



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:07 PM UTC

PDB ID : 6U9D / pdb_00006u9d
Title : Saccharomyces cerevisiae acetohydroxyacid synthase
Authors : Guddat, L.W.; Lonhienne, T.
Deposited on : 2019-09-08
Resolution : 3.19 Å(reported)

This is a 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 types of validation reports are described at

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

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

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

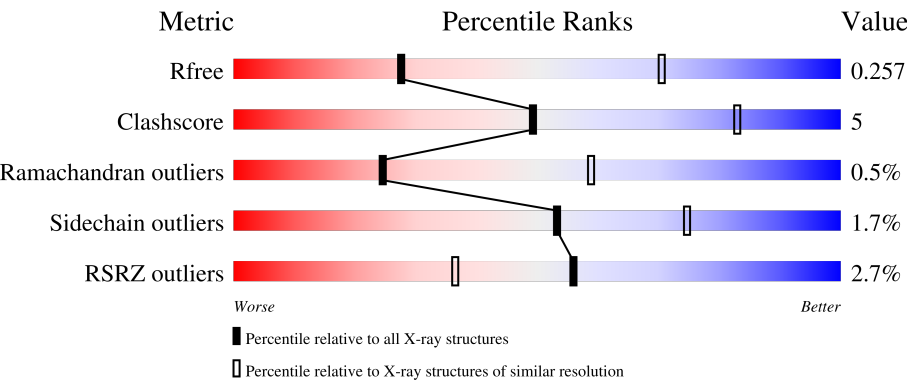
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



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

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

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

Continued on next page...

Continued from previous page...

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

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetolactate synthase catalytic subunit, mitochondrial.

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

There are 168 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

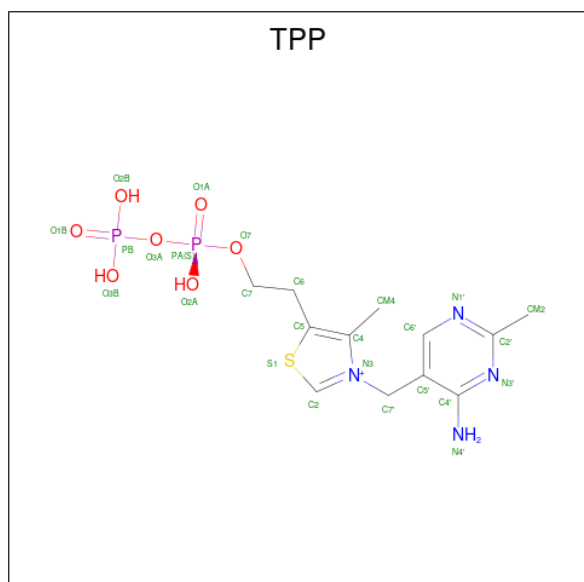
Chain	Residue	Modelled	Actual	Comment	Reference
T	30	GLY	-	expression tag	UNP B3LU66
T	31	SER	-	expression tag	UNP B3LU66
T	32	HIS	-	expression tag	UNP B3LU66
T	33	MET	-	expression tag	UNP B3LU66
T	34	GLU	-	expression tag	UNP B3LU66
T	35	ASN	-	expression tag	UNP B3LU66
T	36	LEU	-	expression tag	UNP B3LU66
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

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

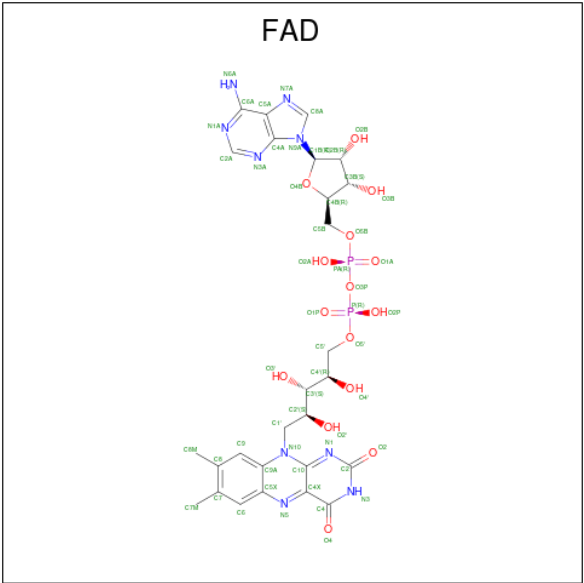
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

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



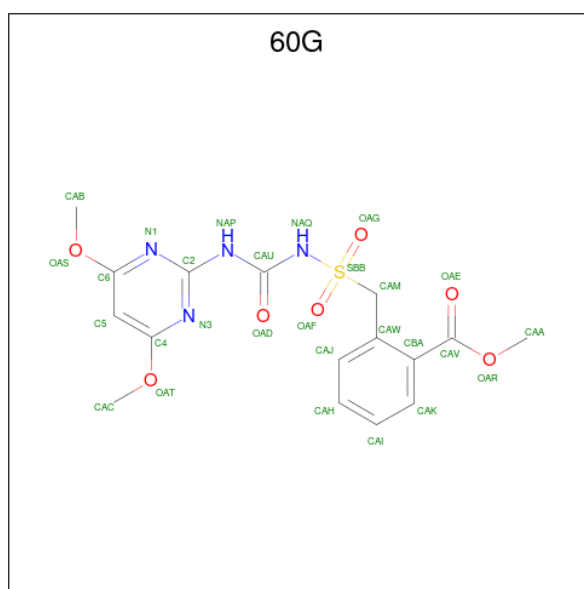
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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

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



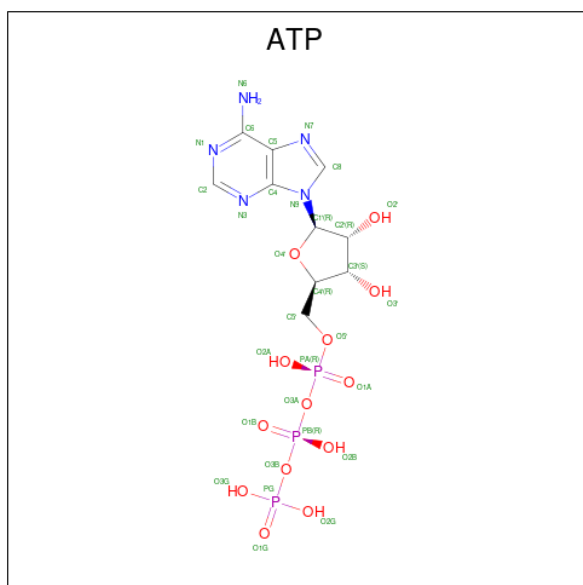
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	B	1	Total	C	N	O	S	0	0
			28	16	4	7	1		
6	E	1	Total	C	N	O	S	0	0
			28	16	4	7	1		

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

Continued from previous page...

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

- Molecule 8 is water.

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

Continued on next page...

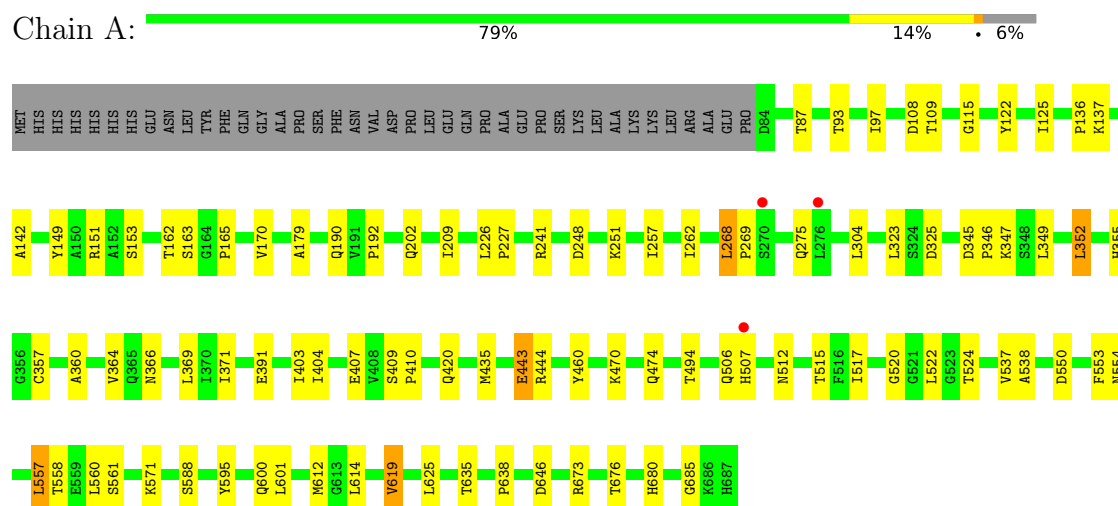
Continued from previous page...

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

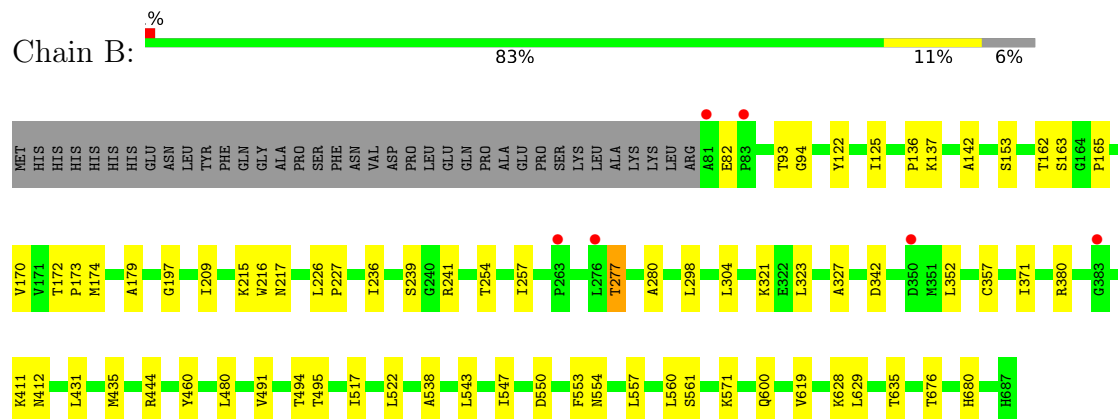
3 Residue-property plots

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.

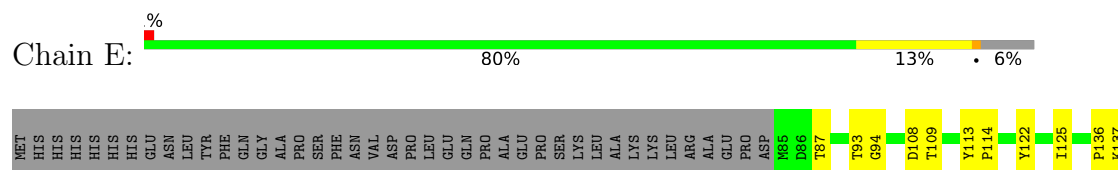
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

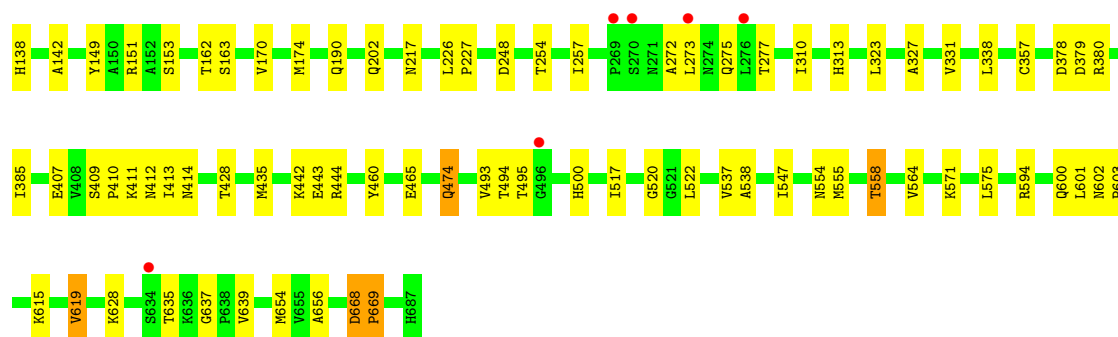


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

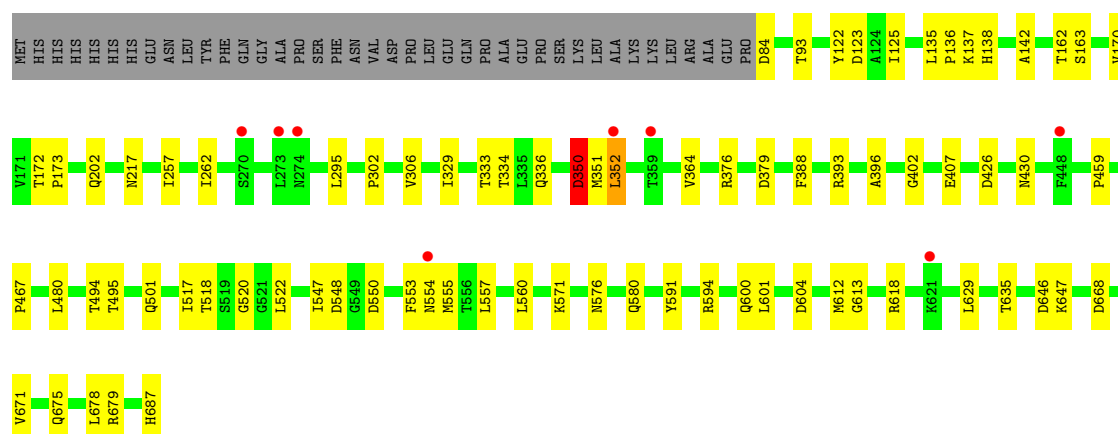
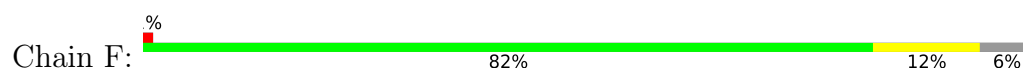


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

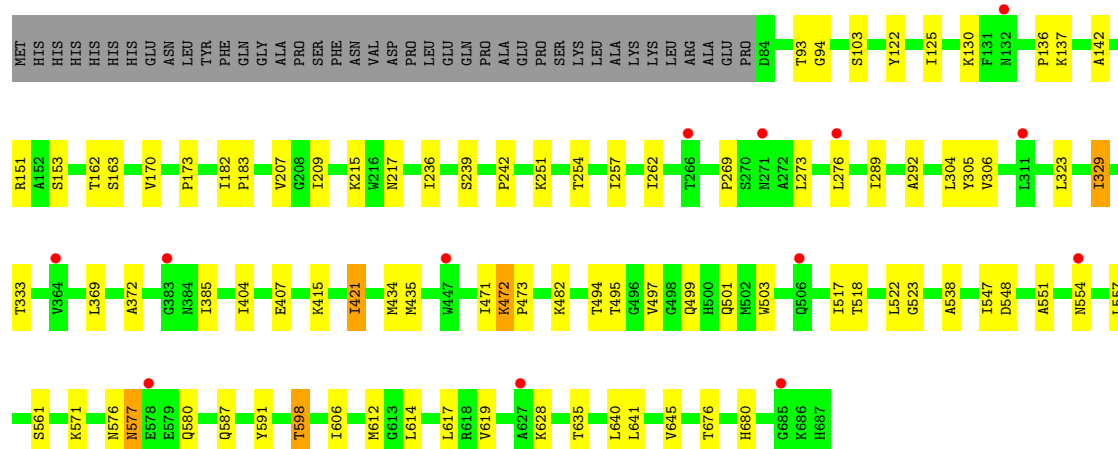




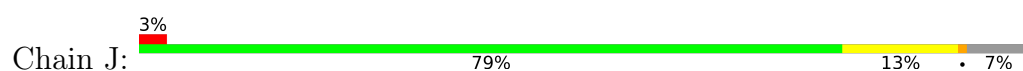
• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

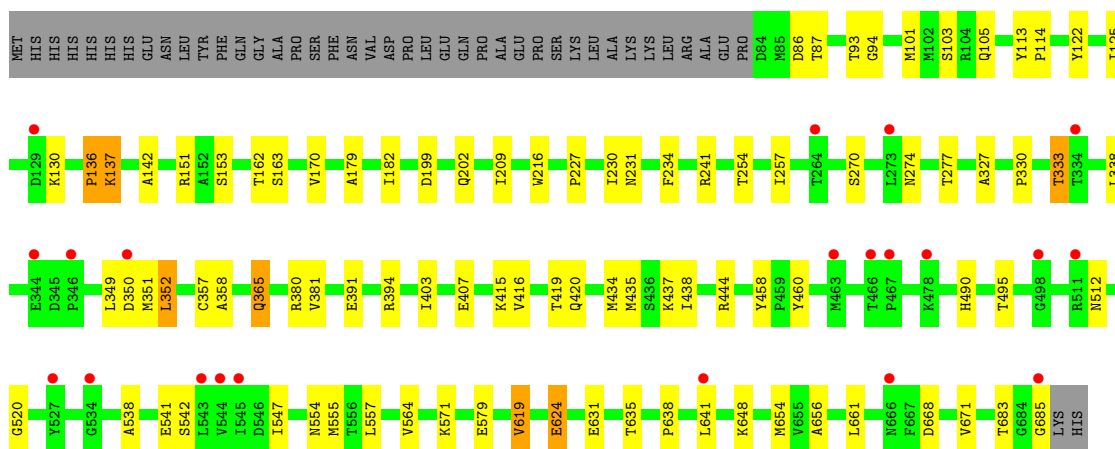


• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial



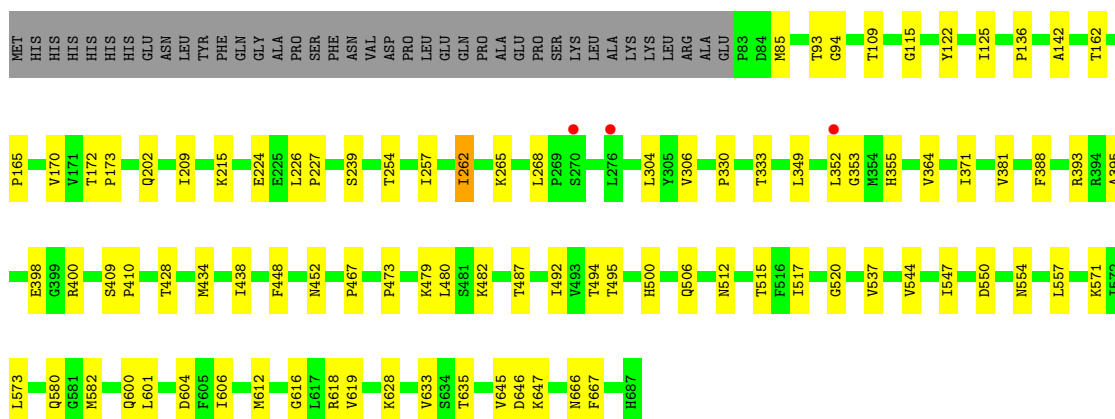
• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





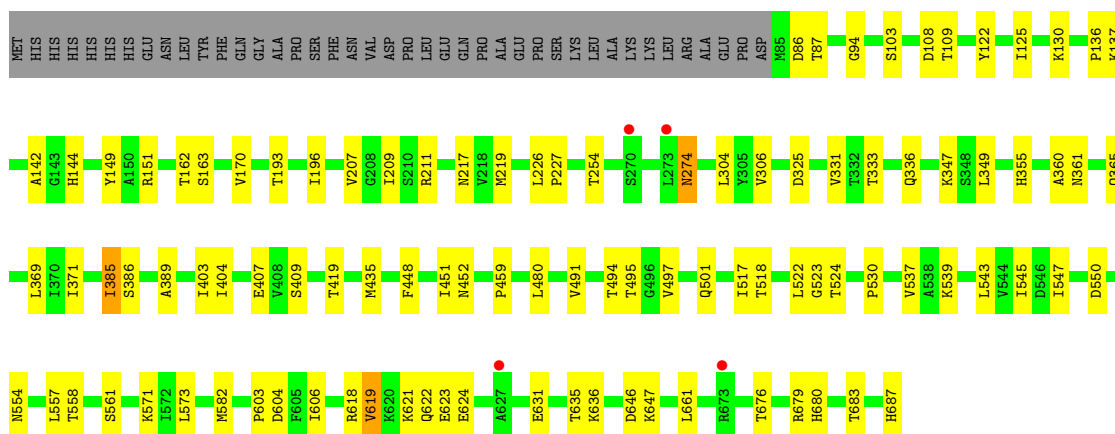
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain M: 80% 14% 6%

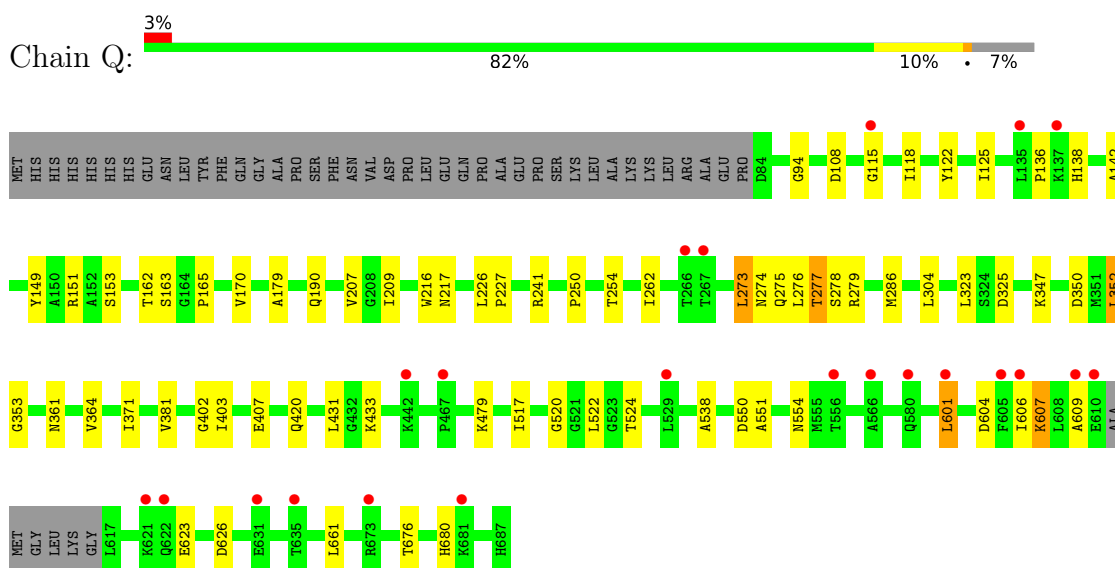


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

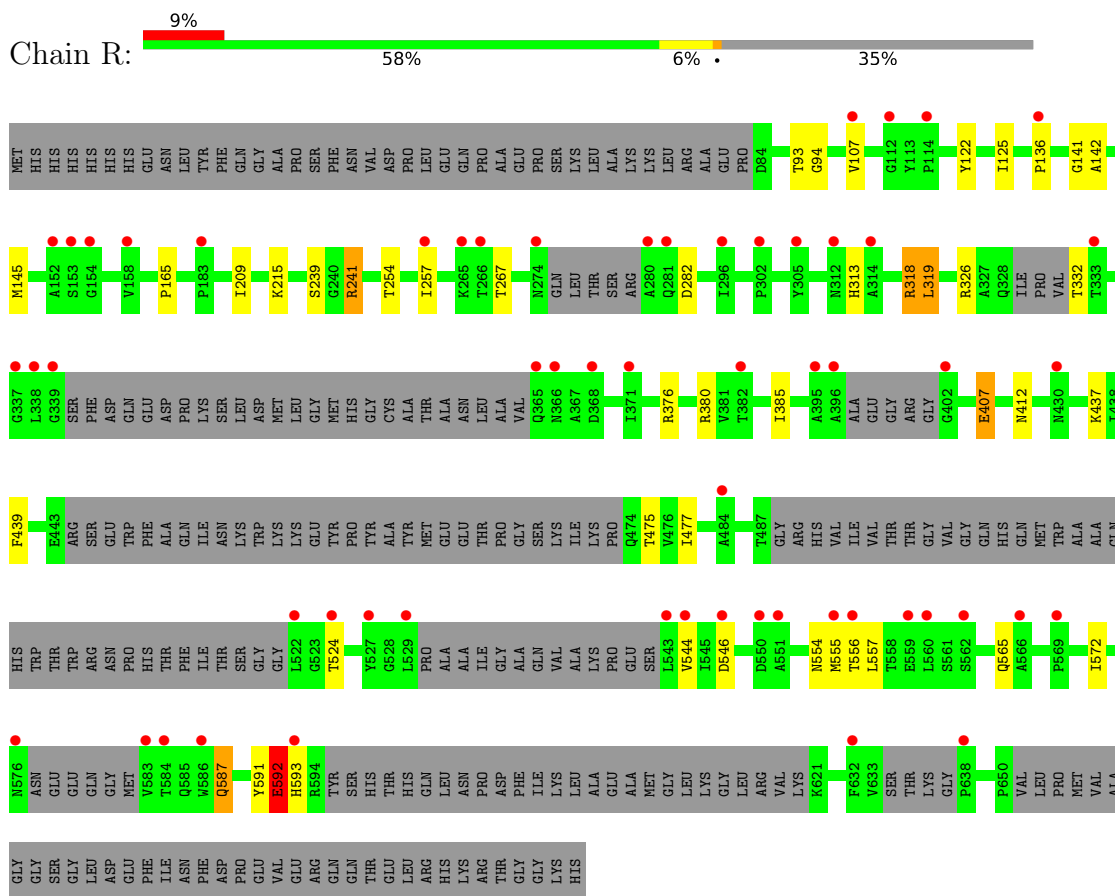
Chain N: 78% 15% 6%



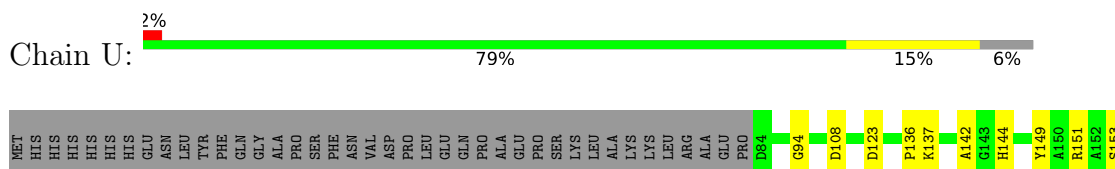
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

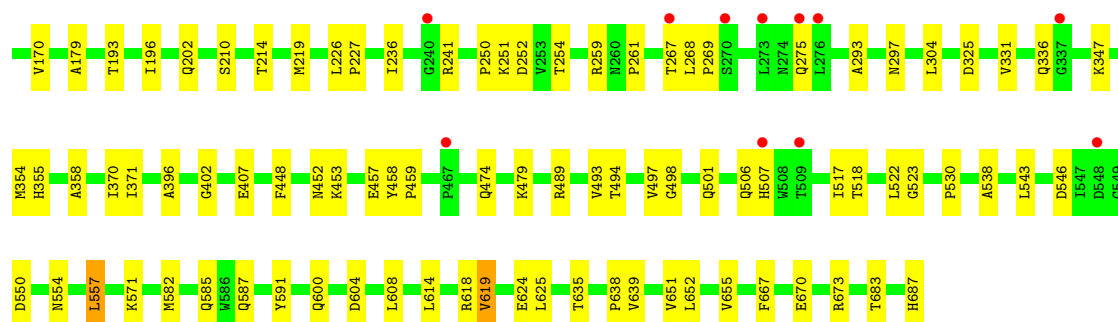


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial



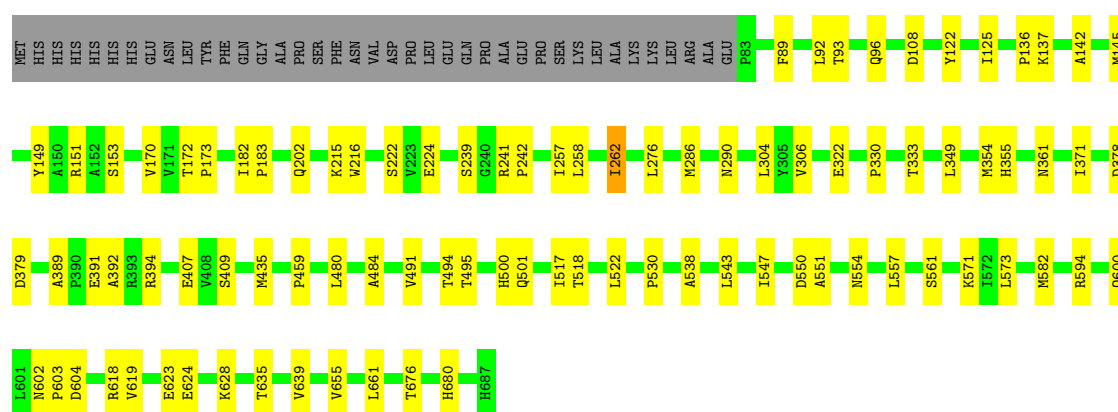
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





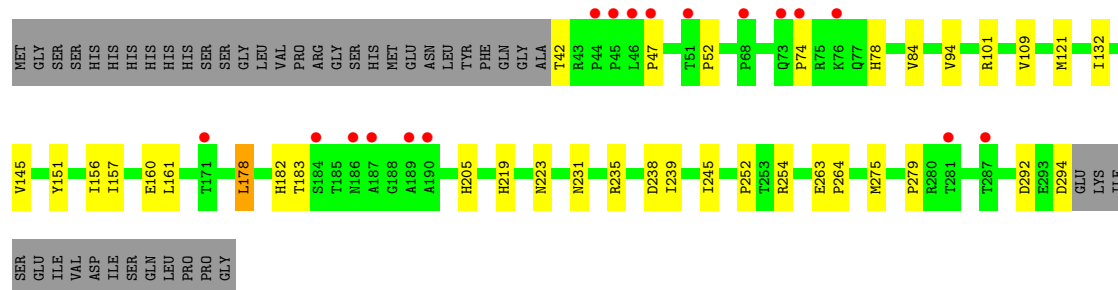
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain V: 80% 14% 6%



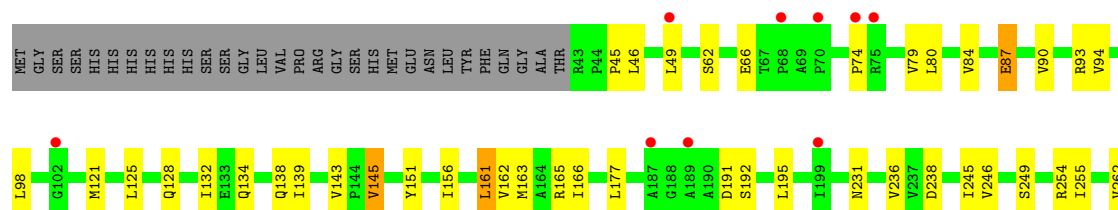
- Molecule 2: Acetolactate synthase small subunit, mitochondrial

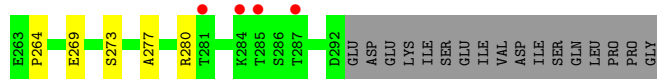
Chain C: 6% 73% 12% 15%



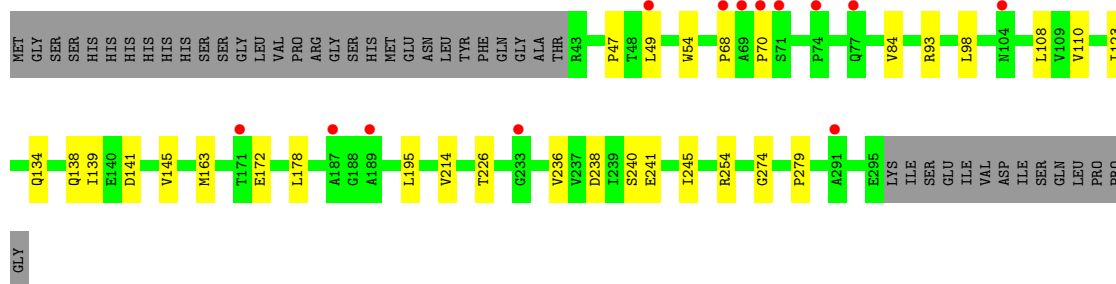
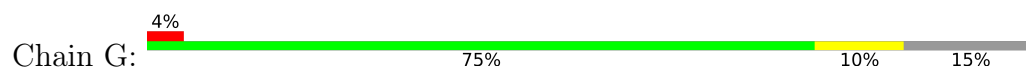
- Molecule 2: Acetolactate synthase small subunit, mitochondrial

Chain D: 4% 68% 15% 16%

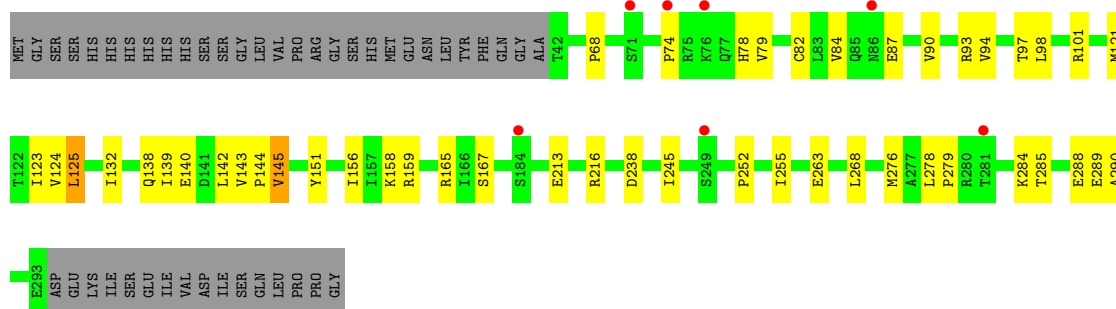




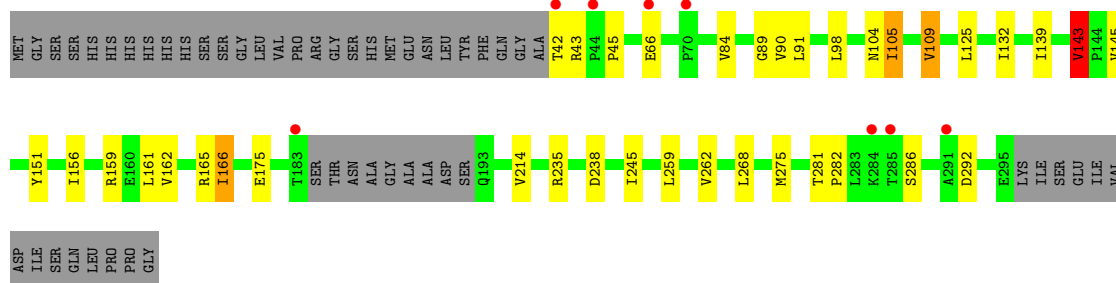
- Molecule 2: Acetolactate synthase small subunit, mitochondrial



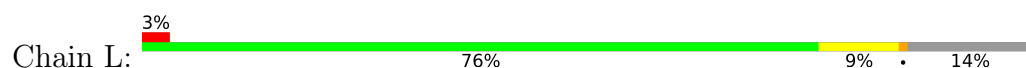
- Molecule 2: Acetolactate synthase small subunit, mitochondrial

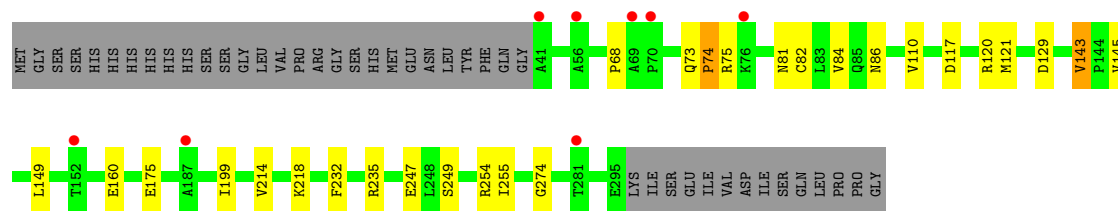


- Molecule 2: Acetolactate synthase small subunit, mitochondrial

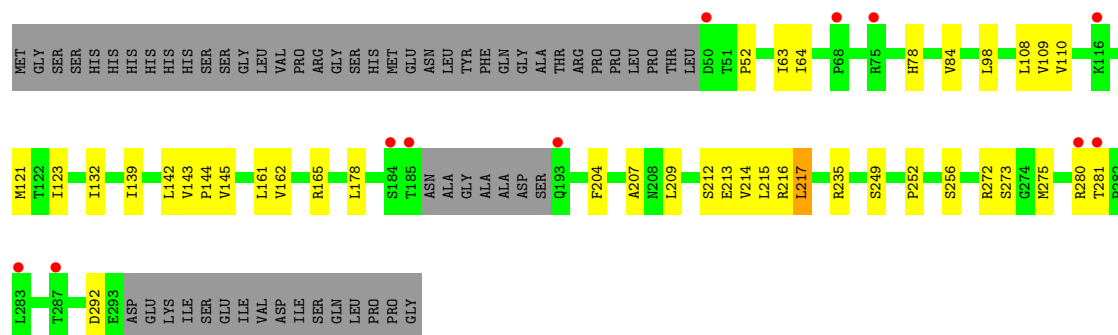


- Molecule 2: Acetolactate synthase small subunit, mitochondrial

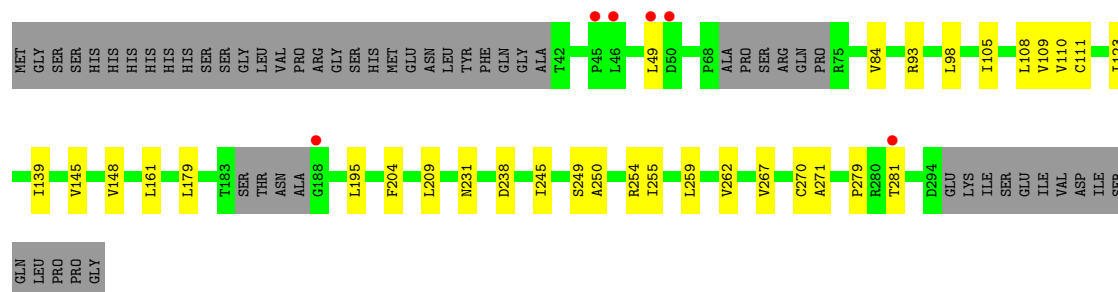




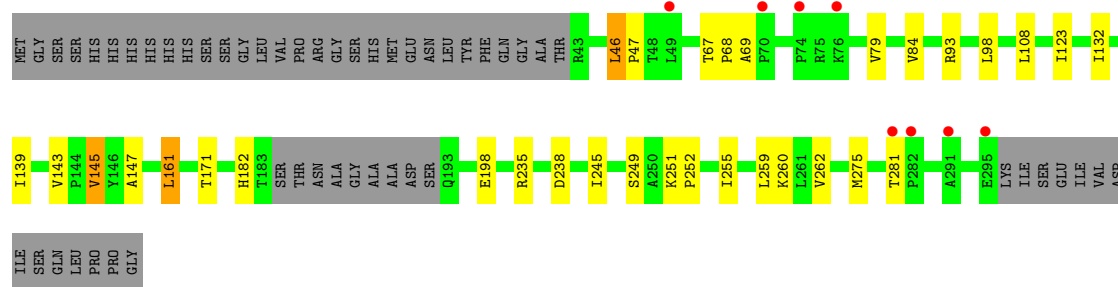
• Molecule 2: Acetolactate synthase small subunit, mitochondrial



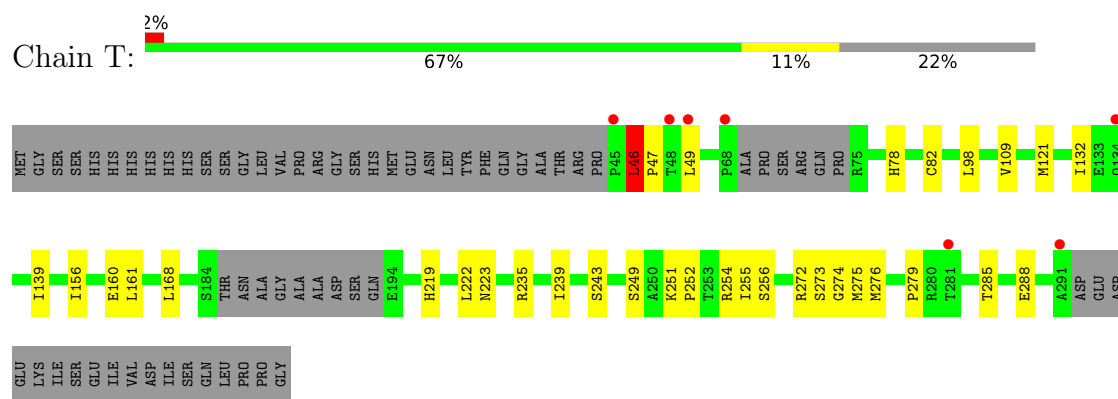
• Molecule 2: Acetolactate synthase small subunit, mitochondrial



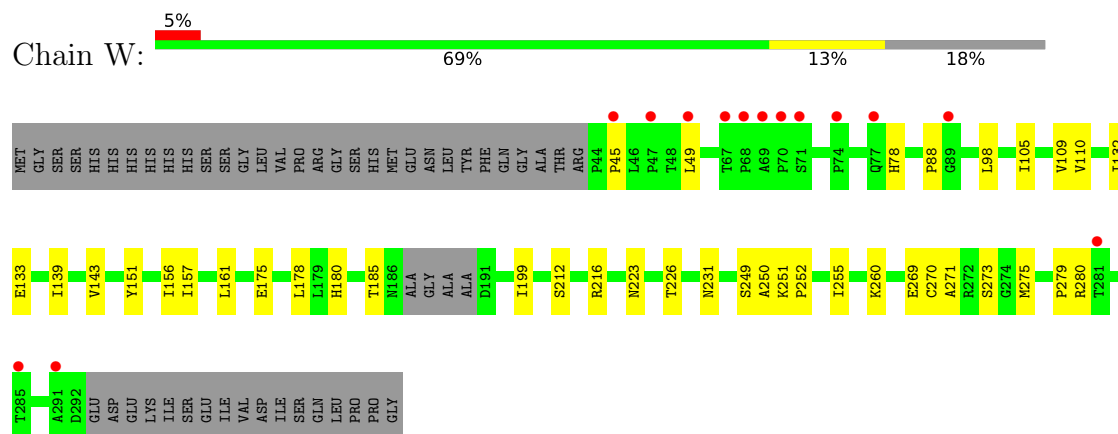
• Molecule 2: Acetolactate synthase small subunit, mitochondrial



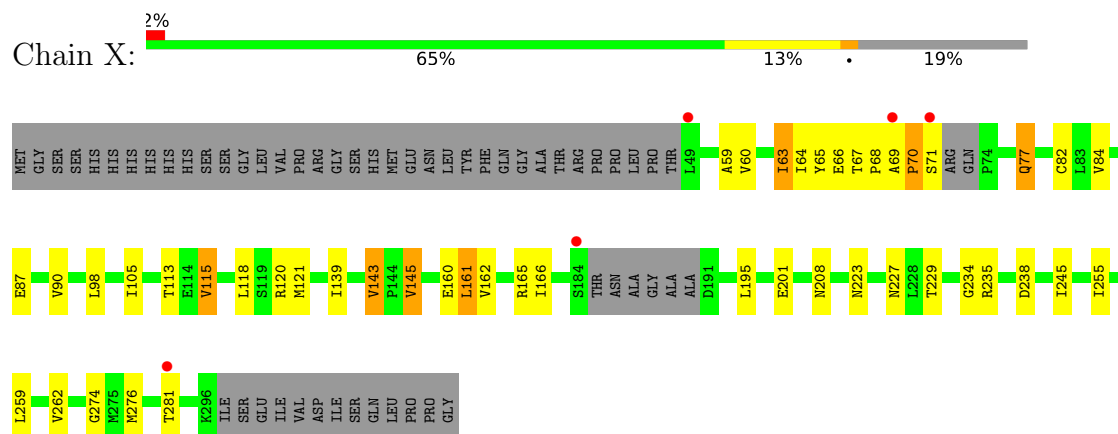
• Molecule 2: Acetolactate synthase small subunit, mitochondrial



- 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 0.212 , 0.257	Depositor DCC
R_{free} test set	1998 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	77705	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	143	VAL	CA-C-N	-7.97	111.75	121.00
2	O	143	VAL	C-N-CA	-7.97	111.75	121.00
2	H	143	VAL	CA-C-N	-7.75	111.84	120.45
2	H	143	VAL	C-N-CA	-7.75	111.84	120.45
2	D	143	VAL	CA-C-N	-7.48	112.15	120.45
2	D	143	VAL	C-N-CA	-7.48	112.15	120.45
2	K	143	VAL	CA-C-N	-7.02	112.39	120.89
2	K	143	VAL	C-N-CA	-7.02	112.39	120.89
1	E	668	ASP	CA-C-N	6.67	128.18	119.84
1	E	668	ASP	C-N-CA	6.67	128.18	119.84
1	U	275	GLN	CB-CA-C	-6.30	109.32	116.63
1	Q	609	ALA	N-CA-C	6.28	119.32	109.96
1	M	268	LEU	CA-C-N	5.59	125.69	119.32
1	M	268	LEU	C-N-CA	5.59	125.69	119.32
1	E	275	GLN	CB-CA-C	-5.57	109.65	117.23
2	K	281	THR	CA-C-N	5.38	126.56	119.84
2	K	281	THR	C-N-CA	5.38	126.56	119.84
1	I	472	LYS	CA-C-N	5.29	124.92	119.05
1	I	472	LYS	C-N-CA	5.29	124.92	119.05
1	N	622	GLN	N-CA-C	5.29	116.73	110.97
1	M	262	ILE	N-CA-C	5.24	113.49	109.19
1	B	82	GLU	CA-C-N	-5.19	113.35	119.84
1	B	82	GLU	C-N-CA	-5.19	113.35	119.84
1	Q	350	ASP	CB-CA-C	-5.19	110.61	116.63
1	Q	607	LYS	N-CA-C	-5.17	106.48	112.89
1	N	539	LYS	CA-C-N	5.14	125.43	119.47
1	N	539	LYS	C-N-CA	5.14	125.43	119.47
2	T	46	LEU	CA-C-N	-5.13	114.95	120.03
2	T	46	LEU	C-N-CA	-5.13	114.95	120.03
2	X	77	GLN	N-CA-C	-5.09	100.11	108.41
2	L	143	VAL	CA-C-N	-5.04	115.69	120.83
2	L	143	VAL	C-N-CA	-5.04	115.69	120.83
1	A	268	LEU	CA-C-N	5.01	124.18	118.97
1	A	268	LEU	C-N-CA	5.01	124.18	118.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4606	0	4614	61	0
1	B	4621	0	4621	48	0
1	E	4580	0	4578	63	0
1	F	4572	0	4540	48	0
1	I	4540	0	4503	47	0
1	J	4533	0	4486	48	0
1	M	4613	0	4622	53	0
1	N	4589	0	4602	62	0
1	Q	4508	0	4439	48	0
1	R	3014	0	2909	29	0
1	U	4554	0	4503	59	0
1	V	4601	0	4601	57	0
2	C	1938	0	1925	27	0
2	D	1915	0	1917	32	0
2	G	1938	0	1928	18	0
2	H	1944	0	1951	29	0
2	K	1889	0	1883	21	0
2	L	1957	0	1952	16	0
2	O	1818	0	1811	28	0
2	P	1881	0	1885	18	0
2	S	1872	0	1854	20	0
2	T	1792	0	1805	22	0
2	W	1894	0	1901	24	0
2	X	1846	0	1823	28	0
3	A	26	0	16	1	0
3	B	26	0	16	2	0
3	E	26	0	16	3	0
3	F	26	0	16	2	0
3	I	26	0	16	2	0
3	J	26	0	16	1	0
3	M	26	0	16	3	0
3	N	26	0	16	1	0
3	Q	26	0	16	2	0
3	U	26	0	16	1	0
3	V	26	0	16	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

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	4	0
5	I	53	0	30	1	0
5	J	53	0	31	4	0
5	M	53	0	30	2	0
5	N	53	0	30	2	0
5	Q	53	0	30	3	0
5	R	53	0	30	7	0
5	U	53	0	30	2	0
5	V	53	0	30	1	0
6	A	28	0	0	0	0
6	B	28	0	0	2	0
6	E	28	0	0	1	0
6	F	28	0	0	0	0
6	I	28	0	0	0	0
6	J	28	0	0	2	0
6	N	56	0	0	0	0
6	Q	28	0	0	0	0
6	R	28	0	0	1	0
6	U	28	0	0	0	0
6	V	28	0	0	1	0
7	C	31	0	12	2	0
7	D	31	0	10	2	0
7	G	31	0	10	3	0
7	H	31	0	11	1	0
7	K	31	0	11	1	0

Continued on next page...

Continued from previous page...

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

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

All (824) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:635:THR:HG21	1:E:639:VAL:HG11	1.27	1.08
1:R:241:ARG:HD3	5:R:701:FAD:H2B	1.57	0.85
1:E:635:THR:CG2	1:E:639:VAL:HG11	2.08	0.81
1:Q:273:LEU:O	1:Q:273:LEU:HD22	1.85	0.76
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.71	0.73
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
2:D:94:VAL:HG21	2:D:121:MET:HE1	1.75	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:V:322:GLU:HG2	1:V:435:MET:HE2	1.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:THR:HG22	1:B:165:PRO:HB3	1.74	0.68
1:A:557:LEU:HD23	1:A:557:LEU:C	2.18	0.68
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: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:217:ASN:OD1	2:D:93:ARG:NH2	2.32	0.63
1:B:411:LYS:HG3	2:D:138:GLN:HG2	1.79	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:ILE:O	7:G:401:ATP:N6	2.32	0.62
1:M:165:PRO:HB3	1:N:524:THR:HG22	1.79	0.62
1:M:571:LYS:NZ	1:M:635:THR:O	2.31	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
1:U:325:ASP:OD1	1:U:347:LYS:NZ	2.32	0.61
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:A:87:THR:HG21	1:U:261:PRO:HD3	1.83	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: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
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
1:J:434:MET:HE3	1:J:438:ILE:HD11	1.83	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
2:C:252:PRO:HG2	2:C:275:MET:HE2	1.83	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:M:434:MET:HE2	1:M:438:ILE:HD11	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:84:VAL:HG21	2:C:121:MET:HE2	1.83	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
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
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:B:170:VAL:HG23	1:B:174:MET:HE2	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:A:601:LEU:O	1:B:137:LYS:NZ	2.36	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:N:355:HIS:HE1	1:N:582:MET:HE1	1.72	0.54
2:P:98:LEU:HD21	2:P:139:ILE:HD11	1.89	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
1:Q:479:LYS:NZ	1:Q:626:ASP:OD1	2.36	0.54
2:D:231:ASN:O	7:D:401:ATP:O2'	2.25	0.54
1:E:138:HIS:HA	1:F:555:MET:HE3	1.89	0.54
1:E:407:GLU:OE2	5:E:703:FAD:O3B	2.25	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
1:U:219:MET:HE3	1:U:250:PRO:HG3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:A:571:LYS:NZ	1:A:635:THR:O	2.39	0.53
2:G:163:MET:HE2	2:H:276:MET:HE2	1.90	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
2:C:264:PRO:HB3	2:G:49:LEU:HD11	1.91	0.53
1:E:603:PRO:HB3	1:F:612:MET:HA	1.89	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:S:161:LEU:HD13	2:T:276:MET:HE2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:ARG:NH2	2:D:269:GLU:OE2	2.29	0.52
2:D:166:ILE:HD13	2:D:262:VAL:HG21	1.91	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:T:252:PRO:HG2	2:T:275:MET:HE2	1.90	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
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: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:J:631:GLU:O	1:J:635:THR:OG1	2.25	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
1:A:87:THR:OG1	1:U:259:ARG:O	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	2:G:49:LEU:HD23	1.75	0.51
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
1:U:407:GLU:OE2	5:U:703:FAD:O2B	2.28	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
2:T:285:THR:HA	2:W:260:LYS:HG2	1.92	0.50
1:V:551:ALA:HB3	3:V:701:TPP:H72	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:170:VAL:HG13	1:E:174:MET:HE2	1.92	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:O:84:VAL:HG21	2:O:121:MET:HE3	1.94	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
1:N:679:ARG:O	1:N:683:THR:OG1	2.26	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
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:D:87:GLU:HG2	2:D:90:VAL:HG23	1.94	0.49
2:D:191:ASP:OD1	2:D:192:SER:N	2.41	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:304:LEU:HD12	1:N:371:ILE:HB	1.95	0.48
1:Q:94:GLY:HA3	1:Q:254:THR:HA	1.95	0.48
1:Q:153:SER:HB3	1:Q:538:ALA:HB1	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:HN42	3:I:701:TPP:H2	1.78	0.48
5:R:701:FAD:H4'	5:R:701:FAD:H1'2	1.57	0.48
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:HN42	3:J:701:TPP:H2	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:555:MET:HB3	1:F:138:HIS:HD2	1.79	0.48
1:E:619:VAL:HG12	1:E:628:LYS:HD2	1.95	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
1:A:323:LEU:HB2	1:A:435:MET:HE1	1.96	0.47
3:V:701:TPP:H2	3:V:701:TPP:HN42	1.79	0.47
2:C:151:TYR:HB3	2:C:156:ILE:HD13	1.96	0.47
2:D:84:VAL:HA	2:D:145:VAL:HA	1.96	0.47
2:D:128:GLN:O	2:D:132:ILE:HG12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:VAL:HB	2:D:255:ILE:HD11	1.96	0.47
1:E:615:LYS:HB2	1:E:639:VAL:HG12	1.96	0.47
1:F:555:MET:HE2	1:F:555:MET:HB3	1.85	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:U:251:LYS:NZ	6:V:704:60G:OAD	2.32	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:165:PRO:HD3	1:B:522:LEU:HG	1.97	0.47
1:A:676:THR:O	1:A:680:HIS:ND1	2.46	0.47
2:C:94:VAL:HG21	2:C:121:MET:HE1	1.96	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
2:T:254:ARG:NH2	7:T:401:ATP:O4'	2.48	0.47
2:C:157:ILE:HB	2:D:163:MET:HE1	1.96	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: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: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
2:W:252:PRO:HG2	2:W:275:MET:HE2	1.95	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:N:274:ASN:N	2.48	0.46
3:N:701:TPP:HN42	3:N:701:TPP:H2	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:Q:277:THR:C	1:Q:279:ARG:N	2.72	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:I:323:LEU:HB2	1:I:435:MET:HE1	1.98	0.46
1:J:153:SER:HB3	1:J:538:ALA:HB1	1.96	0.46
1:N:355:HIS:CE1	1:N:582:MET:HE1	2.49	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
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
2:L:235:ARG:HH21	2:L:247:GLU:CD	2.23	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
1:E:654:MET:HE2	1:E:656:ALA:HB2	1.97	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
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:HE2	1:I:472:LYS:HB3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:273:LEU:HD22	1:Q:273:LEU:C	2.39	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:H2	3:U:701:TPP:HN42	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:I:497:VAL:HG21	1:I:523:GLY:C	2.41	0.45
1:J:330:PRO:HB2	1:J:349:LEU:HD11	1.98	0.45
2:X:65:TYR:C	2:X:65:TYR:CD2	2.95	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
1:A:190:GLN:NE2	1:A:248:ASP:OD2	2.46	0.45
1:E:153:SER:HB3	1:E:538:ALA:HB1	1.98	0.45
1:E:226:LEU:HB3	1:E:227:PRO:HD3	1.99	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:161:LEU:HB2	2:D:161:LEU:HD12	1.98	0.45
2:C:182:HIS:O	2:C:182:HIS:ND1	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:579:GLU:OE1	1:J:648:LYS:NZ	2.41	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:M:170:VAL:C	1:M:173:PRO:HD2	2.43	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
1:B:122:TYR:HA	1:B:125:ILE:HG12	1.97	0.44
3:B:701:TPP:HN42	3:B:701:TPP:H2	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:E:162:THR:OG1	1:E:163:SER:N	2.48	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:I:170:VAL:C	1:I:173:PRO:HD2	2.42	0.44
2:S:171:THR:HG21	2:W:49:LEU:HD13	2.00	0.44
1:U:474:GLN:HB2	1:U:507:HIS:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H9	5:M:703:FAD:H1'1	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:Q:274:ASN:C	1:Q:276:LEU:N	2.73	0.44
1:I:151:ARG:HH11	1:I:182:ILE:HD11	1.83	0.43
1:J:407:GLU:OE2	5:J:703:FAD:O2B	2.36	0.43
2:O:98:LEU:HD11	2:O:123:ILE:HD13	2.00	0.43
1:A:153:SER:HB3	1:A:538:ALA:HB1	1.99	0.43
1:A:357:CYS:HB3	1:A:460:TYR:CZ	2.54	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:H	1:E:474:GLN:HG2	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
1:M:550:ASP:OD1	1:M:550:ASP:N	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:V:170:VAL:C	1:V:173:PRO:HD2	2.43	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:Q:286:MET:HE1	1:Q:433:LYS:HD3	2.00	0.43
1:A:209:ILE:HG23	1:B:209:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:170:VAL:C	1:F:173:PRO:HD2	2.43	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:170:VAL:C	1:B:173:PRO:HD2	2.44	0.43
1:B:676:THR:O	1:B:680:HIS:ND1	2.50	0.43
1:F:84:ASP:OD1	1:F:84:ASP:N	2.52	0.43
1:F:302:PRO:HG2	1:F:329:ILE:HG22	1.99	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
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:62:SER:O	2:D:66:GLU:HG2	2.19	0.43
2:D:238:ASP:HB3	2:D:245:ILE:HB	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:N:636:LYS:HA	1.89	0.43
1:A:588:SER:HG	1:A:595:TYR:HH	1.66	0.42
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:HN42	3:A:701:TPP:H2	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:HD13	1:I:329:ILE:H	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:323:LEU:HB2	1:E:435:MET:HE1	2.00	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
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:HN42	3:B:701:TPP:C2	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:585:GLN:CD	1:U:651:VAL:H	2.28	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
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:H	2.26	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:H8	7:W:402:ATP:H2'	1.68	0.42
1:A:192:PRO:HG3	1:A:251:LYS:HB3	2.02	0.42
5:A:703:FAD:H9	5:A:703:FAD:H1'1	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
1:R:141:GLY:O	1:R:145:MET:N	2.46	0.42
1:R:592:GLU:CD	1:R:592:GLU:H	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:334:THR:OG1	5:F:703:FAD:O1P	2.29	0.41
1:J:654:MET:HE2	1:J:656:ALA:HB2	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
1:U:497:VAL:HG21	1:U:523:GLY:C	2.45	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: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:HE2	1:J:137:LYS:HB3	1.89	0.41
1:J:333:THR:O	1:J:351:MET:HA	2.19	0.41
1:N:497:VAL:HG21	1:N:523:GLY:C	2.45	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
1:R:407:GLU:CD	5:R:701:FAD:H1B	2.45	0.41
1:B:323:LEU:HB2	1:B:435:MET:HE1	2.01	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:M:355:HIS:NE2	1:M:582:MET:HE1	2.36	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
1:J:490:HIS:O	1:J:542:SER:OG	2.30	0.41
5:J:703:FAD:H4'	5:J:703:FAD:H1'2	1.74	0.41
2:L:73:GLN:HA	2:L:74:PRO:HD3	1.93	0.41
7:L:401:ATP:H8	7:L:401:ATP:H2'	1.71	0.41

Continued on next page...

Continued from previous page...

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
1:V:355:HIS:CE1	1:V:582:MET:HE1	2.56	0.41
2:X:70:PRO:O	2:X:71:SER:HB2	2.20	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
2:O:252:PRO:HG2	2:O:275:MET:HE2	2.03	0.41
1:V:89:PHE:HA	1:V:92:LEU:HD12	2.01	0.41
1:A:557:LEU:H	1:A:557:LEU:HD22	1.85	0.41
2:C:205:HIS:CE1	2:K:45:PRO:HG2	2.54	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
1:J:435:MET:C	1:J:437:LYS:H	2.29	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:A:409:SER:HA	1:A:410:PRO:HD3	1.88	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:HD12	1:I:385:ILE:H	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:N:196:ILE:HG12	1:N:219:MET:HE1	2.02	0.41
1:Q:227:PRO:HG2	1:Q:262:ILE:HD12	2.02	0.41
1:Q:522:LEU:HG	1:R:165:PRO:HD3	2.03	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:HB3	1:U:479:LYS:HE2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:101:MET:HG3	1:J:230:ILE:HD12	2.03	0.40
1:U:336:GLN:HE22	1:U:518:THR:HG23	1.86	0.40
2:X:162:VAL:HG21	2:X:259:LEU:HD21	2.02	0.40
2:X:201:GLU:HA	2:X:208:ASN:HD21	1.86	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:R:587:GLN:HE21	1:R:587:GLN:HB2	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:HN42	3:E:701:TPP:C2	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%)	36	68
1	F	602/644 (94%)	572 (95%)	26 (4%)	4 (1%)	18	52
1	I	602/644 (94%)	582 (97%)	20 (3%)	0	100	100
1	J	600/644 (93%)	569 (95%)	28 (5%)	3 (0%)	24	59
1	M	603/644 (94%)	566 (94%)	36 (6%)	1 (0%)	43	73
1	N	601/644 (93%)	569 (95%)	31 (5%)	1 (0%)	43	73
1	Q	594/644 (92%)	570 (96%)	22 (4%)	2 (0%)	36	68
1	R	394/644 (61%)	369 (94%)	21 (5%)	4 (1%)	12	45
1	U	602/644 (94%)	569 (94%)	31 (5%)	2 (0%)	36	68
1	V	603/644 (94%)	574 (95%)	28 (5%)	1 (0%)	43	73
2	C	251/297 (84%)	243 (97%)	7 (3%)	1 (0%)	30	62
2	D	248/297 (84%)	235 (95%)	10 (4%)	3 (1%)	10	42
2	G	251/297 (84%)	237 (94%)	13 (5%)	1 (0%)	30	62
2	H	250/297 (84%)	235 (94%)	13 (5%)	2 (1%)	16	50
2	K	241/297 (81%)	221 (92%)	15 (6%)	5 (2%)	5	31
2	L	253/297 (85%)	237 (94%)	13 (5%)	3 (1%)	10	42
2	O	233/297 (78%)	221 (95%)	11 (5%)	1 (0%)	30	62
2	P	237/297 (80%)	228 (96%)	9 (4%)	0	100	100
2	S	240/297 (81%)	227 (95%)	12 (5%)	1 (0%)	30	62
2	T	226/297 (76%)	214 (95%)	11 (5%)	1 (0%)	30	62
2	W	241/297 (81%)	228 (95%)	10 (4%)	3 (1%)	10	42
2	X	234/297 (79%)	216 (92%)	14 (6%)	4 (2%)	7	35
All	All	9914/11292 (88%)	9412 (95%)	457 (5%)	45 (0%)	24	59

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	477	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
2	W	45	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	488 (99%)	7 (1%)	59	77
1	B	496/531 (93%)	493 (99%)	3 (1%)	78	84
1	E	490/531 (92%)	482 (98%)	8 (2%)	55	75
1	F	487/531 (92%)	480 (99%)	7 (1%)	59	77
1	I	481/531 (91%)	468 (97%)	13 (3%)	39	68
1	J	481/531 (91%)	470 (98%)	11 (2%)	44	70
1	M	496/531 (93%)	493 (99%)	3 (1%)	78	84
1	N	493/531 (93%)	488 (99%)	5 (1%)	68	80
1	Q	475/531 (90%)	468 (98%)	7 (2%)	57	76
1	R	307/531 (58%)	292 (95%)	15 (5%)	22	55
1	U	483/531 (91%)	477 (99%)	6 (1%)	63	79
1	V	493/531 (93%)	490 (99%)	3 (1%)	78	84
2	C	217/260 (84%)	211 (97%)	6 (3%)	38	68
2	D	215/260 (83%)	209 (97%)	6 (3%)	38	68
2	G	218/260 (84%)	213 (98%)	5 (2%)	44	70
2	H	220/260 (85%)	217 (99%)	3 (1%)	59	77
2	K	213/260 (82%)	208 (98%)	5 (2%)	44	70
2	L	219/260 (84%)	218 (100%)	1 (0%)	81	85
2	O	204/260 (78%)	203 (100%)	1 (0%)	81	85
2	P	213/260 (82%)	206 (97%)	7 (3%)	33	65
2	S	210/260 (81%)	201 (96%)	9 (4%)	26	59
2	T	203/260 (78%)	199 (98%)	4 (2%)	48	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	216/260 (83%)	214 (99%)	2 (1%)	70	81
2	X	207/260 (80%)	201 (97%)	6 (3%)	37	67
All	All	8232/9492 (87%)	8089 (98%)	143 (2%)	53	75

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	VAL
1	A	275	GLN
1	A	352	LEU
1	A	443	GLU
1	A	557	LEU
1	A	619	VAL
1	A	673	ARG
1	B	277	THR
1	B	298	LEU
1	B	352	LEU
2	C	42	THR
2	C	109	VAL
2	C	178	LEU
2	C	183	THR
2	C	292	ASP
2	C	294	ASP
2	D	49	LEU
2	D	79	VAL
2	D	87	GLU
2	D	145	VAL
2	D	161	LEU
2	D	177	LEU
1	E	87	THR
1	E	331	VAL
1	E	338	LEU
1	E	465	GLU
1	E	474	GLN
1	E	493	VAL
1	E	558	THR
1	E	619	VAL
1	F	135	LEU
1	F	262	ILE
1	F	295	LEU
1	F	350	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	352	LEU
1	F	379	ASP
1	F	548	ASP
2	G	110	VAL
2	G	172	GLU
2	G	178	LEU
2	G	195	LEU
2	G	214	VAL
2	H	94	VAL
2	H	125	LEU
2	H	145	VAL
1	I	262	ILE
1	I	304	LEU
1	I	329	ILE
1	I	421	ILE
1	I	471	ILE
1	I	482	LYS
1	I	548	ASP
1	I	576	ASN
1	I	577	ASN
1	I	598	THR
1	I	606	ILE
1	I	614	LEU
1	I	640	LEU
1	J	137	LYS
1	J	170	VAL
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	619	VAL
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
2	L	110	VAL
1	M	85	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	224	GLU
1	M	428	THR
1	N	170	VAL
1	N	274	ASN
1	N	385	ILE
1	N	435	MET
1	N	619	VAL
2	O	217	LEU
2	P	109	VAL
2	P	110	VAL
2	P	148	VAL
2	P	179	LEU
2	P	195	LEU
2	P	267	VAL
2	P	281	THR
1	Q	170	VAL
1	Q	273	LEU
1	Q	278	SER
1	Q	352	LEU
1	Q	601	LEU
1	Q	606	ILE
1	Q	623	GLU
1	R	107	VAL
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	437	LYS
1	R	475	THR
1	R	544	VAL
1	R	587	GLN
1	R	592	GLU
2	S	46	LEU
2	S	79	VAL
2	S	132	ILE
2	S	145	VAL
2	S	161	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	109	VAL
2	T	161	LEU
1	U	170	VAL
1	U	267	THR
1	U	331	VAL
1	U	493	VAL
1	U	557	LEU
1	U	619	VAL
1	V	262	ILE
1	V	623	GLU
1	V	639	VAL
2	W	110	VAL
2	W	133	GLU
2	X	77	GLN
2	X	115	VAL
2	X	143	VAL
2	X	145	VAL
2	X	161	LEU
2	X	195	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	HIS
1	A	536	GLN
1	B	96	GLN
1	B	271	ASN
1	B	499	GLN
1	B	580	GLN
1	E	343	GLN
1	E	355	HIS
1	E	499	GLN
1	E	512	ASN
1	E	554	ASN
1	F	499	GLN
1	F	580	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	57	ASN
2	G	134	GLN
2	H	81	ASN
2	H	208	ASN
2	H	227	ASN
2	H	231	ASN
1	I	506	GLN
1	I	536	GLN
1	J	499	GLN
1	J	680	HIS
2	K	57	ASN
2	K	208	ASN
2	K	223	ASN
2	L	81	ASN
2	L	104	ASN
2	L	223	ASN
1	M	96	GLN
1	M	275	GLN
1	M	499	GLN
1	N	281	GLN
1	N	343	GLN
1	N	355	HIS
1	N	450	GLN
1	N	490	HIS
1	N	597	HIS
2	O	77	GLN
2	O	85	GLN
2	O	180	HIS
2	P	77	GLN
1	Q	536	GLN
1	Q	687	HIS
1	R	313	HIS
1	R	485	ASN
1	R	587	GLN
2	S	182	HIS
2	T	57	ASN
2	T	134	GLN
1	U	260	ASN
1	U	499	GLN
1	U	536	GLN
1	V	281	GLN
1	V	485	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	219	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	60G	I	704	-	28,29,29	1.45	3 (10%)	37,40,40	3.50	14 (37%)
5	FAD	E	703	-	58,58,58	1.64	14 (24%)	85,89,89	1.63	19 (22%)
6	60G	J	704	-	28,29,29	1.48	4 (14%)	37,40,40	3.51	13 (35%)
3	TPP	B	701	4	26,27,27	1.39	5 (19%)	38,40,40	1.61	10 (26%)
5	FAD	B	703	-	58,58,58	1.63	15 (25%)	85,89,89	1.64	19 (22%)
3	TPP	A	701	4	26,27,27	1.37	5 (19%)	38,40,40	1.60	10 (26%)
7	ATP	T	401	4	32,33,33	3.51	15 (46%)	48,52,52	1.74	10 (20%)
7	ATP	S	401	-	32,33,33	3.52	15 (46%)	48,52,52	1.67	9 (18%)
5	FAD	V	703	-	58,58,58	1.65	15 (25%)	85,89,89	1.64	19 (22%)
3	TPP	I	701	4	26,27,27	1.39	5 (19%)	38,40,40	1.57	10 (26%)
5	FAD	Q	703	-	58,58,58	1.62	13 (22%)	85,89,89	1.63	19 (22%)
6	60G	R	702	-	28,29,29	1.48	3 (10%)	37,40,40	3.48	13 (35%)
3	TPP	M	701	4	26,27,27	1.40	5 (19%)	38,40,40	1.57	10 (26%)
3	TPP	F	701	4	26,27,27	1.41	5 (19%)	38,40,40	1.58	9 (23%)
3	TPP	N	701	4	26,27,27	1.40	5 (19%)	38,40,40	1.57	10 (26%)
6	60G	Q	704	-	28,29,29	1.49	3 (10%)	37,40,40	3.49	12 (32%)
3	TPP	U	701	4	26,27,27	1.36	5 (19%)	38,40,40	1.57	10 (26%)
6	60G	N	705	-	28,29,29	1.46	3 (10%)	37,40,40	3.49	12 (32%)
6	60G	A	704	-	28,29,29	1.47	3 (10%)	37,40,40	3.50	13 (35%)
6	60G	N	704	-	28,29,29	1.44	3 (10%)	37,40,40	3.49	12 (32%)
7	ATP	D	401	4	32,33,33	3.51	15 (46%)	48,52,52	1.79	11 (22%)
7	ATP	G	401	4	32,33,33	3.54	15 (46%)	48,52,52	1.73	10 (20%)
5	FAD	I	703	-	58,58,58	1.62	12 (20%)	85,89,89	1.63	20 (23%)
5	FAD	N	703	-	58,58,58	1.63	15 (25%)	85,89,89	1.63	20 (23%)
6	60G	E	704	-	28,29,29	1.46	5 (17%)	37,40,40	3.52	12 (32%)
7	ATP	W	402	4	32,33,33	3.53	15 (46%)	48,52,52	1.69	9 (18%)
7	ATP	K	401	4	32,33,33	3.52	15 (46%)	48,52,52	1.70	10 (20%)
5	FAD	F	703	-	58,58,58	1.68	14 (24%)	85,89,89	1.66	19 (22%)
3	TPP	Q	701	4	26,27,27	1.36	5 (19%)	38,40,40	1.57	10 (26%)
7	ATP	O	401	4	32,33,33	3.52	15 (46%)	48,52,52	1.69	9 (18%)
3	TPP	J	701	4	26,27,27	1.42	5 (19%)	38,40,40	1.57	7 (18%)
5	FAD	U	703	-	58,58,58	1.63	14 (24%)	85,89,89	1.64	19 (22%)
5	FAD	M	703	-	58,58,58	1.63	14 (24%)	85,89,89	1.63	19 (22%)
5	FAD	J	703	-	58,58,58	1.63	12 (20%)	85,89,89	1.72	23 (27%)
6	60G	B	704	-	28,29,29	1.46	4 (14%)	37,40,40	3.49	13 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ATP	P	401	4	32,33,33	3.52	15 (46%)	48,52,52	1.70	9 (18%)
6	60G	U	704	-	28,29,29	1.45	3 (10%)	37,40,40	3.50	14 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	H	401	4	-	5/22/38/38	0/3/3/3
7	ATP	C	401	4	-	6/22/38/38	0/3/3/3
6	60G	V	704	-	-	7/24/24/24	0/2/2/2
5	FAD	A	703	-	-	3/34/50/50	0/6/6/6
5	FAD	R	701	-	-	13/34/50/50	0/6/6/6
7	ATP	L	401	4	-	4/22/38/38	0/3/3/3
6	60G	F	704	-	-	7/24/24/24	0/2/2/2
7	ATP	W	401	-	-	6/22/38/38	0/3/3/3
3	TPP	E	701	4	-	4/17/17/17	0/2/2/2
3	TPP	V	701	4	-	2/17/17/17	0/2/2/2
6	60G	I	704	-	-	10/24/24/24	0/2/2/2
5	FAD	E	703	-	-	2/34/50/50	0/6/6/6
6	60G	J	704	-	-	7/24/24/24	0/2/2/2
3	TPP	B	701	4	-	4/17/17/17	0/2/2/2
5	FAD	B	703	-	-	4/34/50/50	0/6/6/6
3	TPP	A	701	4	-	6/17/17/17	0/2/2/2
7	ATP	T	401	4	-	3/22/38/38	0/3/3/3
7	ATP	S	401	-	-	10/22/38/38	0/3/3/3
5	FAD	V	703	-	-	13/34/50/50	0/6/6/6
3	TPP	I	701	4	-	4/17/17/17	0/2/2/2
5	FAD	Q	703	-	-	4/34/50/50	0/6/6/6
6	60G	R	702	-	-	10/24/24/24	0/2/2/2
3	TPP	M	701	4	-	4/17/17/17	0/2/2/2
3	TPP	F	701	4	-	4/17/17/17	0/2/2/2
3	TPP	N	701	4	-	4/17/17/17	0/2/2/2
6	60G	Q	704	-	-	7/24/24/24	0/2/2/2
3	TPP	U	701	4	-	4/17/17/17	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	60G	N	705	-	-	8/24/24/24	0/2/2/2
6	60G	A	704	-	-	10/24/24/24	0/2/2/2
6	60G	N	704	-	-	8/24/24/24	0/2/2/2
7	ATP	D	401	4	-	4/22/38/38	0/3/3/3
7	ATP	G	401	4	-	3/22/38/38	0/3/3/3
5	FAD	I	703	-	-	7/34/50/50	0/6/6/6
5	FAD	N	703	-	-	3/34/50/50	0/6/6/6
6	60G	E	704	-	-	8/24/24/24	0/2/2/2
7	ATP	W	402	4	-	4/22/38/38	0/3/3/3
7	ATP	K	401	4	-	7/22/38/38	0/3/3/3
5	FAD	F	703	-	-	8/34/50/50	0/6/6/6
3	TPP	Q	701	4	-	5/17/17/17	0/2/2/2
7	ATP	O	401	4	-	8/22/38/38	0/3/3/3
3	TPP	J	701	4	-	4/17/17/17	0/2/2/2
5	FAD	U	703	-	-	16/34/50/50	0/6/6/6
5	FAD	M	703	-	-	3/34/50/50	0/6/6/6
5	FAD	J	703	-	-	11/34/50/50	0/6/6/6
6	60G	B	704	-	-	9/24/24/24	0/2/2/2
7	ATP	P	401	4	-	2/22/38/38	0/3/3/3
6	60G	U	704	-	-	7/24/24/24	0/2/2/2

All (442) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	401	ATP	C2'-C3'	-11.44	1.22	1.53
7	C	401	ATP	C2'-C3'	-11.37	1.22	1.53
7	W	402	ATP	C2'-C3'	-11.36	1.22	1.53
7	O	401	ATP	C2'-C3'	-11.36	1.22	1.53
7	S	401	ATP	C2'-C3'	-11.35	1.22	1.53
7	P	401	ATP	C2'-C3'	-11.34	1.22	1.53
7	H	401	ATP	C2'-C3'	-11.32	1.22	1.53
7	W	401	ATP	C2'-C3'	-11.30	1.22	1.53
7	T	401	ATP	C2'-C3'	-11.29	1.22	1.53
7	G	401	ATP	C2'-C3'	-11.28	1.22	1.53
7	K	401	ATP	C2'-C3'	-11.21	1.23	1.53
7	D	401	ATP	C2'-C3'	-11.14	1.23	1.53
7	P	401	ATP	O4'-C4'	-7.51	1.28	1.45
7	T	401	ATP	O4'-C4'	-7.48	1.28	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	401	ATP	O4'-C4'	-7.46	1.28	1.45
7	H	401	ATP	O4'-C4'	-7.43	1.28	1.45
7	O	401	ATP	O4'-C4'	-7.43	1.28	1.45
7	L	401	ATP	O4'-C4'	-7.41	1.28	1.45
7	D	401	ATP	O4'-C4'	-7.40	1.28	1.45
7	W	402	ATP	O4'-C4'	-7.40	1.28	1.45
7	W	401	ATP	O4'-C4'	-7.40	1.28	1.45
7	C	401	ATP	O4'-C4'	-7.40	1.28	1.45
7	K	401	ATP	O4'-C4'	-7.38	1.28	1.45
7	S	401	ATP	O4'-C4'	-7.36	1.28	1.45
7	G	401	ATP	PA-O3A	6.63	1.66	1.59
7	W	401	ATP	PA-O3A	6.57	1.66	1.59
7	W	402	ATP	PA-O3A	6.50	1.66	1.59
7	D	401	ATP	PA-O3A	6.42	1.66	1.59
7	H	401	ATP	PA-O3A	6.42	1.66	1.59
7	K	401	ATP	PA-O3A	6.42	1.66	1.59
7	T	401	ATP	PA-O3A	6.34	1.66	1.59
7	P	401	ATP	PA-O3A	6.34	1.66	1.59
7	L	401	ATP	PA-O3A	6.32	1.66	1.59
7	S	401	ATP	PA-O3A	6.31	1.66	1.59
7	O	401	ATP	PA-O3A	6.26	1.66	1.59
7	C	401	ATP	PA-O3A	6.17	1.66	1.59
5	F	703	FAD	C10-N1	5.39	1.44	1.33
5	N	703	FAD	C10-N1	5.34	1.44	1.33
5	J	703	FAD	C10-N1	5.32	1.44	1.33
5	A	703	FAD	C10-N1	5.31	1.44	1.33
5	M	703	FAD	C10-N1	5.29	1.43	1.33
5	V	703	FAD	C10-N1	5.28	1.43	1.33
5	I	703	FAD	C10-N1	5.28	1.43	1.33
5	U	703	FAD	C10-N1	5.28	1.43	1.33
5	Q	703	FAD	C10-N1	5.27	1.43	1.33
5	E	703	FAD	C10-N1	5.26	1.43	1.33
5	B	703	FAD	C10-N1	5.25	1.43	1.33
5	R	701	FAD	C10-N1	5.24	1.43	1.33
7	H	401	ATP	C6-N6	4.82	1.46	1.34
7	S	401	ATP	C6-N6	4.80	1.46	1.34
7	W	401	ATP	C6-N6	4.80	1.46	1.34
7	P	401	ATP	C6-N6	4.79	1.46	1.34
7	D	401	ATP	C6-N6	4.79	1.46	1.34
7	W	402	ATP	C6-N6	4.79	1.46	1.34
7	K	401	ATP	C6-N6	4.79	1.46	1.34
7	C	401	ATP	C6-N6	4.78	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	401	ATP	C6-N6	4.78	1.46	1.34
7	T	401	ATP	C6-N6	4.77	1.46	1.34
7	L	401	ATP	C6-N6	4.77	1.46	1.34
7	O	401	ATP	C6-N6	4.76	1.46	1.34
7	K	401	ATP	O2'-C2'	4.69	1.54	1.43
7	W	401	ATP	O2'-C2'	4.68	1.54	1.43
7	C	401	ATP	O2'-C2'	4.68	1.54	1.43
7	S	401	ATP	O2'-C2'	4.68	1.54	1.43
7	D	401	ATP	C3'-C4'	4.67	1.64	1.53
7	H	401	ATP	O2'-C2'	4.67	1.54	1.43
7	P	401	ATP	O2'-C2'	4.65	1.54	1.43
7	W	402	ATP	O2'-C2'	4.61	1.54	1.43
7	G	401	ATP	O2'-C2'	4.61	1.54	1.43
7	O	401	ATP	O2'-C2'	4.60	1.54	1.43
7	K	401	ATP	C3'-C4'	4.58	1.64	1.53
7	L	401	ATP	O2'-C2'	4.54	1.54	1.43
7	D	401	ATP	O2'-C2'	4.53	1.54	1.43
7	G	401	ATP	C3'-C4'	4.52	1.64	1.53
7	O	401	ATP	C1'-N9	-4.51	1.33	1.46
7	T	401	ATP	O2'-C2'	4.51	1.54	1.43
7	H	401	ATP	C3'-C4'	4.49	1.64	1.53
7	P	401	ATP	C1'-N9	-4.49	1.33	1.46
7	D	401	ATP	C1'-N9	-4.49	1.33	1.46
7	C	401	ATP	C1'-N9	-4.49	1.33	1.46
7	W	402	ATP	C1'-N9	-4.49	1.33	1.46
7	S	401	ATP	C3'-C4'	4.48	1.64	1.53
7	S	401	ATP	C1'-N9	-4.48	1.34	1.46
7	L	401	ATP	C1'-N9	-4.46	1.34	1.46
7	O	401	ATP	C3'-C4'	4.46	1.64	1.53
7	C	401	ATP	C3'-C4'	4.46	1.64	1.53
7	L	401	ATP	C3'-C4'	4.46	1.64	1.53
7	H	401	ATP	C1'-N9	-4.46	1.34	1.46
7	G	401	ATP	C1'-N9	-4.45	1.34	1.46
7	W	401	ATP	C3'-C4'	4.45	1.64	1.53
7	K	401	ATP	C1'-N9	-4.44	1.34	1.46
7	W	401	ATP	C1'-N9	-4.44	1.34	1.46
7	W	402	ATP	C3'-C4'	4.44	1.64	1.53
7	P	401	ATP	C3'-C4'	4.44	1.64	1.53
7	T	401	ATP	C3'-C4'	4.43	1.64	1.53
7	T	401	ATP	C1'-N9	-4.40	1.34	1.46
5	J	703	FAD	C4X-N5	4.22	1.39	1.30
5	V	703	FAD	C4X-N5	4.18	1.39	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	703	FAD	C4X-N5	4.17	1.39	1.30
7	W	401	ATP	PB-O3A	4.16	1.64	1.59
5	E	703	FAD	C4X-N5	4.16	1.39	1.30
5	M	703	FAD	C4X-N5	4.16	1.39	1.30
5	B	703	FAD	C4X-N5	4.15	1.39	1.30
5	R	701	FAD	C4X-N5	4.14	1.39	1.30
5	N	703	FAD	C4X-N5	4.13	1.39	1.30
7	G	401	ATP	PB-O3A	4.12	1.63	1.59
6	Q	704	60G	C2-NAP	4.11	1.44	1.38
5	I	703	FAD	C4X-N5	4.11	1.39	1.30
7	H	401	ATP	PB-O3A	4.11	1.63	1.59
5	Q	703	FAD	C4X-N5	4.11	1.39	1.30
5	A	703	FAD	C4X-N5	4.10	1.39	1.30
7	P	401	ATP	O3'-C3'	4.08	1.53	1.43
7	K	401	ATP	O3'-C3'	4.06	1.53	1.43
7	O	401	ATP	PB-O3A	4.05	1.63	1.59
5	U	703	FAD	C4X-N5	4.05	1.39	1.30
7	D	401	ATP	PB-O3A	4.05	1.63	1.59
7	D	401	ATP	O3'-C3'	4.05	1.53	1.43
7	C	401	ATP	O3'-C3'	4.05	1.53	1.43
7	S	401	ATP	O3'-C3'	4.04	1.53	1.43
7	H	401	ATP	O3'-C3'	4.04	1.53	1.43
7	G	401	ATP	O3'-C3'	4.03	1.52	1.43
6	J	704	60G	C2-NAP	4.02	1.44	1.38
6	R	702	60G	C2-NAP	4.02	1.44	1.38
7	O	401	ATP	O3'-C3'	4.01	1.52	1.43
7	L	401	ATP	O3'-C3'	4.00	1.52	1.43
7	T	401	ATP	O3'-C3'	3.99	1.52	1.43
7	W	402	ATP	O3'-C3'	3.99	1.52	1.43
7	W	401	ATP	O3'-C3'	3.98	1.52	1.43
6	B	704	60G	C2-NAP	3.95	1.44	1.38
7	W	402	ATP	PB-O3A	3.95	1.63	1.59
6	N	705	60G	C2-NAP	3.94	1.44	1.38
7	L	401	ATP	PB-O3A	3.93	1.63	1.59
6	A	704	60G	C2-NAP	3.92	1.44	1.38
7	T	401	ATP	PB-O3A	3.92	1.63	1.59
6	E	704	60G	C2-NAP	3.89	1.44	1.38
7	K	401	ATP	PB-O3A	3.88	1.63	1.59
6	I	704	60G	C2-NAP	3.88	1.44	1.38
6	F	704	60G	C2-NAP	3.84	1.43	1.38
6	U	704	60G	C2-NAP	3.83	1.43	1.38
6	N	704	60G	C2-NAP	3.82	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	401	ATP	PB-O3A	3.81	1.63	1.59
7	S	401	ATP	PB-O3A	3.78	1.63	1.59
7	P	401	ATP	PB-O3A	3.78	1.63	1.59
6	V	704	60G	C2-NAP	3.75	1.43	1.38
7	W	401	ATP	O4'-C1'	3.44	1.50	1.42
7	K	401	ATP	O4'-C1'	3.43	1.49	1.42
7	S	401	ATP	O4'-C1'	3.43	1.49	1.42
5	F	703	FAD	PA-O3P	-3.43	1.55	1.59
7	L	401	ATP	O4'-C1'	3.40	1.49	1.42
7	H	401	ATP	O4'-C1'	3.39	1.49	1.42
7	W	402	ATP	O4'-C1'	3.38	1.49	1.42
7	C	401	ATP	O4'-C1'	3.38	1.49	1.42
7	G	401	ATP	O4'-C1'	3.37	1.49	1.42
7	O	401	ATP	O4'-C1'	3.36	1.49	1.42
7	T	401	ATP	O4'-C1'	3.34	1.49	1.42
7	P	401	ATP	O4'-C1'	3.33	1.49	1.42
3	I	701	TPP	C4'-N4'	3.29	1.42	1.34
3	J	701	TPP	C4'-N4'	3.27	1.42	1.34
3	F	701	TPP	C4'-N4'	3.27	1.42	1.34
3	E	701	TPP	C4'-N4'	3.26	1.42	1.34
3	Q	701	TPP	C4'-N4'	3.26	1.42	1.34
3	U	701	TPP	C4'-N4'	3.25	1.42	1.34
3	M	701	TPP	C4'-N4'	3.25	1.42	1.34
3	V	701	TPP	C4'-N4'	3.25	1.42	1.34
3	B	701	TPP	C4'-N4'	3.23	1.42	1.34
3	A	701	TPP	C4'-N4'	3.22	1.42	1.34
3	N	701	TPP	C4'-N4'	3.22	1.42	1.34
6	F	704	60G	OAR-CAA	-3.18	1.38	1.45
6	E	704	60G	OAR-CAA	-3.16	1.38	1.45
6	B	704	60G	OAR-CAA	-3.14	1.38	1.45
6	J	704	60G	OAR-CAA	-3.13	1.38	1.45
6	Q	704	60G	OAR-CAA	-3.13	1.38	1.45
7	D	401	ATP	O4'-C1'	3.13	1.49	1.42
6	V	704	60G	OAR-CAA	-3.13	1.38	1.45
6	A	704	60G	OAR-CAA	-3.12	1.38	1.45
6	N	705	60G	OAR-CAA	-3.11	1.38	1.45
6	U	704	60G	OAR-CAA	-3.08	1.38	1.45
6	R	702	60G	OAR-CAA	-3.08	1.38	1.45
3	J	701	TPP	C4-N3	-3.08	1.33	1.39
6	N	704	60G	OAR-CAA	-3.06	1.38	1.45
6	I	704	60G	OAR-CAA	-3.05	1.38	1.45
3	N	701	TPP	C4-N3	-3.03	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	701	TPP	C4-N3	-3.02	1.33	1.39
3	E	701	TPP	C4-N3	-3.01	1.33	1.39
3	U	701	TPP	C4-N3	-3.00	1.33	1.39
6	Q	704	60G	CAU-NAP	2.99	1.44	1.37
6	J	704	60G	CAU-NAP	2.98	1.44	1.37
5	J	703	FAD	PA-O3P	-2.98	1.56	1.59
3	B	701	TPP	C4-N3	-2.98	1.33	1.39
6	R	702	60G	CAU-NAP	2.96	1.44	1.37
3	A	701	TPP	C4-N3	-2.96	1.33	1.39
5	J	703	FAD	C2-N1	2.96	1.43	1.36
5	F	703	FAD	C2-N1	2.95	1.43	1.36
6	A	704	60G	CAU-NAP	2.95	1.44	1.37
5	E	703	FAD	C2-N1	2.95	1.43	1.36
3	I	701	TPP	C4-N3	-2.94	1.33	1.39
5	R	701	FAD	C2-N1	2.93	1.43	1.36
3	F	701	TPP	C4-N3	-2.93	1.33	1.39
5	B	703	FAD	C2-N1	2.93	1.43	1.36
3	Q	701	TPP	C4-N3	-2.92	1.33	1.39
5	I	703	FAD	C2-N1	2.92	1.43	1.36
3	V	701	TPP	C4-N3	-2.92	1.33	1.39
6	F	704	60G	CAU-NAP	2.91	1.43	1.37
5	U	703	FAD	C2-N1	2.91	1.43	1.36
6	E	704	60G	CAU-NAP	2.91	1.43	1.37
3	V	701	TPP	C5-C4	2.91	1.41	1.35
5	Q	703	FAD	C2-N1	2.90	1.43	1.36
5	N	703	FAD	C2-N1	2.90	1.43	1.36
5	V	703	FAD	C2-N1	2.89	1.43	1.36
5	M	703	FAD	C2-N1	2.88	1.43	1.36
3	I	701	TPP	C5-C4	2.88	1.41	1.35
6	V	704	60G	CAU-NAP	2.88	1.43	1.37
5	A	703	FAD	C2-N1	2.87	1.43	1.36
6	B	704	60G	CAU-NAP	2.87	1.43	1.37
6	U	704	60G	CAU-NAP	2.86	1.43	1.37
6	N	705	60G	CAU-NAP	2.85	1.43	1.37
3	N	701	TPP	C5-C4	2.85	1.41	1.35
6	I	704	60G	CAU-NAP	2.85	1.43	1.37
7	L	401	ATP	PB-O3B	2.84	1.62	1.59
5	J	703	FAD	C2'-C3'	2.84	1.58	1.53
7	W	402	ATP	C5-N7	-2.83	1.33	1.39
3	B	701	TPP	C5-C4	2.82	1.41	1.35
3	M	701	TPP	C5-C4	2.82	1.41	1.35
7	L	401	ATP	C5-N7	-2.81	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	701	TPP	PA-O3A	-2.81	1.56	1.59
3	Q	701	TPP	C5-C4	2.80	1.41	1.35
7	D	401	ATP	C5-N7	-2.80	1.34	1.39
7	G	401	ATP	C5-N7	-2.80	1.34	1.39
3	A	701	TPP	C5-C4	2.80	1.41	1.35
7	H	401	ATP	C5-N7	-2.80	1.34	1.39
7	W	401	ATP	C5-N7	-2.80	1.34	1.39
6	N	704	60G	CAU-NAP	2.80	1.43	1.37
5	U	703	FAD	C8A-N9A	-2.79	1.32	1.37
7	T	401	ATP	C5-N7	-2.79	1.34	1.39
5	A	703	FAD	C8A-N9A	-2.79	1.32	1.37
5	Q	703	FAD	C8A-N9A	-2.79	1.32	1.37
3	F	701	TPP	C5-C4	2.78	1.41	1.35
7	K	401	ATP	C5-N7	-2.78	1.34	1.39
5	M	703	FAD	C8A-N9A	-2.77	1.32	1.37
3	F	701	TPP	PA-O3A	-2.77	1.56	1.59
7	S	401	ATP	C5-N7	-2.75	1.34	1.39
7	P	401	ATP	C5-N7	-2.75	1.34	1.39
5	B	703	FAD	C8A-N9A	-2.75	1.32	1.37
5	V	703	FAD	C8A-N9A	-2.75	1.32	1.37
7	S	401	ATP	PB-O3B	2.75	1.62	1.59
5	E	703	FAD	C8A-N9A	-2.74	1.32	1.37
7	C	401	ATP	C5-N7	-2.73	1.34	1.39
3	U	701	TPP	C5-C4	2.73	1.40	1.35
5	R	701	FAD	C8A-N9A	-2.72	1.32	1.37
5	N	703	FAD	C8A-N9A	-2.71	1.32	1.37
5	F	703	FAD	O3'-C3'	-2.71	1.36	1.43
5	I	703	FAD	C8A-N9A	-2.70	1.33	1.37
3	E	701	TPP	C5-C4	2.69	1.40	1.35
7	O	401	ATP	C5-N7	-2.69	1.34	1.39
7	T	401	ATP	PB-O3B	2.69	1.62	1.59
5	M	703	FAD	O3'-C3'	-2.67	1.36	1.43
5	B	703	FAD	O3'-C3'	-2.67	1.36	1.43
5	E	703	FAD	O3'-C3'	-2.66	1.36	1.43
5	I	703	FAD	O3'-C3'	-2.65	1.36	1.43
5	Q	703	FAD	O3'-C3'	-2.64	1.36	1.43
7	K	401	ATP	PB-O3B	2.63	1.62	1.59
5	V	703	FAD	O3'-C3'	-2.63	1.36	1.43
5	E	703	FAD	PA-O3P	-2.62	1.56	1.59
5	A	703	FAD	O3'-C3'	-2.61	1.36	1.43
5	V	703	FAD	PA-O3P	-2.60	1.56	1.59
5	U	703	FAD	O3'-C3'	-2.60	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	703	FAD	O3'-C3'	-2.60	1.36	1.43
7	D	401	ATP	PB-O3B	2.59	1.62	1.59
5	R	701	FAD	O3'-C3'	-2.59	1.36	1.43
5	F	703	FAD	P-O3P	-2.55	1.56	1.59
5	U	703	FAD	PA-O3P	-2.55	1.56	1.59
5	R	701	FAD	C1'-N10	-2.53	1.41	1.47
5	U	703	FAD	C2'-C3'	2.52	1.57	1.53
7	G	401	ATP	PB-O3B	2.51	1.62	1.59
3	J	701	TPP	C5-C4	2.51	1.40	1.35
7	H	401	ATP	PB-O3B	2.50	1.62	1.59
5	A	703	FAD	C1'-N10	-2.50	1.41	1.47
5	F	703	FAD	C2'-C3'	2.50	1.57	1.53
5	V	703	FAD	C1'-N10	-2.50	1.41	1.47
5	R	701	FAD	PA-O3P	-2.48	1.56	1.59
7	P	401	ATP	PB-O3B	2.48	1.62	1.59
5	B	703	FAD	PA-O3P	-2.48	1.56	1.59
5	N	703	FAD	PA-O3P	-2.48	1.56	1.59
5	E	703	FAD	C1'-N10	-2.47	1.41	1.47
5	N	703	FAD	C1'-N10	-2.47	1.41	1.47
7	C	401	ATP	PB-O3B	2.47	1.62	1.59
5	U	703	FAD	C1'-N10	-2.47	1.41	1.47
5	I	703	FAD	C2'-C3'	2.46	1.57	1.53
5	M	703	FAD	C2'-C3'	2.46	1.57	1.53
5	F	703	FAD	C1'-N10	-2.45	1.41	1.47
7	O	401	ATP	PB-O3B	2.45	1.62	1.59
5	J	703	FAD	C1'-N10	-2.45	1.41	1.47
5	R	701	FAD	C2'-C3'	2.45	1.57	1.53
5	I	703	FAD	C1'-N10	-2.44	1.41	1.47
5	I	703	FAD	PA-O3P	-2.44	1.56	1.59
5	M	703	FAD	PA-O3P	-2.44	1.56	1.59
7	W	402	ATP	PB-O3B	2.43	1.62	1.59
5	Q	703	FAD	C2'-C3'	2.43	1.57	1.53
5	B	703	FAD	C2'-C3'	2.42	1.57	1.53
5	B	703	FAD	C1'-N10	-2.42	1.42	1.47
5	N	703	FAD	C2'-C3'	2.42	1.57	1.53
7	W	401	ATP	PB-O3B	2.41	1.62	1.59
5	A	703	FAD	C2'-C3'	2.41	1.57	1.53
5	Q	703	FAD	C1'-N10	-2.41	1.42	1.47
5	V	703	FAD	C2'-C3'	2.41	1.57	1.53
5	A	703	FAD	PA-O3P	-2.40	1.56	1.59
5	E	703	FAD	C2'-C3'	2.39	1.57	1.53
5	Q	703	FAD	PA-O3P	-2.38	1.56	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	703	FAD	C1'-N10	-2.38	1.42	1.47
5	J	703	FAD	O3'-C3'	-2.37	1.37	1.43
3	J	701	TPP	C5'-C4'	-2.29	1.39	1.42
5	F	703	FAD	C8A-N9A	-2.28	1.33	1.37
3	M	701	TPP	PA-O3A	-2.26	1.57	1.59
5	V	703	FAD	P-O3P	-2.25	1.57	1.59
5	R	701	FAD	C2B-C3B	-2.24	1.47	1.53
3	E	701	TPP	PA-O3A	-2.23	1.57	1.59
7	G	401	ATP	C4-N9	-2.23	1.33	1.37
7	H	401	ATP	C4-N9	-2.22	1.33	1.37
7	O	401	ATP	C4-N9	-2.22	1.33	1.37
3	Q	701	TPP	PA-O3A	-2.21	1.57	1.59
5	V	703	FAD	C2B-C3B	-2.21	1.47	1.53
5	Q	703	FAD	C2B-C3B	-2.21	1.47	1.53
5	R	701	FAD	C2B-C1B	-2.21	1.46	1.53
7	L	401	ATP	C4-N9	-2.21	1.33	1.37
7	D	401	ATP	C4-N9	-2.20	1.33	1.37
5	U	703	FAD	C2B-C3B	-2.20	1.47	1.53
7	C	401	ATP	C4-N9	-2.20	1.33	1.37
7	S	401	ATP	C4-N9	-2.20	1.33	1.37
7	W	401	ATP	C4-N9	-2.20	1.33	1.37
5	A	703	FAD	C2B-C3B	-2.20	1.47	1.53
7	W	401	ATP	PG-O2G	-2.19	1.46	1.54
5	N	703	FAD	C2B-C3B	-2.19	1.47	1.53
7	K	401	ATP	C4-N9	-2.19	1.33	1.37
7	W	402	ATP	PG-O2G	-2.19	1.46	1.54
5	B	703	FAD	C2B-C3B	-2.19	1.47	1.53
5	J	703	FAD	C4X-C4	2.18	1.52	1.44
3	B	701	TPP	PA-O3A	-2.18	1.57	1.59
7	T	401	ATP	PG-O2G	-2.18	1.46	1.54
7	D	401	ATP	PG-O2G	-2.17	1.46	1.54
7	H	401	ATP	PG-O2G	-2.17	1.46	1.54
7	P	401	ATP	PG-O2G	-2.17	1.46	1.54
7	C	401	ATP	PG-O2G	-2.17	1.46	1.54
7	G	401	ATP	PG-O2G	-2.17	1.46	1.54
7	P	401	ATP	C4-N9	-2.17	1.33	1.37
5	M	703	FAD	C1'-C2'	2.16	1.55	1.52
7	S	401	ATP	PG-O2G	-2.16	1.46	1.54
5	E	703	FAD	C2B-C3B	-2.16	1.47	1.53
5	M	703	FAD	C2B-C3B	-2.16	1.47	1.53
7	T	401	ATP	C4-N9	-2.16	1.33	1.37
7	K	401	ATP	PG-O2G	-2.16	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	701	FAD	C4X-C4	2.16	1.52	1.44
7	P	401	ATP	C8-N9	-2.15	1.33	1.37
3	Q	701	TPP	C5'-C4'	-2.15	1.39	1.42
3	I	701	TPP	PA-O3A	-2.15	1.57	1.59
7	W	402	ATP	C4-N9	-2.15	1.33	1.37
7	L	401	ATP	C8-N9	-2.15	1.33	1.37
7	O	401	ATP	PG-O2G	-2.15	1.46	1.54
5	J	703	FAD	C8A-N9A	-2.15	1.33	1.37
5	J	703	FAD	O2B-C2B	2.14	1.48	1.43
5	F	703	FAD	C6A-N6A	2.14	1.39	1.34
7	W	401	ATP	C8-N9	-2.14	1.33	1.37
5	R	701	FAD	C1'-C2'	2.14	1.55	1.52
7	H	401	ATP	C8-N9	-2.13	1.33	1.37
5	B	703	FAD	C4X-C4	2.13	1.52	1.44
7	W	402	ATP	C8-N9	-2.13	1.33	1.37
7	S	401	ATP	C8-N9	-2.13	1.33	1.37
5	V	703	FAD	C4X-C4	2.13	1.52	1.44
5	U	703	FAD	C2B-C1B	-2.12	1.46	1.53
7	L	401	ATP	PG-O2G	-2.12	1.46	1.54
7	T	401	ATP	C8-N9	-2.12	1.33	1.37
5	I	703	FAD	C4X-C4	2.11	1.52	1.44
5	N	703	FAD	C4X-C4	2.11	1.52	1.44
5	M	703	FAD	C4X-C4	2.11	1.52	1.44
3	V	701	TPP	PA-O3A	-2.11	1.57	1.59
3	U	701	TPP	PA-O3A	-2.11	1.57	1.59
7	G	401	ATP	C8-N9	-2.10	1.34	1.37
5	Q	703	FAD	C4X-C4	2.10	1.52	1.44
5	E	703	FAD	P-O3P	-2.10	1.57	1.59
7	C	401	ATP	C8-N9	-2.10	1.34	1.37
5	F	703	FAD	C4X-C10	-2.09	1.38	1.44
5	E	703	FAD	C4X-C4	2.09	1.52	1.44
5	I	703	FAD	C6A-N6A	2.09	1.39	1.34
5	E	703	FAD	C6A-N6A	2.09	1.39	1.34
5	U	703	FAD	C4X-C4	2.09	1.52	1.44
3	F	701	TPP	C5'-C4'	-2.09	1.39	1.42
5	V	703	FAD	C7M-C7	2.09	1.54	1.51
3	U	701	TPP	C5'-C4'	-2.09	1.39	1.42
7	K	401	ATP	C8-N9	-2.08	1.34	1.37
5	A	703	FAD	C4X-C4	2.08	1.52	1.44
5	A	703	FAD	C6A-N6A	2.08	1.39	1.34
3	N	701	TPP	C5'-C4'	-2.08	1.39	1.42
3	I	701	TPP	C5'-C4'	-2.08	1.39	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	701	TPP	PA-O3A	-2.08	1.57	1.59
5	U	703	FAD	C1'-C2'	2.08	1.55	1.52
3	M	701	TPP	C5'-C4'	-2.07	1.39	1.42
5	V	703	FAD	C1'-C2'	2.07	1.55	1.52
5	E	703	FAD	C1'-C2'	2.07	1.55	1.52
5	F	703	FAD	C1'-C2'	2.07	1.55	1.52
5	I	703	FAD	C2B-C3B	-2.06	1.47	1.53
5	E	703	FAD	C2B-C1B	-2.06	1.47	1.53
5	N	703	FAD	C6A-N6A	2.06	1.39	1.34
5	N	703	FAD	P-O3P	-2.06	1.57	1.59
5	Q	703	FAD	C6A-N6A	2.06	1.39	1.34
7	D	401	ATP	C8-N9	-2.06	1.34	1.37
5	M	703	FAD	C6A-N6A	2.05	1.39	1.34
5	U	703	FAD	C6A-N6A	2.05	1.39	1.34
3	V	701	TPP	C5'-C4'	-2.05	1.39	1.42
5	U	703	FAD	P-O3P	-2.05	1.57	1.59
5	B	703	FAD	C6A-N6A	2.05	1.39	1.34
5	V	703	FAD	C2B-C1B	-2.05	1.47	1.53
3	A	701	TPP	PA-O3A	-2.05	1.57	1.59
5	A	703	FAD	C2B-C1B	-2.05	1.47	1.53
5	J	703	FAD	C1'-C2'	2.05	1.55	1.52
5	R	701	FAD	C6A-N6A	2.05	1.39	1.34
7	O	401	ATP	C8-N9	-2.05	1.34	1.37
5	A	703	FAD	C1'-C2'	2.04	1.55	1.52
5	I	703	FAD	C7M-C7	2.04	1.54	1.51
5	V	703	FAD	C6A-N6A	2.04	1.39	1.34
5	B	703	FAD	P-O3P	-2.03	1.57	1.59
5	N	703	FAD	C2B-C1B	-2.03	1.47	1.53
5	M	703	FAD	C2B-C1B	-2.03	1.47	1.53
5	Q	703	FAD	C1'-C2'	2.03	1.55	1.52
3	E	701	TPP	C5'-C4'	-2.03	1.39	1.42
5	B	703	FAD	C1'-C2'	2.02	1.55	1.52
5	J	703	FAD	C6A-N6A	2.02	1.39	1.34
5	N	703	FAD	C1'-C2'	2.02	1.55	1.52
5	M	703	FAD	C7M-C7	2.02	1.54	1.51
5	R	701	FAD	C7M-C7	2.02	1.54	1.51
5	Q	703	FAD	C2B-C1B	-2.02	1.47	1.53
5	F	703	FAD	C4X-C4	2.02	1.52	1.44
5	F	703	FAD	O2B-C2B	2.01	1.47	1.43
5	A	703	FAD	C4X-C10	-2.01	1.38	1.44
6	F	704	60G	OAR-CAV	2.01	1.37	1.33
5	B	703	FAD	C7M-C7	2.01	1.54	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	704	60G	OAR-CAV	2.01	1.37	1.33
3	B	701	TPP	C5'-C4'	-2.01	1.39	1.42
6	E	704	60G	CAU-NAQ	2.00	1.43	1.39
5	B	703	FAD	C2B-C1B	-2.00	1.47	1.53
5	N	703	FAD	C7M-C7	2.00	1.54	1.51
3	A	701	TPP	C5'-C4'	-2.00	1.39	1.42
6	B	704	60G	C6-N1	2.00	1.36	1.33
6	J	704	60G	OAR-CAV	2.00	1.37	1.33

All (605) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	704	60G	OAG-SBB-OAF	-13.79	100.05	119.34
6	A	704	60G	OAG-SBB-OAF	-13.76	100.09	119.34
6	I	704	60G	OAG-SBB-OAF	-13.71	100.17	119.34
6	E	704	60G	OAG-SBB-OAF	-13.70	100.17	119.34
6	Q	704	60G	OAG-SBB-OAF	-13.66	100.23	119.34
6	B	704	60G	OAG-SBB-OAF	-13.66	100.24	119.34
6	N	705	60G	OAG-SBB-OAF	-13.60	100.31	119.34
6	J	704	60G	OAG-SBB-OAF	-13.60	100.32	119.34
6	U	704	60G	OAG-SBB-OAF	-13.59	100.33	119.34
6	N	704	60G	OAG-SBB-OAF	-13.55	100.39	119.34
6	R	702	60G	OAG-SBB-OAF	-13.47	100.50	119.34
6	V	704	60G	OAG-SBB-OAF	-13.30	100.74	119.34
6	F	704	60G	C6-C5-C4	7.51	121.70	115.20
6	E	704	60G	C6-C5-C4	7.30	121.52	115.20
6	U	704	60G	C6-C5-C4	7.29	121.51	115.20
6	V	704	60G	C6-C5-C4	7.28	121.51	115.20
6	I	704	60G	C6-C5-C4	7.27	121.49	115.20
6	J	704	60G	C6-C5-C4	7.27	121.49	115.20
6	R	702	60G	C6-C5-C4	7.26	121.48	115.20
6	A	704	60G	C6-C5-C4	7.24	121.47	115.20
6	N	704	60G	C6-C5-C4	7.20	121.44	115.20
6	N	705	60G	C6-C5-C4	7.20	121.43	115.20
6	B	704	60G	C6-C5-C4	7.19	121.42	115.20
6	Q	704	60G	C6-C5-C4	7.05	121.31	115.20
6	Q	704	60G	C2-N3-C4	5.72	121.54	115.00
5	U	703	FAD	C5A-C4A-N3A	-5.51	119.13	126.72
6	B	704	60G	C2-N3-C4	5.50	121.29	115.00
5	I	703	FAD	C5A-C4A-N3A	-5.46	119.20	126.72
5	J	703	FAD	C5A-C4A-N3A	-5.46	119.20	126.72
5	R	701	FAD	C5A-C4A-N3A	-5.45	119.22	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	703	FAD	C5A-C4A-N3A	-5.44	119.23	126.72
5	Q	703	FAD	C5A-C4A-N3A	-5.44	119.23	126.72
6	A	704	60G	C2-N1-C6	5.44	121.21	115.00
5	N	703	FAD	C5A-C4A-N3A	-5.42	119.25	126.72
5	A	703	FAD	C5A-C4A-N3A	-5.41	119.26	126.72
5	B	703	FAD	C5A-C4A-N3A	-5.41	119.26	126.72
5	V	703	FAD	C5A-C4A-N3A	-5.40	119.28	126.72
6	R	702	60G	C2-N1-C6	5.38	121.16	115.00
6	N	705	60G	C2-N1-C6	5.35	121.12	115.00
5	E	703	FAD	C5A-C4A-N3A	-5.35	119.35	126.72
5	F	703	FAD	C5A-C4A-N3A	-5.34	119.36	126.72
6	V	704	60G	C2-N3-C4	5.34	121.10	115.00
6	J	704	60G	C2-N1-C6	5.33	121.09	115.00
6	N	704	60G	C2-N3-C4	5.32	121.09	115.00
6	F	704	60G	C5-C6-N1	-5.32	117.94	124.16
6	I	704	60G	C2-N3-C4	5.30	121.06	115.00
6	E	704	60G	C2-N1-C6	5.30	121.05	115.00
6	U	704	60G	C2-N1-C6	5.27	121.02	115.00
7	T	401	ATP	C5-C4-N3	-5.27	119.47	126.72
7	C	401	ATP	C5-C4-N3	-5.25	119.49	126.72
7	K	401	ATP	C5-C4-N3	-5.25	119.49	126.72
7	L	401	ATP	C5-C4-N3	-5.23	119.51	126.72
7	P	401	ATP	C5-C4-N3	-5.23	119.51	126.72
7	W	401	ATP	C5-C4-N3	-5.18	119.58	126.72
7	W	402	ATP	C5-C4-N3	-5.18	119.58	126.72
7	D	401	ATP	C5-C4-N3	-5.18	119.59	126.72
7	S	401	ATP	C5-C4-N3	-5.14	119.64	126.72
7	G	401	ATP	C5-C4-N3	-5.14	119.64	126.72
6	F	704	60G	NAQ-CAU-NAP	5.13	123.03	114.87
6	R	702	60G	C5-C4-N3	-5.13	118.16	124.16
7	H	401	ATP	C5-C4-N3	-5.12	119.67	126.72
6	U	704	60G	NAQ-CAU-NAP	5.11	123.00	114.87
6	Q	704	60G	C5-C4-N3	-5.08	118.22	124.16
6	J	704	60G	C5-C4-N3	-5.08	118.22	124.16
6	U	704	60G	C5-C4-N3	-5.08	118.22	124.16
6	E	704	60G	C5-C4-N3	-5.07	118.23	124.16
6	I	704	60G	C5-C6-N1	-5.07	118.24	124.16
7	O	401	ATP	C5-C4-N3	-5.06	119.75	126.72
6	N	704	60G	C5-C6-N1	-5.02	118.29	124.16
6	V	704	60G	C5-C6-N1	-5.01	118.31	124.16
6	N	705	60G	C5-C4-N3	-4.99	118.33	124.16
6	B	704	60G	C5-C6-N1	-4.98	118.34	124.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	704	60G	C5-C4-N3	-4.98	118.34	124.16
6	V	704	60G	NAQ-CAU-NAP	4.97	122.77	114.87
6	E	704	60G	NAQ-CAU-NAP	4.93	122.70	114.87
6	A	704	60G	C5-C6-N1	-4.92	118.42	124.16
6	F	704	60G	C2-N3-C4	4.89	120.59	115.00
6	E	704	60G	C5-C6-N1	-4.88	118.45	124.16
6	B	704	60G	C5-C4-N3	-4.88	118.45	124.16
6	V	704	60G	C5-C4-N3	-4.88	118.46	124.16
6	Q	704	60G	NAQ-CAU-NAP	4.86	122.59	114.87
6	U	704	60G	C5-C6-N1	-4.86	118.48	124.16
6	J	704	60G	C5-C6-N1	-4.85	118.49	124.16
6	R	702	60G	C5-C6-N1	-4.85	118.49	124.16
6	N	705	60G	NAQ-CAU-NAP	4.85	122.58	114.87
6	J	704	60G	NAQ-CAU-NAP	4.83	122.55	114.87
6	I	704	60G	C5-C4-N3	-4.83	118.51	124.16
6	N	705	60G	C5-C6-N1	-4.83	118.52	124.16
6	A	704	60G	NAQ-CAU-NAP	4.83	122.55	114.87
6	N	704	60G	C5-C4-N3	-4.83	118.52	124.16
6	Q	704	60G	C5-C6-N1	-4.82	118.53	124.16
6	J	704	60G	OAR-CAV-CBA	4.77	120.23	112.31
6	B	704	60G	NAQ-CAU-NAP	4.75	122.42	114.87
6	N	705	60G	OAR-CAV-CBA	4.73	120.17	112.31
6	R	702	60G	NAQ-CAU-NAP	4.71	122.36	114.87
6	I	704	60G	NAQ-CAU-NAP	4.71	122.36	114.87
6	N	704	60G	NAQ-CAU-NAP	4.70	122.35	114.87
6	E	704	60G	OAR-CAV-CBA	4.70	120.11	112.31
6	F	704	60G	C5-C4-N3	-4.62	118.76	124.16
6	N	704	60G	OAR-CAV-CBA	4.61	119.97	112.31
6	Q	704	60G	OAR-CAV-CBA	4.57	119.89	112.31
6	F	704	60G	OAR-CAV-CBA	4.56	119.89	112.31
6	A	704	60G	OAR-CAV-CBA	4.54	119.85	112.31
6	V	704	60G	OAR-CAV-CBA	4.48	119.74	112.31
6	B	704	60G	OAR-CAV-CBA	4.47	119.73	112.31
6	F	704	60G	C2-NAP-CAU	-4.45	125.76	130.34
6	E	704	60G	C2-NAP-CAU	-4.41	125.80	130.34
6	I	704	60G	C2-NAP-CAU	-4.41	125.80	130.34
7	L	401	ATP	N3-C2-N1	-4.40	121.93	128.58
7	O	401	ATP	N3-C2-N1	-4.33	122.03	128.58
7	H	401	ATP	N3-C2-N1	-4.31	122.06	128.58
6	N	704	60G	C2-NAP-CAU	-4.31	125.91	130.34
7	P	401	ATP	N3-C2-N1	-4.30	122.07	128.58
7	T	401	ATP	N3-C2-N1	-4.29	122.09	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	401	ATP	N3-C2-N1	-4.28	122.11	128.58
7	C	401	ATP	N3-C2-N1	-4.27	122.11	128.58
7	G	401	ATP	N3-C2-N1	-4.27	122.12	128.58
7	W	401	ATP	N3-C2-N1	-4.26	122.13	128.58
7	K	401	ATP	N3-C2-N1	-4.26	122.13	128.58
7	S	401	ATP	N3-C2-N1	-4.26	122.14	128.58
5	R	701	FAD	N3A-C4A-N9A	4.25	134.40	127.17
7	W	402	ATP	N3-C2-N1	-4.25	122.15	128.58
5	U	703	FAD	N3A-C4A-N9A	4.24	134.38	127.17
6	R	702	60G	C2-NAP-CAU	-4.24	125.98	130.34
5	Q	703	FAD	N3A-C4A-N9A	4.23	134.37	127.17
6	I	704	60G	OAR-CAV-CBA	4.23	119.33	112.31
5	I	703	FAD	N3A-C4A-N9A	4.20	134.31	127.17
5	N	703	FAD	N3A-C4A-N9A	4.20	134.31	127.17
5	B	703	FAD	N3A-C4A-N9A	4.19	134.28	127.17
5	A	703	FAD	N3A-C4A-N9A	4.18	134.28	127.17
6	U	704	60G	OAR-CAV-CBA	4.16	119.22	112.31
6	U	704	60G	C2-NAP-CAU	-4.15	126.07	130.34
5	F	703	FAD	N3A-C4A-N9A	4.13	134.20	127.17
5	M	703	FAD	N3A-C4A-N9A	4.13	134.19	127.17
5	V	703	FAD	N3A-C4A-N9A	4.13	134.19	127.17
5	E	703	FAD	N3A-C4A-N9A	4.11	134.16	127.17
6	R	702	60G	C2-N3-C4	4.06	119.63	115.00
5	U	703	FAD	N3A-C2A-N1A	-4.05	122.45	128.58
5	V	703	FAD	N3A-C2A-N1A	-4.04	122.47	128.58
6	J	704	60G	C2-NAP-CAU	-4.03	126.19	130.34
6	F	704	60G	C2-N1-C6	4.03	119.60	115.00
5	N	703	FAD	N3A-C2A-N1A	-4.00	122.53	128.58
5	B	703	FAD	N3A-C2A-N1A	-3.99	122.54	128.58
5	I	703	FAD	N3A-C2A-N1A	-3.98	122.56	128.58
6	J	704	60G	C2-N3-C4	3.97	119.54	115.00
5	R	701	FAD	N3A-C2A-N1A	-3.97	122.57	128.58
5	J	703	FAD	N3A-C4A-N9A	3.97	133.91	127.17
5	E	703	FAD	N3A-C2A-N1A	-3.96	122.59	128.58
6	R	702	60G	OAR-CAV-CBA	3.95	118.87	112.31
5	M	703	FAD	N3A-C2A-N1A	-3.95	122.61	128.58
5	Q	703	FAD	N3A-C2A-N1A	-3.93	122.63	128.58
5	A	703	FAD	N3A-C2A-N1A	-3.92	122.65	128.58
6	N	705	60G	C2-NAP-CAU	-3.87	126.36	130.34
6	V	704	60G	C2-NAP-CAU	-3.86	126.37	130.34
5	J	703	FAD	N3A-C2A-N1A	-3.85	122.75	128.58
6	B	704	60G	C2-NAP-CAU	-3.84	126.39	130.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	704	60G	C2-N1-C6	3.84	119.38	115.00
6	U	704	60G	C2-N3-C4	3.84	119.38	115.00
6	E	704	60G	C2-N3-C4	3.83	119.37	115.00
5	M	703	FAD	C4A-C5A-N7A	-3.82	106.22	110.58
6	N	704	60G	C2-N1-C6	3.81	119.35	115.00
7	L	401	ATP	N3-C4-N9	3.79	133.62	127.17
6	Q	704	60G	C2-N1-C6	3.79	119.33	115.00
7	D	401	ATP	N3-C4-N9	3.79	133.62	127.17
6	B	704	60G	C2-N1-C6	3.79	119.33	115.00
6	N	705	60G	C2-N3-C4	3.78	119.32	115.00
6	V	704	60G	C2-N1-C6	3.76	119.30	115.00
5	B	703	FAD	C4A-C5A-N7A	-3.75	106.29	110.58
7	P	401	ATP	N3-C4-N9	3.75	133.55	127.17
6	A	704	60G	C2-N3-C4	3.75	119.28	115.00
6	A	704	60G	C2-NAP-CAU	-3.74	126.49	130.34
7	W	402	ATP	N3-C4-N9	3.74	133.53	127.17
5	J	703	FAD	C2A-N3A-C4A	3.74	120.97	111.83
5	U	703	FAD	C2A-N3A-C4A	3.74	120.96	111.83
5	U	703	FAD	C4A-C5A-N7A	-3.74	106.31	110.58
5	R	701	FAD	C4A-C5A-N7A	-3.74	106.31	110.58
5	V	703	FAD	C4A-C5A-N7A	-3.73	106.31	110.58
7	K	401	ATP	N3-C4-N9	3.73	133.51	127.17
5	E	703	FAD	C4A-C5A-N7A	-3.73	106.32	110.58
7	C	401	ATP	N3-C4-N9	3.72	133.50	127.17
5	N	703	FAD	C4A-C5A-N7A	-3.72	106.33	110.58
7	T	401	ATP	N3-C4-N9	3.72	133.49	127.17
5	R	701	FAD	C2A-N3A-C4A	3.71	120.89	111.83
5	V	703	FAD	C2A-N3A-C4A	3.70	120.86	111.83
5	I	703	FAD	C2A-N3A-C4A	3.70	120.86	111.83
5	N	703	FAD	C2A-N3A-C4A	3.70	120.86	111.83
3	M	701	TPP	N1'-C2'-N3'	-3.70	119.38	125.53
5	B	703	FAD	C2A-N3A-C4A	3.69	120.85	111.83
5	M	703	FAD	C2A-N3A-C4A	3.69	120.84	111.83
5	Q	703	FAD	C4A-C5A-N7A	-3.69	106.36	110.58
5	A	703	FAD	C4A-C5A-N7A	-3.69	106.37	110.58
5	E	703	FAD	C2A-N3A-C4A	3.69	120.83	111.83
7	S	401	ATP	N3-C4-N9	3.68	133.43	127.17
7	W	401	ATP	N3-C4-N9	3.67	133.41	127.17
5	Q	703	FAD	C2A-N3A-C4A	3.67	120.79	111.83
5	F	703	FAD	N3A-C2A-N1A	-3.66	123.04	128.58
7	G	401	ATP	N3-C4-N9	3.66	133.40	127.17
5	I	703	FAD	C4A-C5A-N7A	-3.66	106.39	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	703	FAD	C2A-N3A-C4A	3.66	120.77	111.83
3	B	701	TPP	N1'-C2'-N3'	-3.64	119.48	125.53
7	H	401	ATP	N3-C4-N9	3.63	133.33	127.17
3	J	701	TPP	N1'-C2'-N3'	-3.62	119.50	125.53
7	L	401	ATP	C2-N3-C4	3.62	120.67	111.83
3	V	701	TPP	N1'-C2'-N3'	-3.61	119.53	125.53
7	O	401	ATP	N3-C4-N9	3.60	133.30	127.17
3	A	701	TPP	N1'-C2'-N3'	-3.59	119.56	125.53
3	E	701	TPP	N1'-C2'-N3'	-3.57	119.58	125.53
7	P	401	ATP	C2-N3-C4	3.57	120.55	111.83
7	T	401	ATP	C2-N3-C4	3.57	120.55	111.83
7	C	401	ATP	C2-N3-C4	3.57	120.54	111.83
3	I	701	TPP	N1'-C2'-N3'	-3.57	119.60	125.53
3	Q	701	TPP	N1'-C2'-N3'	-3.56	119.60	125.53
3	U	701	TPP	N1'-C2'-N3'	-3.56	119.61	125.53
3	N	701	TPP	N1'-C2'-N3'	-3.56	119.61	125.53
5	F	703	FAD	C2A-N3A-C4A	3.55	120.51	111.83
5	B	703	FAD	C5A-N7A-C8A	3.54	109.02	103.45
7	K	401	ATP	C2-N3-C4	3.53	120.45	111.83
7	D	401	ATP	C2-N3-C4	3.52	120.44	111.83
7	W	401	ATP	C2-N3-C4	3.52	120.44	111.83
5	M	703	FAD	C5A-N7A-C8A	3.52	108.98	103.45
7	G	401	ATP	C2-N3-C4	3.52	120.43	111.83
5	R	701	FAD	C5A-N7A-C8A	3.52	108.98	103.45
7	H	401	ATP	C2-N3-C4	3.52	120.42	111.83
7	O	401	ATP	C2-N3-C4	3.51	120.40	111.83
5	Q	703	FAD	C5A-N7A-C8A	3.50	108.96	103.45
6	Q	704	60G	C2-NAP-CAU	-3.50	126.74	130.34
7	W	402	ATP	C2-N3-C4	3.50	120.38	111.83
7	S	401	ATP	C2-N3-C4	3.50	120.37	111.83
5	E	703	FAD	C5A-N7A-C8A	3.49	108.94	103.45
5	N	703	FAD	C5A-N7A-C8A	3.48	108.92	103.45
5	A	703	FAD	C5A-N7A-C8A	3.47	108.90	103.45
5	V	703	FAD	C5A-N7A-C8A	3.44	108.86	103.45
5	U	703	FAD	C5A-N7A-C8A	3.43	108.84	103.45
6	N	704	60G	OAG-SBB-CAM	3.42	113.58	108.33
5	I	703	FAD	C5A-N7A-C8A	3.42	108.83	103.45
6	B	704	60G	OAG-SBB-CAM	3.41	113.57	108.33
5	J	703	FAD	C4-N3-C2	-3.40	119.61	125.64
3	F	701	TPP	N1'-C2'-N3'	-3.39	119.89	125.53
5	J	703	FAD	O4B-C1B-N9A	3.38	114.57	108.09
5	F	703	FAD	C4-N3-C2	-3.35	119.68	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	703	FAD	C4'-C3'-C2'	-3.33	108.03	113.57
5	E	703	FAD	N9A-C8A-N7A	-3.32	109.22	113.94
6	V	704	60G	OAG-SBB-CAM	3.32	113.43	108.33
5	B	703	FAD	N9A-C8A-N7A	-3.32	109.23	113.94
6	Q	704	60G	OAG-SBB-CAM	3.31	113.42	108.33
6	J	704	60G	OAG-SBB-CAM	3.31	113.42	108.33
5	R	701	FAD	C4-N3-C2	-3.31	119.76	125.64
6	F	704	60G	OAG-SBB-CAM	3.31	113.41	108.33
5	M	703	FAD	N9A-C8A-N7A	-3.30	109.25	113.94
5	J	703	FAD	C4'-C3'-C2'	-3.29	108.09	113.57
5	B	703	FAD	C4-N3-C2	-3.29	119.80	125.64
6	N	705	60G	OAG-SBB-CAM	3.29	113.38	108.33
5	I	703	FAD	C4-N3-C2	-3.28	119.81	125.64
6	A	704	60G	OAG-SBB-CAM	3.28	117.81	123.64
6	F	704	60G	OAG-SBB-CAM	3.28	117.81	123.64
5	Q	703	FAD	N9A-C8A-N7A	-3.27	109.29	113.94
6	A	704	60G	OAG-SBB-CAM	3.27	113.35	108.33
6	U	704	60G	OAG-SBB-CAM	3.26	117.84	123.64
5	U	703	FAD	C4-N3-C2	-3.26	119.85	125.64
5	V	703	FAD	C4-N3-C2	-3.26	119.86	125.64
5	V	703	FAD	N9A-C8A-N7A	-3.25	109.33	113.94
5	Q	703	FAD	C4-N3-C2	-3.25	119.87	125.64
5	M	703	FAD	C4-N3-C2	-3.24	119.89	125.64
6	E	704	60G	OAG-SBB-CAM	3.23	113.29	108.33
5	R	701	FAD	N9A-C8A-N7A	-3.23	109.36	113.94
5	I	703	FAD	N9A-C8A-N7A	-3.23	109.36	113.94
5	N	703	FAD	N9A-C8A-N7A	-3.23	109.36	113.94
6	I	704	60G	OAG-SBB-CAM	3.22	113.28	108.33
5	A	703	FAD	C4-N3-C2	-3.22	119.92	125.64
5	A	703	FAD	N9A-C8A-N7A	-3.22	109.37	113.94
6	I	704	60G	OAG-SBB-CAM	3.21	117.93	123.64
5	U	703	FAD	N9A-C8A-N7A	-3.21	109.38	113.94
6	U	704	60G	OAG-SBB-CAM	3.21	113.26	108.33
5	E	703	FAD	C4-N3-C2	-3.20	119.95	125.64
6	E	704	60G	OAG-SBB-CAM	3.20	117.95	123.64
6	N	705	60G	OAG-SBB-CAM	3.20	117.96	123.64
6	V	704	60G	OAG-SBB-CAM	3.19	117.97	123.64
6	N	704	60G	OAG-SBB-CAM	3.19	117.97	123.64
5	F	703	FAD	C5A-N7A-C8A	3.18	108.45	103.45
5	F	703	FAD	C4A-C5A-N7A	-3.18	106.95	110.58
5	J	703	FAD	C4A-C5A-N7A	-3.17	106.95	110.58
7	W	401	ATP	C4-C5-N7	-3.17	106.95	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	703	FAD	C4-N3-C2	-3.17	120.02	125.64
7	H	401	ATP	C4-C5-N7	-3.17	106.96	110.58
6	Q	704	60G	N1-C2-N3	-3.16	121.07	126.26
6	R	702	60G	N1-C2-N3	-3.16	121.07	126.26
7	C	401	ATP	C4-C5-N7	-3.16	106.97	110.58
5	F	703	FAD	C4X-C4-N3	3.14	121.25	113.25
7	D	401	ATP	N9-C8-N7	-3.14	109.48	113.94
5	E	703	FAD	C4A-N9A-C8A	3.14	109.03	105.74
7	T	401	ATP	C4-C5-N7	-3.13	107.00	110.58
7	H	401	ATP	N9-C8-N7	-3.12	109.50	113.94
7	G	401	ATP	C4-C5-N7	-3.12	107.02	110.58
6	B	704	60G	OAD-CAU-NAP	-3.12	118.10	123.64
6	B	704	60G	N1-C2-N3	-3.11	121.15	126.26
5	B	703	FAD	C4A-N9A-C8A	3.11	109.01	105.74
7	O	401	ATP	N9-C8-N7	-3.11	109.52	113.94
6	J	704	60G	N1-C2-N3	-3.11	121.17	126.26
7	K	401	ATP	C4-C5-N7	-3.10	107.03	110.58
7	G	401	ATP	N9-C8-N7	-3.10	109.54	113.94
7	L	401	ATP	N9-C8-N7	-3.10	109.54	113.94
5	Q	703	FAD	C4A-N9A-C8A	3.09	108.98	105.74
7	T	401	ATP	N9-C8-N7	-3.09	109.56	113.94
6	Q	704	60G	OAD-CAU-NAP	-3.08	118.16	123.64
5	V	703	FAD	C4A-N9A-C8A	3.08	108.98	105.74
5	U	703	FAD	C4A-N9A-C8A	3.08	108.97	105.74
5	R	701	FAD	C4A-N9A-C8A	3.08	108.97	105.74
7	C	401	ATP	N9-C8-N7	-3.08	109.57	113.94
5	M	703	FAD	C4A-N9A-C8A	3.07	108.96	105.74
7	S	401	ATP	C4-C5-N7	-3.07	107.07	110.58
7	W	402	ATP	N9-C8-N7	-3.07	109.58	113.94
5	N	703	FAD	C4A-N9A-C8A	3.06	108.95	105.74
6	R	702	60G	OAG-SBB-CAM	3.06	113.03	108.33
7	O	401	ATP	C4-C5-N7	-3.06	107.09	110.58
5	I	703	FAD	C4A-N9A-C8A	3.04	108.93	105.74
6	A	704	60G	N1-C2-N3	-3.04	121.27	126.26
6	R	702	60G	OAD-CAU-NAP	-3.04	118.24	123.64
7	D	401	ATP	C4-C5-N7	-3.03	107.11	110.58
5	J	703	FAD	C4X-C4-N3	3.03	120.98	113.25
7	P	401	ATP	C4-C5-N7	-3.03	107.11	110.58
6	N	705	60G	N1-C2-N3	-3.03	121.29	126.26
3	J	701	TPP	CM2-C2'-N1'	3.03	120.43	117.20
3	M	701	TPP	C6'-N1'-C2'	3.03	121.05	116.07
7	W	402	ATP	C4-C5-N7	-3.03	107.12	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	401	ATP	C4-C5-N7	-3.02	107.13	110.58
6	I	704	60G	N1-C2-N3	-3.01	121.32	126.26
6	N	704	60G	N1-C2-N3	-3.01	121.32	126.26
3	J	701	TPP	C6'-N1'-C2'	3.01	121.02	116.07
7	W	401	ATP	N9-C8-N7	-3.01	109.67	113.94
6	V	704	60G	N1-C2-N3	-3.01	121.33	126.26
7	H	401	ATP	C5-N7-C8	3.01	108.17	103.45
5	A	703	FAD	C4A-N9A-C8A	3.01	108.89	105.74
7	D	401	ATP	C5-N7-C8	2.99	108.15	103.45
3	F	701	TPP	C6'-C5'-C4'	2.99	119.22	115.55
6	E	704	60G	N1-C2-N3	-2.98	121.37	126.26
6	U	704	60G	N1-C2-N3	-2.98	121.38	126.26
6	J	704	60G	OAD-CAU-NAP	-2.98	118.35	123.64
7	W	401	ATP	C5-N7-C8	2.97	108.12	103.45
3	M	701	TPP	CM2-C2'-N1'	2.97	120.36	117.20
3	B	701	TPP	C6'-N1'-C2'	2.97	120.95	116.07
7	K	401	ATP	N9-C8-N7	-2.97	109.72	113.94
7	T	401	ATP	C5-N7-C8	2.97	108.12	103.45
7	G	401	ATP	C5-N7-C8	2.97	108.11	103.45
6	F	704	60G	N1-C2-N3	-2.96	121.41	126.26
7	C	401	ATP	C5-N7-C8	2.96	108.10	103.45
7	S	401	ATP	N9-C8-N7	-2.96	109.74	113.94
7	W	402	ATP	C5-N7-C8	2.94	108.08	103.45
5	R	701	FAD	C4X-C4-N3	2.94	120.74	113.25
3	A	701	TPP	C6'-N1'-C2'	2.93	120.89	116.07
7	P	401	ATP	N9-C8-N7	-2.93	109.78	113.94
7	L	401	ATP	C5-N7-C8	2.92	108.04	103.45
7	O	401	ATP	C5-N7-C8	2.91	108.03	103.45
5	B	703	FAD	C4X-C4-N3	2.91	120.65	113.25
7	K	401	ATP	C5-N7-C8	2.91	108.02	103.45
5	A	703	FAD	C4X-C4-N3	2.89	120.62	113.25
5	U	703	FAD	C4X-C4-N3	2.89	120.61	113.25
3	N	701	TPP	C6'-N1'-C2'	2.89	120.82	116.07
5	I	703	FAD	C4X-C4-N3	2.89	120.60	113.25
3	I	701	TPP	CM2-C2'-N1'	2.89	120.27	117.20
5	J	703	FAD	C5A-N7A-C8A	2.89	107.99	103.45
7	S	401	ATP	C5-N7-C8	2.88	107.98	103.45
5	V	703	FAD	C4X-C4-N3	2.88	120.59	113.25
5	F	703	FAD	N9A-C8A-N7A	-2.88	109.85	113.94
3	V	701	TPP	CM2-C2'-N1'	2.87	120.26	117.20
5	E	703	FAD	C4X-C4-N3	2.87	120.56	113.25
5	Q	703	FAD	C4X-C4-N3	2.87	120.56	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	703	FAD	C4X-C4-N3	2.87	120.55	113.25
3	E	701	TPP	C6'-N1'-C2'	2.87	120.78	116.07
3	V	701	TPP	C6'-N1'-C2'	2.86	120.77	116.07
3	U	701	TPP	C6'-N1'-C2'	2.86	120.77	116.07
3	I	701	TPP	C6'-N1'-C2'	2.85	120.76	116.07
3	E	701	TPP	CM2-C2'-N1'	2.85	120.23	117.20
7	P	401	ATP	C5-N7-C8	2.84	107.92	103.45
3	Q	701	TPP	C6'-N1'-C2'	2.84	120.74	116.07
3	F	701	TPP	C6'-N1'-C2'	2.84	120.74	116.07
3	U	701	TPP	CM2-C2'-N1'	2.84	120.22	117.20
5	F	703	FAD	O4-C4-C4X	-2.84	119.05	126.53
5	N	703	FAD	C4X-C4-N3	2.83	120.46	113.25
7	T	401	ATP	C4'-O4'-C1'	-2.82	103.25	109.47
3	B	701	TPP	CM2-C2'-N1'	2.81	120.19	117.20
3	J	701	TPP	C6'-C5'-C4'	2.80	118.99	115.55
3	F	701	TPP	CM2-C2'-N1'	2.79	120.17	117.20
7	D	401	ATP	C3'-C2'-C1'	2.78	106.72	101.46
3	N	701	TPP	CM2-C2'-N1'	2.76	120.14	117.20
3	A	701	TPP	CM2-C2'-N1'	2.72	120.09	117.20
3	Q	701	TPP	CM2-C2'-N1'	2.72	120.09	117.20
3	Q	701	TPP	C6'-C5'-C4'	2.70	118.87	115.55
3	N	701	TPP	C6'-C5'-C4'	2.69	118.85	115.55
7	P	401	ATP	C4'-O4'-C1'	-2.68	103.54	109.47
5	J	703	FAD	C4X-C10-N1	-2.68	118.03	124.59
7	O	401	ATP	C4'-O4'-C1'	-2.68	103.56	109.47
7	W	402	ATP	C4'-O4'-C1'	-2.66	103.60	109.47
3	I	701	TPP	C6'-C5'-C4'	2.64	118.79	115.55
5	N	703	FAD	C9A-C5X-N5	-2.63	119.67	122.45
5	N	703	FAD	C4-C4X-N5	2.62	121.83	118.21
5	E	703	FAD	C4-C4X-N5	2.62	121.82	118.21
5	V	703	FAD	C4-C4X-N5	2.61	121.82	118.21
5	J	703	FAD	N9A-C8A-N7A	-2.61	110.23	113.94
5	U	703	FAD	C4-C4X-N5	2.60	121.80	118.21
5	R	701	FAD	O4-C4-C4X	-2.60	119.67	126.53
5	U	703	FAD	C9A-C5X-N5	-2.60	119.70	122.45
5	B	703	FAD	C4-C4X-N5	2.59	121.79	118.21
7	G	401	ATP	C4'-O4'-C1'	-2.59	103.74	109.47
7	D	401	ATP	C4-N9-C8	2.59	108.46	105.74
7	D	401	ATP	C2'-C3'-C4'	2.59	107.61	102.61
5	A	703	FAD	O4-C4-C4X	-2.59	119.70	126.53
3	B	701	TPP	C6'-C5'-C4'	2.59	118.73	115.55
5	N	703	FAD	C10-C4X-N5	-2.58	119.54	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	703	FAD	C10-C4X-N5	-2.57	119.56	124.81
5	U	703	FAD	O4-C4-C4X	-2.57	119.75	126.53
5	J	703	FAD	C9A-C5X-N5	-2.57	119.73	122.45
3	U	701	TPP	C6'-C5'-C4'	2.57	118.70	115.55
5	F	703	FAD	O4B-C1B-N9A	2.56	113.00	108.09
7	L	401	ATP	C4-N9-C8	2.56	108.42	105.74
7	D	401	ATP	C4'-O4'-C1'	-2.55	103.83	109.47
5	U	703	FAD	C10-C4X-N5	-2.55	119.59	124.81
5	V	703	FAD	O4-C4-C4X	-2.55	119.79	126.53
5	E	703	FAD	C10-C4X-N5	-2.55	119.60	124.81
3	A	701	TPP	C6'-C5'-C4'	2.55	118.68	115.55
5	E	703	FAD	O4-C4-C4X	-2.55	119.80	126.53
7	O	401	ATP	C4-N9-C8	2.55	108.41	105.74
5	M	703	FAD	O4-C4-C4X	-2.54	119.82	126.53
5	R	701	FAD	C4-C4X-N5	2.54	121.72	118.21
5	A	703	FAD	C4-C4X-N5	2.54	121.72	118.21
5	I	703	FAD	O4-C4-C4X	-2.54	119.83	126.53
5	N	703	FAD	O4-C4-C4X	-2.54	119.83	126.53
3	E	701	TPP	C6'-C5'-C4'	2.54	118.67	115.55
5	B	703	FAD	O4-C4-C4X	-2.53	119.85	126.53
5	Q	703	FAD	O4-C4-C4X	-2.53	119.85	126.53
3	U	701	TPP	CM4-C4-C5	-2.53	121.26	127.75
5	V	703	FAD	C9A-C5X-N5	-2.53	119.77	122.45
5	E	703	FAD	C9A-C5X-N5	-2.53	119.77	122.45
5	J	703	FAD	O4-C4-C4X	-2.53	119.86	126.53
5	F	703	FAD	C4-C4X-N5	2.52	121.69	118.21
7	G	401	ATP	C4-N9-C8	2.51	108.38	105.74
3	V	701	TPP	C6'-C5'-C4'	2.51	118.63	115.55
5	B	703	FAD	C10-C4X-N5	-2.51	119.69	124.81
7	H	401	ATP	C4-N9-C8	2.50	108.36	105.74
5	F	703	FAD	C4X-C10-N1	-2.50	118.46	124.59
3	M	701	TPP	C6'-C5'-C4'	2.49	118.61	115.55
3	A	701	TPP	CM4-C4-C5	-2.49	121.36	127.75
5	J	703	FAD	C4-C4X-N5	2.49	121.65	118.21
5	J	703	FAD	C10-C4X-N5	-2.49	119.73	124.81
3	Q	701	TPP	CM4-C4-C5	-2.49	121.38	127.75
7	C	401	ATP	C4-N9-C8	2.48	108.35	105.74
7	L	401	ATP	C4'-O4'-C1'	-2.48	104.00	109.47
5	Q	703	FAD	C10-C4X-N5	-2.48	119.75	124.81
7	W	402	ATP	C4-N9-C8	2.48	108.34	105.74
5	R	701	FAD	C10-C4X-N5	-2.46	119.79	124.81
5	Q	703	FAD	C4-C4X-N5	2.46	121.60	118.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	703	FAD	C10-C4X-N5	-2.46	119.80	124.81
5	F	703	FAD	C4A-N9A-C8A	2.44	108.31	105.74
3	J	701	TPP	C5'-C6'-N1'	-2.44	119.86	123.83
3	F	701	TPP	C5'-C6'-N1'	-2.43	119.87	123.83
5	M	703	FAD	C4X-C10-N1	-2.43	118.63	124.59
7	T	401	ATP	C4-N9-C8	2.43	108.29	105.74
5	R	701	FAD	C4X-C10-N1	-2.43	118.63	124.59
3	E	701	TPP	CM4-C4-C5	-2.43	121.52	127.75
5	V	703	FAD	C4X-C10-N1	-2.43	118.64	124.59
5	Q	703	FAD	C4X-C10-N1	-2.42	118.65	124.59
7	G	401	ATP	C3'-C2'-C1'	2.42	106.04	101.46
5	F	703	FAD	C10-N1-C2	2.42	122.08	116.85
5	I	703	FAD	C4X-C10-N1	-2.42	118.67	124.59
5	U	703	FAD	C4X-C10-N1	-2.42	118.67	124.59
7	S	401	ATP	C4-N9-C8	2.41	108.27	105.74
7	K	401	ATP	C4'-O4'-C1'	-2.41	104.14	109.47
5	J	703	FAD	C10-N1-C2	2.40	122.04	116.85
7	P	401	ATP	C4-N9-C8	2.39	108.25	105.74
5	B	703	FAD	C9A-C5X-N5	-2.39	119.91	122.45
7	W	401	ATP	C4-N9-C8	2.39	108.25	105.74
6	R	702	60G	OAR-CAV-OAE	-2.39	118.81	123.46
5	M	703	FAD	C10-C4X-N5	-2.38	119.94	124.81
5	E	703	FAD	C4X-C10-N1	-2.38	118.75	124.59
5	B	703	FAD	C4X-C10-N1	-2.38	118.75	124.59
5	I	703	FAD	C10-C4X-N5	-2.38	119.94	124.81
3	J	701	TPP	CM4-C4-C5	-2.38	121.65	127.75
7	K	401	ATP	C4-N9-C8	2.38	108.23	105.74
3	M	701	TPP	CM4-C4-C5	-2.37	121.67	127.75
5	N	703	FAD	C4X-C10-N1	-2.37	118.79	124.59
5	A	703	FAD	C4X-C10-N1	-2.36	118.81	124.59
7	C	401	ATP	C4'-O4'-C1'	-2.35	104.27	109.47
3	B	701	TPP	CM4-C4-C5	-2.35	121.73	127.75
5	E	703	FAD	C5'-C4'-C3'	-2.35	107.79	112.22
5	F	703	FAD	C10-C4X-N5	-2.34	120.02	124.81
5	F	703	FAD	C9A-C5X-N5	-2.34	119.97	122.45
5	I	703	FAD	C4-C4X-N5	2.34	121.44	118.21
3	I	701	TPP	CM4-C4-C5	-2.33	121.77	127.75
5	R	701	FAD	C4X-C10-N10	2.33	119.82	116.48
3	N	701	TPP	CM4-C4-C5	-2.33	121.77	127.75
5	M	703	FAD	C4X-C10-N10	2.33	119.81	116.48
3	F	701	TPP	CM4-C4-C5	-2.33	121.78	127.75
7	T	401	ATP	C3'-C2'-C1'	2.32	105.86	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	703	FAD	C4-C4X-N5	2.32	121.41	118.21
3	B	701	TPP	C7'-N3-C2	-2.32	118.65	123.48
5	V	703	FAD	C4'-C3'-C2'	-2.32	109.72	113.57
5	R	701	FAD	C9A-C5X-N5	-2.31	120.00	122.45
3	Q	701	TPP	C7'-N3-C2	-2.31	118.67	123.48
7	W	401	ATP	C4'-O4'-C1'	-2.31	104.37	109.47
3	V	701	TPP	C7'-N3-C2	-2.31	118.67	123.48
5	I	703	FAD	C4X-C10-N10	2.30	119.78	116.48
3	I	701	TPP	C7'-N3-C2	-2.30	118.68	123.48
3	F	701	TPP	C7'-N3-C2	-2.30	118.69	123.48
7	H	401	ATP	C4'-O4'-C1'	-2.30	104.39	109.47
5	R	701	FAD	C10-N1-C2	2.30	121.82	116.85
5	J	703	FAD	C4X-C10-N10	2.29	119.76	116.48
3	B	701	TPP	O3B-PB-O3A	2.28	112.30	104.64
5	A	703	FAD	C5'-C4'-C3'	-2.28	107.91	112.22
5	B	703	FAD	C5'-C4'-C3'	-2.28	107.91	112.22
5	Q	703	FAD	C9A-C5X-N5	-2.28	120.04	122.45
5	U	703	FAD	C4'-C3'-C2'	-2.27	109.79	113.57
3	B	701	TPP	C5'-C6'-N1'	-2.27	120.14	123.83
3	A	701	TPP	C7'-N3-C2	-2.27	118.75	123.48
3	N	701	TPP	C5'-C6'-N1'	-2.26	120.15	123.83
3	M	701	TPP	C5'-C6'-N1'	-2.26	120.16	123.83
3	N	701	TPP	C7'-N3-C2	-2.25	118.78	123.48
5	A	703	FAD	C4X-C10-N10	2.25	119.70	116.48
3	E	701	TPP	PA-O7-C7	-2.25	110.55	121.26
3	V	701	TPP	CM4-C4-C5	-2.25	122.00	127.75
3	B	701	TPP	PA-O7-C7	-2.24	110.61	121.26
3	A	701	TPP	O3B-PB-O3A	2.23	112.12	104.64
3	Q	701	TPP	PA-O7-C7	-2.22	110.67	121.26
3	Q	701	TPP	C5'-C6'-N1'	-2.22	120.22	123.83
3	I	701	TPP	C5'-C6'-N1'	-2.22	120.22	123.83
5	M	703	FAD	C5'-C4'-C3'	-2.22	108.03	112.22
5	I	703	FAD	C9A-C5X-N5	-2.21	120.11	122.45
3	A	701	TPP	C5'-C6'-N1'	-2.21	120.24	123.83
5	R	701	FAD	C4'-C3'-C2'	-2.21	109.89	113.57
5	A	703	FAD	C9A-C5X-N5	-2.21	120.11	122.45
3	I	701	TPP	PA-O7-C7	-2.21	110.75	121.26
3	E	701	TPP	C7'-N3-C2	-2.21	118.88	123.48
3	U	701	TPP	C5'-C6'-N1'	-2.20	120.25	123.83
5	Q	703	FAD	C4X-C10-N10	2.20	119.63	116.48
5	J	703	FAD	O4B-C1B-C2B	-2.20	101.91	106.62
3	M	701	TPP	C7'-N3-C2	-2.20	118.90	123.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	703	FAD	C9A-C5X-N5	-2.19	120.13	122.45
3	A	701	TPP	PA-O7-C7	-2.19	110.85	121.26
5	I	703	FAD	C10-N1-C2	2.19	121.58	116.85
5	V	703	FAD	C10-N1-C2	2.18	121.58	116.85
5	U	703	FAD	C10-N1-C2	2.18	121.57	116.85
5	E	703	FAD	C6A-C5A-N7A	2.17	136.28	132.09
3	N	701	TPP	C5'-C7'-N3	-2.17	108.28	112.97
3	J	701	TPP	C7'-N3-C2	-2.17	118.95	123.48
7	K	401	ATP	C3'-C2'-C1'	2.17	105.57	101.46
5	M	703	FAD	C10-N1-C2	2.17	121.55	116.85
5	E	703	FAD	C10-N1-C2	2.17	121.55	116.85
3	E	701	TPP	C5'-C6'-N1'	-2.17	120.30	123.83
5	B	703	FAD	C4X-C10-N10	2.17	119.59	116.48
5	Q	703	FAD	C10-N1-C2	2.17	121.54	116.85
6	U	704	60G	OAR-CAV-OAE	-2.17	119.24	123.46
5	J	703	FAD	C5X-C9A-N10	2.17	119.93	117.97
5	R	701	FAD	C6A-C5A-N7A	2.16	136.26	132.09
5	U	703	FAD	C4X-C10-N10	2.16	119.58	116.48
5	M	703	FAD	C6A-C5A-N7A	2.16	136.26	132.09
3	U	701	TPP	C7'-N3-C2	-2.16	118.97	123.48
5	B	703	FAD	C10-N1-C2	2.16	121.52	116.85
3	V	701	TPP	C5'-C6'-N1'	-2.15	120.33	123.83
3	A	701	TPP	CM2-C2'-N3'	2.15	120.34	117.13
3	N	701	TPP	PA-O7-C7	-2.15	111.05	121.26
3	B	701	TPP	CM2-C2'-N3'	2.14	120.33	117.13
5	A	703	FAD	C10-N1-C2	2.13	121.47	116.85
5	V	703	FAD	C6A-C5A-N7A	2.13	136.21	132.09
7	S	401	ATP	C4'-O4'-C1'	-2.13	104.76	109.47
5	V	703	FAD	C4X-C10-N10	2.13	119.53	116.48
5	B	703	FAD	C6A-C5A-N7A	2.13	136.19	132.09
3	I	701	TPP	O2B-PB-O3A	2.12	111.76	104.64
5	N	703	FAD	C6A-C5A-N7A	2.12	136.18	132.09
3	Q	701	TPP	CM2-C2'-N3'	2.12	120.30	117.13
3	U	701	TPP	C5'-C7'-N3	-2.12	108.40	112.97
5	U	703	FAD	C6A-C5A-N7A	2.12	136.17	132.09
3	V	701	TPP	PA-O7-C7	-2.11	111.22	121.26
6	F	704	60G	CAA-OAR-CAV	2.10	119.85	115.81
5	F	703	FAD	C4X-C10-N10	2.10	119.49	116.48
5	N	703	FAD	C10-N1-C2	2.09	121.38	116.85
5	J	703	FAD	C4A-N9A-C8A	2.09	107.94	105.74
5	N	703	FAD	C4'-C3'-C2'	-2.09	110.09	113.57
5	I	703	FAD	C3B-C2B-C1B	2.09	105.42	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	701	TPP	CM2-C2'-N3'	2.09	120.25	117.13
3	M	701	TPP	CM2-C2'-N3'	2.09	120.25	117.13
5	J	703	FAD	C5A-C6A-N6A	-2.09	118.12	123.29
3	M	701	TPP	PA-O7-C7	-2.08	111.34	121.26
6	I	704	60G	OAR-CAV-OAE	-2.08	119.41	123.46
5	A	703	FAD	C6A-C5A-N7A	2.07	136.09	132.09
3	F	701	TPP	PA-O7-C7	-2.06	111.44	121.26
5	J	703	FAD	O2B-C2B-C1B	2.06	117.20	110.10
3	V	701	TPP	CM2-C2'-N3'	2.06	120.21	117.13
3	M	701	TPP	O3B-PB-O3A	2.06	111.53	104.64
5	I	703	FAD	C6A-C5A-N7A	2.06	136.05	132.09
6	I	704	60G	CAA-OAR-CAV	2.06	119.76	115.81
5	E	703	FAD	C4X-C10-N10	2.05	119.42	116.48
5	N	703	FAD	C5'-C4'-C3'	-2.05	108.35	112.22
6	U	704	60G	CAA-OAR-CAV	2.04	119.74	115.81
3	E	701	TPP	CM2-C2'-N3'	2.04	120.19	117.13
6	J	704	60G	CAA-OAR-CAV	2.04	119.72	115.81
3	U	701	TPP	PA-O7-C7	-2.04	111.57	121.26
5	Q	703	FAD	C6A-C5A-N7A	2.04	136.01	132.09
3	U	701	TPP	CM2-C2'-N3'	2.04	120.17	117.13
5	N	703	FAD	C4X-C10-N10	2.03	119.39	116.48
6	B	704	60G	CAA-OAR-CAV	2.03	119.71	115.81
5	I	703	FAD	C5'-C4'-C3'	-2.03	108.39	112.22
6	V	704	60G	OAR-CAV-OAE	-2.03	119.51	123.46
5	Q	703	FAD	C5'-C4'-C3'	-2.02	108.40	112.22
3	Q	701	TPP	C5'-C7'-N3	-2.02	108.61	112.97
3	F	701	TPP	O2B-PB-O3A	2.01	111.37	104.64
3	I	701	TPP	CM2-C2'-N3'	2.01	120.13	117.13
6	A	704	60G	OAR-CAV-OAE	-2.00	119.56	123.46

There are no chirality outliers.

All (292) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	701	TPP	C7-O7-PA-O3A
3	E	701	TPP	C7-O7-PA-O1A
3	E	701	TPP	C7-O7-PA-O2A
3	E	701	TPP	C7-O7-PA-O3A
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	F	701	TPP	C7-O7-PA-O3A
3	I	701	TPP	C5-C6-C7-O7
3	I	701	TPP	C7-O7-PA-O2A
3	I	701	TPP	C7-O7-PA-O3A
3	J	701	TPP	C7-O7-PA-O1A
3	J	701	TPP	C7-O7-PA-O2A
3	J	701	TPP	C7-O7-PA-O3A
3	N	701	TPP	C5-C6-C7-O7
3	N	701	TPP	C7-O7-PA-O3A
3	Q	701	TPP	C5-C6-C7-O7
3	Q	701	TPP	C7-O7-PA-O2A
3	Q	701	TPP	C7-O7-PA-O3A
3	U	701	TPP	C5-C6-C7-O7
3	U	701	TPP	C7-O7-PA-O1A
3	U	701	TPP	C7-O7-PA-O2A
3	U	701	TPP	C7-O7-PA-O3A
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	J	703	FAD	C5B-O5B-PA-O2A
5	J	703	FAD	C5B-O5B-PA-O3P
5	J	703	FAD	C3'-C4'-C5'-O5'
5	J	703	FAD	O4'-C4'-C5'-O5'
5	R	701	FAD	N10-C1'-C2'-O2'
5	U	703	FAD	C5B-O5B-PA-O1A
5	U	703	FAD	C5B-O5B-PA-O3P
5	U	703	FAD	C1'-C2'-C3'-C4'
5	U	703	FAD	C3'-C4'-C5'-O5'
5	U	703	FAD	O4'-C4'-C5'-O5'
5	V	703	FAD	C1'-C2'-C3'-C4'
5	V	703	FAD	C3'-C4'-C5'-O5'
5	V	703	FAD	O4'-C4'-C5'-O5'
6	A	704	60G	C5-C6-OAS-CAB
6	A	704	60G	N1-C6-OAS-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
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	E	704	60G	CAW-CAM-SBB-NAQ
6	F	704	60G	C5-C4-OAT-CAC
6	F	704	60G	N3-C4-OAT-CAC
6	F	704	60G	CAW-CAM-SBB-OAF
6	F	704	60G	CAW-CAM-SBB-NAQ
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	J	704	60G	C5-C6-OAS-CAB
6	J	704	60G	N1-C6-OAS-CAB
6	J	704	60G	CAW-CAM-SBB-OAF
6	J	704	60G	CAW-CAM-SBB-NAQ
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	N	704	60G	CAW-CAM-SBB-NAQ
6	N	705	60G	CAW-CAM-SBB-OAF
6	N	705	60G	CAW-CAM-SBB-NAQ
6	Q	704	60G	C5-C6-OAS-CAB
6	Q	704	60G	N1-C6-OAS-CAB
6	Q	704	60G	CAW-CAM-SBB-OAF
6	Q	704	60G	CAW-CAM-SBB-NAQ
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
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	V	704	60G	CAW-CAM-SBB-OAF
6	V	704	60G	CAW-CAM-SBB-NAQ
7	C	401	ATP	C2'-C1'-N9-C8
7	D	401	ATP	C2'-C1'-N9-C8
7	D	401	ATP	C2'-C1'-N9-C4
7	G	401	ATP	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	H	401	ATP	C2'-C1'-N9-C8
7	K	401	ATP	C5'-O5'-PA-O1A
7	K	401	ATP	C5'-O5'-PA-O2A
7	K	401	ATP	C5'-O5'-PA-O3A
7	L	401	ATP	C2'-C1'-N9-C8
7	O	401	ATP	C5'-O5'-PA-O1A
7	O	401	ATP	C5'-O5'-PA-O3A
7	O	401	ATP	O4'-C4'-C5'-O5'
7	O	401	ATP	C3'-C4'-C5'-O5'
7	O	401	ATP	C2'-C1'-N9-C8
7	O	401	ATP	C2'-C1'-N9-C4
7	P	401	ATP	C2'-C1'-N9-C8
7	S	401	ATP	PB-O3B-PG-O3G
7	S	401	ATP	C2'-C1'-N9-C8
7	S	401	ATP	C2'-C1'-N9-C4
7	T	401	ATP	C2'-C1'-N9-C8
7	T	401	ATP	C2'-C1'-N9-C4
7	W	401	ATP	C5'-O5'-PA-O2A
7	W	401	ATP	C5'-O5'-PA-O3A
7	W	401	ATP	C2'-C1'-N9-C8
7	W	402	ATP	C2'-C1'-N9-C8
6	R	702	60G	CBA-CAV-OAR-CAA
6	A	704	60G	C5-C4-OAT-CAC
6	E	704	60G	C5-C4-OAT-CAC
6	I	704	60G	C5-C6-OAS-CAB
6	J	704	60G	C5-C4-OAT-CAC
6	N	704	60G	C5-C6-OAS-CAB
6	N	705	60G	C5-C4-OAT-CAC
6	N	705	60G	C5-C6-OAS-CAB
6	Q	704	60G	C5-C4-OAT-CAC
6	V	704	60G	C5-C4-OAT-CAC
6	V	704	60G	C5-C6-OAS-CAB
6	A	704	60G	N3-C4-OAT-CAC
6	B	704	60G	N1-C6-OAS-CAB
6	E	704	60G	N3-C4-OAT-CAC
6	F	704	60G	N1-C6-OAS-CAB
6	I	704	60G	N1-C6-OAS-CAB
6	J	704	60G	N3-C4-OAT-CAC
6	N	704	60G	N1-C6-OAS-CAB
6	N	705	60G	N3-C4-OAT-CAC
6	N	705	60G	N1-C6-OAS-CAB
6	Q	704	60G	N3-C4-OAT-CAC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	V	704	60G	N3-C4-OAT-CAC
6	V	704	60G	N1-C6-OAS-CAB
5	J	703	FAD	C3B-C4B-C5B-O5B
6	U	704	60G	CBA-CAV-OAR-CAA
6	B	704	60G	C5-C6-OAS-CAB
6	F	704	60G	C5-C6-OAS-CAB
7	C	401	ATP	C2'-C1'-N9-C4
7	G	401	ATP	C2'-C1'-N9-C4
7	H	401	ATP	C2'-C1'-N9-C4
7	L	401	ATP	C2'-C1'-N9-C4
7	P	401	ATP	C2'-C1'-N9-C4
7	W	401	ATP	C2'-C1'-N9-C4
7	W	402	ATP	C2'-C1'-N9-C4
6	A	704	60G	CBA-CAV-OAR-CAA
7	S	401	ATP	C3'-C4'-C5'-O5'
6	B	704	60G	CBA-CAV-OAR-CAA
6	I	704	60G	CBA-CAV-OAR-CAA
5	R	701	FAD	O4B-C4B-C5B-O5B
7	S	401	ATP	O4'-C4'-C5'-O5'
5	U	703	FAD	O2'-C2'-C3'-O3'
5	J	703	FAD	O4B-C4B-C5B-O5B
5	R	701	FAD	C3B-C4B-C5B-O5B
7	K	401	ATP	C2'-C1'-N9-C8
5	U	703	FAD	O2'-C2'-C3'-C4'
6	R	702	60G	CAW-CAM-SBB-OAF
5	E	703	FAD	PA-O3P-P-O1P
5	F	703	FAD	PA-O3P-P-O1P
5	I	703	FAD	PA-O3P-P-O1P
5	M	703	FAD	PA-O3P-P-O1P
5	Q	703	FAD	PA-O3P-P-O1P
5	R	701	FAD	P-O3P-PA-O1A
7	S	401	ATP	PG-O3B-PB-O1B
3	Q	701	TPP	PB-O3A-PA-O7
5	J	703	FAD	P-O3P-PA-O5B
5	U	703	FAD	P-O3P-PA-O5B
5	V	703	FAD	O2'-C2'-C3'-C4'
5	V	703	FAD	C2'-C3'-C4'-O4'
5	U	703	FAD	C1'-C2'-C3'-O3'
3	A	701	TPP	PA-O3A-PB-O2B
5	V	703	FAD	O3'-C3'-C4'-C5'
5	I	703	FAD	C2'-C3'-C4'-O4'
7	K	401	ATP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	701	TPP	C5-C6-C7-O7
3	J	701	TPP	C5-C6-C7-O7
3	M	701	TPP	C5-C6-C7-O7
3	V	701	TPP	C5-C6-C7-O7
6	A	704	60G	CAW-CAM-SBB-NAQ
6	B	704	60G	CAW-CAM-SBB-NAQ
6	I	704	60G	CAW-CAM-SBB-NAQ
6	U	704	60G	CAW-CAM-SBB-NAQ
5	B	703	FAD	O4B-C4B-C5B-O5B
7	C	401	ATP	C3'-C4'-C5'-O5'
5	Q	703	FAD	C2B-C1B-N9A-C8A
5	A	703	FAD	PA-O3P-P-O1P
5	J	703	FAD	PA-O3P-P-O1P
7	L	401	ATP	PB-O3A-PA-O2A
7	W	402	ATP	PG-O3B-PB-O2B
6	U	704	60G	OAR-CAV-CBA-CAK
6	I	704	60G	OAR-CAV-CBA-CAK
5	R	701	FAD	N10-C1'-C2'-C3'
7	K	401	ATP	C4'-C5'-O5'-PA
6	R	702	60G	OAR-CAV-CBA-CAK
5	I	703	FAD	O3'-C3'-C4'-O4'
5	B	703	FAD	C3B-C4B-C5B-O5B
3	I	701	TPP	C7-O7-PA-O1A
3	M	701	TPP	C7-O7-PA-O1A
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	F	703	FAD	C5'-O5'-P-O3P
5	J	703	FAD	C5'-O5'-P-O1P
5	J	703	FAD	C5'-O5'-P-O2P
5	J	703	FAD	C5'-O5'-P-O3P
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
5	U	703	FAD	C5'-O5'-P-O3P
5	V	703	FAD	C5'-O5'-P-O1P
7	O	401	ATP	C5'-O5'-PA-O2A
7	S	401	ATP	PB-O3B-PG-O1G
5	V	703	FAD	O2'-C2'-C3'-O3'
6	R	702	60G	OAR-CAV-CBA-CAW
5	I	703	FAD	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	703	FAD	O3'-C3'-C4'-C5'
3	M	701	TPP	PB-O3A-PA-O1A
3	N	701	TPP	PB-O3A-PA-O2A
3	V	701	TPP	PB-O3A-PA-O1A
5	B	703	FAD	PA-O3P-P-O1P
5	N	703	FAD	PA-O3P-P-O1P
7	C	401	ATP	PG-O3B-PB-O2B
7	H	401	ATP	PG-O3B-PB-O2B
7	O	401	ATP	PA-O3A-PB-O1B
7	S	401	ATP	PA-O3A-PB-O2B
5	V	703	FAD	C2'-C3'-C4'-C5'
5	A	703	FAD	C2B-C1B-N9A-C8A
5	V	703	FAD	C2B-C1B-N9A-C8A
7	G	401	ATP	C3'-C4'-C5'-O5'
5	I	703	FAD	C2'-C3'-C4'-C5'
6	I	704	60G	OAR-CAV-CBA-CAW
6	U	704	60G	OAR-CAV-CBA-CAW
5	R	701	FAD	O3'-C3'-C4'-C5'
5	R	701	FAD	C2'-C3'-C4'-O4'
5	R	701	FAD	C4'-C5'-O5'-P
5	R	701	FAD	O3'-C3'-C4'-O4'
5	A	703	FAD	PA-O3P-P-O2P
5	R	701	FAD	PA-O3P-P-O1P
5	V	703	FAD	PA-O3P-P-O1P
5	V	703	FAD	O3'-C3'-C4'-O4'
6	A	704	60G	OAR-CAV-CBA-CAK
6	B	704	60G	CAW-CAM-SBB-OAG
6	E	704	60G	CAW-CAM-SBB-OAG
6	F	704	60G	CAW-CAM-SBB-OAG
6	J	704	60G	CAW-CAM-SBB-OAG
6	N	704	60G	CAW-CAM-SBB-OAG
6	N	705	60G	CAW-CAM-SBB-OAG
6	Q	704	60G	CAW-CAM-SBB-OAG
6	V	704	60G	CAW-CAM-SBB-OAG
5	V	703	FAD	C1'-C2'-C3'-O3'
5	M	703	FAD	O4B-C4B-C5B-O5B
5	N	703	FAD	C2B-C1B-N9A-C8A
7	S	401	ATP	C4'-C5'-O5'-PA
5	I	703	FAD	C3B-C4B-C5B-O5B
6	R	702	60G	CAW-CAM-SBB-NAQ
5	E	703	FAD	O4B-C4B-C5B-O5B
7	D	401	ATP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	W	401	ATP	C3'-C4'-C5'-O5'
7	W	402	ATP	C3'-C4'-C5'-O5'
5	U	703	FAD	C2B-C1B-N9A-C8A
3	N	701	TPP	PB-O3A-PA-O1A
5	B	703	FAD	PA-O3P-P-O2P
5	R	701	FAD	P-O3P-PA-O2A
7	C	401	ATP	PG-O3B-PB-O1B
7	H	401	ATP	PG-O3B-PB-O1B
7	S	401	ATP	PA-O3A-PB-O1B
7	T	401	ATP	PB-O3A-PA-O2A
7	W	401	ATP	PB-O3A-PA-O2A
6	E	704	60G	OAR-CAV-CBA-CAK
6	N	704	60G	OAR-CAV-CBA-CAK
5	M	703	FAD	C2B-C1B-N9A-C8A
6	B	704	60G	OAR-CAV-CBA-CAK
5	U	703	FAD	N10-C1'-C2'-O2'
5	Q	703	FAD	O4B-C1B-N9A-C8A
7	K	401	ATP	O4'-C1'-N9-C8
5	R	701	FAD	C2'-C3'-C4'-C5'
6	R	702	60G	OAE-CAV-CBA-CAK
6	N	705	60G	OAR-CAV-CBA-CAK
7	D	401	ATP	C4'-C5'-O5'-PA
6	A	704	60G	CAW-CAM-SBB-OAG
7	H	401	ATP	O4'-C1'-N9-C8
3	M	701	TPP	PB-O3A-PA-O2A
5	N	703	FAD	PA-O3P-P-O2P
5	Q	703	FAD	PA-O3P-P-O2P
5	U	703	FAD	P-O3P-PA-O2A
7	C	401	ATP	PB-O3A-PA-O2A
7	L	401	ATP	PB-O3A-PA-O1A
6	A	704	60G	OAR-CAV-CBA-CAW
6	I	704	60G	OAE-CAV-CBA-CAK

There are no ring outliers.

38 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	401	ATP	1	0
7	C	401	ATP	2	0
6	V	704	60G	1	0
5	A	703	FAD	3	0
5	R	701	FAD	7	0

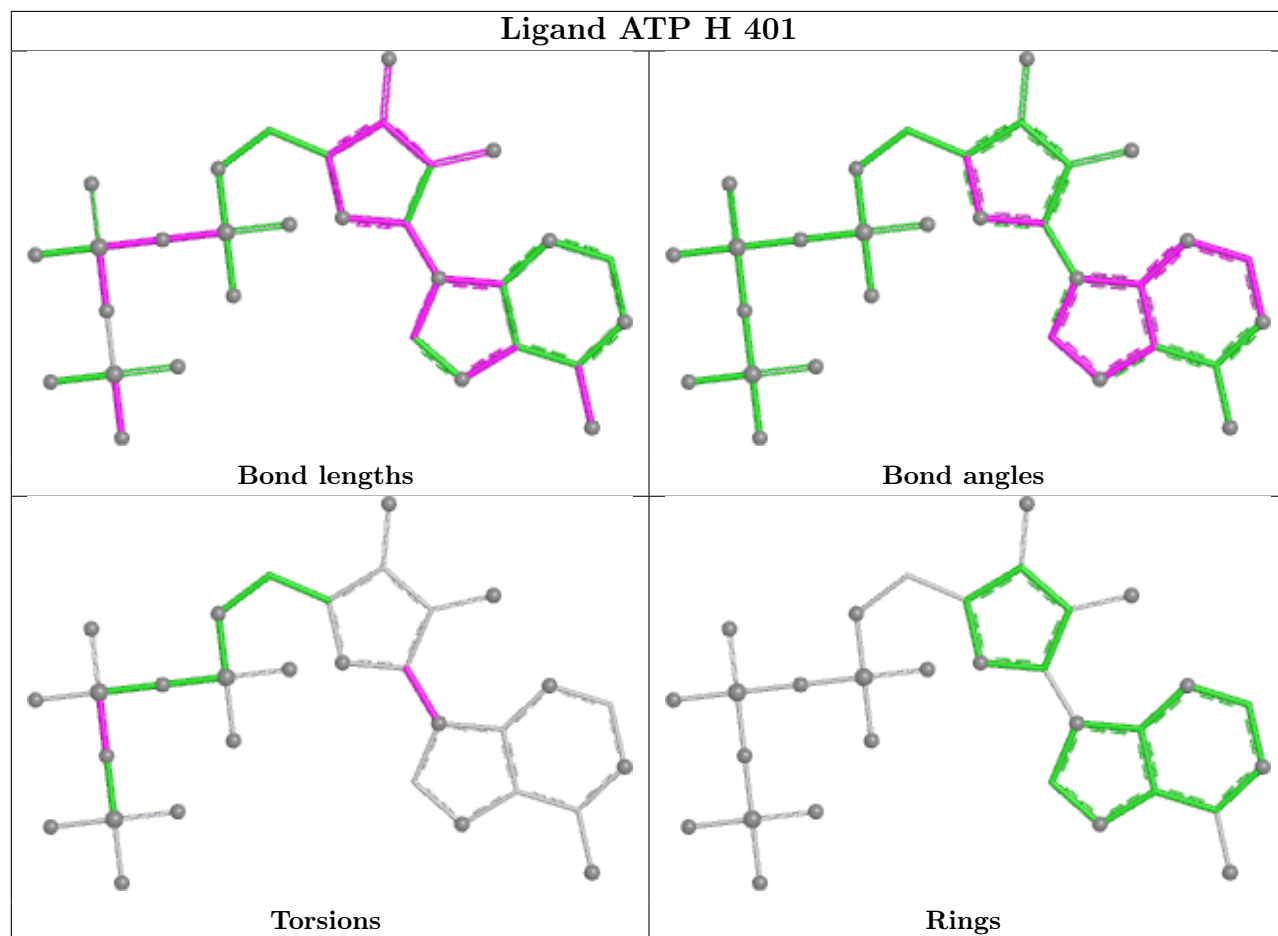
Continued on next page...

Continued from previous page...

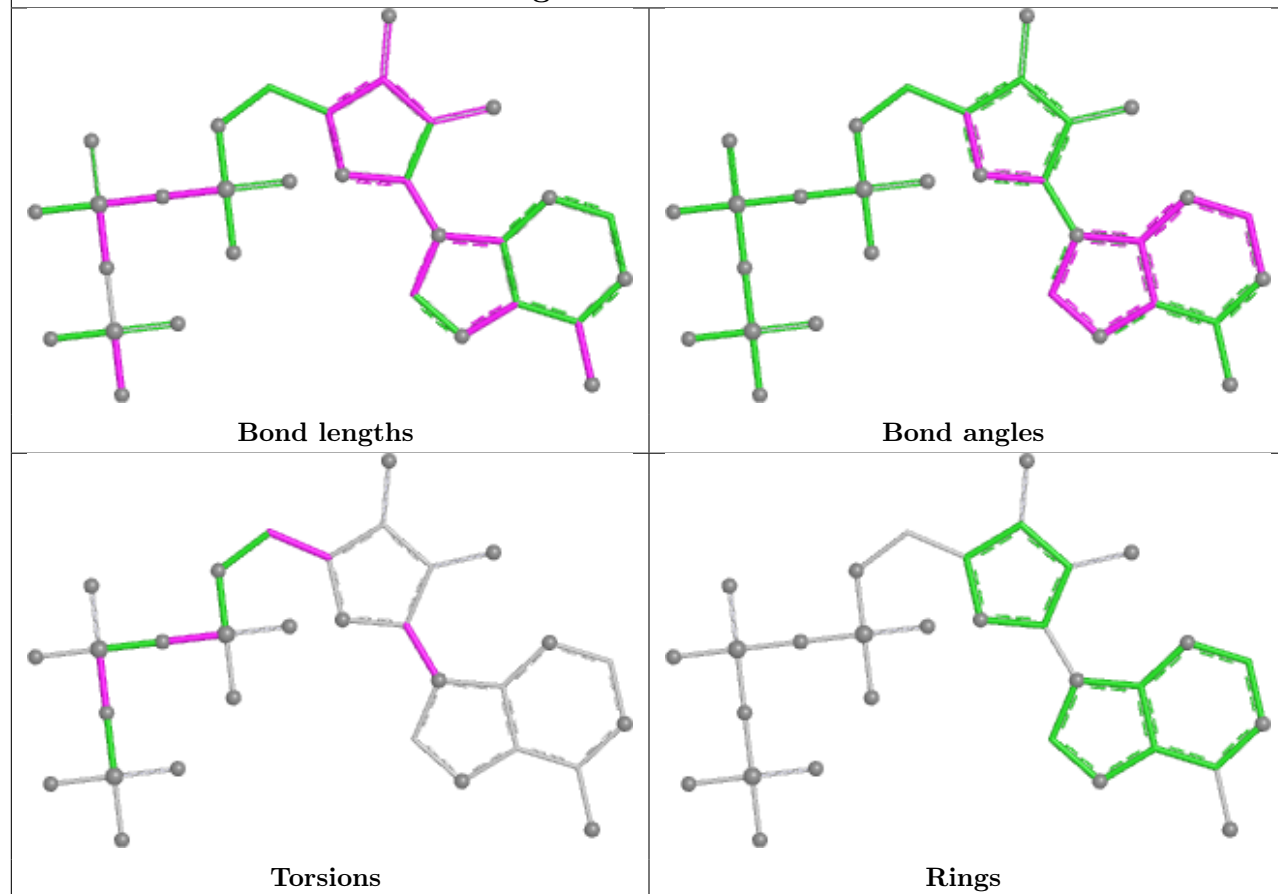
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	401	ATP	4	0
3	E	701	TPP	3	0
3	V	701	TPP	3	0
5	E	703	FAD	3	0
6	J	704	60G	2	0
3	B	701	TPP	2	0
5	B	703	FAD	1	0
3	A	701	TPP	1	0
7	T	401	ATP	1	0
7	S	401	ATP	2	0
5	V	703	FAD	1	0
3	I	701	TPP	2	0
5	Q	703	FAD	3	0
6	R	702	60G	1	0
3	M	701	TPP	3	0
3	F	701	TPP	2	0
3	N	701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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

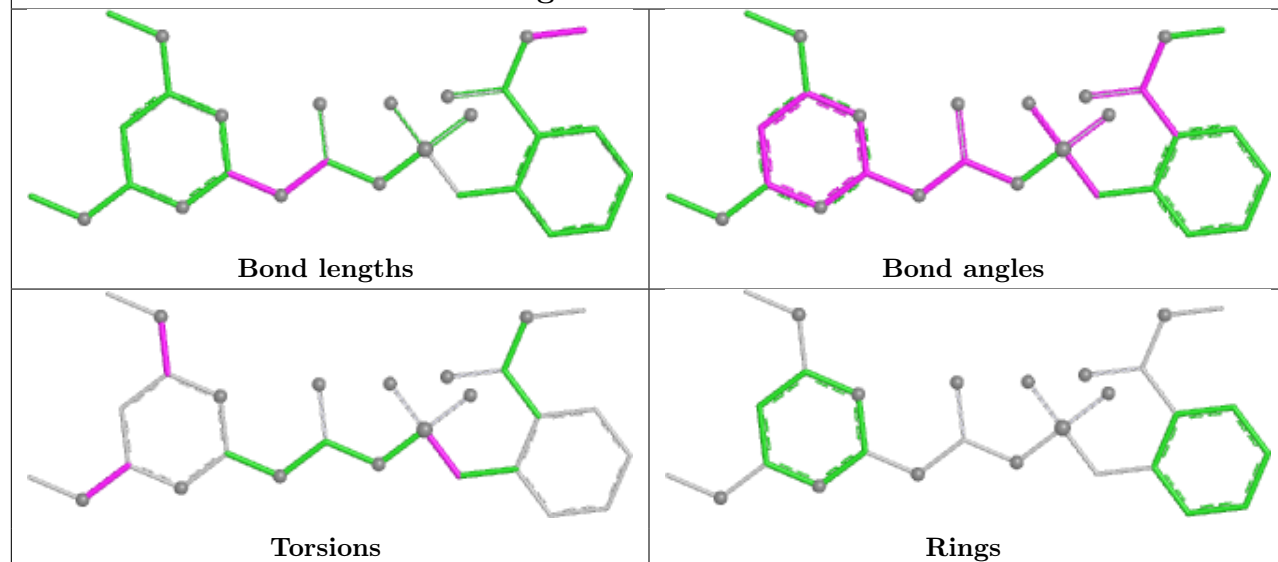
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

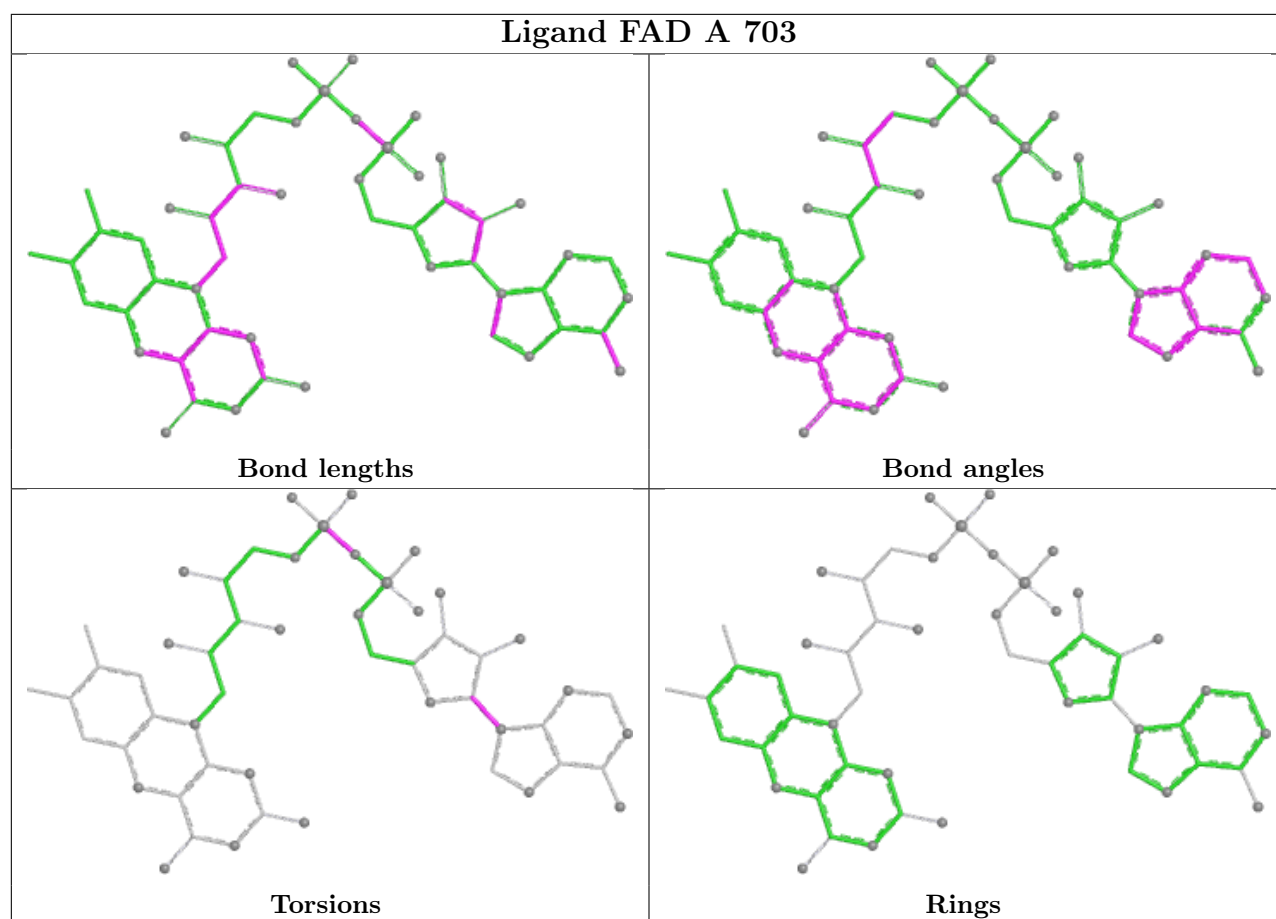


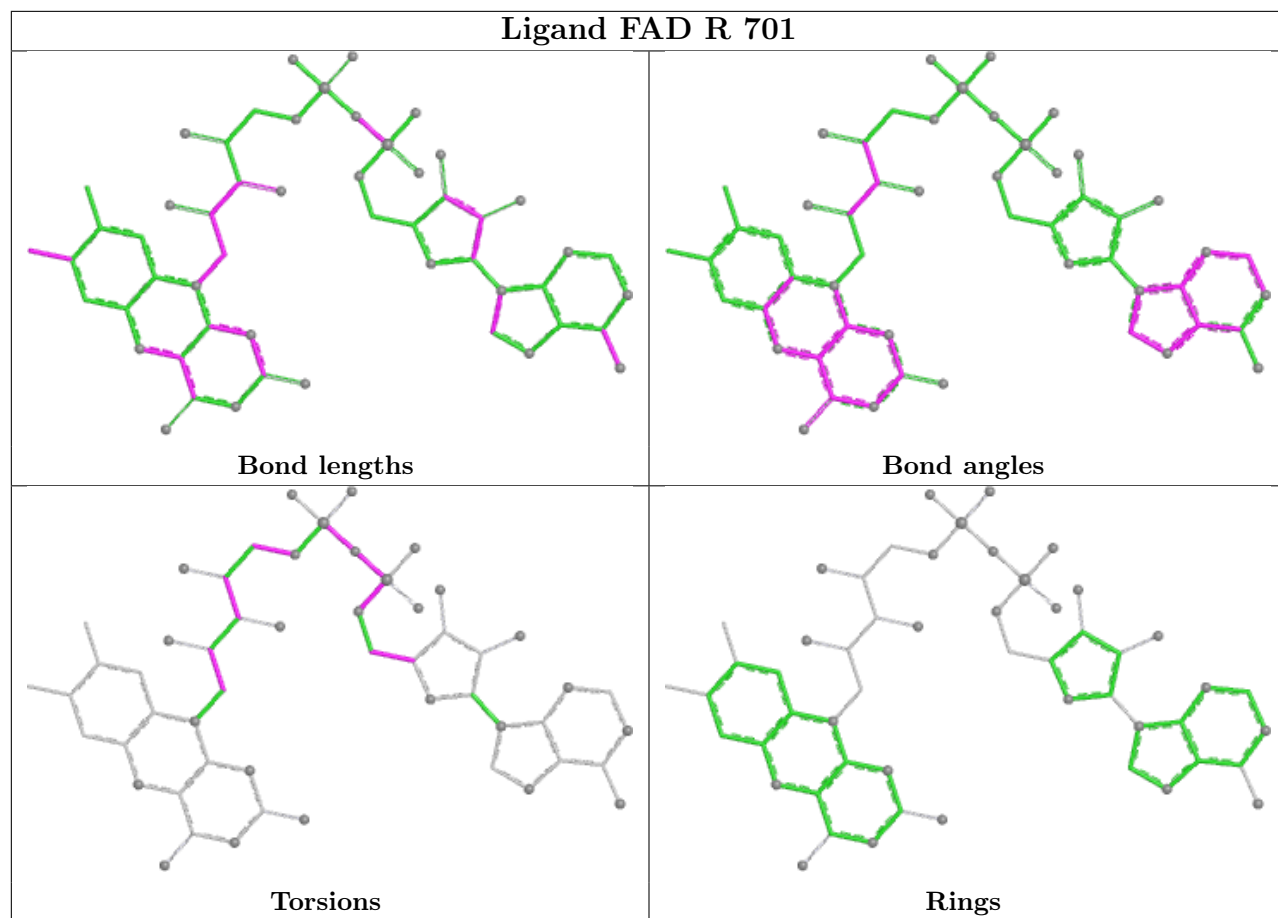
Ligand ATP C 401



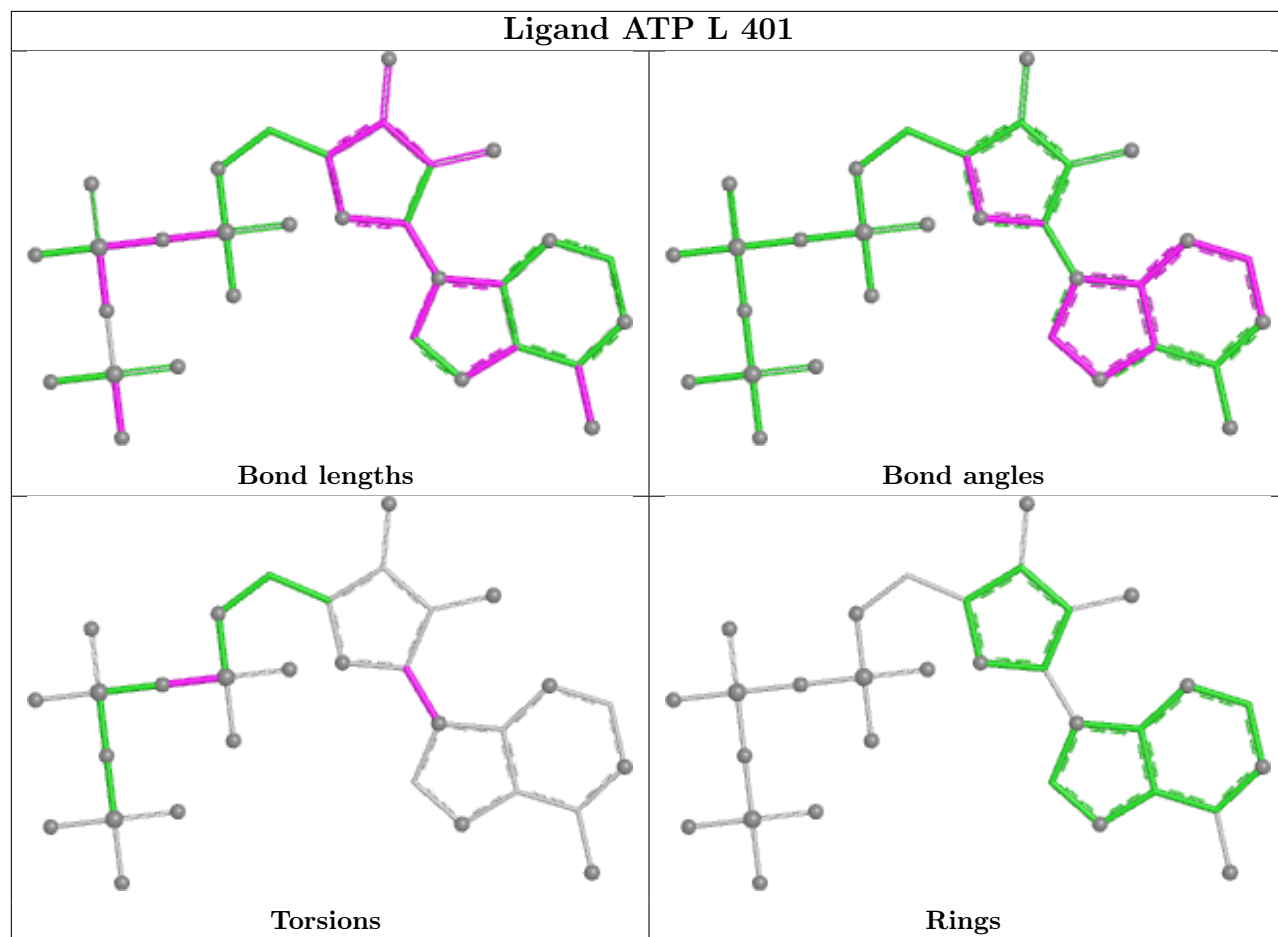
Ligand 60G V 704



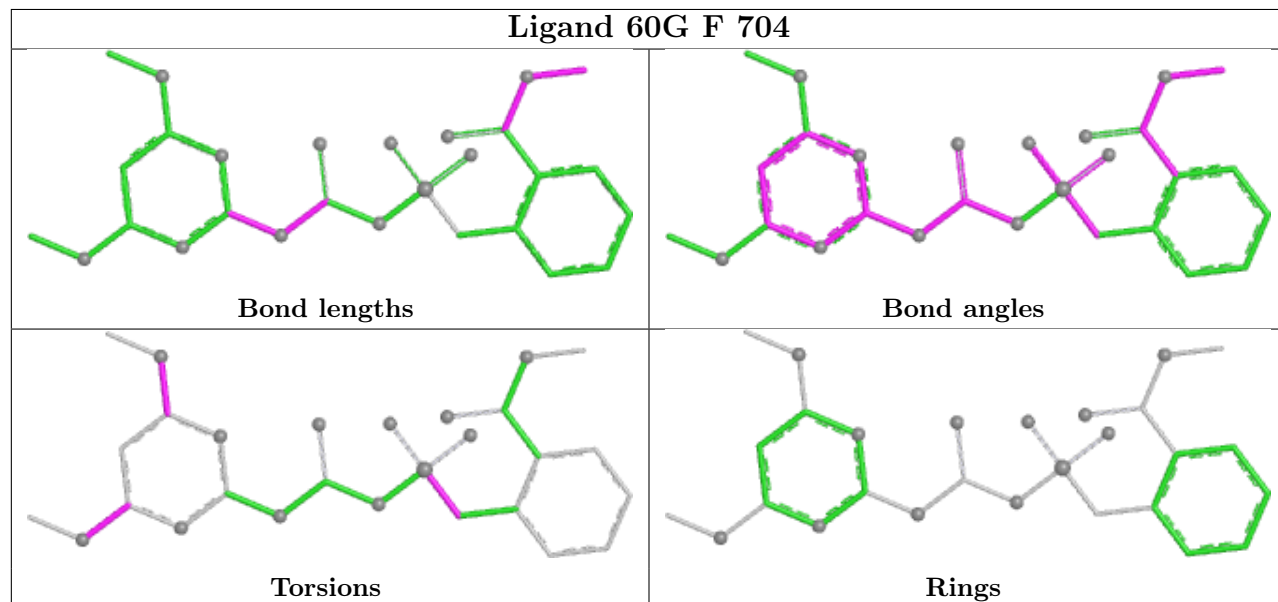


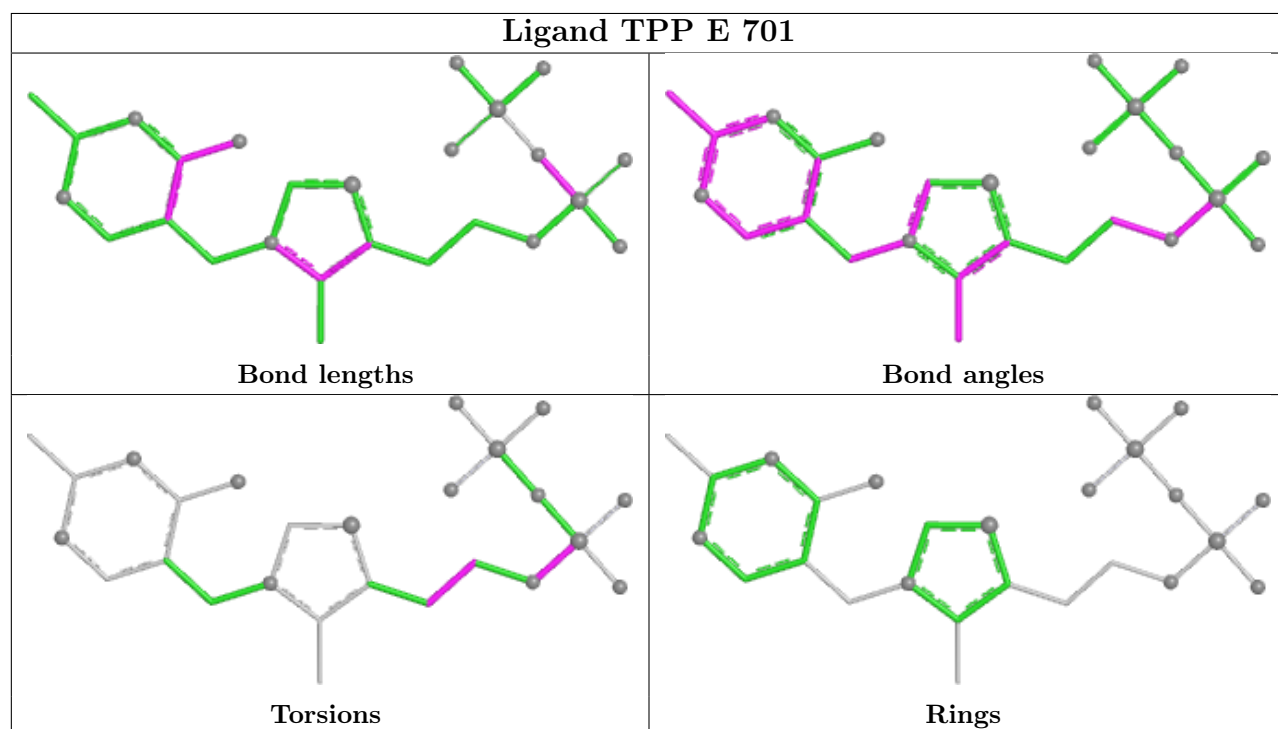
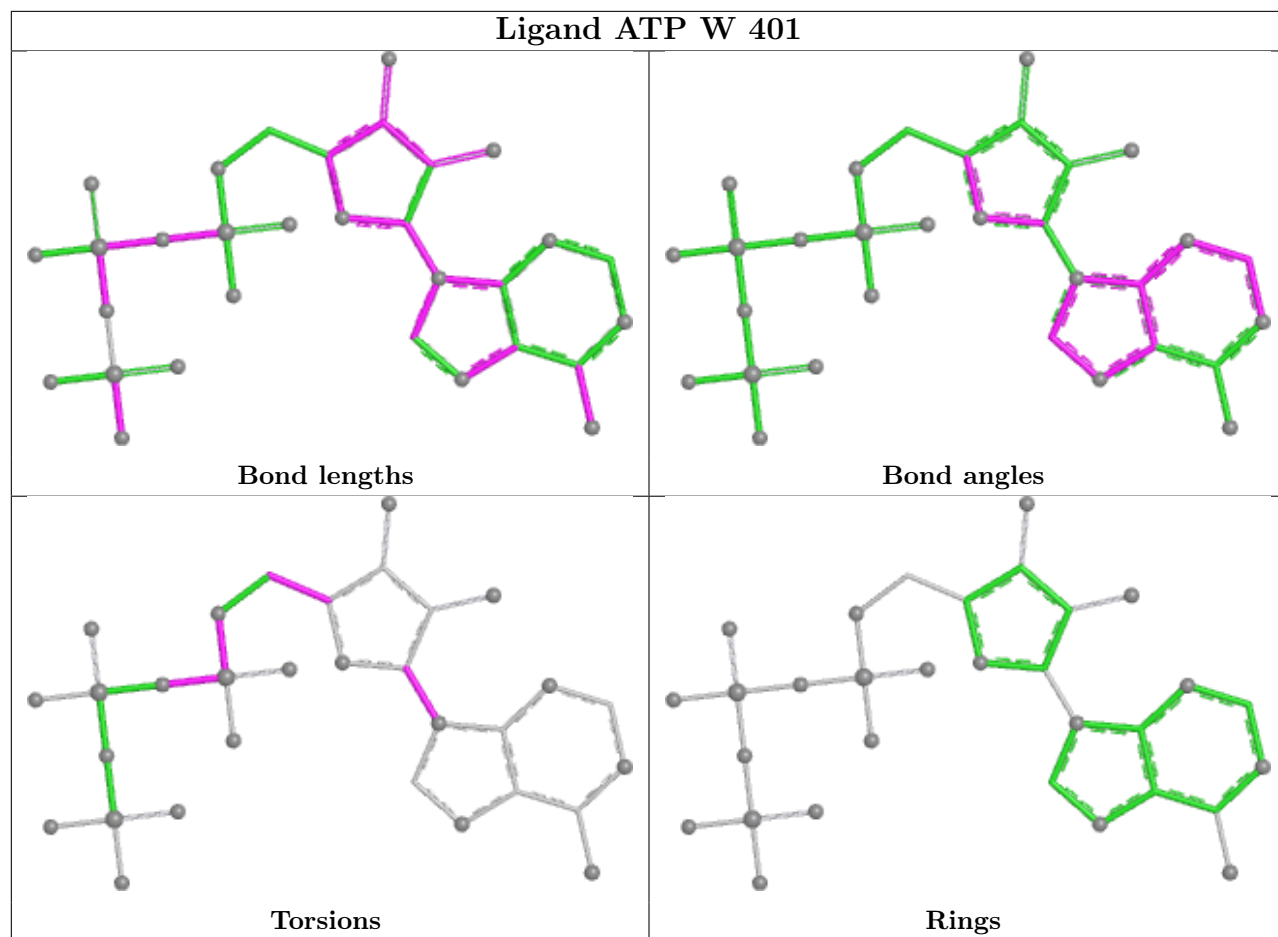


Ligand ATP L 401

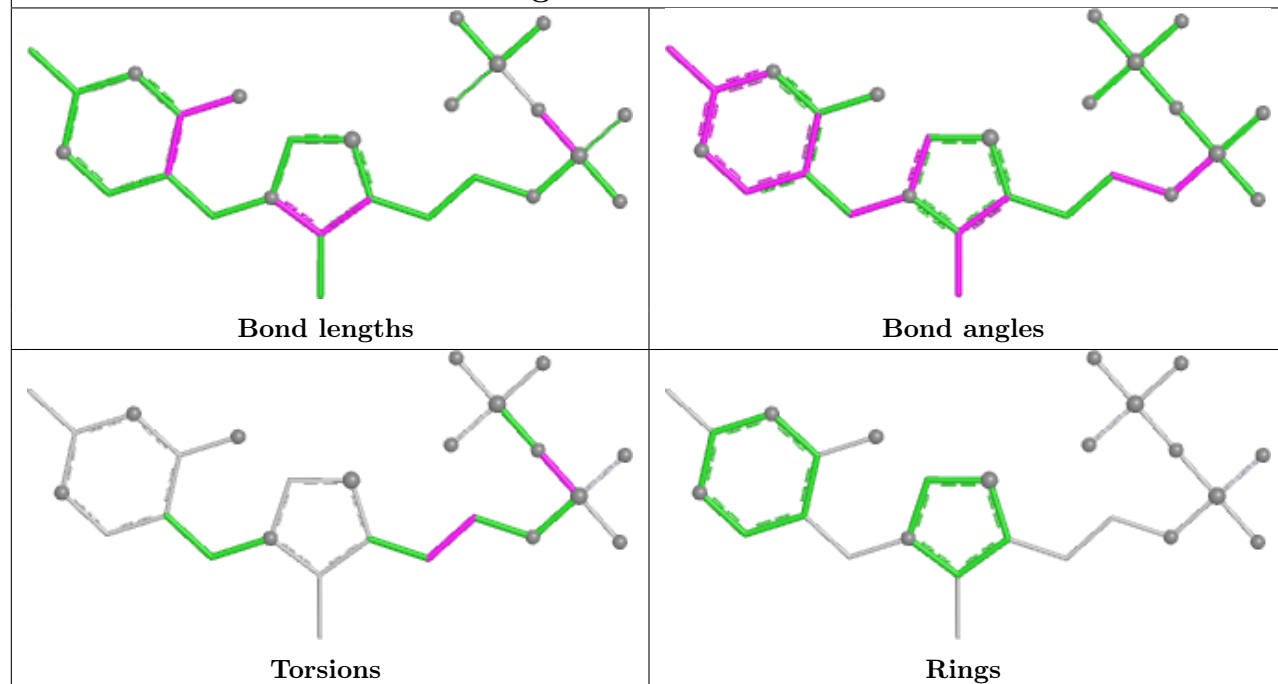


Ligand 60G F 704

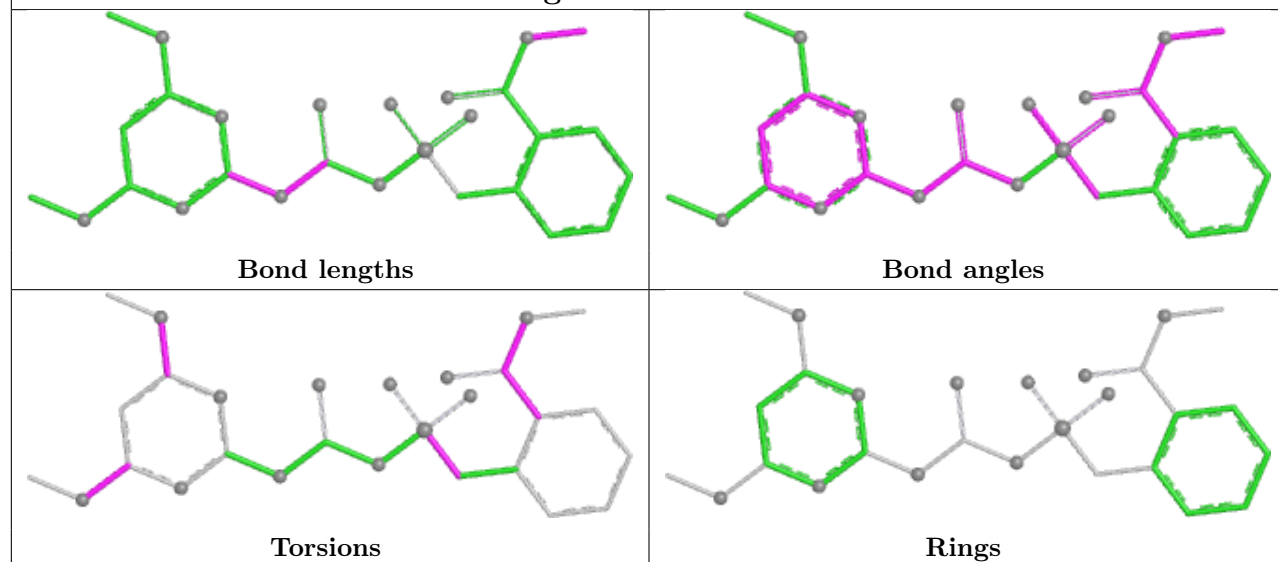




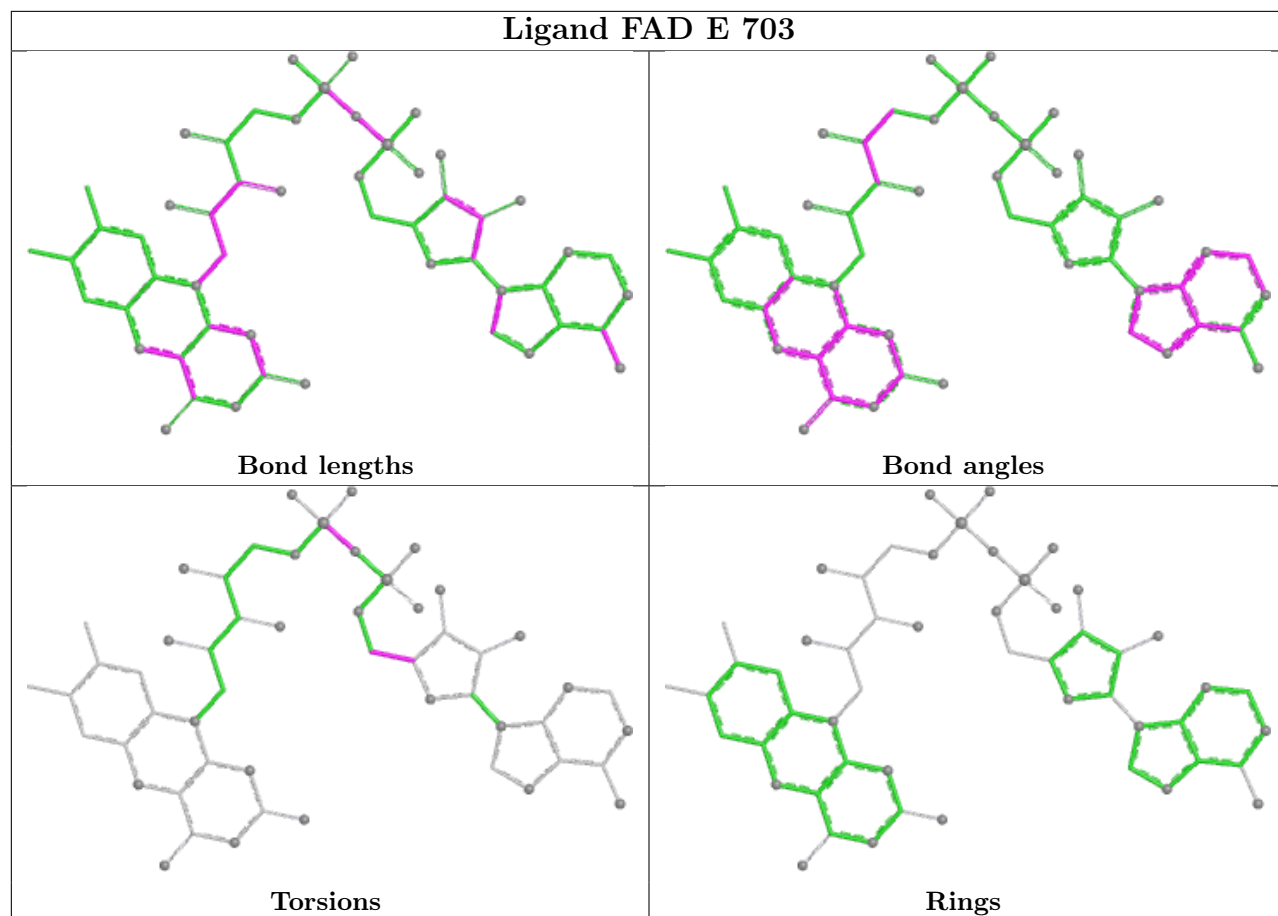
Ligand TPP V 701



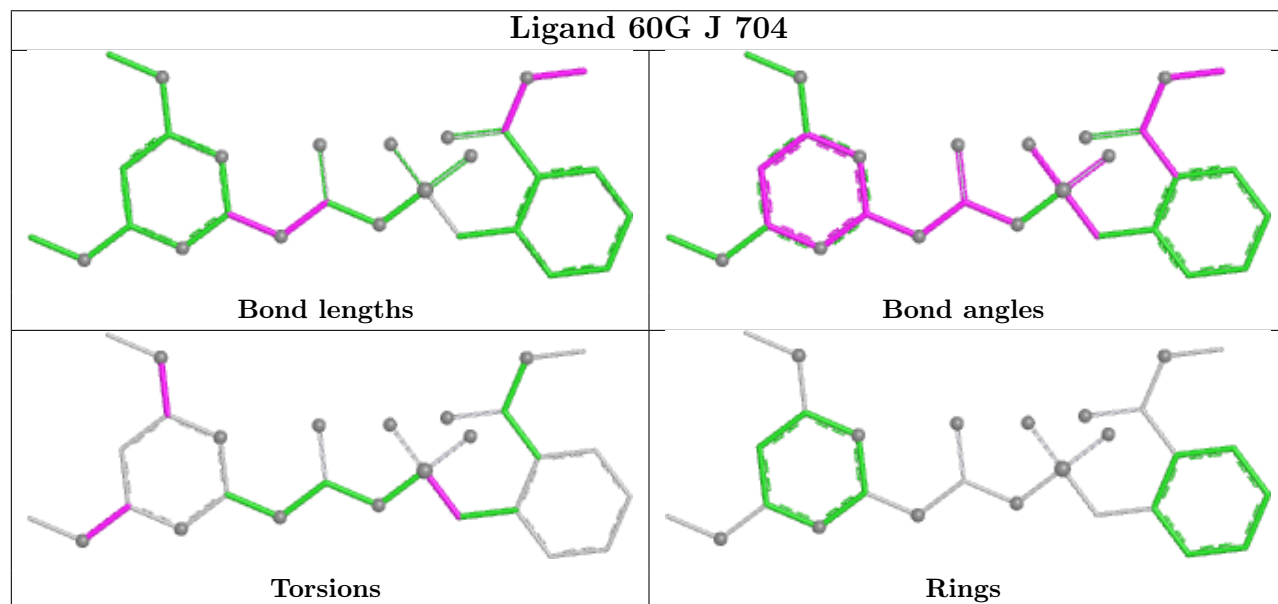
Ligand 60G I 704



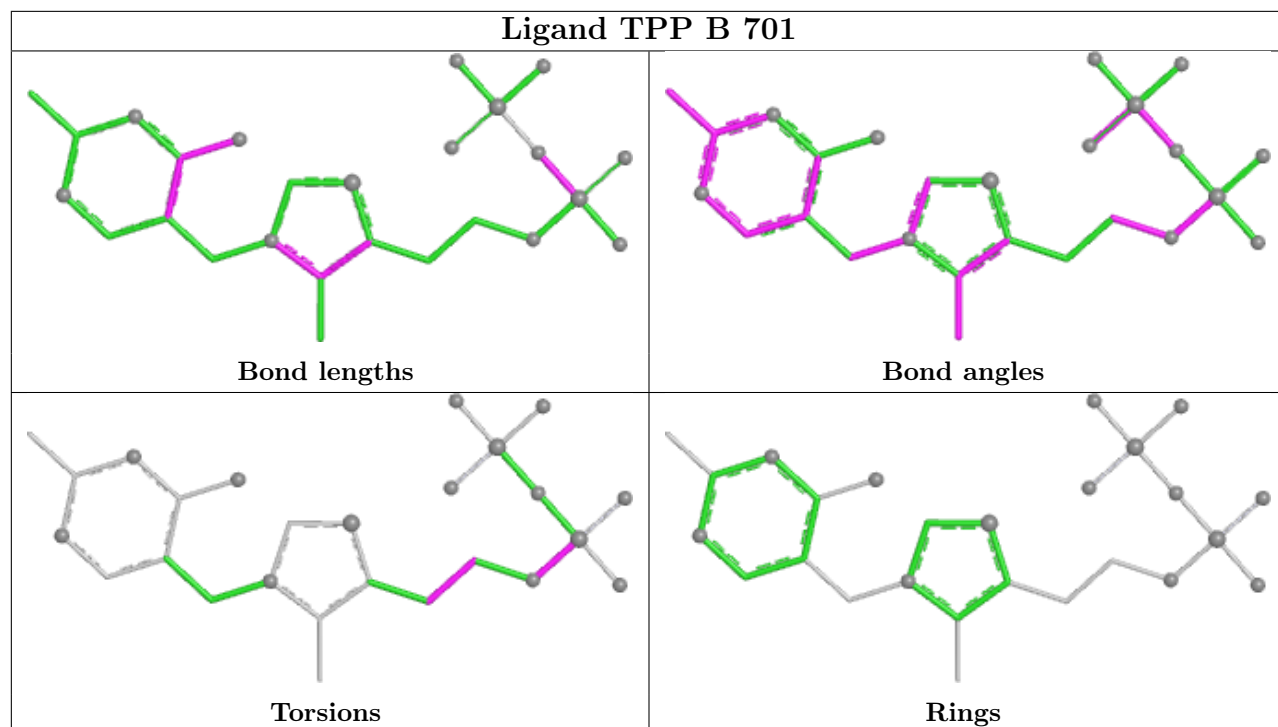
Ligand FAD E 703



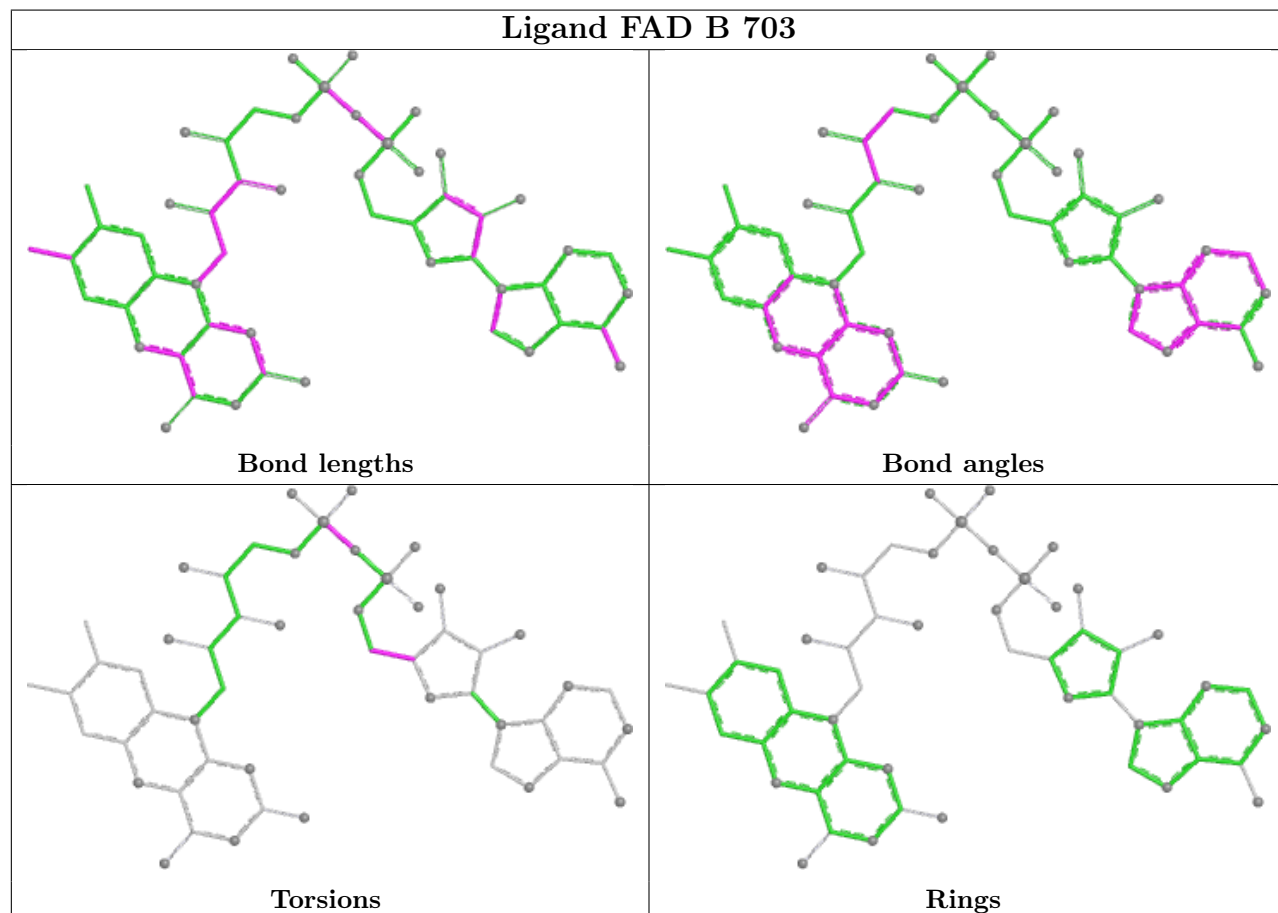
Ligand 60G J 704



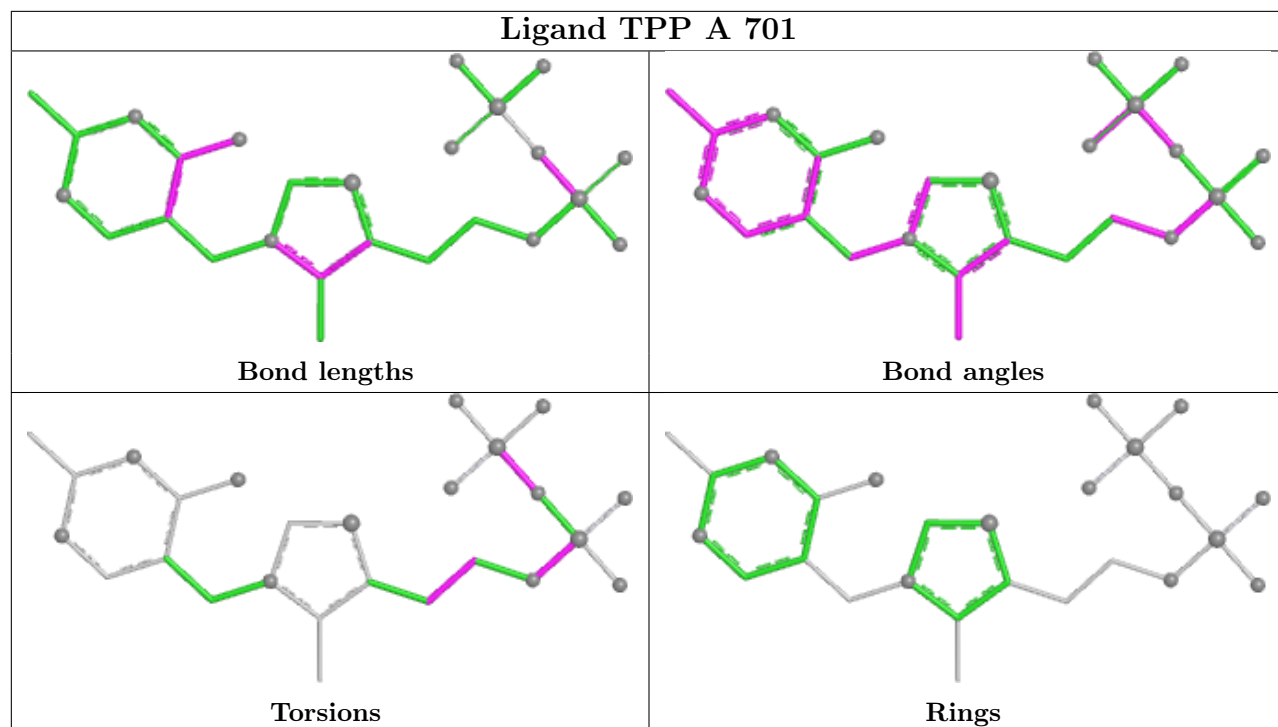
Ligand TPP B 701



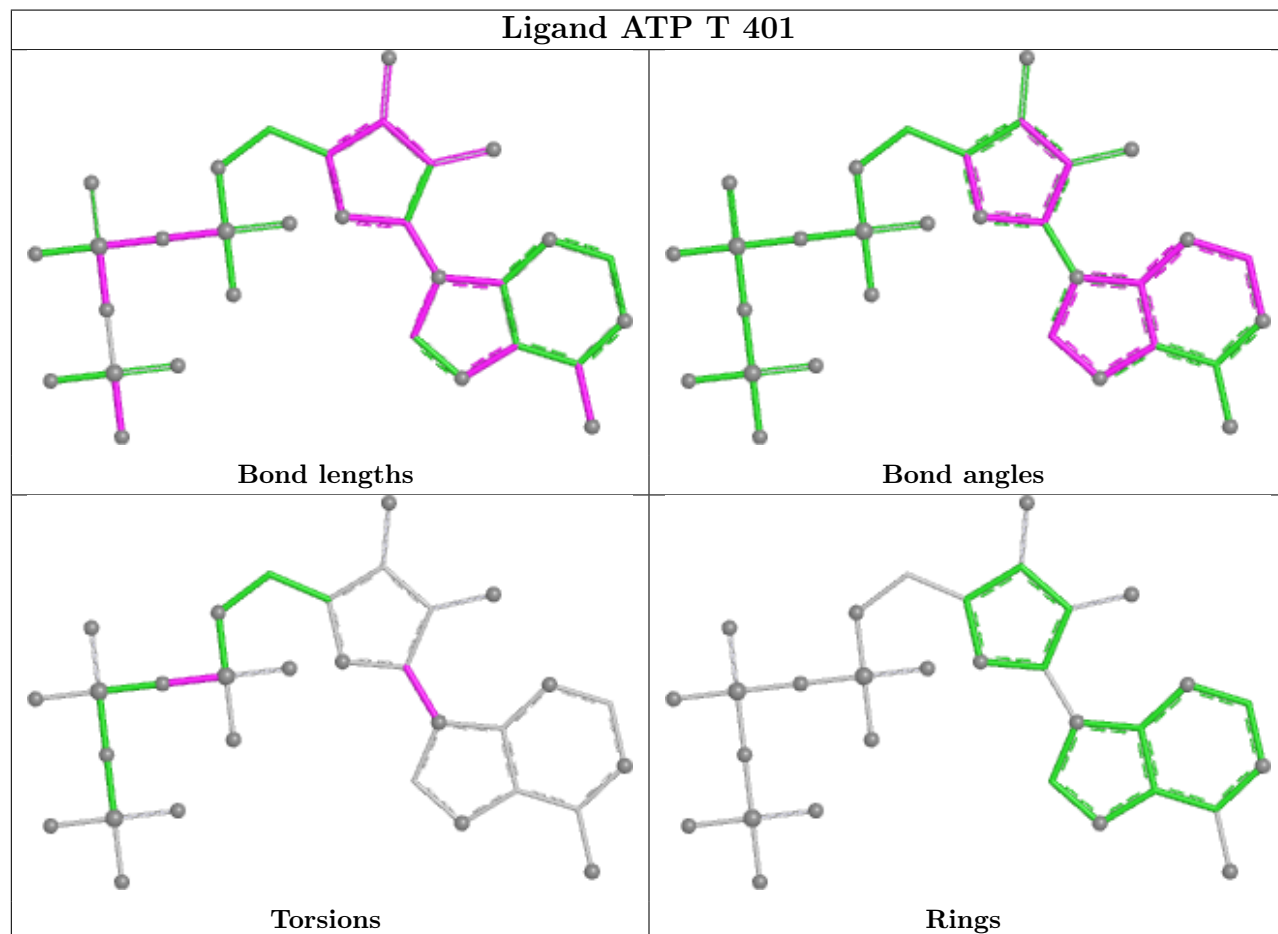
Ligand FAD B 703



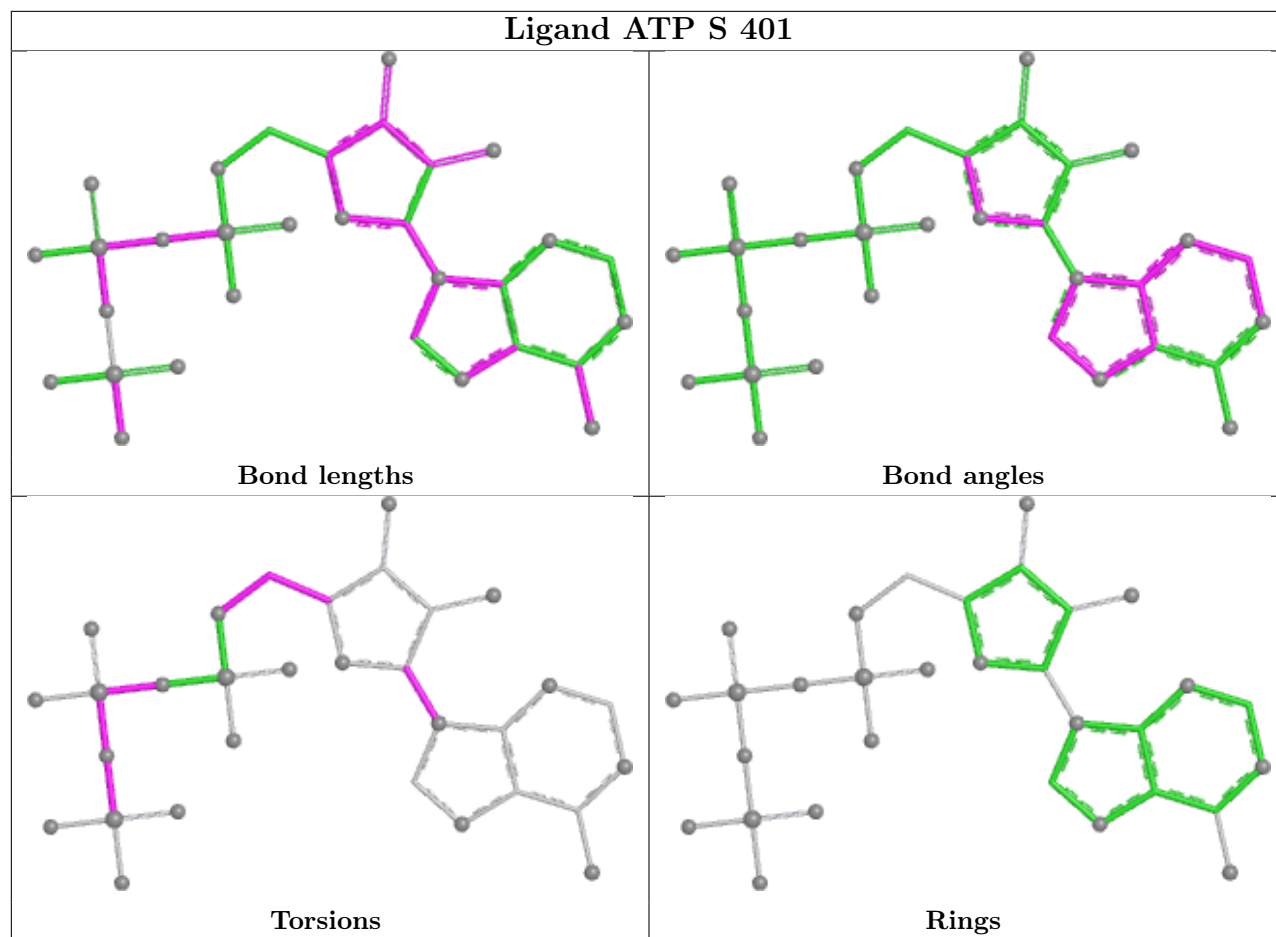
Ligand TPP A 701



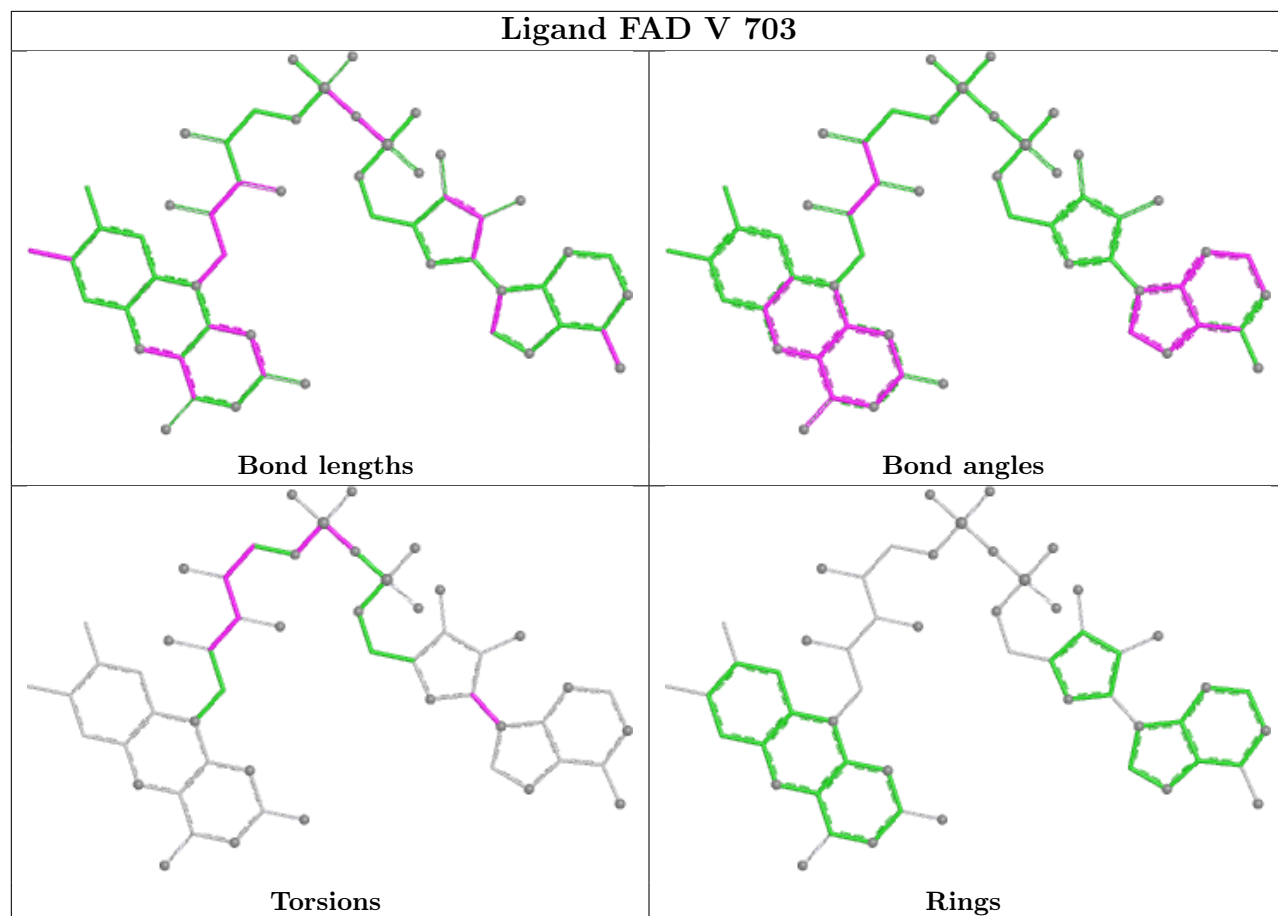
Ligand ATP T 401



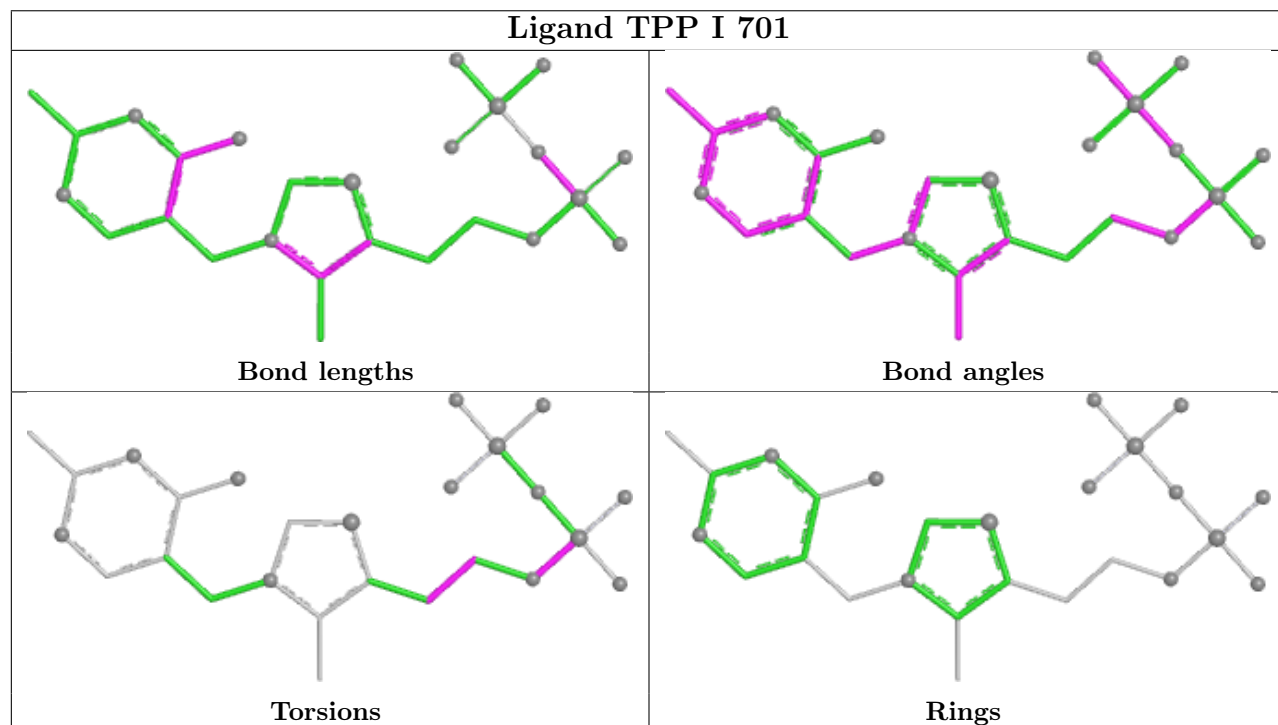
Ligand ATP S 401



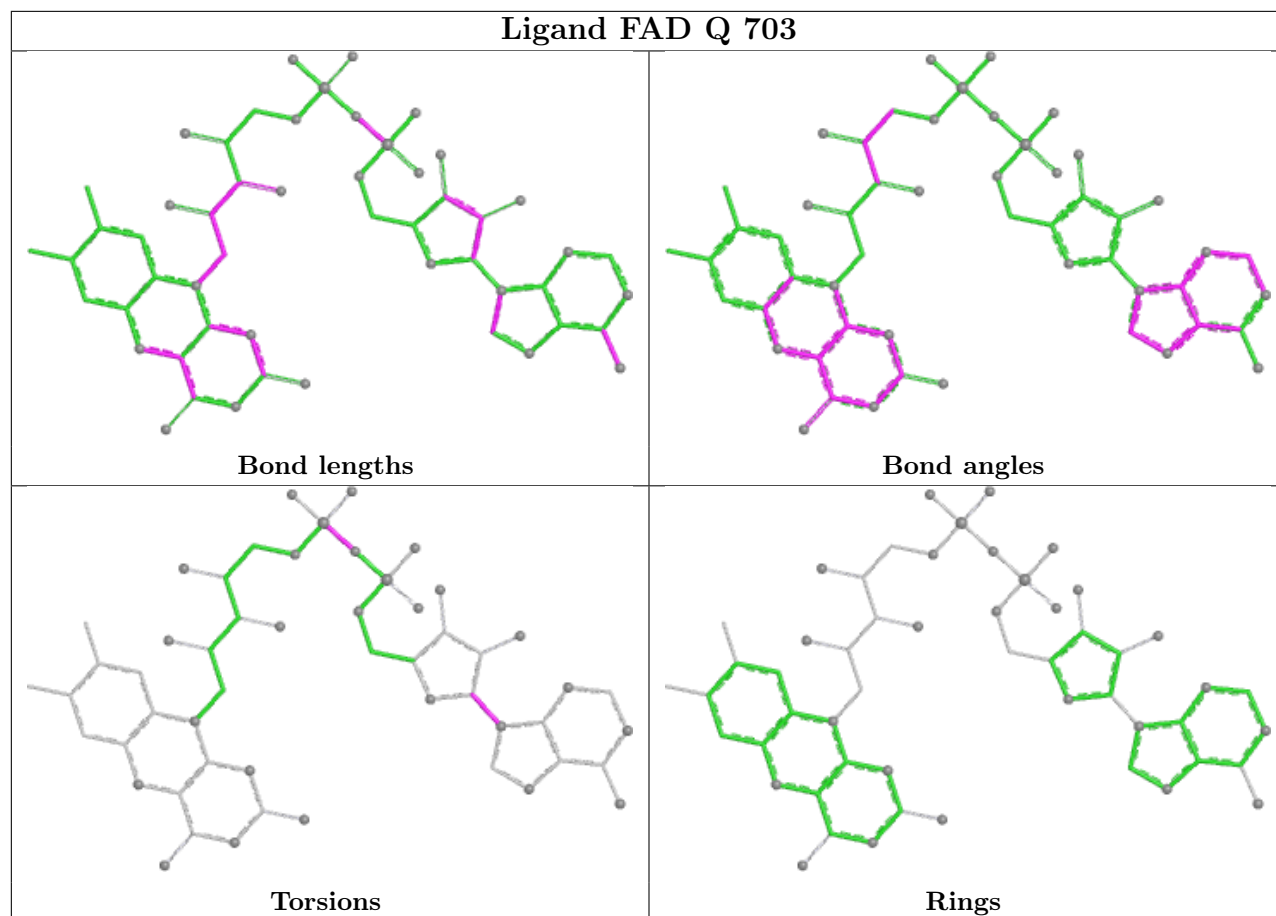
Ligand FAD V 703



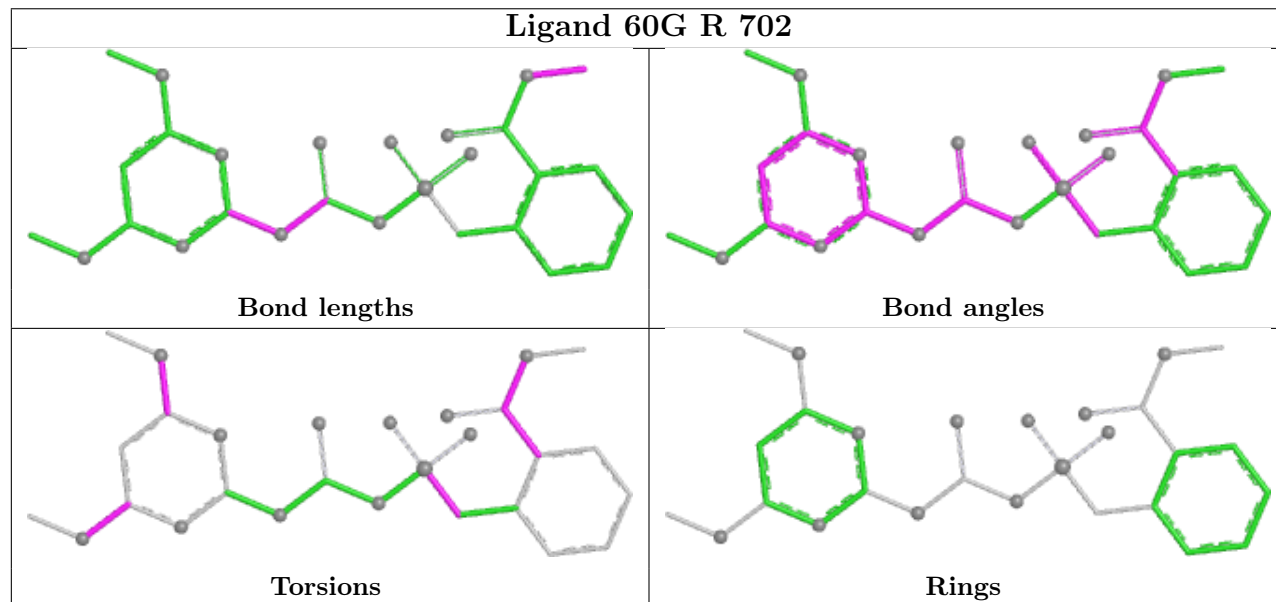
Ligand TPP I 701

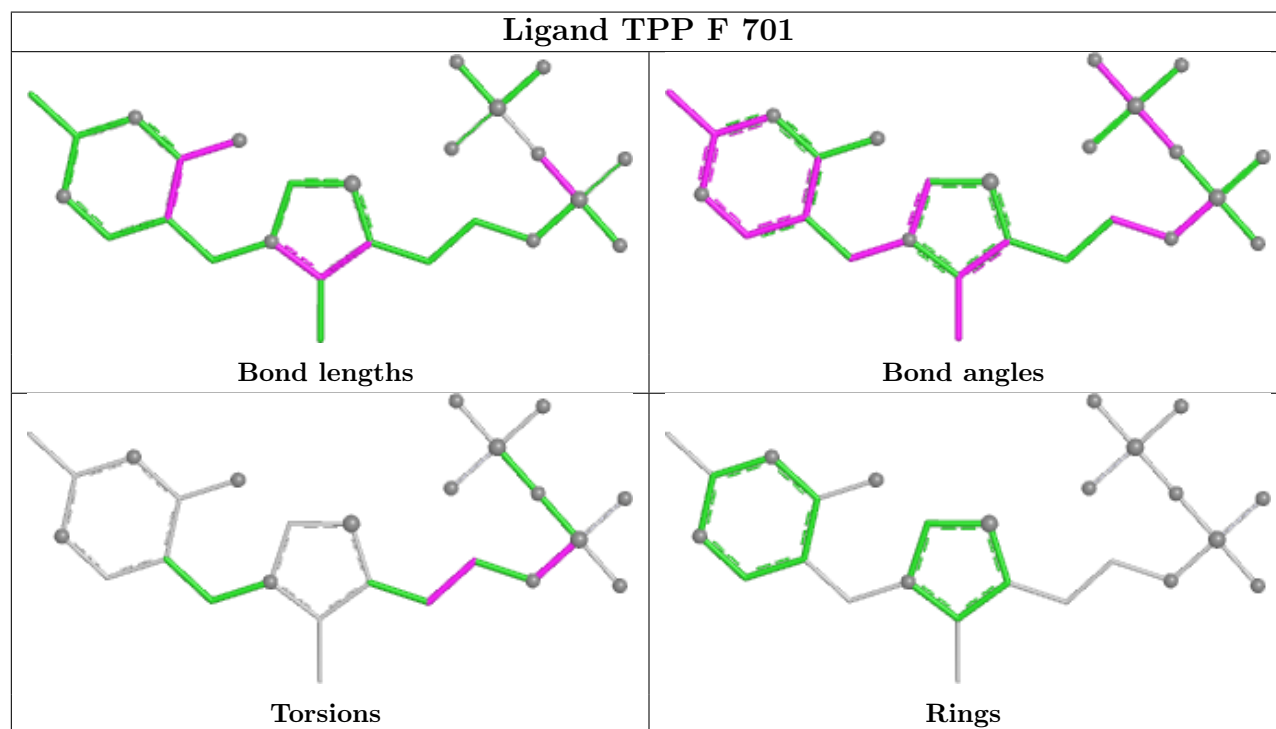
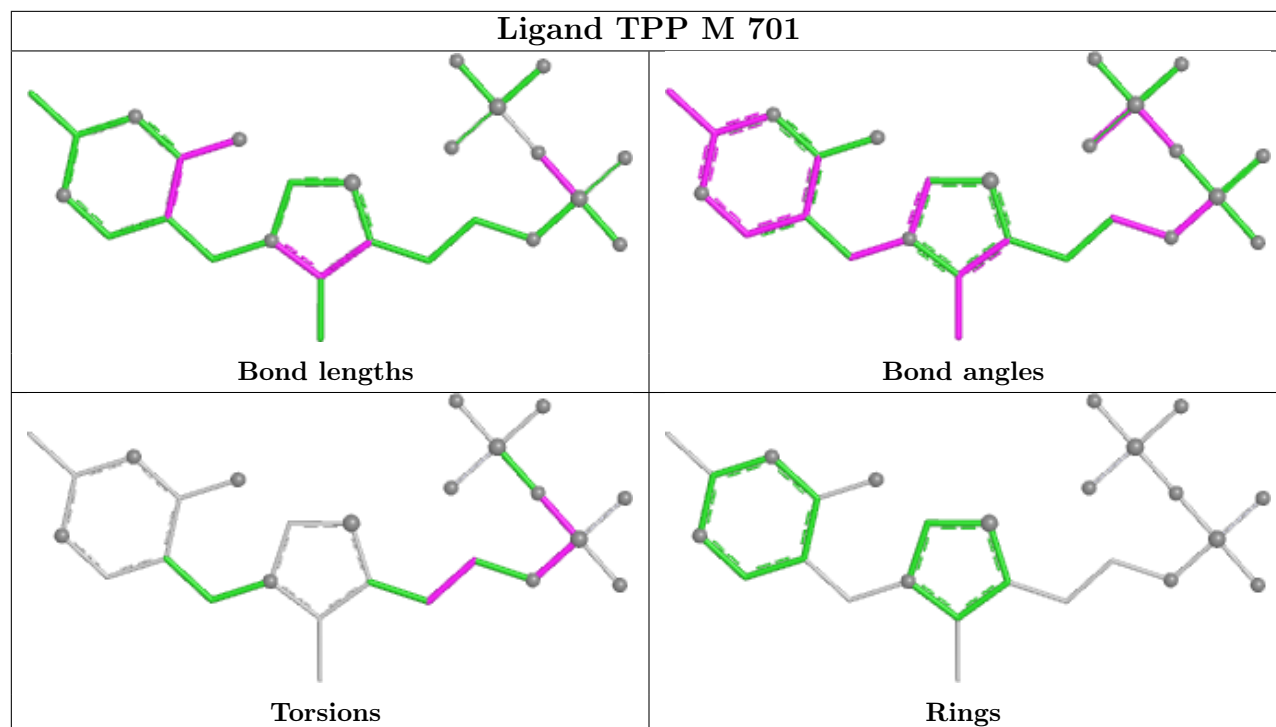


Ligand FAD Q 703

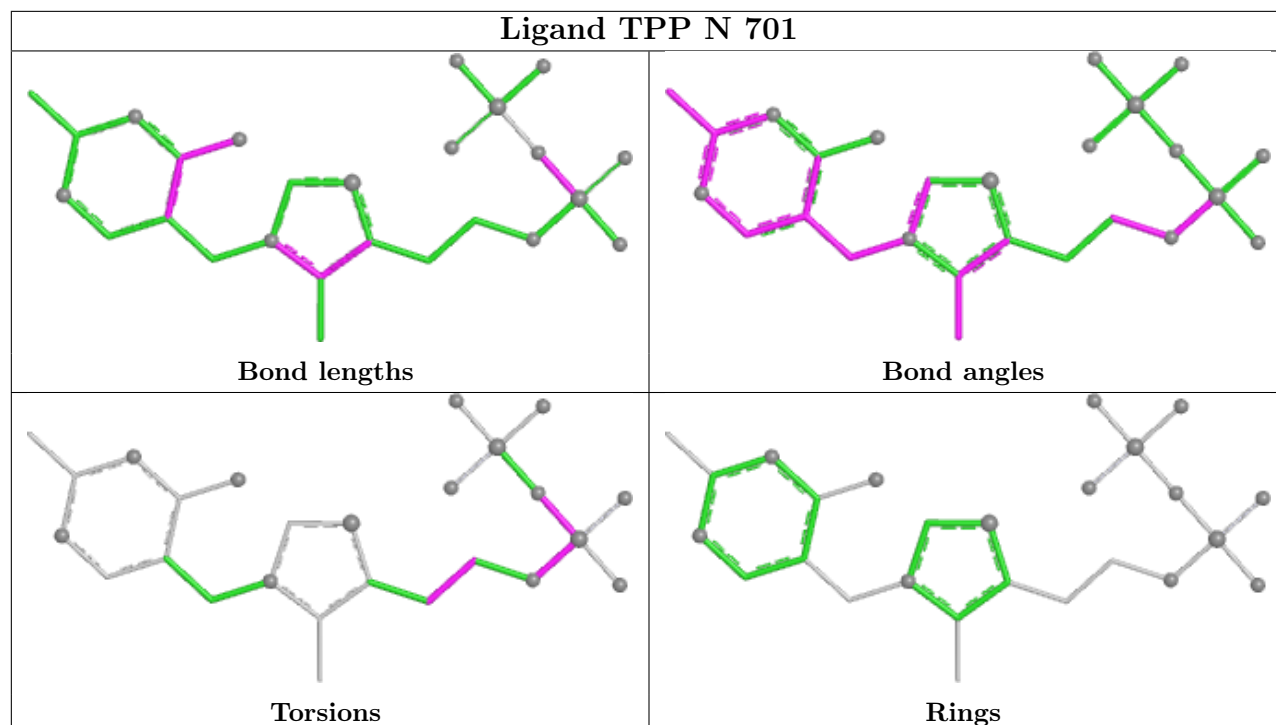


Ligand 60G R 702

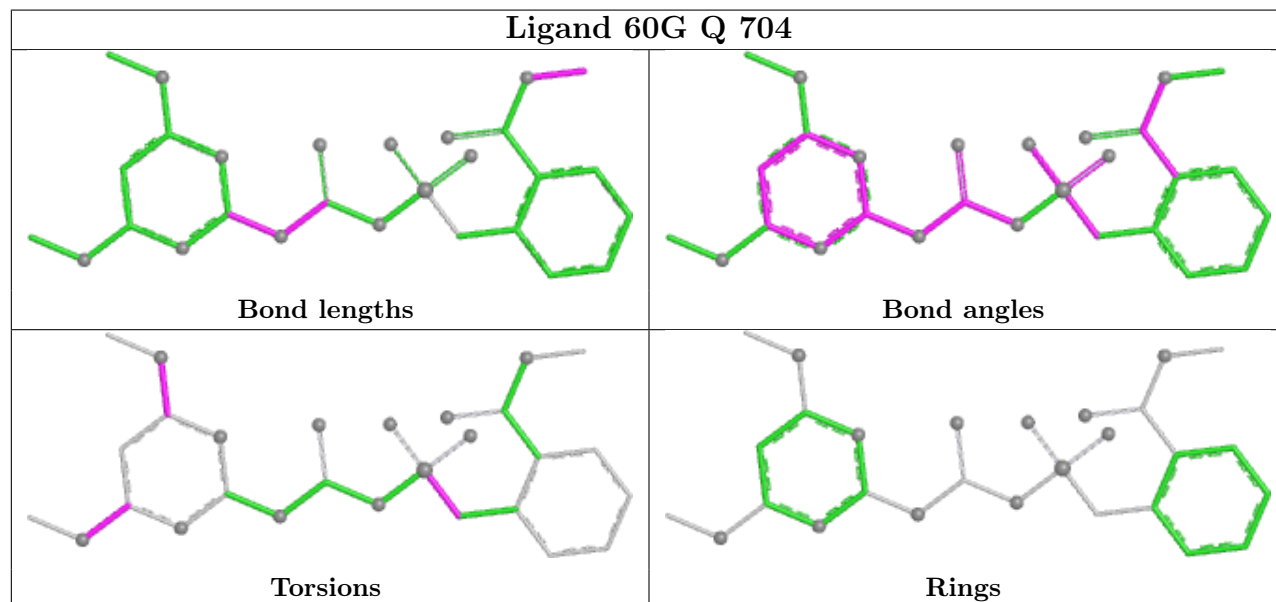




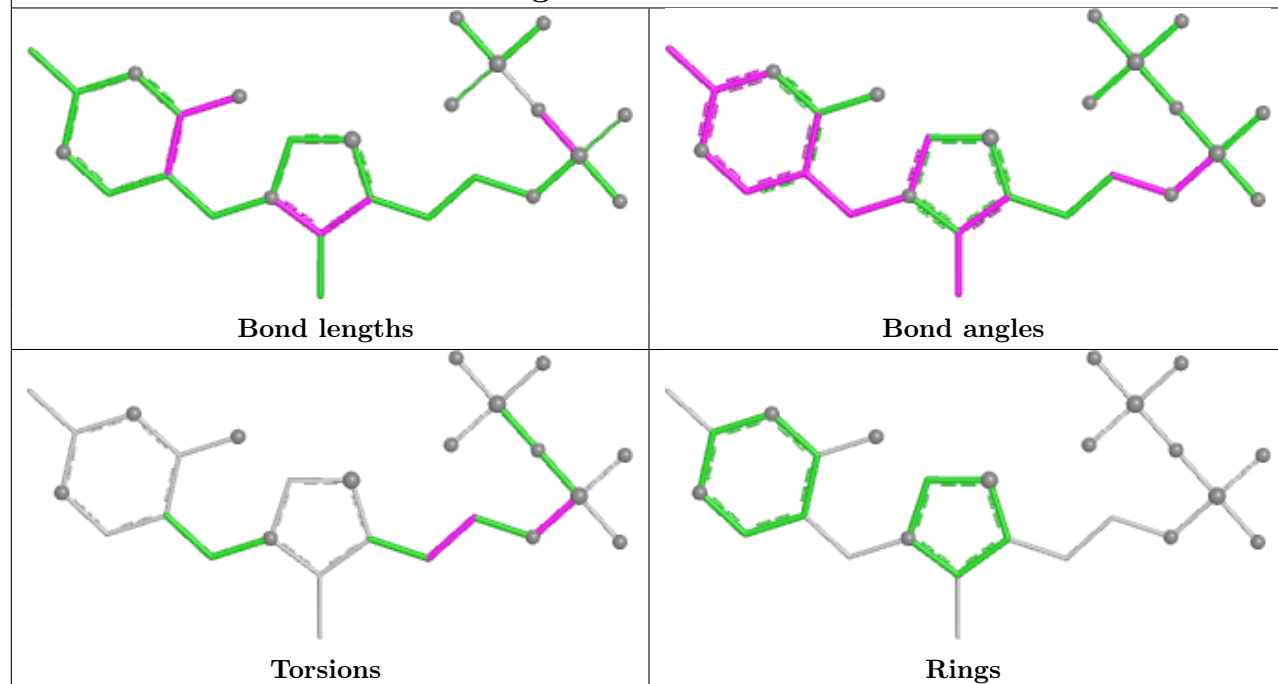
Ligand TPP N 701



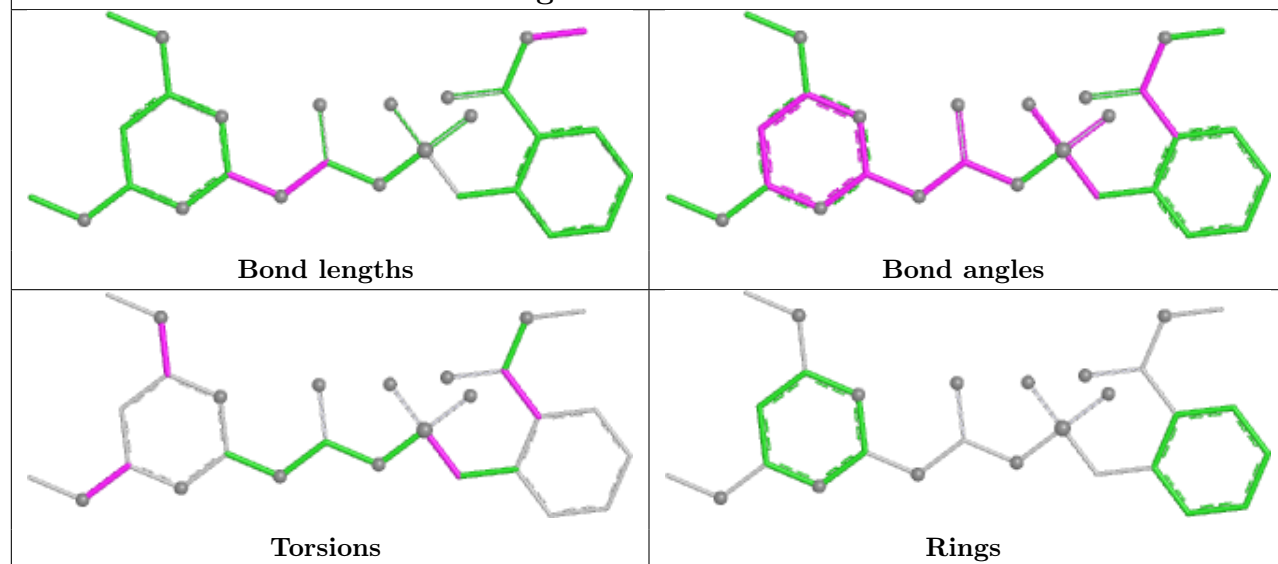
Ligand 60G Q 704



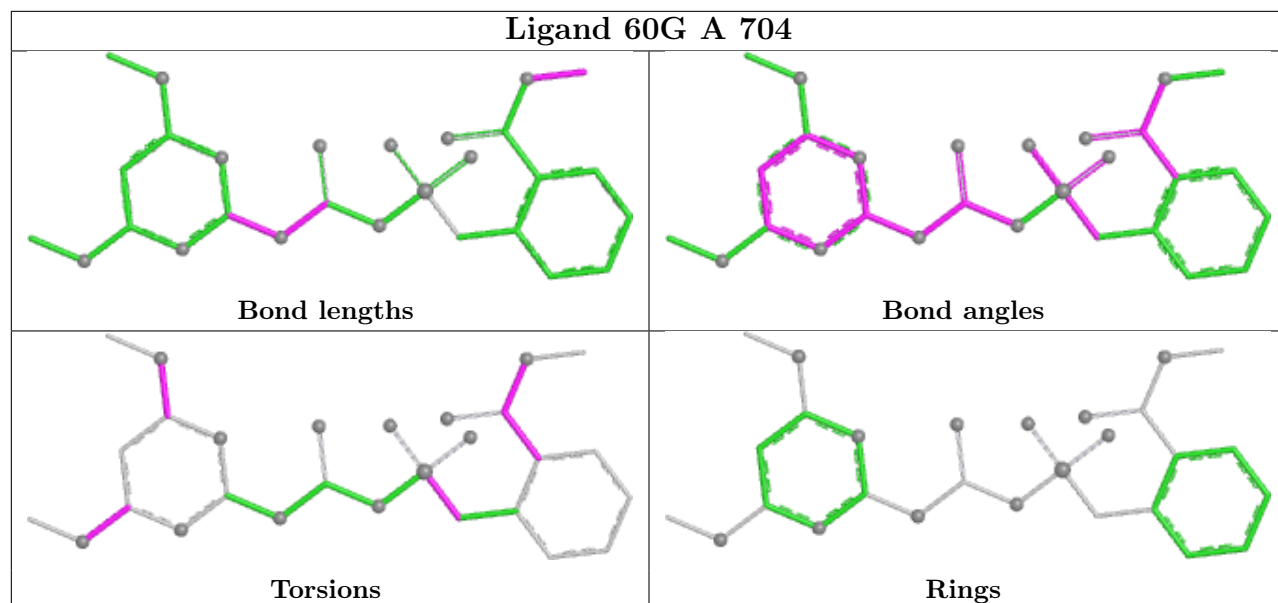
Ligand TPP U 701



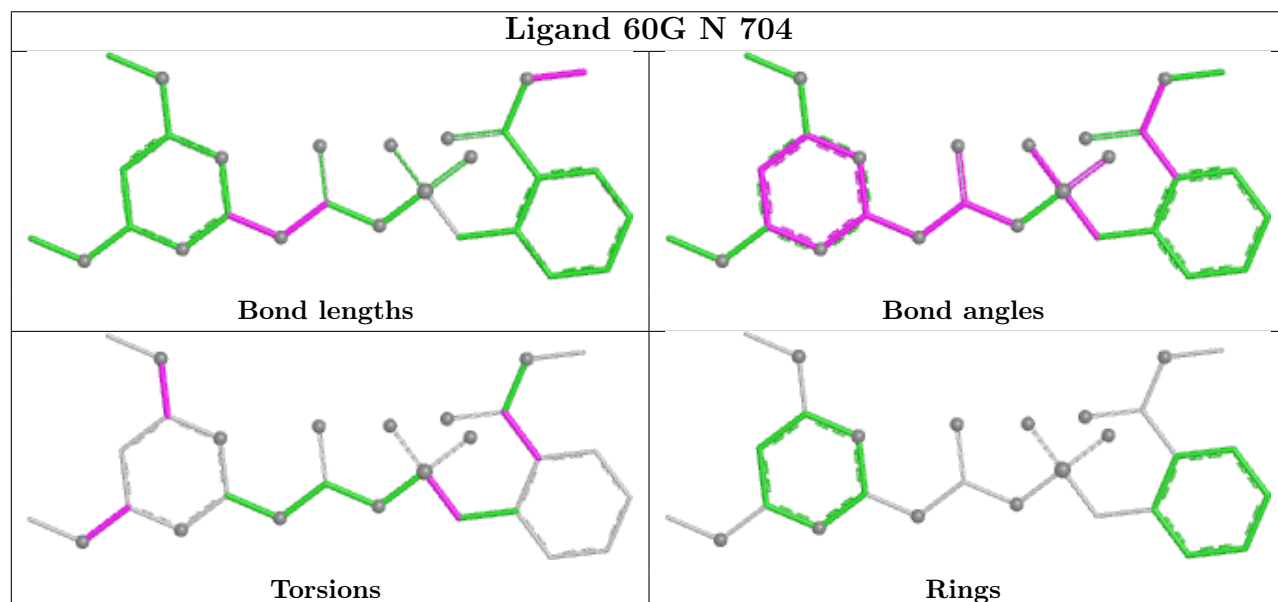
Ligand 60G N 705

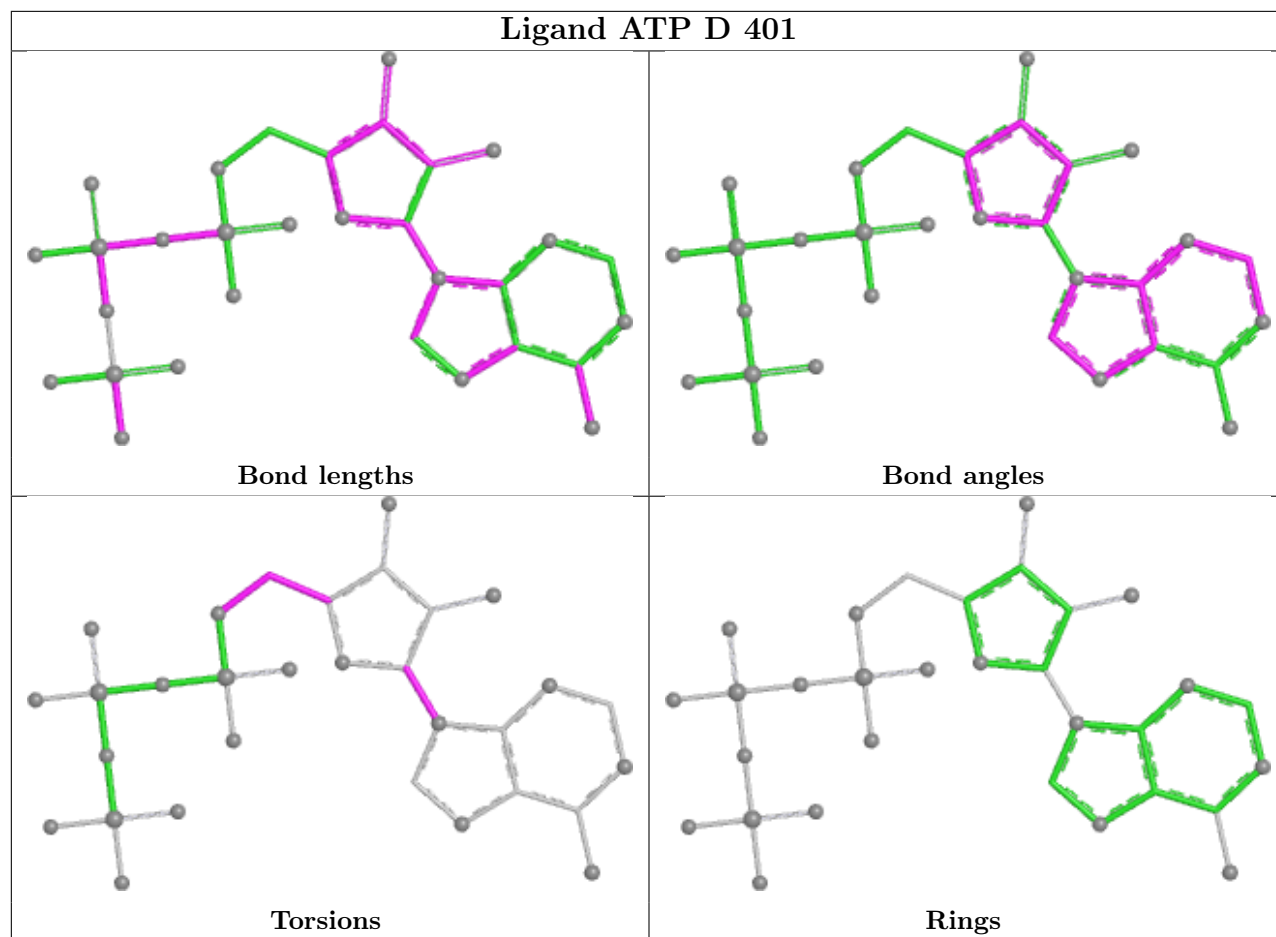


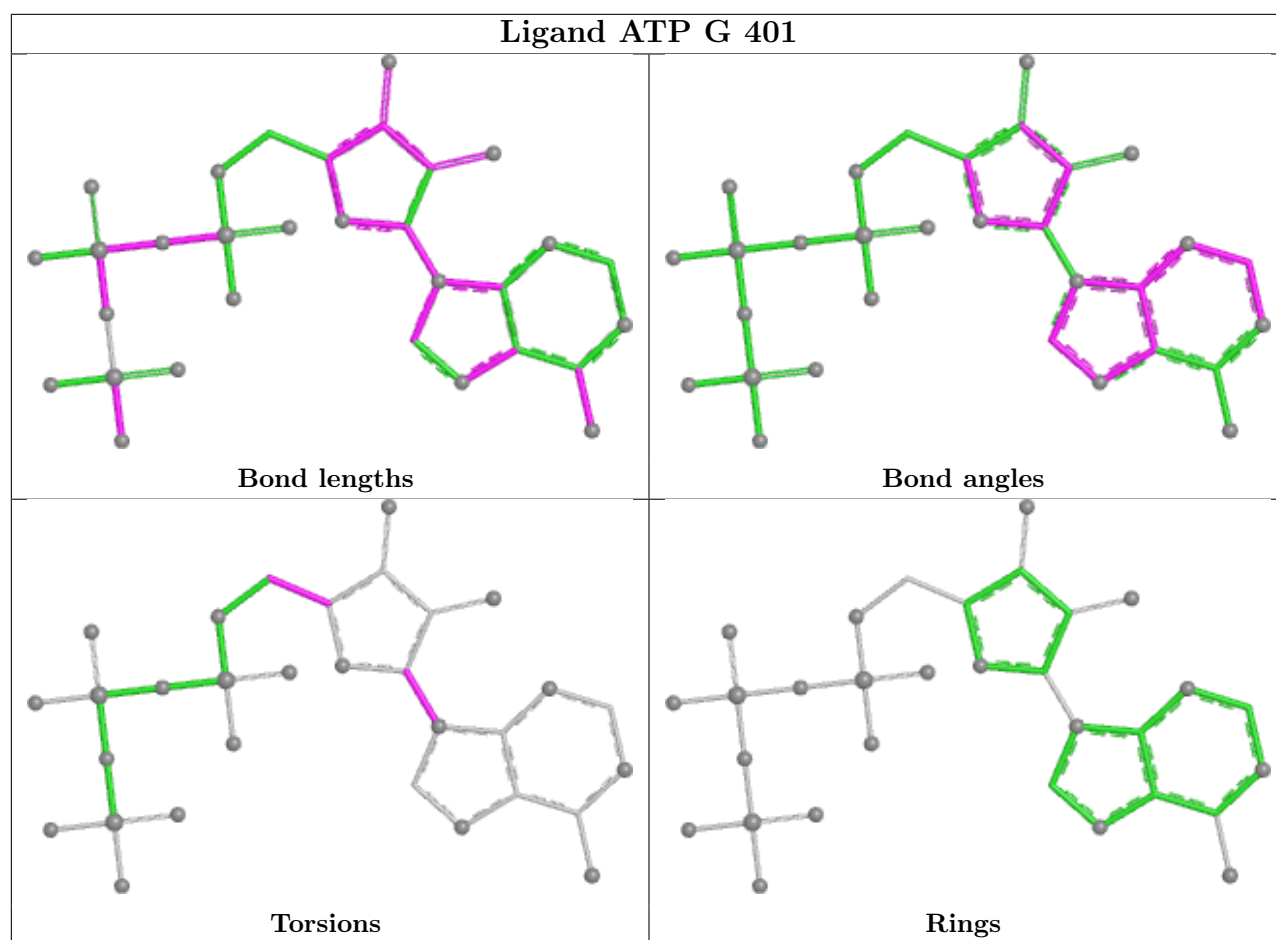
Ligand 60G A 704



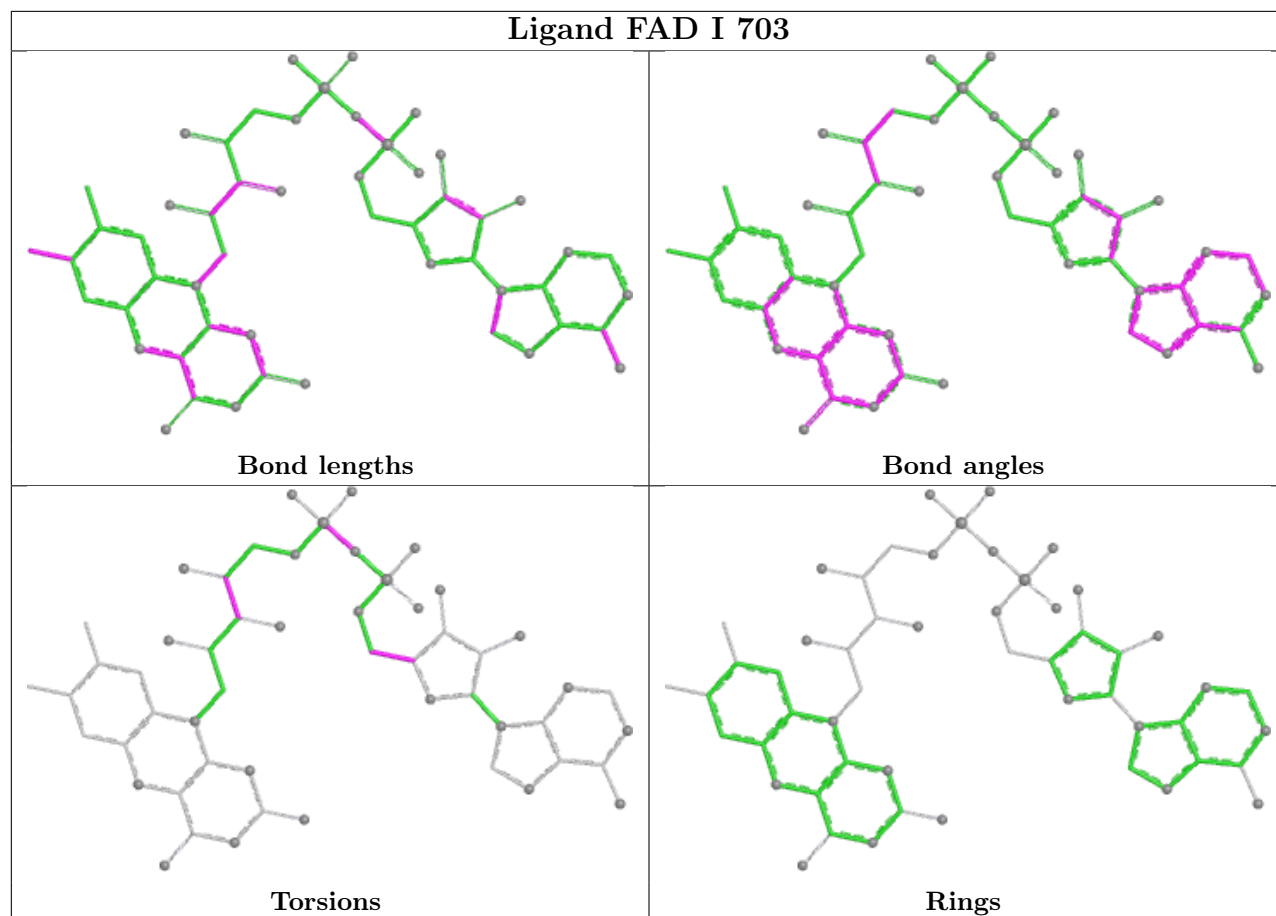
Ligand 60G N 704



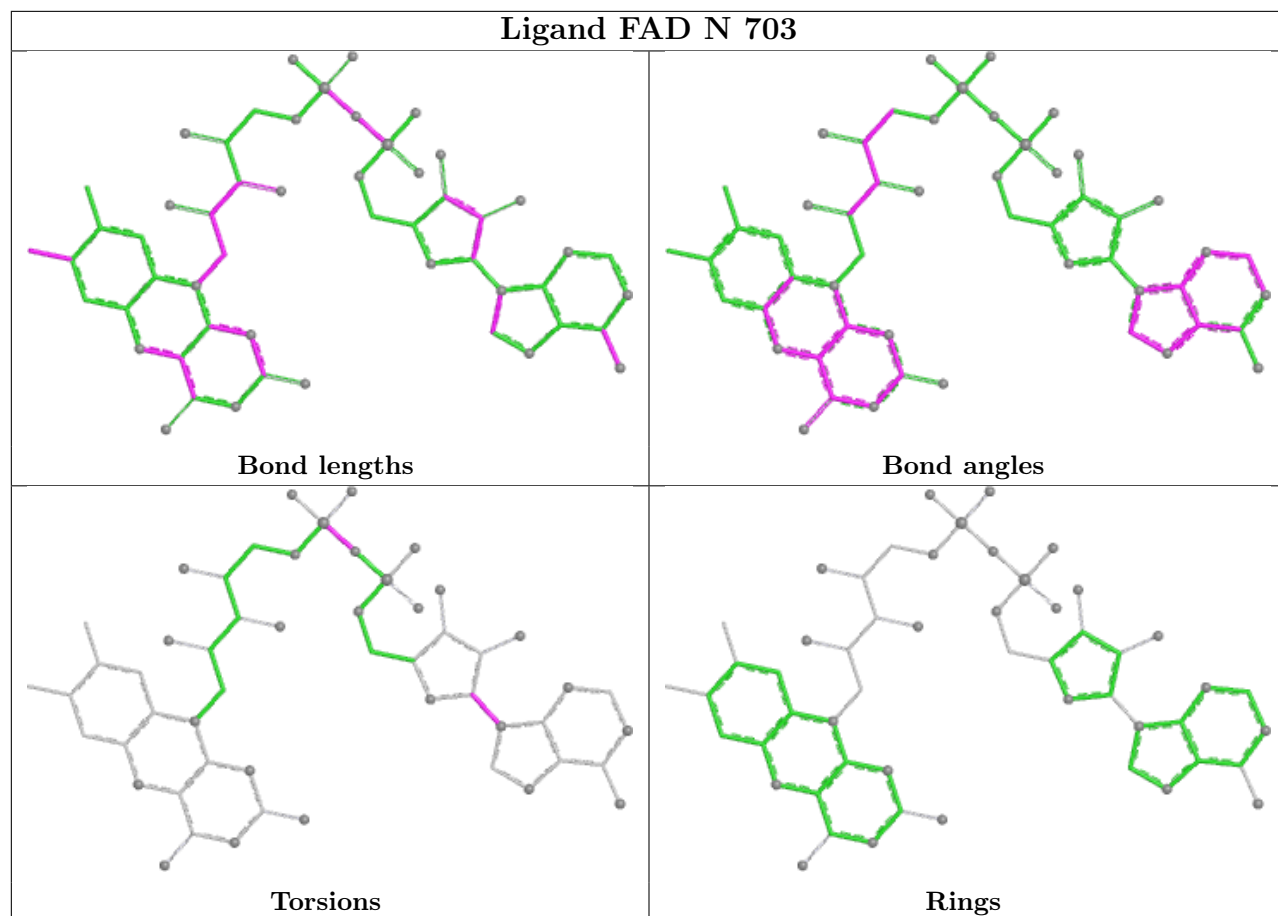




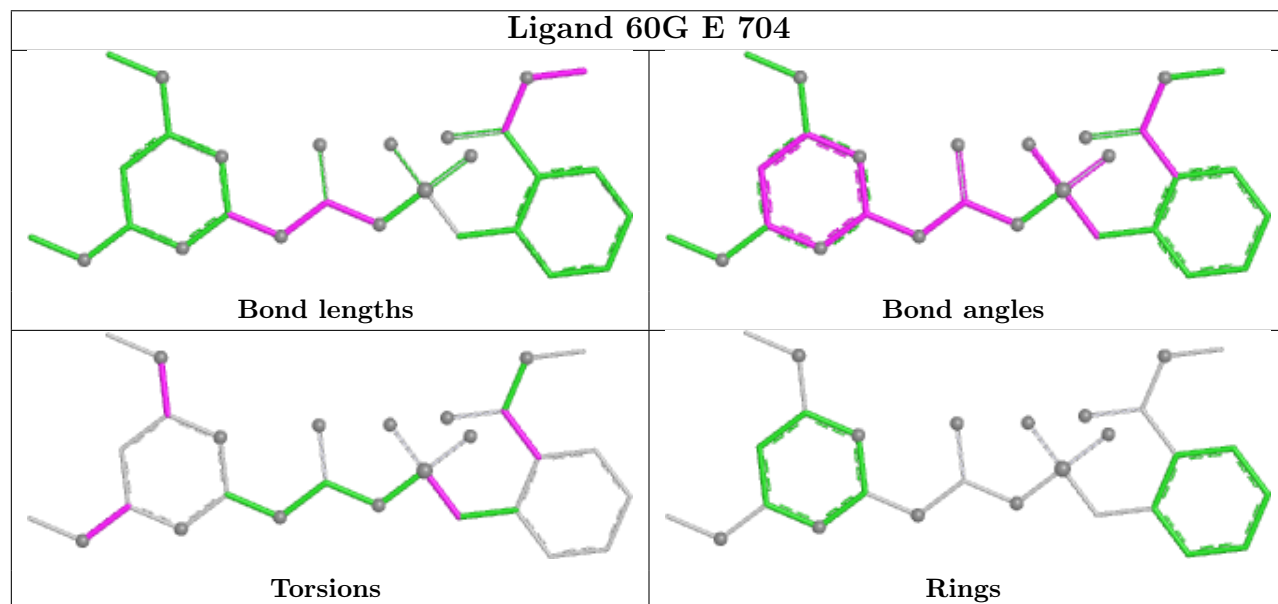
Ligand FAD I 703

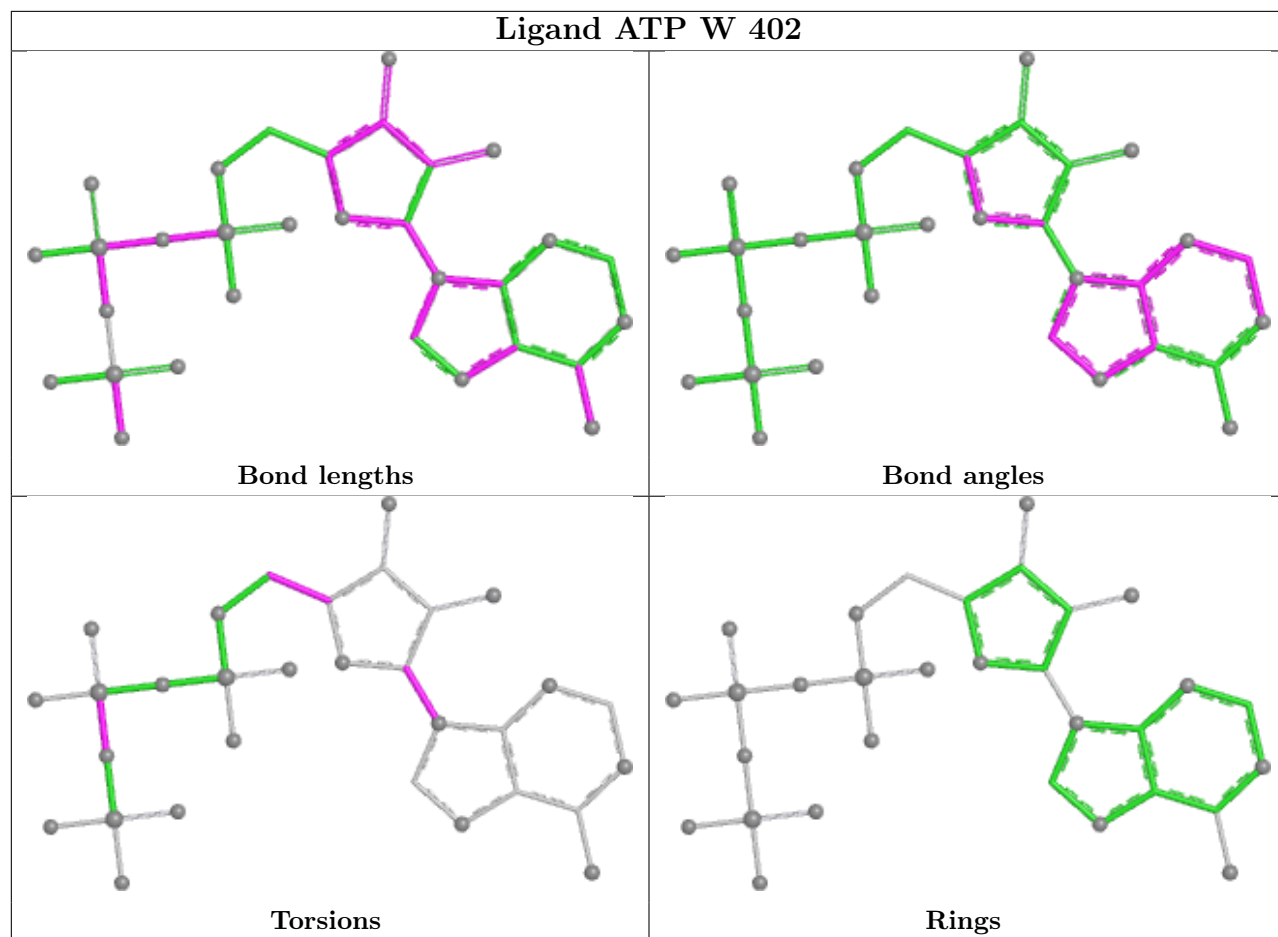


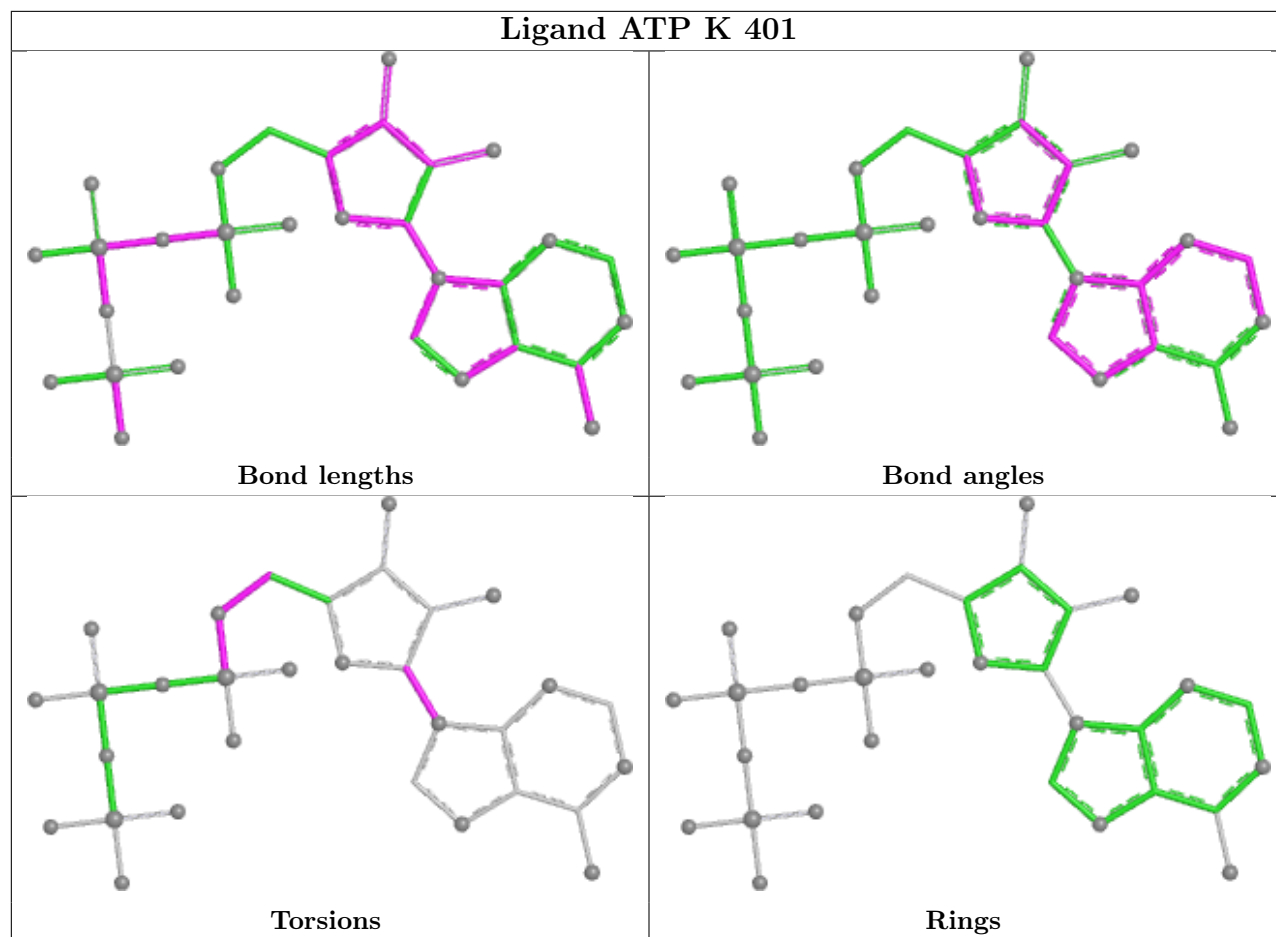
Ligand FAD N 703



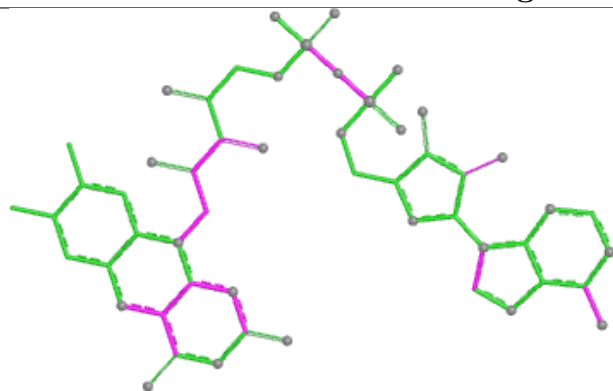
Ligand 60G E 704



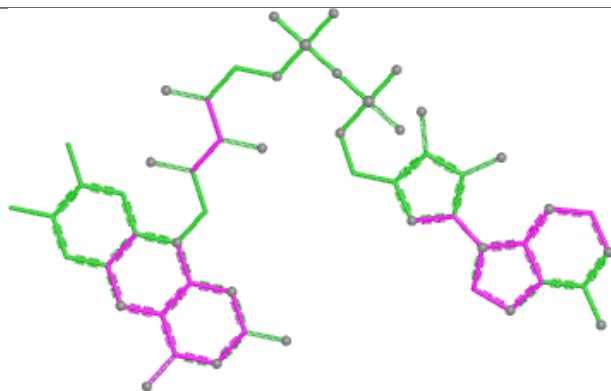




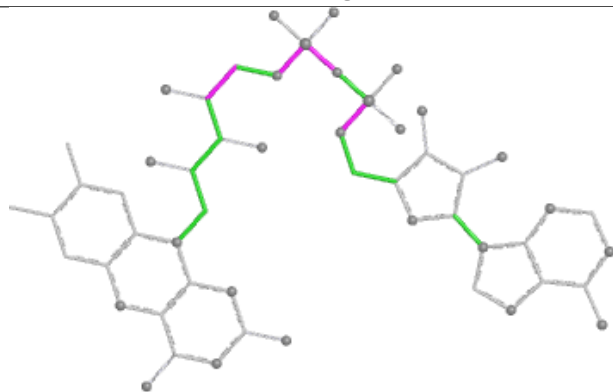
Ligand FAD F 703



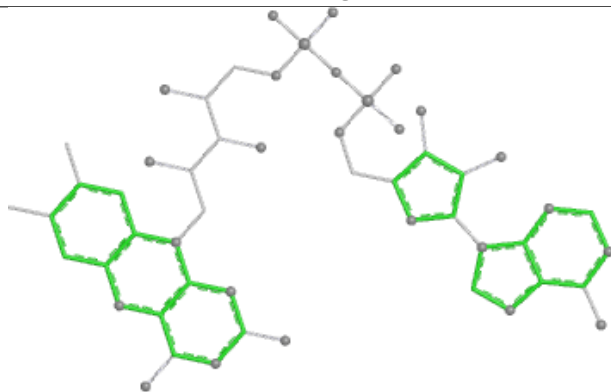
Bond lengths



Bond angles

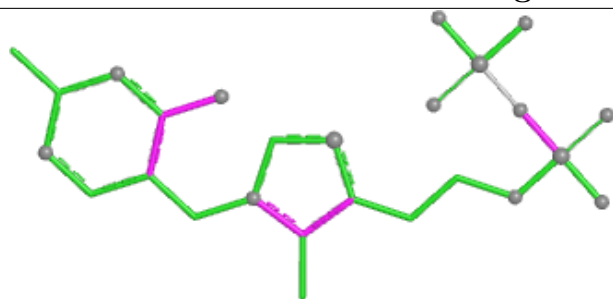


Torsions

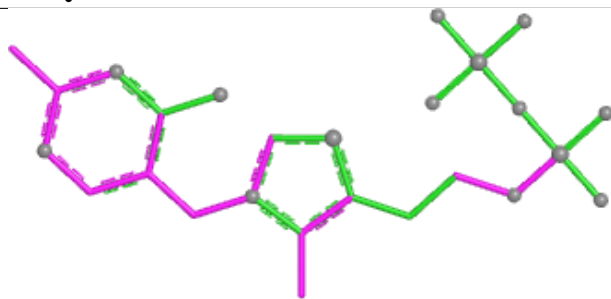


Rings

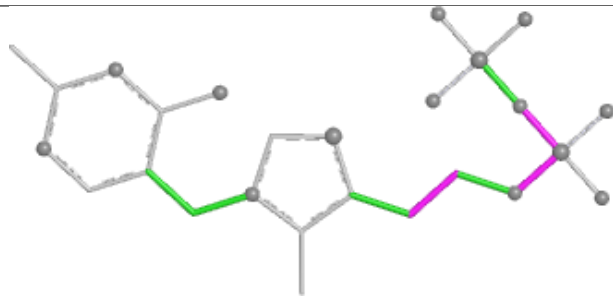
Ligand TPP Q 701



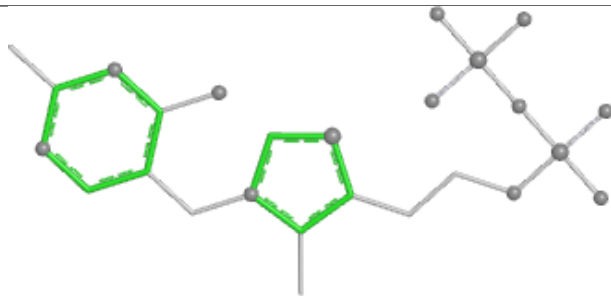
Bond lengths



Bond angles

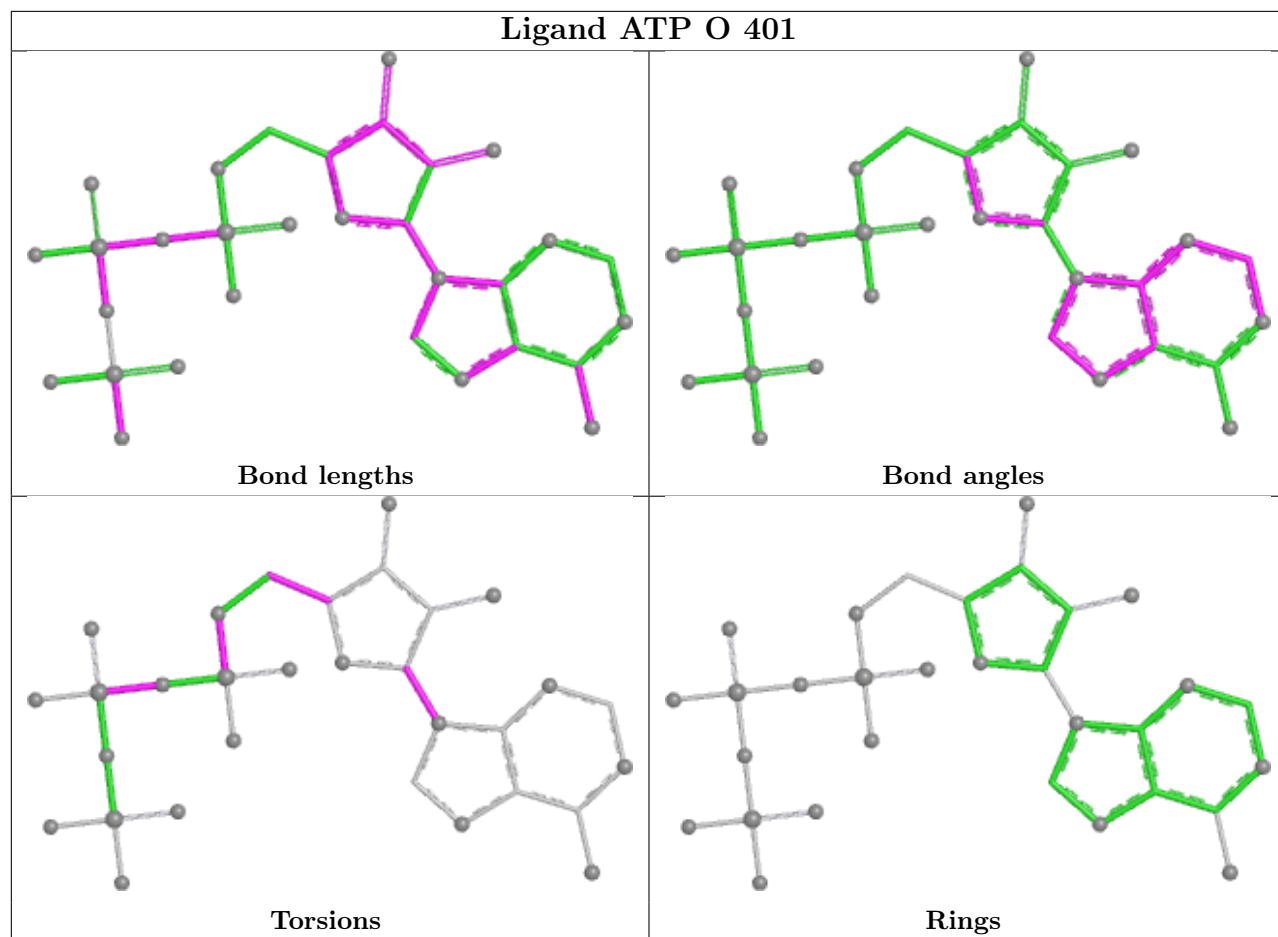


Torsions

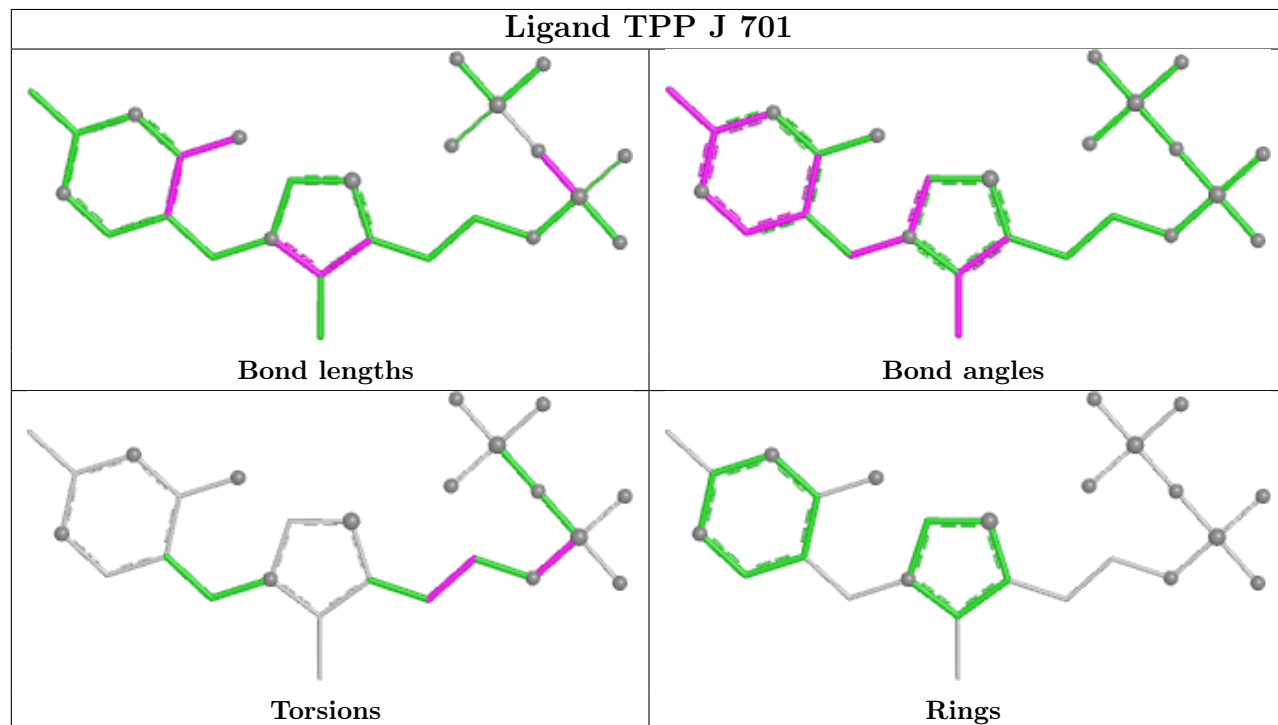


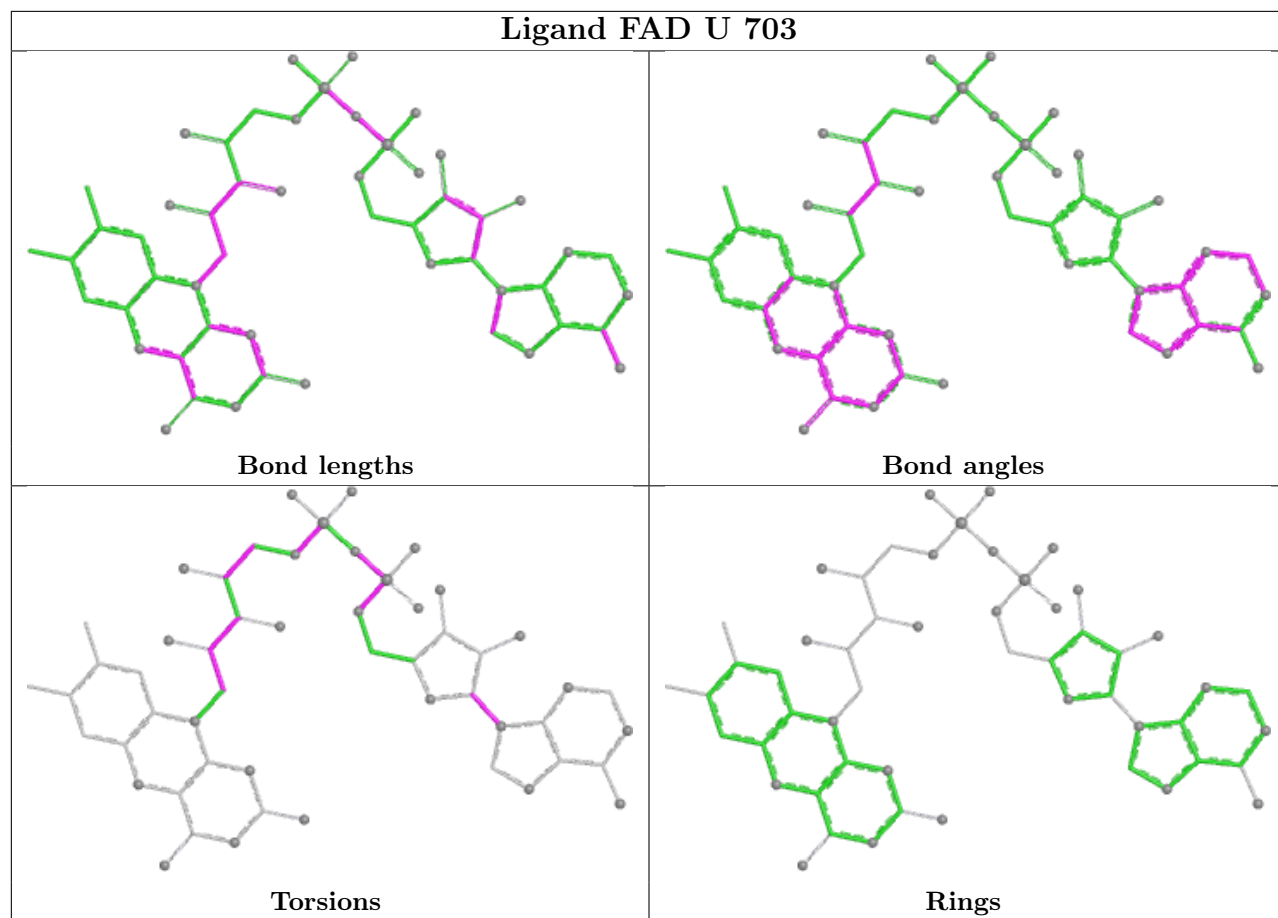
Rings

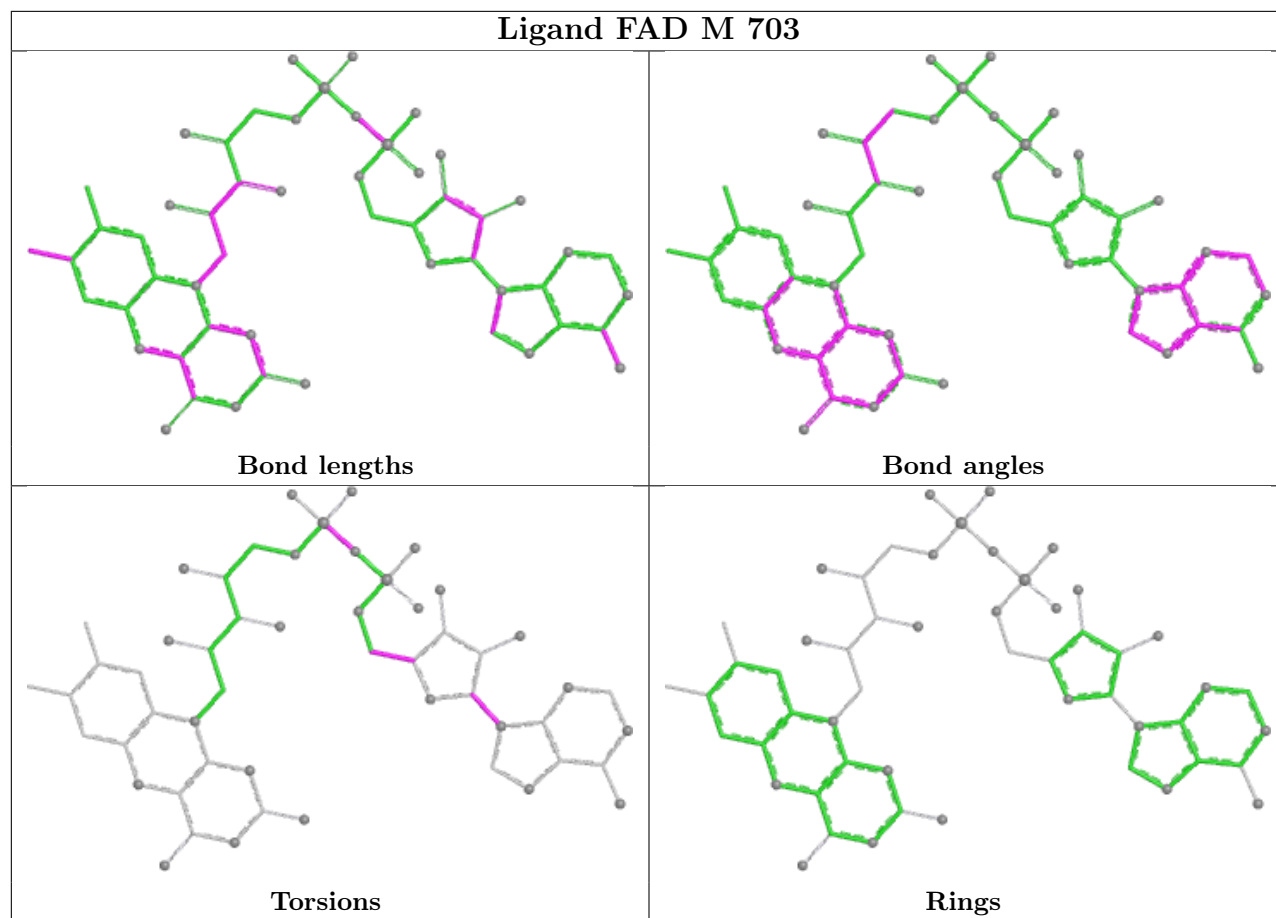
Ligand ATP O 401



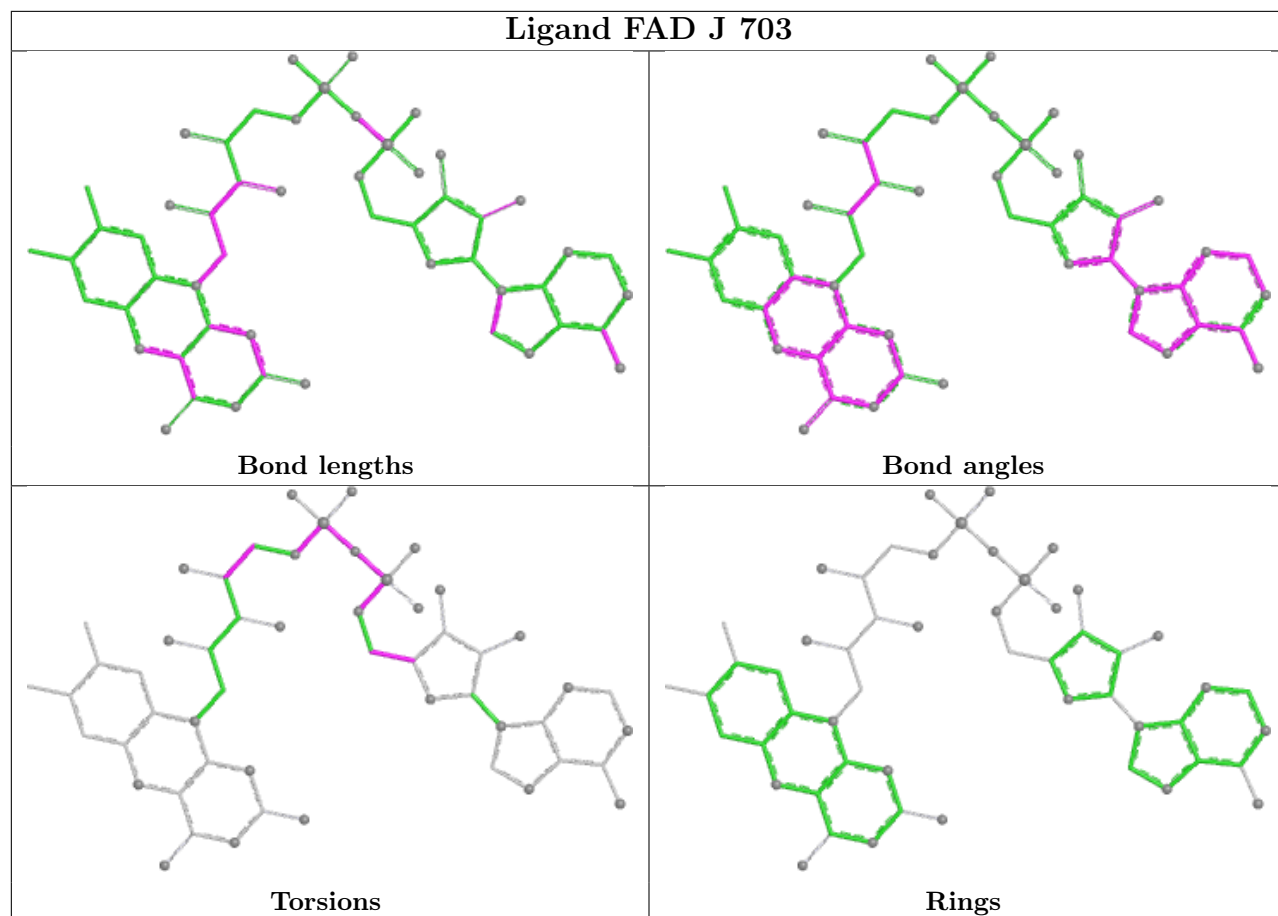
Ligand TPP J 701



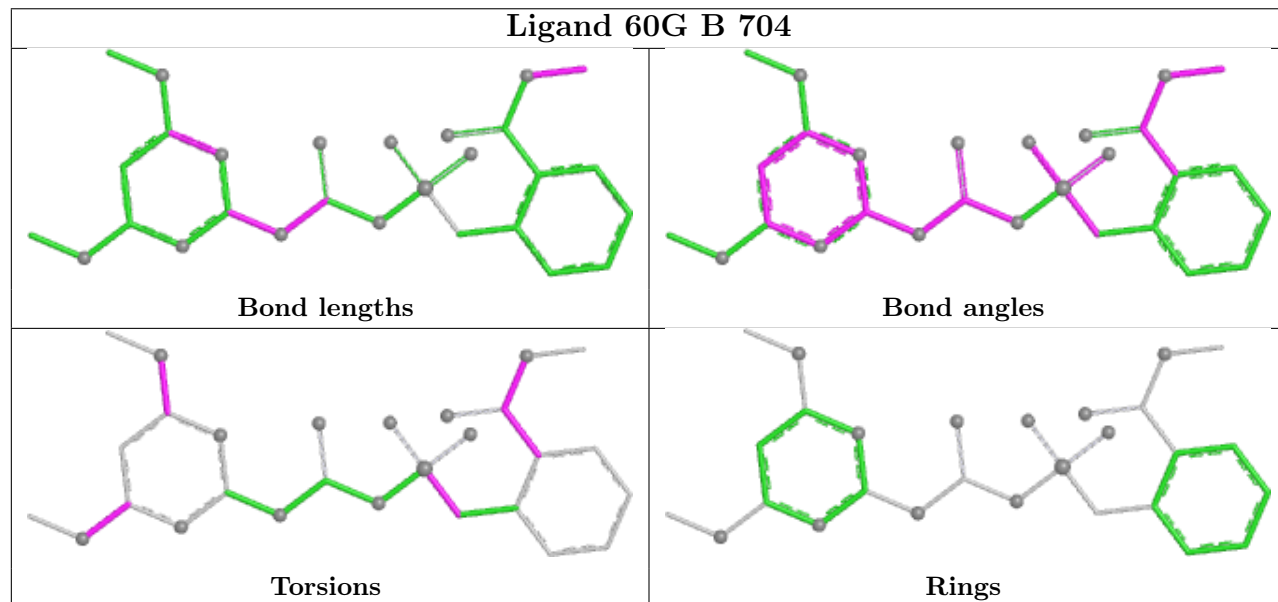


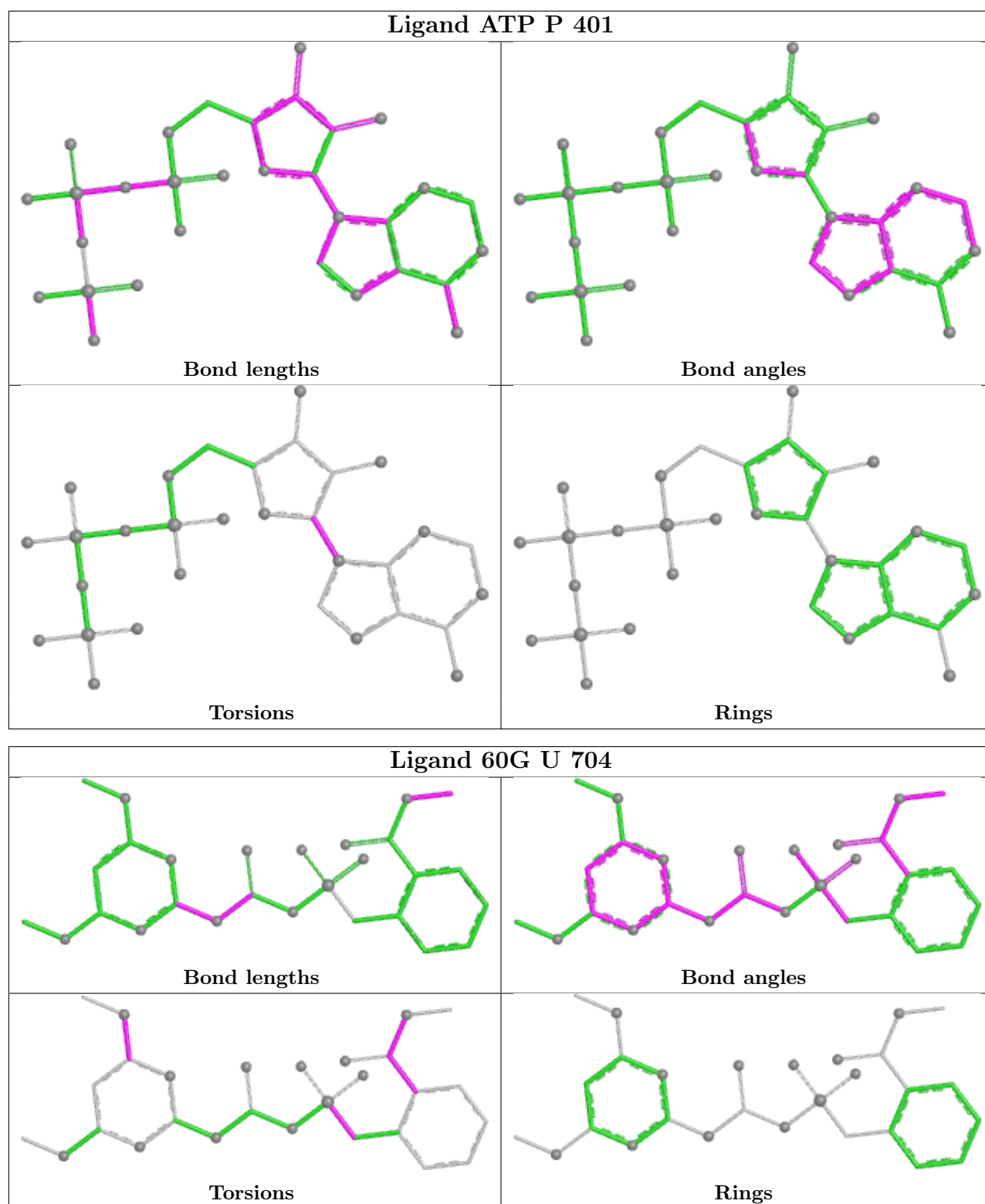


Ligand FAD J 703



Ligand 60G B 704





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

Continued on next page...

Continued from previous page...

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

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	281	THR	5.3
1	J	685	GLY	4.9
1	R	402	GLY	4.8
1	R	559	GLU	4.7
2	C	281	THR	4.6
2	D	281	THR	4.5
1	F	270	SER	4.4
1	R	153	SER	4.3
1	R	562	SER	4.3
1	Q	556	THR	4.2
2	W	69	ALA	4.1
2	T	281	THR	4.0
2	K	285	THR	4.0
1	R	583	VAL	3.9
2	O	185	THR	3.9
1	Q	610	GLU	3.9
1	R	566	ALA	3.9
1	R	152	ALA	3.8
2	G	69	ALA	3.7
1	I	271	ASN	3.7
2	P	281	THR	3.7
2	K	44	PRO	3.7
1	R	338	LEU	3.7
1	R	522	LEU	3.6
2	D	102	GLY	3.5
2	O	283	LEU	3.5
1	R	333	THR	3.5
2	C	51	THR	3.5
2	X	69	ALA	3.5
1	Q	135	LEU	3.5
1	N	273	LEU	3.4
2	T	291	ALA	3.4
1	R	274	ASN	3.3
1	R	314	ALA	3.3
1	J	666	ASN	3.3
1	U	270	SER	3.3
1	R	339	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	276	LEU	3.2
2	L	281	THR	3.2
1	R	302	PRO	3.2
1	R	543	LEU	3.2
2	O	193	GLN	3.2
2	D	285	THR	3.2
2	G	49	LEU	3.1
2	C	44	PRO	3.1
2	W	47	PRO	3.1
1	R	395	ALA	3.1
1	J	334	THR	3.0
1	A	276	LEU	3.0
1	B	276	LEU	3.0
1	I	383	GLY	2.9
2	S	49	LEU	2.9
1	I	554	ASN	2.9
2	S	281	THR	2.9
1	R	529	LEU	2.9
2	T	49	LEU	2.9
1	F	274	ASN	2.9
2	W	281	THR	2.9
2	D	70	PRO	2.9
2	W	71	SER	2.9
1	B	350	ASP	2.9
1	J	350	ASP	2.9
1	F	359	THR	2.8
2	G	68	PRO	2.8
1	R	280	ALA	2.8
2	P	49	LEU	2.8
1	J	463	MET	2.8
1	N	270	SER	2.8
2	K	70	PRO	2.8
2	P	50	ASP	2.8
1	B	383	GLY	2.8
2	C	186	ASN	2.8
1	F	352	LEU	2.8
2	X	71	SER	2.8
1	R	638	PRO	2.7
1	J	466	THR	2.7
1	E	276	LEU	2.7
2	S	74	PRO	2.7
1	R	524	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	171	THR	2.7
2	H	76	LYS	2.7
1	U	267	THR	2.7
1	J	527	TYR	2.7
1	R	544	VAL	2.7
2	S	70	PRO	2.6
1	Q	442	LYS	2.6
2	K	66	GLU	2.6
1	R	265	LYS	2.6
2	S	76	LYS	2.6
1	Q	115	GLY	2.6
1	U	240	GLY	2.6
1	Q	631	GLU	2.6
1	R	484	ALA	2.6
1	R	560	LEU	2.6
1	F	554	ASN	2.6
1	J	344	GLU	2.6
1	F	273	LEU	2.6
1	B	81	ALA	2.6
1	R	551	ALA	2.6
1	J	543	LEU	2.6
2	C	189	ALA	2.6
1	A	270	SER	2.6
2	D	189	ALA	2.6
2	W	45	PRO	2.5
1	E	270	SER	2.5
2	D	68	PRO	2.5
2	L	70	PRO	2.5
1	R	584	THR	2.5
1	R	593	HIS	2.5
2	C	74	PRO	2.5
2	X	184	SER	2.5
1	Q	566	ALA	2.5
2	C	68	PRO	2.5
1	Q	601	LEU	2.5
1	R	365	GLN	2.5
1	E	634	SER	2.5
1	R	382	THR	2.5
2	D	74	PRO	2.5
2	O	68	PRO	2.5
1	R	368	ASP	2.4
1	R	546	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	76	LYS	2.4
2	O	75	ARG	2.4
1	M	352	LEU	2.4
2	D	287	THR	2.4
2	G	187	ALA	2.4
2	K	42	THR	2.4
1	B	83	PRO	2.4
2	T	68	PRO	2.4
2	G	74	PRO	2.4
2	T	45	PRO	2.4
1	R	154	GLY	2.4
1	R	305	TYR	2.4
1	J	511	ARG	2.4
1	M	270	SER	2.4
1	U	467	PRO	2.4
2	W	67	THR	2.4
1	J	545	ILE	2.4
2	C	184	SER	2.4
1	J	544	VAL	2.4
1	R	586	TRP	2.4
2	W	70	PRO	2.4
1	J	498	GLY	2.3
1	U	509	THR	2.3
1	Q	609	ALA	2.3
1	U	275	GLN	2.3
2	X	49	LEU	2.3
1	I	578	GLU	2.3
1	R	107	VAL	2.3
1	I	447	TRP	2.3
1	Q	467	PRO	2.3
2	H	184	SER	2.3
1	J	478	LYS	2.3
2	H	281	THR	2.3
2	W	285	THR	2.3
1	R	396	ALA	2.3
2	C	190	ALA	2.3
1	U	273	LEU	2.3
1	Q	580	GLN	2.3
2	W	89	GLY	2.3
2	D	187	ALA	2.3
2	K	183	THR	2.3
1	R	555	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	312	ASN	2.3
1	R	550	ASP	2.3
1	J	264	THR	2.3
2	H	71	SER	2.3
1	R	576	ASN	2.3
1	J	467	PRO	2.3
1	E	496	GLY	2.3
1	N	627	ALA	2.3
2	P	188	GLY	2.3
1	J	641	LEU	2.3
2	C	287	THR	2.3
1	Q	605	PHE	2.3
1	F	621	LYS	2.3
1	Q	621	LYS	2.3
1	R	527	TYR	2.2
1	Q	673	ARG	2.2
1	B	263	PRO	2.2
1	I	311	LEU	2.2
2	C	171	THR	2.2
1	I	506	GLN	2.2
1	R	112	GLY	2.2
1	R	136	PRO	2.2
2	L	69	ALA	2.2
2	D	284	LYS	2.2
2	K	284	LYS	2.2
1	N	673	ARG	2.2
2	O	280	ARG	2.2
1	Q	635	THR	2.2
2	O	184	SER	2.2
2	C	73	GLN	2.2
2	C	47	PRO	2.2
2	G	233	GLY	2.2
1	Q	266	THR	2.2
1	R	371	ILE	2.2
1	E	273	LEU	2.2
1	I	627	ALA	2.2
1	R	366	ASN	2.2
2	H	86	ASN	2.2
1	E	269	PRO	2.2
1	J	346	PRO	2.2
1	R	183	PRO	2.2
1	R	337	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	74	PRO	2.2
1	J	129	ASP	2.2
2	O	50	ASP	2.2
1	R	257	ILE	2.1
1	R	296	ILE	2.1
2	D	199	ILE	2.1
1	Q	622	GLN	2.1
2	T	134	GLN	2.1
2	W	77	GLN	2.1
1	Q	137	LYS	2.1
2	K	291	ALA	2.1
1	R	569	PRO	2.1
2	C	45	PRO	2.1
2	W	68	PRO	2.1
1	R	632	PHE	2.1
1	U	548	ASP	2.1
1	Q	267	THR	2.1
1	R	556	THR	2.1
2	G	77	GLN	2.1
2	G	70	PRO	2.1
2	G	71	SER	2.1
2	S	282	PRO	2.1
1	I	132	ASN	2.1
2	G	104	ASN	2.1
1	I	364	VAL	2.1
2	O	116	LYS	2.1
2	X	281	THR	2.1
2	D	75	ARG	2.1
2	L	187	ALA	2.1
2	P	45	PRO	2.1
1	Q	606	ILE	2.1
2	D	49	LEU	2.1
2	W	49	LEU	2.1
1	J	534	GLY	2.1
1	U	337	GLY	2.1
2	W	74	PRO	2.1
1	I	276	LEU	2.1
1	U	276	LEU	2.1
2	C	46	LEU	2.1
1	A	507	HIS	2.1
1	U	507	HIS	2.1
2	G	291	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	S	291	ALA	2.1
1	I	685	GLY	2.1
2	H	249	SER	2.0
1	Q	529	LEU	2.0
1	I	266	THR	2.0
2	C	187	ALA	2.0
2	G	189	ALA	2.0
2	L	56	ALA	2.0
2	L	152	THR	2.0
2	T	48	THR	2.0
2	W	291	ALA	2.0
1	F	448	PHE	2.0
1	R	281	GLN	2.0
1	Q	681	LYS	2.0
2	L	76	LYS	2.0
2	S	295	GLU	2.0
2	P	46	LEU	2.0
1	R	430	ASN	2.0
1	R	266	THR	2.0
2	L	41	ALA	2.0
2	O	287	THR	2.0
1	R	114	PRO	2.0
1	R	158	VAL	2.0
1	J	273	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	MG	Q	702	1/1	0.76	0.12	137,137,137,137	0
6	60G	R	702	28/28	0.80	0.17	66,105,122,137	0
6	60G	I	704	28/28	0.84	0.16	53,75,91,104	0
5	FAD	R	701	53/53	0.84	0.14	79,105,131,145	0
3	TPP	Q	701	26/26	0.90	0.14	42,108,149,232	0
7	ATP	L	401	31/31	0.90	0.12	22,56,127,136	0
3	TPP	N	701	26/26	0.91	0.12	32,50,92,109	0
3	TPP	E	701	26/26	0.91	0.13	47,67,103,136	0
6	60G	J	704	28/28	0.91	0.12	51,75,90,104	0
3	TPP	I	701	26/26	0.91	0.13	46,91,106,154	0
4	MG	V	702	1/1	0.91	0.15	63,63,63,63	0
3	TPP	J	701	26/26	0.92	0.11	54,91,135,145	0
7	ATP	D	401	31/31	0.92	0.10	37,56,84,94	0
6	60G	E	704	28/28	0.92	0.12	60,70,88,99	0
7	ATP	W	401	31/31	0.92	0.10	10,42,76,83	0
3	TPP	U	701	26/26	0.93	0.13	26,64,105,143	0
5	FAD	I	703	53/53	0.93	0.11	32,74,100,132	0
6	60G	N	704	28/28	0.93	0.12	37,54,80,91	0
5	FAD	J	703	53/53	0.93	0.10	37,55,88,132	0
4	MG	E	702	1/1	0.93	0.06	77,77,77,77	0
7	ATP	H	401	31/31	0.93	0.10	8,58,82,105	0
7	ATP	K	401	31/31	0.93	0.09	36,65,75,82	0
3	TPP	F	701	26/26	0.93	0.12	36,68,92,132	0
7	ATP	S	401	31/31	0.93	0.09	25,51,71,75	0
6	60G	F	704	28/28	0.93	0.12	35,68,81,88	0
4	MG	W	403	1/1	0.94	0.15	29,29,29,29	0
7	ATP	G	401	31/31	0.94	0.09	27,55,82,116	0
5	FAD	E	703	53/53	0.94	0.09	39,60,85,134	0
5	FAD	F	703	53/53	0.94	0.09	43,69,84,102	0
6	60G	N	705	28/28	0.94	0.11	34,58,68,74	0
7	ATP	O	401	31/31	0.94	0.10	9,66,87,104	0
4	MG	F	702	1/1	0.94	0.07	50,50,50,50	0
6	60G	U	704	28/28	0.94	0.11	24,56,73,75	0
3	TPP	M	701	26/26	0.95	0.11	11,50,91,103	0
7	ATP	P	401	31/31	0.95	0.09	24,49,73,128	0
5	FAD	U	703	53/53	0.95	0.09	25,52,75,121	0
7	ATP	T	401	31/31	0.95	0.10	21,44,78,82	0
5	FAD	N	703	53/53	0.95	0.10	42,63,86,102	0
7	ATP	W	402	31/31	0.95	0.08	11,46,70,78	0
7	ATP	C	401	31/31	0.96	0.08	16,43,86,94	0
6	60G	B	704	28/28	0.96	0.09	11,40,62,69	0
5	FAD	B	703	53/53	0.96	0.08	10,42,56,61	0
5	FAD	M	703	53/53	0.96	0.08	25,41,59,63	0

Continued on next page...

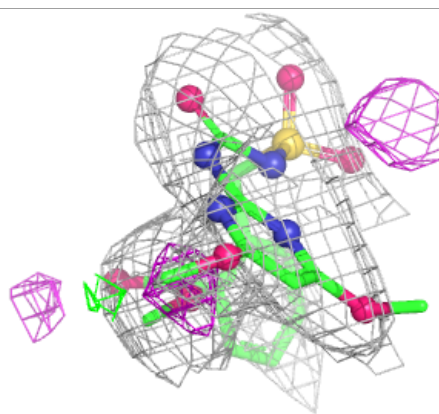
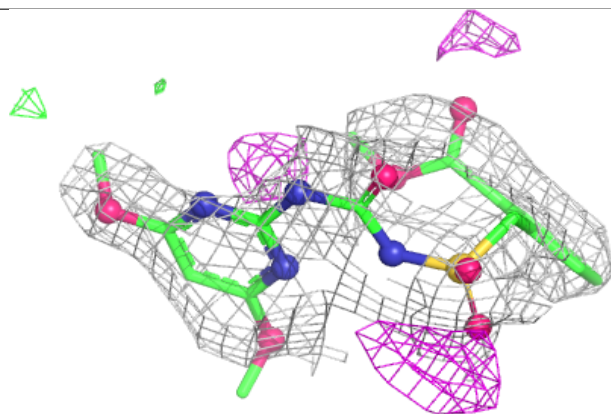
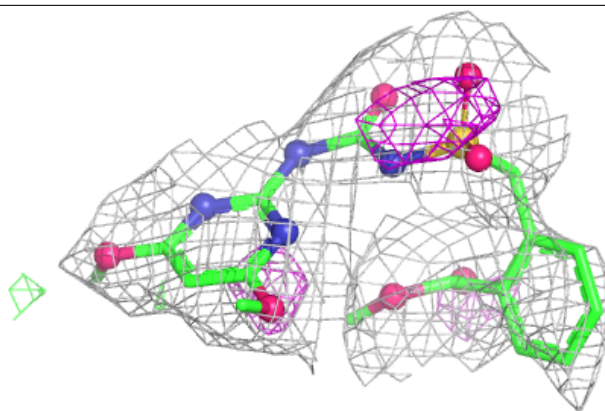
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TPP	B	701	26/26	0.96	0.09	15,41,63,74	0
5	FAD	Q	703	53/53	0.96	0.08	17,44,71,74	0
3	TPP	V	701	26/26	0.96	0.09	9,50,69,119	0
4	MG	H	402	1/1	0.96	0.10	53,53,53,53	0
6	60G	Q	704	28/28	0.96	0.11	45,63,75,82	0
5	FAD	V	703	53/53	0.96	0.08	22,37,50,57	0
6	60G	A	704	28/28	0.96	0.10	18,45,64,79	0
6	60G	V	704	28/28	0.96	0.10	17,48,64,82	0
5	FAD	A	703	53/53	0.97	0.07	19,37,51,65	0
4	MG	C	402	1/1	0.97	0.09	61,61,61,61	0
3	TPP	A	701	26/26	0.97	0.08	13,41,66,77	0
4	MG	N	702	1/1	0.97	0.04	84,84,84,84	0
4	MG	J	702	1/1	0.98	0.04	99,99,99,99	0
4	MG	L	402	1/1	0.98	0.07	74,74,74,74	0
4	MG	B	702	1/1	0.98	0.10	30,30,30,30	0
4	MG	A	702	1/1	0.98	0.06	19,19,19,19	0
4	MG	D	402	1/1	0.98	0.06	40,40,40,40	0
4	MG	I	702	1/1	0.98	0.04	49,49,49,49	0
4	MG	M	702	1/1	0.99	0.04	27,27,27,27	0
4	MG	U	702	1/1	0.99	0.02	44,44,44,44	0

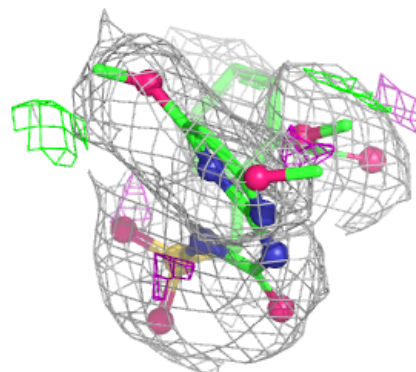
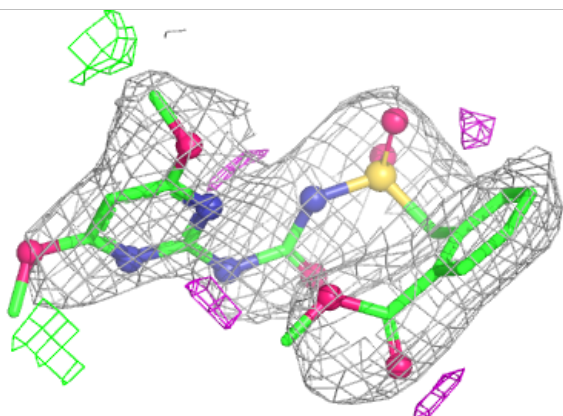
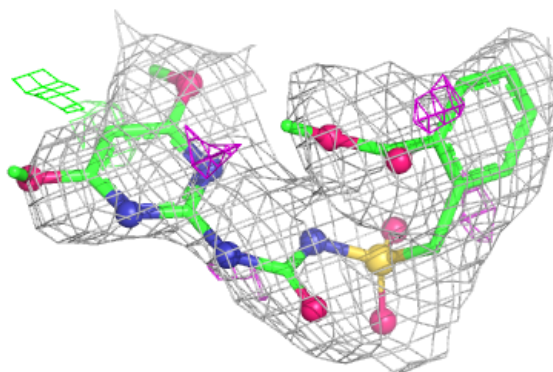
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 60G R 702:

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

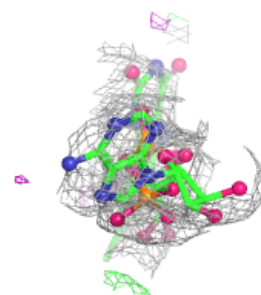
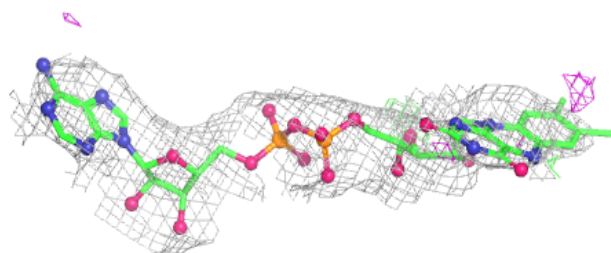
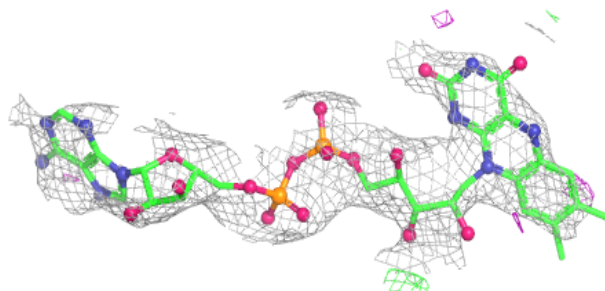
**Electron density around 60G I 704:**

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

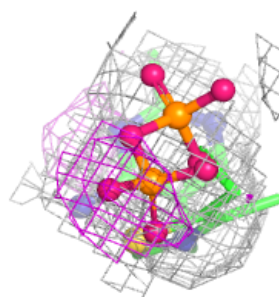
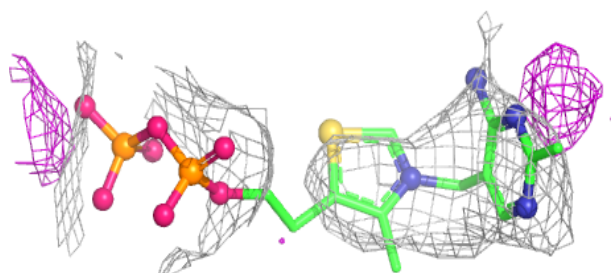
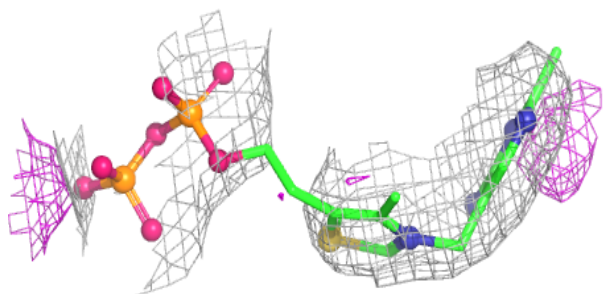


Electron density around FAD R 701:

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

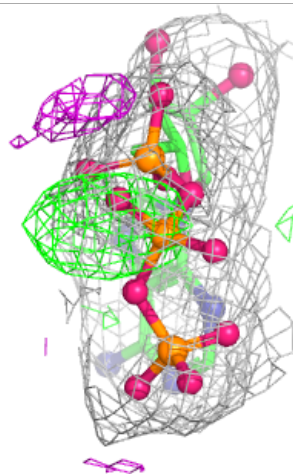
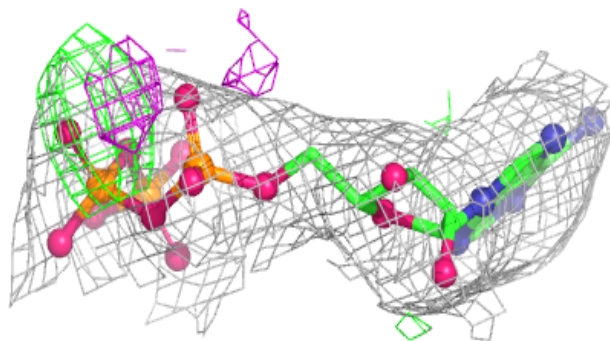
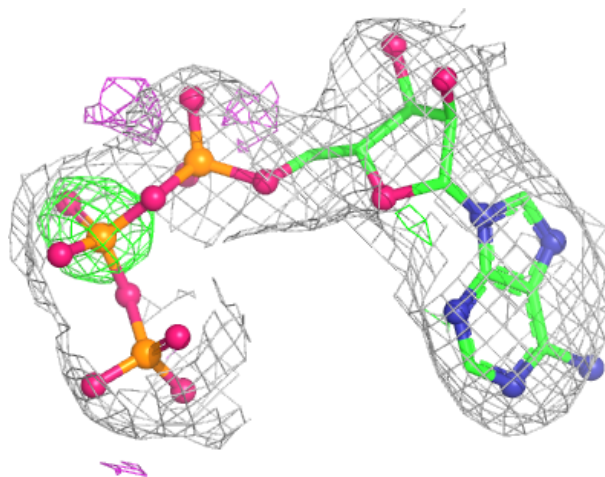
**Electron density around TPP Q 701:**

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



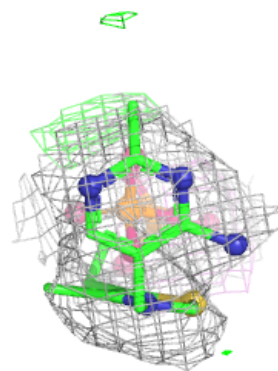
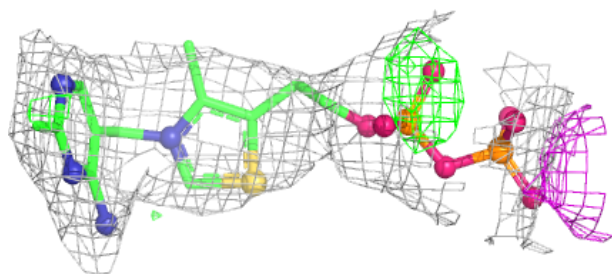
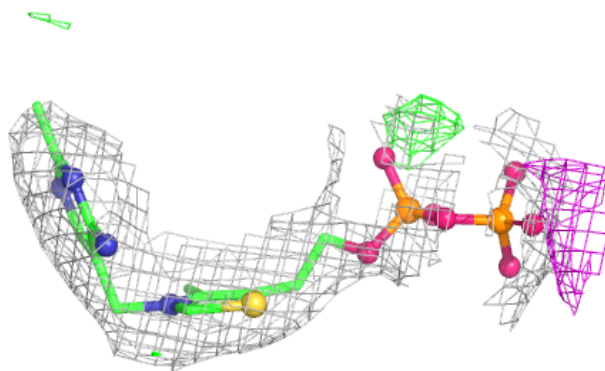
Electron density around ATP L 401:

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

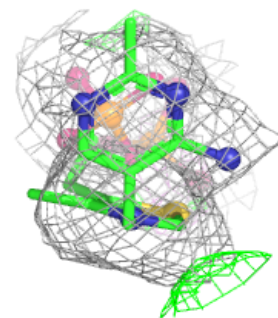
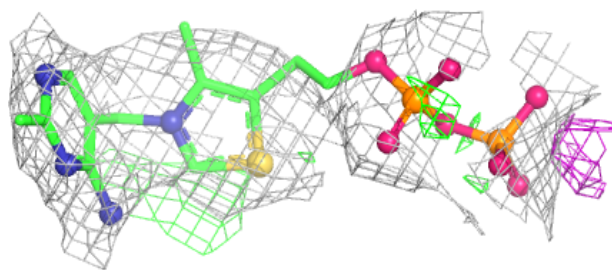
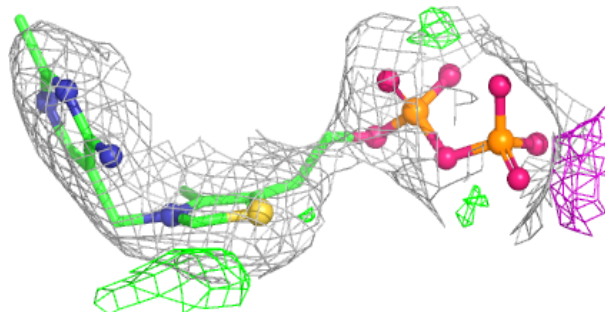


Electron density around TPP N 701:

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

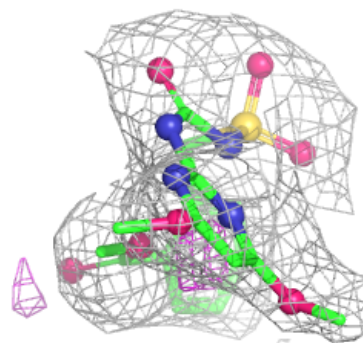
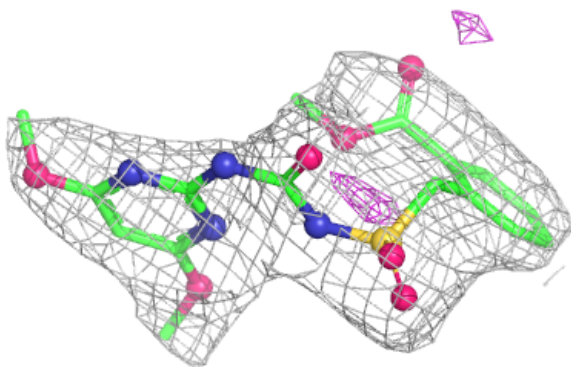
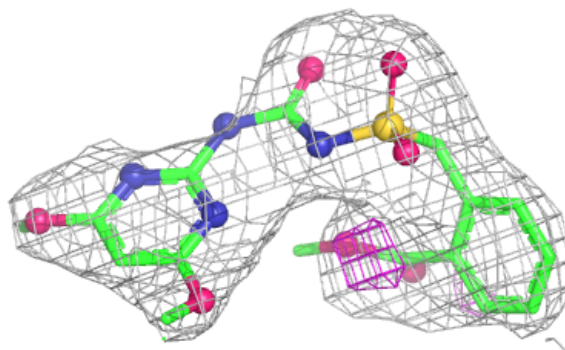
**Electron density around TPP E 701:**

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

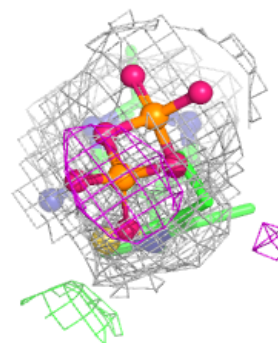
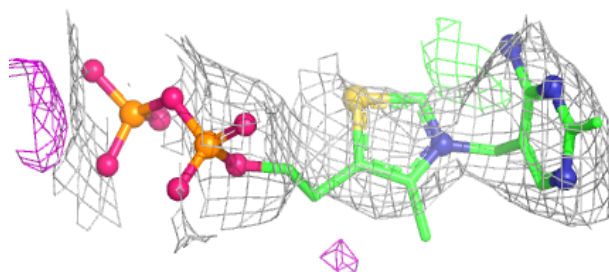
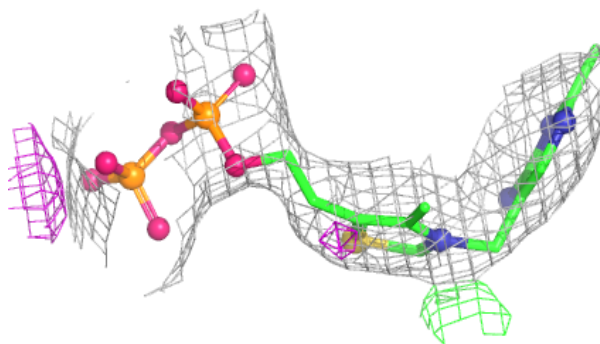


Electron density around 60G J 704:

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

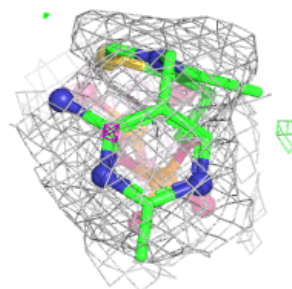
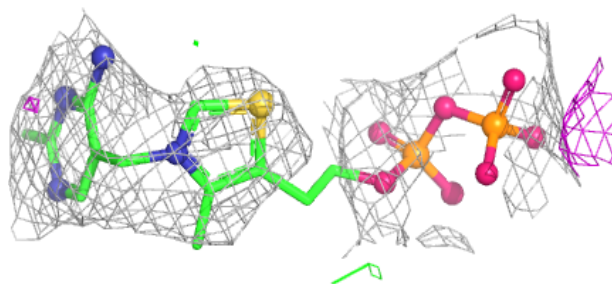
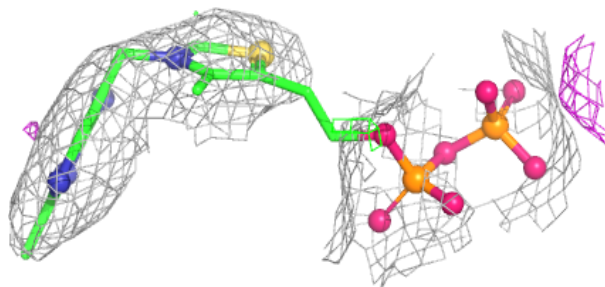
**Electron density around TPP I 701:**

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

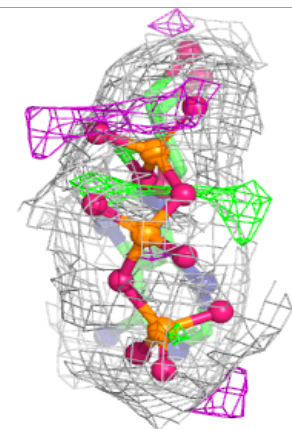
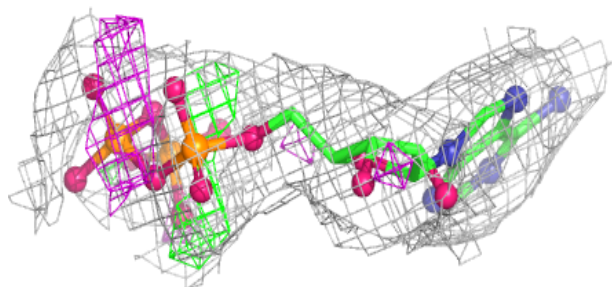
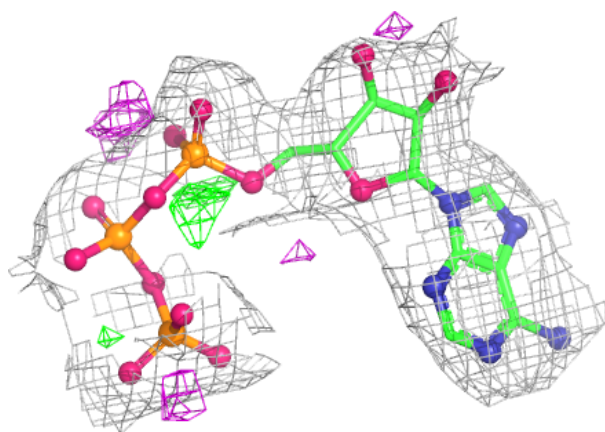


Electron density around TPP J 701:

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

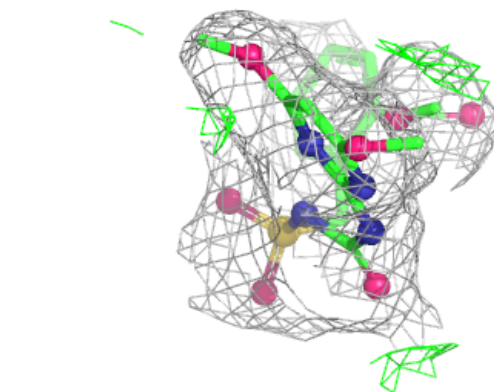
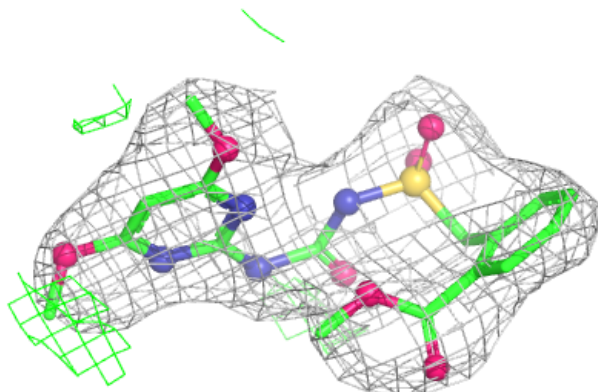
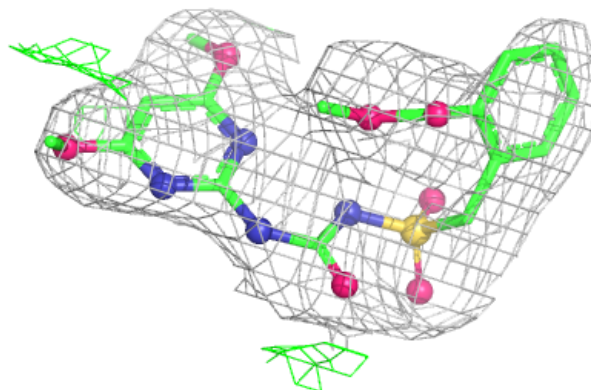
**Electron density around ATP D 401:**

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

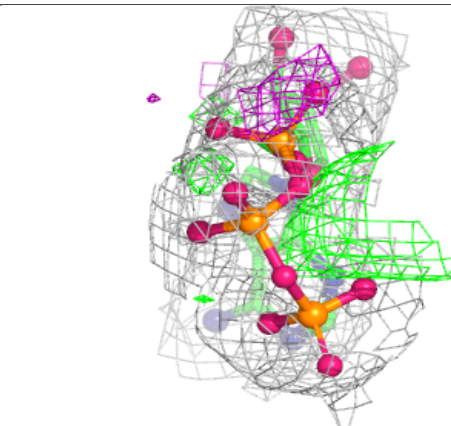
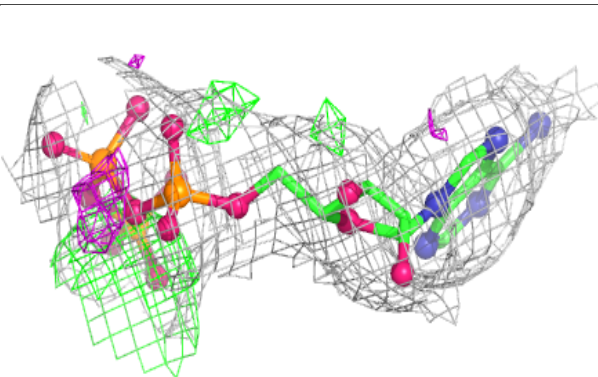
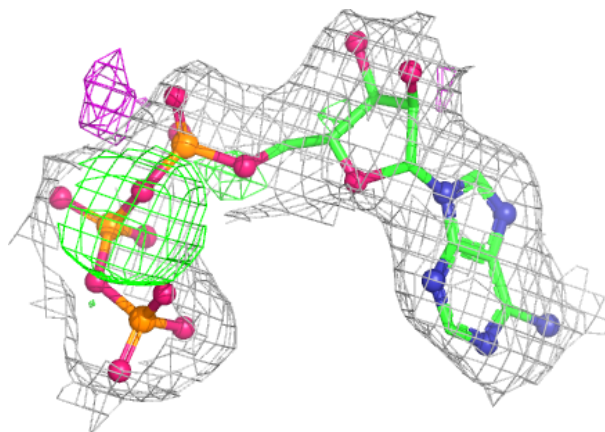


Electron density around 60G E 704:

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

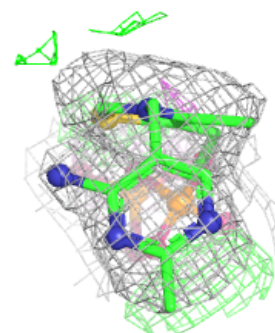
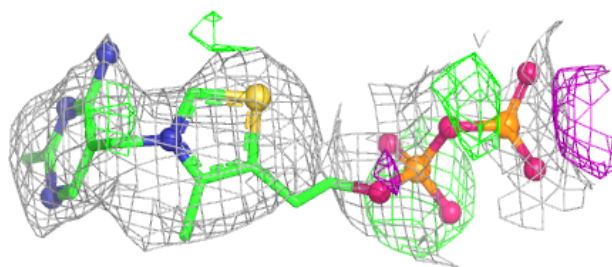
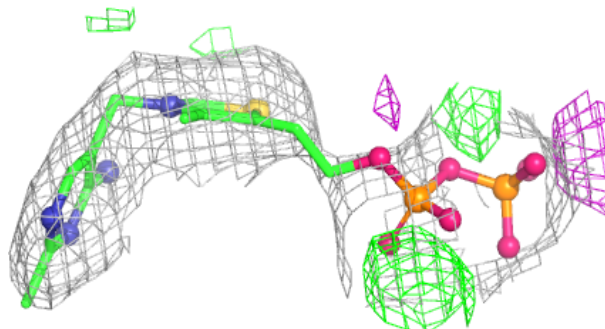
**Electron density around ATP W 401:**

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

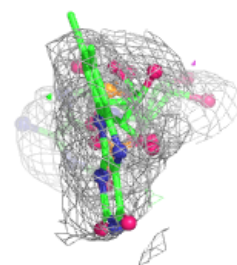
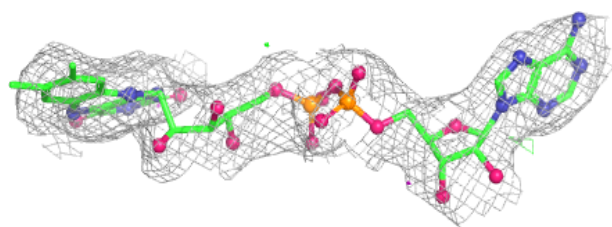
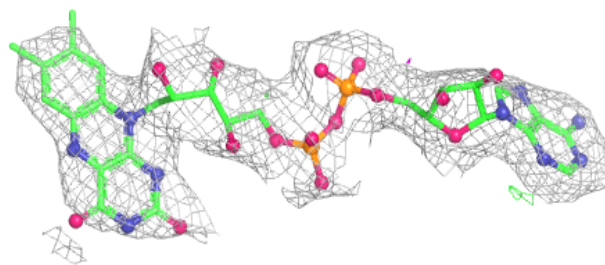


Electron density around TPP U 701:

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

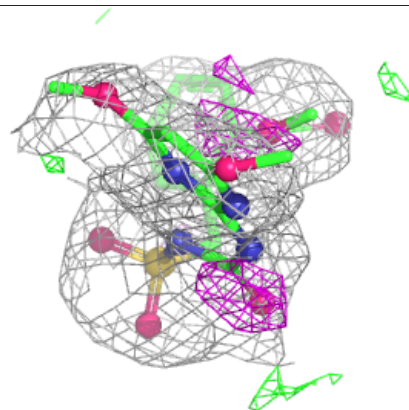
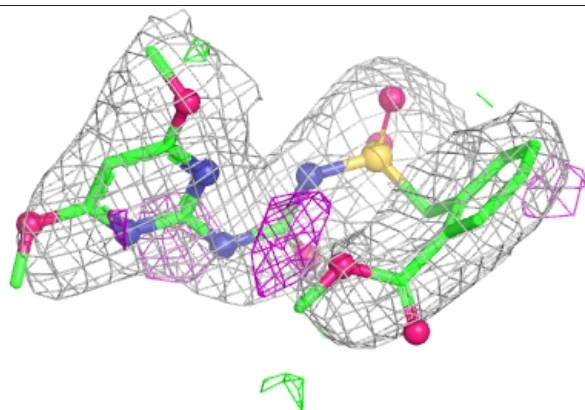
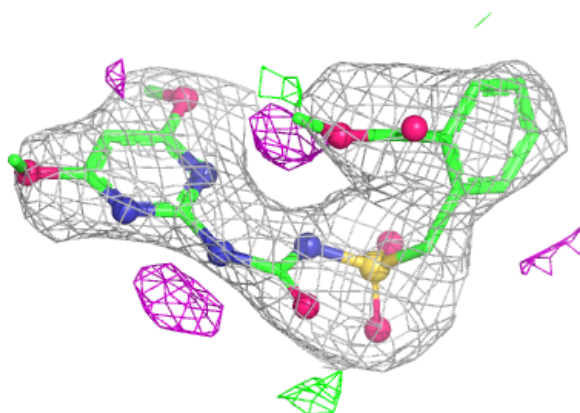
**Electron density around FAD I 703:**

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

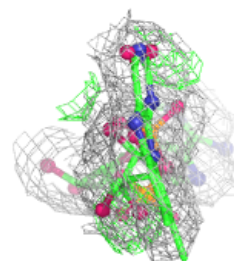
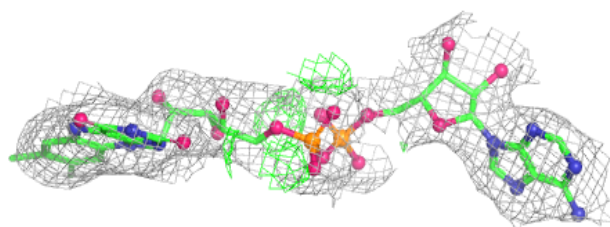
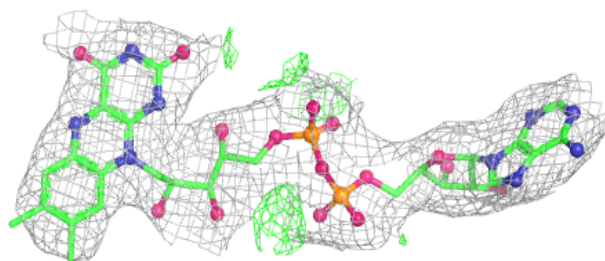


Electron density around 60G N 704:

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

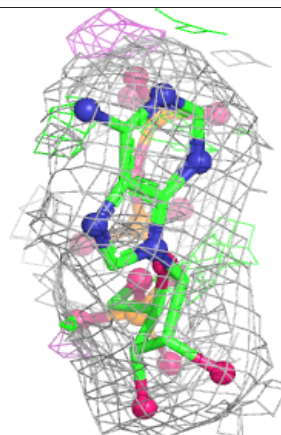
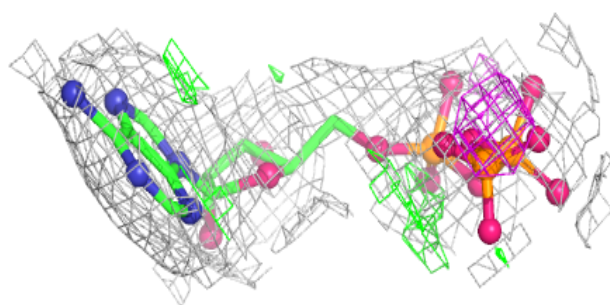
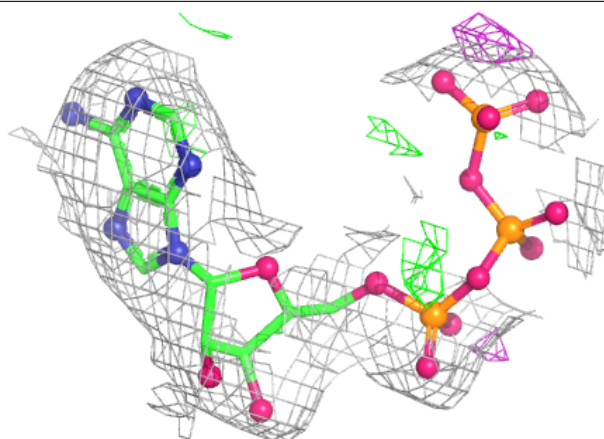
**Electron density around FAD J 703:**

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



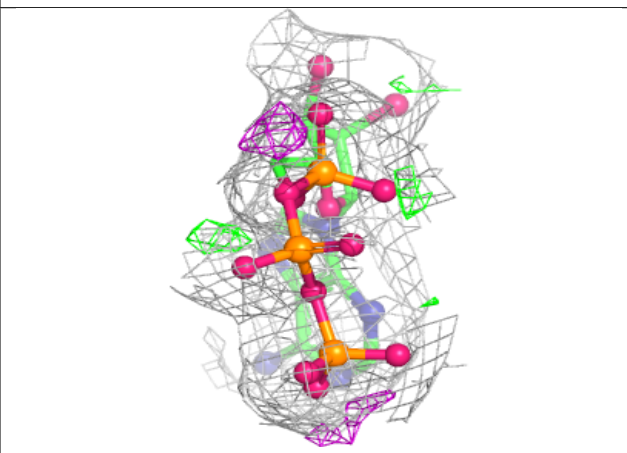
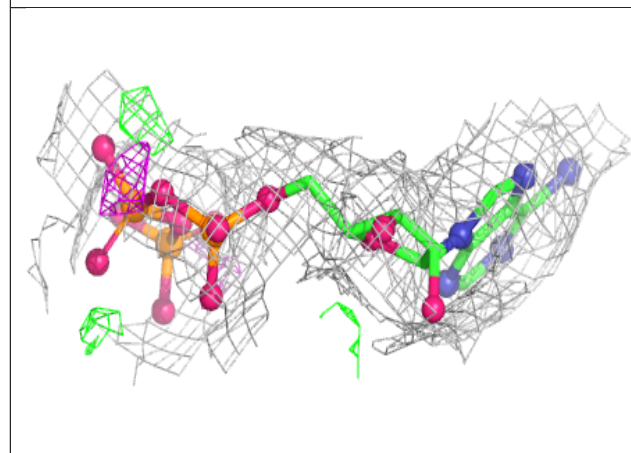
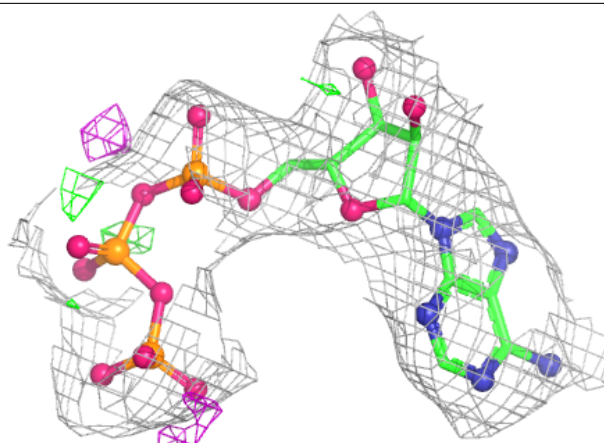
Electron density around ATP H 401:

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

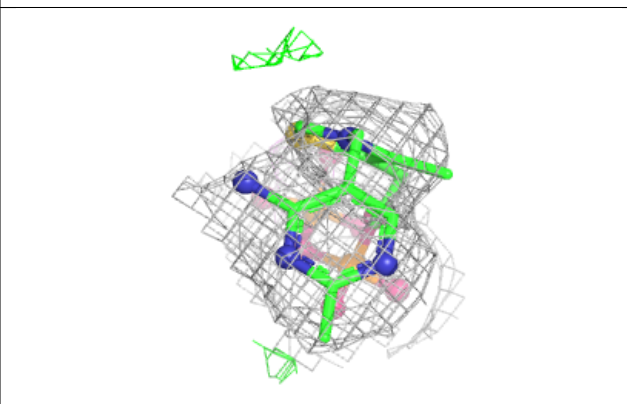
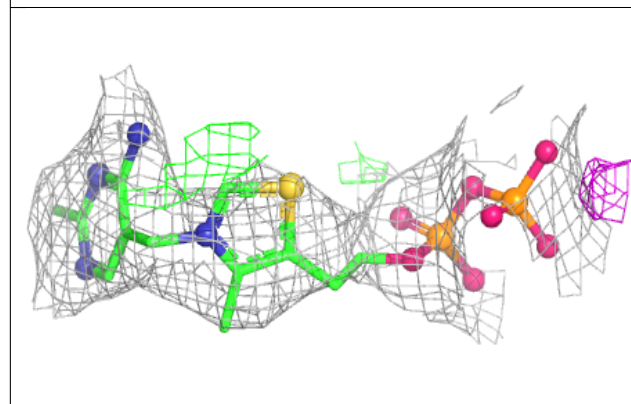
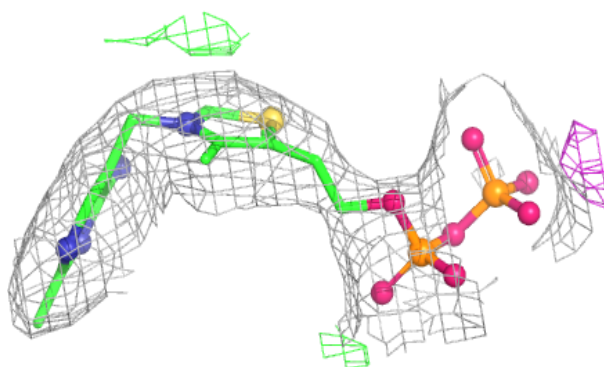


Electron density around ATP K 401:

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

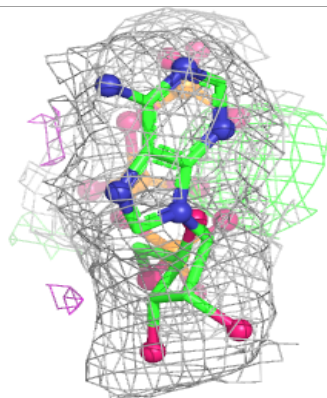
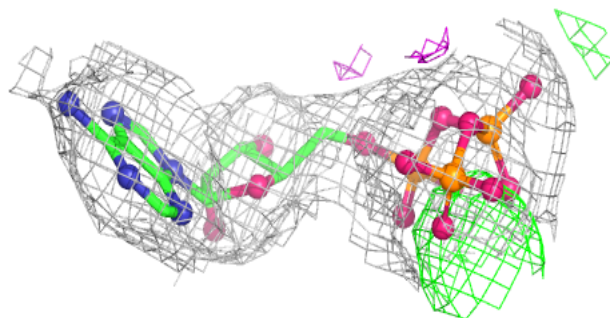
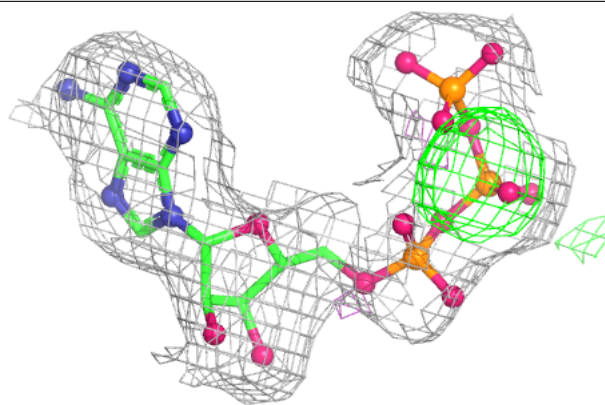
**Electron density around TPP F 701:**

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

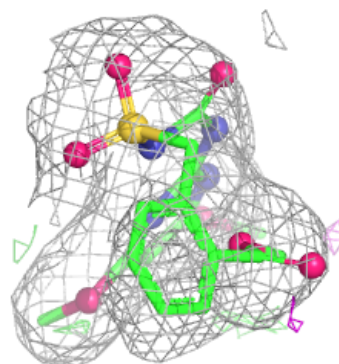
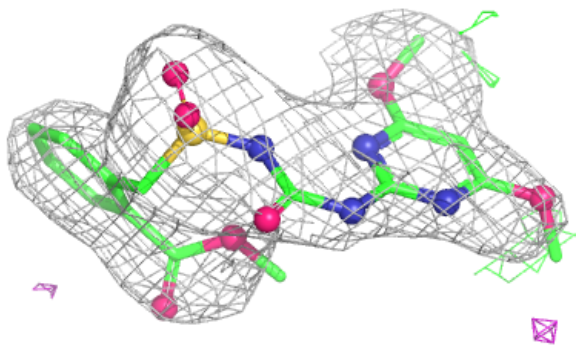
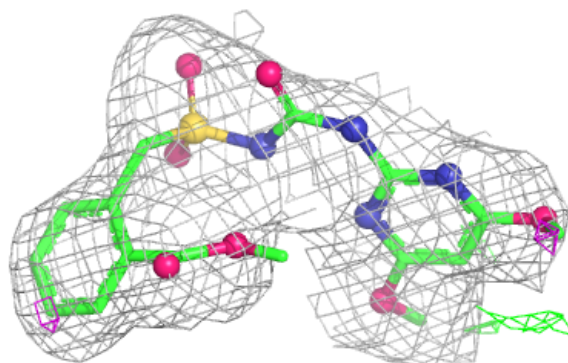


Electron density around ATP S 401:

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

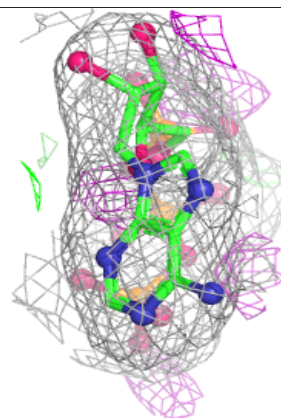
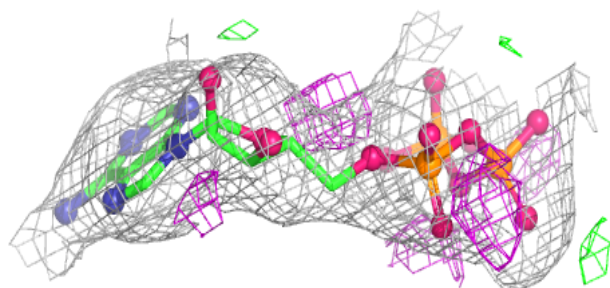
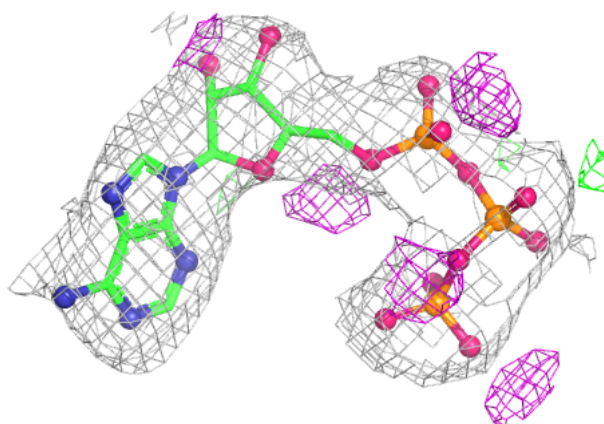
**Electron density around 60G F 704:**

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

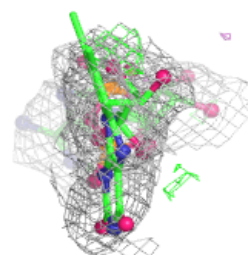
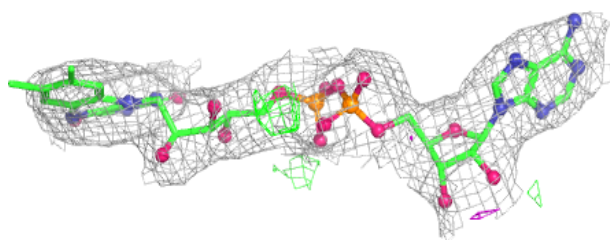


Electron density around ATP G 401:

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

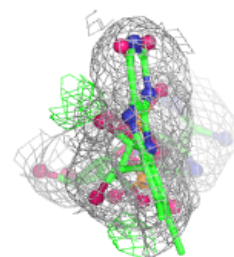
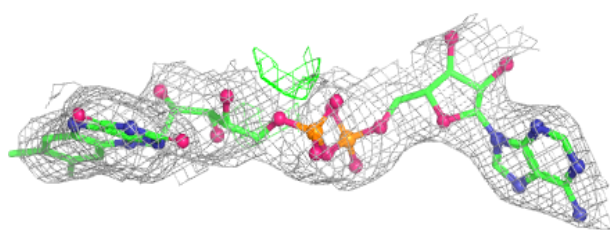
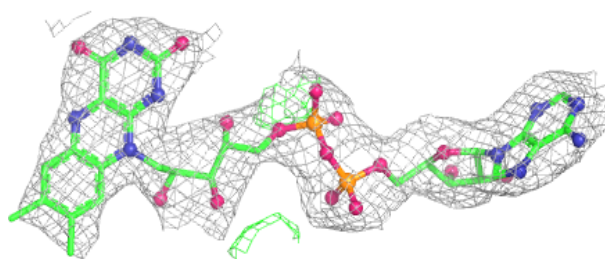
**Electron density around FAD E 703:**

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

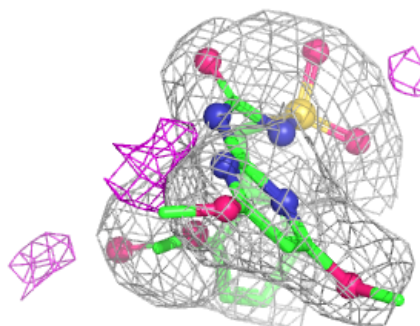
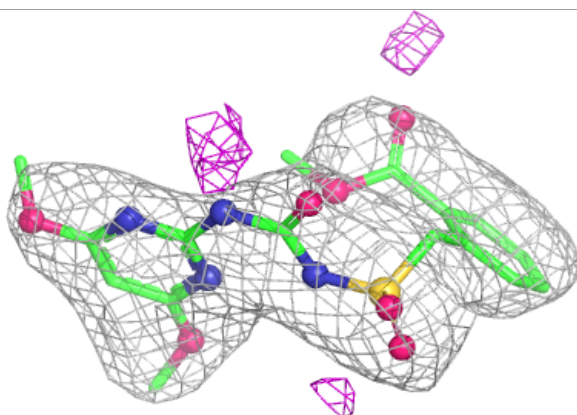
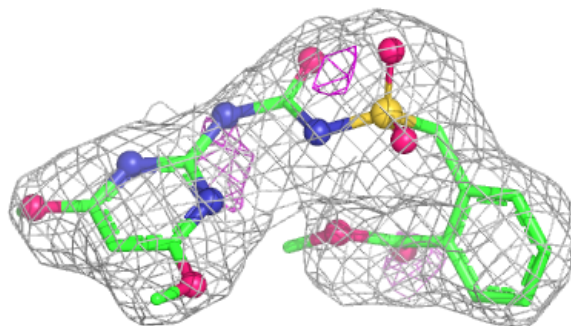


Electron density around FAD F 703:

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

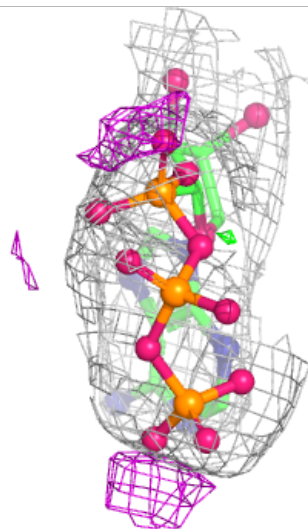
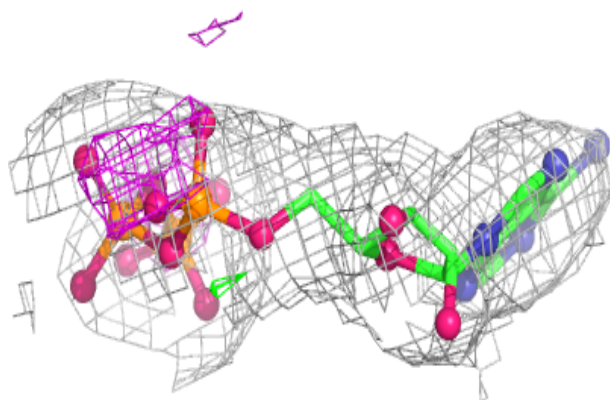
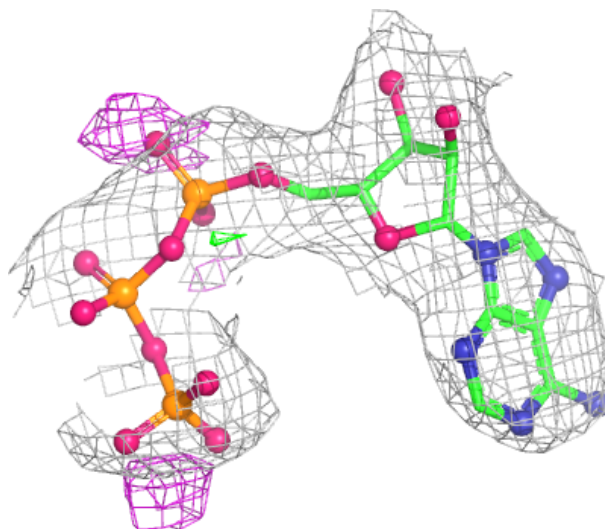
**Electron density around 60G N 705:**

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



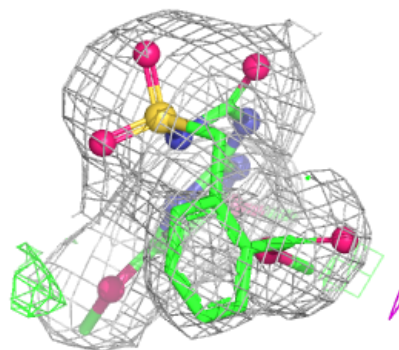
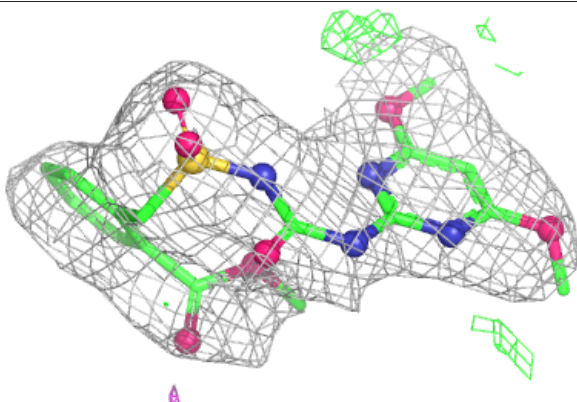
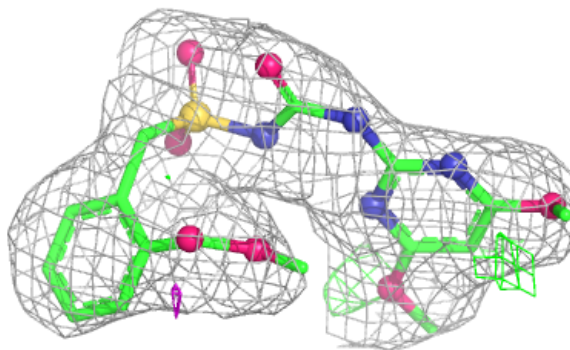
Electron density around ATP O 401:

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

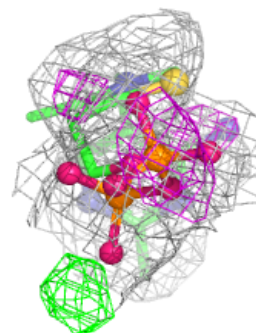
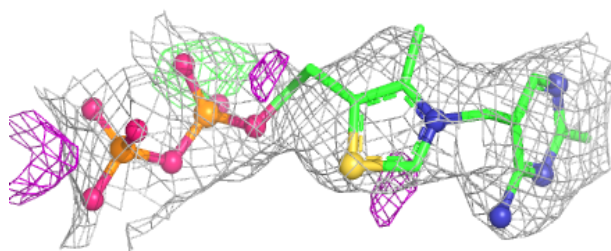
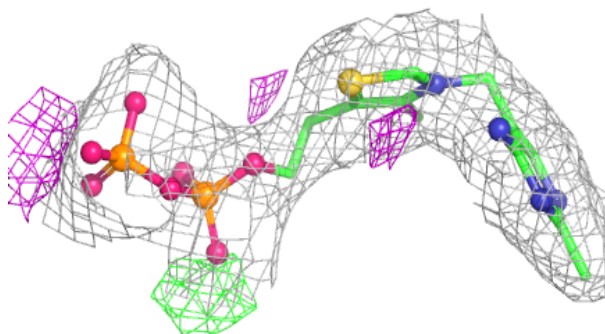


Electron density around 60G U 704:

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

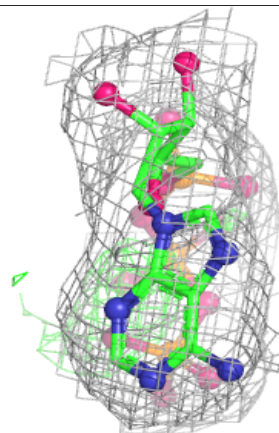
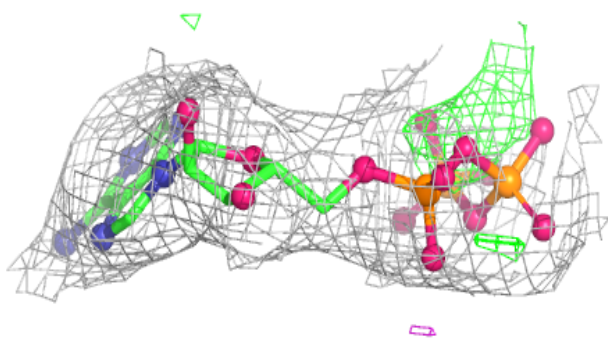
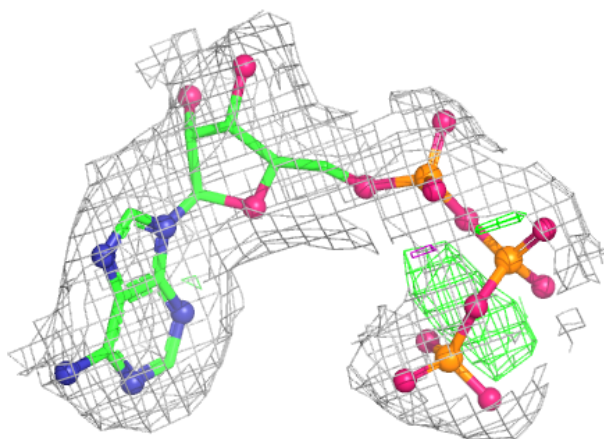
**Electron density around TPP M 701:**

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

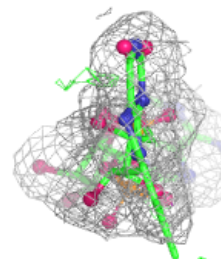
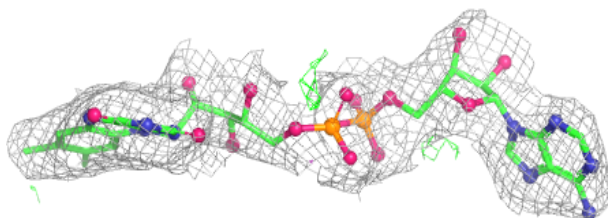
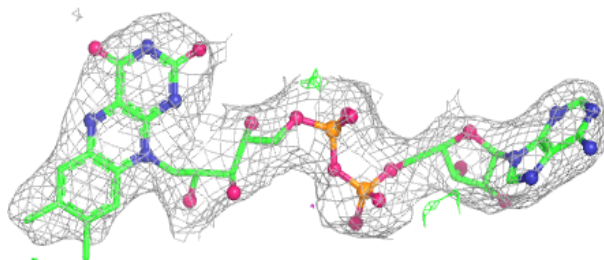


Electron density around ATP P 401:

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

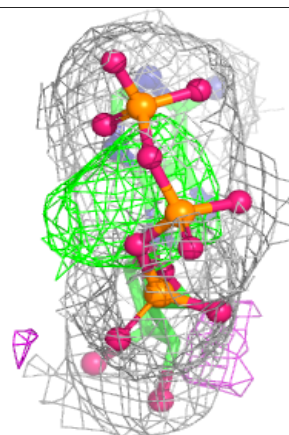
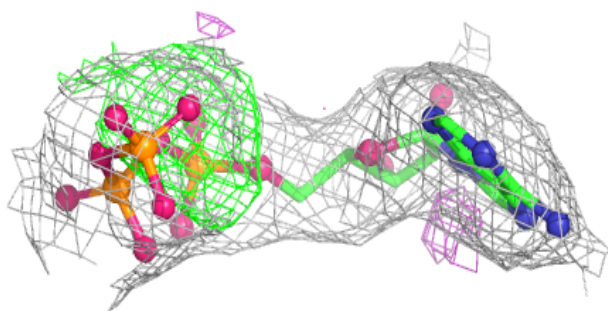
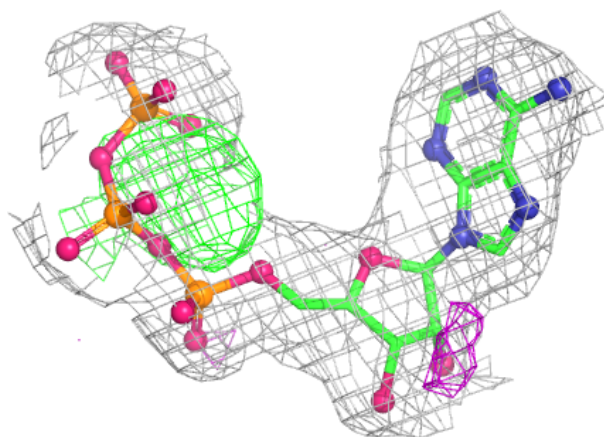
**Electron density around FAD U 703:**

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

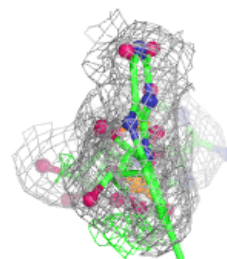
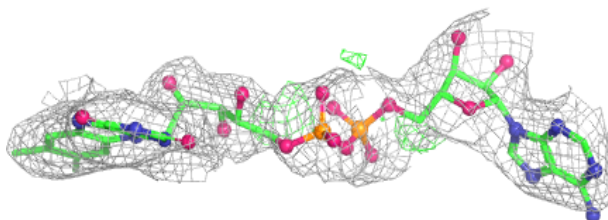
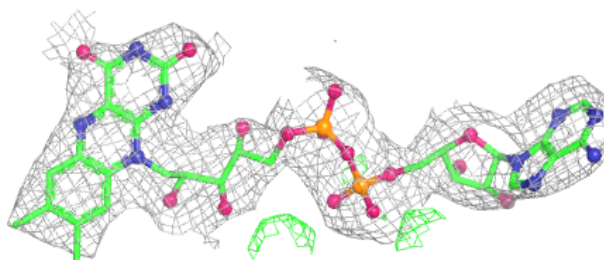


Electron density around ATP T 401:

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

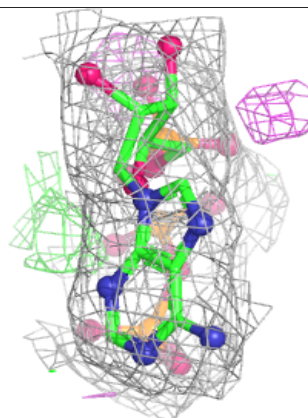
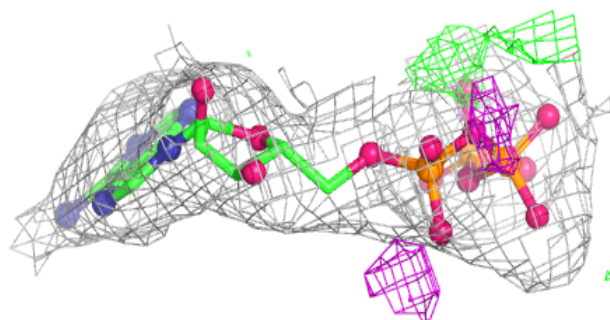
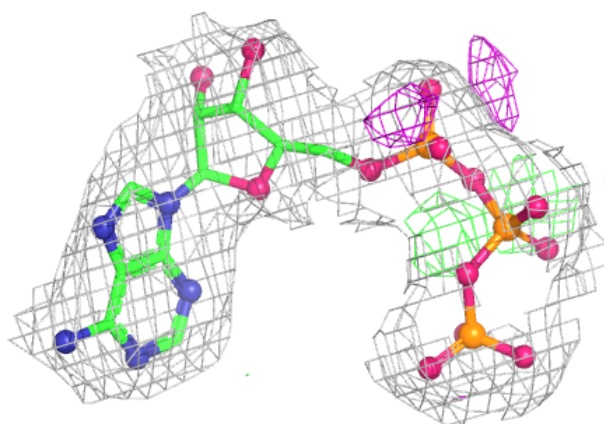
**Electron density around FAD N 703:**

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



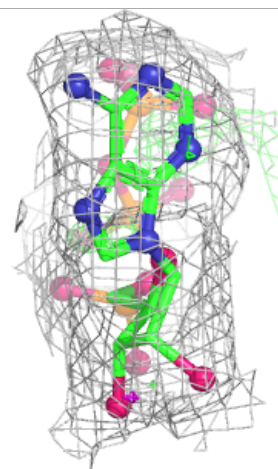
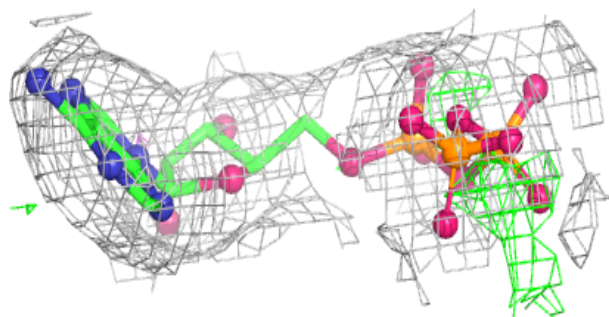
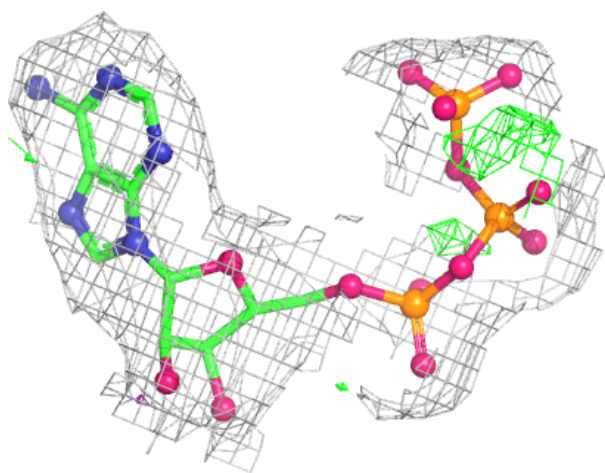
Electron density around ATP W 402:

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



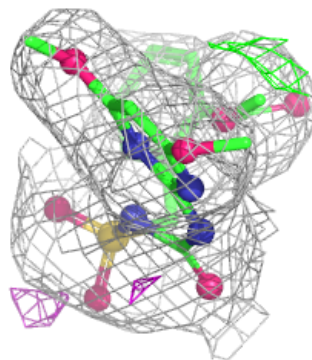
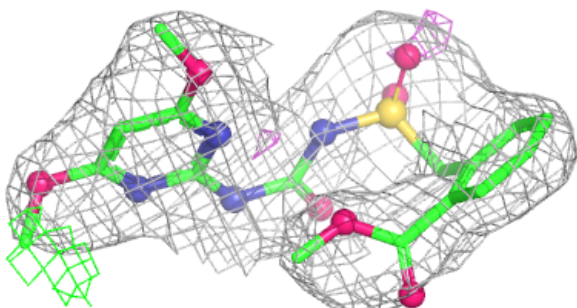
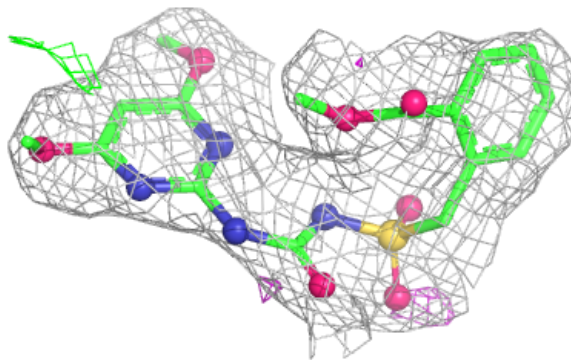
Electron density around ATP C 401:

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

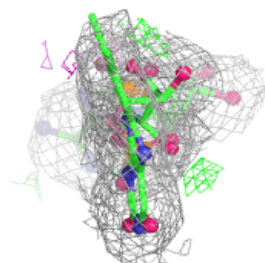
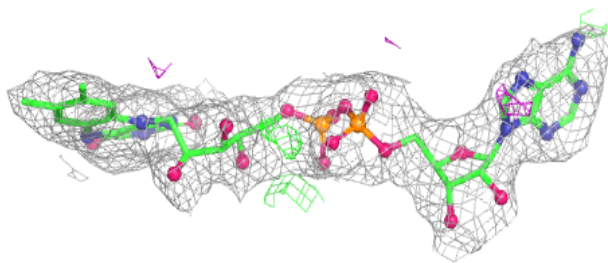
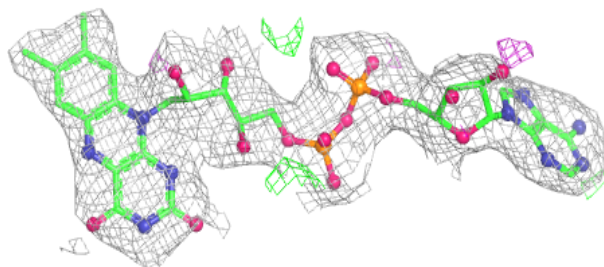


Electron density around 60G B 704:

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

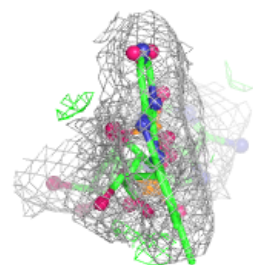
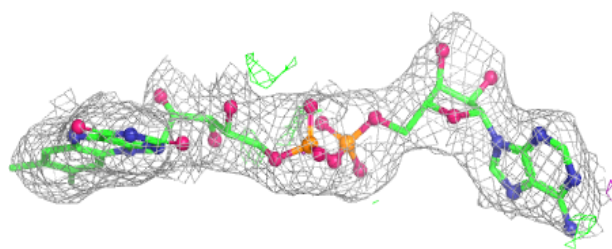
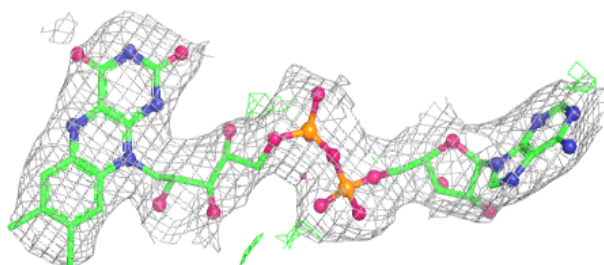
**Electron density around FAD B 703:**

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

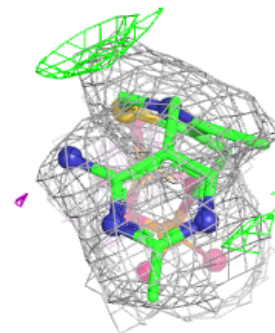
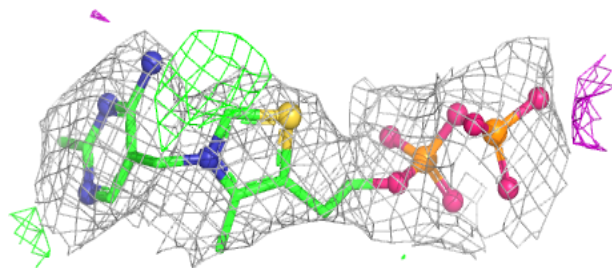
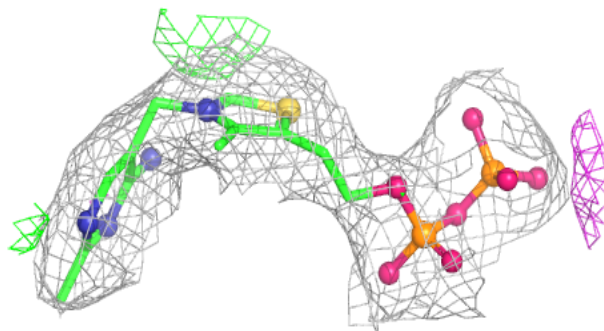


Electron density around FAD M 703:

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

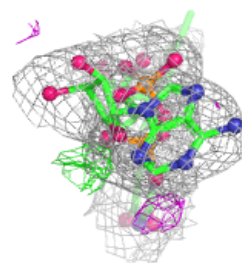
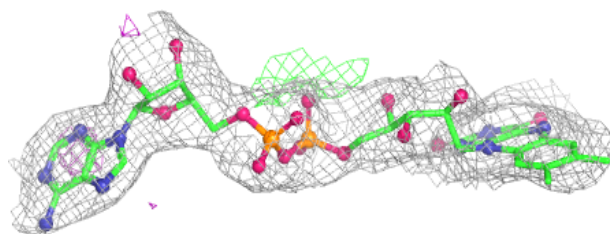
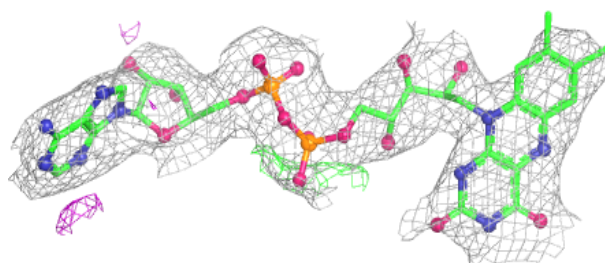
**Electron density around TPP B 701:**

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

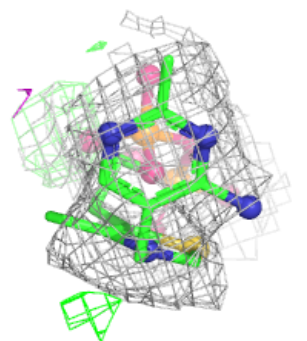
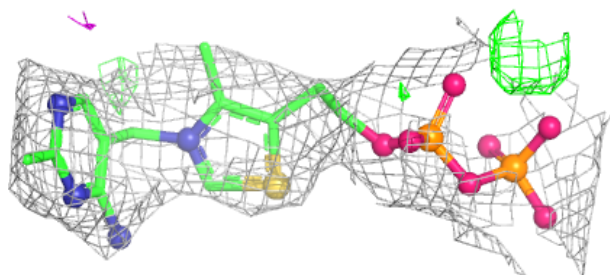
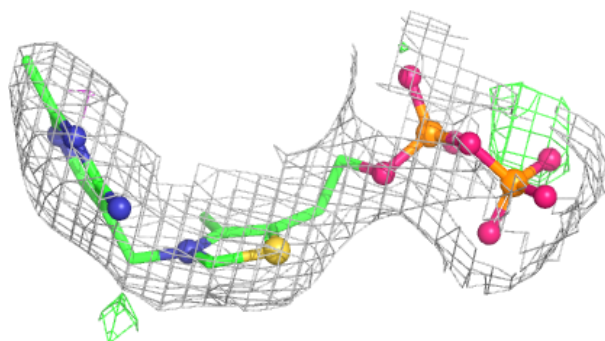


Electron density around FAD Q 703:

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

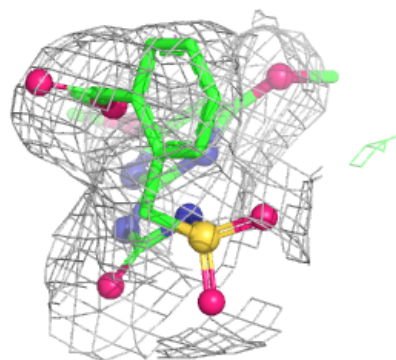
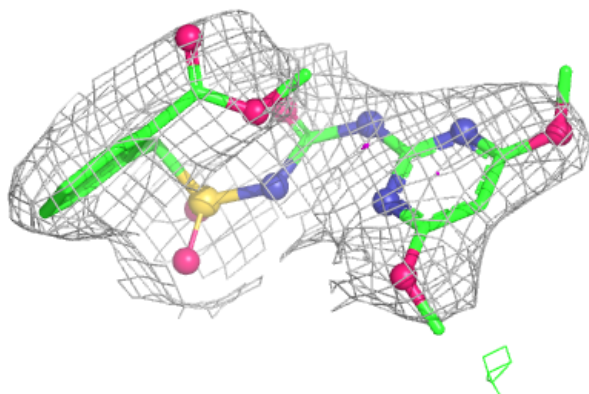
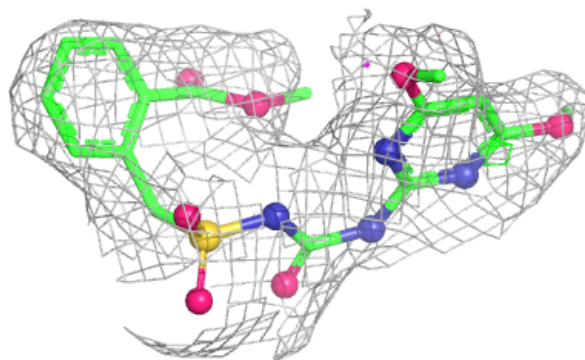
**Electron density around TPP V 701:**

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

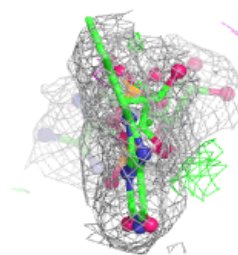
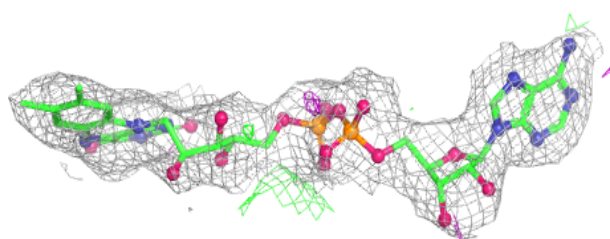
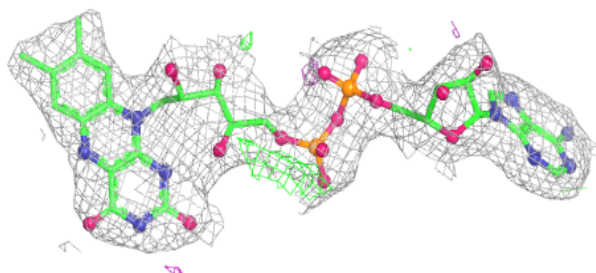


Electron density around 60G Q 704:

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

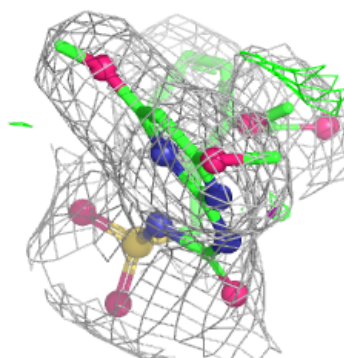
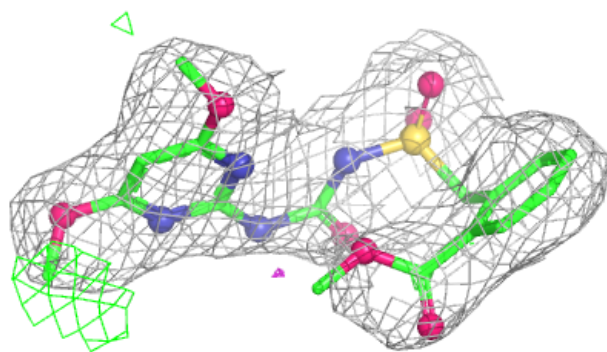
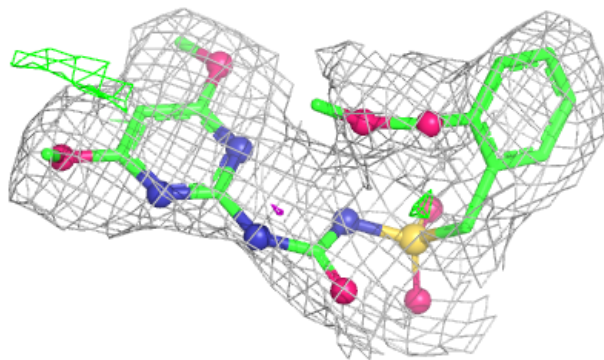
**Electron density around FAD V 703:**

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

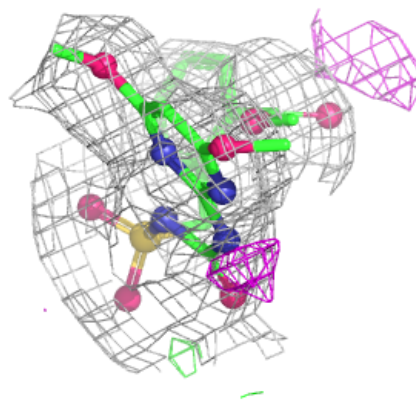
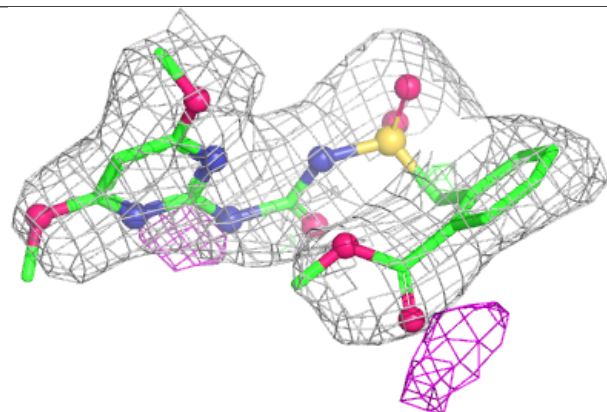
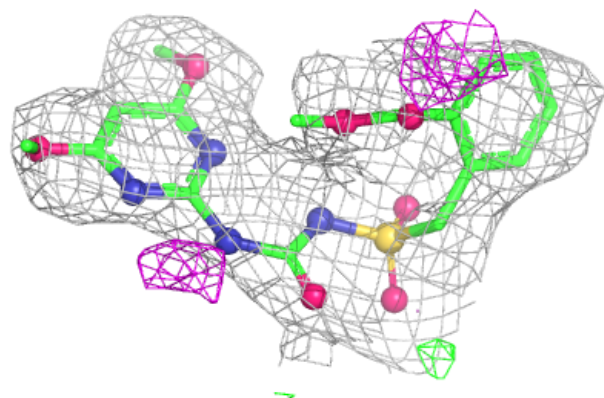


Electron density around 60G A 704:

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

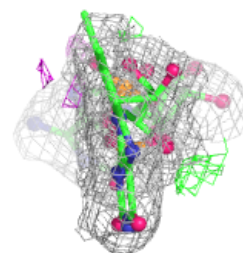
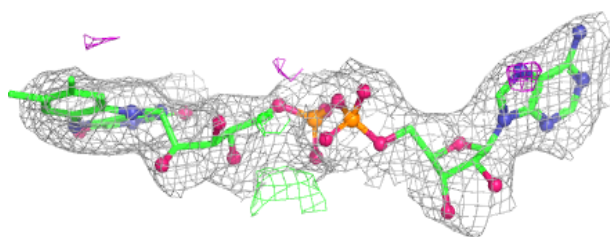
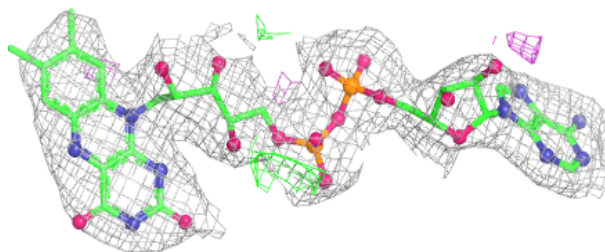
**Electron density around 60G V 704:**

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

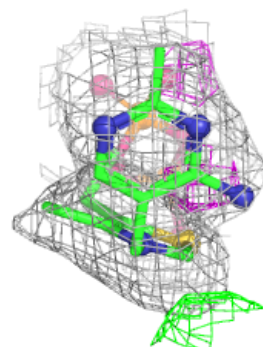
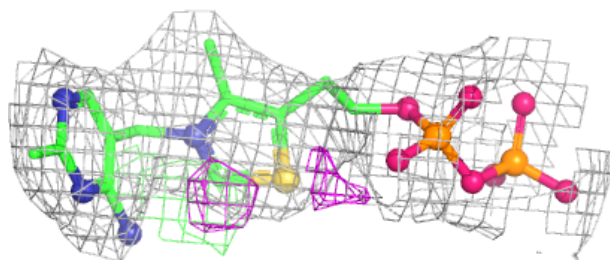
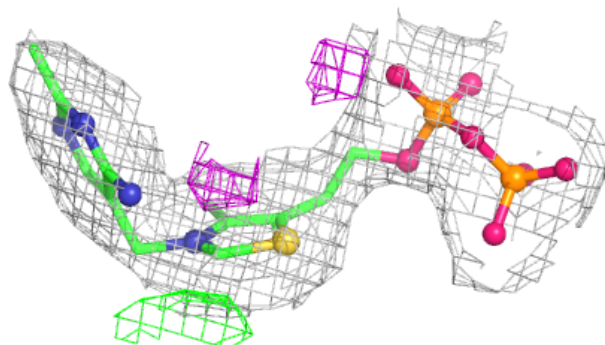


Electron density around FAD A 703:

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

**Electron density around TPP A 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.