B:137:LYS:HE2	1.97	0.47
1:B:412:ASN:ND2	5:B:703:FAD:O3B	2.40	0.47
1:E:554:ASN:ND2	1:E:602:ASN:OD1	2.47	0.47
1:N:604:ASP:OD1	1:N:618:ARG:NH2	2.48	0.47
1:Q:402:GLY:HA3	1:Q:420:GLN:HG3	1.97	0.47
1:R:546:ASP:HB3	1:R:572:ILE:HG22	1.96	0.47
2:D:254:ARG:NH2	7:D:401:ATP:O4'	2.48	0.47
1:F:520:GLY:HA2	5:F:703:FAD:H9	1.97	0.47
1:V:676:THR:O	1:V:680:HIS:ND1	2.47	0.47
1:E:668:ASP:HA	1:E:669:PRO:HD2	1.72	0.47
2:H:285:THR:HG23	2:H:288:GLU:H	1.80	0.47
1:I:209:ILE:HG23	1:J:209:ILE:HG23	1.95	0.47
1:M:480:LEU:HD22	1:M:573:LEU:HD22	1.96	0.47
2:O:142:LEU:HB3	2:O:144:PRO:HD2	1.95	0.47
7:S:401:ATP:N6	2:T:239:ILE:O	2.48	0.47
1:V:151:ARG:HD3	1:V:182:ILE:HG12	1.97	0.47
1:E:109:THR:HG21	1:E:537:VAL:HG11	1.97	0.46
2:H:78:HIS:CG	2:H:132:ILE:HG12	2.50	0.46
1:J:495:THR:HG22	1:J:547:ILE:HB	1.97	0.46
1:M:520:GLY:HA2	5:M:703:FAD:H9	1.97	0.46
1:N:274:ASN:N	1:N:274:ASN:OD1	2.48	0.46
3:N:701:TPP:H2	3:N:701:TPP:HN42	1.80	0.46
2:O:78:HIS:CG	2:O:132:ILE:HG12	2.49	0.46
2:P:231:ASN:O	7:P:401:ATP:O2'	2.26	0.46
1:Q:217:ASN:H	2:S:93:ARG:HH22	1.63	0.46
1:A:614:LEU:HG	1:A:638:PRO:HB2	1.96	0.46
1:E:202:GLN:HG2	1:F:522:LEU:O	2.16	0.46
1:M:604:ASP:OD1	1:M:618:ARG:NH2	2.46	0.46
1:E:520:GLY:HA2	5:E:703:FAD:H9	1.97	0.46
2:O:165:ARG:NH1	2:P:279:PRO:O	2.46	0.46
2:T:160:GLU:HB2	2:T:255:ILE:HD12	1.97	0.46
1:J:153:SER:HB3	1:J:538:ALA:HB1	1.96	0.46
1:U:144:HIS:HB2	1:U:530:PRO:HB2	1.98	0.46
1:J:564:VAL:HG12	1:J:638:PRO:HG2	1.98	0.46
1:Q:216:TRP:HB2	2:S:143:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:LEU:HD21	2:G:139:ILE:HD11	1.98	0.46
1:J:415:LYS:HG3	1:J:416:VAL:HG23	1.98	0.46
1:N:94:GLY:HA3	1:N:254:THR:HA	1.98	0.46
1:Q:162:THR:OG1	1:Q:163:SER:N	2.48	0.46
2:S:251:LYS:HE3	7:S:401:ATP:PB	2.56	0.46
1:U:670:GLU:OE1	1:U:673:ARG:NH2	2.49	0.46
2:D:264:PRO:HB3	2:P:49:LEU:HD13	1.96	0.46
2:C:238:ASP:HB3	2:C:245:ILE:HB	1.97	0.46
1:F:501:GLN:NE2	1:F:518:THR:OG1	2.48	0.46
1:F:553:PHE:HZ	1:F:560:LEU:HD11	1.80	0.46
2:L:231:ASN:O	7:L:401:ATP:O2'	2.28	0.46
3:M:701:TPP:H2	3:M:701:TPP:HN42	1.80	0.46
2:O:256:SER:HB3	2:O:272:ARG:HH12	1.79	0.46
2:H:125:LEU:HD13	2:H:132:ILE:HG13	1.97	0.46
1:I:306:VAL:HB	1:I:333:THR:HG22	1.98	0.46
1:I:472:LYS:HB3	1:I:472:LYS:HE2	1.78	0.46
2:S:67:THR:HA	2:S:68:PRO:HD3	1.85	0.46
1:U:501:GLN:NE2	1:U:518:THR:OG1	2.49	0.46
1:E:594:ARG:NH2	1:F:123:ASP:OD1	2.47	0.46
2:H:263:GLU:OE1	2:K:286:SER:OG	2.34	0.46
1:M:330:PRO:HB2	1:M:349:LEU:HD11	1.97	0.46
1:Q:361:ASN:HB3	1:Q:661:LEU:HB3	1.98	0.46
1:B:137:LYS:NZ	1:B:561:SER:OG	2.39	0.45
1:N:109:THR:HG21	1:N:537:VAL:HG11	1.96	0.45
2:O:292:ASP:OD1	2:O:292:ASP:N	2.48	0.45
5:U:703:FAD:H9	5:U:703:FAD:H1'1	1.71	0.45
2:W:157:ILE:HD11	2:W:280:ARG:NE	2.31	0.45
1:I:561:SER:OG	1:I:612:MET:SD	2.72	0.45
1:U:268:LEU:HA	1:U:269:PRO:HD3	1.87	0.45
1:U:554:ASN:HA	1:U:557:LEU:HD12	1.97	0.45
3:U:701:TPP:HN42	3:U:701:TPP:H2	1.81	0.45
1:I:587:GLN:HA	1:I:591:TYR:HB2	1.99	0.45
2:P:98:LEU:HD11	2:P:123:ILE:HD13	1.97	0.45
1:Q:179:ALA:O	1:Q:241:ARG:NH2	2.45	0.45
1:V:151:ARG:HH11	1:V:182:ILE:HD11	1.81	0.45
1:E:162:THR:OG1	1:E:163:SER:N	2.48	0.45
1:J:330:PRO:HB2	1:J:349:LEU:HD11	1.98	0.45
1:E:635:THR:CG2	1:E:639:VAL:CG1	2.87	0.45
1:I:551:ALA:HB3	3:I:701:TPP:H72	1.99	0.45
1:J:391:GLU:OE1	1:J:394:ARG:NH1	2.49	0.45
1:N:545:ILE:HA	1:N:571:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:NE2	1:A:248:ASP:OD2	2.46	0.45
1:E:226:LEU:HB3	1:E:227:PRO:HD3	1.99	0.45
1:E:323:LEU:HD13	1:E:435:MET:HE1	1.98	0.45
1:E:153:SER:HB3	1:E:538:ALA:HB1	1.98	0.45
1:N:480:LEU:HD21	1:N:545:ILE:HG21	1.99	0.45
1:Q:209:ILE:HG23	1:R:209:ILE:HG23	1.98	0.45
2:C:182:HIS:O	2:C:182:HIS:ND1	2.48	0.45
2:C:161:LEU:HB2	2:D:161:LEU:HD12	1.98	0.45
2:H:140:GLU:HA	2:H:145:VAL:HG21	1.99	0.45
1:N:347:LYS:HG2	1:N:448:PHE:CE1	2.52	0.45
2:X:64:ILE:O	2:X:67:THR:CB	2.64	0.45
1:F:646:ASP:OD2	1:F:647:LYS:N	2.50	0.45
1:J:103:SER:HB3	1:J:130:LYS:HD2	1.98	0.45
2:P:259:LEU:HA	2:P:262:VAL:HG12	1.99	0.45
1:Q:604:ASP:HB2	1:Q:607:LYS:HE2	1.99	0.45
1:U:202:GLN:HG2	1:V:522:LEU:O	2.17	0.45
1:U:474:GLN:HB2	1:U:507:HIS:ND1	2.31	0.45
1:A:560:LEU:HD23	1:A:612:MET:HG3	1.99	0.45
1:F:352:LEU:HD11	1:F:364:VAL:HG21	1.98	0.45
1:U:619:VAL:HG21	1:U:625:LEU:HA	1.98	0.45
1:I:292:ALA:HA	1:I:421:ILE:HD12	1.99	0.44
1:J:520:GLY:HA2	5:J:703:FAD:H9	1.99	0.44
1:U:210:SER:O	1:U:214:THR:OG1	2.24	0.44
1:U:358:ALA:HB3	1:U:458:TYR:HB3	1.98	0.44
1:U:587:GLN:HA	1:U:591:TYR:HD2	1.82	0.44
1:A:137:LYS:HB3	1:B:554:ASN:O	2.17	0.44
1:E:385:ILE:HD12	1:E:385:ILE:H	1.82	0.44
1:E:407:GLU:HG3	1:E:409:SER:H	1.82	0.44
1:J:162:THR:OG1	1:J:163:SER:N	2.50	0.44
1:Q:676:THR:O	1:Q:680:HIS:ND1	2.42	0.44
1:U:489:ARG:HH21	1:U:543:LEU:HD13	1.82	0.44
1:V:137:LYS:NZ	1:V:561:SER:OG	2.50	0.44
1:A:122:TYR:HA	1:A:125:ILE:HG12	1.98	0.44
1:B:226:LEU:HB3	1:B:227:PRO:HD3	2.00	0.44
1:F:480:LEU:HD13	1:F:629:LEU:HD22	2.00	0.44
2:G:108:LEU:HD13	2:G:123:ILE:HG12	1.98	0.44
2:K:105:ILE:H	2:K:125:LEU:HD23	1.81	0.44
1:M:580:GLN:HB3	3:M:701:TPP:H61	1.98	0.44
1:V:304:LEU:HD23	1:V:371:ILE:HB	2.00	0.44
1:V:550:ASP:O	1:V:554:ASN:ND2	2.32	0.44
2:W:78:HIS:CG	2:W:132:ILE:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:TYR:HA	1:B:125:ILE:HG12	1.97	0.44
3:B:701:TPP:H2	3:B:701:TPP:HN42	1.83	0.44
2:G:47:PRO:HD3	2:O:207:ALA:HA	1.98	0.44
2:H:98:LEU:HD11	2:H:123:ILE:HD13	2.00	0.44
2:O:273:SER:HA	2:P:111:CYS:HA	1.98	0.44
2:P:108:LEU:HG	2:P:123:ILE:HG12	1.99	0.44
1:V:619:VAL:HG22	1:V:628:LYS:HG2	1.99	0.44
2:W:151:TYR:HB3	2:W:156:ILE:HD13	2.00	0.44
2:W:273:SER:HB3	2:X:276:MET:SD	2.57	0.44
2:X:113:THR:HG21	2:X:118:LEU:HD23	2.00	0.44
2:H:238:ASP:HB3	2:H:245:ILE:HB	2.00	0.44
1:U:474:GLN:HB2	1:U:507:HIS:CE1	2.52	0.44
2:S:171:THR:HG21	2:W:49:LEU:HD13	2.00	0.44
1:E:94:GLY:HA3	1:E:254:THR:HA	2.00	0.44
3:E:701:TPP:H2	3:E:701:TPP:HN42	1.82	0.44
1:F:550:ASP:O	1:F:554:ASN:ND2	2.37	0.44
1:F:591:TYR:O	1:F:594:ARG:HG2	2.17	0.44
2:H:139:ILE:HA	2:H:142:LEU:HD13	2.00	0.44
1:I:183:PRO:HB3	1:I:242:PRO:HB3	2.00	0.44
5:M:703:FAD:H1'	5:M:703:FAD:H9	1.77	0.44
1:R:385:ILE:HD12	1:R:385:ILE:H	1.83	0.44
1:V:183:PRO:HB3	1:V:242:PRO:HB3	1.98	0.44
1:A:304:LEU:HD23	1:A:371:ILE:HB	2.00	0.44
1:A:347:LYS:HB2	1:A:347:LYS:HE3	1.83	0.44
1:I:137:LYS:O	1:J:555:MET:HG2	2.18	0.44
1:U:546:ASP:N	1:U:571:LYS:O	2.41	0.44
1:M:355:HIS:O	1:M:506:GLN:NE2	2.47	0.44
1:I:151:ARG:HH11	1:I:182:ILE:HD11	1.83	0.43
2:O:98:LEU:HD11	2:O:123:ILE:HD13	2.00	0.43
1:A:357:CYS:HB3	1:A:460:TYR:CZ	2.54	0.43
1:A:153:SER:HB3	1:A:538:ALA:HB1	1.99	0.43
1:M:115:GLY:HA3	1:M:162:THR:HB	2.00	0.43
1:Q:407:GLU:OE2	5:Q:703:FAD:O2B	2.33	0.43
1:U:226:LEU:HB3	1:U:227:PRO:HD3	2.00	0.43
1:V:93:THR:HG22	1:V:257:ILE:HG12	2.01	0.43
2:X:238:ASP:HB3	2:X:245:ILE:HB	2.00	0.43
2:C:52:PRO:HB2	2:O:178:LEU:HD23	2.00	0.43
1:E:190:GLN:NE2	1:E:248:ASP:OD2	2.48	0.43
1:E:474:GLN:HG2	1:E:474:GLN:H	1.52	0.43
2:G:254:ARG:NH2	7:G:401:ATP:O4'	2.52	0.43
1:M:306:VAL:HB	1:M:333:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:550:ASP:N	1:M:550:ASP:OD1	2.51	0.43
1:M:612:MET:HA	1:N:603:PRO:HB3	2.00	0.43
3:Q:701:TPP:HN42	3:Q:701:TPP:H2	1.83	0.43
2:T:78:HIS:CG	2:T:132:ILE:HG12	2.53	0.43
1:E:122:TYR:HA	1:E:125:ILE:HG12	2.00	0.43
2:G:238:ASP:HB3	2:G:245:ILE:HB	2.00	0.43
2:L:82:CYS:HB2	2:L:121:MET:HB2	1.99	0.43
1:M:473:PRO:HG3	1:M:645:VAL:HB	2.01	0.43
1:A:209:ILE:HG23	1:B:209:ILE:HG23	2.00	0.43
1:B:495:THR:HG22	1:B:547:ILE:HB	2.00	0.43
1:E:558:THR:HG23	1:F:557:LEU:HD21	2.00	0.43
1:M:512:ASN:HB2	1:M:515:THR:HG21	2.00	0.43
1:Q:216:TRP:HA	2:S:93:ARG:HH21	1.83	0.43
1:U:252:ASP:OD1	1:U:252:ASP:N	2.52	0.43
1:U:683:THR:HG21	1:U:687:HIS:HB2	2.00	0.43
1:A:137:LYS:HE2	1:B:600:GLN:HB2	2.00	0.43
1:A:680:HIS:O	1:A:685:GLY:N	2.50	0.43
1:B:676:THR:O	1:B:680:HIS:ND1	2.50	0.43
1:F:302:PRO:HG2	1:F:329:ILE:HG22	1.99	0.43
1:F:84:ASP:OD1	1:F:84:ASP:N	2.52	0.43
1:I:522:LEU:O	1:J:202:GLN:HG2	2.18	0.43
1:R:587:GLN:O	1:R:587:GLN:NE2	2.52	0.43
1:V:241:ARG:HG3	5:V:703:FAD:H2B	2.00	0.43
1:E:357:CYS:HB3	1:E:460:TYR:CZ	2.53	0.43
1:N:606:ILE:HD13	1:N:618:ARG:HE	1.84	0.43
2:S:238:ASP:HB3	2:S:245:ILE:HB	2.00	0.43
1:U:236:ILE:HD13	2:W:143:VAL:HG21	2.01	0.43
1:V:276:LEU:HD21	2:W:185:THR:HG22	2.00	0.43
1:A:226:LEU:HB3	1:A:227:PRO:HD3	2.01	0.43
1:A:268:LEU:HA	1:A:269:PRO:HD3	1.85	0.43
1:E:522:LEU:O	1:F:202:GLN:HG2	2.19	0.43
1:E:635:THR:O	1:E:635:THR:HG23	2.19	0.43
1:J:554:ASN:HA	1:J:557:LEU:HD23	2.00	0.43
2:L:214:VAL:HG12	2:L:218:LYS:HE3	1.99	0.43
1:U:619:VAL:HG23	1:U:624:GLU:HB2	2.00	0.43
1:V:153:SER:HB3	1:V:538:ALA:HB1	2.01	0.43
2:X:229:THR:O	2:X:234:GLY:N	2.49	0.43
1:A:93:THR:HG22	1:A:257:ILE:HG12	2.00	0.43
2:C:178:LEU:HD21	2:G:54:TRP:HA	2.00	0.43
1:I:273:LEU:HA	1:I:276:LEU:HD23	2.01	0.43
1:I:305:TYR:HB3	1:I:372:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:522:LEU:O	1:V:202:GLN:HG2	2.19	0.43
1:B:357:CYS:HB3	1:B:460:TYR:CZ	2.54	0.43
2:D:238:ASP:HB3	2:D:245:ILE:HB	2.00	0.43
2:D:62:SER:O	2:D:66:GLU:HG2	2.19	0.43
1:I:269:PRO:HG2	2:K:143:VAL:O	2.19	0.43
2:K:151:TYR:HB3	2:K:156:ILE:HG21	2.01	0.43
2:K:166:ILE:HD13	2:K:262:VAL:HG21	2.01	0.43
1:M:265:LYS:H	1:M:265:LYS:HG3	1.62	0.43
1:M:352:LEU:HD11	1:M:364:VAL:HG21	2.00	0.43
1:N:349:LEU:O	1:N:360:ALA:HB2	2.19	0.43
1:N:636:LYS:HA	1:N:636:LYS:HD2	1.89	0.43
1:F:396:ALA:HB2	1:F:402:GLY:HA2	2.01	0.42
1:F:550:ASP:HB3	1:F:576:ASN:HA	2.01	0.42
1:M:487:THR:HG21	1:M:633:VAL:HG11	2.00	0.42
1:V:258:LEU:HD21	1:V:262:ILE:HG12	2.00	0.42
2:H:139:ILE:O	2:H:142:LEU:HB2	2.19	0.42
2:K:162:VAL:HG21	2:K:259:LEU:HD21	2.01	0.42
2:L:81:ASN:HD21	2:L:120:ARG:HD3	1.83	0.42
1:N:646:ASP:OD1	1:N:647:LYS:N	2.49	0.42
2:O:280:ARG:HG2	2:O:281:THR:H	1.84	0.42
2:P:84:VAL:HG22	2:P:145:VAL:HG12	2.01	0.42
1:Q:323:LEU:HD22	1:Q:431:LEU:HD22	2.01	0.42
1:A:443:GLU:OE2	1:A:444:ARG:N	2.52	0.42
3:A:701:TPP:H2	3:A:701:TPP:HN42	1.84	0.42
2:C:78:HIS:CG	2:C:132:ILE:HG13	2.55	0.42
1:E:564:VAL:HG23	1:F:601:LEU:HD23	2.01	0.42
1:E:571:LYS:NZ	1:E:637:GLY:O	2.51	0.42
1:I:329:ILE:H	1:I:329:ILE:HD13	1.84	0.42
1:I:554:ASN:HA	1:I:557:LEU:HB2	2.00	0.42
2:P:161:LEU:HD23	2:P:249:SER:HB3	2.01	0.42
1:V:330:PRO:HB2	1:V:349:LEU:HD11	1.99	0.42
2:W:270:CYS:SG	2:W:271:ALA:N	2.92	0.42
2:X:166:ILE:HD13	2:X:262:VAL:HG21	2.02	0.42
1:E:407:GLU:OE2	5:E:703:FAD:O3B	2.25	0.42
1:M:500:HIS:N	3:M:701:TPP:O2B	2.45	0.42
1:V:602:ASN:HA	1:V:603:PRO:HD3	1.89	0.42
1:A:202:GLN:HG2	1:B:522:LEU:O	2.20	0.42
1:A:522:LEU:HG	1:B:165:PRO:HD3	2.01	0.42
1:B:619:VAL:HG22	1:B:628:LYS:HG3	2.01	0.42
1:F:675:GLN:HA	1:F:678:LEU:HB3	2.01	0.42
1:I:369:LEU:HD11	1:I:404:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:499:GLN:HB3	1:I:503:TRP:CZ3	2.54	0.42
1:M:226:LEU:HB3	1:M:227:PRO:HD3	2.01	0.42
2:P:270:CYS:SG	2:P:271:ALA:N	2.93	0.42
1:Q:138:HIS:HD2	1:R:555:MET:HB2	1.84	0.42
1:A:553:PHE:O	1:A:557:LEU:HB3	2.20	0.42
3:B:701:TPP:C2	3:B:701:TPP:HN42	2.32	0.42
2:C:263:GLU:N	2:C:264:PRO:HD2	2.34	0.42
2:D:156:ILE:HD12	2:D:277:ALA:HB1	2.01	0.42
1:I:289:ILE:HG23	1:I:434:MET:HG3	2.02	0.42
1:I:617:LEU:HB3	1:I:628:LYS:HE3	2.01	0.42
1:M:109:THR:HG21	1:M:537:VAL:HG11	2.01	0.42
1:N:226:LEU:HB3	1:N:227:PRO:HD3	2.02	0.42
2:O:204:PHE:HA	2:O:209:LEU:HD11	2.01	0.42
1:U:354:MET:HG3	1:U:655:VAL:O	2.19	0.42
1:V:145:MET:HG2	1:V:530:PRO:O	2.19	0.42
1:V:554:ASN:HA	1:V:557:LEU:HD23	2.01	0.42
2:W:98:LEU:HD22	2:W:105:ILE:HD11	2.01	0.42
1:E:615:LYS:HD2	1:E:639:VAL:HG12	2.01	0.42
1:J:403:ILE:N	1:J:420:GLN:OE1	2.48	0.42
1:J:579:GLU:OE1	1:J:648:LYS:NZ	2.41	0.42
5:J:703:FAD:H9	5:J:703:FAD:H1'1	1.72	0.42
1:M:352:LEU:HD23	1:M:353:GLY:N	2.34	0.42
1:A:109:THR:HG21	1:A:537:VAL:HG11	2.01	0.42
2:C:78:HIS:CD2	2:C:132:ILE:HG13	2.54	0.42
2:C:84:VAL:HG22	2:C:145:VAL:HG12	2.02	0.42
1:J:105:GLN:HG2	1:J:234:PHE:CG	2.54	0.42
2:K:292:ASP:OD1	2:K:292:ASP:N	2.50	0.42
1:N:306:VAL:HB	1:N:333:THR:HG22	2.01	0.42
1:Q:277:THR:C	1:Q:279:ARG:N	2.72	0.42
2:T:156:ILE:HG22	2:T:279:PRO:HA	2.02	0.42
1:I:501:GLN:NE2	1:I:518:THR:OG1	2.52	0.42
1:J:113:TYR:HA	1:J:114:PRO:HD3	1.88	0.42
1:M:646:ASP:OD1	1:M:647:LYS:N	2.52	0.42
7:W:402:ATP:H2'	7:W:402:ATP:H8	1.68	0.42
1:A:192:PRO:HG3	1:A:251:LYS:HB3	2.02	0.42
5:A:703:FAD:H1'1	5:A:703:FAD:H9	1.78	0.42
1:B:277:THR:HG22	1:B:280:ALA:HB3	2.02	0.42
2:C:156:ILE:HA	2:C:279:PRO:HA	2.01	0.42
1:F:426:ASP:O	1:F:430:ASN:ND2	2.37	0.42
1:M:606:ILE:HG23	1:M:616:GLY:HA3	2.02	0.42
1:N:304:LEU:HD23	1:N:331:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:141:GLY:O	1:R:145:MET:N	2.46	0.42
2:S:251:LYS:O	2:S:255:ILE:HG12	2.20	0.42
2:S:259:LEU:HA	2:S:262:VAL:HG12	2.02	0.42
1:A:407:GLU:OE2	5:A:703:FAD:O2B	2.28	0.41
1:B:491:VAL:HG22	1:B:543:LEU:HD23	2.02	0.41
2:D:161:LEU:H	2:D:273:SER:HB3	1.85	0.41
1:E:409:SER:HA	1:E:410:PRO:HD3	1.92	0.41
2:H:97:THR:O	2:H:101:ARG:HG2	2.20	0.41
1:M:202:GLN:HG2	1:N:522:LEU:O	2.20	0.41
1:B:553:PHE:HZ	1:B:560:LEU:HD11	1.85	0.41
1:E:500:HIS:HB2	1:E:575:LEU:HD12	2.02	0.41
2:L:175:GLU:HB3	2:L:199:ILE:HD13	2.02	0.41
1:R:376:ARG:HB3	5:R:701:FAD:O3B	2.20	0.41
2:W:156:ILE:HG22	2:W:279:PRO:HA	2.03	0.41
1:A:619:VAL:HG21	1:A:625:LEU:HA	2.02	0.41
1:B:480:LEU:HD13	1:B:629:LEU:HD22	2.02	0.41
1:F:172:THR:HB	1:F:173:PRO:HD3	2.02	0.41
1:J:435:MET:O	1:J:436:SER:OG	2.34	0.41
2:L:235:ARG:HH21	2:L:247:GLU:CD	2.23	0.41
1:N:361:ASN:HB3	1:N:661:LEU:HB3	2.01	0.41
1:V:172:THR:HB	1:V:173:PRO:HD3	2.02	0.41
1:A:474:GLN:HB3	1:A:507:HIS:CE1	2.55	0.41
1:B:172:THR:HB	1:B:173:PRO:HD3	2.03	0.41
1:I:577:ASN:HB3	1:I:645:VAL:HG23	2.02	0.41
1:J:137:LYS:HB3	1:J:137:LYS:HE2	1.89	0.41
1:J:333:THR:O	1:J:351:MET:HA	2.19	0.41
1:Q:190:GLN:HB3	1:Q:250:PRO:HA	2.02	0.41
1:Q:226:LEU:HB3	1:Q:227:PRO:HD3	2.02	0.41
1:R:318:ARG:HG3	1:R:319:LEU:N	2.35	0.41
2:C:160:GLU:HG3	2:C:252:PRO:HG3	2.03	0.41
1:J:357:CYS:HB3	1:J:460:TYR:CZ	2.55	0.41
1:N:385:ILE:HG22	1:N:386:SER:H	1.86	0.41
5:N:703:FAD:H9	5:N:703:FAD:H1'1	1.78	0.41
1:Q:115:GLY:O	1:Q:118:ILE:HG22	2.21	0.41
1:V:491:VAL:HG22	1:V:543:LEU:HD23	2.01	0.41
1:A:349:LEU:O	1:A:360:ALA:HB2	2.20	0.41
1:F:350:ASP:HB3	1:F:351:MET:H	1.69	0.41
5:J:703:FAD:H1'2	5:J:703:FAD:H4'	1.74	0.41
7:L:401:ATP:H8	7:L:401:ATP:H2'	1.71	0.41
2:L:73:GLN:HA	2:L:74:PRO:HD3	1.93	0.41
1:M:296:ILE:HD12	1:M:434:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:557:LEU:HG	1:N:558:THR:HG22	2.02	0.41
1:Q:520:GLY:HA2	5:Q:703:FAD:H9	2.02	0.41
2:T:251:LYS:HE2	2:T:254:ARG:NH1	2.36	0.41
1:U:396:ALA:HB2	1:U:402:GLY:HA2	2.02	0.41
2:X:70:PRO:O	2:X:71:SER:HB2	2.20	0.41
1:J:407:GLU:OE2	5:J:703:FAD:O2B	2.36	0.41
1:M:409:SER:HA	1:M:410:PRO:HD3	1.88	0.41
2:O:110:VAL:HG22	2:O:121:MET:HG2	2.03	0.41
2:O:235:ARG:NH2	2:P:249:SER:O	2.54	0.41
1:V:89:PHE:HA	1:V:92:LEU:HD12	2.01	0.41
1:A:557:LEU:HD22	1:A:557:LEU:H	1.85	0.41
1:E:413:ILE:HG22	1:E:414:ASN:ND2	2.36	0.41
1:E:555:MET:HG2	1:F:137:LYS:O	2.21	0.41
1:F:376:ARG:HD3	5:F:703:FAD:H51A	2.03	0.41
2:H:158:LYS:O	2:H:159:ARG:NE	2.53	0.41
2:C:205:HIS:CE1	2:K:45:PRO:HG2	2.54	0.41
1:N:448:PHE:HA	1:N:451:ILE:HG12	2.03	0.41
1:V:354:MET:HA	1:V:655:VAL:HB	2.03	0.41
1:A:345:ASP:HA	1:A:346:PRO:HD3	1.97	0.41
1:A:366:ASN:HA	1:A:391:GLU:HG3	2.03	0.41
1:B:197:GLY:HA3	2:C:101:ARG:HA	2.02	0.41
1:F:580:GLN:HB3	3:F:701:TPP:H61	2.01	0.41
1:I:385:ILE:H	1:I:385:ILE:HD12	1.85	0.41
1:J:365:GLN:NE2	1:J:661:LEU:HB2	2.35	0.41
1:J:380:ARG:NH2	6:J:704:60G:OAG	2.35	0.41
2:L:86:ASN:HB3	2:L:117:ASP:HA	2.02	0.41
2:L:232:PHE:HA	7:L:401:ATP:O2'	2.21	0.41
1:M:172:THR:HB	1:M:173:PRO:HD3	2.03	0.41
1:Q:522:LEU:HG	1:R:165:PRO:HD3	2.03	0.41
1:A:409:SER:HA	1:A:410:PRO:HD3	1.88	0.41
1:Q:227:PRO:HG2	1:Q:262:ILE:HD12	2.02	0.41
1:Q:273:LEU:C	1:Q:273:LEU:HD22	2.39	0.41
2:T:256:SER:HA	2:T:272:ARG:HH12	1.86	0.41
1:U:453:LYS:O	1:U:457:GLU:HG2	2.20	0.41
1:U:479:LYS:HE2	1:U:479:LYS:HB3	1.84	0.41
2:G:240:SER:OG	2:G:241:GLU:N	2.54	0.41
1:Q:217:ASN:H	2:S:93:ARG:NH2	2.19	0.41
1:V:500:HIS:N	3:V:701:TPP:O2B	2.51	0.41
1:A:97:ILE:HG21	1:A:227:PRO:HG3	2.03	0.40
1:I:497:VAL:HG21	1:I:523:GLY:C	2.41	0.40
1:J:101:MET:HG3	1:J:230:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:336:GLN:HE22	1:U:518:THR:HG23	1.86	0.40
2:X:201:GLU:HA	2:X:208:ASN:HD21	1.86	0.40
2:X:162:VAL:HG21	2:X:259:LEU:HD21	2.02	0.40
2:X:65:TYR:CD2	2:X:65:TYR:C	2.95	0.40
1:B:323:LEU:HD22	1:B:431:LEU:HD22	2.02	0.40
2:H:167:SER:HB2	2:H:268:LEU:HD21	2.03	0.40
1:Q:274:ASN:C	1:Q:276:LEU:N	2.73	0.40
1:R:587:GLN:HB2	1:R:587:GLN:HE21	1.64	0.40
1:V:495:THR:HG22	1:V:547:ILE:HB	2.02	0.40
1:A:115:GLY:HA3	1:A:162:THR:HB	2.02	0.40
1:B:217:ASN:H	2:D:93:ARG:NH2	2.16	0.40
2:D:192:SER:HB3	2:D:195:LEU:HD12	2.03	0.40
3:E:701:TPP:C2	3:E:701:TPP:HN42	2.35	0.40
1:F:336:GLN:NE2	1:F:520:GLY:H	2.19	0.40
2:L:120:ARG:HH21	2:O:63:ILE:HD13	1.86	0.40
1:U:123:ASP:O	1:V:594:ARG:NH2	2.46	0.40
1:V:122:TYR:HA	1:V:125:ILE:HG12	2.02	0.40
1:V:407:GLU:HG3	1:V:409:SER:H	1.86	0.40
1:A:369:LEU:HD11	1:A:404:ILE:HG13	2.04	0.40
1:A:512:ASN:HB2	1:A:515:THR:HG21	2.04	0.40
1:B:162:THR:OG1	1:B:163:SER:N	2.52	0.40
1:B:216:TRP:CE3	1:B:236:ILE:HD12	2.57	0.40
1:E:113:TYR:HA	1:E:114:PRO:HD3	1.90	0.40
1:E:600:GLN:HB2	1:F:137:LYS:HE2	2.03	0.40
1:F:162:THR:OG1	1:F:163:SER:N	2.54	0.40
2:G:68:PRO:HG2	2:G:70:PRO:HD3	2.03	0.40
1:F:217:ASN:OD1	2:H:93:ARG:NH1	2.54	0.40
1:J:94:GLY:HA3	1:J:254:THR:HA	2.02	0.40
2:L:160:GLU:HB3	2:L:255:ILE:HD12	2.04	0.40
1:N:501:GLN:NE2	1:N:518:THR:OG1	2.48	0.40
1:R:93:THR:HG22	1:R:257:ILE:HG12	2.03	0.40
1:U:498:GLY:HA2	1:U:582:MET:HB2	2.03	0.40
1:V:108:ASP:OD1	1:V:149:TYR:OH	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	41	74
1	F	602/644 (94%)	572 (95%)	26 (4%)	4 (1%)	22	61
1	I	602/644 (94%)	582 (97%)	20 (3%)	0	100	100
1	J	600/644 (93%)	569 (95%)	28 (5%)	3 (0%)	29	67
1	M	603/644 (94%)	566 (94%)	36 (6%)	1 (0%)	47	79
1	N	601/644 (93%)	569 (95%)	31 (5%)	1 (0%)	47	79
1	Q	594/644 (92%)	570 (96%)	22 (4%)	2 (0%)	41	74
1	R	394/644 (61%)	369 (94%)	21 (5%)	4 (1%)	15	54
1	U	602/644 (94%)	569 (94%)	31 (5%)	2 (0%)	41	74
1	V	603/644 (94%)	574 (95%)	28 (5%)	1 (0%)	47	79
2	C	251/297 (84%)	243 (97%)	7 (3%)	1 (0%)	34	69
2	D	248/297 (84%)	235 (95%)	10 (4%)	3 (1%)	13	49
2	G	251/297 (84%)	237 (94%)	13 (5%)	1 (0%)	34	69
2	H	250/297 (84%)	235 (94%)	13 (5%)	2 (1%)	19	58
2	K	241/297 (81%)	221 (92%)	15 (6%)	5 (2%)	7	37
2	L	253/297 (85%)	237 (94%)	13 (5%)	3 (1%)	13	49
2	O	233/297 (78%)	221 (95%)	11 (5%)	1 (0%)	34	69
2	P	237/297 (80%)	228 (96%)	9 (4%)	0	100	100
2	S	240/297 (81%)	227 (95%)	12 (5%)	1 (0%)	34	69
2	T	226/297 (76%)	214 (95%)	11 (5%)	1 (0%)	34	69
2	W	241/297 (81%)	228 (95%)	10 (4%)	3 (1%)	13	49
2	X	234/297 (79%)	216 (92%)	14 (6%)	4 (2%)	9	42
All	All	9914/11292 (88%)	9412 (95%)	457 (5%)	45 (0%)	29	67

All (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
1	Q	275	GLN
1	R	592	GLU
2	C	74	PRO
2	D	45	PRO
1	F	467	PRO
1	J	350	ASP
2	L	68	PRO
2	L	74	PRO
1	N	459	PRO
1	V	459	PRO
2	W	88	PRO
1	F	350	ASP
1	F	459	PRO
2	K	166	ILE
2	K	282	PRO
1	M	467	PRO
1	Q	277	THR
1	R	556	THR
1	U	459	PRO
2	X	63	ILE
1	E	272	ALA
2	G	274	GLY
1	J	136	PRO
1	J	512	ASN
2	K	90	VAL
2	K	105	ILE
2	K	109	VAL
2	O	109	VAL
2	X	281	THR
1	E	669	PRO
2	S	69	ALA
1	U	370	ILE
2	D	46	LEU
1	F	613	GLY
2	H	74	PRO
2	L	274	GLY
1	R	439	PHE

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Mol	Chain	Res	Type
2	W	45	PRO
2	H	68	PRO
2	D	74	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%)	490 (99%)	5 (1%)	76	90
1	B	496/531 (93%)	493 (99%)	3 (1%)	86	94
1	E	490/531 (92%)	485 (99%)	5 (1%)	76	90
1	F	487/531 (92%)	483 (99%)	4 (1%)	81	93
1	I	481/531 (91%)	472 (98%)	9 (2%)	57	81
1	J	481/531 (91%)	470 (98%)	11 (2%)	50	78
1	M	496/531 (93%)	494 (100%)	2 (0%)	91	95
1	N	493/531 (93%)	490 (99%)	3 (1%)	86	94
1	Q	475/531 (90%)	470 (99%)	5 (1%)	73	88
1	R	307/531 (58%)	293 (95%)	14 (5%)	27	63
1	U	483/531 (91%)	478 (99%)	5 (1%)	76	90
1	V	493/531 (93%)	490 (99%)	3 (1%)	86	94
2	C	217/260 (84%)	213 (98%)	4 (2%)	59	82
2	D	215/260 (83%)	211 (98%)	4 (2%)	57	81
2	G	218/260 (84%)	215 (99%)	3 (1%)	67	86
2	H	220/260 (85%)	216 (98%)	4 (2%)	59	82
2	K	213/260 (82%)	208 (98%)	5 (2%)	50	78
2	L	219/260 (84%)	219 (100%)	0	100	100
2	O	204/260 (78%)	202 (99%)	2 (1%)	76	90
2	P	213/260 (82%)	210 (99%)	3 (1%)	67	86
2	S	210/260 (81%)	203 (97%)	7 (3%)	38	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	203/260 (78%)	198 (98%)	5 (2%)	47	77
2	W	216/260 (83%)	216 (100%)	0	100	100
2	X	207/260 (80%)	203 (98%)	4 (2%)	57	81
All	All	8232/9492 (87%)	8122 (99%)	110 (1%)	69	87

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	350	ASP
1	A	352	LEU
1	A	443	GLU
1	A	557	LEU
1	B	277	THR
1	B	298	LEU
1	B	352	LEU
2	C	42	THR
2	C	178	LEU
2	C	183	THR
2	C	294	ASP
2	D	49	LEU
2	D	87	GLU
2	D	145	VAL
2	D	161	LEU
1	E	87	THR
1	E	331	VAL
1	E	465	GLU
1	E	474	GLN
1	E	558	THR
1	F	295	LEU
1	F	350	ASP
1	F	352	LEU
1	F	548	ASP
2	G	172	GLU
2	G	178	LEU
2	G	195	LEU
2	H	94	VAL
2	H	125	LEU
2	H	129	ASP
2	H	145	VAL
1	I	131	PHE

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Mol	Chain	Res	Type
1	I	304	LEU
1	I	329	ILE
1	I	471	ILE
1	I	548	ASP
1	I	576	ASN
1	I	598	THR
1	I	614	LEU
1	I	640	LEU
1	J	137	LYS
1	J	248	ASP
1	J	275	GLN
1	J	277	THR
1	J	333	THR
1	J	338	LEU
1	J	352	LEU
1	J	365	GLN
1	J	541	GLU
1	J	624	GLU
1	J	641	LEU
2	K	66	GLU
2	K	104	ASN
2	K	132	ILE
2	K	143	VAL
2	K	161	LEU
1	M	265	LYS
1	M	428	THR
1	N	274	ASN
1	N	435	MET
1	N	619	VAL
2	O	76	LYS
2	O	284	LYS
2	P	179	LEU
2	P	195	LEU
2	P	281	THR
1	Q	273	LEU
1	Q	278	SER
1	Q	352	LEU
1	Q	606	ILE
1	Q	623	GLU
1	R	104	ARG
1	R	113	TYR
1	R	151	ARG

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Mol	Chain	Res	Type
1	R	241	ARG
1	R	267	THR
1	R	282	ASP
1	R	313	HIS
1	R	318	ARG
1	R	319	LEU
1	R	326	ARG
1	R	332	THR
1	R	407	GLU
1	R	475	THR
1	R	587	GLN
2	S	46	LEU
2	S	145	VAL
2	S	161	LEU
2	S	182	HIS
2	S	198	GLU
2	S	260	LYS
2	S	281	THR
2	T	46	LEU
2	T	49	LEU
2	T	50	ASP
2	T	109	VAL
2	T	161	LEU
1	U	267	THR
1	U	286	MET
1	U	493	VAL
1	U	557	LEU
1	U	619	VAL
1	V	286	MET
1	V	442	LYS
1	V	623	GLU
2	X	143	VAL
2	X	145	VAL
2	X	161	LEU
2	X	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	HIS
2	G	134	GLN
2	L	81	ASN

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Mol	Chain	Res	Type
1	R	587	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 monosaccharides 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	S	401	-	26,33,33	3.54	9 (34%)	31,52,52	1.36	5 (16%)
6	60G	E	704	-	28,29,29	1.45	4 (14%)	38,40,40	3.43	13 (34%)
6	60G	A	704	-	28,29,29	1.46	4 (14%)	38,40,40	3.41	13 (34%)
6	60G	B	704	-	28,29,29	1.45	3 (10%)	38,40,40	3.40	13 (34%)
3	TPP	A	701	4	22,27,27	1.86	2 (9%)	29,40,40	2.15	13 (44%)
7	ATP	T	401	4	26,33,33	3.52	9 (34%)	31,52,52	1.44	5 (16%)
3	TPP	J	701	4	22,27,27	1.87	3 (13%)	29,40,40	2.13	11 (37%)
6	60G	I	704	-	28,29,29	1.43	4 (14%)	38,40,40	3.41	15 (39%)
7	ATP	P	401	4	26,33,33	3.54	9 (34%)	31,52,52	1.38	5 (16%)
6	60G	U	704	-	28,29,29	1.44	4 (14%)	38,40,40	3.41	14 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	60G	Q	704	-	28,29,29	1.48	4 (14%)	38,40,40	3.40	12 (31%)
3	TPP	Q	701	4	22,27,27	1.83	3 (13%)	29,40,40	2.15	12 (41%)
5	FAD	F	703	-	51,58,58	2.25	10 (19%)	60,89,89	1.52	13 (21%)
5	FAD	R	701	-	51,58,58	2.28	11 (21%)	60,89,89	1.48	11 (18%)
5	FAD	B	703	-	51,58,58	2.26	11 (21%)	60,89,89	1.53	13 (21%)
5	FAD	U	703	-	51,58,58	2.26	11 (21%)	60,89,89	1.47	12 (20%)
3	TPP	I	701	4	22,27,27	1.85	3 (13%)	29,40,40	2.12	12 (41%)
5	FAD	V	703	-	51,58,58	2.27	11 (21%)	60,89,89	1.52	12 (20%)
3	TPP	U	701	4	22,27,27	1.85	3 (13%)	29,40,40	2.15	11 (37%)
7	ATP	H	401	4	26,33,33	3.54	9 (34%)	31,52,52	1.38	5 (16%)
5	FAD	N	703	-	51,58,58	2.27	11 (21%)	60,89,89	1.55	12 (20%)
5	FAD	M	703	-	51,58,58	2.25	11 (21%)	60,89,89	1.53	12 (20%)
7	ATP	O	401	4	26,33,33	3.53	9 (34%)	31,52,52	1.39	5 (16%)
5	FAD	E	703	-	51,58,58	2.26	11 (21%)	60,89,89	1.53	13 (21%)
6	60G	R	702	-	28,29,29	1.47	4 (14%)	38,40,40	3.38	13 (34%)
7	ATP	K	401	4	26,33,33	3.53	9 (34%)	31,52,52	1.40	5 (16%)
3	TPP	M	701	4	22,27,27	1.88	2 (9%)	29,40,40	2.11	11 (37%)
7	ATP	C	401	4	26,33,33	3.53	9 (34%)	31,52,52	1.38	5 (16%)
3	TPP	F	701	4	22,27,27	1.83	3 (13%)	29,40,40	2.13	12 (41%)
7	ATP	L	401	4	26,33,33	3.54	9 (34%)	31,52,52	1.37	5 (16%)
7	ATP	W	402	4	26,33,33	3.53	9 (34%)	31,52,52	1.36	5 (16%)
3	TPP	N	701	4	22,27,27	1.88	3 (13%)	29,40,40	2.11	11 (37%)
7	ATP	W	401	-	26,33,33	3.54	9 (34%)	31,52,52	1.40	5 (16%)
7	ATP	D	401	4	26,33,33	3.48	9 (34%)	31,52,52	1.55	7 (22%)
5	FAD	J	703	-	51,58,58	2.22	10 (19%)	60,89,89	1.62	14 (23%)
5	FAD	I	703	-	51,58,58	2.25	11 (21%)	60,89,89	1.52	12 (20%)
3	TPP	V	701	4	22,27,27	1.83	2 (9%)	29,40,40	2.09	11 (37%)
6	60G	F	704	-	28,29,29	1.44	4 (14%)	38,40,40	3.46	13 (34%)
3	TPP	E	701	4	22,27,27	1.85	2 (9%)	29,40,40	2.15	11 (37%)
3	TPP	B	701	4	22,27,27	1.86	2 (9%)	29,40,40	2.14	13 (44%)
5	FAD	A	703	-	51,58,58	2.26	11 (21%)	60,89,89	1.53	13 (21%)
6	60G	N	705	-	28,29,29	1.45	3 (10%)	38,40,40	3.40	12 (31%)
7	ATP	G	401	4	26,33,33	3.53	9 (34%)	31,52,52	1.44	5 (16%)
6	60G	N	704	-	28,29,29	1.43	3 (10%)	38,40,40	3.40	12 (31%)
5	FAD	Q	703	-	51,58,58	2.25	11 (21%)	60,89,89	1.52	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	60G	J	704	-	28,29,29	1.47	4 (14%)	38,40,40	3.42	13 (34%)
6	60G	V	704	-	28,29,29	1.43	3 (10%)	38,40,40	3.37	13 (34%)

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	S	401	-	-	8/18/38/38	0/3/3/3
6	60G	E	704	-	-	7/24/24/24	0/2/2/2
6	60G	A	704	-	-	7/24/24/24	0/2/2/2
6	60G	B	704	-	-	8/24/24/24	0/2/2/2
3	TPP	A	701	4	-	7/16/17/17	0/2/2/2
7	ATP	T	401	4	-	1/18/38/38	0/3/3/3
3	TPP	J	701	4	-	5/16/17/17	0/2/2/2
6	60G	I	704	-	-	8/24/24/24	0/2/2/2
7	ATP	P	401	4	-	1/18/38/38	0/3/3/3
6	60G	U	704	-	-	6/24/24/24	0/2/2/2
6	60G	Q	704	-	-	7/24/24/24	0/2/2/2
3	TPP	Q	701	4	-	6/16/17/17	0/2/2/2
5	FAD	F	703	-	-	8/30/50/50	0/6/6/6
5	FAD	R	701	-	-	13/30/50/50	0/6/6/6
5	FAD	B	703	-	-	5/30/50/50	0/6/6/6
5	FAD	U	703	-	-	16/30/50/50	0/6/6/6
3	TPP	I	701	4	-	5/16/17/17	0/2/2/2
5	FAD	V	703	-	-	15/30/50/50	0/6/6/6
3	TPP	U	701	4	-	5/16/17/17	0/2/2/2
7	ATP	H	401	4	-	2/18/38/38	0/3/3/3
5	FAD	N	703	-	-	2/30/50/50	0/6/6/6
5	FAD	M	703	-	-	3/30/50/50	0/6/6/6
7	ATP	O	401	4	-	6/18/38/38	0/3/3/3
5	FAD	E	703	-	-	4/30/50/50	0/6/6/6
6	60G	R	702	-	-	9/24/24/24	0/2/2/2
7	ATP	K	401	4	-	4/18/38/38	0/3/3/3
3	TPP	M	701	4	-	3/16/17/17	0/2/2/2

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

All (310) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	401	ATP	C2'-C3'	-11.31	1.22	1.53
7	C	401	ATP	C2'-C3'	-11.25	1.22	1.53
7	W	402	ATP	C2'-C3'	-11.24	1.22	1.53
7	O	401	ATP	C2'-C3'	-11.24	1.22	1.53
7	S	401	ATP	C2'-C3'	-11.23	1.22	1.53
7	P	401	ATP	C2'-C3'	-11.22	1.22	1.53
7	H	401	ATP	C2'-C3'	-11.20	1.22	1.53
7	W	401	ATP	C2'-C3'	-11.18	1.22	1.53
7	T	401	ATP	C2'-C3'	-11.17	1.22	1.53
7	G	401	ATP	C2'-C3'	-11.16	1.22	1.53
7	K	401	ATP	C2'-C3'	-11.09	1.23	1.53
7	D	401	ATP	C2'-C3'	-11.02	1.23	1.53
5	F	703	FAD	C10-N1	8.48	1.44	1.33
5	N	703	FAD	C10-N1	8.40	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	703	FAD	C10-N1	8.37	1.44	1.33
5	A	703	FAD	C10-N1	8.36	1.44	1.33
5	M	703	FAD	C10-N1	8.32	1.43	1.33
5	V	703	FAD	C10-N1	8.31	1.43	1.33
5	I	703	FAD	C10-N1	8.31	1.43	1.33
5	U	703	FAD	C10-N1	8.31	1.43	1.33
5	Q	703	FAD	C10-N1	8.29	1.43	1.33
5	E	703	FAD	C10-N1	8.27	1.43	1.33
5	B	703	FAD	C10-N1	8.27	1.43	1.33
5	R	701	FAD	C10-N1	8.24	1.43	1.33
7	P	401	ATP	O4'-C4'	-7.48	1.28	1.45
7	T	401	ATP	O4'-C4'	-7.45	1.28	1.45
7	G	401	ATP	O4'-C4'	-7.42	1.28	1.45
7	H	401	ATP	O4'-C4'	-7.39	1.28	1.45
7	O	401	ATP	O4'-C4'	-7.39	1.28	1.45
7	L	401	ATP	O4'-C4'	-7.37	1.28	1.45
7	D	401	ATP	O4'-C4'	-7.37	1.28	1.45
7	W	402	ATP	O4'-C4'	-7.37	1.28	1.45
7	W	401	ATP	O4'-C4'	-7.36	1.28	1.45
7	C	401	ATP	O4'-C4'	-7.36	1.28	1.45
7	K	401	ATP	O4'-C4'	-7.34	1.28	1.45
7	S	401	ATP	O4'-C4'	-7.33	1.28	1.45
3	J	701	TPP	C4-N3	-7.07	1.33	1.39
3	N	701	TPP	C4-N3	-6.97	1.33	1.39
3	M	701	TPP	C4-N3	-6.94	1.33	1.39
3	E	701	TPP	C4-N3	-6.93	1.33	1.39
3	U	701	TPP	C4-N3	-6.89	1.33	1.39
3	B	701	TPP	C4-N3	-6.84	1.33	1.39
3	A	701	TPP	C4-N3	-6.79	1.33	1.39
3	I	701	TPP	C4-N3	-6.75	1.33	1.39
3	F	701	TPP	C4-N3	-6.72	1.33	1.39
3	Q	701	TPP	C4-N3	-6.71	1.33	1.39
3	V	701	TPP	C4-N3	-6.70	1.33	1.39
5	J	703	FAD	C4-C4X	6.51	1.52	1.41
5	R	701	FAD	C4-C4X	6.45	1.52	1.41
5	B	703	FAD	C4-C4X	6.40	1.52	1.41
5	V	703	FAD	C4-C4X	6.39	1.52	1.41
7	W	401	ATP	O4'-C1'	6.36	1.50	1.41
5	I	703	FAD	C4-C4X	6.36	1.52	1.41
5	N	703	FAD	C4-C4X	6.36	1.52	1.41
5	M	703	FAD	C4-C4X	6.36	1.52	1.41
7	K	401	ATP	O4'-C1'	6.34	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	401	ATP	O4'-C1'	6.34	1.49	1.41
5	Q	703	FAD	C4-C4X	6.34	1.52	1.41
5	R	701	FAD	C1'-N10	-6.32	1.41	1.48
5	E	703	FAD	C4-C4X	6.32	1.52	1.41
5	U	703	FAD	C4-C4X	6.31	1.52	1.41
5	A	703	FAD	C4-C4X	6.30	1.52	1.41
7	L	401	ATP	O4'-C1'	6.29	1.49	1.41
7	H	401	ATP	O4'-C1'	6.27	1.49	1.41
5	A	703	FAD	C1'-N10	-6.26	1.41	1.48
7	W	402	ATP	O4'-C1'	6.25	1.49	1.41
7	C	401	ATP	O4'-C1'	6.25	1.49	1.41
5	V	703	FAD	C1'-N10	-6.25	1.41	1.48
7	G	401	ATP	O4'-C1'	6.23	1.49	1.41
7	O	401	ATP	O4'-C1'	6.23	1.49	1.41
5	E	703	FAD	C1'-N10	-6.20	1.41	1.48
5	N	703	FAD	C1'-N10	-6.20	1.41	1.48
7	T	401	ATP	O4'-C1'	6.19	1.49	1.41
5	U	703	FAD	C1'-N10	-6.18	1.41	1.48
7	P	401	ATP	O4'-C1'	6.17	1.49	1.41
5	F	703	FAD	C4-C4X	6.15	1.52	1.41
5	F	703	FAD	C1'-N10	-6.15	1.41	1.48
5	J	703	FAD	C1'-N10	-6.14	1.41	1.48
5	I	703	FAD	C1'-N10	-6.12	1.41	1.48
5	B	703	FAD	C1'-N10	-6.07	1.42	1.48
5	Q	703	FAD	C1'-N10	-6.04	1.42	1.48
5	M	703	FAD	C1'-N10	-5.98	1.42	1.48
7	D	401	ATP	O4'-C1'	5.84	1.49	1.41
7	K	401	ATP	O2'-C2'	4.92	1.54	1.43
7	W	401	ATP	O2'-C2'	4.91	1.54	1.43
7	C	401	ATP	O2'-C2'	4.91	1.54	1.43
7	S	401	ATP	O2'-C2'	4.91	1.54	1.43
7	H	401	ATP	O2'-C2'	4.90	1.54	1.43
7	P	401	ATP	O2'-C2'	4.88	1.54	1.43
7	W	402	ATP	O2'-C2'	4.84	1.54	1.43
7	G	401	ATP	O2'-C2'	4.84	1.54	1.43
7	O	401	ATP	O2'-C2'	4.83	1.54	1.43
7	L	401	ATP	O2'-C2'	4.77	1.54	1.43
5	R	701	FAD	C2B-C1B	-4.76	1.46	1.53
7	D	401	ATP	O2'-C2'	4.75	1.54	1.43
7	T	401	ATP	O2'-C2'	4.73	1.54	1.43
7	D	401	ATP	C3'-C4'	4.64	1.64	1.53
5	U	703	FAD	C2B-C1B	-4.58	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	703	FAD	C4X-N5	4.56	1.39	1.33
7	K	401	ATP	C3'-C4'	4.54	1.64	1.53
5	V	703	FAD	C4X-N5	4.52	1.39	1.33
5	F	703	FAD	C4X-N5	4.50	1.39	1.33
7	G	401	ATP	C3'-C4'	4.49	1.64	1.53
5	E	703	FAD	C4X-N5	4.48	1.39	1.33
5	M	703	FAD	C4X-N5	4.48	1.39	1.33
5	B	703	FAD	C4X-N5	4.47	1.39	1.33
7	H	401	ATP	C3'-C4'	4.46	1.64	1.53
5	R	701	FAD	C4X-N5	4.46	1.39	1.33
5	E	703	FAD	C2B-C1B	-4.46	1.47	1.53
7	S	401	ATP	C3'-C4'	4.45	1.64	1.53
5	V	703	FAD	C2B-C1B	-4.43	1.47	1.53
7	O	401	ATP	C3'-C4'	4.43	1.64	1.53
5	N	703	FAD	C4X-N5	4.43	1.39	1.33
5	A	703	FAD	C2B-C1B	-4.43	1.47	1.53
7	C	401	ATP	C3'-C4'	4.43	1.64	1.53
7	L	401	ATP	C3'-C4'	4.42	1.64	1.53
7	W	401	ATP	C3'-C4'	4.42	1.64	1.53
7	W	402	ATP	C3'-C4'	4.40	1.64	1.53
5	I	703	FAD	C4X-N5	4.40	1.39	1.33
7	P	401	ATP	C3'-C4'	4.40	1.64	1.53
5	Q	703	FAD	C4X-N5	4.40	1.39	1.33
7	T	401	ATP	C3'-C4'	4.40	1.64	1.53
5	A	703	FAD	C4X-N5	4.40	1.39	1.33
5	N	703	FAD	C2B-C1B	-4.39	1.47	1.53
5	M	703	FAD	C2B-C1B	-4.39	1.47	1.53
5	Q	703	FAD	C2B-C1B	-4.36	1.47	1.53
5	B	703	FAD	C2B-C1B	-4.33	1.47	1.53
5	I	703	FAD	C2B-C1B	-4.32	1.47	1.53
5	U	703	FAD	C4X-N5	4.32	1.39	1.33
7	P	401	ATP	O3'-C3'	4.29	1.53	1.43
7	K	401	ATP	O3'-C3'	4.26	1.53	1.43
7	D	401	ATP	O3'-C3'	4.25	1.53	1.43
7	C	401	ATP	O3'-C3'	4.25	1.53	1.43
7	S	401	ATP	O3'-C3'	4.24	1.53	1.43
7	H	401	ATP	O3'-C3'	4.24	1.53	1.43
7	G	401	ATP	O3'-C3'	4.23	1.52	1.43
7	O	401	ATP	O3'-C3'	4.21	1.52	1.43
7	L	401	ATP	O3'-C3'	4.20	1.52	1.43
7	T	401	ATP	O3'-C3'	4.19	1.52	1.43
7	W	402	ATP	O3'-C3'	4.19	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	401	ATP	O3'-C3'	4.17	1.52	1.43
6	Q	704	60G	C2-NAP	4.17	1.44	1.38
5	F	703	FAD	C2B-C1B	-4.11	1.47	1.53
6	J	704	60G	C2-NAP	4.08	1.44	1.38
6	R	702	60G	C2-NAP	4.07	1.44	1.38
6	B	704	60G	C2-NAP	4.01	1.44	1.38
6	N	705	60G	C2-NAP	3.99	1.44	1.38
6	A	704	60G	C2-NAP	3.98	1.44	1.38
6	E	704	60G	C2-NAP	3.94	1.44	1.38
6	I	704	60G	C2-NAP	3.93	1.44	1.38
6	F	704	60G	C2-NAP	3.90	1.43	1.38
6	U	704	60G	C2-NAP	3.88	1.43	1.38
6	N	704	60G	C2-NAP	3.87	1.43	1.38
6	V	704	60G	C2-NAP	3.81	1.43	1.38
5	J	703	FAD	C2B-C1B	-3.49	1.48	1.53
7	H	401	ATP	C6-N6	3.42	1.46	1.34
7	S	401	ATP	C6-N6	3.41	1.46	1.34
7	W	401	ATP	C6-N6	3.40	1.46	1.34
7	P	401	ATP	C6-N6	3.40	1.46	1.34
7	D	401	ATP	C6-N6	3.40	1.46	1.34
7	W	402	ATP	C6-N6	3.40	1.46	1.34
7	K	401	ATP	C6-N6	3.39	1.46	1.34
7	C	401	ATP	C6-N6	3.39	1.46	1.34
7	G	401	ATP	C6-N6	3.39	1.46	1.34
7	T	401	ATP	C6-N6	3.39	1.46	1.34
7	L	401	ATP	C6-N6	3.38	1.46	1.34
7	O	401	ATP	C6-N6	3.38	1.46	1.34
3	I	701	TPP	C4'-N4'	3.38	1.42	1.34
3	J	701	TPP	C4'-N4'	3.36	1.42	1.34
3	F	701	TPP	C4'-N4'	3.36	1.42	1.34
3	E	701	TPP	C4'-N4'	3.34	1.42	1.34
3	Q	701	TPP	C4'-N4'	3.34	1.42	1.34
3	U	701	TPP	C4'-N4'	3.34	1.42	1.34
3	M	701	TPP	C4'-N4'	3.34	1.42	1.34
3	V	701	TPP	C4'-N4'	3.34	1.42	1.34
5	R	701	FAD	C4-N3	3.32	1.38	1.33
3	B	701	TPP	C4'-N4'	3.32	1.42	1.34
5	I	703	FAD	C4-N3	3.31	1.38	1.33
3	A	701	TPP	C4'-N4'	3.31	1.42	1.34
3	N	701	TPP	C4'-N4'	3.31	1.42	1.34
5	E	703	FAD	C4-N3	3.29	1.38	1.33
5	U	703	FAD	C4-N3	3.27	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	703	FAD	C4-N3	3.26	1.38	1.33
5	B	703	FAD	C4-N3	3.25	1.38	1.33
5	A	703	FAD	C4-N3	3.25	1.38	1.33
5	Q	703	FAD	C4-N3	3.24	1.38	1.33
7	O	401	ATP	C2'-C1'	3.22	1.58	1.53
5	V	703	FAD	C4-N3	3.20	1.38	1.33
7	K	401	ATP	C2'-C1'	3.20	1.58	1.53
7	W	402	ATP	C2'-C1'	3.20	1.58	1.53
5	N	703	FAD	C4-N3	3.20	1.38	1.33
5	M	703	FAD	C4-N3	3.20	1.38	1.33
6	Q	704	60G	CAU-NAP	3.16	1.44	1.37
7	G	401	ATP	C2'-C1'	3.16	1.58	1.53
6	J	704	60G	CAU-NAP	3.15	1.44	1.37
7	T	401	ATP	C2'-C1'	3.14	1.58	1.53
6	R	702	60G	CAU-NAP	3.13	1.44	1.37
7	H	401	ATP	C2'-C1'	3.13	1.58	1.53
6	A	704	60G	CAU-NAP	3.12	1.44	1.37
7	W	401	ATP	C2'-C1'	3.11	1.58	1.53
7	S	401	ATP	C2'-C1'	3.11	1.58	1.53
6	F	704	60G	CAU-NAP	3.08	1.43	1.37
6	E	704	60G	CAU-NAP	3.07	1.43	1.37
7	L	401	ATP	C2'-C1'	3.06	1.58	1.53
5	N	703	FAD	O4B-C1B	3.06	1.45	1.41
7	P	401	ATP	C2'-C1'	3.06	1.58	1.53
5	I	703	FAD	O4B-C1B	3.06	1.45	1.41
5	M	703	FAD	O4B-C1B	3.05	1.45	1.41
6	V	704	60G	CAU-NAP	3.05	1.43	1.37
5	B	703	FAD	O4B-C1B	3.04	1.45	1.41
5	A	703	FAD	O4B-C1B	3.04	1.45	1.41
7	C	401	ATP	C2'-C1'	3.04	1.58	1.53
5	J	703	FAD	C4-N3	3.03	1.38	1.33
6	B	704	60G	CAU-NAP	3.03	1.43	1.37
6	F	704	60G	OAR-CAA	-3.03	1.38	1.45
6	U	704	60G	CAU-NAP	3.02	1.43	1.37
6	N	705	60G	CAU-NAP	3.01	1.43	1.37
6	I	704	60G	CAU-NAP	3.01	1.43	1.37
5	Q	703	FAD	O4B-C1B	3.01	1.45	1.41
6	E	704	60G	OAR-CAA	-3.00	1.38	1.45
5	E	703	FAD	O4B-C1B	3.00	1.45	1.41
6	B	704	60G	OAR-CAA	-2.98	1.38	1.45
6	J	704	60G	OAR-CAA	-2.98	1.38	1.45
6	Q	704	60G	OAR-CAA	-2.98	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	703	FAD	O4B-C1B	2.97	1.45	1.41
6	V	704	60G	OAR-CAA	-2.97	1.38	1.45
7	D	401	ATP	C2'-C1'	2.97	1.58	1.53
6	A	704	60G	OAR-CAA	-2.97	1.38	1.45
5	V	703	FAD	O4B-C1B	2.96	1.45	1.41
6	N	705	60G	OAR-CAA	-2.96	1.38	1.45
6	N	704	60G	CAU-NAP	2.95	1.43	1.37
6	U	704	60G	OAR-CAA	-2.93	1.38	1.45
5	R	701	FAD	O4B-C1B	2.92	1.45	1.41
6	R	702	60G	OAR-CAA	-2.92	1.38	1.45
6	N	704	60G	OAR-CAA	-2.91	1.38	1.45
6	I	704	60G	OAR-CAA	-2.90	1.38	1.45
5	F	703	FAD	O3'-C3'	-2.85	1.36	1.43
5	M	703	FAD	O3'-C3'	-2.81	1.36	1.43
5	B	703	FAD	O3'-C3'	-2.81	1.36	1.43
5	E	703	FAD	O3'-C3'	-2.81	1.36	1.43
5	I	703	FAD	O3'-C3'	-2.79	1.36	1.43
5	Q	703	FAD	O3'-C3'	-2.78	1.36	1.43
5	V	703	FAD	O3'-C3'	-2.77	1.36	1.43
5	A	703	FAD	O3'-C3'	-2.75	1.36	1.43
5	U	703	FAD	O3'-C3'	-2.74	1.36	1.43
5	N	703	FAD	O3'-C3'	-2.74	1.36	1.43
5	R	701	FAD	O3'-C3'	-2.73	1.36	1.43
5	J	703	FAD	C2'-C3'	2.61	1.58	1.53
5	J	703	FAD	C2-N1	2.60	1.43	1.38
5	F	703	FAD	C2-N1	2.60	1.43	1.38
5	E	703	FAD	C2-N1	2.60	1.43	1.38
5	R	701	FAD	C2-N1	2.57	1.43	1.38
5	B	703	FAD	C2-N1	2.57	1.43	1.38
5	I	703	FAD	C2-N1	2.56	1.43	1.38
5	U	703	FAD	C2-N1	2.55	1.43	1.38
5	Q	703	FAD	C2-N1	2.54	1.43	1.38
5	N	703	FAD	C2-N1	2.54	1.43	1.38
5	V	703	FAD	C2-N1	2.53	1.43	1.38
5	M	703	FAD	C2-N1	2.52	1.43	1.38
5	A	703	FAD	C2-N1	2.51	1.43	1.38
5	J	703	FAD	O3'-C3'	-2.50	1.37	1.43
5	U	703	FAD	C2'-C3'	2.32	1.57	1.53
5	F	703	FAD	C2'-C3'	2.29	1.57	1.53
5	I	703	FAD	C2'-C3'	2.26	1.57	1.53
5	M	703	FAD	C2'-C3'	2.26	1.57	1.53
5	J	703	FAD	O2B-C2B	2.25	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	701	FAD	C2'-C3'	2.25	1.57	1.53
5	Q	703	FAD	C2'-C3'	2.23	1.57	1.53
5	B	703	FAD	C2'-C3'	2.22	1.57	1.53
5	N	703	FAD	C2'-C3'	2.22	1.57	1.53
5	A	703	FAD	C2'-C3'	2.22	1.57	1.53
5	V	703	FAD	C2'-C3'	2.21	1.57	1.53
3	J	701	TPP	C5'-C4'	-2.21	1.39	1.42
5	R	701	FAD	C2B-C3B	-2.20	1.47	1.53
5	E	703	FAD	C2'-C3'	2.20	1.57	1.53
5	V	703	FAD	C2B-C3B	-2.18	1.47	1.53
5	Q	703	FAD	C2B-C3B	-2.18	1.47	1.53
5	U	703	FAD	C2B-C3B	-2.17	1.47	1.53
5	A	703	FAD	C2B-C3B	-2.16	1.47	1.53
5	N	703	FAD	C2B-C3B	-2.16	1.47	1.53
5	B	703	FAD	C2B-C3B	-2.16	1.47	1.53
5	E	703	FAD	C2B-C3B	-2.13	1.47	1.53
5	M	703	FAD	C2B-C3B	-2.13	1.47	1.53
7	W	401	ATP	PG-O2G	-2.13	1.46	1.54
7	W	402	ATP	PG-O2G	-2.12	1.46	1.54
7	T	401	ATP	PG-O2G	-2.11	1.46	1.54
5	F	703	FAD	O2B-C2B	2.11	1.47	1.43
7	D	401	ATP	PG-O2G	-2.11	1.46	1.54
7	H	401	ATP	PG-O2G	-2.10	1.46	1.54
7	P	401	ATP	PG-O2G	-2.10	1.46	1.54
7	C	401	ATP	PG-O2G	-2.10	1.46	1.54
7	G	401	ATP	PG-O2G	-2.10	1.46	1.54
7	S	401	ATP	PG-O2G	-2.09	1.46	1.54
7	K	401	ATP	PG-O2G	-2.09	1.46	1.54
7	O	401	ATP	PG-O2G	-2.08	1.46	1.54
3	Q	701	TPP	C5'-C4'	-2.07	1.39	1.42
6	F	704	60G	OAR-CAV	2.06	1.37	1.33
7	L	401	ATP	PG-O2G	-2.06	1.46	1.54
6	E	704	60G	OAR-CAV	2.06	1.37	1.33
6	J	704	60G	OAR-CAV	2.05	1.37	1.33
6	R	702	60G	OAR-CAV	2.04	1.37	1.33
5	I	703	FAD	C2B-C3B	-2.03	1.47	1.53
6	U	704	60G	OAR-CAV	2.02	1.37	1.33
6	Q	704	60G	OAR-CAV	2.01	1.37	1.33
3	F	701	TPP	C5'-C4'	-2.01	1.39	1.42
3	U	701	TPP	C5'-C4'	-2.01	1.39	1.42
6	I	704	60G	OAR-CAV	2.00	1.37	1.33
3	N	701	TPP	C5'-C4'	-2.00	1.39	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	704	60G	OAR-CAV	2.00	1.37	1.33
3	I	701	TPP	C5'-C4'	-2.00	1.39	1.42

All (495) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	704	60G	OAG-SBB-OAF	-13.32	100.05	119.35
6	A	704	60G	OAG-SBB-OAF	-13.30	100.09	119.35
6	I	704	60G	OAG-SBB-OAF	-13.24	100.17	119.35
6	E	704	60G	OAG-SBB-OAF	-13.24	100.17	119.35
6	Q	704	60G	OAG-SBB-OAF	-13.20	100.23	119.35
6	B	704	60G	OAG-SBB-OAF	-13.19	100.24	119.35
6	N	705	60G	OAG-SBB-OAF	-13.14	100.31	119.35
6	J	704	60G	OAG-SBB-OAF	-13.14	100.32	119.35
6	U	704	60G	OAG-SBB-OAF	-13.13	100.33	119.35
6	N	704	60G	OAG-SBB-OAF	-13.09	100.39	119.35
6	R	702	60G	OAG-SBB-OAF	-13.01	100.50	119.35
6	V	704	60G	OAG-SBB-OAF	-12.85	100.74	119.35
6	F	704	60G	C6-C5-C4	7.14	121.70	115.21
6	E	704	60G	C6-C5-C4	6.94	121.52	115.21
6	U	704	60G	C6-C5-C4	6.93	121.51	115.21
6	V	704	60G	C6-C5-C4	6.93	121.51	115.21
6	I	704	60G	C6-C5-C4	6.91	121.49	115.21
6	J	704	60G	C6-C5-C4	6.91	121.49	115.21
6	R	702	60G	C6-C5-C4	6.90	121.48	115.21
6	A	704	60G	C6-C5-C4	6.89	121.47	115.21
6	N	704	60G	C6-C5-C4	6.85	121.44	115.21
6	N	705	60G	C6-C5-C4	6.84	121.43	115.21
6	B	704	60G	C6-C5-C4	6.84	121.42	115.21
6	Q	704	60G	C6-C5-C4	6.71	121.31	115.21
6	F	704	60G	NAQ-CAU-NAP	6.11	123.03	114.93
6	U	704	60G	NAQ-CAU-NAP	6.09	123.00	114.93
6	V	704	60G	NAQ-CAU-NAP	5.92	122.77	114.93
3	E	701	TPP	PA-O3A-PB	-5.89	112.61	132.83
3	J	701	TPP	PA-O3A-PB	-5.87	112.68	132.83
6	E	704	60G	NAQ-CAU-NAP	5.86	122.70	114.93
3	V	701	TPP	PA-O3A-PB	-5.80	112.93	132.83
6	Q	704	60G	NAQ-CAU-NAP	5.78	122.59	114.93
6	N	705	60G	NAQ-CAU-NAP	5.77	122.58	114.93
5	N	703	FAD	C4-N3-C2	5.77	120.02	115.14
6	J	704	60G	NAQ-CAU-NAP	5.75	122.55	114.93
6	A	704	60G	NAQ-CAU-NAP	5.75	122.55	114.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	701	TPP	PA-O3A-PB	-5.73	113.16	132.83
5	E	703	FAD	C4-N3-C2	5.70	119.95	115.14
3	U	701	TPP	PA-O3A-PB	-5.69	113.30	132.83
5	A	703	FAD	C4-N3-C2	5.66	119.92	115.14
6	B	704	60G	NAQ-CAU-NAP	5.65	122.42	114.93
5	M	703	FAD	C4-N3-C2	5.62	119.89	115.14
6	R	702	60G	NAQ-CAU-NAP	5.61	122.36	114.93
6	I	704	60G	NAQ-CAU-NAP	5.61	122.36	114.93
5	Q	703	FAD	C4-N3-C2	5.60	119.87	115.14
6	N	704	60G	NAQ-CAU-NAP	5.60	122.35	114.93
3	F	701	TPP	PA-O3A-PB	-5.60	113.62	132.83
3	M	701	TPP	PA-O3A-PB	-5.59	113.65	132.83
5	V	703	FAD	C4-N3-C2	5.59	119.86	115.14
5	U	703	FAD	C4-N3-C2	5.58	119.85	115.14
3	I	701	TPP	PA-O3A-PB	-5.57	113.71	132.83
6	Q	704	60G	C2-N3-C4	5.57	121.54	114.99
5	I	703	FAD	C4-N3-C2	5.53	119.81	115.14
5	B	703	FAD	C4-N3-C2	5.52	119.80	115.14
3	N	701	TPP	PA-O3A-PB	-5.51	113.91	132.83
3	A	701	TPP	PA-O3A-PB	-5.50	113.94	132.83
5	R	701	FAD	C4-N3-C2	5.47	119.76	115.14
3	B	701	TPP	PA-O3A-PB	-5.44	114.17	132.83
5	F	703	FAD	C4-N3-C2	5.38	119.68	115.14
6	B	704	60G	C2-N3-C4	5.36	121.29	114.99
6	A	704	60G	C2-N1-C6	5.29	121.21	114.99
5	J	703	FAD	C4-N3-C2	5.29	119.61	115.14
6	F	704	60G	C5-C6-N1	-5.26	117.94	124.08
6	R	702	60G	C2-N1-C6	5.24	121.16	114.99
6	N	705	60G	C2-N1-C6	5.21	121.12	114.99
6	V	704	60G	C2-N3-C4	5.19	121.10	114.99
6	J	704	60G	C2-N1-C6	5.19	121.09	114.99
6	N	704	60G	C2-N3-C4	5.18	121.09	114.99
6	I	704	60G	C2-N3-C4	5.16	121.06	114.99
6	E	704	60G	C2-N1-C6	5.15	121.05	114.99
6	U	704	60G	C2-N1-C6	5.13	121.02	114.99
6	R	702	60G	C5-C4-N3	-5.07	118.16	124.08
6	Q	704	60G	C5-C4-N3	-5.02	118.22	124.08
6	U	704	60G	C5-C4-N3	-5.02	118.22	124.08
6	J	704	60G	C5-C4-N3	-5.02	118.22	124.08
6	E	704	60G	C5-C4-N3	-5.01	118.23	124.08
6	I	704	60G	C5-C6-N1	-5.00	118.24	124.08
6	N	704	60G	C5-C6-N1	-4.96	118.29	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	704	60G	C5-C6-N1	-4.95	118.31	124.08
6	N	705	60G	C5-C4-N3	-4.93	118.33	124.08
6	B	704	60G	C5-C6-N1	-4.92	118.34	124.08
6	A	704	60G	C5-C4-N3	-4.91	118.34	124.08
6	A	704	60G	C5-C6-N1	-4.85	118.42	124.08
6	E	704	60G	C5-C6-N1	-4.82	118.45	124.08
6	B	704	60G	C5-C4-N3	-4.82	118.45	124.08
6	V	704	60G	C5-C4-N3	-4.82	118.46	124.08
6	U	704	60G	C5-C6-N1	-4.79	118.48	124.08
6	J	704	60G	C5-C6-N1	-4.79	118.49	124.08
6	R	702	60G	C5-C6-N1	-4.79	118.49	124.08
6	J	704	60G	OAR-CAV-CBA	4.78	120.23	112.30
6	I	704	60G	C5-C4-N3	-4.77	118.51	124.08
6	N	705	60G	C5-C6-N1	-4.77	118.52	124.08
6	N	704	60G	C5-C4-N3	-4.77	118.52	124.08
6	F	704	60G	C2-N3-C4	4.76	120.59	114.99
6	Q	704	60G	C5-C6-N1	-4.75	118.53	124.08
6	N	705	60G	OAR-CAV-CBA	4.74	120.17	112.30
6	E	704	60G	OAR-CAV-CBA	4.70	120.11	112.30
6	N	704	60G	OAR-CAV-CBA	4.62	119.97	112.30
6	Q	704	60G	OAR-CAV-CBA	4.58	119.89	112.30
6	F	704	60G	OAR-CAV-CBA	4.57	119.89	112.30
6	F	704	60G	C5-C4-N3	-4.56	118.76	124.08
6	A	704	60G	OAR-CAV-CBA	4.55	119.85	112.30
6	V	704	60G	OAR-CAV-CBA	4.48	119.74	112.30
6	B	704	60G	OAR-CAV-CBA	4.48	119.73	112.30
6	F	704	60G	C2-NAP-CAU	-4.35	125.76	130.40
7	L	401	ATP	N3-C2-N1	-4.32	121.93	128.68
6	E	704	60G	C2-NAP-CAU	-4.32	125.80	130.40
6	I	704	60G	C2-NAP-CAU	-4.31	125.80	130.40
7	O	401	ATP	N3-C2-N1	-4.25	122.03	128.68
6	I	704	60G	OAR-CAV-CBA	4.24	119.33	112.30
7	H	401	ATP	N3-C2-N1	-4.23	122.06	128.68
7	P	401	ATP	N3-C2-N1	-4.23	122.07	128.68
7	T	401	ATP	N3-C2-N1	-4.22	122.09	128.68
6	N	704	60G	C2-NAP-CAU	-4.21	125.91	130.40
7	D	401	ATP	N3-C2-N1	-4.20	122.11	128.68
7	C	401	ATP	N3-C2-N1	-4.20	122.11	128.68
7	G	401	ATP	N3-C2-N1	-4.20	122.12	128.68
7	W	401	ATP	N3-C2-N1	-4.19	122.13	128.68
7	K	401	ATP	N3-C2-N1	-4.19	122.13	128.68
7	S	401	ATP	N3-C2-N1	-4.19	122.14	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	402	ATP	N3-C2-N1	-4.17	122.15	128.68
6	U	704	60G	OAR-CAV-CBA	4.17	119.22	112.30
6	R	702	60G	C2-NAP-CAU	-4.14	125.98	130.40
6	U	704	60G	C2-NAP-CAU	-4.06	126.07	130.40
5	U	703	FAD	N3A-C2A-N1A	-3.99	122.45	128.68
5	V	703	FAD	N3A-C2A-N1A	-3.98	122.47	128.68
6	R	702	60G	OAR-CAV-CBA	3.96	118.87	112.30
6	R	702	60G	C2-N3-C4	3.95	119.63	114.99
6	J	704	60G	C2-NAP-CAU	-3.94	126.19	130.40
5	N	703	FAD	N3A-C2A-N1A	-3.94	122.53	128.68
5	B	703	FAD	N3A-C2A-N1A	-3.93	122.54	128.68
6	F	704	60G	C2-N1-C6	3.92	119.60	114.99
5	I	703	FAD	N3A-C2A-N1A	-3.91	122.56	128.68
5	R	701	FAD	N3A-C2A-N1A	-3.91	122.57	128.68
5	E	703	FAD	N3A-C2A-N1A	-3.89	122.59	128.68
5	M	703	FAD	N3A-C2A-N1A	-3.88	122.61	128.68
5	Q	703	FAD	N3A-C2A-N1A	-3.87	122.63	128.68
6	J	704	60G	C2-N3-C4	3.87	119.54	114.99
5	A	703	FAD	N3A-C2A-N1A	-3.86	122.65	128.68
7	D	401	ATP	C3'-C2'-C1'	3.82	106.72	100.98
5	J	703	FAD	N3A-C2A-N1A	-3.79	122.75	128.68
6	N	705	60G	C2-NAP-CAU	-3.79	126.36	130.40
6	V	704	60G	C2-NAP-CAU	-3.78	126.37	130.40
6	B	704	60G	C2-NAP-CAU	-3.76	126.39	130.40
6	I	704	60G	C2-N1-C6	3.74	119.38	114.99
6	U	704	60G	C2-N3-C4	3.73	119.38	114.99
6	E	704	60G	C2-N3-C4	3.73	119.37	114.99
3	B	701	TPP	C7'-N3-C2	-3.71	118.65	125.35
6	N	704	60G	C2-N1-C6	3.71	119.35	114.99
3	Q	701	TPP	C7'-N3-C2	-3.70	118.67	125.35
3	V	701	TPP	C7'-N3-C2	-3.70	118.67	125.35
5	A	703	FAD	C1'-N10-C9A	3.70	121.20	118.29
6	Q	704	60G	C2-N1-C6	3.69	119.33	114.99
3	I	701	TPP	C7'-N3-C2	-3.69	118.68	125.35
6	B	704	60G	C2-N1-C6	3.69	119.33	114.99
3	F	701	TPP	C7'-N3-C2	-3.69	118.69	125.35
6	N	705	60G	C2-N3-C4	3.68	119.32	114.99
6	A	704	60G	C2-NAP-CAU	-3.67	126.49	130.40
6	V	704	60G	C2-N1-C6	3.67	119.30	114.99
3	A	701	TPP	C7'-N3-C2	-3.66	118.75	125.35
6	A	704	60G	C2-N3-C4	3.65	119.28	114.99
3	N	701	TPP	C7'-N3-C2	-3.64	118.78	125.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	703	FAD	N3A-C2A-N1A	-3.61	123.04	128.68
3	E	701	TPP	C7'-N3-C2	-3.58	118.88	125.35
3	M	701	TPP	N1'-C2'-N3'	-3.58	119.38	125.54
3	M	701	TPP	C7'-N3-C2	-3.57	118.90	125.35
3	J	701	TPP	C7'-N3-C2	-3.54	118.95	125.35
3	U	701	TPP	C7'-N3-C2	-3.53	118.97	125.35
3	B	701	TPP	N1'-C2'-N3'	-3.52	119.48	125.54
5	N	703	FAD	C1'-N10-C9A	3.52	121.06	118.29
5	M	703	FAD	C1'-N10-C9A	3.52	121.06	118.29
3	J	701	TPP	N1'-C2'-N3'	-3.51	119.50	125.54
3	V	701	TPP	N1'-C2'-N3'	-3.49	119.53	125.54
3	A	701	TPP	N1'-C2'-N3'	-3.47	119.56	125.54
6	N	704	60G	OAG-SBB-CAM	3.47	113.58	108.30
3	E	701	TPP	N1'-C2'-N3'	-3.46	119.58	125.54
6	B	704	60G	OAG-SBB-CAM	3.46	113.57	108.30
3	I	701	TPP	N1'-C2'-N3'	-3.45	119.60	125.54
3	Q	701	TPP	N1'-C2'-N3'	-3.45	119.60	125.54
3	U	701	TPP	N1'-C2'-N3'	-3.45	119.61	125.54
3	N	701	TPP	N1'-C2'-N3'	-3.45	119.61	125.54
5	Q	703	FAD	C1'-N10-C9A	3.44	121.00	118.29
6	A	704	60G	OAD-CAU-NAP	-3.44	117.81	123.62
6	F	704	60G	OAD-CAU-NAP	-3.44	117.81	123.62
6	Q	704	60G	C2-NAP-CAU	-3.43	126.74	130.40
5	J	703	FAD	O4B-C1B-C2B	-3.43	101.91	106.93
6	U	704	60G	OAD-CAU-NAP	-3.42	117.84	123.62
5	I	703	FAD	C1'-N10-C9A	3.41	120.97	118.29
6	V	704	60G	OAG-SBB-CAM	3.37	113.43	108.30
6	I	704	60G	OAD-CAU-NAP	-3.37	117.93	123.62
7	G	401	ATP	C3'-C2'-C1'	3.36	106.04	100.98
6	Q	704	60G	OAG-SBB-CAM	3.36	113.42	108.30
6	J	704	60G	OAG-SBB-CAM	3.36	113.42	108.30
6	F	704	60G	OAG-SBB-CAM	3.35	113.41	108.30
6	E	704	60G	OAD-CAU-NAP	-3.35	117.95	123.62
6	N	705	60G	OAD-CAU-NAP	-3.35	117.96	123.62
6	V	704	60G	OAD-CAU-NAP	-3.34	117.97	123.62
6	N	704	60G	OAD-CAU-NAP	-3.34	117.97	123.62
6	N	705	60G	OAG-SBB-CAM	3.34	113.38	108.30
6	A	704	60G	OAG-SBB-CAM	3.32	113.35	108.30
5	B	703	FAD	C1'-N10-C9A	3.32	120.90	118.29
3	F	701	TPP	N1'-C2'-N3'	-3.28	119.89	125.54
6	E	704	60G	OAG-SBB-CAM	3.28	113.29	108.30
7	W	401	ATP	PB-O3B-PG	-3.27	121.60	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	704	60G	OAG-SBB-CAM	3.27	113.28	108.30
6	B	704	60G	OAD-CAU-NAP	-3.26	118.10	123.62
6	Q	704	60G	N1-C2-N3	-3.26	121.07	126.23
6	R	702	60G	N1-C2-N3	-3.26	121.07	126.23
6	U	704	60G	OAG-SBB-CAM	3.25	113.26	108.30
7	T	401	ATP	C3'-C2'-C1'	3.24	105.86	100.98
6	Q	704	60G	OAD-CAU-NAP	-3.23	118.16	123.62
6	B	704	60G	N1-C2-N3	-3.21	121.15	126.23
6	J	704	60G	N1-C2-N3	-3.20	121.17	126.23
6	R	702	60G	OAD-CAU-NAP	-3.18	118.24	123.62
5	E	703	FAD	C1'-N10-C9A	3.17	120.79	118.29
3	M	701	TPP	C5-C4-N3	3.16	113.89	107.57
5	U	703	FAD	C9A-N10-C10	-3.15	117.78	121.91
6	A	704	60G	N1-C2-N3	-3.14	121.27	126.23
7	K	401	ATP	PA-O3A-PB	-3.13	122.08	132.83
3	Q	701	TPP	C5-C4-N3	3.13	113.83	107.57
6	N	705	60G	N1-C2-N3	-3.13	121.29	126.23
6	J	704	60G	OAD-CAU-NAP	-3.12	118.35	123.62
3	U	701	TPP	C5-C4-N3	3.12	113.81	107.57
3	A	701	TPP	C5-C4-N3	3.11	113.80	107.57
6	I	704	60G	N1-C2-N3	-3.11	121.32	126.23
6	N	704	60G	N1-C2-N3	-3.11	121.32	126.23
6	R	702	60G	OAG-SBB-CAM	3.10	113.03	108.30
6	V	704	60G	N1-C2-N3	-3.10	121.33	126.23
6	E	704	60G	N1-C2-N3	-3.07	121.37	126.23
3	F	701	TPP	C5-C4-N3	3.07	113.72	107.57
6	U	704	60G	N1-C2-N3	-3.07	121.38	126.23
3	E	701	TPP	C5-C4-N3	3.06	113.70	107.57
5	M	703	FAD	C4A-C5A-N7A	-3.05	106.22	109.40
7	K	401	ATP	C3'-C2'-C1'	3.05	105.57	100.98
5	J	703	FAD	C5X-C9A-N10	3.05	119.93	117.72
6	F	704	60G	N1-C2-N3	-3.05	121.41	126.23
3	N	701	TPP	C5-C4-N3	3.05	113.68	107.57
7	D	401	ATP	PB-O3B-PG	-3.04	122.38	132.83
3	B	701	TPP	C5-C4-N3	3.04	113.66	107.57
7	P	401	ATP	PB-O3B-PG	-3.02	122.46	132.83
3	I	701	TPP	C5-C4-N3	3.02	113.62	107.57
7	T	401	ATP	PB-O3B-PG	-3.02	122.48	132.83
3	N	701	TPP	C5'-C7'-N3	-3.00	108.28	113.28
3	V	701	TPP	C5-C4-N3	2.99	113.56	107.57
7	C	401	ATP	PA-O3A-PB	-2.99	122.56	132.83
3	J	701	TPP	CM2-C2'-N1'	2.99	120.43	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	401	ATP	PA-O3A-PB	-2.99	122.56	132.83
3	M	701	TPP	C6'-N1'-C2'	2.99	121.05	115.96
7	O	401	ATP	PA-O3A-PB	-2.98	122.59	132.83
5	B	703	FAD	C4A-C5A-N7A	-2.98	106.29	109.40
3	J	701	TPP	C6'-N1'-C2'	2.97	121.02	115.96
5	U	703	FAD	C4A-C5A-N7A	-2.96	106.31	109.40
5	R	701	FAD	C4A-C5A-N7A	-2.96	106.31	109.40
5	V	703	FAD	C4A-C5A-N7A	-2.96	106.31	109.40
5	E	703	FAD	C4A-C5A-N7A	-2.95	106.32	109.40
5	I	703	FAD	C3B-C2B-C1B	2.95	105.42	100.98
7	O	401	ATP	PB-O3B-PG	-2.95	122.72	132.83
5	N	703	FAD	C4A-C5A-N7A	-2.95	106.33	109.40
3	M	701	TPP	CM2-C2'-N1'	2.93	120.36	117.14
3	B	701	TPP	C6'-N1'-C2'	2.93	120.95	115.96
3	U	701	TPP	C5'-C7'-N3	-2.93	108.40	113.28
5	F	703	FAD	P-O3P-PA	-2.92	122.80	132.83
5	Q	703	FAD	C4A-C5A-N7A	-2.91	106.36	109.40
5	A	703	FAD	C4A-C5A-N7A	-2.91	106.37	109.40
3	U	701	TPP	CM4-C4-C5	-2.90	121.26	127.60
3	A	701	TPP	C6'-N1'-C2'	2.90	120.89	115.96
7	P	401	ATP	PA-O3A-PB	-2.89	122.91	132.83
7	W	402	ATP	PA-O3A-PB	-2.89	122.91	132.83
5	I	703	FAD	C4A-C5A-N7A	-2.88	106.39	109.40
7	L	401	ATP	PA-O3A-PB	-2.87	122.99	132.83
7	C	401	ATP	PB-O3B-PG	-2.86	123.00	132.83
3	N	701	TPP	C6'-N1'-C2'	2.86	120.82	115.96
3	A	701	TPP	CM4-C4-C5	-2.85	121.36	127.60
3	I	701	TPP	CM2-C2'-N1'	2.85	120.27	117.14
3	Q	701	TPP	CM4-C4-C5	-2.85	121.38	127.60
7	H	401	ATP	PB-O3B-PG	-2.84	123.07	132.83
3	V	701	TPP	CM2-C2'-N1'	2.84	120.26	117.14
3	E	701	TPP	C6'-N1'-C2'	2.83	120.78	115.96
5	J	703	FAD	C1'-N10-C10	2.83	120.94	118.41
5	N	703	FAD	C4-C4X-N5	2.83	121.83	118.60
3	J	701	TPP	C5-C4-N3	2.83	113.23	107.57
3	V	701	TPP	C6'-N1'-C2'	2.82	120.77	115.96
3	U	701	TPP	C6'-N1'-C2'	2.82	120.77	115.96
5	E	703	FAD	C4-C4X-N5	2.82	121.82	118.60
3	I	701	TPP	C6'-N1'-C2'	2.82	120.76	115.96
5	V	703	FAD	C4-C4X-N5	2.82	121.82	118.60
7	W	402	ATP	PB-O3B-PG	-2.81	123.17	132.83
7	G	401	ATP	PB-O3B-PG	-2.81	123.18	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	701	TPP	CM2-C2'-N1'	2.81	120.23	117.14
5	F	703	FAD	C1'-N10-C9A	2.81	120.50	118.29
3	Q	701	TPP	C6'-N1'-C2'	2.81	120.74	115.96
3	F	701	TPP	C6'-N1'-C2'	2.81	120.74	115.96
5	U	703	FAD	C4-C4X-N5	2.80	121.80	118.60
3	Q	701	TPP	C5'-C7'-N3	-2.80	108.61	113.28
3	U	701	TPP	CM2-C2'-N1'	2.80	120.22	117.14
7	T	401	ATP	PA-O3A-PB	-2.80	123.21	132.83
5	B	703	FAD	C4-C4X-N5	2.79	121.79	118.60
5	V	703	FAD	C1'-N10-C9A	2.78	120.48	118.29
3	E	701	TPP	CM4-C4-C5	-2.78	121.52	127.60
3	B	701	TPP	CM2-C2'-N1'	2.77	120.19	117.14
3	F	701	TPP	CM2-C2'-N1'	2.76	120.17	117.14
5	V	703	FAD	C9A-N10-C10	-2.75	118.31	121.91
5	E	703	FAD	C9A-N10-C10	-2.74	118.32	121.91
3	A	701	TPP	C5'-C7'-N3	-2.73	108.72	113.28
5	R	701	FAD	C4-C4X-N5	2.73	121.72	118.60
5	A	703	FAD	C4-C4X-N5	2.73	121.72	118.60
3	N	701	TPP	CM2-C2'-N1'	2.73	120.14	117.14
7	G	401	ATP	PA-O3A-PB	-2.72	123.48	132.83
3	J	701	TPP	CM4-C4-C5	-2.72	121.65	127.60
5	M	703	FAD	C5X-C9A-N10	2.72	119.68	117.72
7	L	401	ATP	PB-O3B-PG	-2.72	123.51	132.83
7	H	401	ATP	C3'-C2'-C1'	2.71	105.06	100.98
5	B	703	FAD	C3B-C2B-C1B	2.71	105.06	100.98
3	M	701	TPP	CM4-C4-C5	-2.71	121.67	127.60
5	R	701	FAD	C5X-C9A-N10	2.71	119.68	117.72
5	F	703	FAD	C4-C4X-N5	2.71	121.69	118.60
7	H	401	ATP	PA-O3A-PB	-2.70	123.55	132.83
5	B	703	FAD	P-O3P-PA	-2.70	123.55	132.83
3	A	701	TPP	CM2-C2'-N1'	2.69	120.09	117.14
7	W	401	ATP	PA-O3A-PB	-2.69	123.60	132.83
3	Q	701	TPP	CM2-C2'-N1'	2.69	120.09	117.14
3	B	701	TPP	CM4-C4-C5	-2.68	121.73	127.60
5	N	703	FAD	C9A-N10-C10	-2.68	118.39	121.91
3	I	701	TPP	CM4-C4-C5	-2.67	121.77	127.60
5	J	703	FAD	C4-C4X-N5	2.67	121.65	118.60
3	N	701	TPP	CM4-C4-C5	-2.67	121.77	127.60
5	V	703	FAD	P-O3P-PA	-2.66	123.69	132.83
3	E	701	TPP	C5'-C7'-N3	-2.66	108.84	113.28
3	F	701	TPP	CM4-C4-C5	-2.66	121.78	127.60
7	P	401	ATP	C3'-C2'-C1'	2.63	104.94	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	703	FAD	C4-C4X-N5	2.63	121.60	118.60
7	W	401	ATP	C3'-C2'-C1'	2.62	104.92	100.98
5	N	703	FAD	P-O3P-PA	-2.61	123.86	132.83
5	A	703	FAD	P-O3P-PA	-2.60	123.90	132.83
5	Q	703	FAD	P-O3P-PA	-2.60	123.91	132.83
7	W	402	ATP	C3'-C2'-C1'	2.60	104.89	100.98
7	K	401	ATP	PB-O3B-PG	-2.60	123.92	132.83
5	J	703	FAD	P-O3P-PA	-2.59	123.93	132.83
5	M	703	FAD	C3B-C2B-C1B	2.58	104.86	100.98
5	R	701	FAD	C1'-N10-C9A	2.58	120.32	118.29
3	F	701	TPP	C6'-C5'-C4'	2.57	119.22	115.72
5	F	703	FAD	C4'-C3'-C2'	-2.57	108.03	113.36
3	V	701	TPP	CM4-C4-C5	-2.56	122.00	127.60
5	E	703	FAD	P-O3P-PA	-2.56	124.03	132.83
7	D	401	ATP	C2'-C3'-C4'	2.56	107.61	102.64
5	I	703	FAD	C5X-C9A-N10	2.56	119.57	117.72
7	D	401	ATP	PA-O3A-PB	-2.53	124.13	132.83
5	J	703	FAD	C4'-C3'-C2'	-2.53	108.09	113.36
7	C	401	ATP	C3'-C2'-C1'	2.52	104.77	100.98
5	F	703	FAD	C4-C4X-C10	-2.51	118.29	119.95
5	I	703	FAD	P-O3P-PA	-2.51	124.21	132.83
5	M	703	FAD	P-O3P-PA	-2.51	124.23	132.83
7	S	401	ATP	PB-O3B-PG	-2.50	124.24	132.83
3	V	701	TPP	C5'-C7'-N3	-2.50	109.12	113.28
3	I	701	TPP	C5'-C7'-N3	-2.50	109.12	113.28
3	B	701	TPP	C5'-C7'-N3	-2.50	109.12	113.28
5	U	703	FAD	C5X-C9A-N10	2.49	119.52	117.72
5	I	703	FAD	C4-C4X-N5	2.48	121.44	118.60
5	N	703	FAD	C10-C4X-N5	-2.48	119.54	121.26
7	L	401	ATP	C3'-C2'-C1'	2.47	104.69	100.98
7	O	401	ATP	C3'-C2'-C1'	2.47	104.69	100.98
5	M	703	FAD	C4-C4X-N5	2.46	121.41	118.60
5	V	703	FAD	C10-C4X-N5	-2.46	119.56	121.26
5	B	703	FAD	C9A-N10-C10	-2.45	118.70	121.91
5	Q	703	FAD	C5X-C9A-N10	2.41	119.46	117.72
5	U	703	FAD	C10-C4X-N5	-2.41	119.59	121.26
3	J	701	TPP	C6'-C5'-C4'	2.40	118.99	115.72
5	E	703	FAD	C10-C4X-N5	-2.40	119.60	121.26
5	J	703	FAD	C1'-N10-C9A	2.39	120.17	118.29
3	J	701	TPP	C5'-C6'-N1'	-2.38	119.86	123.82
6	R	702	60G	OAR-CAV-OAE	-2.37	118.81	123.45
3	F	701	TPP	C5'-C6'-N1'	-2.37	119.87	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	701	FAD	P-O3P-PA	-2.36	124.73	132.83
5	J	703	FAD	C4X-N5-C5X	2.36	119.13	116.77
5	A	703	FAD	C9A-N10-C10	-2.36	118.82	121.91
5	J	703	FAD	C9A-N10-C10	-2.35	118.83	121.91
5	F	703	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
5	Q	703	FAD	C9A-N10-C10	-2.35	118.83	121.91
5	J	703	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
7	W	401	ATP	C4-C5-N7	-2.35	106.95	109.40
7	S	401	ATP	C3'-C2'-C1'	2.34	104.51	100.98
5	R	701	FAD	C9A-N10-C10	-2.34	118.84	121.91
7	H	401	ATP	C4-C5-N7	-2.34	106.96	109.40
7	C	401	ATP	C4-C5-N7	-2.33	106.97	109.40
5	B	703	FAD	C5X-C9A-N10	2.32	119.40	117.72
3	Q	701	TPP	C6'-C5'-C4'	2.32	118.87	115.72
5	M	703	FAD	C4X-N5-C5X	2.31	119.08	116.77
7	T	401	ATP	C4-C5-N7	-2.30	107.00	109.40
3	N	701	TPP	C6'-C5'-C4'	2.30	118.85	115.72
5	F	703	FAD	C5X-C9A-N10	2.30	119.38	117.72
5	V	703	FAD	C5X-C9A-N10	2.29	119.38	117.72
3	F	701	TPP	C5'-C7'-N3	-2.29	109.46	113.28
3	B	701	TPP	O3B-PB-O3A	2.28	112.30	104.64
7	G	401	ATP	C4-C5-N7	-2.28	107.02	109.40
5	E	703	FAD	C5'-C4'-C3'	-2.28	107.79	112.20
5	I	703	FAD	C9A-N10-C10	-2.27	118.94	121.91
7	K	401	ATP	C4-C5-N7	-2.27	107.03	109.40
5	M	703	FAD	C9A-N10-C10	-2.27	118.94	121.91
5	B	703	FAD	C10-C4X-N5	-2.26	119.69	121.26
5	A	703	FAD	C3B-C2B-C1B	2.26	104.39	100.98
5	A	703	FAD	C5X-C9A-N10	2.26	119.35	117.72
3	I	701	TPP	C6'-C5'-C4'	2.25	118.79	115.72
5	E	703	FAD	C5X-C9A-N10	2.25	119.35	117.72
3	E	701	TPP	PA-O7-C7	-2.24	110.55	121.59
3	A	701	TPP	O3B-PB-O3A	2.23	112.12	104.64
7	S	401	ATP	C4-C5-N7	-2.23	107.07	109.40
5	F	703	FAD	C3B-C2B-C1B	2.23	104.34	100.98
3	B	701	TPP	PA-O7-C7	-2.23	110.61	121.59
5	A	703	FAD	C5'-C4'-C3'	-2.22	107.91	112.20
5	B	703	FAD	C5'-C4'-C3'	-2.22	107.91	112.20
7	O	401	ATP	C4-C5-N7	-2.22	107.09	109.40
3	Q	701	TPP	PA-O7-C7	-2.22	110.67	121.59
5	N	703	FAD	C5X-C9A-N10	2.21	119.32	117.72
3	B	701	TPP	C6'-C5'-C4'	2.21	118.73	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	TPP	C5'-C6'-N1'	-2.21	120.14	123.82
5	A	703	FAD	C4-C4X-C10	-2.21	118.49	119.95
5	J	703	FAD	C10-C4X-N5	-2.21	119.73	121.26
5	R	701	FAD	C4-C4X-C10	-2.20	118.49	119.95
3	I	701	TPP	PA-O7-C7	-2.20	110.75	121.59
5	R	701	FAD	C4X-N5-C5X	2.20	118.97	116.77
3	N	701	TPP	C5'-C6'-N1'	-2.20	120.15	123.82
5	Q	703	FAD	C3B-C2B-C1B	2.20	104.29	100.98
3	M	701	TPP	C5'-C6'-N1'	-2.20	120.16	123.82
5	U	703	FAD	C1'-N10-C9A	2.20	120.02	118.29
7	D	401	ATP	C4-C5-N7	-2.19	107.11	109.40
3	U	701	TPP	C6'-C5'-C4'	2.19	118.70	115.72
7	P	401	ATP	C4-C5-N7	-2.19	107.11	109.40
7	W	402	ATP	C4-C5-N7	-2.19	107.12	109.40
3	J	701	TPP	C5'-C7'-N3	-2.19	109.64	113.28
3	A	701	TPP	PA-O7-C7	-2.18	110.85	121.59
7	L	401	ATP	C4-C5-N7	-2.18	107.13	109.40
5	Q	703	FAD	C10-C4X-N5	-2.18	119.75	121.26
3	A	701	TPP	C6'-C5'-C4'	2.18	118.68	115.72
5	N	703	FAD	C4X-C4-N3	-2.17	120.46	123.43
5	I	703	FAD	C4X-N5-C5X	2.16	118.94	116.77
5	B	703	FAD	C4-C4X-C10	-2.16	118.52	119.95
3	E	701	TPP	C6'-C5'-C4'	2.16	118.67	115.72
3	Q	701	TPP	C5'-C6'-N1'	-2.16	120.22	123.82
5	M	703	FAD	C5'-C4'-C3'	-2.16	108.03	112.20
3	I	701	TPP	C5'-C6'-N1'	-2.16	120.22	123.82
6	U	704	60G	OAR-CAV-OAE	-2.15	119.24	123.45
3	A	701	TPP	C5'-C6'-N1'	-2.15	120.24	123.82
3	U	701	TPP	C5'-C6'-N1'	-2.14	120.25	123.82
3	N	701	TPP	PA-O7-C7	-2.14	111.05	121.59
3	V	701	TPP	C6'-C5'-C4'	2.14	118.63	115.72
5	V	703	FAD	C3B-C2B-C1B	2.13	104.19	100.98
3	M	701	TPP	C6'-C5'-C4'	2.13	118.61	115.72
5	R	701	FAD	C10-C4X-N5	-2.13	119.79	121.26
3	I	701	TPP	O2B-PB-O3A	2.12	111.76	104.64
5	A	703	FAD	C10-C4X-N5	-2.12	119.80	121.26
3	E	701	TPP	C5'-C6'-N1'	-2.11	120.30	123.82
5	U	703	FAD	P-O3P-PA	-2.11	125.58	132.83
3	V	701	TPP	PA-O7-C7	-2.11	111.22	121.59
5	M	703	FAD	C4X-C4-N3	-2.10	120.55	123.43
5	Q	703	FAD	C4X-C4-N3	-2.10	120.56	123.43
5	E	703	FAD	C4X-C4-N3	-2.10	120.56	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	704	60G	CAM-SBB-NAQ	2.10	110.87	105.07
3	V	701	TPP	C5'-C6'-N1'	-2.09	120.33	123.82
6	F	704	60G	CAA-OAR-CAV	2.08	119.85	115.83
3	M	701	TPP	PA-O7-C7	-2.08	111.34	121.59
5	V	703	FAD	C4X-C4-N3	-2.08	120.59	123.43
7	D	401	ATP	O4'-C1'-C2'	-2.08	103.89	106.93
5	E	703	FAD	C4-C4X-C10	-2.07	118.58	119.95
5	I	703	FAD	C4X-C4-N3	-2.07	120.60	123.43
6	I	704	60G	OAR-CAV-OAE	-2.07	119.41	123.45
3	F	701	TPP	PA-O7-C7	-2.06	111.44	121.59
5	U	703	FAD	C4X-C4-N3	-2.06	120.61	123.43
5	Q	703	FAD	C4X-N5-C5X	2.06	118.83	116.77
3	M	701	TPP	O3B-PB-O3A	2.06	111.53	104.64
5	A	703	FAD	C4X-C4-N3	-2.06	120.62	123.43
3	A	701	TPP	CM2-C2'-N3'	2.05	120.34	117.15
5	E	703	FAD	C3B-C2B-C1B	2.05	104.06	100.98
5	F	703	FAD	C1'-N10-C10	2.04	120.24	118.41
5	N	703	FAD	C3B-C2B-C1B	2.04	104.05	100.98
3	B	701	TPP	CM2-C2'-N3'	2.04	120.33	117.15
3	U	701	TPP	PA-O7-C7	-2.04	111.57	121.59
6	I	704	60G	CAA-OAR-CAV	2.04	119.76	115.83
5	U	703	FAD	C4-C4X-C10	-2.03	118.60	119.95
5	F	703	FAD	C4X-N5-C5X	2.03	118.80	116.77
5	B	703	FAD	C4X-C4-N3	-2.03	120.65	123.43
3	J	701	TPP	CM4-C4-N3	2.03	125.12	122.53
5	F	703	FAD	C9A-N10-C10	-2.03	119.25	121.91
6	U	704	60G	CAA-OAR-CAV	2.02	119.74	115.83
3	Q	701	TPP	CM2-C2'-N3'	2.02	120.30	117.15
6	A	704	60G	CAM-SBB-NAQ	2.02	110.65	105.07
6	J	704	60G	CAA-OAR-CAV	2.02	119.72	115.83
5	U	703	FAD	C3B-C2B-C1B	2.02	104.02	100.98
6	V	704	60G	OAR-CAV-OAE	-2.01	119.51	123.45
5	J	703	FAD	C4-C4X-C10	-2.01	118.62	119.95
6	B	704	60G	CAA-OAR-CAV	2.01	119.71	115.83
3	F	701	TPP	O2B-PB-O3A	2.01	111.37	104.64
5	I	703	FAD	C4-C4X-C10	-2.01	118.62	119.95
5	N	703	FAD	C4-C4X-C10	-2.01	118.62	119.95
5	V	703	FAD	C4-C4X-C10	-2.00	118.62	119.95
6	E	704	60G	CAM-SBB-NAQ	2.00	110.60	105.07

There are no chirality outliers.

All (265) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	401	ATP	PB-O3B-PG-O3G
7	W	401	ATP	C5'-O5'-PA-O3A
6	E	704	60G	C5-C6-OAS-CAB
6	E	704	60G	N1-C6-OAS-CAB
6	E	704	60G	CAW-CAM-SBB-OAF
6	A	704	60G	C5-C6-OAS-CAB
6	A	704	60G	N1-C6-OAS-CAB
6	A	704	60G	CAW-CAM-SBB-OAF
6	B	704	60G	C5-C4-OAT-CAC
6	B	704	60G	N3-C4-OAT-CAC
6	B	704	60G	CAW-CAM-SBB-OAF
3	A	701	TPP	C5-C6-C7-O7
3	A	701	TPP	C7-O7-PA-O1A
3	A	701	TPP	C7-O7-PA-O2A
3	A	701	TPP	PA-O3A-PB-O3B
3	J	701	TPP	C5-C6-C7-O7
3	J	701	TPP	C7-O7-PA-O1A
3	J	701	TPP	C7-O7-PA-O2A
6	I	704	60G	C5-C4-OAT-CAC
6	I	704	60G	N3-C4-OAT-CAC
6	I	704	60G	CAW-CAM-SBB-OAF
6	U	704	60G	C5-C6-OAS-CAB
6	U	704	60G	N1-C6-OAS-CAB
6	U	704	60G	CAW-CAM-SBB-OAF
6	Q	704	60G	C5-C6-OAS-CAB
6	Q	704	60G	N1-C6-OAS-CAB
6	Q	704	60G	CAW-CAM-SBB-OAF
3	Q	701	TPP	C4-C5-C6-C7
3	Q	701	TPP	C5-C6-C7-O7
3	Q	701	TPP	C7-O7-PA-O2A
5	F	703	FAD	C5B-O5B-PA-O1A
5	F	703	FAD	C5B-O5B-PA-O3P
5	F	703	FAD	C3'-C4'-C5'-O5'
5	F	703	FAD	O4'-C4'-C5'-O5'
5	F	703	FAD	C5'-O5'-P-O3P
5	R	701	FAD	O4B-C4B-C5B-O5B
5	R	701	FAD	N10-C1'-C2'-O2'
5	B	703	FAD	C2'-C1'-N10-C9A
5	U	703	FAD	C5B-O5B-PA-O1A
5	U	703	FAD	C2'-C1'-N10-C9A
5	U	703	FAD	C1'-C2'-C3'-C4'
5	U	703	FAD	C3'-C4'-C5'-O5'
5	U	703	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	U	703	FAD	C5'-O5'-P-O3P
3	I	701	TPP	C5-C6-C7-O7
3	I	701	TPP	C7-O7-PA-O2A
5	V	703	FAD	C2'-C1'-N10-C9A
5	V	703	FAD	C1'-C2'-C3'-C4'
5	V	703	FAD	C3'-C4'-C5'-O5'
5	V	703	FAD	O4'-C4'-C5'-O5'
3	U	701	TPP	C4-C5-C6-C7
3	U	701	TPP	C5-C6-C7-O7
3	U	701	TPP	C7-O7-PA-O1A
3	U	701	TPP	C7-O7-PA-O2A
7	O	401	ATP	C5'-O5'-PA-O1A
7	O	401	ATP	O4'-C4'-C5'-O5'
7	O	401	ATP	C3'-C4'-C5'-O5'
5	E	703	FAD	C2'-C1'-N10-C9A
7	K	401	ATP	C5'-O5'-PA-O1A
7	K	401	ATP	C5'-O5'-PA-O2A
3	M	701	TPP	C5-C6-C7-O7
3	F	701	TPP	C5-C6-C7-O7
3	F	701	TPP	C7-O7-PA-O1A
3	F	701	TPP	C7-O7-PA-O2A
3	N	701	TPP	C5-C6-C7-O7
3	N	701	TPP	C7-O7-PA-O3A
6	R	702	60G	C5-C4-OAT-CAC
6	R	702	60G	N3-C4-OAT-CAC
6	R	702	60G	C5-C6-OAS-CAB
6	R	702	60G	N1-C6-OAS-CAB
5	J	703	FAD	C5B-O5B-PA-O2A
5	J	703	FAD	C5B-O5B-PA-O3P
5	J	703	FAD	C3B-C4B-C5B-O5B
5	J	703	FAD	C3'-C4'-C5'-O5'
5	J	703	FAD	O4'-C4'-C5'-O5'
5	J	703	FAD	C5'-O5'-P-O3P
3	V	701	TPP	C5-C6-C7-O7
6	F	704	60G	C5-C4-OAT-CAC
6	F	704	60G	N3-C4-OAT-CAC
6	F	704	60G	CAW-CAM-SBB-OAF
3	E	701	TPP	C4-C5-C6-C7
3	E	701	TPP	C7-O7-PA-O1A
3	E	701	TPP	C7-O7-PA-O2A
3	B	701	TPP	C5-C6-C7-O7
3	B	701	TPP	C7-O7-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	B	701	TPP	C7-O7-PA-O2A
6	N	705	60G	CAW-CAM-SBB-OAF
6	N	704	60G	C5-C4-OAT-CAC
6	N	704	60G	N3-C4-OAT-CAC
6	N	704	60G	CAW-CAM-SBB-OAF
6	J	704	60G	C5-C6-OAS-CAB
6	J	704	60G	N1-C6-OAS-CAB
6	J	704	60G	CAW-CAM-SBB-OAF
6	V	704	60G	CAW-CAM-SBB-OAF
6	R	702	60G	CBA-CAV-OAR-CAA
6	E	704	60G	C5-C4-OAT-CAC
6	A	704	60G	C5-C4-OAT-CAC
6	I	704	60G	C5-C6-OAS-CAB
6	Q	704	60G	C5-C4-OAT-CAC
6	N	705	60G	C5-C4-OAT-CAC
6	N	705	60G	C5-C6-OAS-CAB
6	N	704	60G	C5-C6-OAS-CAB
6	J	704	60G	C5-C4-OAT-CAC
6	V	704	60G	C5-C4-OAT-CAC
6	V	704	60G	C5-C6-OAS-CAB
6	E	704	60G	N3-C4-OAT-CAC
6	A	704	60G	N3-C4-OAT-CAC
6	B	704	60G	N1-C6-OAS-CAB
6	I	704	60G	N1-C6-OAS-CAB
6	Q	704	60G	N3-C4-OAT-CAC
6	F	704	60G	N1-C6-OAS-CAB
6	N	705	60G	N3-C4-OAT-CAC
6	N	705	60G	N1-C6-OAS-CAB
6	N	704	60G	N1-C6-OAS-CAB
6	J	704	60G	N3-C4-OAT-CAC
6	V	704	60G	N3-C4-OAT-CAC
6	V	704	60G	N1-C6-OAS-CAB
6	U	704	60G	CBA-CAV-OAR-CAA
7	S	401	ATP	O4'-C4'-C5'-O5'
7	S	401	ATP	C3'-C4'-C5'-O5'
6	B	704	60G	C5-C6-OAS-CAB
6	F	704	60G	C5-C6-OAS-CAB
6	A	704	60G	CBA-CAV-OAR-CAA
5	R	701	FAD	C3B-C4B-C5B-O5B
6	B	704	60G	CBA-CAV-OAR-CAA
6	I	704	60G	CBA-CAV-OAR-CAA
5	U	703	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
5	U	703	FAD	O2'-C2'-C3'-C4'
5	B	703	FAD	O4B-C4B-C5B-O5B
5	J	703	FAD	O4B-C4B-C5B-O5B
5	V	703	FAD	O2'-C2'-C3'-C4'
6	R	702	60G	CAW-CAM-SBB-OAF
7	S	401	ATP	PG-O3B-PB-O1B
5	F	703	FAD	PA-O3P-P-O1P
5	R	701	FAD	P-O3P-PA-O1A
5	Q	703	FAD	PA-O3P-P-O1P
5	E	703	FAD	PA-O3P-P-O1P
5	M	703	FAD	PA-O3P-P-O1P
5	I	703	FAD	PA-O3P-P-O1P
5	I	703	FAD	O4B-C4B-C5B-O5B
3	Q	701	TPP	PB-O3A-PA-O7
5	U	703	FAD	P-O3P-PA-O5B
5	J	703	FAD	P-O3P-PA-O5B
5	B	703	FAD	C3B-C4B-C5B-O5B
3	E	701	TPP	C5-C6-C7-O7
7	K	401	ATP	C4'-C5'-O5'-PA
3	A	701	TPP	PA-O3A-PB-O2B
3	J	701	TPP	C7-O7-PA-O3A
5	U	703	FAD	C5B-O5B-PA-O3P
5	V	703	FAD	C5'-O5'-P-O3P
7	O	401	ATP	C5'-O5'-PA-O3A
3	E	701	TPP	C7-O7-PA-O3A
7	L	401	ATP	PB-O3A-PA-O2A
7	W	402	ATP	PG-O3B-PB-O2B
5	J	703	FAD	PA-O3P-P-O1P
5	A	703	FAD	PA-O3P-P-O1P
5	I	703	FAD	C2'-C3'-C4'-O4'
7	W	401	ATP	C5'-O5'-PA-O2A
3	Q	701	TPP	C7-O7-PA-O1A
5	F	703	FAD	C5'-O5'-P-O1P
5	F	703	FAD	C5'-O5'-P-O2P
5	R	701	FAD	C5B-O5B-PA-O2A
5	U	703	FAD	C5B-O5B-PA-O2A
5	U	703	FAD	C5'-O5'-P-O1P
5	U	703	FAD	C5'-O5'-P-O2P
3	I	701	TPP	C7-O7-PA-O1A
5	V	703	FAD	C5'-O5'-P-O1P
7	O	401	ATP	C5'-O5'-PA-O2A
5	J	703	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
5	J	703	FAD	C5'-O5'-P-O2P
6	I	704	60G	OAR-CAV-CBA-CAK
6	U	704	60G	OAR-CAV-CBA-CAK
5	U	703	FAD	C1'-C2'-C3'-O3'
6	R	702	60G	OAR-CAV-CBA-CAK
5	V	703	FAD	O2'-C2'-C3'-O3'
3	A	701	TPP	C4-C5-C6-C7
3	J	701	TPP	C4-C5-C6-C7
3	I	701	TPP	C4-C5-C6-C7
7	C	401	ATP	C3'-C4'-C5'-O5'
3	B	701	TPP	C4-C5-C6-C7
5	R	701	FAD	N10-C1'-C2'-C3'
6	R	702	60G	OAR-CAV-CBA-CAW
5	V	703	FAD	C2'-C3'-C4'-O4'
7	S	401	ATP	PB-O3B-PG-O1G
5	V	703	FAD	O3'-C3'-C4'-C5'
5	M	703	FAD	O4B-C4B-C5B-O5B
7	S	401	ATP	PA-O3A-PB-O2B
5	B	703	FAD	PA-O3P-P-O1P
7	H	401	ATP	PG-O3B-PB-O2B
5	N	703	FAD	PA-O3P-P-O1P
7	O	401	ATP	PA-O3A-PB-O1B
3	M	701	TPP	PB-O3A-PA-O1A
7	C	401	ATP	PG-O3B-PB-O2B
3	N	701	TPP	PB-O3A-PA-O2A
3	V	701	TPP	PB-O3A-PA-O1A
5	R	701	FAD	C4'-C5'-O5'-P
5	I	703	FAD	O3'-C3'-C4'-O4'
5	E	703	FAD	O4B-C4B-C5B-O5B
6	I	704	60G	OAR-CAV-CBA-CAW
6	U	704	60G	OAR-CAV-CBA-CAW
5	I	703	FAD	O3'-C3'-C4'-C5'
7	G	401	ATP	C3'-C4'-C5'-O5'
5	V	703	FAD	C2'-C3'-C4'-C5'
7	S	401	ATP	C4'-C5'-O5'-PA
6	J	704	60G	CAW-CAM-SBB-NAQ
5	I	703	FAD	C2'-C3'-C4'-C5'
5	R	701	FAD	PA-O3P-P-O1P
5	V	703	FAD	PA-O3P-P-O1P
5	A	703	FAD	PA-O3P-P-O2P
6	A	704	60G	OAR-CAV-CBA-CAK
5	I	703	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
5	R	701	FAD	O3'-C3'-C4'-C5'
5	R	701	FAD	C2'-C3'-C4'-O4'
6	E	704	60G	CAW-CAM-SBB-OAG
6	B	704	60G	CAW-CAM-SBB-OAG
6	Q	704	60G	CAW-CAM-SBB-OAG
6	F	704	60G	CAW-CAM-SBB-OAG
6	N	705	60G	CAW-CAM-SBB-OAG
6	N	704	60G	CAW-CAM-SBB-OAG
6	J	704	60G	CAW-CAM-SBB-OAG
6	V	704	60G	CAW-CAM-SBB-OAG
3	A	701	TPP	C7-O7-PA-O3A
7	P	401	ATP	C5'-O5'-PA-O3A
3	Q	701	TPP	C7-O7-PA-O3A
3	I	701	TPP	C7-O7-PA-O3A
3	U	701	TPP	C7-O7-PA-O3A
7	K	401	ATP	C5'-O5'-PA-O3A
7	C	401	ATP	C5'-O5'-PA-O3A
3	F	701	TPP	C7-O7-PA-O3A
3	B	701	TPP	C7-O7-PA-O3A
5	R	701	FAD	O3'-C3'-C4'-O4'
7	W	401	ATP	C3'-C4'-C5'-O5'
5	U	703	FAD	O4B-C4B-C5B-O5B
5	V	703	FAD	O4B-C4B-C5B-O5B
5	N	703	FAD	O4B-C4B-C5B-O5B
7	D	401	ATP	C3'-C4'-C5'-O5'
7	W	402	ATP	C3'-C4'-C5'-O5'
5	M	703	FAD	C3B-C4B-C5B-O5B
7	S	401	ATP	PA-O3A-PB-O1B
7	T	401	ATP	PB-O3A-PA-O2A
7	W	401	ATP	PB-O3A-PA-O2A
5	R	701	FAD	P-O3P-PA-O2A
5	B	703	FAD	PA-O3P-P-O2P
7	H	401	ATP	PG-O3B-PB-O1B
7	C	401	ATP	PG-O3B-PB-O1B
3	N	701	TPP	PB-O3A-PA-O1A
6	E	704	60G	OAR-CAV-CBA-CAK
6	N	704	60G	OAR-CAV-CBA-CAK
5	V	703	FAD	O3'-C3'-C4'-O4'
6	Q	704	60G	CAW-CAM-SBB-NAQ
5	R	701	FAD	C5'-O5'-P-O1P
3	M	701	TPP	C7-O7-PA-O1A
3	N	701	TPP	C7-O7-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	F	704	60G	CAW-CAM-SBB-NAQ
6	N	704	60G	CAW-CAM-SBB-NAQ
6	V	704	60G	CAW-CAM-SBB-NAQ
5	Q	703	FAD	O4B-C4B-C5B-O5B
5	E	703	FAD	C3B-C4B-C5B-O5B
5	A	703	FAD	O4B-C4B-C5B-O5B
6	B	704	60G	OAR-CAV-CBA-CAK
5	V	703	FAD	C1'-C2'-C3'-O3'
7	D	401	ATP	C4'-C5'-O5'-PA
5	U	703	FAD	N10-C1'-C2'-O2'
6	R	702	60G	OAE-CAV-CBA-CAK
6	N	705	60G	OAR-CAV-CBA-CAK

There are no ring outliers.

38 monomers are involved in 80 short contacts:

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

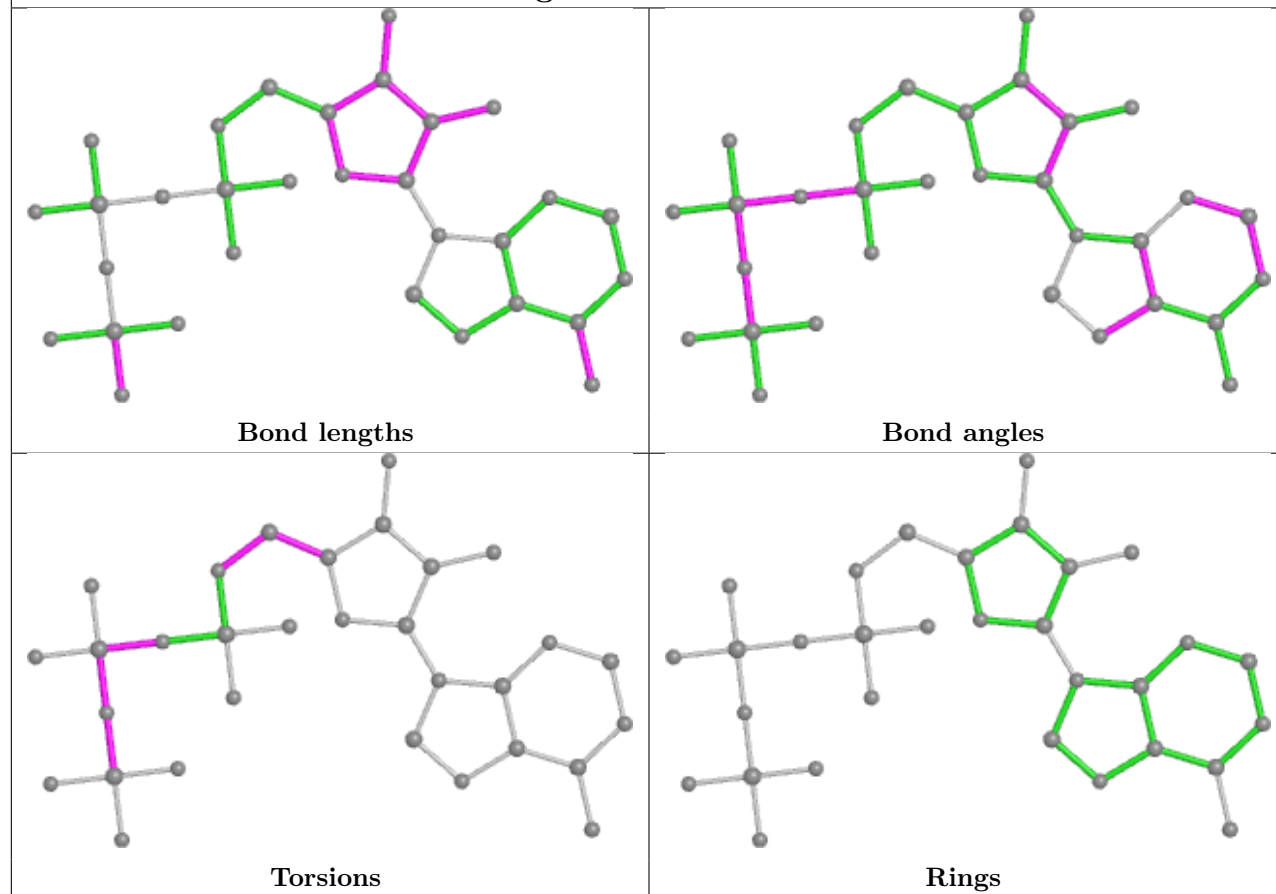
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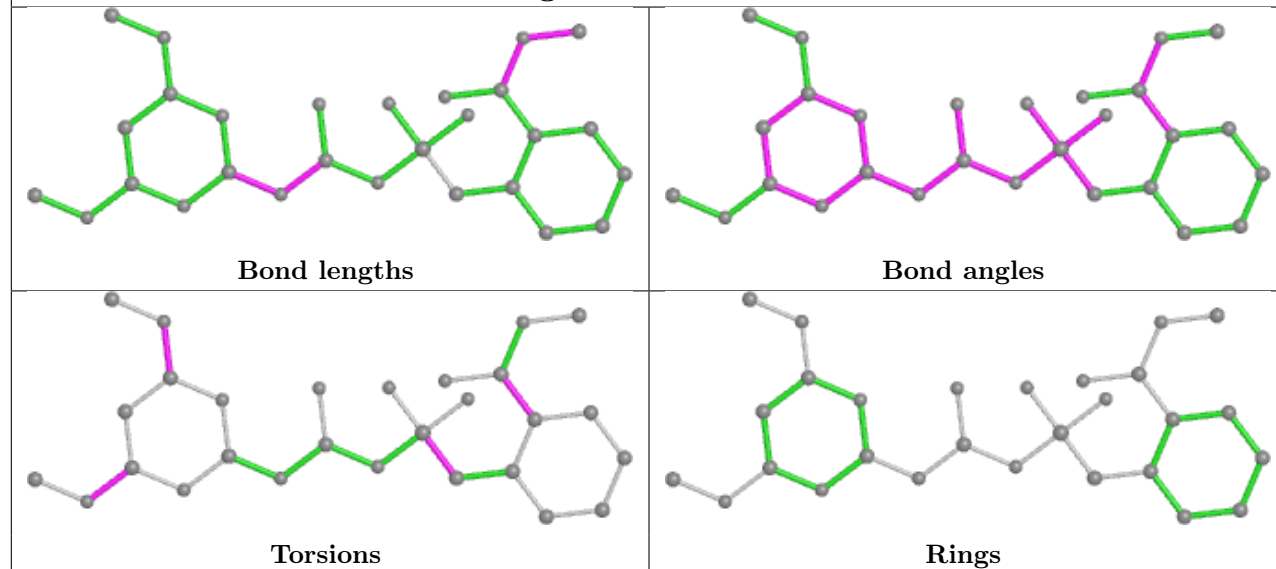
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	401	ATP	5	0
7	W	402	ATP	3	0
3	N	701	TPP	1	0
7	D	401	ATP	2	0
5	J	703	FAD	4	0
5	I	703	FAD	1	0
3	V	701	TPP	3	0
3	E	701	TPP	3	0
3	B	701	TPP	2	0
5	A	703	FAD	3	0
7	G	401	ATP	3	0
5	Q	703	FAD	3	0
6	J	704	60G	2	0

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.

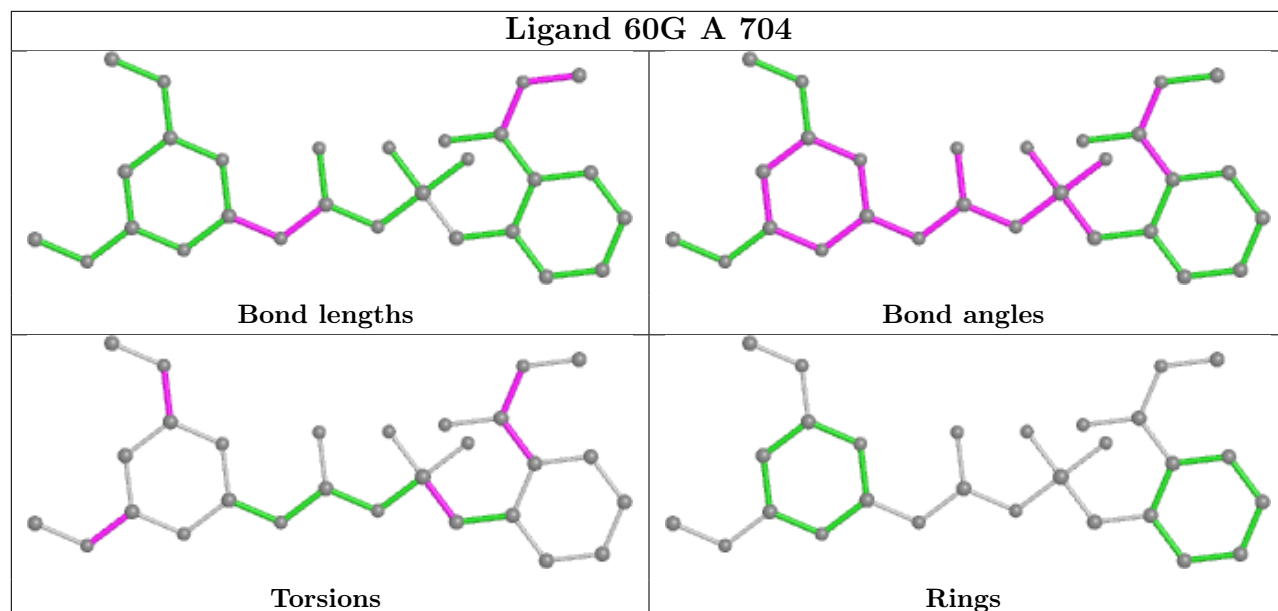
Ligand ATP S 401



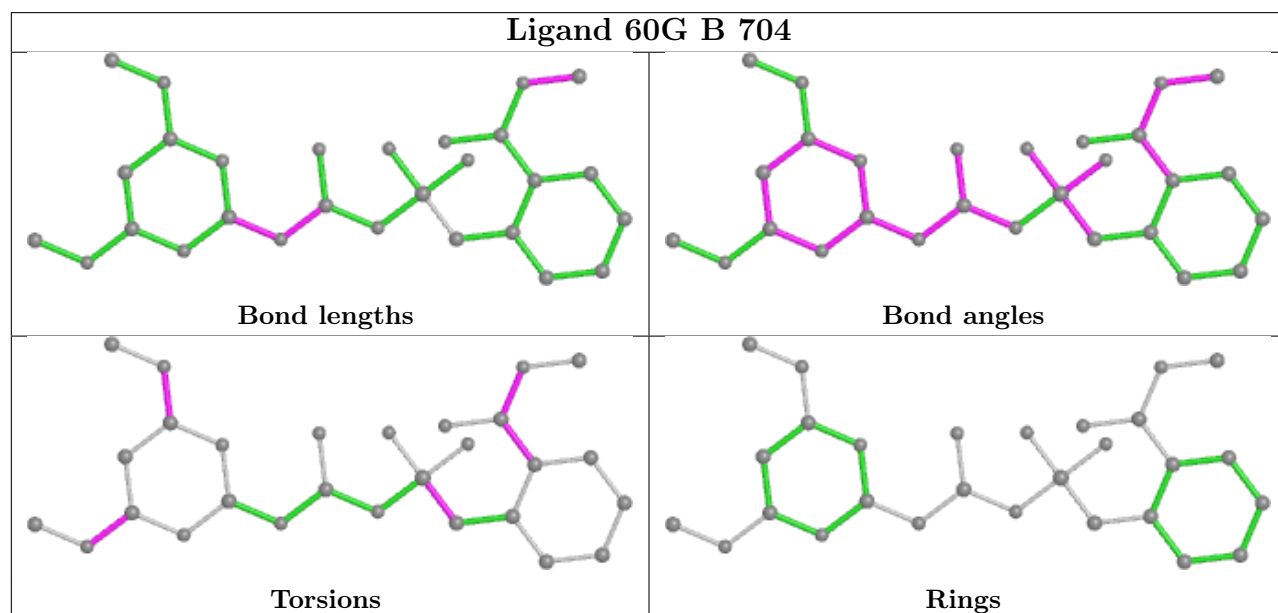
Ligand 60G E 704



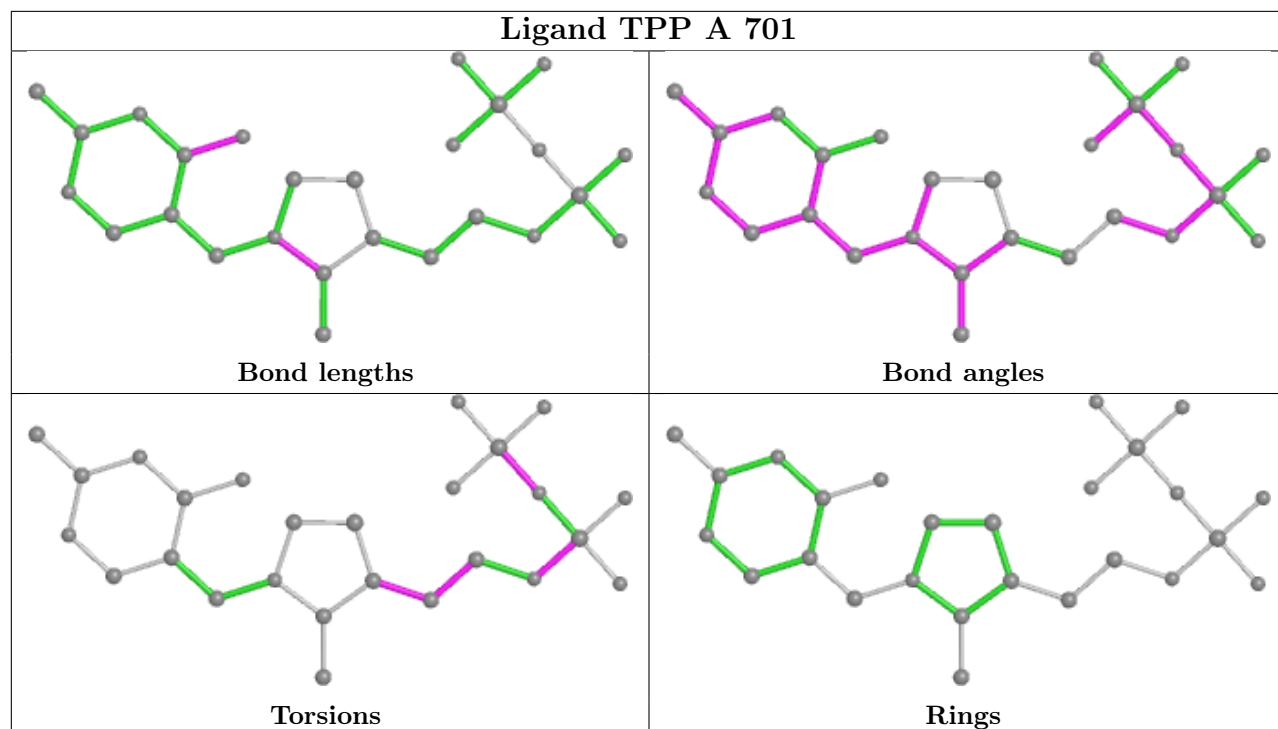
Ligand 60G A 704



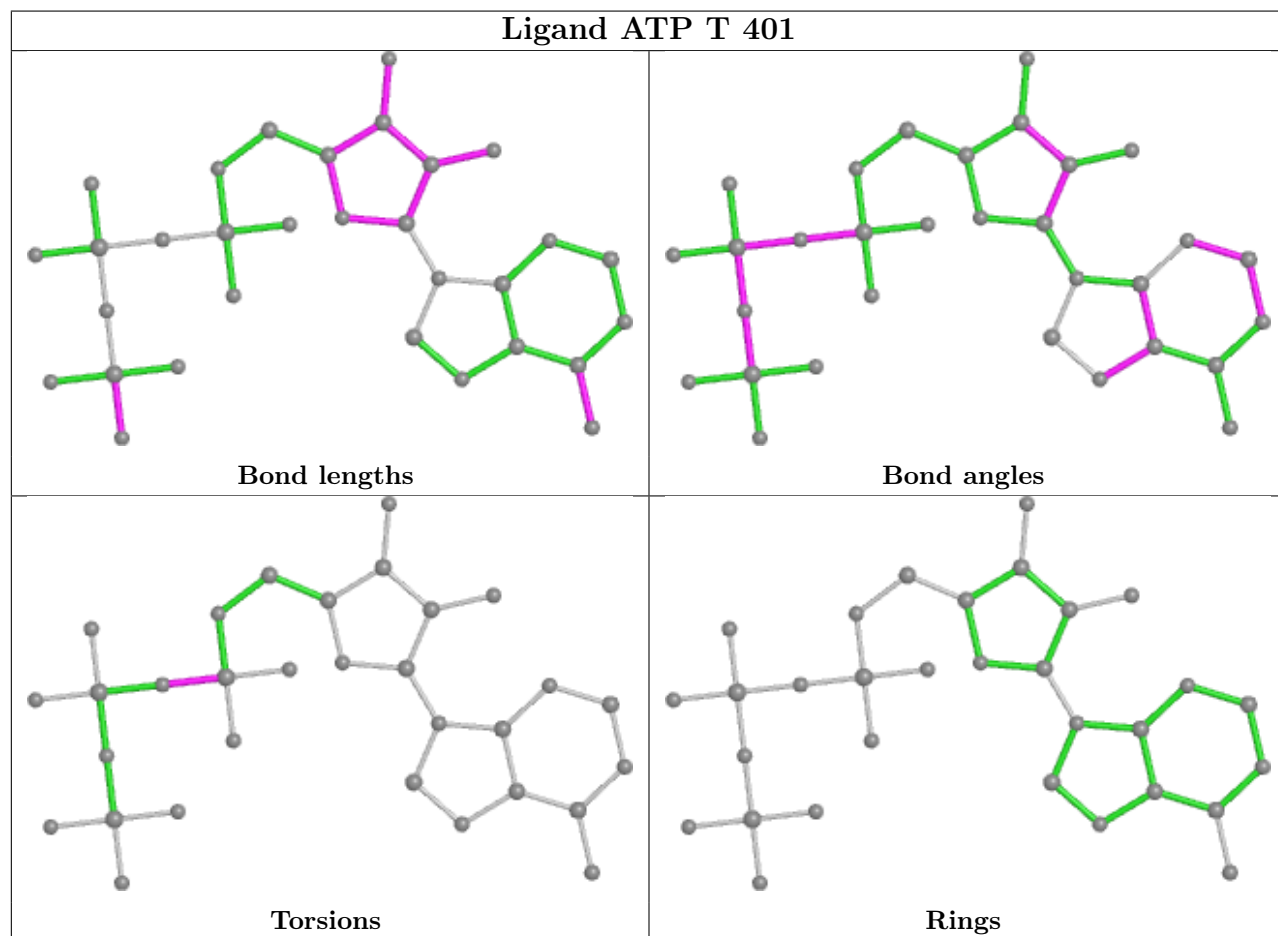
Ligand 60G B 704



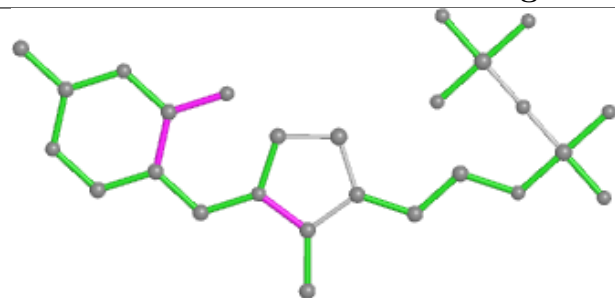
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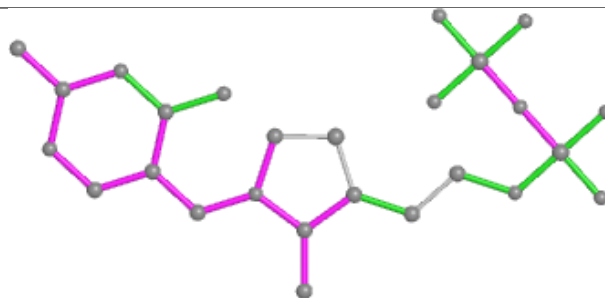
Ligand ATP T 401



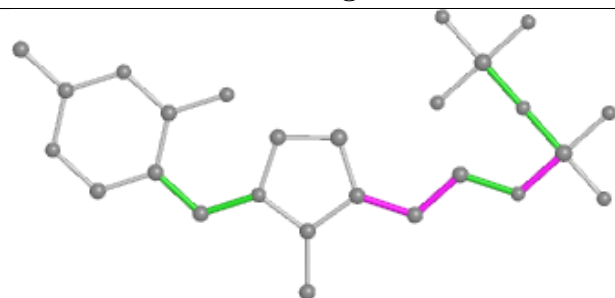
Ligand TPP J 701



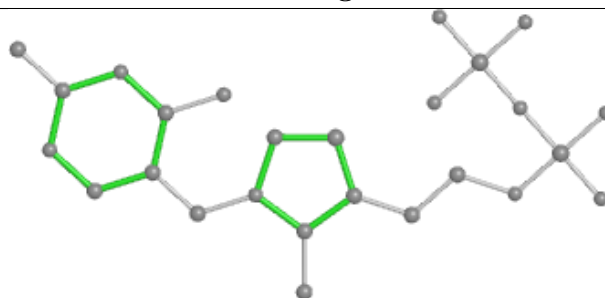
Bond lengths



Bond angles

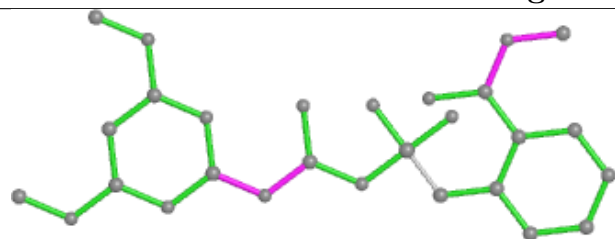


Torsions

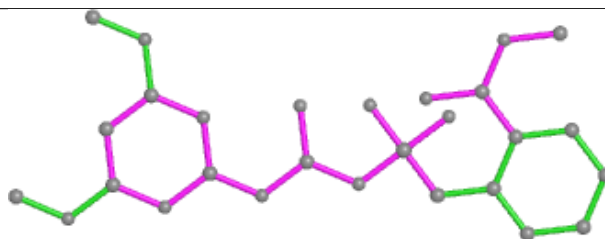


Rings

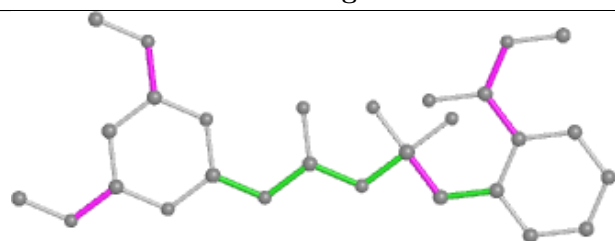
Ligand 60G I 704



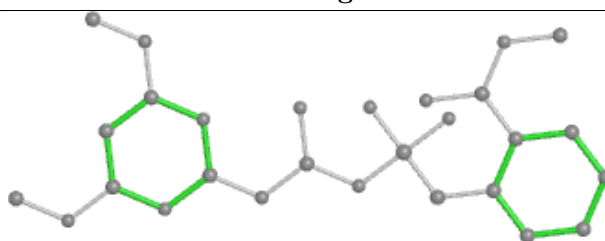
Bond lengths



Bond angles

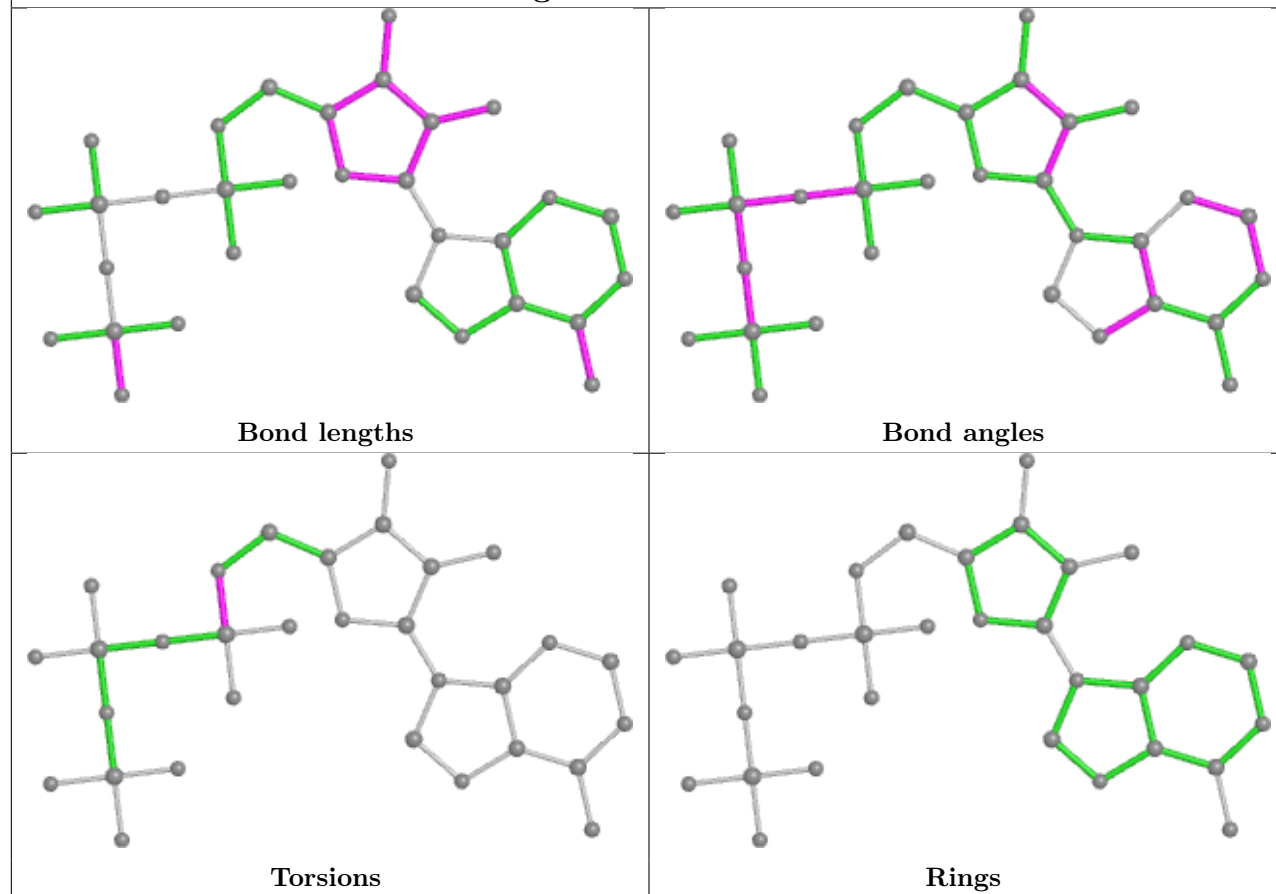


Torsions

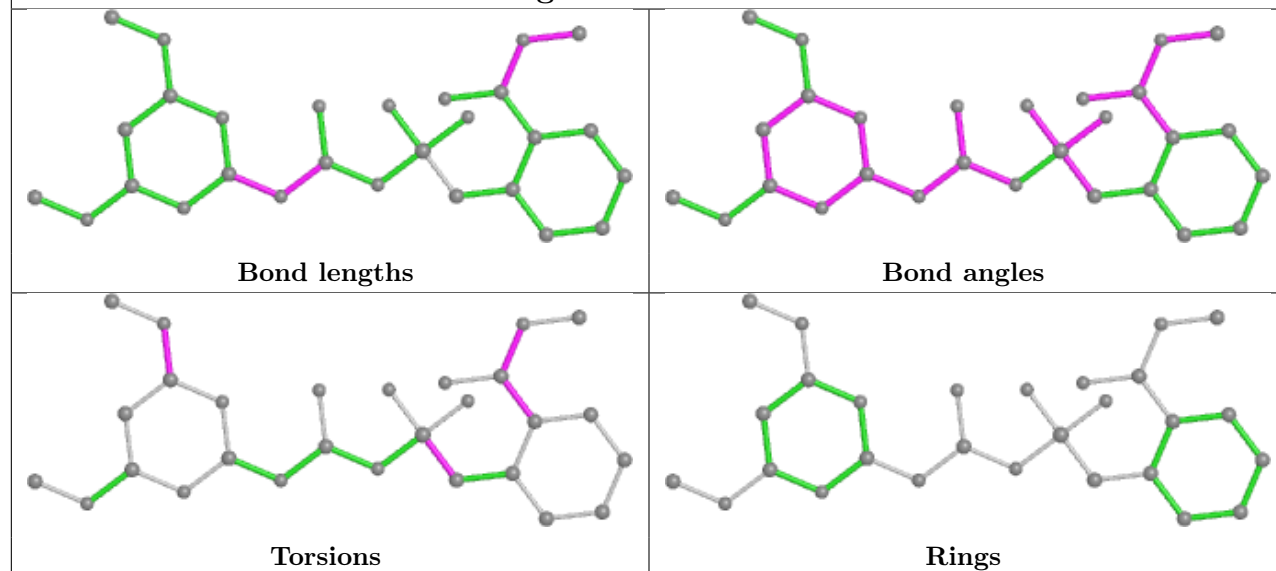


Rings

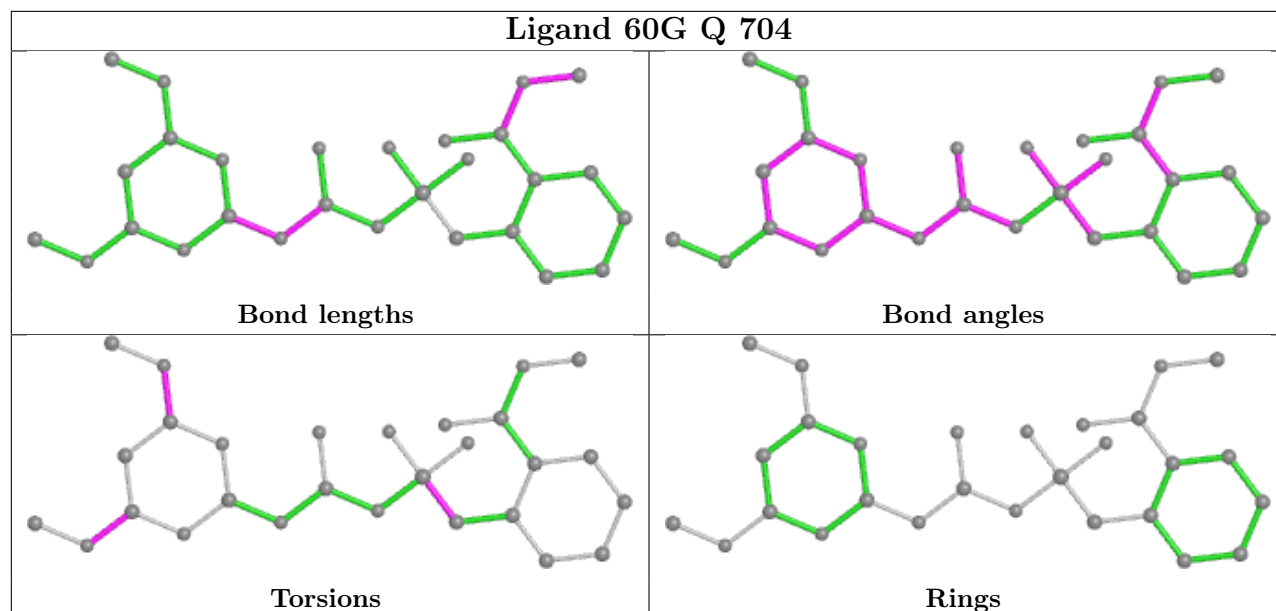
Ligand ATP P 401



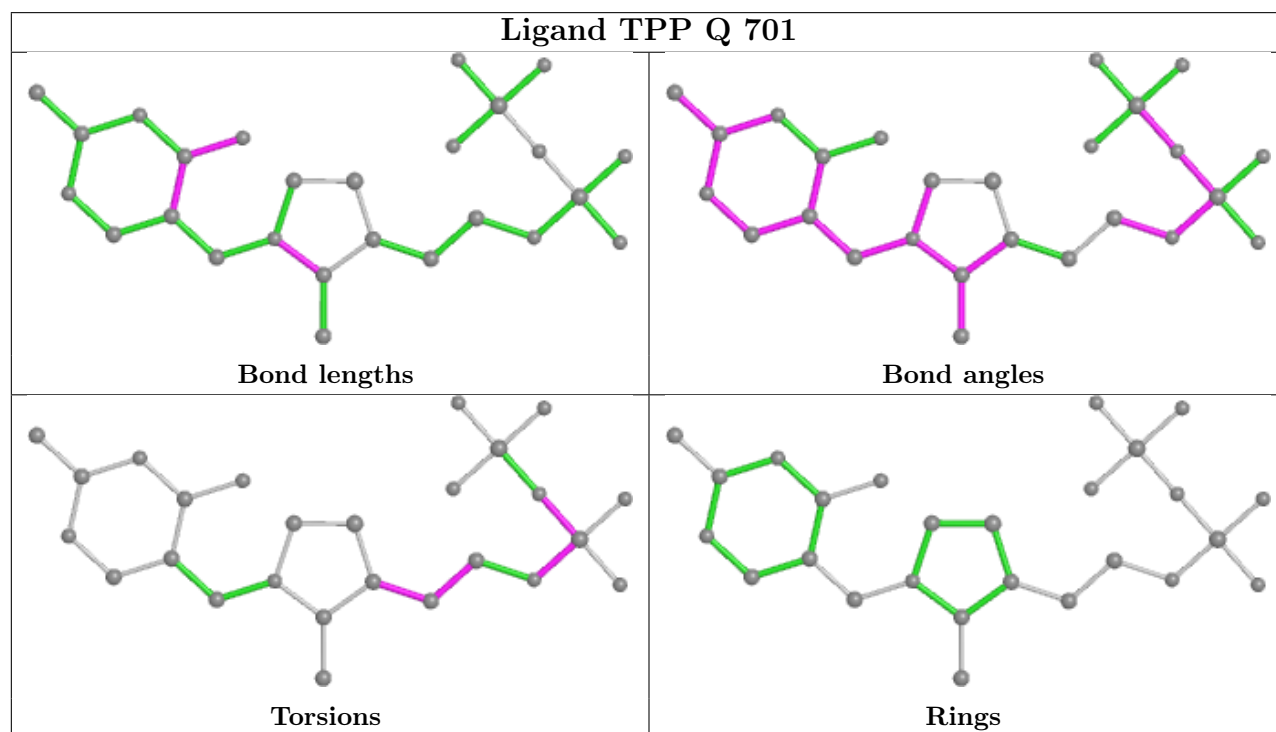
Ligand 60G U 704



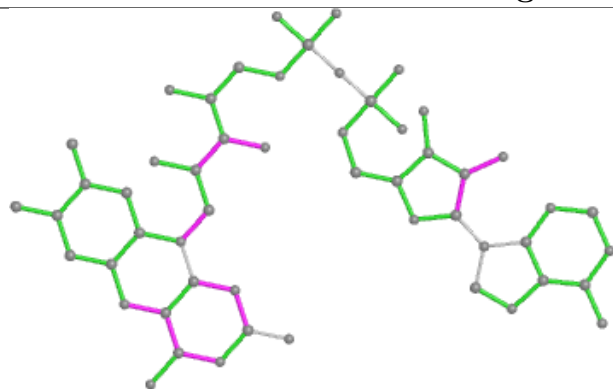
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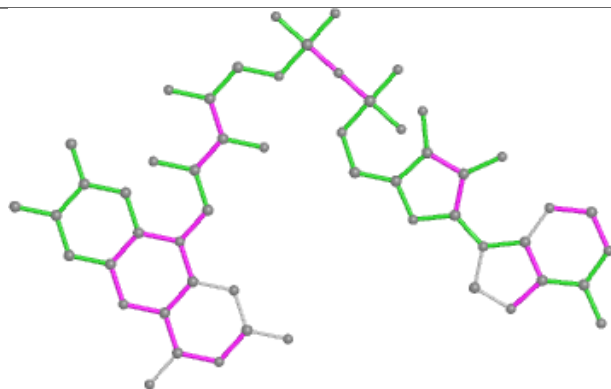
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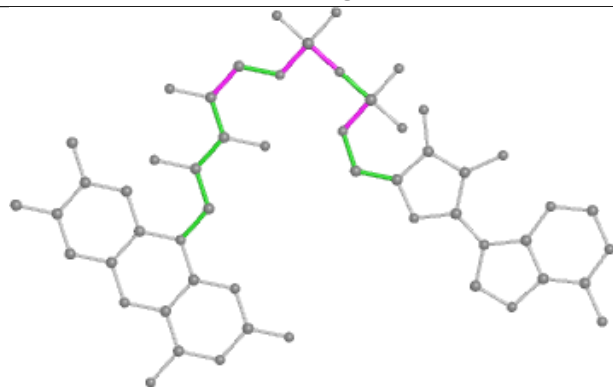
Ligand FAD F 703



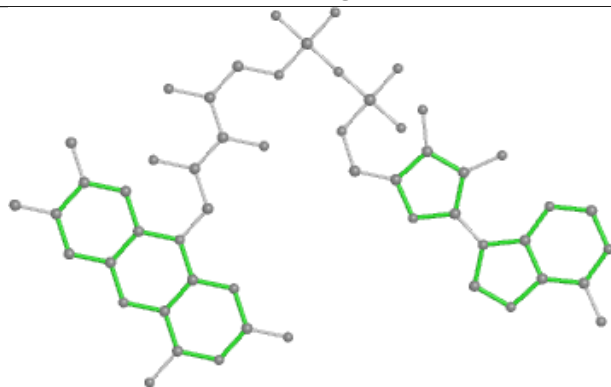
Bond lengths



Bond angles

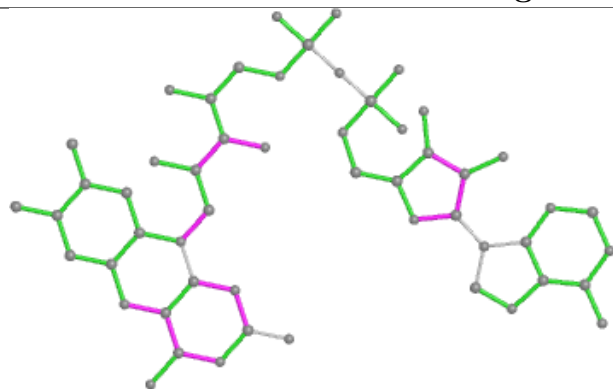


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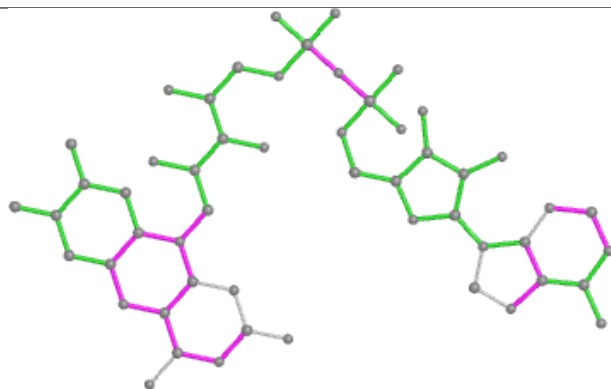


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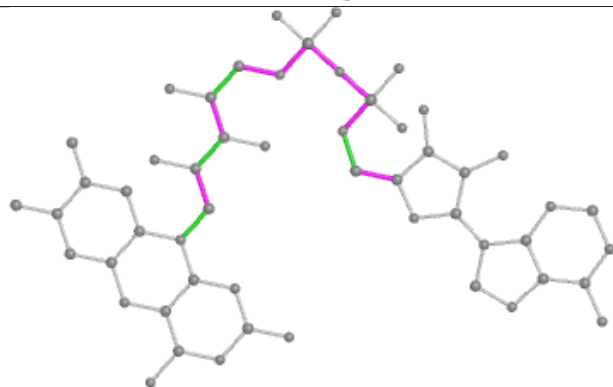
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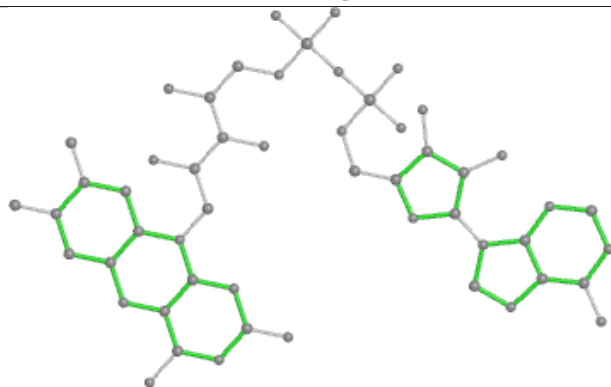
Bond lengths



Bond angles

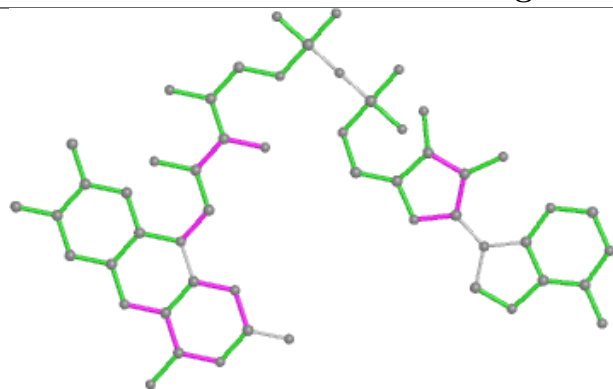


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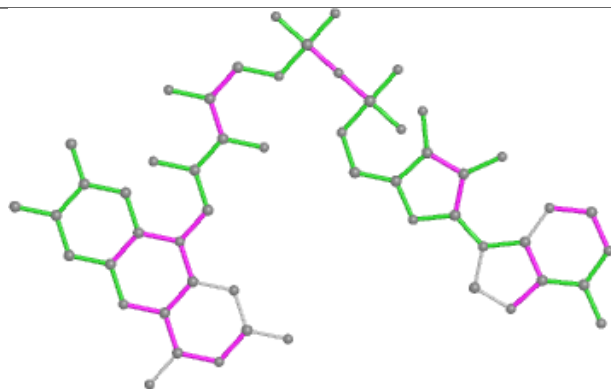


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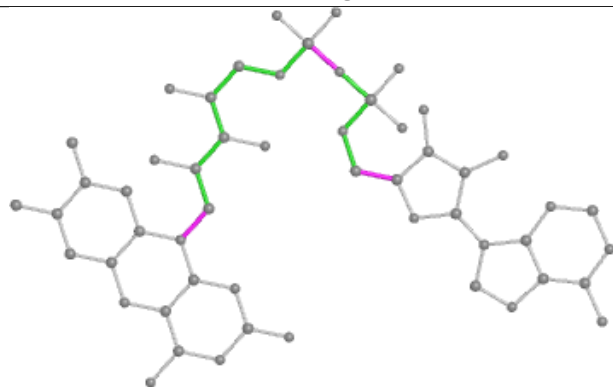
Ligand FAD B 703



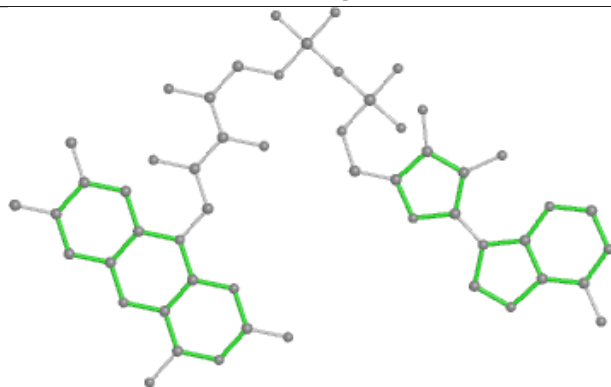
Bond lengths



Bond angles

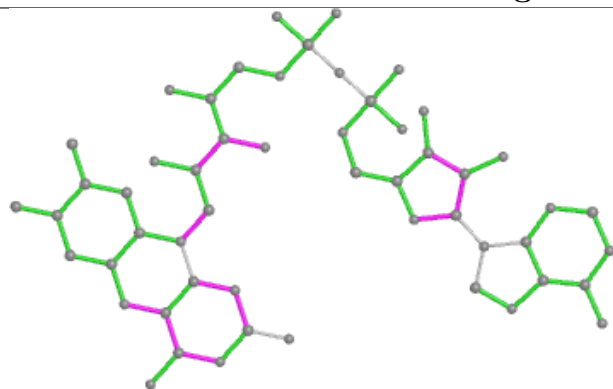


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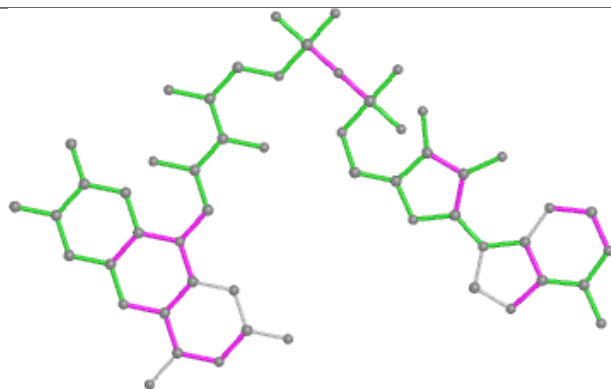


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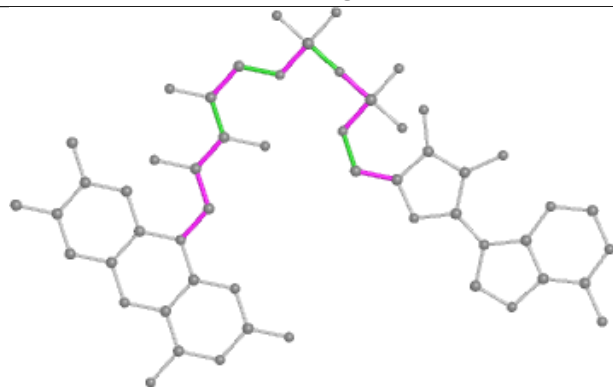
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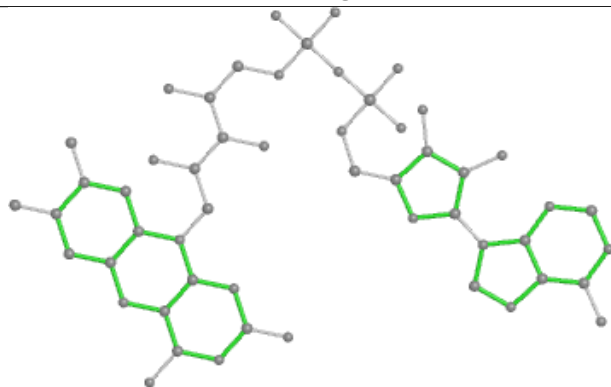
Bond lengths



Bond angles

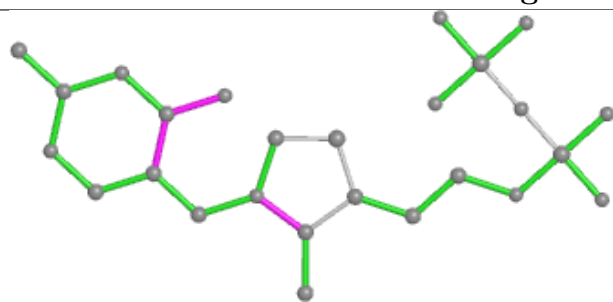


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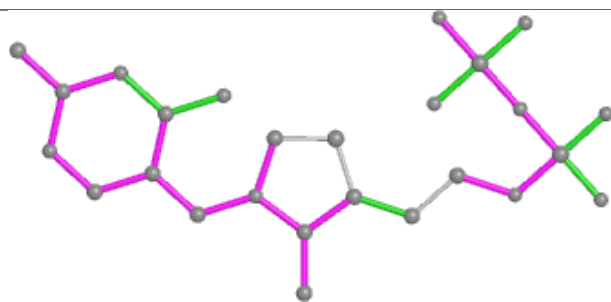


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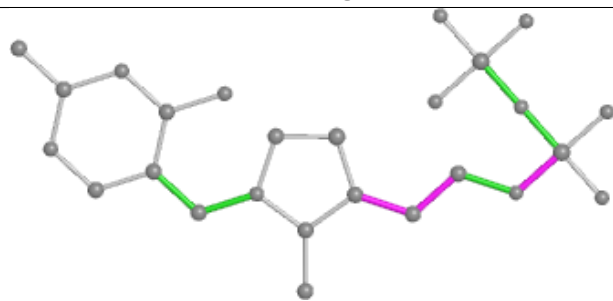
Ligand TPP I 701



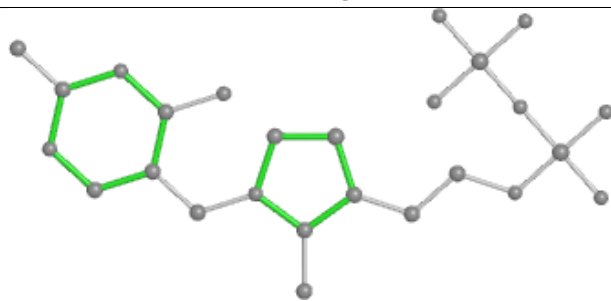
Bond lengths



Bond angles

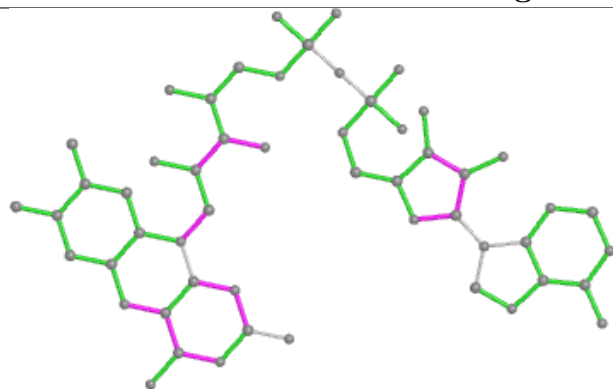


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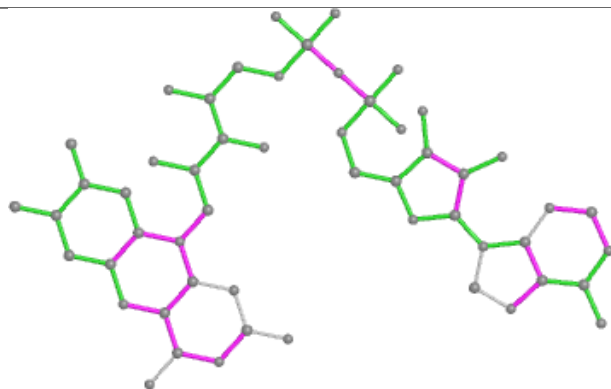


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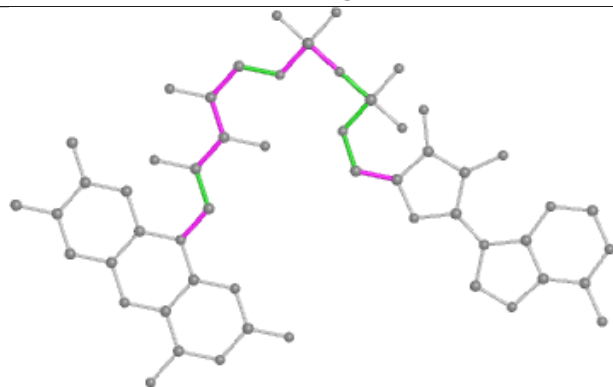
Ligand FAD V 703



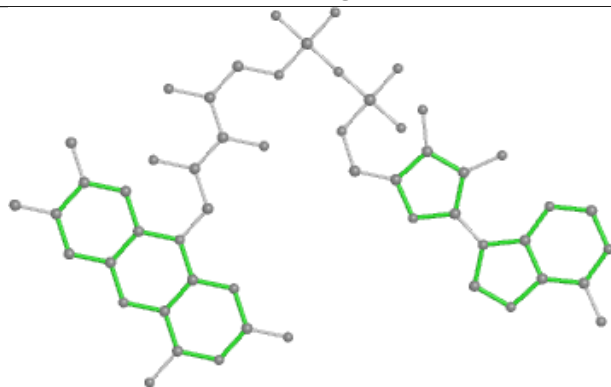
Bond lengths



Bond angles

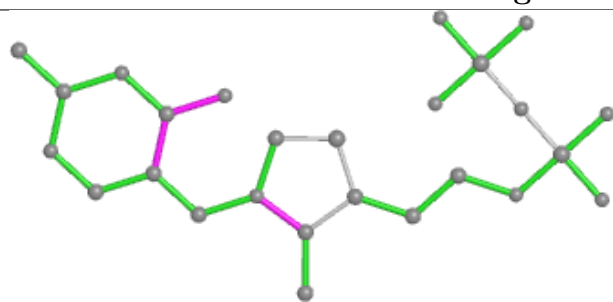


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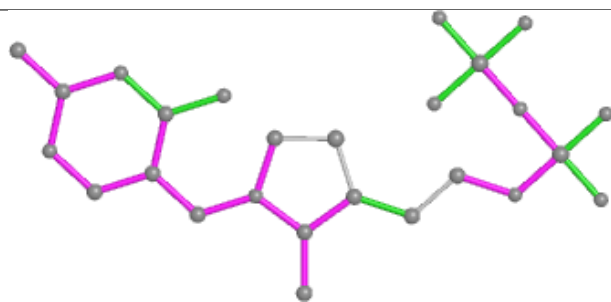


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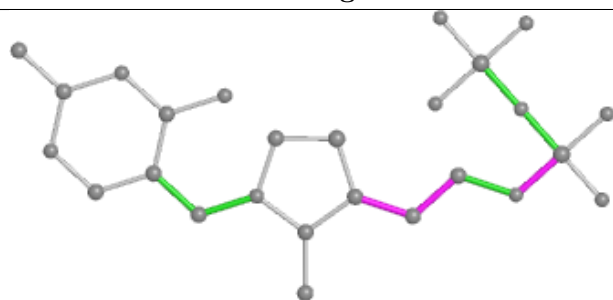
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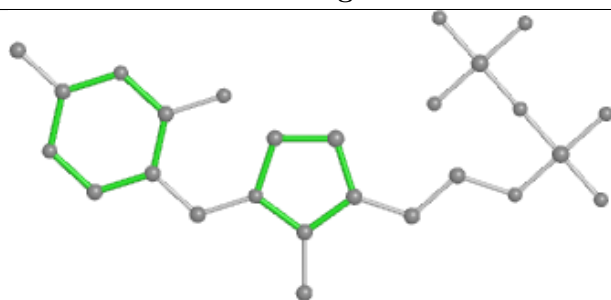
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Bond angles

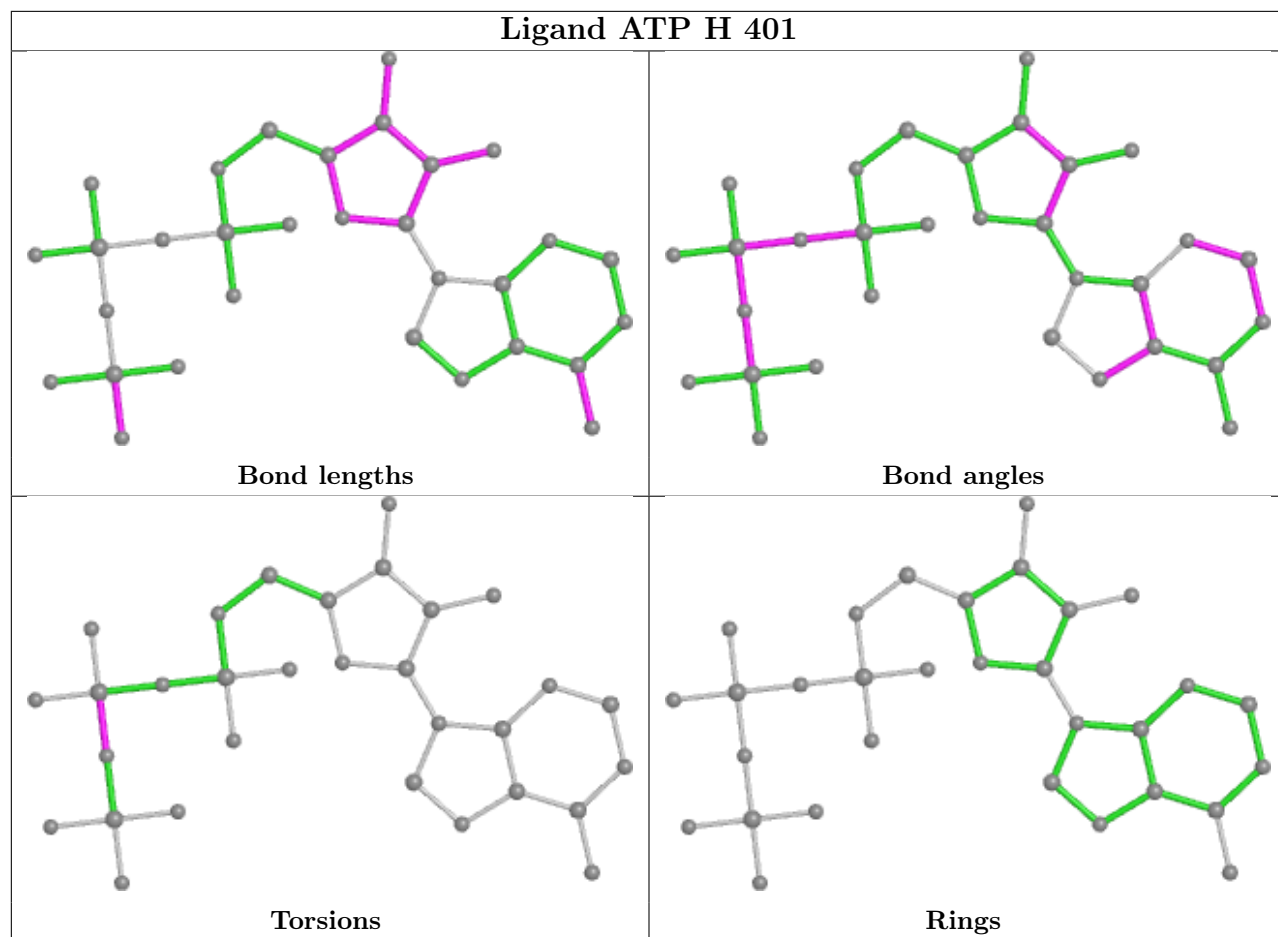


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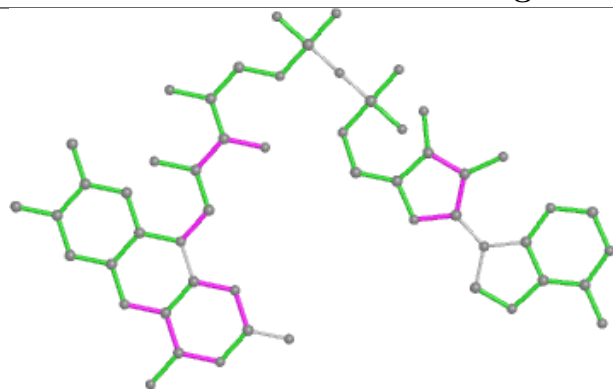


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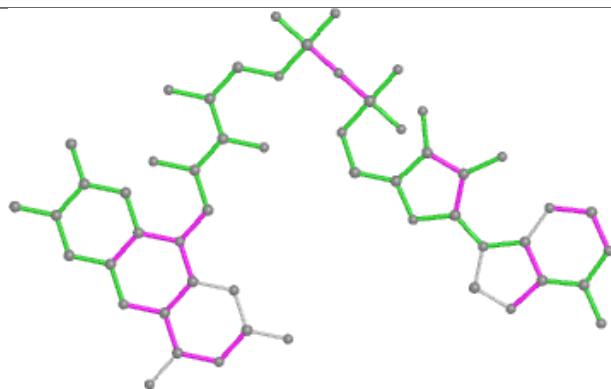
Ligand ATP H 401



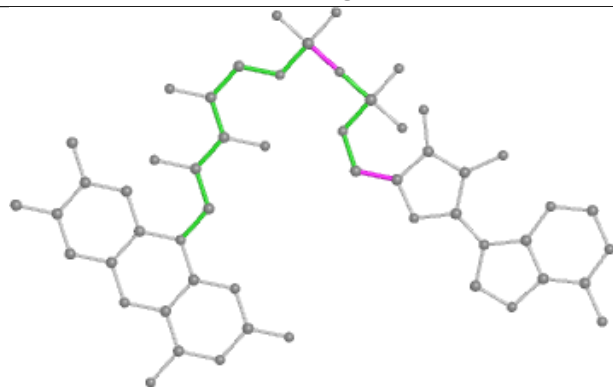
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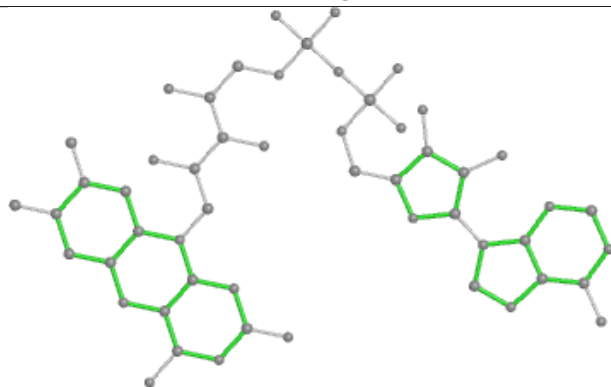
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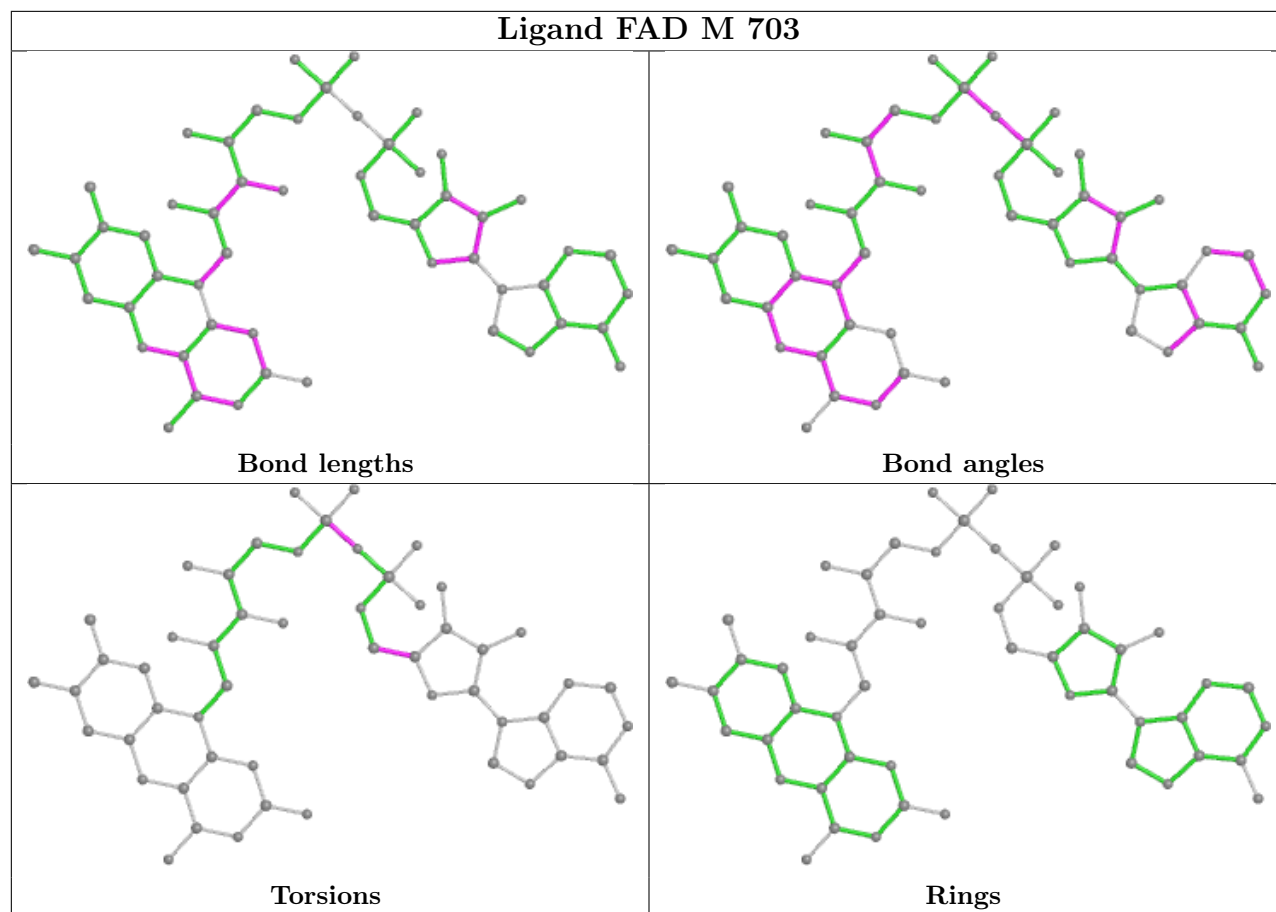
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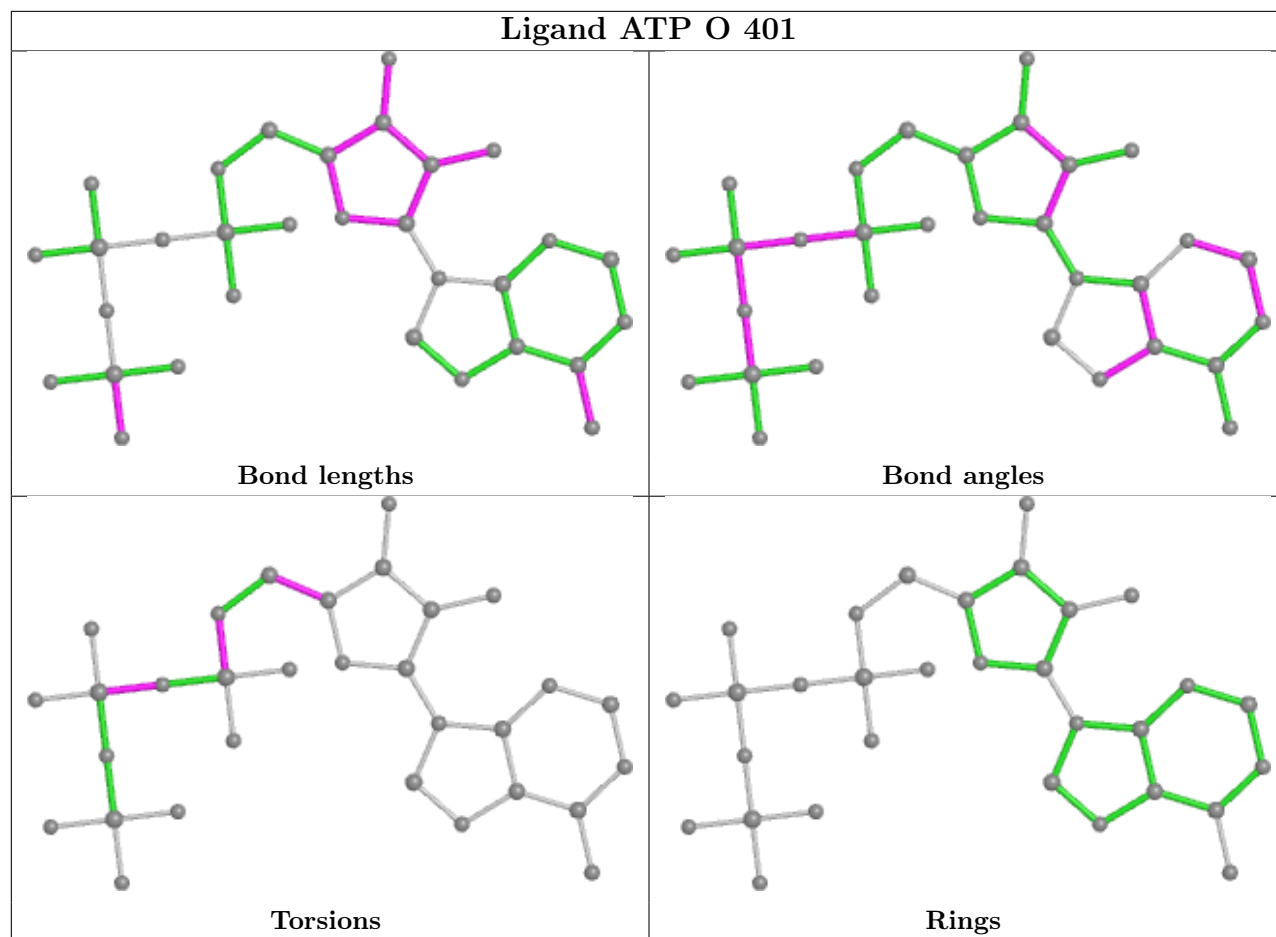


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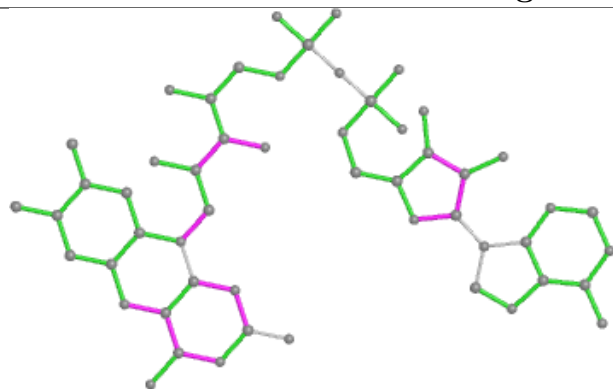


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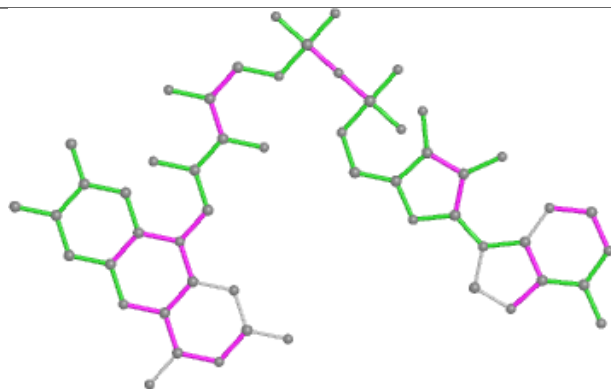




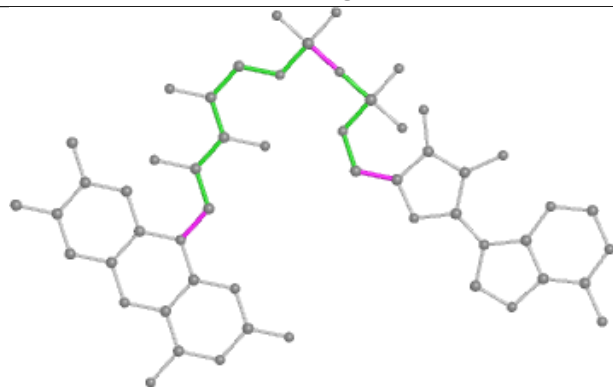
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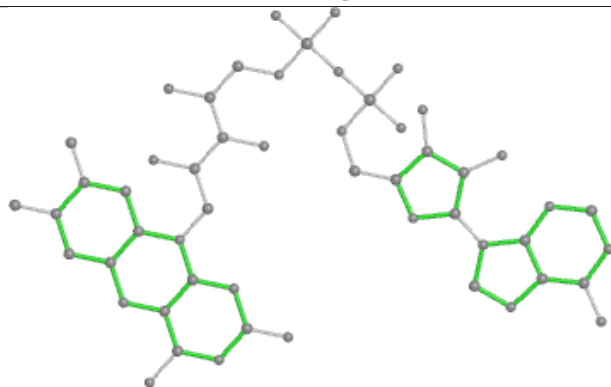
Bond lengths



Bond angles

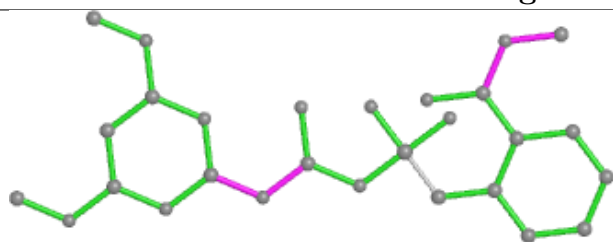


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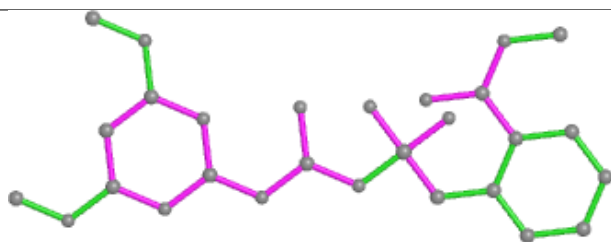


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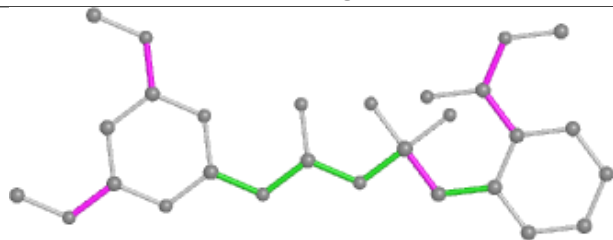
Ligand 60G R 702



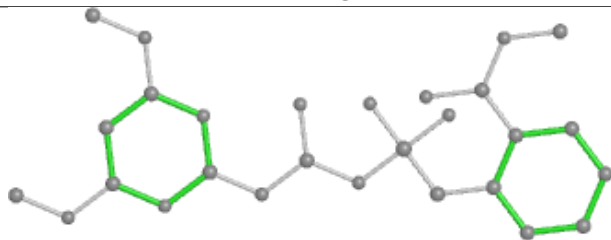
Bond lengths



Bond angles

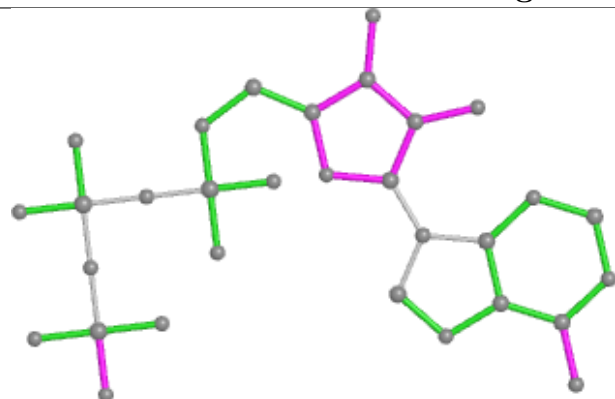


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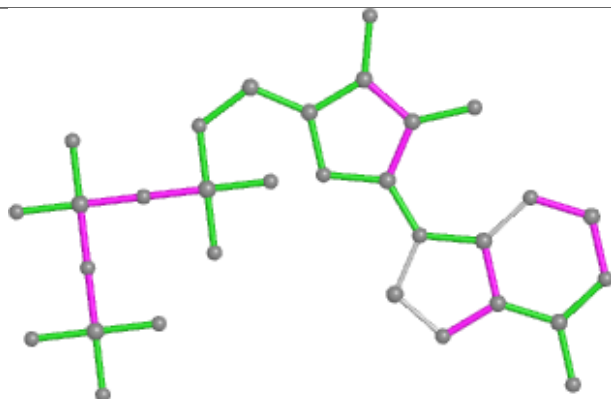


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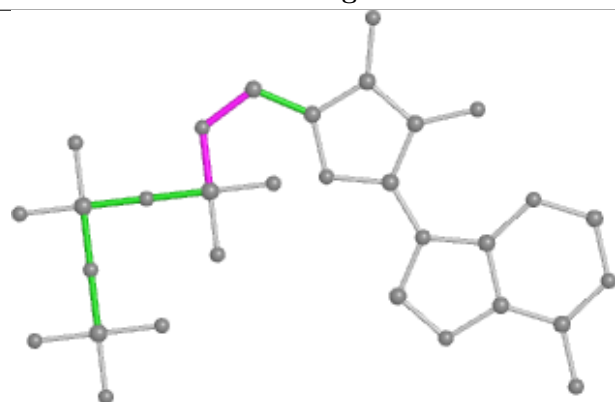
Ligand ATP K 401



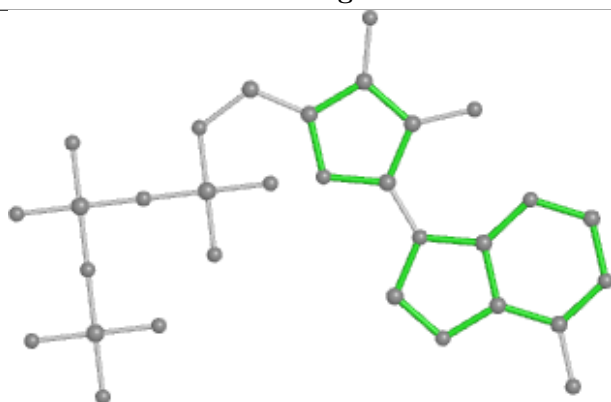
Bond lengths



Bond angles

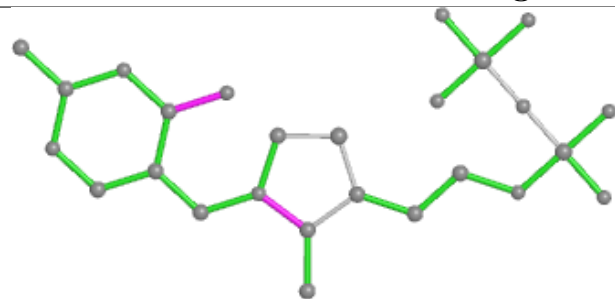


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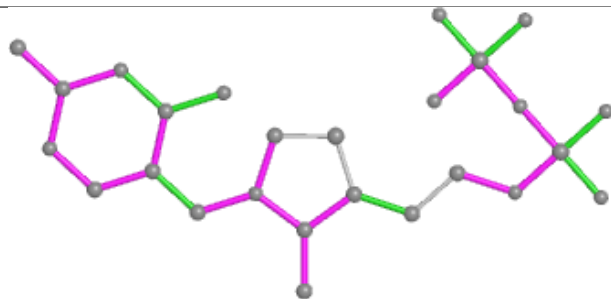


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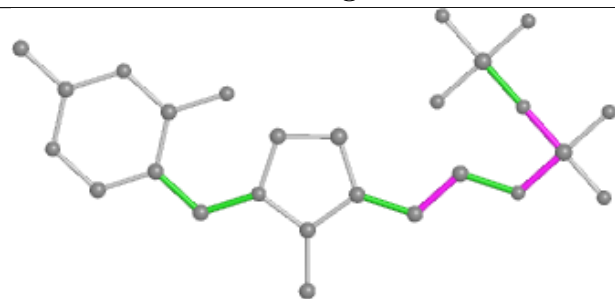
Ligand TPP M 701



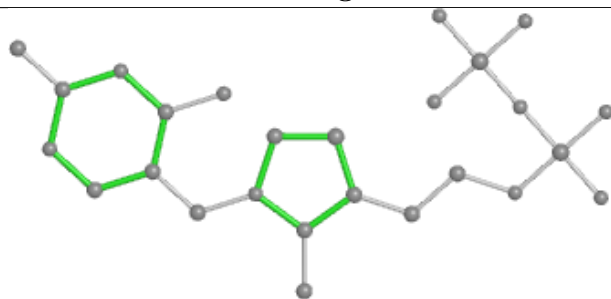
Bond lengths



Bond angles

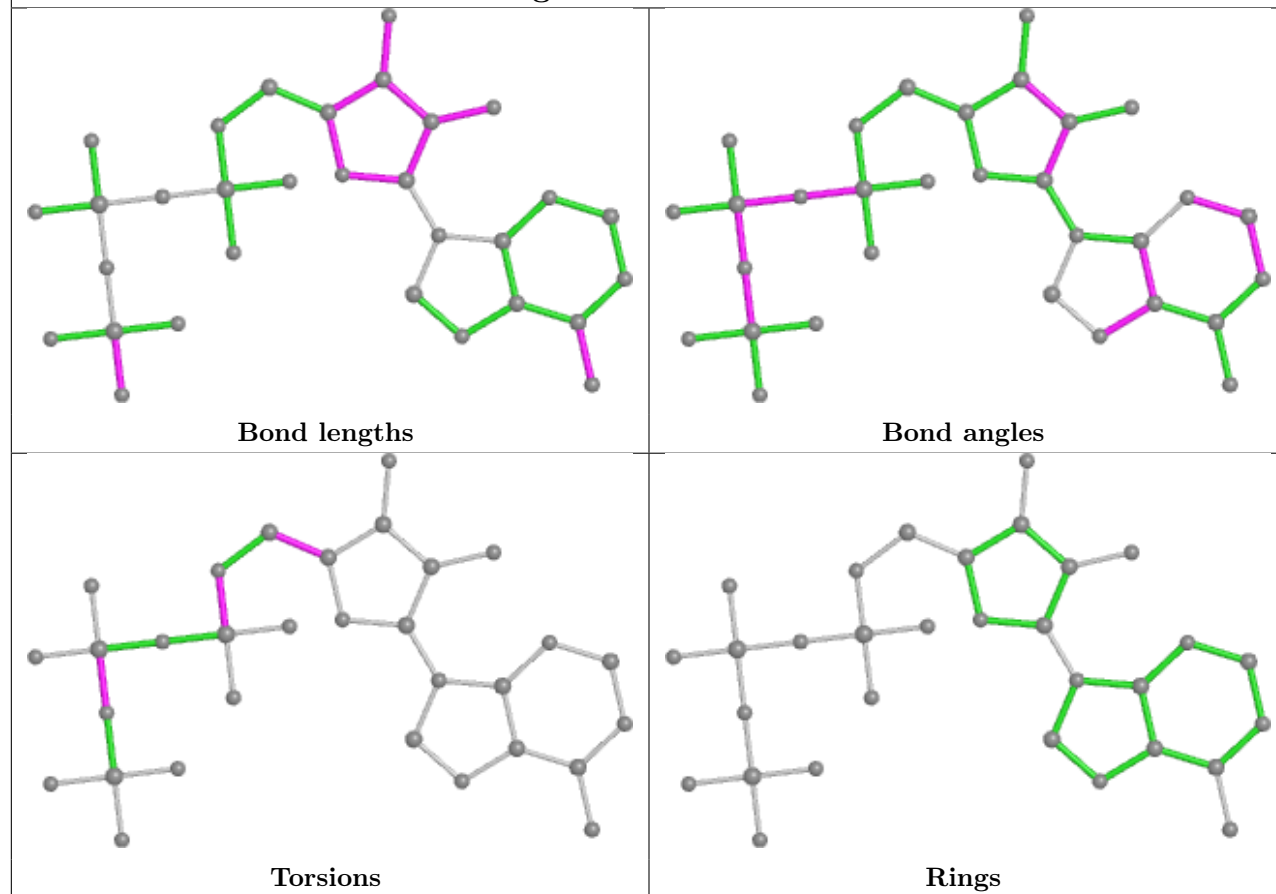


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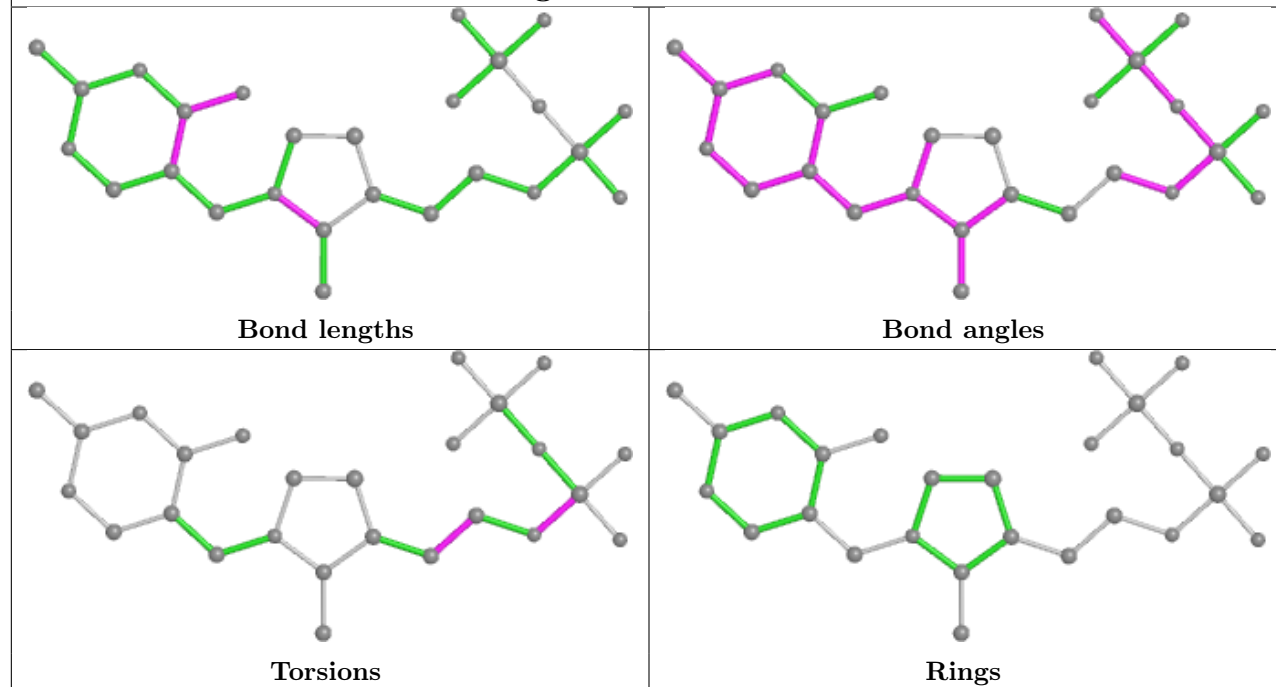


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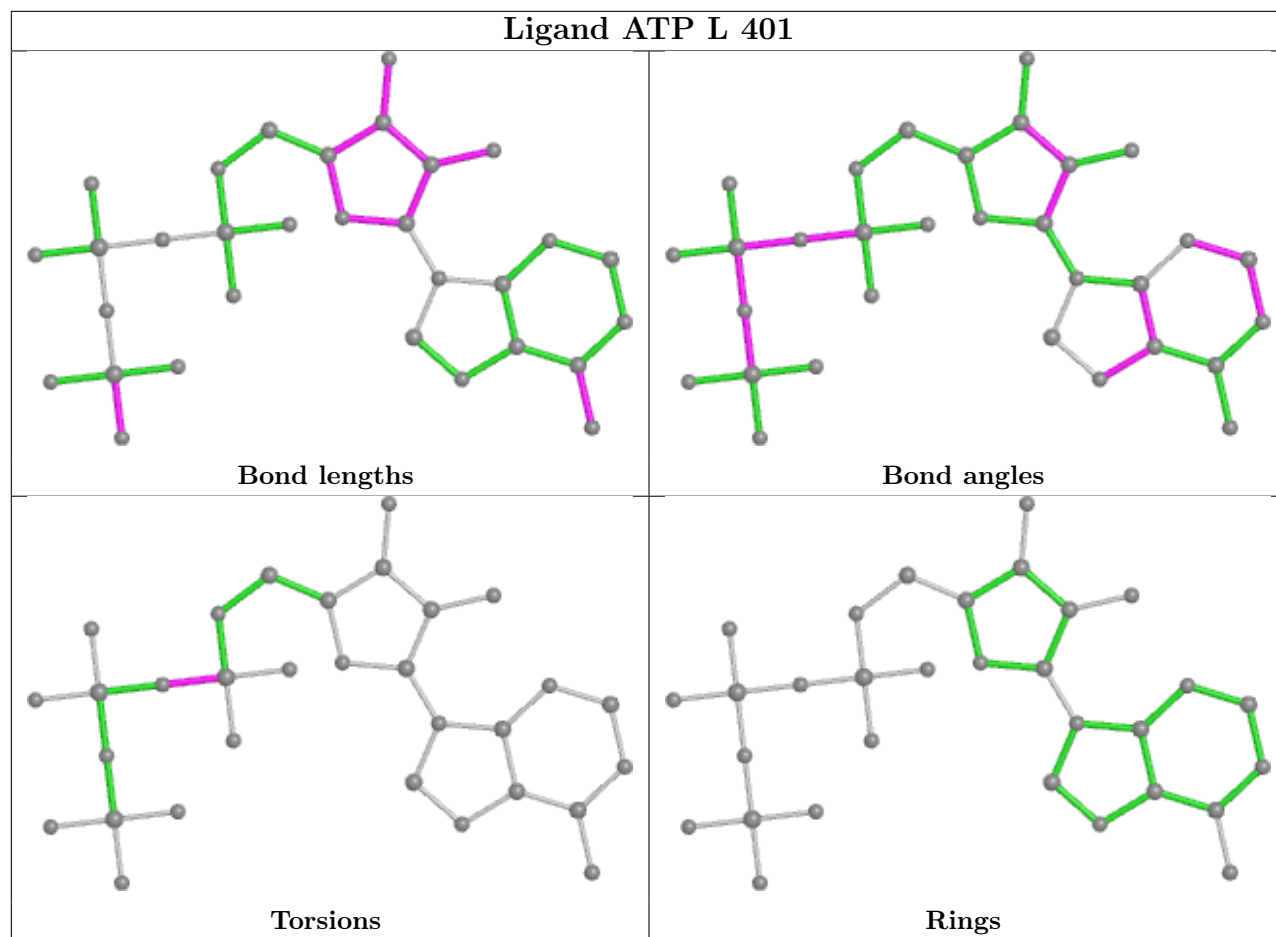
Ligand ATP C 401

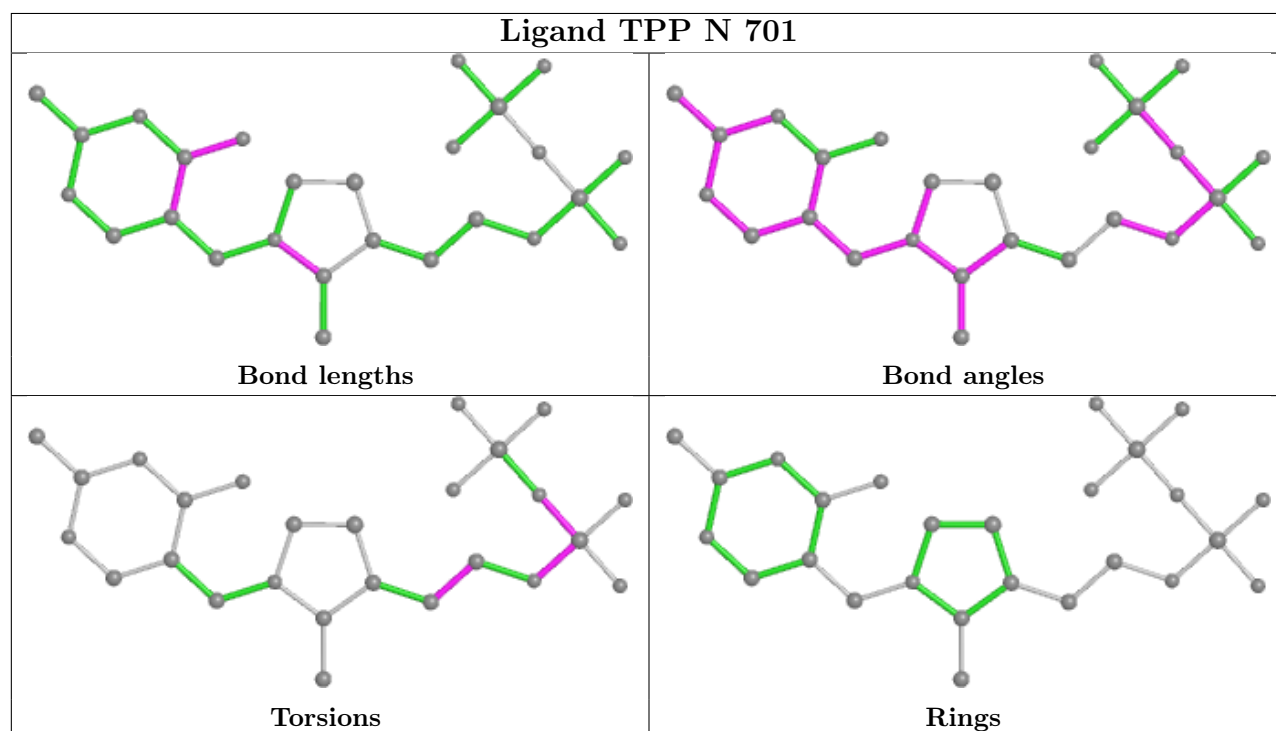
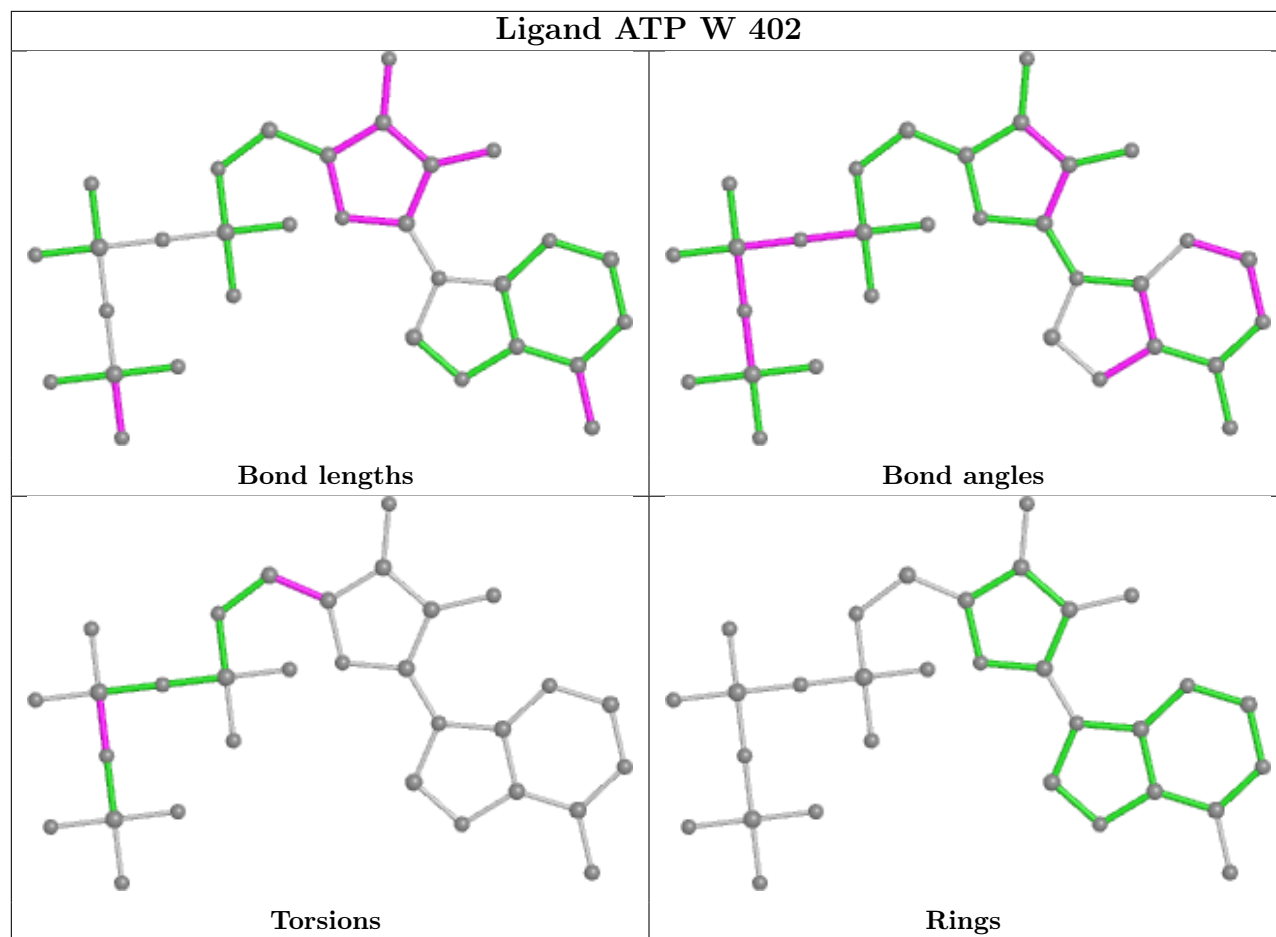


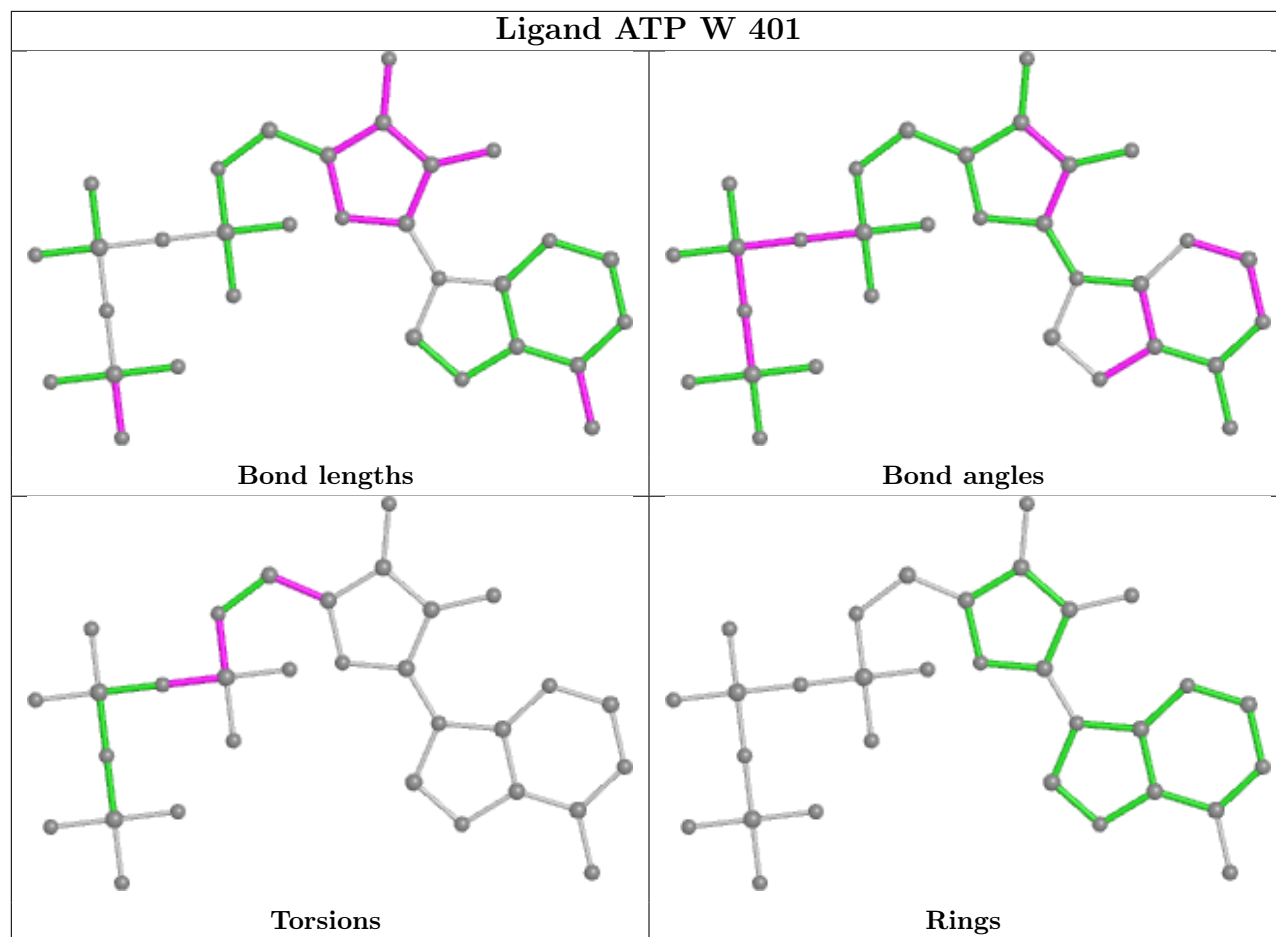
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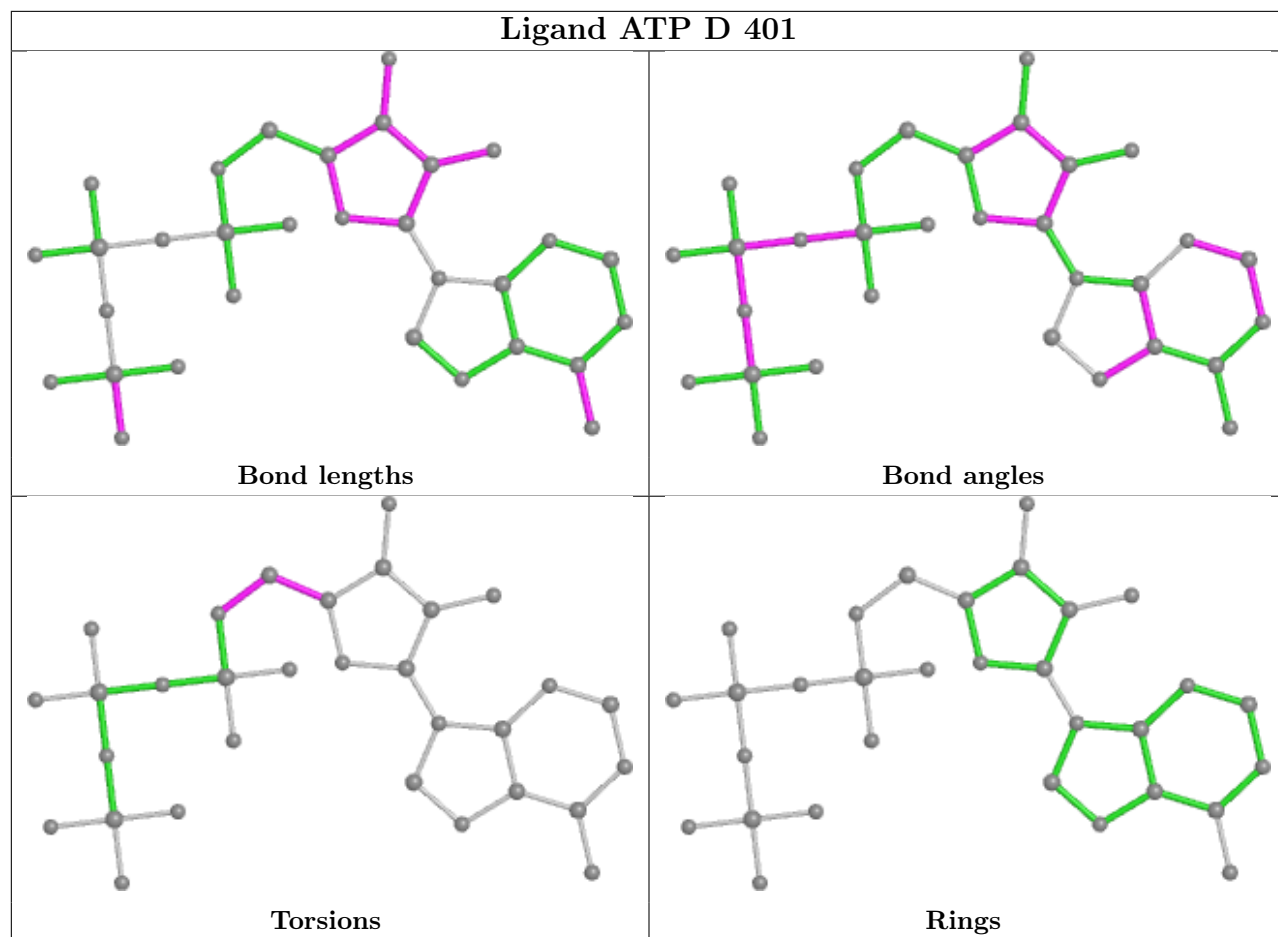


Ligand ATP L 401

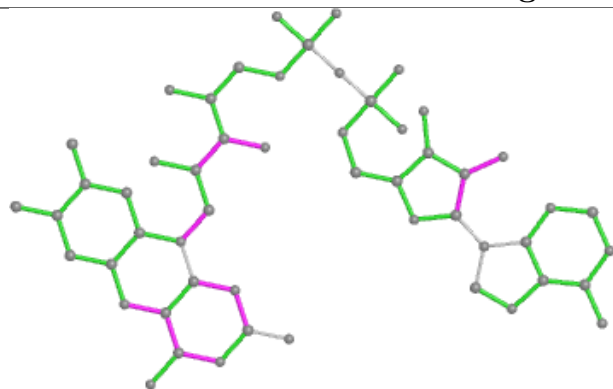




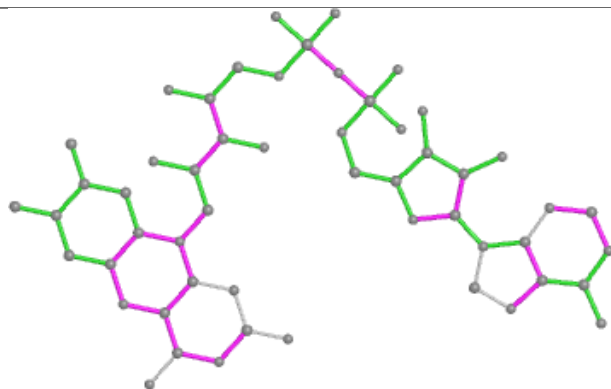




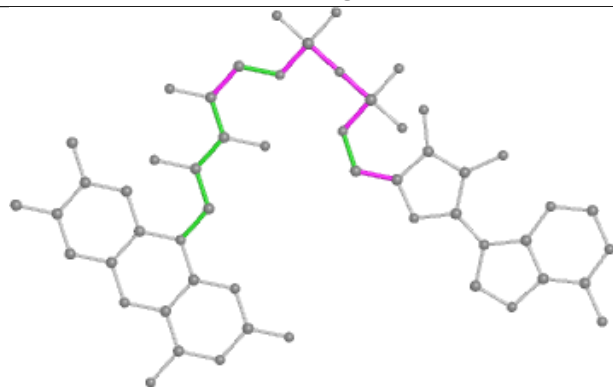
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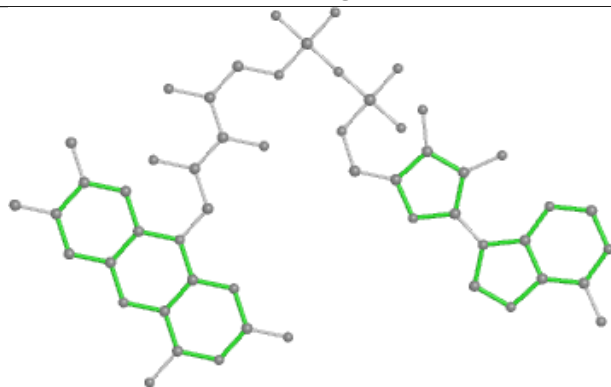
Bond lengths



Bond angles

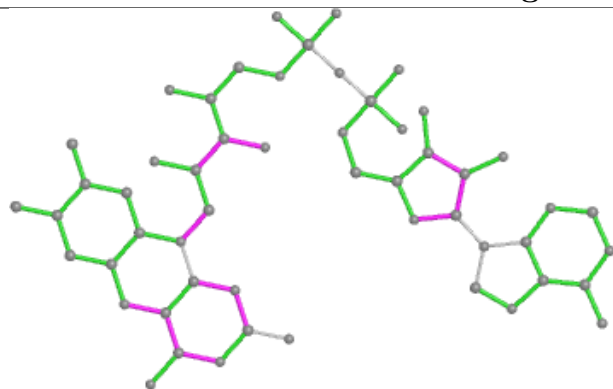


Torsions

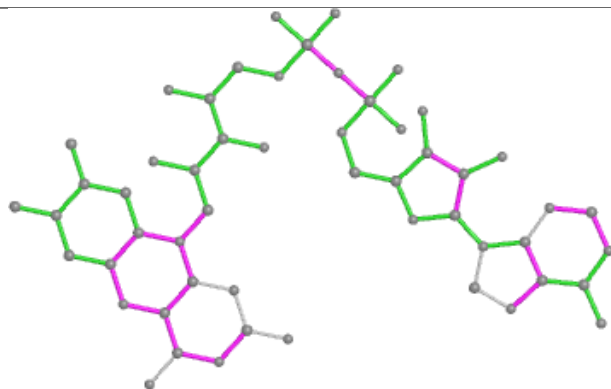


Rings

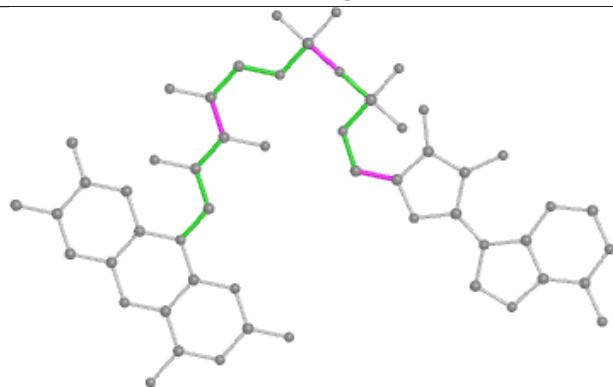
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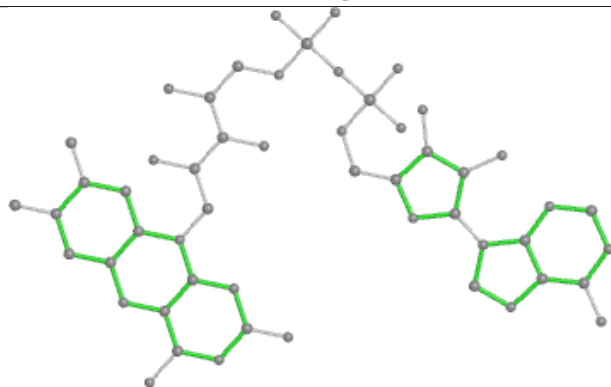
Bond lengths



Bond angles

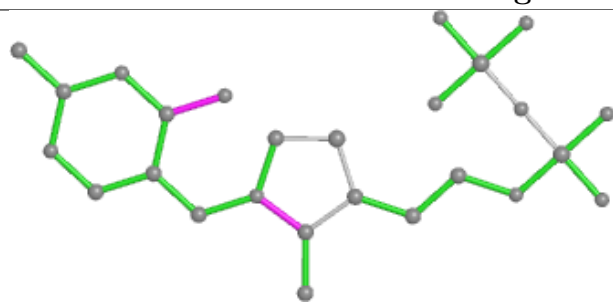


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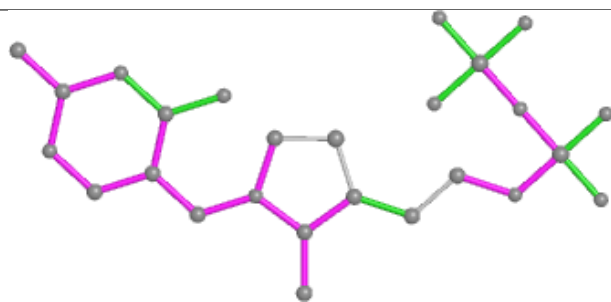


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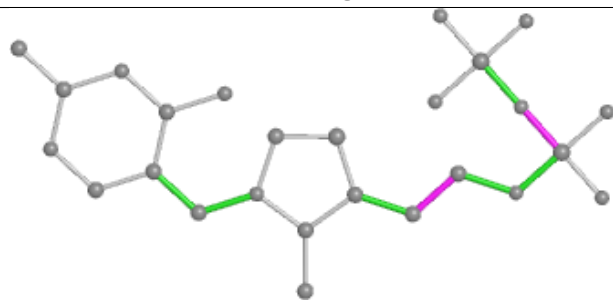
Ligand TPP V 701



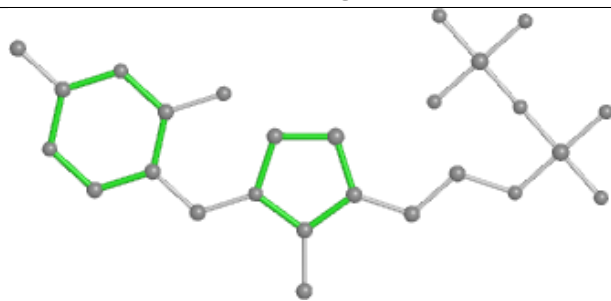
Bond lengths



Bond angles

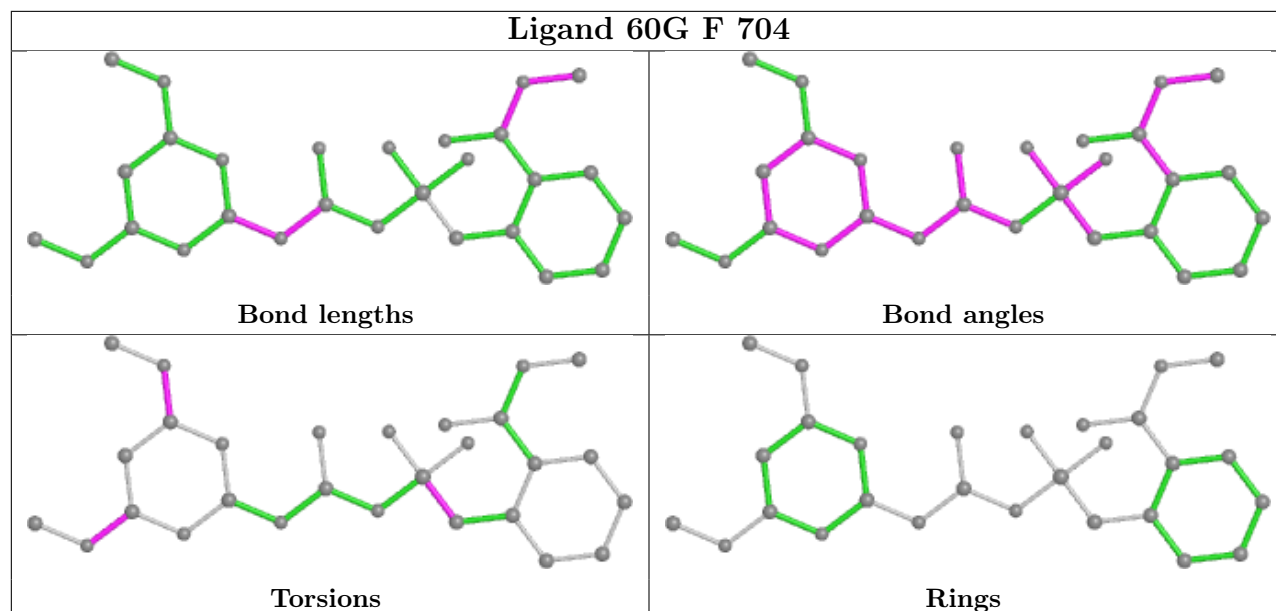


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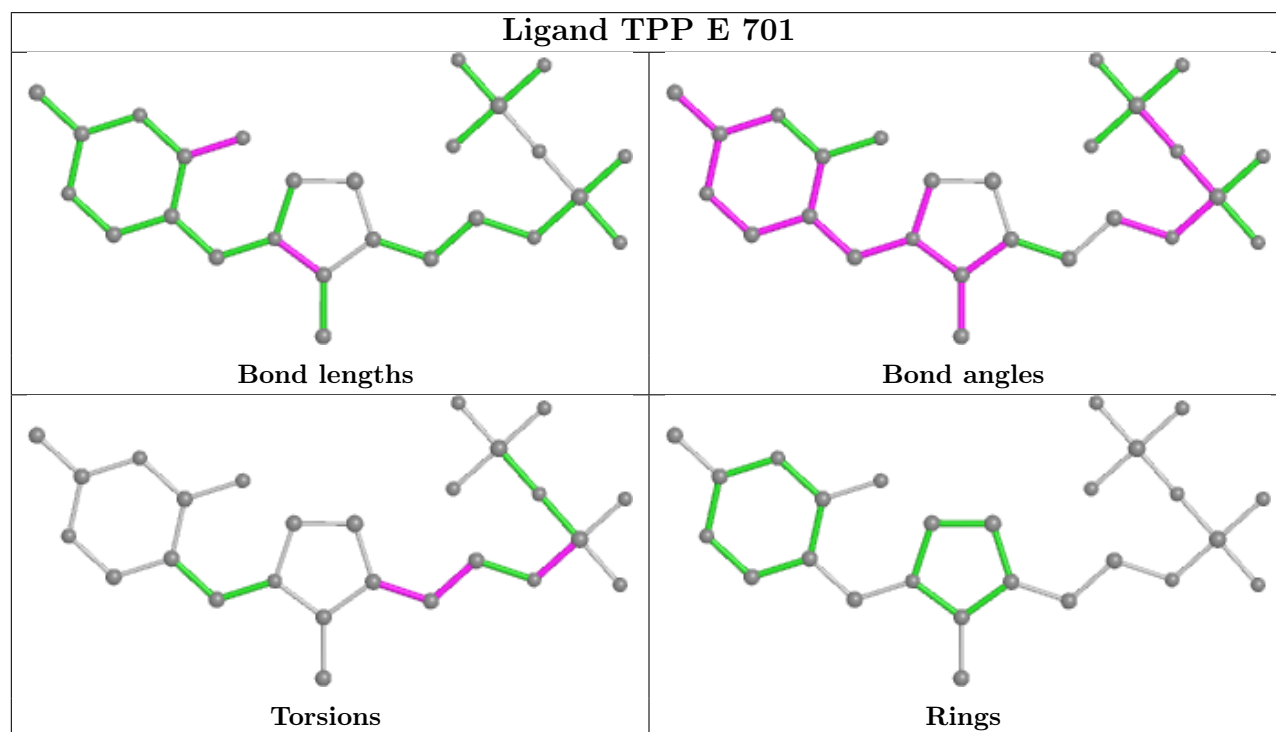


Rings

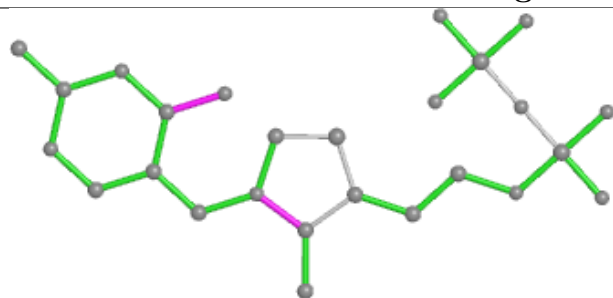
Ligand 60G F 704



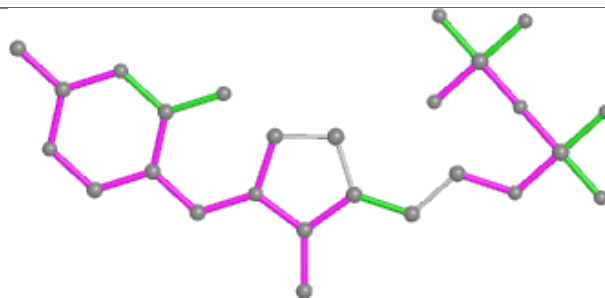
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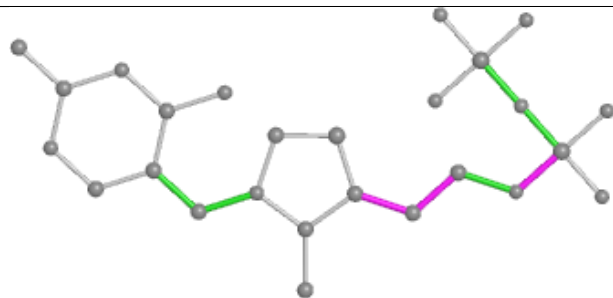
Ligand TPP B 701



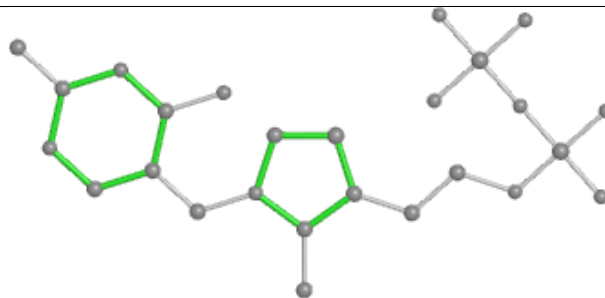
Bond lengths



Bond angles

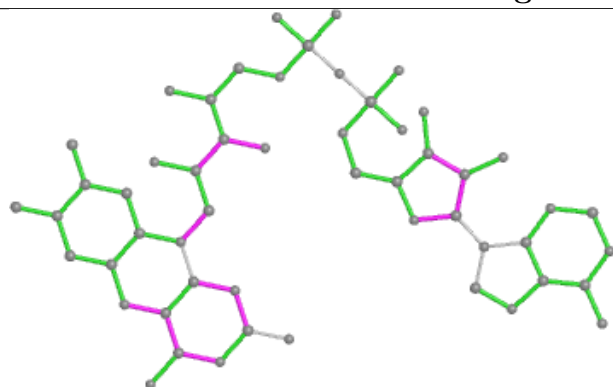


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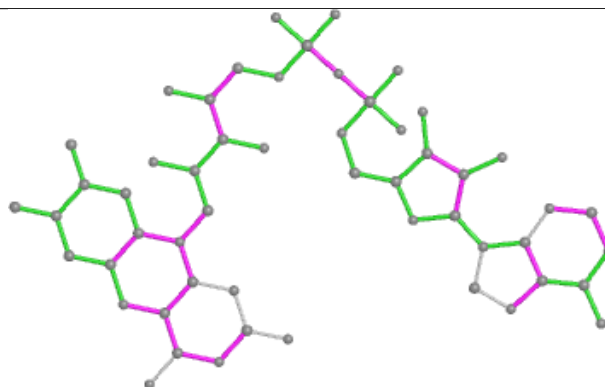


Rings

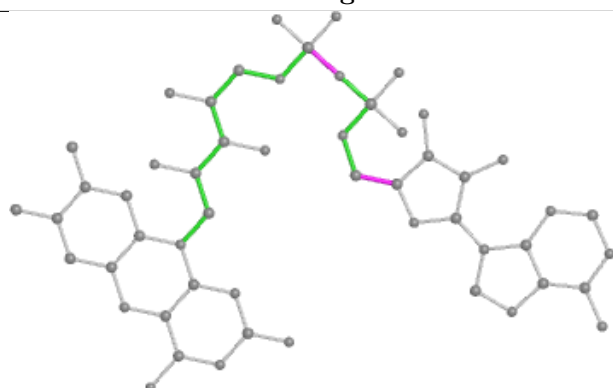
Ligand FAD A 703



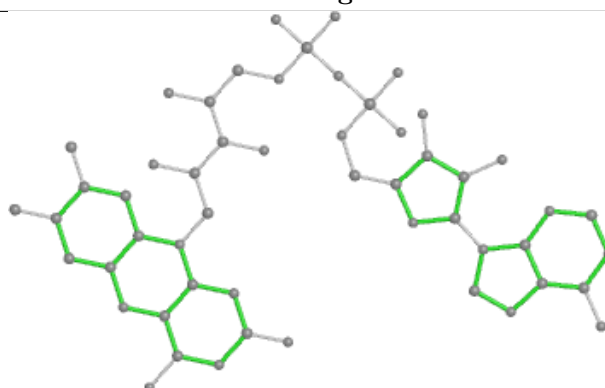
Bond lengths



Bond angles

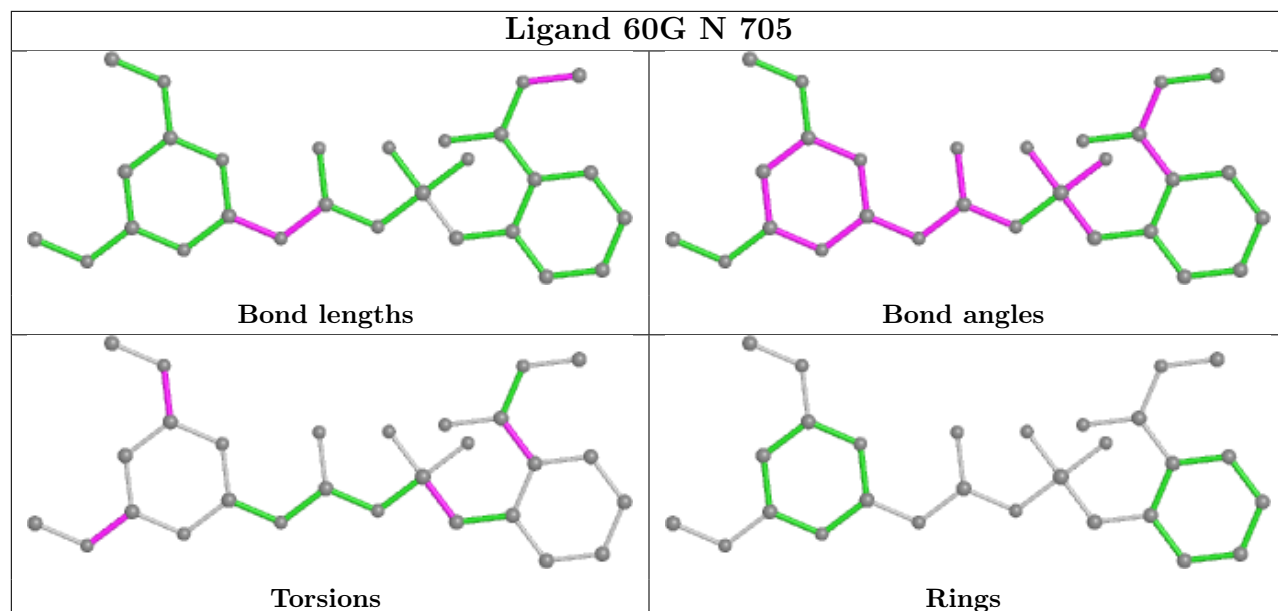


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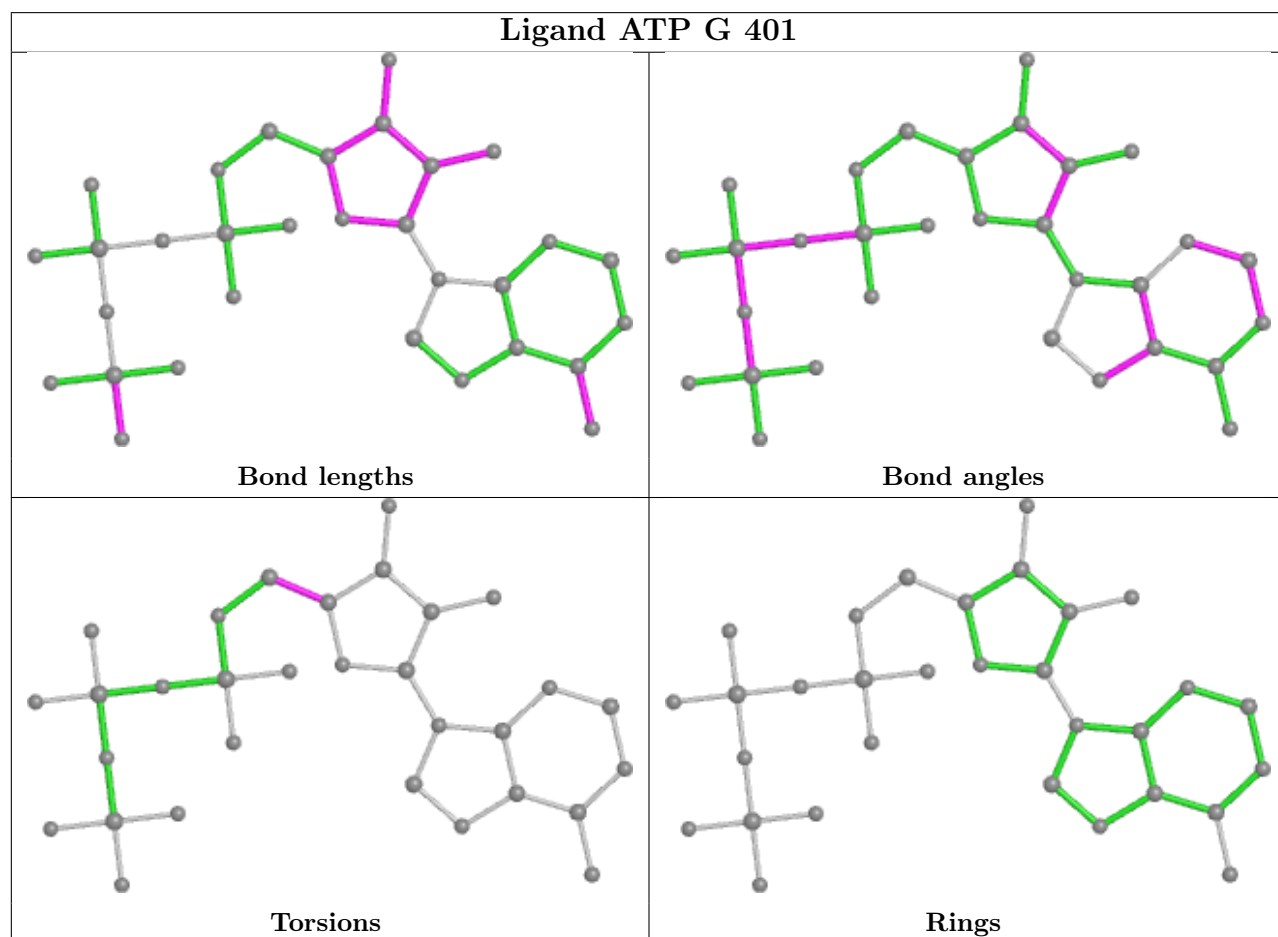


Rings

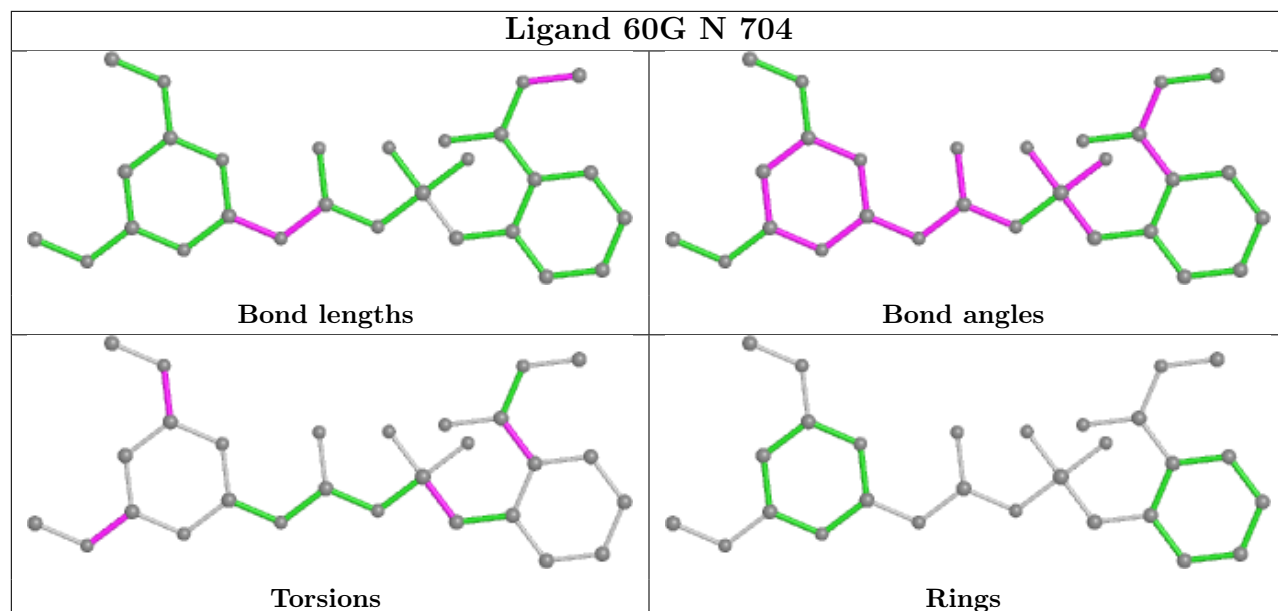
Ligand 60G N 705



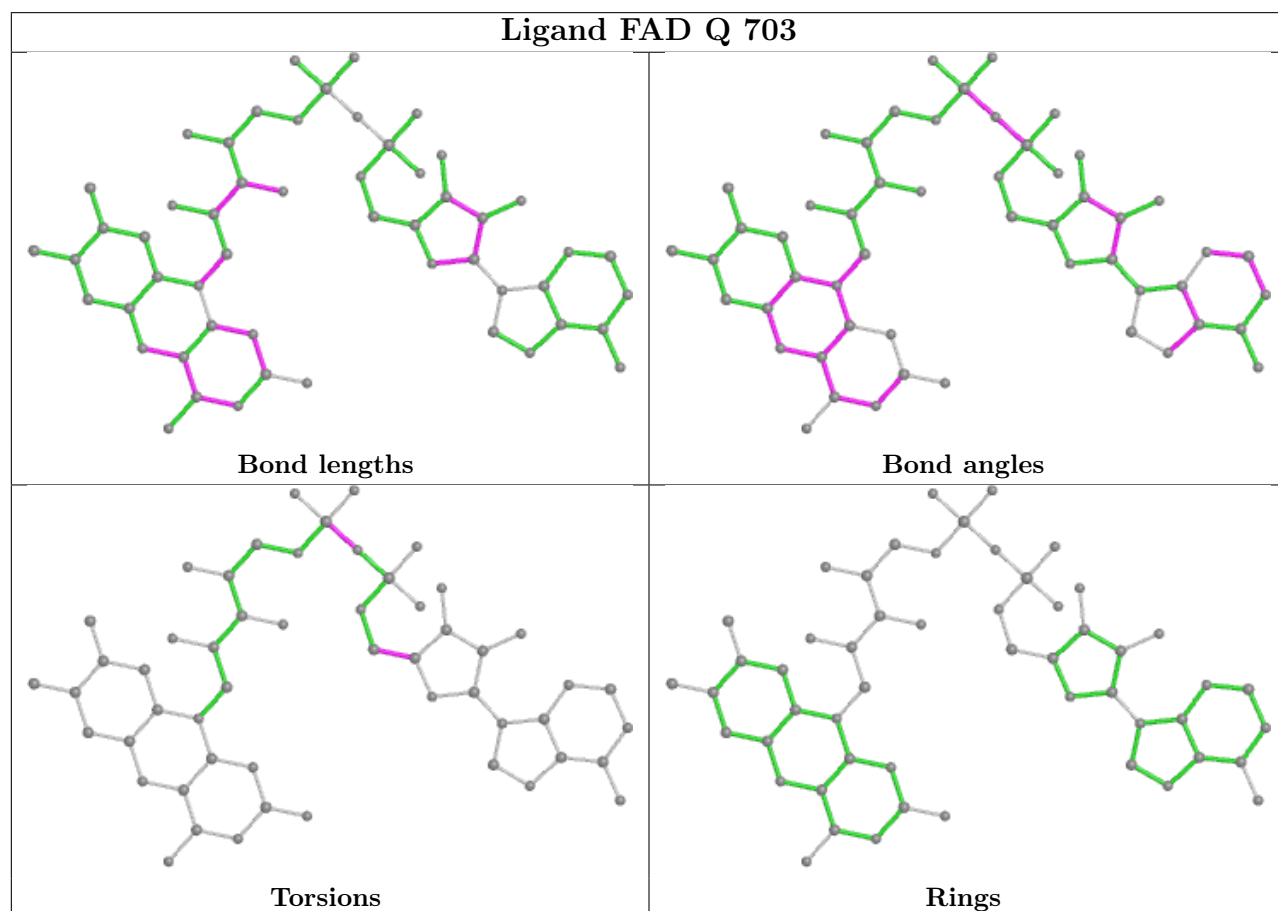
Ligand ATP G 401

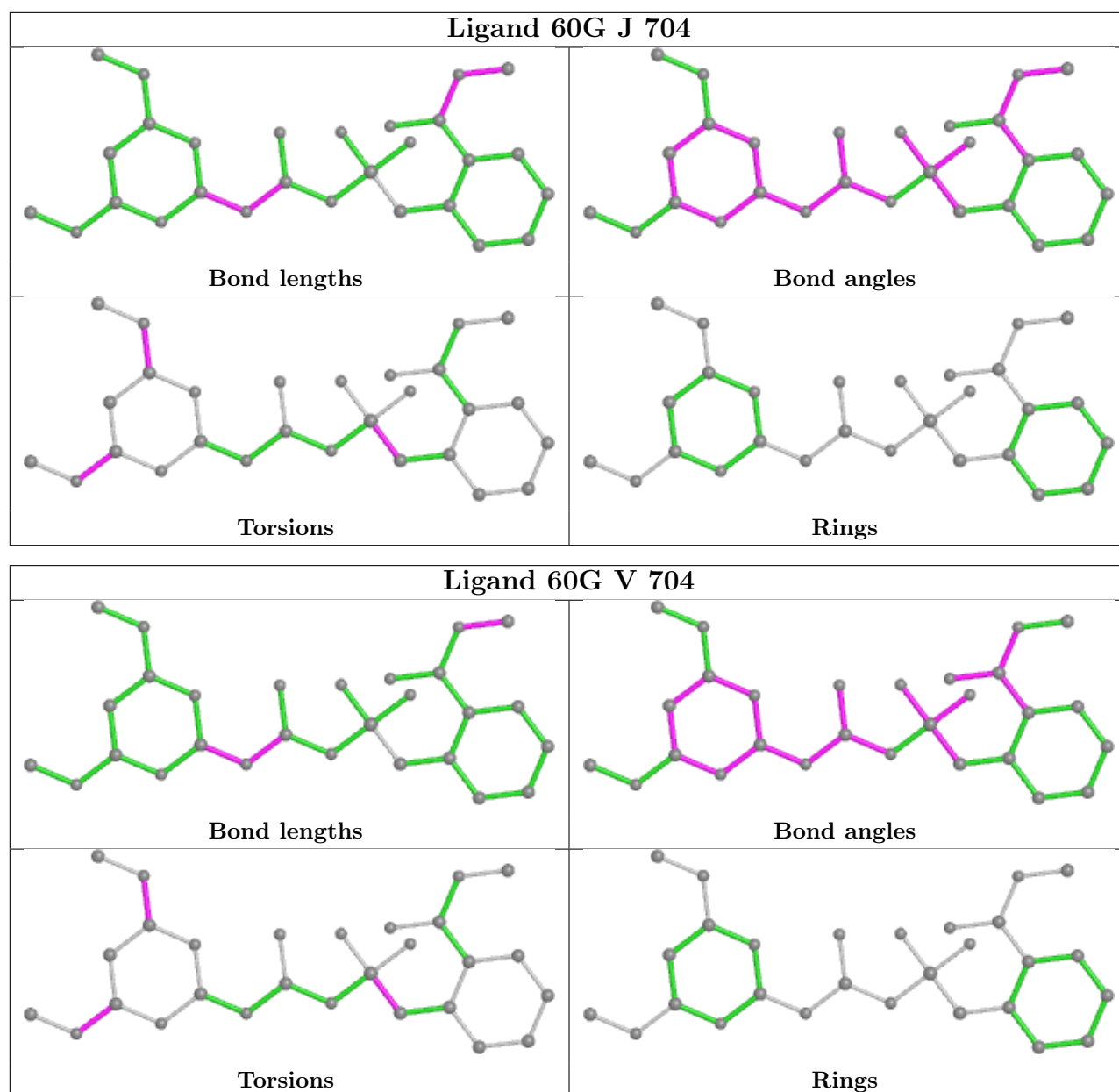


Ligand 60G N 704



Ligand FAD Q 703





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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%)	-0.28	0 100 100	25, 48, 86, 163	0
1	B	607/644 (94%)	-0.25	5 (0%) 86 78	26, 50, 90, 174	0
1	E	603/644 (93%)	0.07	14 (2%) 60 47	50, 74, 111, 191	0
1	F	604/644 (93%)	0.06	5 (0%) 86 78	50, 79, 121, 210	0
1	I	604/644 (93%)	0.14	9 (1%) 73 61	54, 93, 134, 205	0
1	J	602/644 (93%)	0.16	15 (2%) 57 43	56, 93, 135, 174	0
1	M	605/644 (93%)	-0.25	5 (0%) 86 78	29, 57, 101, 174	0
1	N	603/644 (93%)	-0.01	6 (0%) 82 72	34, 73, 119, 197	0
1	Q	598/644 (92%)	-0.03	10 (1%) 70 57	32, 82, 134, 168	0
1	R	416/644 (64%)	0.71	51 (12%) 4 2	46, 109, 161, 185	0
1	U	604/644 (93%)	-0.08	6 (0%) 82 72	27, 64, 105, 175	0
1	V	605/644 (93%)	-0.24	3 (0%) 91 86	27, 50, 85, 149	0
2	C	253/297 (85%)	0.01	15 (5%) 22 13	36, 61, 164, 226	0
2	D	250/297 (84%)	0.07	21 (8%) 11 6	39, 60, 157, 222	0
2	G	253/297 (85%)	0.04	9 (3%) 42 27	48, 75, 151, 202	0
2	H	252/297 (84%)	0.11	14 (5%) 24 13	44, 76, 144, 187	0
2	K	245/297 (82%)	0.11	10 (4%) 37 24	48, 74, 150, 220	0
2	L	255/297 (85%)	-0.00	10 (3%) 39 25	47, 72, 142, 183	0
2	O	237/297 (79%)	0.01	13 (5%) 25 14	40, 63, 154, 215	0
2	P	243/297 (81%)	-0.18	5 (2%) 63 49	36, 61, 117, 156	0
2	S	244/297 (82%)	-0.18	7 (2%) 51 36	34, 57, 133, 193	0
2	T	232/297 (78%)	-0.11	1 (0%) 92 89	36, 61, 118, 159	0
2	W	245/297 (82%)	-0.00	10 (4%) 37 24	31, 58, 140, 219	0
2	X	240/297 (80%)	-0.26	3 (1%) 77 65	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%)	-0.02	247 (2%) 57 43	25, 69, 131, 226	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	402	GLY	8.6
2	K	73	GLN	6.5
2	W	69	ALA	6.4
2	O	74	PRO	6.1
2	C	189	ALA	5.8
2	L	41	ALA	5.7
2	O	185	THR	5.6
2	D	73	GLN	5.2
1	U	276	LEU	5.2
2	G	74	PRO	5.2
2	K	72	ARG	5.1
2	D	74	PRO	5.1
1	N	275	GLN	5.1
2	C	74	PRO	5.0
2	K	74	PRO	5.0
1	R	314	ALA	4.8
2	H	71	SER	4.7
2	H	189	ALA	4.7
2	D	71	SER	4.5
2	H	183	THR	4.4
2	O	72	ARG	4.4
2	G	187	ALA	4.4
1	R	333	THR	4.3
1	R	371	ILE	4.3
1	E	272	ALA	4.3
2	C	49	LEU	4.3
2	S	70	PRO	4.3
2	H	70	PRO	4.2
2	G	71	SER	4.1
2	O	73	GLN	4.0
2	C	185	THR	4.0
2	D	72	ARG	4.0
2	K	71	SER	3.9
2	O	286	SER	3.9
2	H	188	GLY	3.8
1	Q	684	GLY	3.8
2	G	192	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	276	LEU	3.8
1	U	84	ASP	3.7
2	G	191	ASP	3.7
1	E	276	LEU	3.7
1	R	373	VAL	3.7
1	I	447	TRP	3.7
1	M	264	THR	3.6
2	W	71	SER	3.6
1	R	485	ASN	3.6
1	I	84	ASP	3.5
2	G	69	ALA	3.5
2	H	73	GLN	3.5
2	C	50	ASP	3.5
1	R	304	LEU	3.5
1	R	406	PHE	3.5
2	W	70	PRO	3.4
1	B	81	ALA	3.4
2	W	74	PRO	3.4
2	W	285	THR	3.4
2	H	74	PRO	3.3
2	H	187	ALA	3.3
2	K	285	THR	3.3
1	R	302	PRO	3.3
1	E	346	PRO	3.3
1	R	296	ILE	3.3
1	J	666	ASN	3.2
2	C	71	SER	3.2
1	J	90	VAL	3.2
1	M	276	LEU	3.2
1	R	129	ASP	3.2
2	K	284	LYS	3.2
1	B	83	PRO	3.2
2	C	188	GLY	3.2
1	Q	127	ASN	3.2
1	R	337	GLY	3.1
2	K	75	ARG	3.1
2	S	295	GLU	3.1
1	M	83	PRO	3.1
2	D	189	ALA	3.1
1	R	566	ALA	3.1
1	R	303	VAL	3.1
2	G	73	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	186	ASN	3.0
2	O	287	THR	3.0
2	H	72	ARG	3.0
1	B	82	GLU	3.0
1	Q	99	ASN	3.0
1	N	673	ARG	3.0
1	E	634	SER	3.0
2	W	48	THR	3.0
1	R	306	VAL	2.9
1	J	260	ASN	2.9
2	D	187	ALA	2.9
2	P	50	ASP	2.9
2	L	42	THR	2.9
2	L	43	ARG	2.9
2	C	68	PRO	2.9
2	S	74	PRO	2.9
1	R	265	LYS	2.9
2	O	196	VAL	2.8
1	R	430	ASN	2.8
1	N	402	GLY	2.8
2	C	70	PRO	2.8
1	R	257	ILE	2.8
1	R	567	GLY	2.8
2	D	190	ALA	2.8
2	W	47	PRO	2.8
2	H	284	LYS	2.7
2	L	187	ALA	2.7
1	F	85	MET	2.7
2	P	45	PRO	2.7
2	D	45	PRO	2.7
1	I	264	THR	2.7
1	J	274	ASN	2.7
1	U	275	GLN	2.7
2	C	72	ARG	2.7
2	L	70	PRO	2.7
1	U	402	GLY	2.7
2	D	186	ASN	2.7
2	C	47	PRO	2.7
2	H	69	ALA	2.7
1	R	266	THR	2.7
2	S	49	LEU	2.7
2	P	192	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	284	LYS	2.6
2	T	48	THR	2.6
2	O	283	LEU	2.6
1	I	129	ASP	2.6
1	R	593	HIS	2.6
2	D	188	GLY	2.6
1	V	83	PRO	2.6
1	R	382	THR	2.6
2	D	185	THR	2.6
1	E	85	MET	2.6
2	D	50	ASP	2.6
2	D	292	ASP	2.6
2	L	192	SER	2.6
2	S	282	PRO	2.5
1	J	84	ASP	2.5
1	F	274	ASN	2.5
1	R	475	THR	2.5
1	R	633	VAL	2.5
1	B	265	LYS	2.5
1	R	338	LEU	2.5
1	E	91	GLY	2.5
1	I	303	VAL	2.5
1	I	271	ASN	2.4
1	M	275	GLN	2.4
1	R	625	LEU	2.4
2	X	49	LEU	2.4
1	E	260	ASN	2.4
1	I	625	LEU	2.4
1	V	212	SER	2.4
1	J	629	LEU	2.4
1	J	646	ASP	2.4
2	O	50	ASP	2.4
1	N	330	PRO	2.4
1	Q	685	GLY	2.4
1	I	212	SER	2.4
2	O	71	SER	2.4
1	J	373	VAL	2.4
1	R	87	THR	2.4
2	S	69	ALA	2.4
1	N	303	VAL	2.4
1	Q	673	ARG	2.4
2	H	186	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	43	ARG	2.3
1	U	526	GLY	2.3
2	D	184	SER	2.3
1	E	258	LEU	2.3
1	J	277	THR	2.3
1	Q	84	ASP	2.3
1	R	298	LEU	2.3
1	R	100	GLU	2.3
1	R	325	ASP	2.3
1	E	264	THR	2.3
1	R	369	LEU	2.3
1	R	421	ILE	2.3
1	R	479	LYS	2.3
1	R	484	ALA	2.3
1	J	129	ASP	2.2
1	R	319	LEU	2.2
1	R	393	ARG	2.2
1	R	646	ASP	2.2
1	I	89	PHE	2.2
2	H	283	LEU	2.2
2	P	46	LEU	2.2
1	J	404	ILE	2.2
2	K	129	ASP	2.2
2	D	194	GLU	2.2
1	E	172	THR	2.2
2	S	73	GLN	2.2
1	R	481	SER	2.2
1	E	556	THR	2.2
2	L	77	GLN	2.2
2	X	192	SER	2.2
1	E	402	GLY	2.2
1	R	626	ASP	2.2
1	V	264	THR	2.2
2	D	199	ILE	2.2
1	M	261	PRO	2.2
1	R	261	PRO	2.2
2	C	73	GLN	2.2
2	O	68	PRO	2.2
2	C	75	ARG	2.2
2	D	70	PRO	2.1
2	G	188	GLY	2.1
1	R	264	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	262	ILE	2.1
2	P	153	ASN	2.1
1	R	312	ASN	2.1
2	D	69	ALA	2.1
1	R	295	LEU	2.1
1	R	630	LYS	2.1
2	L	191	ASP	2.1
2	L	190	ALA	2.1
1	F	666	ASN	2.1
1	Q	683	THR	2.1
1	F	140	GLN	2.1
1	J	261	PRO	2.1
1	Q	266	THR	2.1
1	F	402	GLY	2.1
2	L	73	GLN	2.1
2	O	57	ASN	2.1
1	R	288	SER	2.1
1	R	405	HIS	2.1
1	J	91	GLY	2.1
1	R	332	THR	2.1
2	D	285	THR	2.1
2	H	42	THR	2.1
1	U	270	SER	2.1
2	G	104	ASN	2.1
2	W	183	THR	2.1
2	W	286	SER	2.1
2	C	187	ALA	2.1
1	E	496	GLY	2.1
1	J	212	SER	2.1
1	J	85	MET	2.1
1	N	270	SER	2.1
1	R	268	LEU	2.0
1	R	403	ILE	2.0
2	O	69	ALA	2.0
1	Q	262	ILE	2.0
2	D	201	GLU	2.0
1	R	293	ALA	2.0
2	X	69	ALA	2.0
2	W	284	LYS	2.0
2	K	70	PRO	2.0
1	E	205	ASP	2.0
1	Q	223	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	MG	I	702	1/1	0.85	0.10	49,49,49,49	0
4	MG	V	702	1/1	0.88	0.32	63,63,63,63	0
5	FAD	R	701	53/53	0.88	0.26	79,105,131,145	0
6	60G	R	702	28/28	0.89	0.28	66,105,122,137	0
4	MG	F	702	1/1	0.90	0.20	50,50,50,50	0
4	MG	N	702	1/1	0.91	0.10	84,84,84,84	0
4	MG	E	702	1/1	0.91	0.13	77,77,77,77	0
6	60G	I	704	28/28	0.92	0.22	53,75,91,104	0
4	MG	M	702	1/1	0.93	0.13	27,27,27,27	0
3	TPP	Q	701	26/26	0.94	0.23	42,108,149,232	0
7	ATP	W	401	31/31	0.94	0.21	10,42,76,83	0
3	TPP	I	701	26/26	0.94	0.21	46,91,106,154	0
5	FAD	I	703	53/53	0.94	0.21	32,74,100,132	0
6	60G	E	704	28/28	0.94	0.20	60,70,88,99	0
6	60G	J	704	28/28	0.94	0.21	51,75,90,104	0
7	ATP	L	401	31/31	0.95	0.19	22,56,127,136	0
5	FAD	E	703	53/53	0.95	0.19	39,60,85,134	0
4	MG	B	702	1/1	0.95	0.21	30,30,30,30	0
7	ATP	K	401	31/31	0.95	0.18	36,65,75,82	0
7	ATP	D	401	31/31	0.95	0.20	37,56,84,94	0
5	FAD	F	703	53/53	0.95	0.19	43,69,84,102	0
4	MG	C	402	1/1	0.95	0.17	61,61,61,61	0
4	MG	J	702	1/1	0.95	0.06	99,99,99,99	0
5	FAD	J	703	53/53	0.95	0.18	37,55,88,132	0
5	FAD	U	703	53/53	0.95	0.21	25,52,75,121	0
6	60G	F	704	28/28	0.95	0.19	35,68,81,88	0
3	TPP	E	701	26/26	0.95	0.26	47,67,103,136	0

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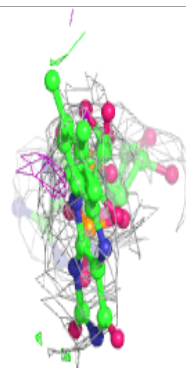
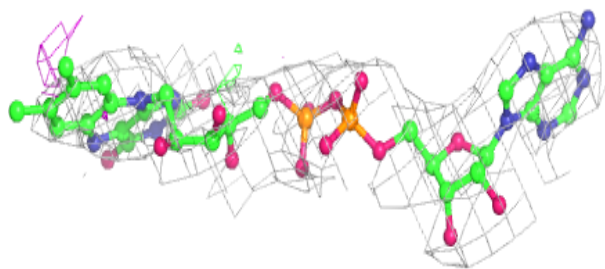
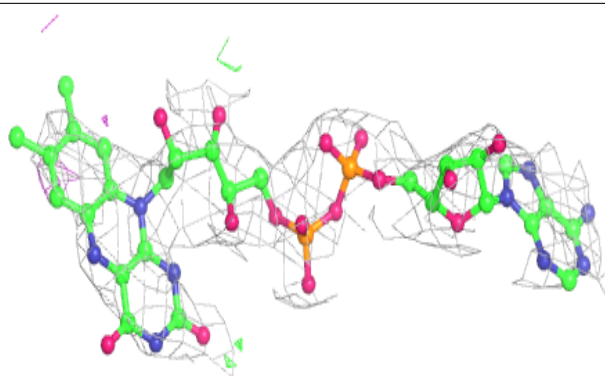
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	60G	N	704	28/28	0.95	0.22	37,54,80,91	0
7	ATP	S	401	31/31	0.95	0.17	25,51,71,75	0
3	TPP	J	701	26/26	0.95	0.17	54,91,135,145	0
4	MG	Q	702	1/1	0.96	0.14	137,137,137,137	0
7	ATP	C	401	31/31	0.96	0.17	16,43,86,94	0
7	ATP	T	401	31/31	0.96	0.17	21,44,78,82	0
6	60G	A	704	28/28	0.96	0.18	18,45,64,79	0
3	TPP	F	701	26/26	0.96	0.22	36,68,92,132	0
5	FAD	V	703	53/53	0.96	0.18	22,37,50,57	0
3	TPP	N	701	26/26	0.96	0.19	32,50,92,109	0
3	TPP	U	701	26/26	0.96	0.23	26,64,105,143	0
5	FAD	M	703	53/53	0.96	0.18	25,41,59,63	0
4	MG	U	702	1/1	0.96	0.13	44,44,44,44	0
7	ATP	H	401	31/31	0.96	0.19	8,58,82,105	0
7	ATP	P	401	31/31	0.96	0.15	24,49,73,128	0
5	FAD	N	703	53/53	0.96	0.20	42,63,86,102	0
7	ATP	O	401	31/31	0.96	0.18	9,66,87,104	0
6	60G	N	705	28/28	0.96	0.18	34,58,68,74	0
7	ATP	G	401	31/31	0.96	0.17	27,55,82,116	0
6	60G	U	704	28/28	0.96	0.18	24,56,73,75	0
5	FAD	B	703	53/53	0.96	0.17	10,42,56,61	0
6	60G	Q	704	28/28	0.96	0.21	45,63,75,82	0
6	60G	V	704	28/28	0.96	0.21	17,48,64,82	0
6	60G	B	704	28/28	0.97	0.17	11,40,62,69	0
5	FAD	Q	703	53/53	0.97	0.16	17,44,71,74	0
3	TPP	V	701	26/26	0.97	0.22	9,50,69,119	0
3	TPP	M	701	26/26	0.97	0.19	11,50,91,103	0
7	ATP	W	402	31/31	0.97	0.16	11,46,70,78	0
5	FAD	A	703	53/53	0.97	0.18	19,37,51,65	0
4	MG	D	402	1/1	0.98	0.19	40,40,40,40	0
4	MG	H	402	1/1	0.98	0.20	53,53,53,53	0
3	TPP	A	701	26/26	0.98	0.18	13,41,66,77	0
4	MG	W	403	1/1	0.98	0.24	29,29,29,29	0
3	TPP	B	701	26/26	0.98	0.19	15,41,63,74	0
4	MG	A	702	1/1	0.98	0.15	19,19,19,19	0
4	MG	L	402	1/1	0.99	0.20	74,74,74,74	0

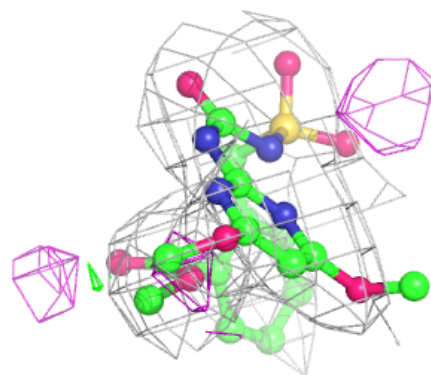
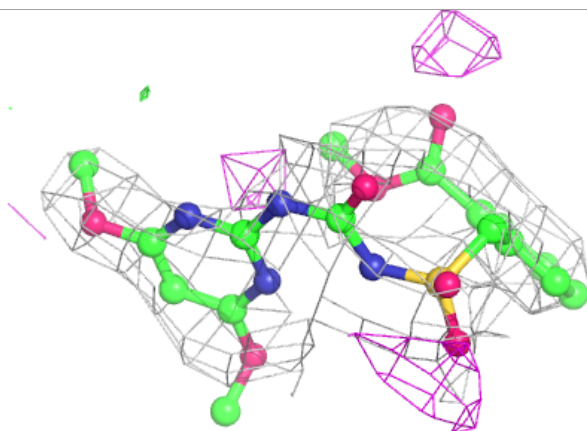
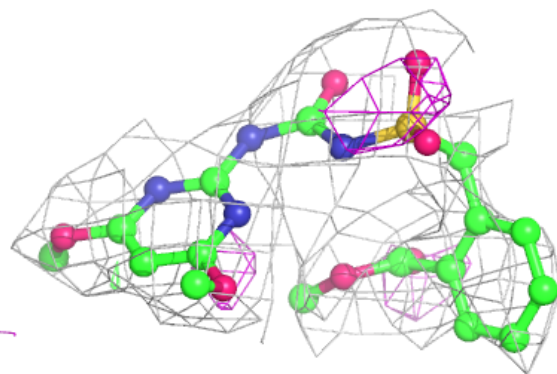
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD R 701:

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

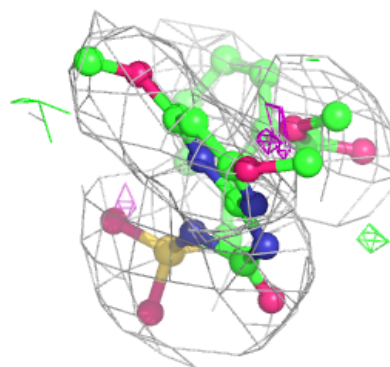
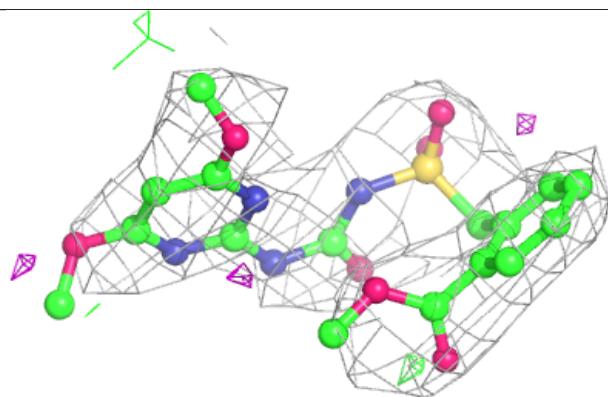
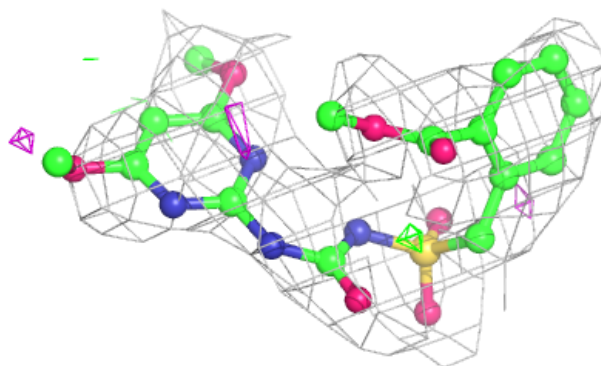
**Electron density around 60G R 702:**

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

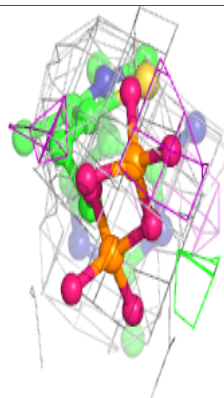
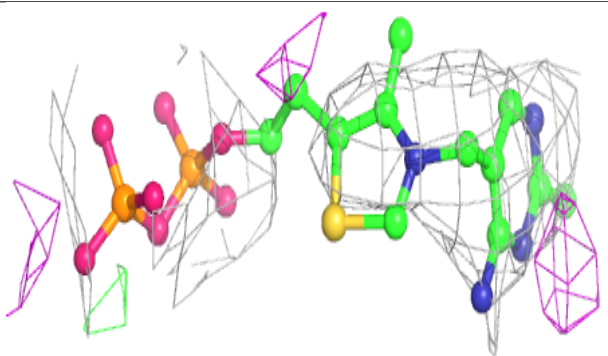
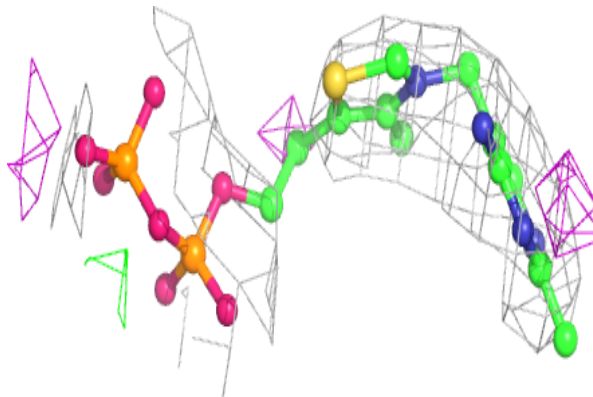


Electron density around 60G I 704:

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

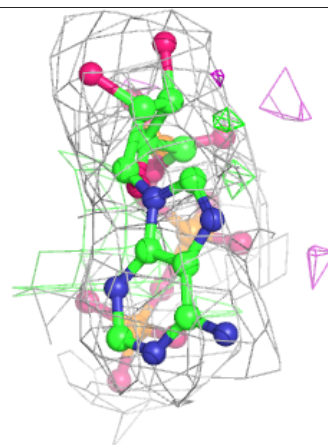
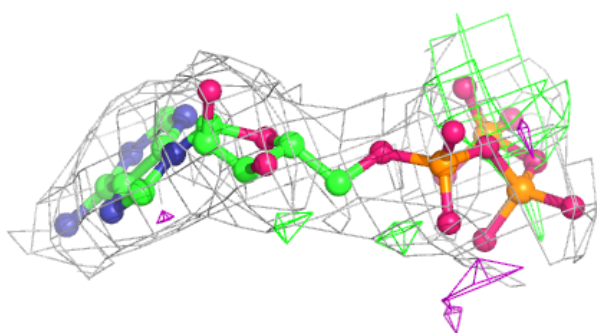
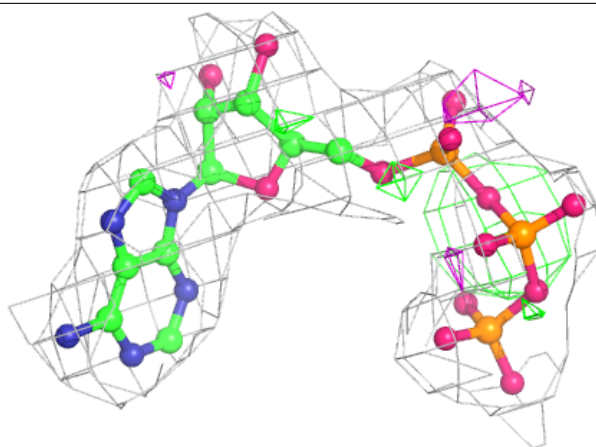
**Electron density around TPP Q 701:**

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

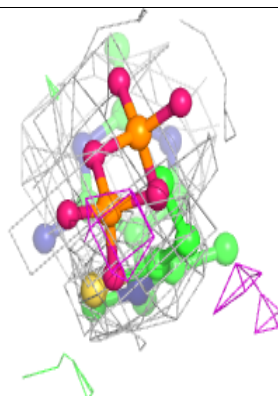
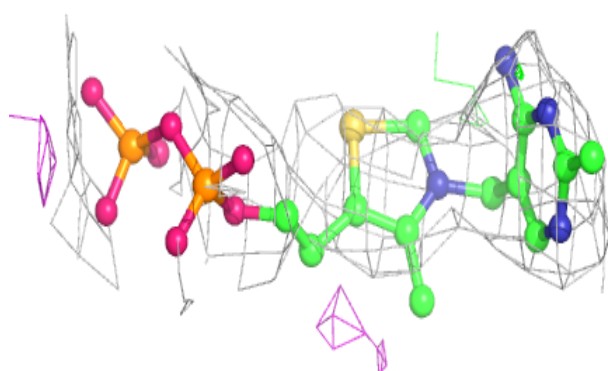
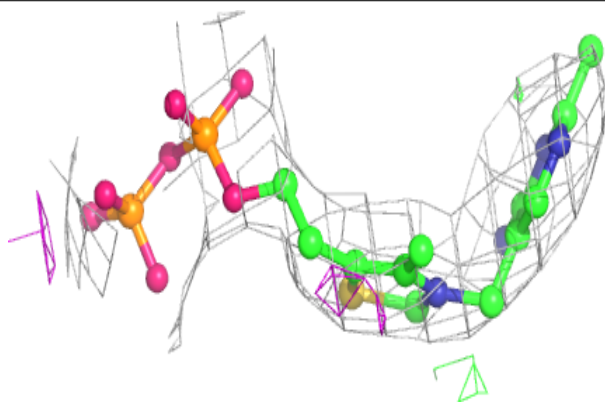


Electron density around ATP W 401:

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

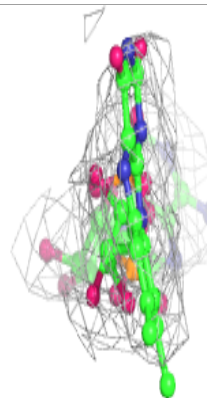
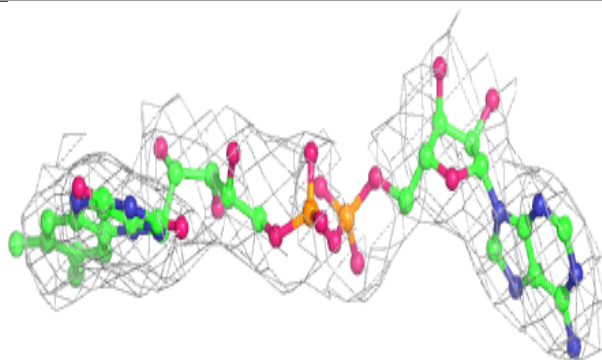
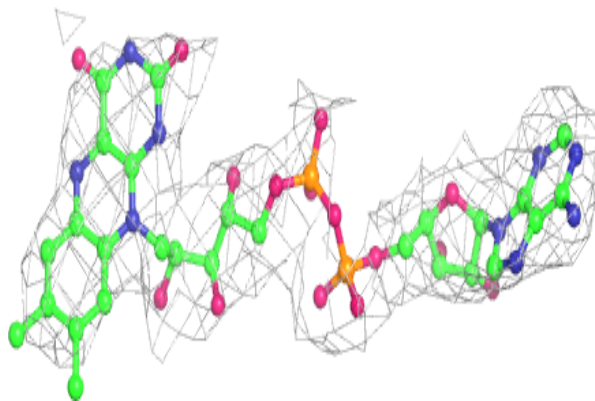
**Electron density around TPP I 701:**

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



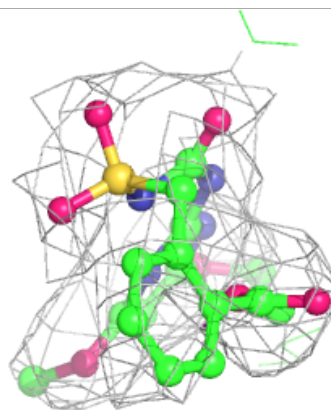
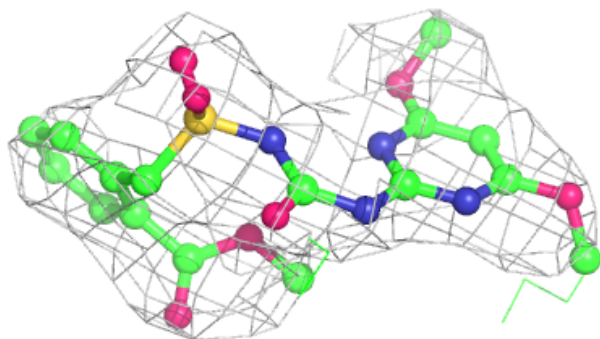
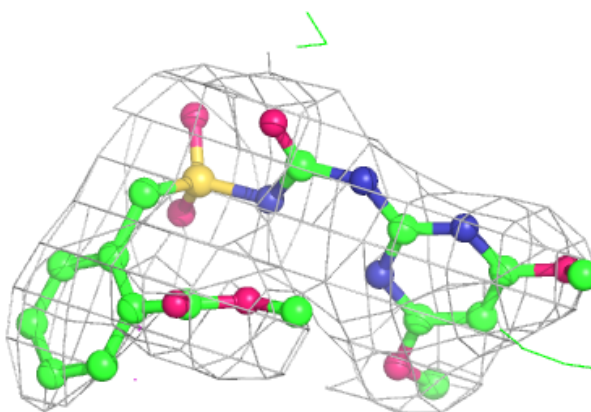
Electron density around FAD I 703:

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



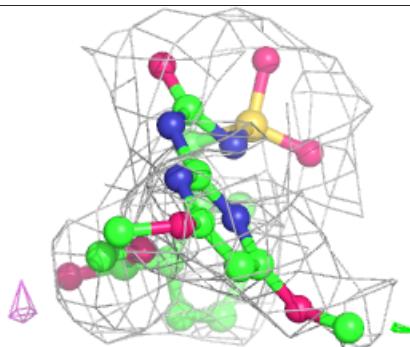
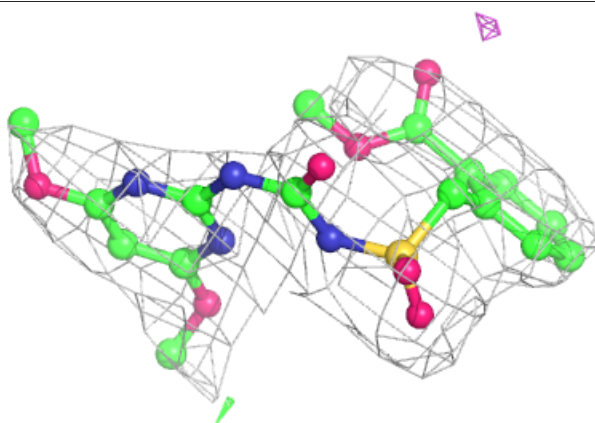
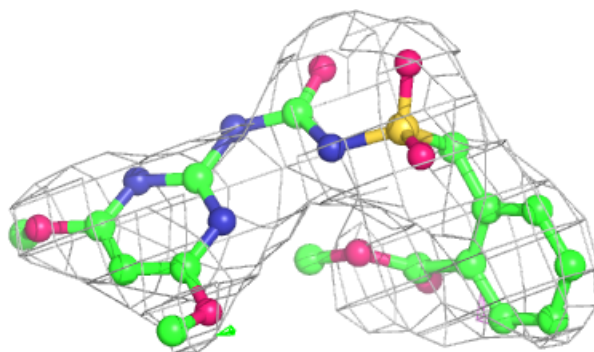
Electron density around 60G E 704:

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



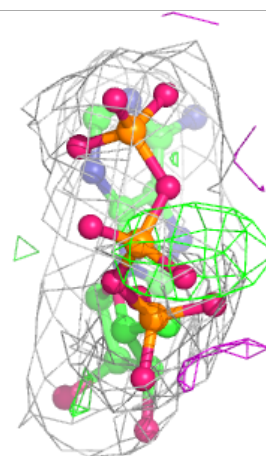
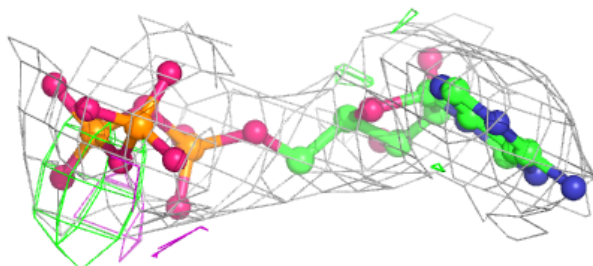
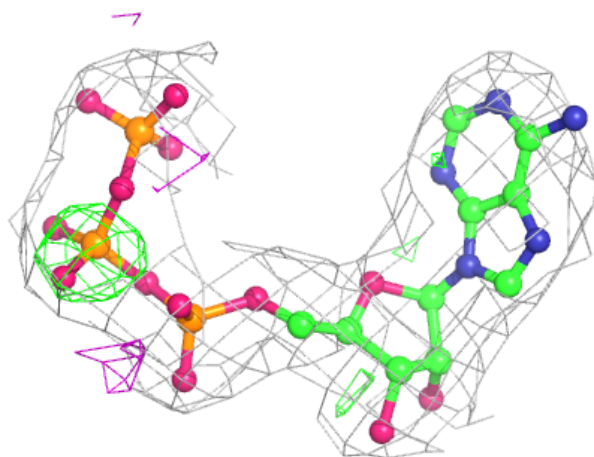
Electron density around 60G J 704:

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



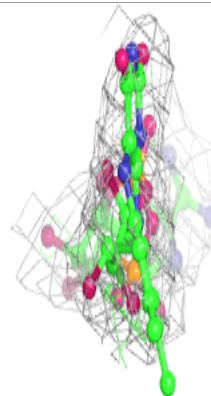
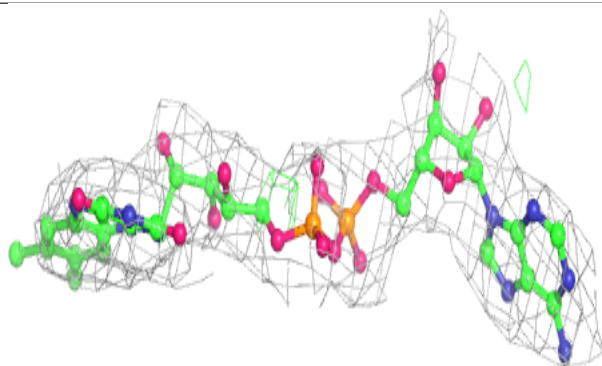
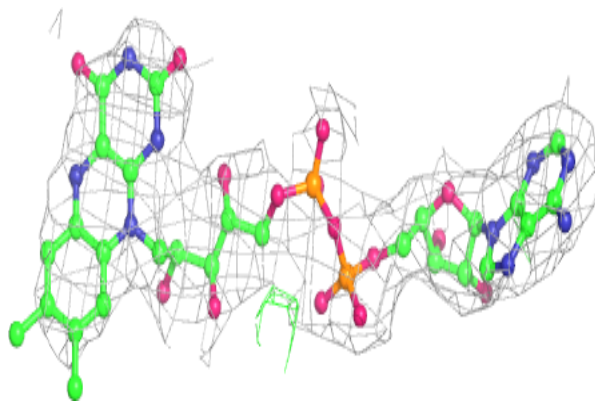
Electron density around ATP L 401:

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



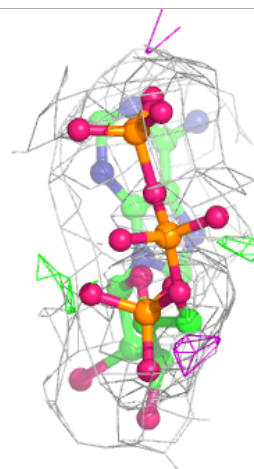
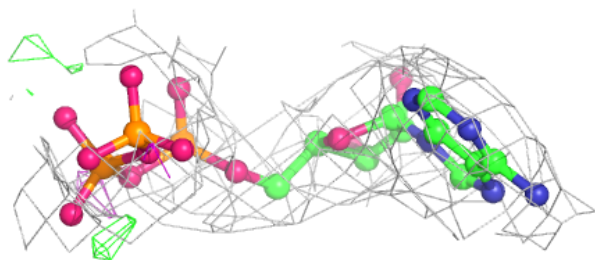
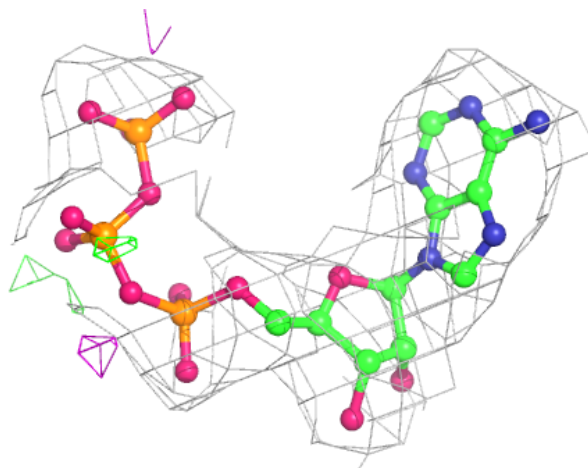
Electron density around FAD E 703:

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



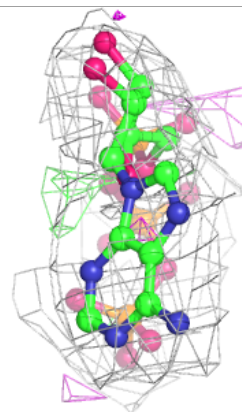
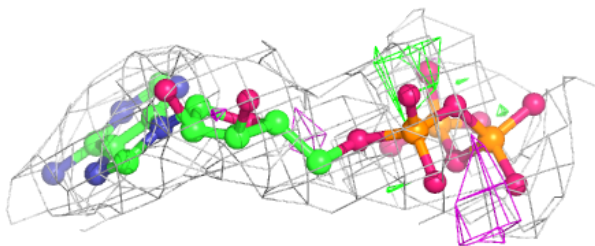
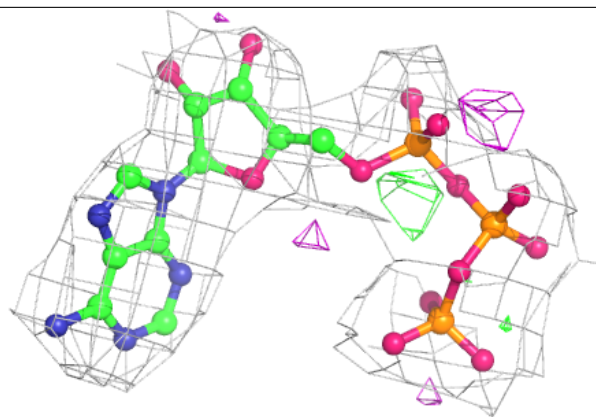
Electron density around ATP K 401:

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

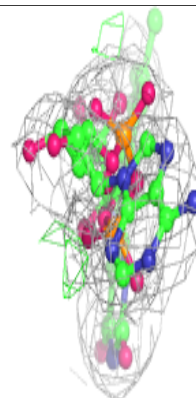
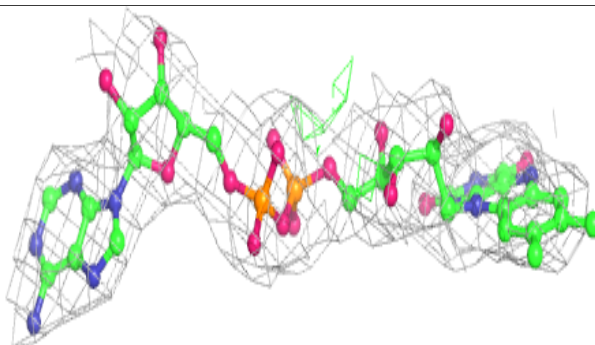
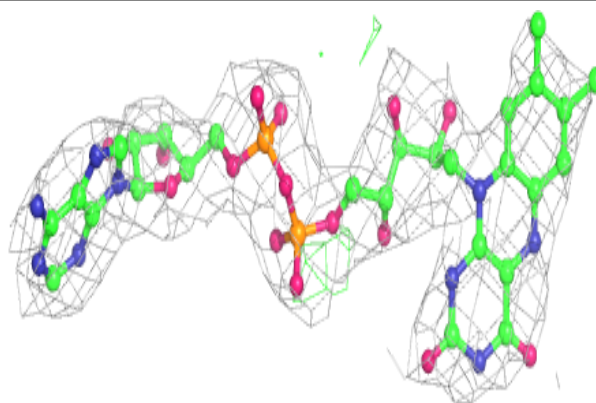


Electron density around ATP D 401:

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

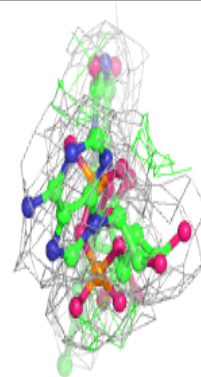
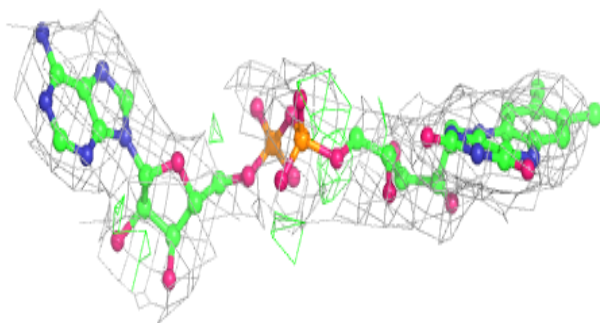
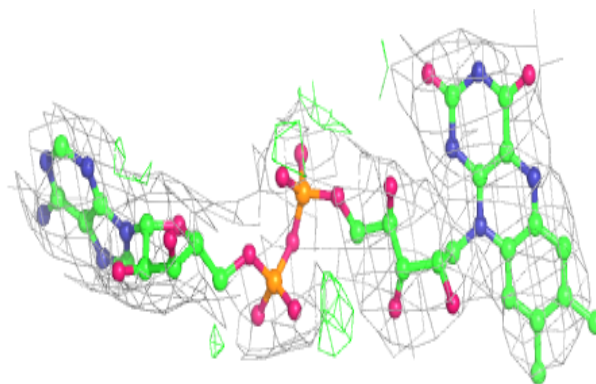
**Electron density around FAD F 703:**

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

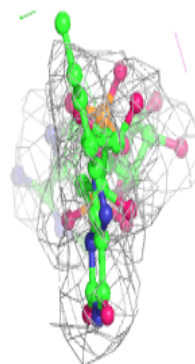
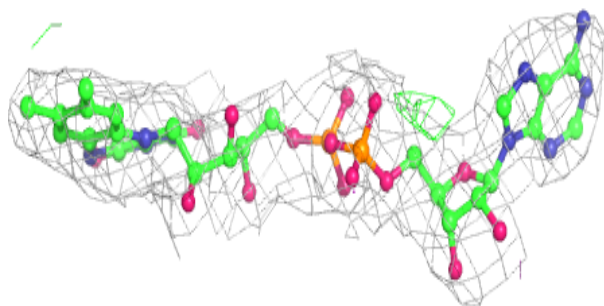
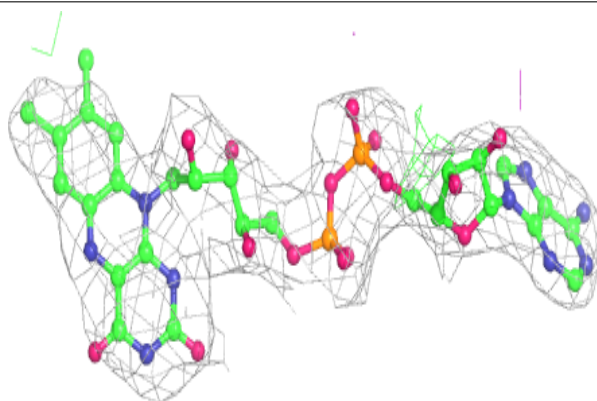


Electron density around FAD J 703:

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

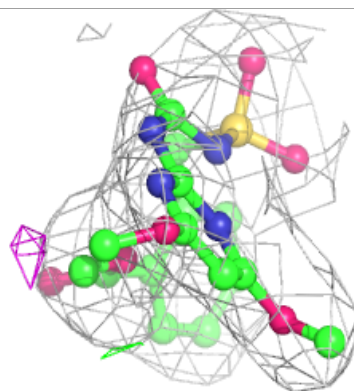
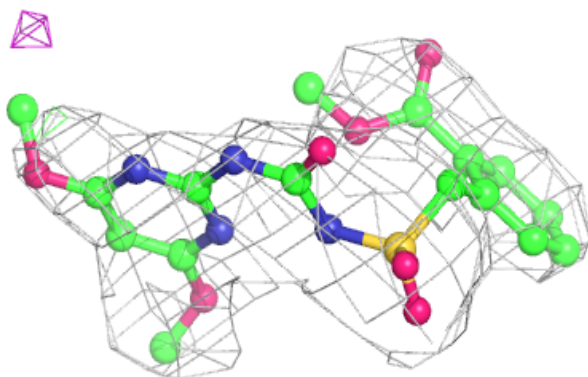
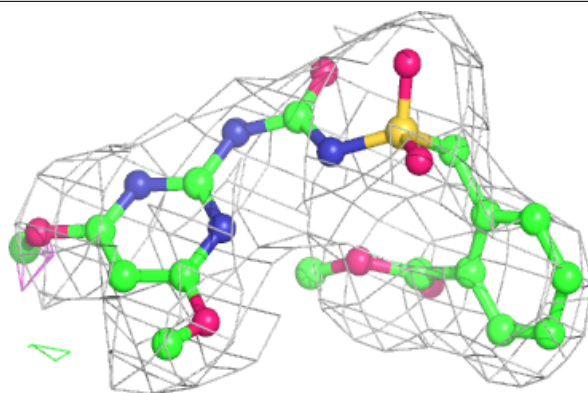
**Electron density around FAD U 703:**

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

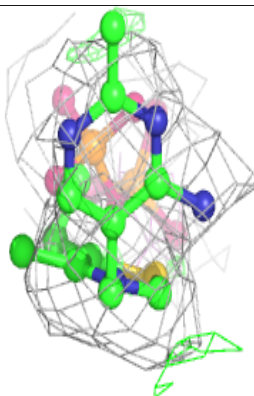
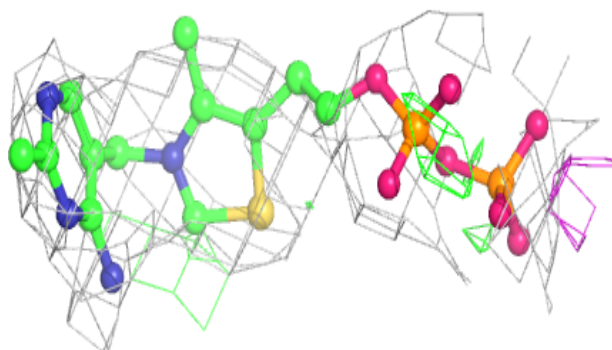
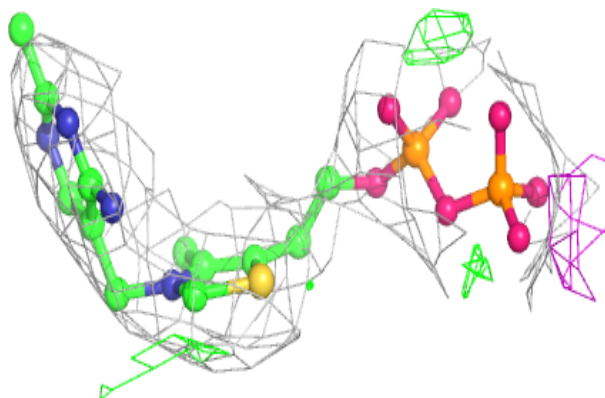


Electron density around 60G F 704:

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

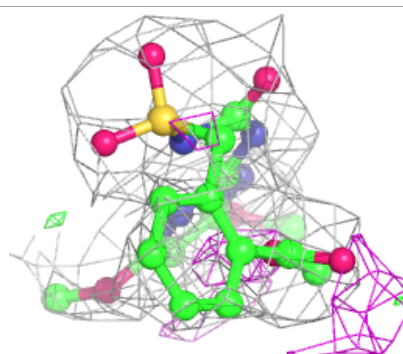
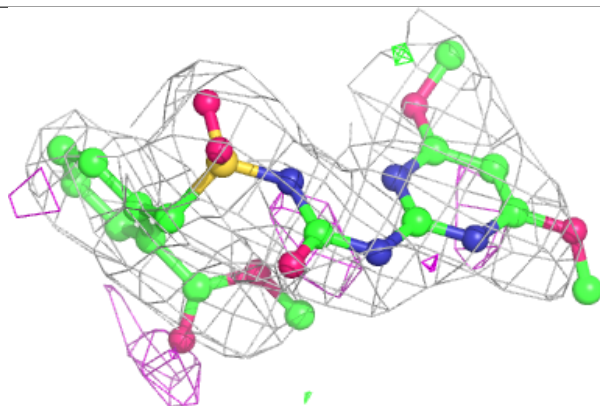
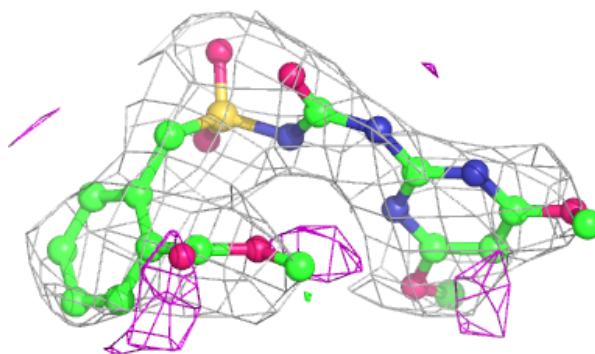
**Electron density around TPP E 701:**

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

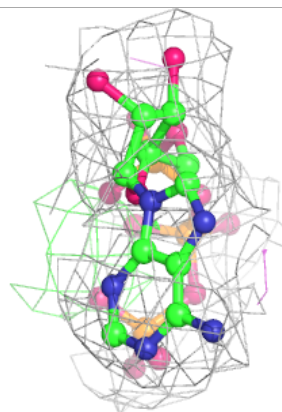
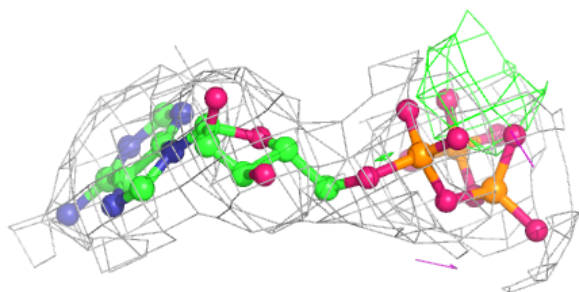
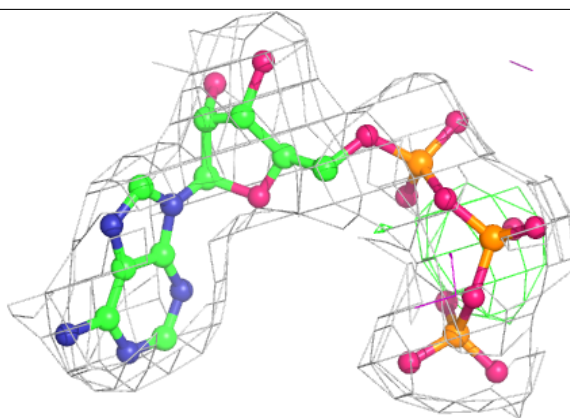


Electron density around 60G N 704:

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

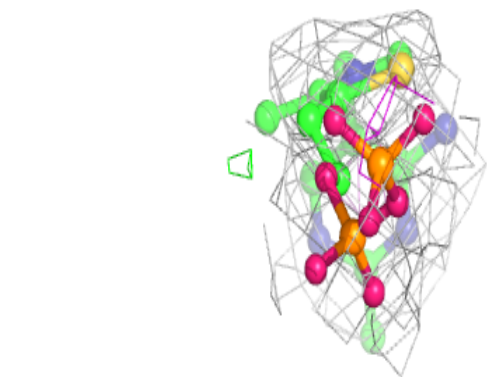
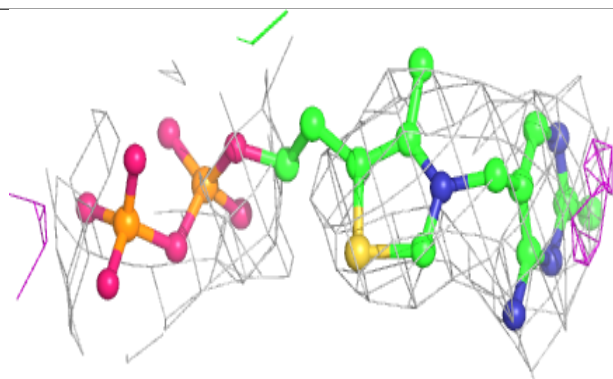
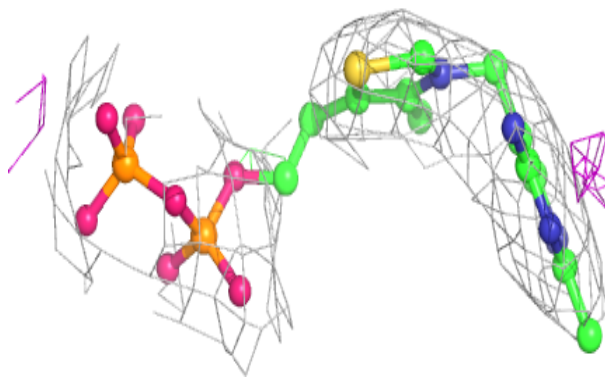
**Electron density around ATP S 401:**

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

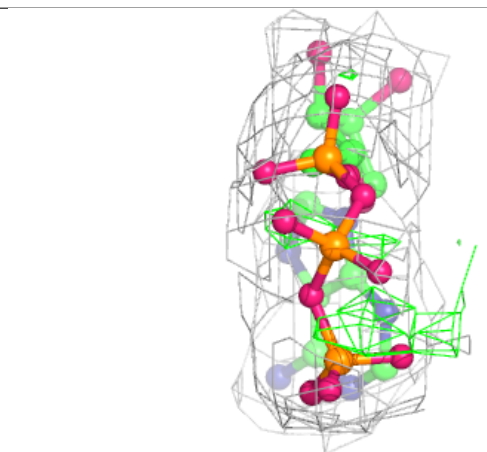
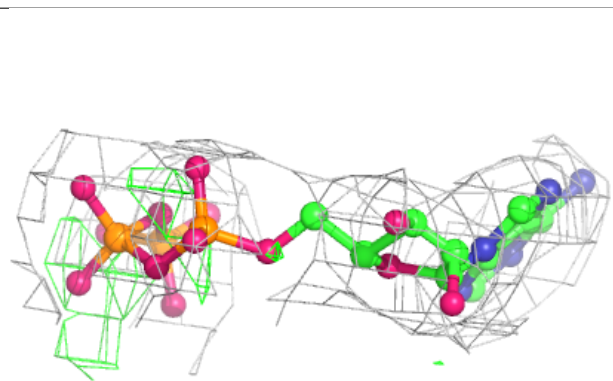
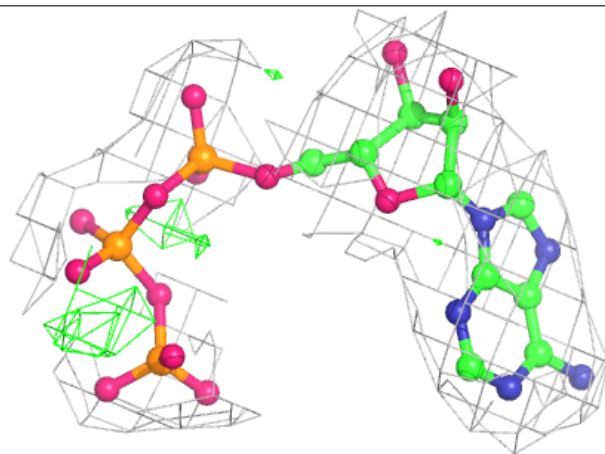


Electron density around TPP J 701:

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

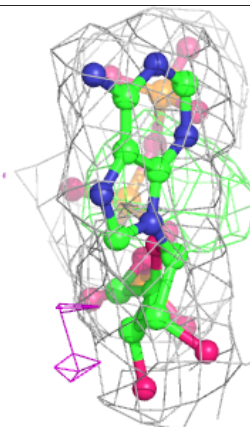
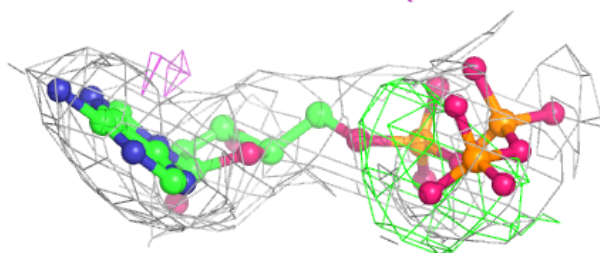
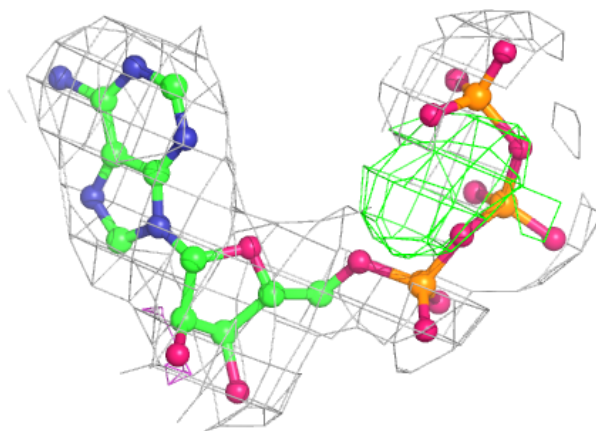
**Electron density around ATP C 401:**

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

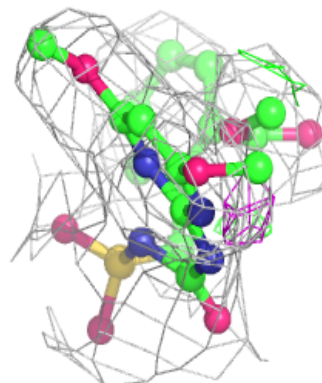
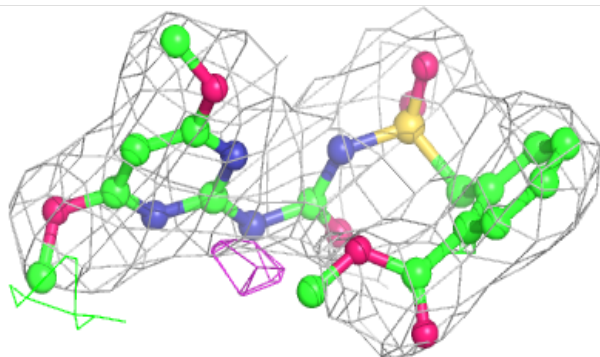
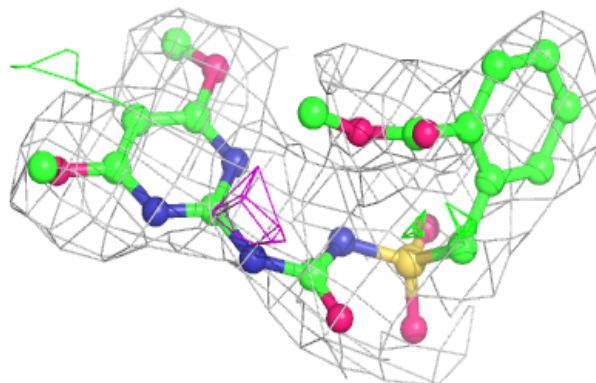


Electron density around ATP T 401:

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

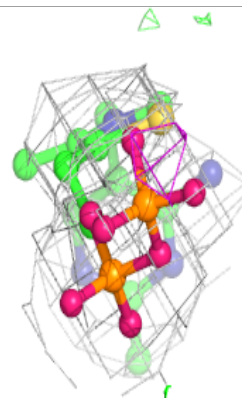
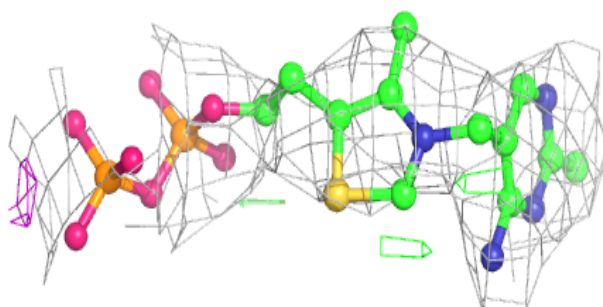
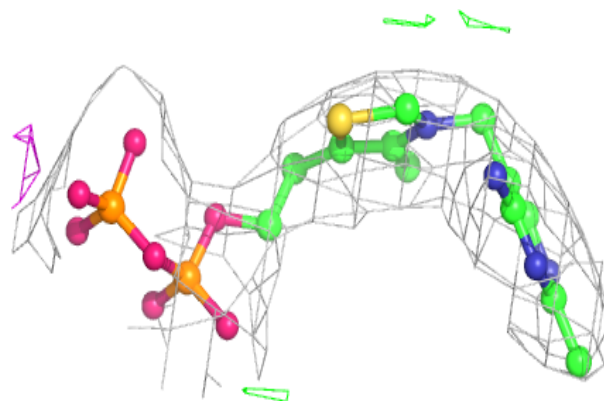
**Electron density around 60G A 704:**

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

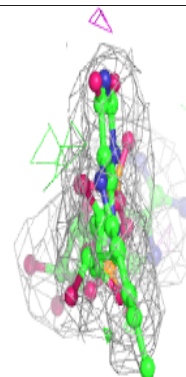
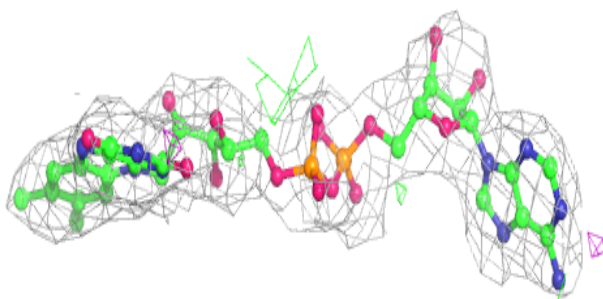
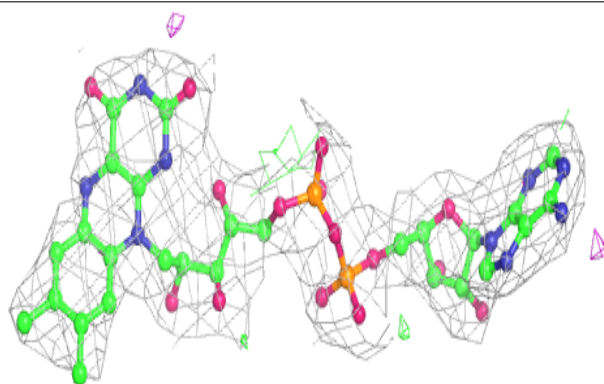


Electron density around TPP F 701:

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

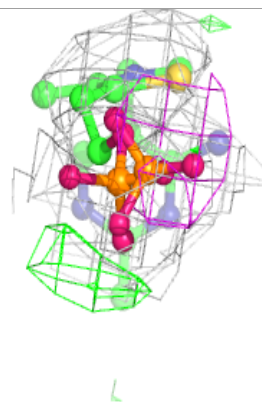
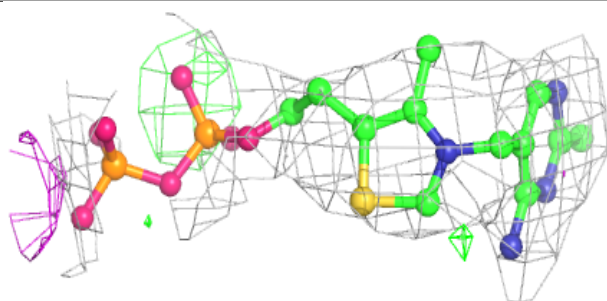
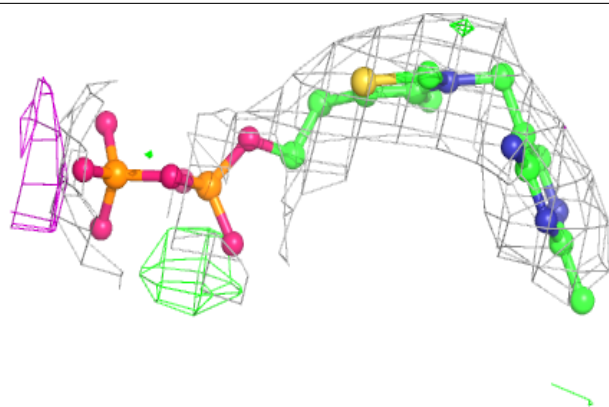
**Electron density around FAD V 703:**

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

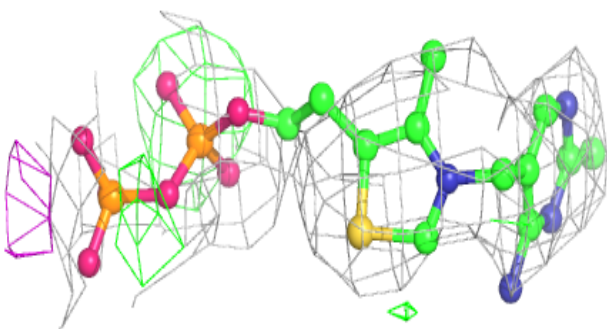
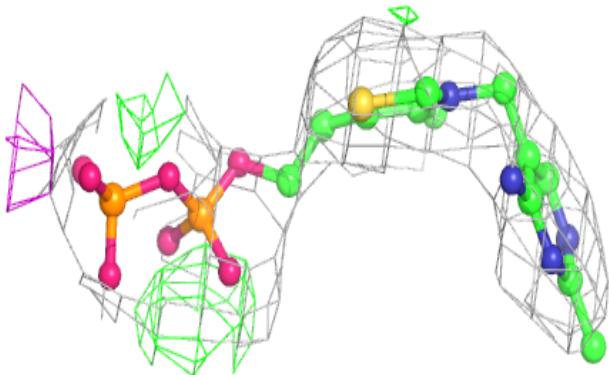


Electron density around TPP N 701:

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

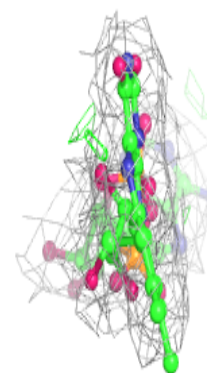
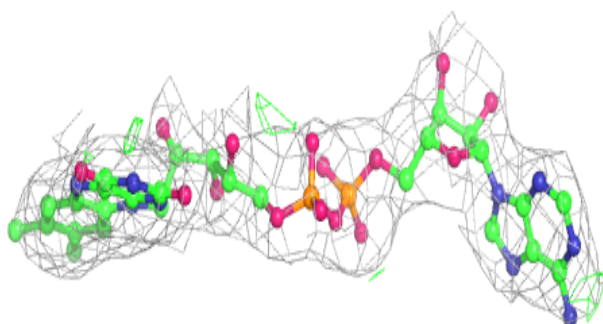
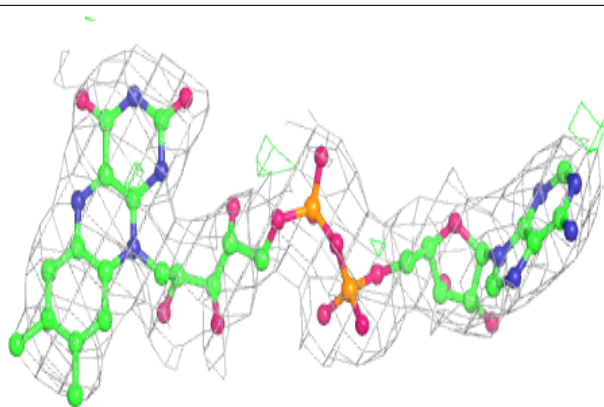
**Electron density around TPP U 701:**

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

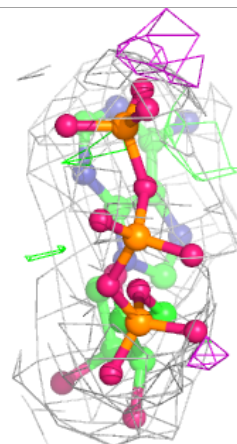
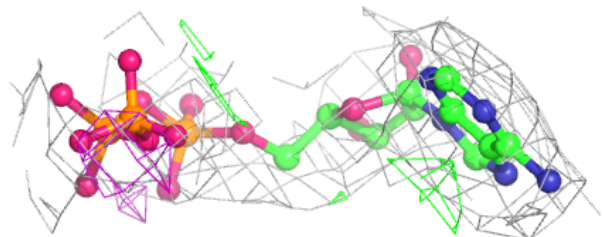
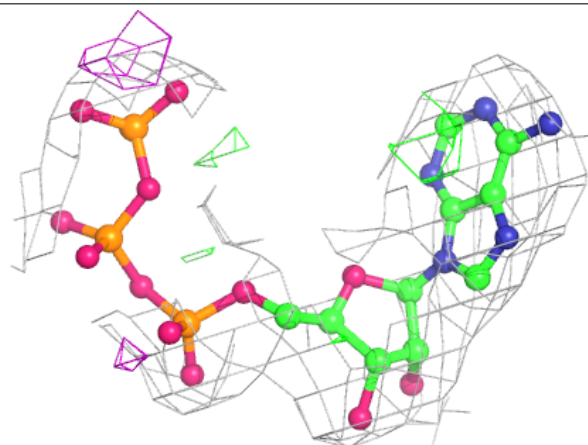


Electron density around FAD M 703:

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

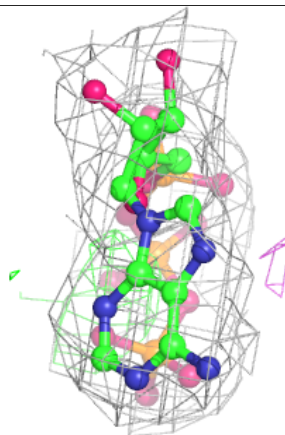
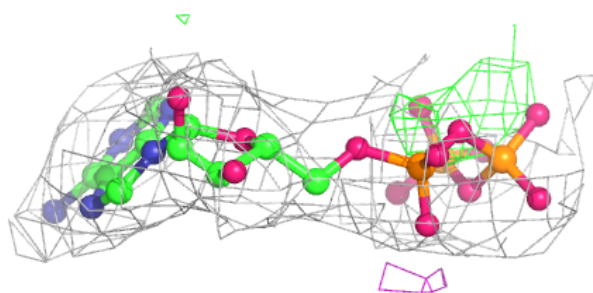
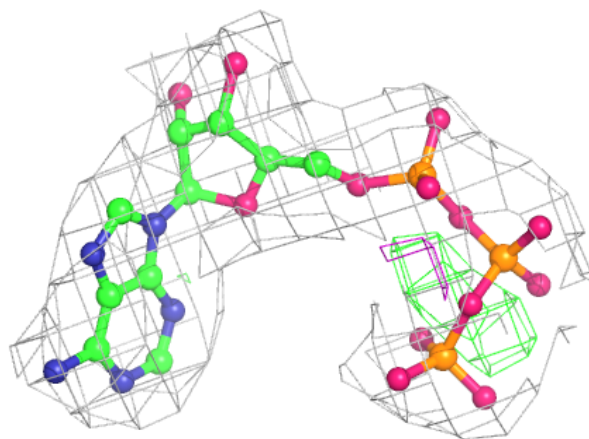
**Electron density around ATP H 401:**

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

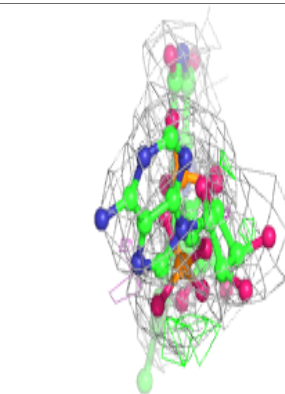
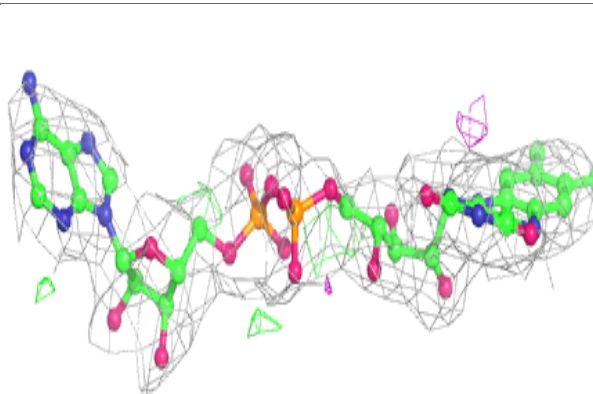
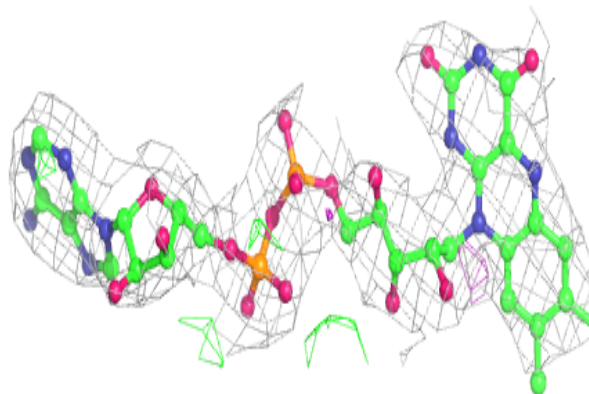


Electron density around ATP P 401:

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

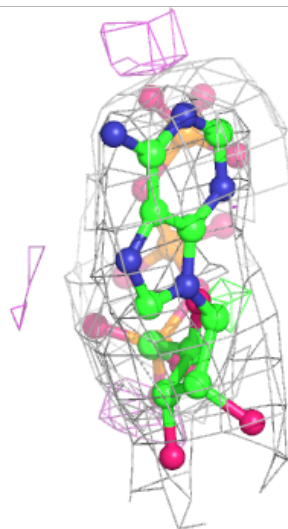
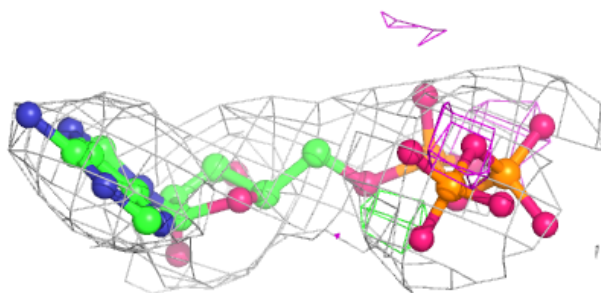
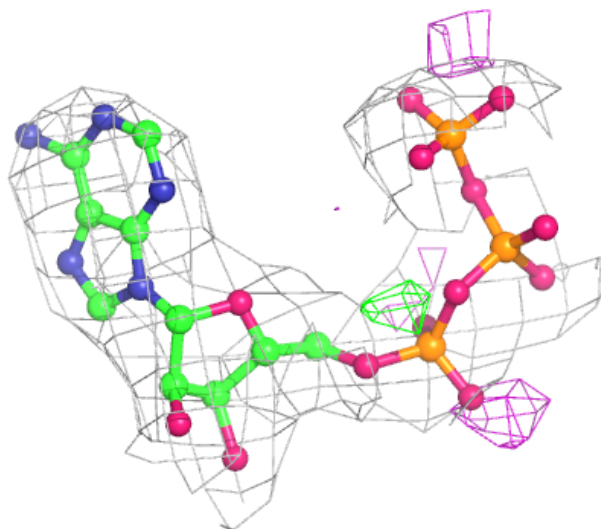
**Electron density around FAD N 703:**

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



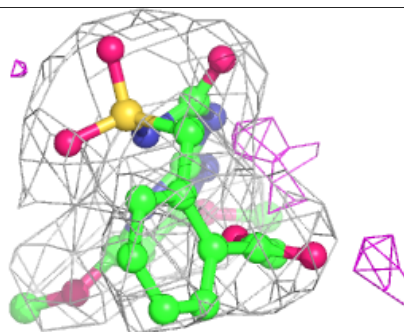
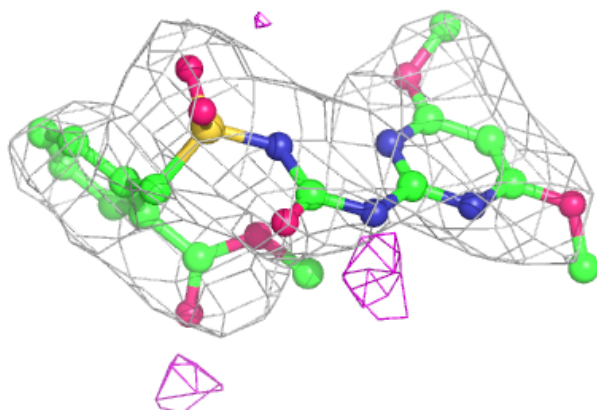
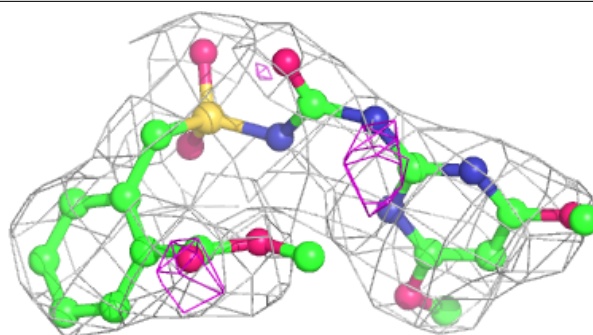
Electron density around ATP O 401:

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

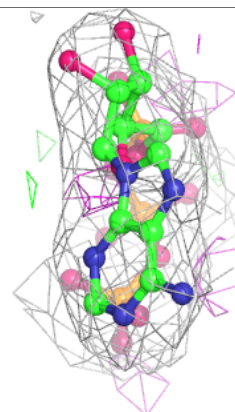
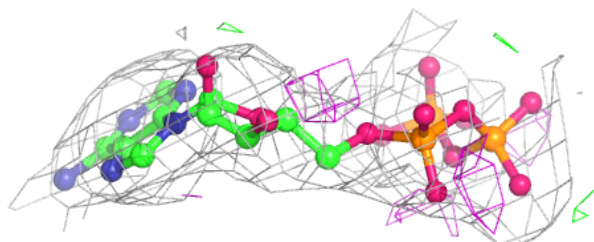
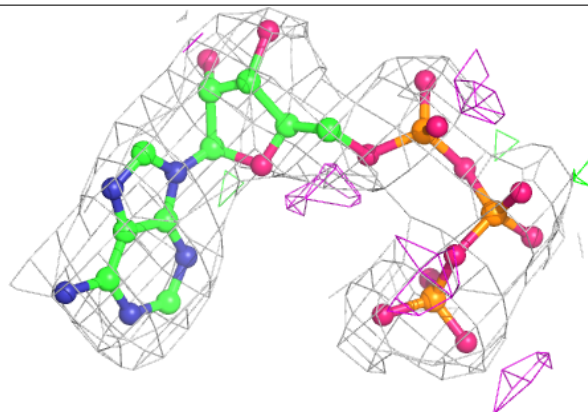


Electron density around 60G N 705:

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

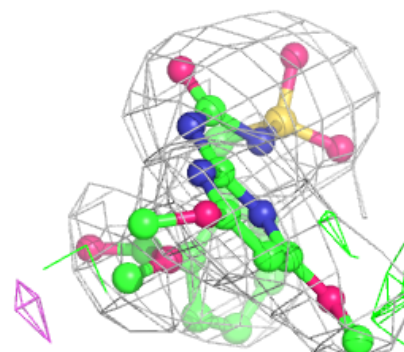
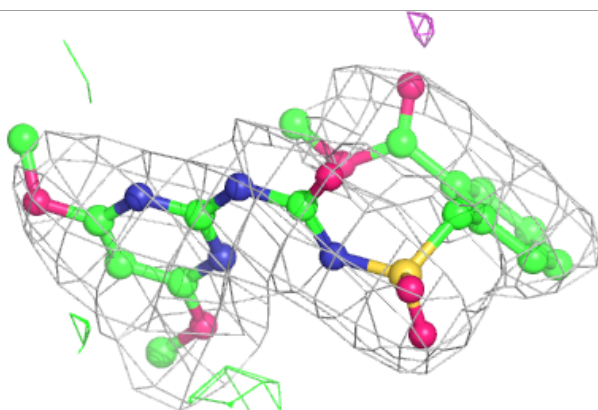
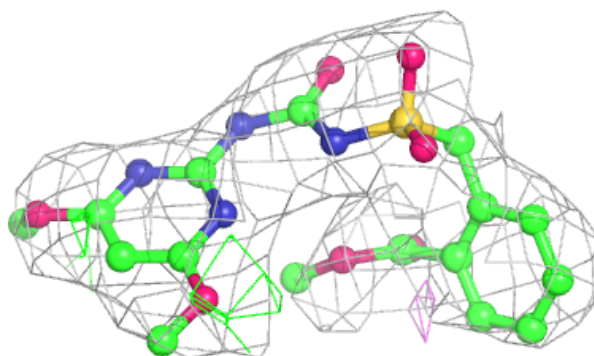
**Electron density around ATP G 401:**

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

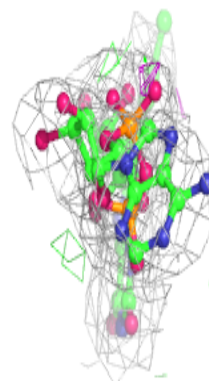
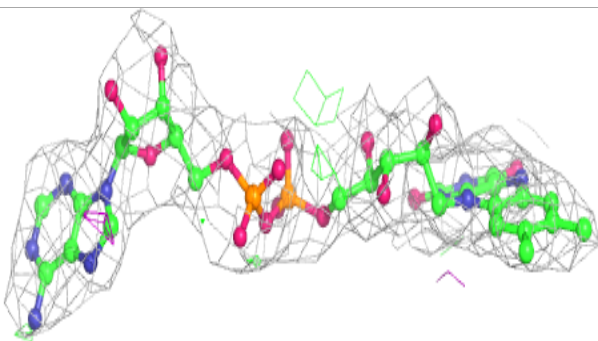
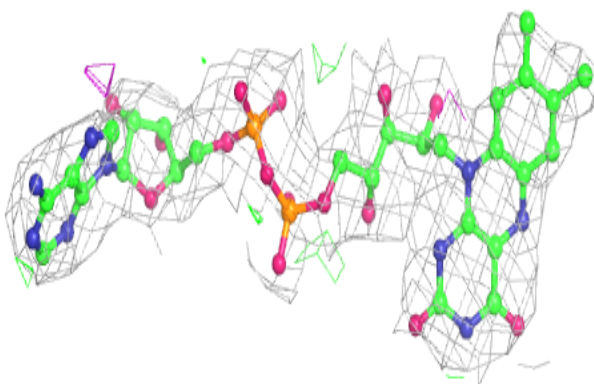


Electron density around 60G U 704:

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

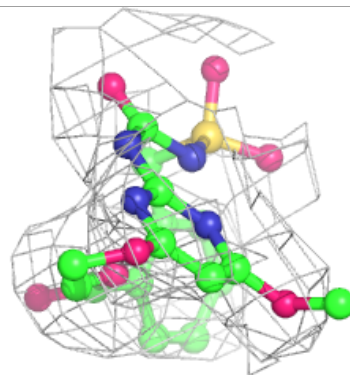
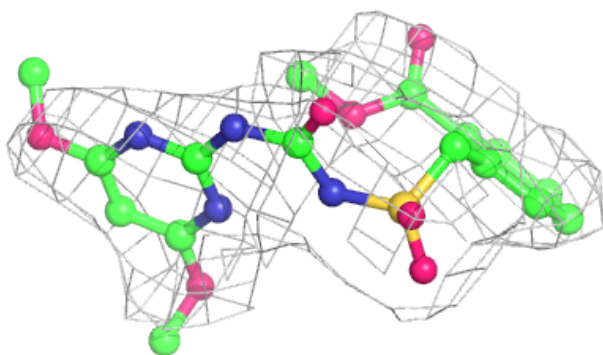
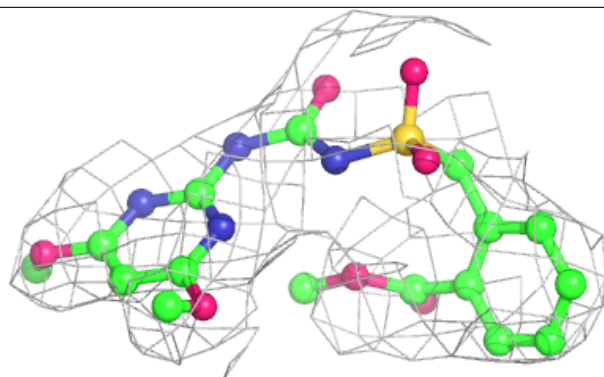
**Electron density around FAD B 703:**

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

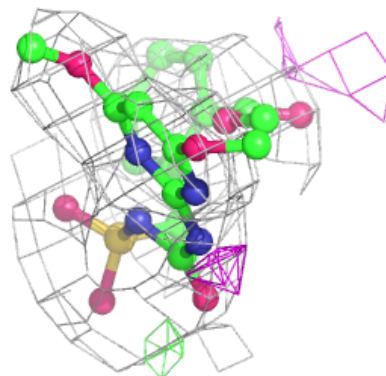
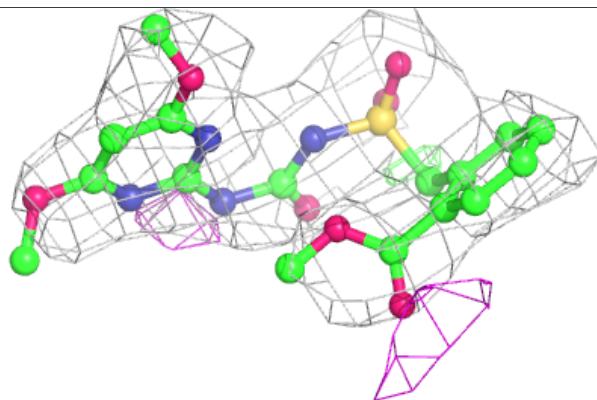
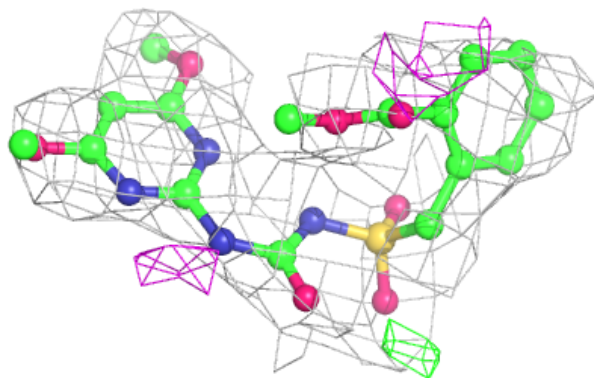


Electron density around 60G Q 704:

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

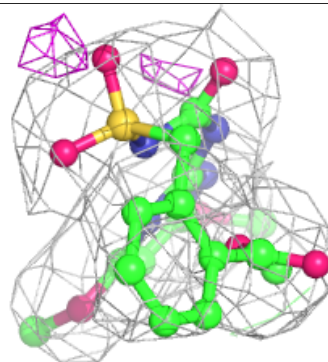
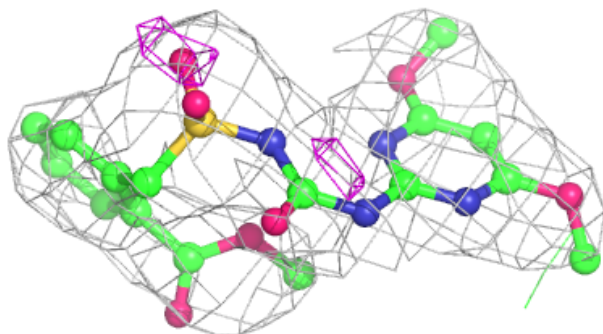
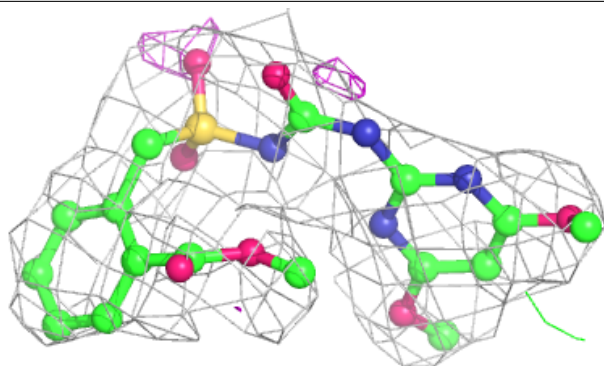
**Electron density around 60G V 704:**

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

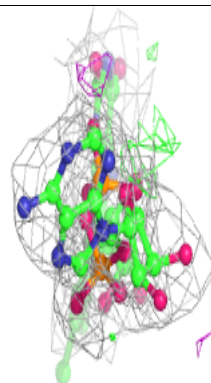
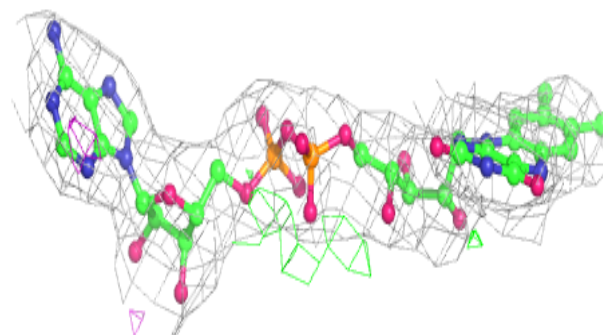
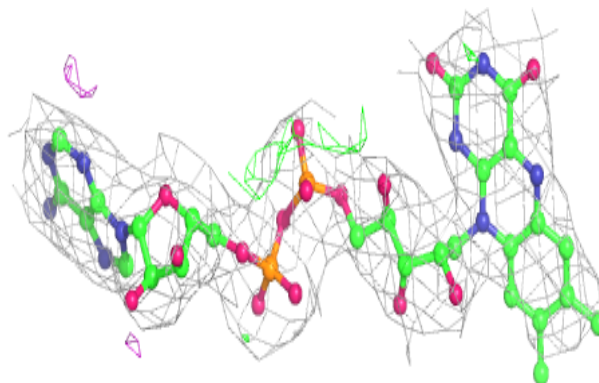


Electron density around 60G B 704:

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

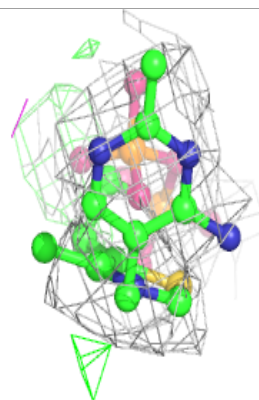
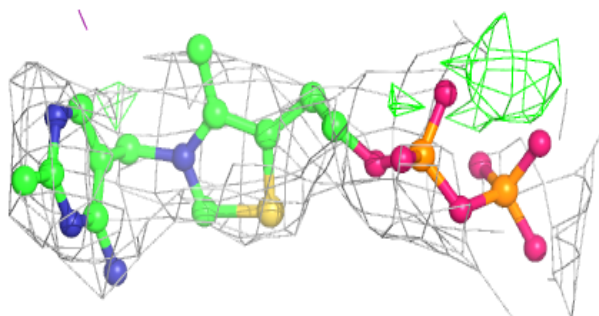
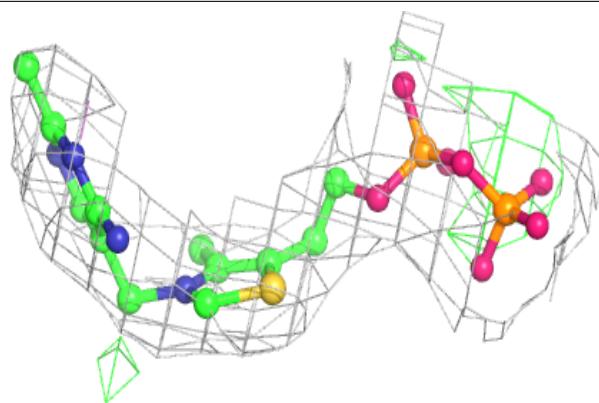
**Electron density around FAD Q 703:**

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

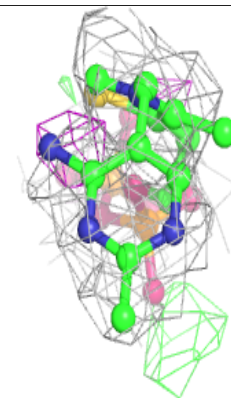
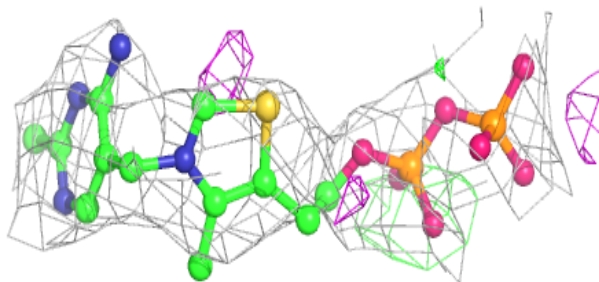
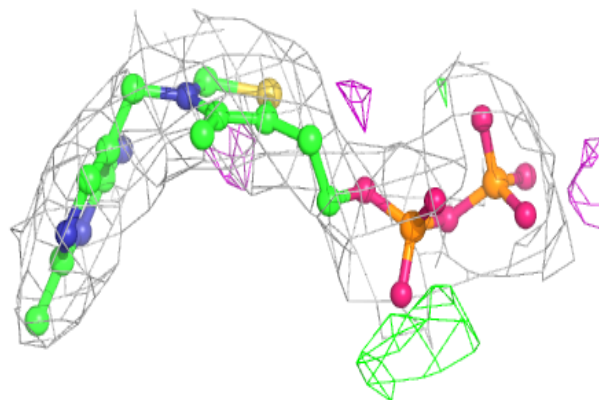


Electron density around TPP V 701:

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

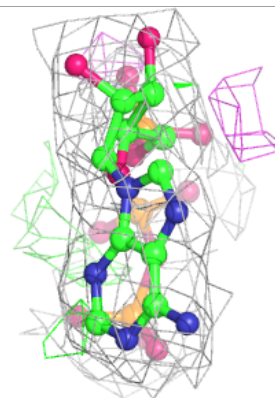
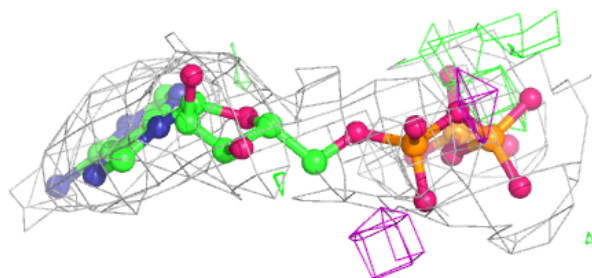
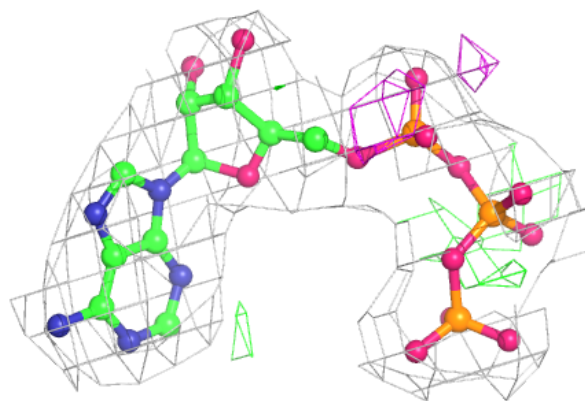
**Electron density around TPP M 701:**

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

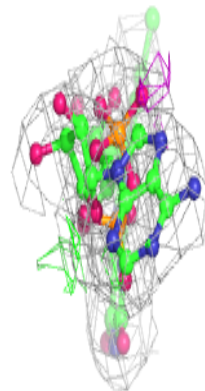
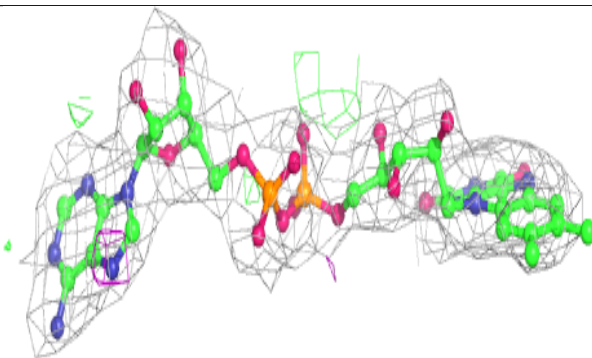
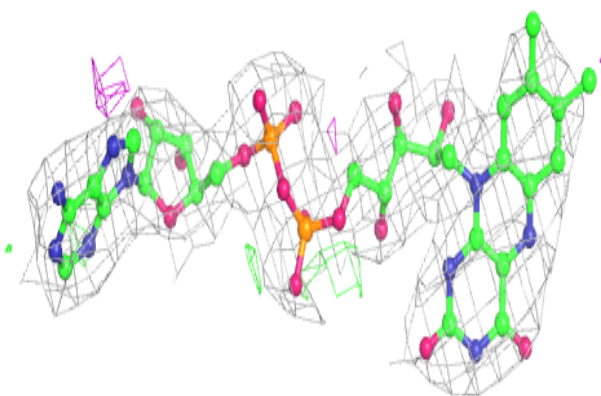


Electron density around ATP W 402:

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

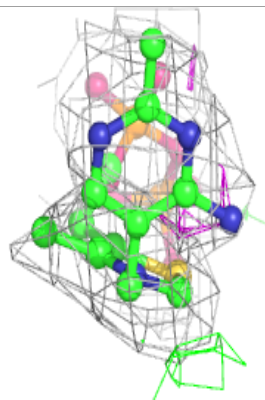
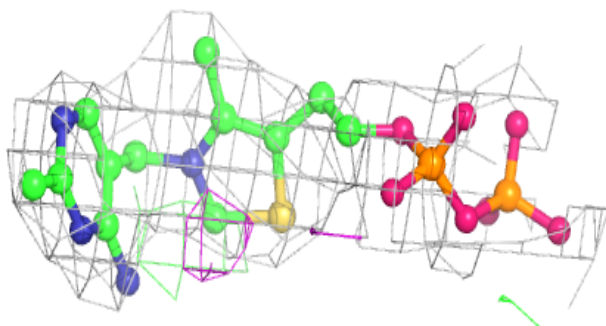
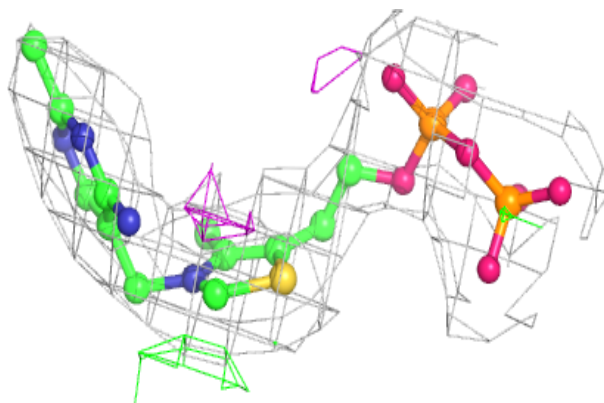
**Electron density around FAD A 703:**

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

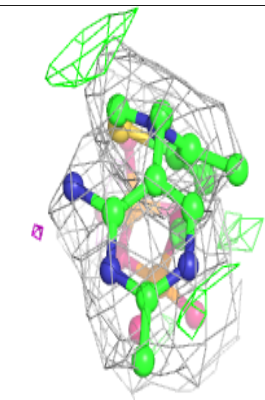
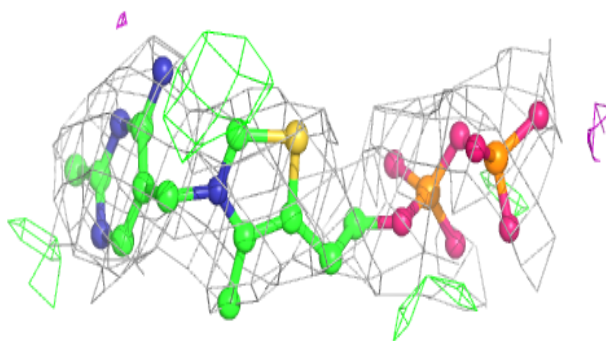
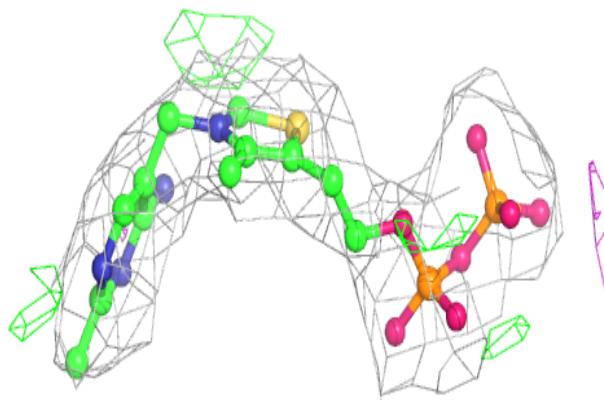


Electron density around TPP A 701:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.