



Full wwPDB X-ray Structure Validation Report i

Oct 2, 2023 – 11:56 PM EDT

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

This is a 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 i symbol.

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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

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

2 Entry composition (i)

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

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

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

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

There are 168 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

There are 336 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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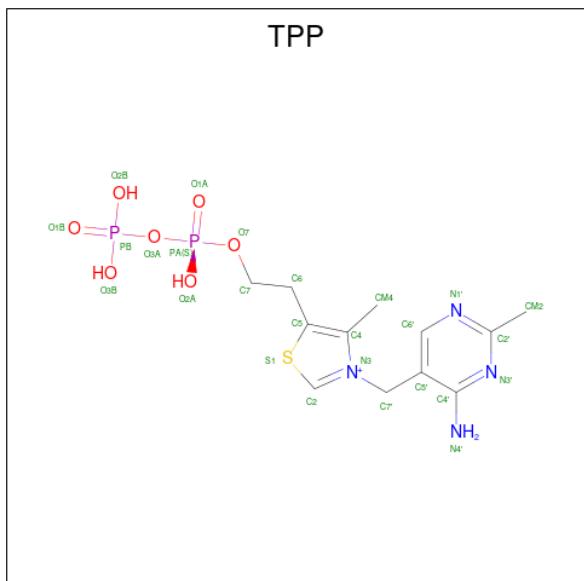
Chain	Residue	Modelled	Actual	Comment	Reference
T	30	GLY	-	expression tag	UNP B3LU66
T	31	SER	-	expression tag	UNP B3LU66
T	32	HIS	-	expression tag	UNP B3LU66
T	33	MET	-	expression tag	UNP B3LU66
T	34	GLU	-	expression tag	UNP B3LU66
T	35	ASN	-	expression tag	UNP B3LU66
T	36	LEU	-	expression tag	UNP B3LU66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

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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

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

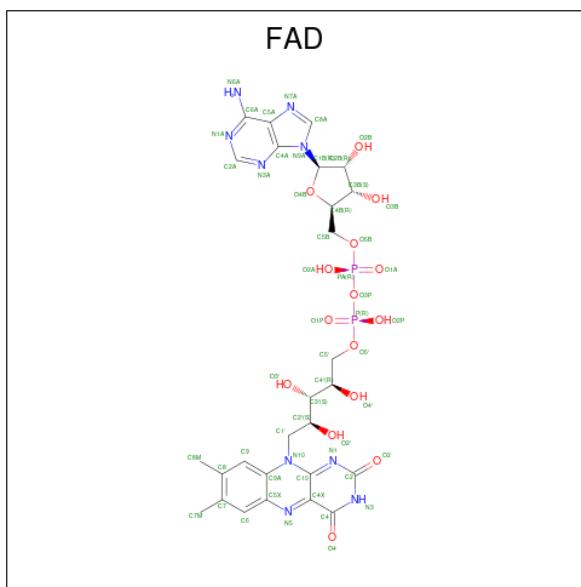
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg		
			1	1	0	0
4	B	1	Total	Mg		
			1	1	0	0
4	C	1	Total	Mg		
			1	1	0	0
4	D	1	Total	Mg		
			1	1	0	0
4	E	1	Total	Mg		
			1	1	0	0
4	F	1	Total	Mg		
			1	1	0	0
4	H	1	Total	Mg		
			1	1	0	0
4	I	1	Total	Mg		
			1	1	0	0
4	J	1	Total	Mg		
			1	1	0	0

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

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



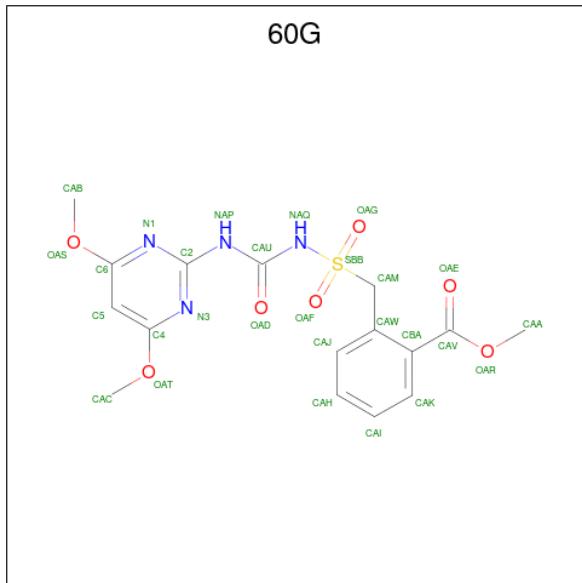
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	Total 53	27	9	15	2	0	0
5	B	1	Total 53	27	9	15	2	0	0
5	E	1	Total 53	27	9	15	2	0	0
5	F	1	Total 53	27	9	15	2	0	0

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

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



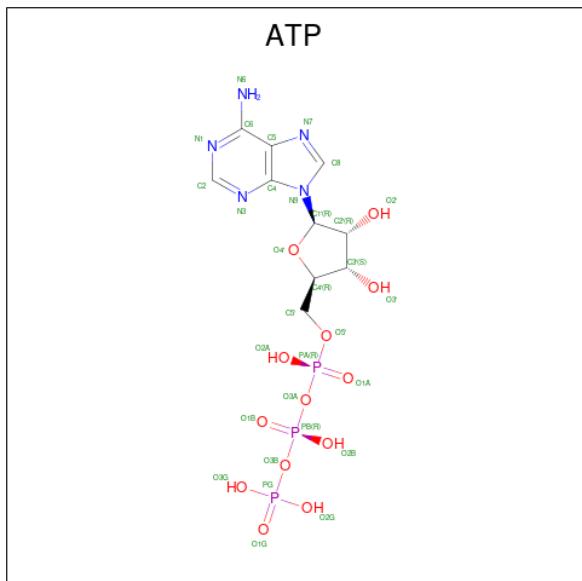
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 28 16 4 7 1	0	0
6	B	1	Total C N O S 28 16 4 7 1	0	0

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

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 8 is water.

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

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

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

3 Data and refinement statistics i

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

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

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

¹Intensities estimated from amplitudes.

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

4 Model quality [\(i\)](#)

4.1 Standard geometry [\(i\)](#)

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

4.2 Too-close contacts [\(i\)](#)

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

4.3 Torsion angles [\(i\)](#)

4.3.1 Protein backbone [\(i\)](#)

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

4.3.2 Protein sidechains [\(i\)](#)

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

4.3.3 RNA [\(i\)](#)

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

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

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

4.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [\(i\)](#)

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

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

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

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

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

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

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

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

All (307) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	401	ATP	C2'-C3'	-11.31	1.22	1.53
7	C	401	ATP	C2'-C3'	-11.25	1.22	1.53
7	W	402	ATP	C2'-C3'	-11.24	1.22	1.53
7	O	401	ATP	C2'-C3'	-11.24	1.22	1.53
7	S	401	ATP	C2'-C3'	-11.23	1.22	1.53
7	P	401	ATP	C2'-C3'	-11.22	1.22	1.53
7	H	401	ATP	C2'-C3'	-11.20	1.22	1.53
7	W	401	ATP	C2'-C3'	-11.18	1.22	1.53
7	T	401	ATP	C2'-C3'	-11.17	1.22	1.53
7	G	401	ATP	C2'-C3'	-11.16	1.22	1.53
7	K	401	ATP	C2'-C3'	-11.09	1.23	1.53
7	D	401	ATP	C2'-C3'	-11.02	1.23	1.53
7	P	401	ATP	O4'-C4'	-7.48	1.28	1.45
7	T	401	ATP	O4'-C4'	-7.45	1.28	1.45
7	G	401	ATP	O4'-C4'	-7.42	1.28	1.45
7	H	401	ATP	O4'-C4'	-7.39	1.28	1.45
7	O	401	ATP	O4'-C4'	-7.39	1.28	1.45
7	L	401	ATP	O4'-C4'	-7.37	1.28	1.45
7	D	401	ATP	O4'-C4'	-7.37	1.28	1.45
7	W	402	ATP	O4'-C4'	-7.37	1.28	1.45
7	W	401	ATP	O4'-C4'	-7.36	1.28	1.45
7	C	401	ATP	O4'-C4'	-7.36	1.28	1.45
7	K	401	ATP	O4'-C4'	-7.34	1.28	1.45
7	S	401	ATP	O4'-C4'	-7.33	1.28	1.45
3	J	701	TPP	C4-N3	-7.07	1.33	1.39
3	N	701	TPP	C4-N3	-6.97	1.33	1.39
3	M	701	TPP	C4-N3	-6.94	1.33	1.39
3	E	701	TPP	C4-N3	-6.93	1.33	1.39
3	U	701	TPP	C4-N3	-6.89	1.33	1.39
3	B	701	TPP	C4-N3	-6.84	1.33	1.39
3	A	701	TPP	C4-N3	-6.79	1.33	1.39
3	I	701	TPP	C4-N3	-6.75	1.33	1.39
3	F	701	TPP	C4-N3	-6.72	1.33	1.39
3	Q	701	TPP	C4-N3	-6.71	1.33	1.39
3	V	701	TPP	C4-N3	-6.70	1.33	1.39
7	W	401	ATP	O4'-C1'	6.36	1.50	1.41
7	K	401	ATP	O4'-C1'	6.34	1.49	1.41
7	S	401	ATP	O4'-C1'	6.34	1.49	1.41
7	L	401	ATP	O4'-C1'	6.29	1.49	1.41
7	H	401	ATP	O4'-C1'	6.27	1.49	1.41
7	W	402	ATP	O4'-C1'	6.25	1.49	1.41
7	C	401	ATP	O4'-C1'	6.25	1.49	1.41
7	G	401	ATP	O4'-C1'	6.23	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	401	ATP	O4'-C1'	6.23	1.49	1.41
7	T	401	ATP	O4'-C1'	6.19	1.49	1.41
7	P	401	ATP	O4'-C1'	6.17	1.49	1.41
7	D	401	ATP	O4'-C1'	5.84	1.49	1.41
5	F	703	FAD	C10-N1	5.32	1.44	1.33
5	N	703	FAD	C10-N1	5.27	1.44	1.33
5	J	703	FAD	C10-N1	5.26	1.44	1.33
5	A	703	FAD	C10-N1	5.25	1.44	1.33
5	M	703	FAD	C10-N1	5.22	1.43	1.33
5	V	703	FAD	C10-N1	5.22	1.43	1.33
5	I	703	FAD	C10-N1	5.22	1.43	1.33
5	U	703	FAD	C10-N1	5.21	1.43	1.33
5	Q	703	FAD	C10-N1	5.21	1.43	1.33
5	E	703	FAD	C10-N1	5.19	1.43	1.33
5	B	703	FAD	C10-N1	5.19	1.43	1.33
5	R	701	FAD	C10-N1	5.17	1.43	1.33
7	K	401	ATP	O2'-C2'	4.92	1.54	1.43
7	W	401	ATP	O2'-C2'	4.91	1.54	1.43
7	C	401	ATP	O2'-C2'	4.91	1.54	1.43
7	S	401	ATP	O2'-C2'	4.91	1.54	1.43
7	H	401	ATP	O2'-C2'	4.90	1.54	1.43
7	P	401	ATP	O2'-C2'	4.88	1.54	1.43
7	W	402	ATP	O2'-C2'	4.84	1.54	1.43
7	G	401	ATP	O2'-C2'	4.84	1.54	1.43
7	O	401	ATP	O2'-C2'	4.83	1.54	1.43
7	L	401	ATP	O2'-C2'	4.77	1.54	1.43
5	R	701	FAD	C2B-C1B	-4.76	1.46	1.53
7	D	401	ATP	O2'-C2'	4.75	1.54	1.43
7	T	401	ATP	O2'-C2'	4.73	1.54	1.43
5	J	703	FAD	C4X-N5	4.68	1.39	1.30
5	V	703	FAD	C4X-N5	4.65	1.39	1.30
7	D	401	ATP	C3'-C4'	4.64	1.64	1.53
5	F	703	FAD	C4X-N5	4.64	1.39	1.30
5	E	703	FAD	C4X-N5	4.62	1.39	1.30
5	M	703	FAD	C4X-N5	4.62	1.39	1.30
5	B	703	FAD	C4X-N5	4.61	1.39	1.30
5	R	701	FAD	C4X-N5	4.61	1.39	1.30
5	N	703	FAD	C4X-N5	4.59	1.39	1.30
5	U	703	FAD	C2B-C1B	-4.58	1.46	1.53
5	I	703	FAD	C4X-N5	4.57	1.39	1.30
5	Q	703	FAD	C4X-N5	4.57	1.39	1.30
5	A	703	FAD	C4X-N5	4.56	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	401	ATP	C3'-C4'	4.54	1.64	1.53
5	U	703	FAD	C4X-N5	4.50	1.39	1.30
7	G	401	ATP	C3'-C4'	4.49	1.64	1.53
7	H	401	ATP	C3'-C4'	4.46	1.64	1.53
5	E	703	FAD	C2B-C1B	-4.46	1.47	1.53
7	S	401	ATP	C3'-C4'	4.45	1.64	1.53
5	V	703	FAD	C2B-C1B	-4.43	1.47	1.53
7	O	401	ATP	C3'-C4'	4.43	1.64	1.53
5	A	703	FAD	C2B-C1B	-4.43	1.47	1.53
7	C	401	ATP	C3'-C4'	4.43	1.64	1.53
7	L	401	ATP	C3'-C4'	4.42	1.64	1.53
7	W	401	ATP	C3'-C4'	4.42	1.64	1.53
7	W	402	ATP	C3'-C4'	4.40	1.64	1.53
7	P	401	ATP	C3'-C4'	4.40	1.64	1.53
7	T	401	ATP	C3'-C4'	4.40	1.64	1.53
5	N	703	FAD	C2B-C1B	-4.39	1.47	1.53
5	M	703	FAD	C2B-C1B	-4.39	1.47	1.53
5	Q	703	FAD	C2B-C1B	-4.36	1.47	1.53
5	B	703	FAD	C2B-C1B	-4.33	1.47	1.53
5	I	703	FAD	C2B-C1B	-4.32	1.47	1.53
7	P	401	ATP	O3'-C3'	4.29	1.53	1.43
7	K	401	ATP	O3'-C3'	4.26	1.53	1.43
7	D	401	ATP	O3'-C3'	4.25	1.53	1.43
7	C	401	ATP	O3'-C3'	4.25	1.53	1.43
7	S	401	ATP	O3'-C3'	4.24	1.53	1.43
7	H	401	ATP	O3'-C3'	4.24	1.53	1.43
7	G	401	ATP	O3'-C3'	4.23	1.52	1.43
7	O	401	ATP	O3'-C3'	4.21	1.52	1.43
7	L	401	ATP	O3'-C3'	4.20	1.52	1.43
7	T	401	ATP	O3'-C3'	4.19	1.52	1.43
7	W	402	ATP	O3'-C3'	4.19	1.52	1.43
7	W	401	ATP	O3'-C3'	4.17	1.52	1.43
6	Q	704	60G	C2-NAP	4.17	1.44	1.38
5	F	703	FAD	C2B-C1B	-4.11	1.47	1.53
6	J	704	60G	C2-NAP	4.08	1.44	1.38
6	R	702	60G	C2-NAP	4.07	1.44	1.38
6	B	704	60G	C2-NAP	4.01	1.44	1.38
6	N	705	60G	C2-NAP	3.99	1.44	1.38
6	A	704	60G	C2-NAP	3.98	1.44	1.38
6	E	704	60G	C2-NAP	3.94	1.44	1.38
6	I	704	60G	C2-NAP	3.93	1.44	1.38
6	F	704	60G	C2-NAP	3.90	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	704	60G	C2-NAP	3.88	1.43	1.38
6	N	704	60G	C2-NAP	3.87	1.43	1.38
6	V	704	60G	C2-NAP	3.81	1.43	1.38
5	J	703	FAD	C2B-C1B	-3.49	1.48	1.53
7	H	401	ATP	C6-N6	3.42	1.46	1.34
7	S	401	ATP	C6-N6	3.41	1.46	1.34
7	W	401	ATP	C6-N6	3.40	1.46	1.34
7	P	401	ATP	C6-N6	3.40	1.46	1.34
7	D	401	ATP	C6-N6	3.40	1.46	1.34
7	W	402	ATP	C6-N6	3.40	1.46	1.34
7	K	401	ATP	C6-N6	3.39	1.46	1.34
7	C	401	ATP	C6-N6	3.39	1.46	1.34
7	G	401	ATP	C6-N6	3.39	1.46	1.34
7	T	401	ATP	C6-N6	3.39	1.46	1.34
7	L	401	ATP	C6-N6	3.38	1.46	1.34
7	O	401	ATP	C6-N6	3.38	1.46	1.34
3	I	701	TPP	C4'-N4'	3.38	1.42	1.34
3	J	701	TPP	C4'-N4'	3.36	1.42	1.34
3	F	701	TPP	C4'-N4'	3.36	1.42	1.34
3	E	701	TPP	C4'-N4'	3.34	1.42	1.34
3	Q	701	TPP	C4'-N4'	3.34	1.42	1.34
3	U	701	TPP	C4'-N4'	3.34	1.42	1.34
3	M	701	TPP	C4'-N4'	3.34	1.42	1.34
3	V	701	TPP	C4'-N4'	3.34	1.42	1.34
3	B	701	TPP	C4'-N4'	3.32	1.42	1.34
3	A	701	TPP	C4'-N4'	3.31	1.42	1.34
3	N	701	TPP	C4'-N4'	3.31	1.42	1.34
7	O	401	ATP	C2'-C1'	3.22	1.58	1.53
7	K	401	ATP	C2'-C1'	3.20	1.58	1.53
7	W	402	ATP	C2'-C1'	3.20	1.58	1.53
6	Q	704	60G	CAU-NAP	3.16	1.44	1.37
7	G	401	ATP	C2'-C1'	3.16	1.58	1.53
6	J	704	60G	CAU-NAP	3.15	1.44	1.37
7	T	401	ATP	C2'-C1'	3.14	1.58	1.53
6	R	702	60G	CAU-NAP	3.13	1.44	1.37
7	H	401	ATP	C2'-C1'	3.13	1.58	1.53
6	A	704	60G	CAU-NAP	3.12	1.44	1.37
7	W	401	ATP	C2'-C1'	3.11	1.58	1.53
7	S	401	ATP	C2'-C1'	3.11	1.58	1.53
6	F	704	60G	CAU-NAP	3.08	1.43	1.37
6	E	704	60G	CAU-NAP	3.07	1.43	1.37
7	L	401	ATP	C2'-C1'	3.06	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	703	FAD	O4B-C1B	3.06	1.45	1.41
7	P	401	ATP	C2'-C1'	3.06	1.58	1.53
5	I	703	FAD	O4B-C1B	3.06	1.45	1.41
5	M	703	FAD	O4B-C1B	3.05	1.45	1.41
6	V	704	60G	CAU-NAP	3.05	1.43	1.37
5	A	703	FAD	O4B-C1B	3.04	1.45	1.41
5	B	703	FAD	O4B-C1B	3.04	1.45	1.41
7	C	401	ATP	C2'-C1'	3.04	1.58	1.53
6	B	704	60G	CAU-NAP	3.03	1.43	1.37
6	F	704	60G	OAR-CAA	-3.03	1.38	1.45
6	U	704	60G	CAU-NAP	3.02	1.43	1.37
6	N	705	60G	CAU-NAP	3.01	1.43	1.37
6	I	704	60G	CAU-NAP	3.01	1.43	1.37
5	Q	703	FAD	O4B-C1B	3.01	1.45	1.41
6	E	704	60G	OAR-CAA	-3.00	1.38	1.45
5	E	703	FAD	O4B-C1B	3.00	1.45	1.41
6	B	704	60G	OAR-CAA	-2.98	1.38	1.45
6	J	704	60G	OAR-CAA	-2.98	1.38	1.45
6	Q	704	60G	OAR-CAA	-2.98	1.38	1.45
5	U	703	FAD	O4B-C1B	2.97	1.45	1.41
6	V	704	60G	OAR-CAA	-2.97	1.38	1.45
7	D	401	ATP	C2'-C1'	2.97	1.58	1.53
6	A	704	60G	OAR-CAA	-2.97	1.38	1.45
5	V	703	FAD	O4B-C1B	2.96	1.45	1.41
6	N	705	60G	OAR-CAA	-2.96	1.38	1.45
6	N	704	60G	CAU-NAP	2.95	1.43	1.37
6	U	704	60G	OAR-CAA	-2.93	1.38	1.45
5	R	701	FAD	O4B-C1B	2.92	1.45	1.41
6	R	702	60G	OAR-CAA	-2.92	1.38	1.45
6	N	704	60G	OAR-CAA	-2.91	1.38	1.45
6	I	704	60G	OAR-CAA	-2.90	1.38	1.45
5	F	703	FAD	O3'-C3'	-2.85	1.36	1.43
5	M	703	FAD	O3'-C3'	-2.81	1.36	1.43
5	B	703	FAD	O3'-C3'	-2.81	1.36	1.43
5	E	703	FAD	O3'-C3'	-2.81	1.36	1.43
5	I	703	FAD	O3'-C3'	-2.79	1.36	1.43
5	Q	703	FAD	O3'-C3'	-2.78	1.36	1.43
5	V	703	FAD	O3'-C3'	-2.77	1.36	1.43
5	J	703	FAD	C2-N1	2.76	1.43	1.36
5	F	703	FAD	C2-N1	2.76	1.43	1.36
5	E	703	FAD	C2-N1	2.76	1.43	1.36
5	A	703	FAD	O3'-C3'	-2.75	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	703	FAD	O3'-C3'	-2.74	1.36	1.43
5	N	703	FAD	O3'-C3'	-2.74	1.36	1.43
5	R	701	FAD	C2-N1	2.74	1.43	1.36
5	B	703	FAD	C2-N1	2.74	1.43	1.36
5	R	701	FAD	O3'-C3'	-2.73	1.36	1.43
5	I	703	FAD	C2-N1	2.73	1.43	1.36
5	U	703	FAD	C2-N1	2.72	1.43	1.36
5	Q	703	FAD	C2-N1	2.71	1.43	1.36
5	N	703	FAD	C2-N1	2.71	1.43	1.36
5	V	703	FAD	C2-N1	2.70	1.43	1.36
5	M	703	FAD	C2-N1	2.70	1.43	1.36
5	A	703	FAD	C2-N1	2.68	1.43	1.36
5	J	703	FAD	C2'-C3'	2.61	1.58	1.53
5	R	701	FAD	C1'-N10	-2.53	1.41	1.48
5	A	703	FAD	C1'-N10	-2.51	1.41	1.48
5	V	703	FAD	C1'-N10	-2.50	1.41	1.48
5	J	703	FAD	O3'-C3'	-2.50	1.37	1.43
5	E	703	FAD	C1'-N10	-2.48	1.41	1.48
5	N	703	FAD	C1'-N10	-2.48	1.41	1.48
5	U	703	FAD	C1'-N10	-2.48	1.41	1.48
5	F	703	FAD	C1'-N10	-2.47	1.41	1.48
5	J	703	FAD	C1'-N10	-2.46	1.41	1.48
5	I	703	FAD	C1'-N10	-2.45	1.41	1.48
5	B	703	FAD	C1'-N10	-2.43	1.42	1.48
5	Q	703	FAD	C1'-N10	-2.42	1.42	1.48
5	M	703	FAD	C1'-N10	-2.39	1.42	1.48
5	U	703	FAD	C2'-C3'	2.32	1.57	1.53
5	F	703	FAD	C2'-C3'	2.29	1.57	1.53
5	I	703	FAD	C2'-C3'	2.26	1.57	1.53
5	M	703	FAD	C2'-C3'	2.26	1.57	1.53
5	J	703	FAD	O2B-C2B	2.25	1.48	1.43
5	R	701	FAD	C2'-C3'	2.25	1.57	1.53
5	Q	703	FAD	C2'-C3'	2.23	1.57	1.53
5	B	703	FAD	C2'-C3'	2.22	1.57	1.53
5	N	703	FAD	C2'-C3'	2.22	1.57	1.53
5	A	703	FAD	C2'-C3'	2.22	1.57	1.53
5	V	703	FAD	C2'-C3'	2.21	1.57	1.53
3	J	701	TPP	C5'-C4'	-2.21	1.39	1.42
5	R	701	FAD	C2B-C3B	-2.20	1.47	1.53
5	J	703	FAD	C4X-C4	2.20	1.52	1.44
5	E	703	FAD	C2'-C3'	2.20	1.57	1.53
5	V	703	FAD	C2B-C3B	-2.18	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	703	FAD	C2B-C3B	-2.18	1.47	1.53
5	U	703	FAD	C2B-C3B	-2.17	1.47	1.53
5	R	701	FAD	C4X-C4	2.17	1.52	1.44
5	A	703	FAD	C2B-C3B	-2.16	1.47	1.53
5	N	703	FAD	C2B-C3B	-2.16	1.47	1.53
5	B	703	FAD	C2B-C3B	-2.16	1.47	1.53
5	B	703	FAD	C4X-C4	2.15	1.52	1.44
5	V	703	FAD	C4X-C4	2.14	1.52	1.44
5	M	703	FAD	C1'-C2'	2.13	1.55	1.52
5	I	703	FAD	C4X-C4	2.13	1.52	1.44
5	N	703	FAD	C4X-C4	2.13	1.52	1.44
5	M	703	FAD	C4X-C4	2.13	1.52	1.44
5	E	703	FAD	C2B-C3B	-2.13	1.47	1.53
5	M	703	FAD	C2B-C3B	-2.13	1.47	1.53
7	W	401	ATP	PG-O2G	-2.13	1.46	1.54
7	W	402	ATP	PG-O2G	-2.12	1.46	1.54
5	Q	703	FAD	C4X-C4	2.12	1.52	1.44
7	T	401	ATP	PG-O2G	-2.11	1.46	1.54
5	E	703	FAD	C4X-C4	2.11	1.52	1.44
5	F	703	FAD	O2B-C2B	2.11	1.47	1.43
5	U	703	FAD	C4X-C4	2.11	1.52	1.44
7	D	401	ATP	PG-O2G	-2.11	1.46	1.54
7	H	401	ATP	PG-O2G	-2.10	1.46	1.54
5	R	701	FAD	C1'-C2'	2.10	1.55	1.52
7	P	401	ATP	PG-O2G	-2.10	1.46	1.54
7	C	401	ATP	PG-O2G	-2.10	1.46	1.54
7	G	401	ATP	PG-O2G	-2.10	1.46	1.54
5	A	703	FAD	C4X-C4	2.10	1.52	1.44
7	S	401	ATP	PG-O2G	-2.09	1.46	1.54
7	K	401	ATP	PG-O2G	-2.09	1.46	1.54
7	O	401	ATP	PG-O2G	-2.08	1.46	1.54
5	F	703	FAD	C4X-C10	-2.07	1.38	1.44
3	Q	701	TPP	C5'-C4'	-2.07	1.39	1.42
6	F	704	60G	OAR-CAV	2.06	1.37	1.33
7	L	401	ATP	PG-O2G	-2.06	1.46	1.54
6	E	704	60G	OAR-CAV	2.06	1.37	1.33
6	J	704	60G	OAR-CAV	2.05	1.37	1.33
5	U	703	FAD	C1'-C2'	2.05	1.55	1.52
6	R	702	60G	OAR-CAV	2.04	1.37	1.33
5	V	703	FAD	C1'-C2'	2.04	1.55	1.52
5	E	703	FAD	C1'-C2'	2.04	1.55	1.52
5	F	703	FAD	C1'-C2'	2.04	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	703	FAD	C2B-C3B	-2.03	1.47	1.53
5	F	703	FAD	C4X-C4	2.03	1.52	1.44
6	U	704	60G	OAR-CAV	2.02	1.37	1.33
5	J	703	FAD	C1'-C2'	2.01	1.55	1.52
6	Q	704	60G	OAR-CAV	2.01	1.37	1.33
5	A	703	FAD	C1'-C2'	2.01	1.55	1.52
3	F	701	TPP	C5'-C4'	-2.01	1.39	1.42
3	U	701	TPP	C5'-C4'	-2.01	1.39	1.42
6	I	704	60G	OAR-CAV	2.00	1.37	1.33
3	N	701	TPP	C5'-C4'	-2.00	1.39	1.42
6	A	704	60G	OAR-CAV	2.00	1.37	1.33
3	I	701	TPP	C5'-C4'	-2.00	1.39	1.42

All (506) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	704	60G	OAG-SBB-OAF	-13.32	100.05	119.35
6	A	704	60G	OAG-SBB-OAF	-13.30	100.09	119.35
6	I	704	60G	OAG-SBB-OAF	-13.24	100.17	119.35
6	E	704	60G	OAG-SBB-OAF	-13.24	100.17	119.35
6	Q	704	60G	OAG-SBB-OAF	-13.20	100.23	119.35
6	B	704	60G	OAG-SBB-OAF	-13.19	100.24	119.35
6	N	705	60G	OAG-SBB-OAF	-13.14	100.31	119.35
6	J	704	60G	OAG-SBB-OAF	-13.14	100.32	119.35
6	U	704	60G	OAG-SBB-OAF	-13.13	100.33	119.35
6	N	704	60G	OAG-SBB-OAF	-13.09	100.39	119.35
6	R	702	60G	OAG-SBB-OAF	-13.01	100.50	119.35
6	V	704	60G	OAG-SBB-OAF	-12.85	100.74	119.35
6	F	704	60G	C6-C5-C4	7.14	121.70	115.21
6	E	704	60G	C6-C5-C4	6.94	121.52	115.21
6	U	704	60G	C6-C5-C4	6.93	121.51	115.21
6	V	704	60G	C6-C5-C4	6.93	121.51	115.21
6	I	704	60G	C6-C5-C4	6.91	121.49	115.21
6	J	704	60G	C6-C5-C4	6.91	121.49	115.21
6	R	702	60G	C6-C5-C4	6.90	121.48	115.21
6	A	704	60G	C6-C5-C4	6.89	121.47	115.21
6	N	704	60G	C6-C5-C4	6.85	121.44	115.21
6	N	705	60G	C6-C5-C4	6.84	121.43	115.21
6	B	704	60G	C6-C5-C4	6.84	121.42	115.21
6	Q	704	60G	C6-C5-C4	6.71	121.31	115.21
6	F	704	60G	NAQ-CAU-NAP	6.11	123.03	114.93
6	U	704	60G	NAQ-CAU-NAP	6.09	123.00	114.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	704	60G	NAQ-CAU-NAP	5.92	122.77	114.93
3	E	701	TPP	PA-O3A-PB	-5.89	112.61	132.83
3	J	701	TPP	PA-O3A-PB	-5.87	112.68	132.83
6	E	704	60G	NAQ-CAU-NAP	5.86	122.70	114.93
3	V	701	TPP	PA-O3A-PB	-5.80	112.93	132.83
6	Q	704	60G	NAQ-CAU-NAP	5.78	122.59	114.93
6	N	705	60G	NAQ-CAU-NAP	5.77	122.58	114.93
6	J	704	60G	NAQ-CAU-NAP	5.75	122.55	114.93
6	A	704	60G	NAQ-CAU-NAP	5.75	122.55	114.93
3	Q	701	TPP	PA-O3A-PB	-5.73	113.16	132.83
3	U	701	TPP	PA-O3A-PB	-5.69	113.30	132.83
6	B	704	60G	NAQ-CAU-NAP	5.65	122.42	114.93
6	R	702	60G	NAQ-CAU-NAP	5.61	122.36	114.93
6	I	704	60G	NAQ-CAU-NAP	5.61	122.36	114.93
6	N	704	60G	NAQ-CAU-NAP	5.60	122.35	114.93
3	F	701	TPP	PA-O3A-PB	-5.60	113.62	132.83
3	M	701	TPP	PA-O3A-PB	-5.59	113.65	132.83
3	I	701	TPP	PA-O3A-PB	-5.57	113.71	132.83
6	Q	704	60G	C2-N3-C4	5.57	121.54	114.99
3	N	701	TPP	PA-O3A-PB	-5.51	113.91	132.83
3	A	701	TPP	PA-O3A-PB	-5.50	113.94	132.83
3	B	701	TPP	PA-O3A-PB	-5.44	114.17	132.83
6	B	704	60G	C2-N3-C4	5.36	121.29	114.99
6	A	704	60G	C2-N1-C6	5.29	121.21	114.99
6	F	704	60G	C5-C6-N1	-5.26	117.94	124.08
6	R	702	60G	C2-N1-C6	5.24	121.16	114.99
6	N	705	60G	C2-N1-C6	5.21	121.12	114.99
6	V	704	60G	C2-N3-C4	5.19	121.10	114.99
6	J	704	60G	C2-N1-C6	5.19	121.09	114.99
6	N	704	60G	C2-N3-C4	5.18	121.09	114.99
6	I	704	60G	C2-N3-C4	5.16	121.06	114.99
6	E	704	60G	C2-N1-C6	5.15	121.05	114.99
6	U	704	60G	C2-N1-C6	5.13	121.02	114.99
6	R	702	60G	C5-C4-N3	-5.07	118.16	124.08
6	Q	704	60G	C5-C4-N3	-5.02	118.22	124.08
6	J	704	60G	C5-C4-N3	-5.02	118.22	124.08
6	U	704	60G	C5-C4-N3	-5.02	118.22	124.08
6	E	704	60G	C5-C4-N3	-5.01	118.23	124.08
6	I	704	60G	C5-C6-N1	-5.00	118.24	124.08
6	N	704	60G	C5-C6-N1	-4.96	118.29	124.08
6	V	704	60G	C5-C6-N1	-4.95	118.31	124.08
6	N	705	60G	C5-C4-N3	-4.93	118.33	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	704	60G	C5-C6-N1	-4.92	118.34	124.08
6	A	704	60G	C5-C4-N3	-4.91	118.34	124.08
6	A	704	60G	C5-C6-N1	-4.85	118.42	124.08
6	E	704	60G	C5-C6-N1	-4.82	118.45	124.08
6	B	704	60G	C5-C4-N3	-4.82	118.45	124.08
6	V	704	60G	C5-C4-N3	-4.82	118.46	124.08
6	U	704	60G	C5-C6-N1	-4.79	118.48	124.08
6	J	704	60G	C5-C6-N1	-4.79	118.49	124.08
6	R	702	60G	C5-C6-N1	-4.79	118.49	124.08
6	J	704	60G	OAR-CAV-CBA	4.78	120.23	112.30
6	I	704	60G	C5-C4-N3	-4.77	118.51	124.08
6	N	705	60G	C5-C6-N1	-4.77	118.52	124.08
6	N	704	60G	C5-C4-N3	-4.77	118.52	124.08
6	F	704	60G	C2-N3-C4	4.76	120.59	114.99
6	Q	704	60G	C5-C6-N1	-4.75	118.53	124.08
6	N	705	60G	OAR-CAV-CBA	4.74	120.17	112.30
6	E	704	60G	OAR-CAV-CBA	4.70	120.11	112.30
6	N	704	60G	OAR-CAV-CBA	4.62	119.97	112.30
6	Q	704	60G	OAR-CAV-CBA	4.58	119.89	112.30
6	F	704	60G	OAR-CAV-CBA	4.57	119.89	112.30
6	F	704	60G	C5-C4-N3	-4.56	118.76	124.08
6	A	704	60G	OAR-CAV-CBA	4.55	119.85	112.30
6	V	704	60G	OAR-CAV-CBA	4.48	119.74	112.30
6	B	704	60G	OAR-CAV-CBA	4.48	119.73	112.30
6	F	704	60G	C2-NAP-CAU	-4.35	125.76	130.40
7	L	401	ATP	N3-C2-N1	-4.32	121.93	128.68
6	E	704	60G	C2-NAP-CAU	-4.32	125.80	130.40
6	I	704	60G	C2-NAP-CAU	-4.31	125.80	130.40
7	O	401	ATP	N3-C2-N1	-4.25	122.03	128.68
6	I	704	60G	OAR-CAV-CBA	4.24	119.33	112.30
7	H	401	ATP	N3-C2-N1	-4.23	122.06	128.68
7	P	401	ATP	N3-C2-N1	-4.23	122.07	128.68
7	T	401	ATP	N3-C2-N1	-4.22	122.09	128.68
6	N	704	60G	C2-NAP-CAU	-4.21	125.91	130.40
7	D	401	ATP	N3-C2-N1	-4.20	122.11	128.68
7	C	401	ATP	N3-C2-N1	-4.20	122.11	128.68
7	G	401	ATP	N3-C2-N1	-4.20	122.12	128.68
7	W	401	ATP	N3-C2-N1	-4.19	122.13	128.68
7	K	401	ATP	N3-C2-N1	-4.19	122.13	128.68
7	S	401	ATP	N3-C2-N1	-4.19	122.14	128.68
7	W	402	ATP	N3-C2-N1	-4.17	122.15	128.68
6	U	704	60G	OAR-CAV-CBA	4.17	119.22	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	702	60G	C2-NAP-CAU	-4.14	125.98	130.40
6	U	704	60G	C2-NAP-CAU	-4.06	126.07	130.40
5	U	703	FAD	N3A-C2A-N1A	-3.99	122.45	128.68
5	V	703	FAD	N3A-C2A-N1A	-3.98	122.47	128.68
6	R	702	60G	OAR-CAV-CBA	3.96	118.87	112.30
6	R	702	60G	C2-N3-C4	3.95	119.63	114.99
6	J	704	60G	C2-NAP-CAU	-3.94	126.19	130.40
5	N	703	FAD	N3A-C2A-N1A	-3.94	122.53	128.68
5	B	703	FAD	N3A-C2A-N1A	-3.93	122.54	128.68
6	F	704	60G	C2-N1-C6	3.92	119.60	114.99
5	I	703	FAD	N3A-C2A-N1A	-3.91	122.56	128.68
5	R	701	FAD	N3A-C2A-N1A	-3.91	122.57	128.68
5	E	703	FAD	N3A-C2A-N1A	-3.89	122.59	128.68
5	M	703	FAD	N3A-C2A-N1A	-3.88	122.61	128.68
5	Q	703	FAD	N3A-C2A-N1A	-3.87	122.63	128.68
6	J	704	60G	C2-N3-C4	3.87	119.54	114.99
5	A	703	FAD	N3A-C2A-N1A	-3.86	122.65	128.68
7	D	401	ATP	C3'-C2'-C1'	3.82	106.72	100.98
5	J	703	FAD	N3A-C2A-N1A	-3.79	122.75	128.68
6	N	705	60G	C2-NAP-CAU	-3.79	126.36	130.40
6	V	704	60G	C2-NAP-CAU	-3.78	126.37	130.40
6	B	704	60G	C2-NAP-CAU	-3.76	126.39	130.40
6	I	704	60G	C2-N1-C6	3.74	119.38	114.99
6	U	704	60G	C2-N3-C4	3.73	119.38	114.99
6	E	704	60G	C2-N3-C4	3.73	119.37	114.99
3	B	701	TPP	C7'-N3-C2	-3.71	118.65	125.35
6	N	704	60G	C2-N1-C6	3.71	119.35	114.99
3	Q	701	TPP	C7'-N3-C2	-3.70	118.67	125.35
3	V	701	TPP	C7'-N3-C2	-3.70	118.67	125.35
6	Q	704	60G	C2-N1-C6	3.69	119.33	114.99
3	I	701	TPP	C7'-N3-C2	-3.69	118.68	125.35
6	B	704	60G	C2-N1-C6	3.69	119.33	114.99
3	F	701	TPP	C7'-N3-C2	-3.69	118.69	125.35
6	N	705	60G	C2-N3-C4	3.68	119.32	114.99
6	A	704	60G	C2-NAP-CAU	-3.67	126.49	130.40
6	V	704	60G	C2-N1-C6	3.67	119.30	114.99
3	A	701	TPP	C7'-N3-C2	-3.66	118.75	125.35
6	A	704	60G	C2-N3-C4	3.65	119.28	114.99
3	N	701	TPP	C7'-N3-C2	-3.64	118.78	125.35
5	F	703	FAD	N3A-C2A-N1A	-3.61	123.04	128.68
3	E	701	TPP	C7'-N3-C2	-3.58	118.88	125.35
3	M	701	TPP	N1'-C2'-N3'	-3.58	119.38	125.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	701	TPP	C7'-N3-C2	-3.57	118.90	125.35
3	J	701	TPP	C7'-N3-C2	-3.54	118.95	125.35
3	U	701	TPP	C7'-N3-C2	-3.53	118.97	125.35
3	B	701	TPP	N1'-C2'-N3'	-3.52	119.48	125.54
3	J	701	TPP	N1'-C2'-N3'	-3.51	119.50	125.54
3	V	701	TPP	N1'-C2'-N3'	-3.49	119.53	125.54
3	A	701	TPP	N1'-C2'-N3'	-3.47	119.56	125.54
6	N	704	60G	OAG-SBB-CAM	3.47	113.58	108.30
3	E	701	TPP	N1'-C2'-N3'	-3.46	119.58	125.54
6	B	704	60G	OAG-SBB-CAM	3.46	113.57	108.30
3	I	701	TPP	N1'-C2'-N3'	-3.45	119.60	125.54
3	Q	701	TPP	N1'-C2'-N3'	-3.45	119.60	125.54
3	U	701	TPP	N1'-C2'-N3'	-3.45	119.61	125.54
3	N	701	TPP	N1'-C2'-N3'	-3.45	119.61	125.54
6	A	704	60G	OAD-CAU-NAP	-3.44	117.81	123.62
6	F	704	60G	OAD-CAU-NAP	-3.44	117.81	123.62
6	Q	704	60G	C2-NAP-CAU	-3.43	126.74	130.40
5	J	703	FAD	O4B-C1B-C2B	-3.43	101.91	106.93
6	U	704	60G	OAD-CAU-NAP	-3.42	117.84	123.62
6	V	704	60G	OAG-SBB-CAM	3.37	113.43	108.30
6	I	704	60G	OAD-CAU-NAP	-3.37	117.93	123.62
7	G	401	ATP	C3'-C2'-C1'	3.36	106.04	100.98
6	Q	704	60G	OAG-SBB-CAM	3.36	113.42	108.30
6	J	704	60G	OAG-SBB-CAM	3.36	113.42	108.30
6	F	704	60G	OAG-SBB-CAM	3.35	113.41	108.30
6	E	704	60G	OAD-CAU-NAP	-3.35	117.95	123.62
6	N	705	60G	OAD-CAU-NAP	-3.35	117.96	123.62
6	V	704	60G	OAD-CAU-NAP	-3.34	117.97	123.62
6	N	704	60G	OAD-CAU-NAP	-3.34	117.97	123.62
6	N	705	60G	OAG-SBB-CAM	3.34	113.38	108.30
6	A	704	60G	OAG-SBB-CAM	3.32	113.35	108.30
3	F	701	TPP	N1'-C2'-N3'	-3.28	119.89	125.54
6	E	704	60G	OAG-SBB-CAM	3.28	113.29	108.30
7	W	401	ATP	PB-O3B-PG	-3.27	121.60	132.83
6	I	704	60G	OAG-SBB-CAM	3.27	113.28	108.30
5	J	703	FAD	C4-N3-C2	-3.27	119.61	125.64
6	B	704	60G	OAD-CAU-NAP	-3.26	118.10	123.62
6	Q	704	60G	N1-C2-N3	-3.26	121.07	126.23
6	R	702	60G	N1-C2-N3	-3.26	121.07	126.23
6	U	704	60G	OAG-SBB-CAM	3.25	113.26	108.30
7	T	401	ATP	C3'-C2'-C1'	3.24	105.86	100.98
6	Q	704	60G	OAD-CAU-NAP	-3.23	118.16	123.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	703	FAD	C4-N3-C2	-3.22	119.68	125.64
6	B	704	60G	N1-C2-N3	-3.21	121.15	126.23
6	J	704	60G	N1-C2-N3	-3.20	121.17	126.23
6	R	702	60G	OAD-CAU-NAP	-3.18	118.24	123.62
5	R	701	FAD	C4-N3-C2	-3.18	119.76	125.64
5	F	703	FAD	C4X-C4-N3	3.17	121.25	113.19
5	B	703	FAD	C4-N3-C2	-3.16	119.80	125.64
3	M	701	TPP	C5-C4-N3	3.16	113.89	107.57
5	I	703	FAD	C4-N3-C2	-3.16	119.81	125.64
6	A	704	60G	N1-C2-N3	-3.14	121.27	126.23
5	U	703	FAD	C4-N3-C2	-3.13	119.85	125.64
7	K	401	ATP	PA-O3A-PB	-3.13	122.08	132.83
5	V	703	FAD	C4-N3-C2	-3.13	119.86	125.64
3	Q	701	TPP	C5-C4-N3	3.13	113.83	107.57
6	N	705	60G	N1-C2-N3	-3.13	121.29	126.23
5	Q	703	FAD	C4-N3-C2	-3.12	119.87	125.64
6	J	704	60G	OAD-CAU-NAP	-3.12	118.35	123.62
3	U	701	TPP	C5-C4-N3	3.12	113.81	107.57
5	M	703	FAD	C4-N3-C2	-3.11	119.89	125.64
3	A	701	TPP	C5-C4-N3	3.11	113.80	107.57
6	I	704	60G	N1-C2-N3	-3.11	121.32	126.23
6	N	704	60G	N1-C2-N3	-3.11	121.32	126.23
6	R	702	60G	OAG-SBB-CAM	3.10	113.03	108.30
6	V	704	60G	N1-C2-N3	-3.10	121.33	126.23
5	A	703	FAD	C4-N3-C2	-3.10	119.92	125.64
5	E	703	FAD	C4-N3-C2	-3.08	119.95	125.64
6	E	704	60G	N1-C2-N3	-3.07	121.37	126.23
3	F	701	TPP	C5-C4-N3	3.07	113.72	107.57
6	U	704	60G	N1-C2-N3	-3.07	121.38	126.23
5	J	703	FAD	C4X-C4-N3	3.07	120.98	113.19
3	E	701	TPP	C5-C4-N3	3.06	113.70	107.57
5	M	703	FAD	C4A-C5A-N7A	-3.05	106.22	109.40
7	K	401	ATP	C3'-C2'-C1'	3.05	105.57	100.98
6	F	704	60G	N1-C2-N3	-3.05	121.41	126.23
3	N	701	TPP	C5-C4-N3	3.05	113.68	107.57
5	N	703	FAD	C4-N3-C2	-3.05	120.02	125.64
7	D	401	ATP	PB-O3B-PG	-3.04	122.38	132.83
3	B	701	TPP	C5-C4-N3	3.04	113.66	107.57
7	P	401	ATP	PB-O3B-PG	-3.02	122.46	132.83
3	I	701	TPP	C5-C4-N3	3.02	113.62	107.57
7	T	401	ATP	PB-O3B-PG	-3.02	122.48	132.83
3	N	701	TPP	C5'-C7'-N3	-3.00	108.28	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	701	TPP	C5-C4-N3	2.99	113.56	107.57
7	C	401	ATP	PA-O3A-PB	-2.99	122.56	132.83
3	J	701	TPP	CM2-C2'-N1'	2.99	120.43	117.14
7	S	401	ATP	PA-O3A-PB	-2.99	122.56	132.83
3	M	701	TPP	C6'-N1'-C2'	2.99	121.05	115.96
7	O	401	ATP	PA-O3A-PB	-2.98	122.59	132.83
5	B	703	FAD	C4A-C5A-N7A	-2.98	106.29	109.40
5	R	701	FAD	C4X-C4-N3	2.97	120.74	113.19
3	J	701	TPP	C6'-N1'-C2'	2.97	121.02	115.96
5	U	703	FAD	C4A-C5A-N7A	-2.96	106.31	109.40
5	R	701	FAD	C4A-C5A-N7A	-2.96	106.31	109.40
5	V	703	FAD	C4A-C5A-N7A	-2.96	106.31	109.40
5	E	703	FAD	C4A-C5A-N7A	-2.95	106.32	109.40
5	I	703	FAD	C3B-C2B-C1B	2.95	105.42	100.98
7	O	401	ATP	PB-O3B-PG	-2.95	122.72	132.83
5	N	703	FAD	C4A-C5A-N7A	-2.95	106.33	109.40
5	B	703	FAD	C4X-C4-N3	2.94	120.65	113.19
3	M	701	TPP	CM2-C2'-N1'	2.93	120.36	117.14
3	B	701	TPP	C6'-N1'-C2'	2.93	120.95	115.96
3	U	701	TPP	C5'-C7'-N3	-2.93	108.40	113.28
5	A	703	FAD	C4X-C4-N3	2.93	120.62	113.19
5	U	703	FAD	C4X-C4-N3	2.92	120.61	113.19
5	F	703	FAD	P-O3P-PA	-2.92	122.80	132.83
5	I	703	FAD	C4X-C4-N3	2.92	120.60	113.19
5	Q	703	FAD	C4A-C5A-N7A	-2.91	106.36	109.40
5	V	703	FAD	C4X-C4-N3	2.91	120.59	113.19
5	A	703	FAD	C4A-C5A-N7A	-2.91	106.37	109.40
5	E	703	FAD	C4X-C4-N3	2.90	120.56	113.19
5	Q	703	FAD	C4X-C4-N3	2.90	120.56	113.19
3	U	701	TPP	CM4-C4-C5	-2.90	121.26	127.60
5	M	703	FAD	C4X-C4-N3	2.90	120.55	113.19
3	A	701	TPP	C6'-N1'-C2'	2.90	120.89	115.96
7	P	401	ATP	PA-O3A-PB	-2.89	122.91	132.83
7	W	402	ATP	PA-O3A-PB	-2.89	122.91	132.83
5	J	703	FAD	C4X-C10-N1	-2.89	118.03	124.73
5	I	703	FAD	C4A-C5A-N7A	-2.88	106.39	109.40
7	L	401	ATP	PA-O3A-PB	-2.87	122.99	132.83
7	C	401	ATP	PB-O3B-PG	-2.86	123.00	132.83
5	N	703	FAD	C4X-C4-N3	2.86	120.46	113.19
3	N	701	TPP	C6'-N1'-C2'	2.86	120.82	115.96
3	A	701	TPP	CM4-C4-C5	-2.85	121.36	127.60
3	I	701	TPP	CM2-C2'-N1'	2.85	120.27	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	703	FAD	O4-C4-C4X	-2.85	119.05	126.60
3	Q	701	TPP	CM4-C4-C5	-2.85	121.38	127.60
7	H	401	ATP	PB-O3B-PG	-2.84	123.07	132.83
3	V	701	TPP	CM2-C2'-N1'	2.84	120.26	117.14
3	E	701	TPP	C6'-N1'-C2'	2.83	120.78	115.96
3	J	701	TPP	C5-C4-N3	2.83	113.23	107.57
3	V	701	TPP	C6'-N1'-C2'	2.82	120.77	115.96
3	U	701	TPP	C6'-N1'-C2'	2.82	120.77	115.96
3	I	701	TPP	C6'-N1'-C2'	2.82	120.76	115.96
7	W	402	ATP	PB-O3B-PG	-2.81	123.17	132.83
7	G	401	ATP	PB-O3B-PG	-2.81	123.18	132.83
3	E	701	TPP	CM2-C2'-N1'	2.81	120.23	117.14
3	Q	701	TPP	C6'-N1'-C2'	2.81	120.74	115.96
3	F	701	TPP	C6'-N1'-C2'	2.81	120.74	115.96
3	Q	701	TPP	C5'-C7'-N3	-2.80	108.61	113.28
3	U	701	TPP	CM2-C2'-N1'	2.80	120.22	117.14
7	T	401	ATP	PA-O3A-PB	-2.80	123.21	132.83
3	E	701	TPP	CM4-C4-C5	-2.78	121.52	127.60
3	B	701	TPP	CM2-C2'-N1'	2.77	120.19	117.14
3	F	701	TPP	CM2-C2'-N1'	2.76	120.17	117.14
3	A	701	TPP	C5'-C7'-N3	-2.73	108.72	113.28
3	N	701	TPP	CM2-C2'-N1'	2.73	120.14	117.14
7	G	401	ATP	PA-O3A-PB	-2.72	123.48	132.83
3	J	701	TPP	CM4-C4-C5	-2.72	121.65	127.60
7	L	401	ATP	PB-O3B-PG	-2.72	123.51	132.83
7	H	401	ATP	C3'-C2'-C1'	2.71	105.06	100.98
5	B	703	FAD	C3B-C2B-C1B	2.71	105.06	100.98
3	M	701	TPP	CM4-C4-C5	-2.71	121.67	127.60
7	H	401	ATP	PA-O3A-PB	-2.70	123.55	132.83
5	B	703	FAD	P-O3P-PA	-2.70	123.55	132.83
5	F	703	FAD	C4X-C10-N1	-2.70	118.46	124.73
3	A	701	TPP	CM2-C2'-N1'	2.69	120.09	117.14
7	W	401	ATP	PA-O3A-PB	-2.69	123.60	132.83
3	Q	701	TPP	CM2-C2'-N1'	2.69	120.09	117.14
3	B	701	TPP	CM4-C4-C5	-2.68	121.73	127.60
3	I	701	TPP	CM4-C4-C5	-2.67	121.77	127.60
3	N	701	TPP	CM4-C4-C5	-2.67	121.77	127.60
5	V	703	FAD	P-O3P-PA	-2.66	123.69	132.83
3	E	701	TPP	C5'-C7'-N3	-2.66	108.84	113.28
3	F	701	TPP	CM4-C4-C5	-2.66	121.78	127.60
5	M	703	FAD	C4X-C10-N1	-2.63	118.63	124.73
7	P	401	ATP	C3'-C2'-C1'	2.63	104.94	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	701	FAD	C4X-C10-N1	-2.63	118.63	124.73
5	V	703	FAD	C4X-C10-N1	-2.62	118.64	124.73
5	Q	703	FAD	C4X-C10-N1	-2.62	118.65	124.73
7	W	401	ATP	C3'-C2'-C1'	2.62	104.92	100.98
5	N	703	FAD	P-O3P-PA	-2.61	123.86	132.83
5	I	703	FAD	C4X-C10-N1	-2.61	118.67	124.73
5	R	701	FAD	O4-C4-C4X	-2.61	119.67	126.60
5	U	703	FAD	C4X-C10-N1	-2.61	118.67	124.73
5	A	703	FAD	P-O3P-PA	-2.60	123.90	132.83
5	A	703	FAD	O4-C4-C4X	-2.60	119.70	126.60
5	Q	703	FAD	P-O3P-PA	-2.60	123.91	132.83
7	W	402	ATP	C3'-C2'-C1'	2.60	104.89	100.98
7	K	401	ATP	PB-O3B-PG	-2.60	123.92	132.83
5	J	703	FAD	P-O3P-PA	-2.59	123.93	132.83
5	F	703	FAD	C10-N1-C2	2.59	122.08	116.90
5	U	703	FAD	O4-C4-C4X	-2.58	119.75	126.60
5	E	703	FAD	C4X-C10-N1	-2.58	118.75	124.73
5	B	703	FAD	C4X-C10-N1	-2.58	118.75	124.73
5	M	703	FAD	C3B-C2B-C1B	2.58	104.86	100.98
3	F	701	TPP	C6'-C5'-C4'	2.57	119.22	115.72
5	J	703	FAD	C10-N1-C2	2.57	122.04	116.90
5	V	703	FAD	O4-C4-C4X	-2.57	119.79	126.60
5	F	703	FAD	C4'-C3'-C2'	-2.57	108.03	113.36
3	V	701	TPP	CM4-C4-C5	-2.56	122.00	127.60
5	E	703	FAD	P-O3P-PA	-2.56	124.03	132.83
5	E	703	FAD	O4-C4-C4X	-2.56	119.80	126.60
5	N	703	FAD	C4X-C10-N1	-2.56	118.79	124.73
7	D	401	ATP	C2'-C3'-C4'	2.56	107.61	102.64
5	M	703	FAD	O4-C4-C4X	-2.56	119.82	126.60
5	I	703	FAD	O4-C4-C4X	-2.55	119.83	126.60
5	N	703	FAD	O4-C4-C4X	-2.55	119.83	126.60
5	A	703	FAD	C4X-C10-N1	-2.55	118.81	124.73
5	B	703	FAD	O4-C4-C4X	-2.55	119.85	126.60
5	Q	703	FAD	O4-C4-C4X	-2.55	119.85	126.60
5	N	703	FAD	C9A-C5X-N5	-2.55	119.67	122.43
5	J	703	FAD	O4-C4-C4X	-2.54	119.86	126.60
7	D	401	ATP	PA-O3A-PB	-2.53	124.13	132.83
5	J	703	FAD	C4'-C3'-C2'	-2.53	108.09	113.36
5	N	703	FAD	C4-C4X-N5	2.53	121.83	118.23
5	E	703	FAD	C4-C4X-N5	2.52	121.82	118.23
7	C	401	ATP	C3'-C2'-C1'	2.52	104.77	100.98
5	V	703	FAD	C4-C4X-N5	2.52	121.82	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	703	FAD	C9A-C5X-N5	-2.51	119.70	122.43
5	I	703	FAD	P-O3P-PA	-2.51	124.21	132.83
5	U	703	FAD	C4-C4X-N5	2.51	121.80	118.23
5	M	703	FAD	P-O3P-PA	-2.51	124.23	132.83
5	N	703	FAD	C10-C4X-N5	-2.50	119.54	124.86
7	S	401	ATP	PB-O3B-PG	-2.50	124.24	132.83
5	B	703	FAD	C4-C4X-N5	2.50	121.79	118.23
3	V	701	TPP	C5'-C7'-N3	-2.50	109.12	113.28
3	I	701	TPP	C5'-C7'-N3	-2.50	109.12	113.28
5	V	703	FAD	C10-C4X-N5	-2.50	119.56	124.86
3	B	701	TPP	C5'-C7'-N3	-2.50	109.12	113.28
5	J	703	FAD	C9A-C5X-N5	-2.49	119.73	122.43
5	U	703	FAD	C10-C4X-N5	-2.48	119.59	124.86
5	E	703	FAD	C10-C4X-N5	-2.48	119.60	124.86
7	L	401	ATP	C3'-C2'-C1'	2.47	104.69	100.98
7	O	401	ATP	C3'-C2'-C1'	2.47	104.69	100.98
5	R	701	FAD	C10-N1-C2	2.46	121.82	116.90
5	V	703	FAD	C9A-C5X-N5	-2.45	119.77	122.43
5	R	701	FAD	C4-C4X-N5	2.45	121.72	118.23
5	A	703	FAD	C4-C4X-N5	2.45	121.72	118.23
5	E	703	FAD	C9A-C5X-N5	-2.45	119.77	122.43
5	B	703	FAD	C10-C4X-N5	-2.43	119.69	124.86
5	F	703	FAD	C4-C4X-N5	2.43	121.69	118.23
5	J	703	FAD	C10-C4X-N5	-2.41	119.73	124.86
5	Q	703	FAD	C10-C4X-N5	-2.41	119.75	124.86
3	J	701	TPP	C6'-C5'-C4'	2.40	118.99	115.72
5	J	703	FAD	C4-C4X-N5	2.40	121.65	118.23
5	R	701	FAD	C10-C4X-N5	-2.39	119.79	124.86
5	A	703	FAD	C10-C4X-N5	-2.39	119.80	124.86
3	J	701	TPP	C5'-C6'-N1'	-2.38	119.86	123.82
6	R	702	60G	OAR-CAV-OAE	-2.37	118.81	123.45
3	F	701	TPP	C5'-C6'-N1'	-2.37	119.87	123.82
5	Q	703	FAD	C4-C4X-N5	2.37	121.60	118.23
5	R	701	FAD	P-O3P-PA	-2.36	124.73	132.83
5	F	703	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
5	J	703	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
7	W	401	ATP	C4-C5-N7	-2.35	106.95	109.40
7	S	401	ATP	C3'-C2'-C1'	2.34	104.51	100.98
5	I	703	FAD	C10-N1-C2	2.34	121.58	116.90
7	H	401	ATP	C4-C5-N7	-2.34	106.96	109.40
5	V	703	FAD	C10-N1-C2	2.34	121.58	116.90
5	U	703	FAD	C10-N1-C2	2.34	121.57	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	401	ATP	C4-C5-N7	-2.33	106.97	109.40
5	M	703	FAD	C10-N1-C2	2.32	121.55	116.90
5	E	703	FAD	C10-N1-C2	2.32	121.55	116.90
5	Q	703	FAD	C10-N1-C2	2.32	121.54	116.90
5	M	703	FAD	C10-C4X-N5	-2.32	119.94	124.86
5	B	703	FAD	C9A-C5X-N5	-2.32	119.91	122.43
3	Q	701	TPP	C6'-C5'-C4'	2.32	118.87	115.72
5	I	703	FAD	C10-C4X-N5	-2.32	119.94	124.86
5	B	703	FAD	C10-N1-C2	2.31	121.52	116.90
7	T	401	ATP	C4-C5-N7	-2.30	107.00	109.40
3	N	701	TPP	C6'-C5'-C4'	2.30	118.85	115.72
3	F	701	TPP	C5'-C7'-N3	-2.29	109.46	113.28
5	R	701	FAD	C4X-C10-N10	2.29	119.82	116.48
3	B	701	TPP	O3B-PB-O3A	2.28	112.30	104.64
5	A	703	FAD	C10-N1-C2	2.28	121.47	116.90
7	G	401	ATP	C4-C5-N7	-2.28	107.02	109.40
5	E	703	FAD	C5'-C4'-C3'	-2.28	107.79	112.20
5	M	703	FAD	C4X-C10-N10	2.28	119.81	116.48
5	F	703	FAD	C10-C4X-N5	-2.28	120.02	124.86
7	K	401	ATP	C4-C5-N7	-2.27	107.03	109.40
5	F	703	FAD	C9A-C5X-N5	-2.27	119.97	122.43
5	A	703	FAD	C3B-C2B-C1B	2.26	104.39	100.98
5	I	703	FAD	C4X-C10-N10	2.26	119.78	116.48
3	I	701	TPP	C6'-C5'-C4'	2.25	118.79	115.72
5	I	703	FAD	C4-C4X-N5	2.25	121.44	118.23
5	J	703	FAD	C4X-C10-N10	2.24	119.76	116.48
3	E	701	TPP	PA-O7-C7	-2.24	110.55	121.59
5	N	703	FAD	C10-N1-C2	2.24	121.38	116.90
5	R	701	FAD	C9A-C5X-N5	-2.23	120.00	122.43
3	A	701	TPP	O3B-PB-O3A	2.23	112.12	104.64
5	M	703	FAD	C4-C4X-N5	2.23	121.41	118.23
7	S	401	ATP	C4-C5-N7	-2.23	107.07	109.40
5	F	703	FAD	C3B-C2B-C1B	2.23	104.34	100.98
3	B	701	TPP	PA-O7-C7	-2.23	110.61	121.59
5	A	703	FAD	C5'-C4'-C3'	-2.22	107.91	112.20
5	B	703	FAD	C5'-C4'-C3'	-2.22	107.91	112.20
7	O	401	ATP	C4-C5-N7	-2.22	107.09	109.40
3	Q	701	TPP	PA-O7-C7	-2.22	110.67	121.59
3	B	701	TPP	C6'-C5'-C4'	2.21	118.73	115.72
3	B	701	TPP	C5'-C6'-N1'	-2.21	120.14	123.82
5	A	703	FAD	C4X-C10-N10	2.20	119.70	116.48
5	Q	703	FAD	C9A-C5X-N5	-2.20	120.04	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	701	TPP	PA-O7-C7	-2.20	110.75	121.59
3	N	701	TPP	C5'-C6'-N1'	-2.20	120.15	123.82
5	Q	703	FAD	C3B-C2B-C1B	2.20	104.29	100.98
3	M	701	TPP	C5'-C6'-N1'	-2.20	120.16	123.82
7	D	401	ATP	C4-C5-N7	-2.19	107.11	109.40
3	U	701	TPP	C6'-C5'-C4'	2.19	118.70	115.72
7	P	401	ATP	C4-C5-N7	-2.19	107.11	109.40
7	W	402	ATP	C4-C5-N7	-2.19	107.12	109.40
3	J	701	TPP	C5'-C7'-N3	-2.19	109.64	113.28
3	A	701	TPP	PA-O7-C7	-2.18	110.85	121.59
7	L	401	ATP	C4-C5-N7	-2.18	107.13	109.40
3	A	701	TPP	C6'-C5'-C4'	2.18	118.68	115.72
3	E	701	TPP	C6'-C5'-C4'	2.16	118.67	115.72
3	Q	701	TPP	C5'-C6'-N1'	-2.16	120.22	123.82
5	M	703	FAD	C5'-C4'-C3'	-2.16	108.03	112.20
3	I	701	TPP	C5'-C6'-N1'	-2.16	120.22	123.82
5	Q	703	FAD	C4X-C10-N10	2.16	119.63	116.48
6	U	704	60G	OAR-CAV-OAE	-2.15	119.24	123.45
3	A	701	TPP	C5'-C6'-N1'	-2.15	120.24	123.82
3	U	701	TPP	C5'-C6'-N1'	-2.14	120.25	123.82
5	I	703	FAD	C9A-C5X-N5	-2.14	120.11	122.43
3	N	701	TPP	PA-O7-C7	-2.14	111.05	121.59
3	V	701	TPP	C6'-C5'-C4'	2.14	118.63	115.72
5	A	703	FAD	C9A-C5X-N5	-2.14	120.11	122.43
5	V	703	FAD	C3B-C2B-C1B	2.13	104.19	100.98
3	M	701	TPP	C6'-C5'-C4'	2.13	118.61	115.72
5	B	703	FAD	C4X-C10-N10	2.13	119.59	116.48
3	I	701	TPP	O2B-PB-O3A	2.12	111.76	104.64
5	M	703	FAD	C9A-C5X-N5	-2.12	120.13	122.43
5	U	703	FAD	C4X-C10-N10	2.12	119.58	116.48
3	E	701	TPP	C5'-C6'-N1'	-2.11	120.30	123.82
5	U	703	FAD	P-O3P-PA	-2.11	125.58	132.83
3	V	701	TPP	PA-O7-C7	-2.11	111.22	121.59
6	I	704	60G	CAM-SBB-NAQ	2.10	110.87	105.07
3	V	701	TPP	C5'-C6'-N1'	-2.09	120.33	123.82
5	V	703	FAD	C4X-C10-N10	2.09	119.53	116.48
6	F	704	60G	CAA-OAR-CAV	2.08	119.85	115.83
3	M	701	TPP	PA-O7-C7	-2.08	111.34	121.59
7	D	401	ATP	O4'-C1'-C2'	-2.08	103.89	106.93
6	I	704	60G	OAR-CAV-OAE	-2.07	119.41	123.45
3	F	701	TPP	PA-O7-C7	-2.06	111.44	121.59
5	F	703	FAD	C4X-C10-N10	2.06	119.49	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	701	TPP	O3B-PB-O3A	2.06	111.53	104.64
3	A	701	TPP	CM2-C2'-N3'	2.05	120.34	117.15
5	E	703	FAD	C3B-C2B-C1B	2.05	104.06	100.98
5	N	703	FAD	C3B-C2B-C1B	2.04	104.05	100.98
3	B	701	TPP	CM2-C2'-N3'	2.04	120.33	117.15
3	U	701	TPP	PA-O7-C7	-2.04	111.57	121.59
6	I	704	60G	CAA-OAR-CAV	2.04	119.76	115.83
3	J	701	TPP	CM4-C4-N3	2.03	125.12	122.53
6	U	704	60G	CAA-OAR-CAV	2.02	119.74	115.83
3	Q	701	TPP	CM2-C2'-N3'	2.02	120.30	117.15
6	A	704	60G	CAM-SBB-NAQ	2.02	110.65	105.07
6	J	704	60G	CAA-OAR-CAV	2.02	119.72	115.83
5	U	703	FAD	C3B-C2B-C1B	2.02	104.02	100.98
6	V	704	60G	OAR-CAV-OAE	-2.01	119.51	123.45
5	E	703	FAD	C4X-C10-N10	2.01	119.42	116.48
6	B	704	60G	CAA-OAR-CAV	2.01	119.71	115.83
3	F	701	TPP	O2B-PB-O3A	2.01	111.37	104.64
6	E	704	60G	CAM-SBB-NAQ	2.00	110.60	105.07

There are no chirality outliers.

All (261) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	TPP	C5-C6-C7-O7
3	A	701	TPP	C7-O7-PA-O1A
3	A	701	TPP	C7-O7-PA-O2A
3	A	701	TPP	PA-O3A-PB-O3B
3	B	701	TPP	C5-C6-C7-O7
3	B	701	TPP	C7-O7-PA-O1A
3	B	701	TPP	C7-O7-PA-O2A
3	E	701	TPP	C4-C5-C6-C7
3	E	701	TPP	C7-O7-PA-O1A
3	E	701	TPP	C7-O7-PA-O2A
3	F	701	TPP	C5-C6-C7-O7
3	F	701	TPP	C7-O7-PA-O1A
3	F	701	TPP	C7-O7-PA-O2A
3	I	701	TPP	C5-C6-C7-O7
3	I	701	TPP	C7-O7-PA-O2A
3	J	701	TPP	C5-C6-C7-O7
3	J	701	TPP	C7-O7-PA-O1A
3	J	701	TPP	C7-O7-PA-O2A
3	M	701	TPP	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
3	N	701	TPP	C5-C6-C7-O7
3	N	701	TPP	C7-O7-PA-O3A
3	Q	701	TPP	C4-C5-C6-C7
3	Q	701	TPP	C5-C6-C7-O7
3	Q	701	TPP	C7-O7-PA-O2A
3	U	701	TPP	C4-C5-C6-C7
3	U	701	TPP	C5-C6-C7-O7
3	U	701	TPP	C7-O7-PA-O1A
3	U	701	TPP	C7-O7-PA-O2A
3	V	701	TPP	C5-C6-C7-O7
5	F	703	FAD	C5B-O5B-PA-O1A
5	F	703	FAD	C5B-O5B-PA-O3P
5	F	703	FAD	C3'-C4'-C5'-O5'
5	F	703	FAD	O4'-C4'-C5'-O5'
5	F	703	FAD	C5'-O5'-P-O3P
5	J	703	FAD	C5B-O5B-PA-O2A
5	J	703	FAD	C5B-O5B-PA-O3P
5	J	703	FAD	C3B-C4B-C5B-O5B
5	J	703	FAD	C3'-C4'-C5'-O5'
5	J	703	FAD	O4'-C4'-C5'-O5'
5	J	703	FAD	C5'-O5'-P-O3P
5	R	701	FAD	O4B-C4B-C5B-O5B
5	R	701	FAD	N10-C1'-C2'-O2'
5	U	703	FAD	C5B-O5B-PA-O1A
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	U	703	FAD	C5'-O5'-P-O3P
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
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	F	704	60G	C5-C4-OAT-CAC
6	F	704	60G	N3-C4-OAT-CAC

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Mol	Chain	Res	Type	Atoms
6	F	704	60G	CAW-CAM-SBB-OAF
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	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	705	60G	CAW-CAM-SBB-OAF
6	Q	704	60G	C5-C6-OAS-CAB
6	Q	704	60G	N1-C6-OAS-CAB
6	Q	704	60G	CAW-CAM-SBB-OAF
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
7	K	401	ATP	C5'-O5'-PA-O1A
7	K	401	ATP	C5'-O5'-PA-O2A
7	O	401	ATP	C5'-O5'-PA-O1A
7	O	401	ATP	O4'-C4'-C5'-O5'
7	O	401	ATP	C3'-C4'-C5'-O5'
7	S	401	ATP	PB-O3B-PG-O3G
7	W	401	ATP	C5'-O5'-PA-O3A
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

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Mol	Chain	Res	Type	Atoms
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
6	V	704	60G	N3-C4-OAT-CAC
6	V	704	60G	N1-C6-OAS-CAB
6	U	704	60G	CBA-CAV-OAR-CAA
7	S	401	ATP	O4'-C4'-C5'-O5'
7	S	401	ATP	C3'-C4'-C5'-O5'
6	B	704	60G	C5-C6-OAS-CAB
6	F	704	60G	C5-C6-OAS-CAB
6	A	704	60G	CBA-CAV-OAR-CAA
5	R	701	FAD	C3B-C4B-C5B-O5B
6	B	704	60G	CBA-CAV-OAR-CAA
6	I	704	60G	CBA-CAV-OAR-CAA
5	U	703	FAD	O2'-C2'-C3'-O3'
5	U	703	FAD	O2'-C2'-C3'-C4'
5	B	703	FAD	O4B-C4B-C5B-O5B
5	J	703	FAD	O4B-C4B-C5B-O5B
5	V	703	FAD	O2'-C2'-C3'-C4'
6	R	702	60G	CAW-CAM-SBB-OAF
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
5	I	703	FAD	O4B-C4B-C5B-O5B
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	B	703	FAD	C3B-C4B-C5B-O5B
3	E	701	TPP	C5-C6-C7-O7
7	K	401	ATP	C4'-C5'-O5'-PA
3	A	701	TPP	PA-O3A-PB-O2B
3	E	701	TPP	C7-O7-PA-O3A
3	J	701	TPP	C7-O7-PA-O3A

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

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Mol	Chain	Res	Type	Atoms
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	R	701	FAD	C4'-C5'-O5'-P
5	I	703	FAD	O3'-C3'-C4'-O4'
5	E	703	FAD	O4B-C4B-C5B-O5B
6	I	704	60G	OAR-CAV-CBA-CAW
6	U	704	60G	OAR-CAV-CBA-CAW
5	I	703	FAD	O3'-C3'-C4'-C5'
7	G	401	ATP	C3'-C4'-C5'-O5'
5	V	703	FAD	C2'-C3'-C4'-C5'
7	S	401	ATP	C4'-C5'-O5'-PA
6	J	704	60G	CAW-CAM-SBB-NAQ
5	I	703	FAD	C2'-C3'-C4'-C5'
5	A	703	FAD	PA-O3P-P-O2P
5	R	701	FAD	PA-O3P-P-O1P
5	V	703	FAD	PA-O3P-P-O1P
6	A	704	60G	OAR-CAV-CBA-CAK
5	I	703	FAD	C3B-C4B-C5B-O5B
5	R	701	FAD	O3'-C3'-C4'-C5'
5	R	701	FAD	C2'-C3'-C4'-O4'
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
3	A	701	TPP	C7-O7-PA-O3A
3	B	701	TPP	C7-O7-PA-O3A
3	F	701	TPP	C7-O7-PA-O3A
3	I	701	TPP	C7-O7-PA-O3A
3	Q	701	TPP	C7-O7-PA-O3A
3	U	701	TPP	C7-O7-PA-O3A
7	C	401	ATP	C5'-O5'-PA-O3A
7	K	401	ATP	C5'-O5'-PA-O3A
7	P	401	ATP	C5'-O5'-PA-O3A
5	R	701	FAD	O3'-C3'-C4'-O4'
5	M	703	FAD	C3B-C4B-C5B-O5B
5	N	703	FAD	O4B-C4B-C5B-O5B

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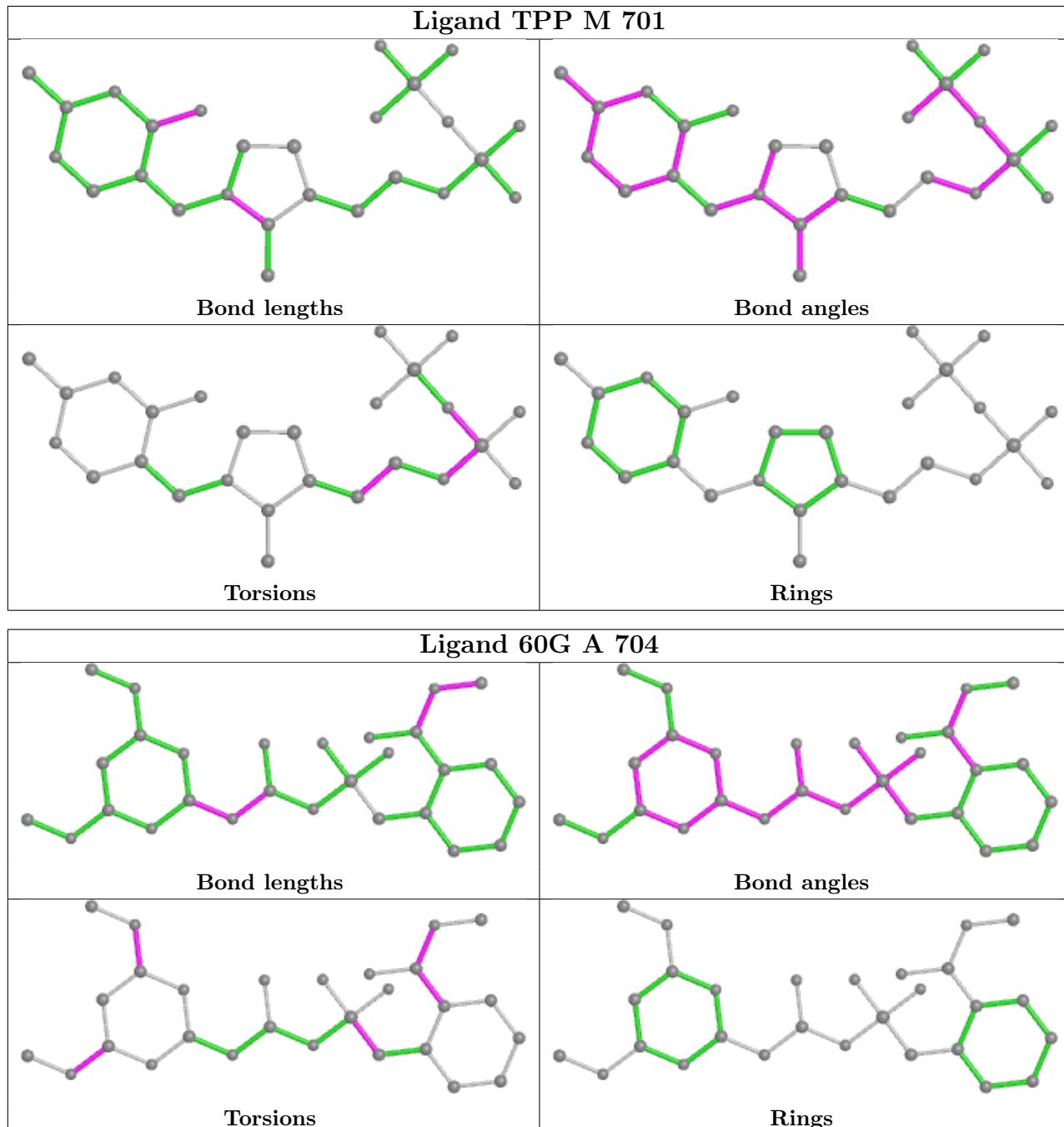
Mol	Chain	Res	Type	Atoms
5	U	703	FAD	O4B-C4B-C5B-O5B
5	V	703	FAD	O4B-C4B-C5B-O5B
7	D	401	ATP	C3'-C4'-C5'-O5'
7	W	401	ATP	C3'-C4'-C5'-O5'
7	W	402	ATP	C3'-C4'-C5'-O5'
3	N	701	TPP	PB-O3A-PA-O1A
5	B	703	FAD	PA-O3P-P-O2P
5	R	701	FAD	P-O3P-PA-O2A
7	C	401	ATP	PG-O3B-PB-O1B
7	H	401	ATP	PG-O3B-PB-O1B
7	S	401	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	V	703	FAD	O3'-C3'-C4'-O4'
3	M	701	TPP	C7-O7-PA-O1A
3	N	701	TPP	C7-O7-PA-O2A
5	R	701	FAD	C5'-O5'-P-O1P
6	F	704	60G	CAW-CAM-SBB-NAQ
6	N	704	60G	CAW-CAM-SBB-NAQ
6	Q	704	60G	CAW-CAM-SBB-NAQ
6	V	704	60G	CAW-CAM-SBB-NAQ
5	A	703	FAD	O4B-C4B-C5B-O5B
5	E	703	FAD	C3B-C4B-C5B-O5B
5	Q	703	FAD	O4B-C4B-C5B-O5B
6	B	704	60G	OAR-CAV-CBA-CAK
5	V	703	FAD	C1'-C2'-C3'-O3'
7	D	401	ATP	C4'-C5'-O5'-PA
5	U	703	FAD	N10-C1'-C2'-O2'
6	R	702	60G	OAE-CAV-CBA-CAK
6	N	705	60G	OAR-CAV-CBA-CAK

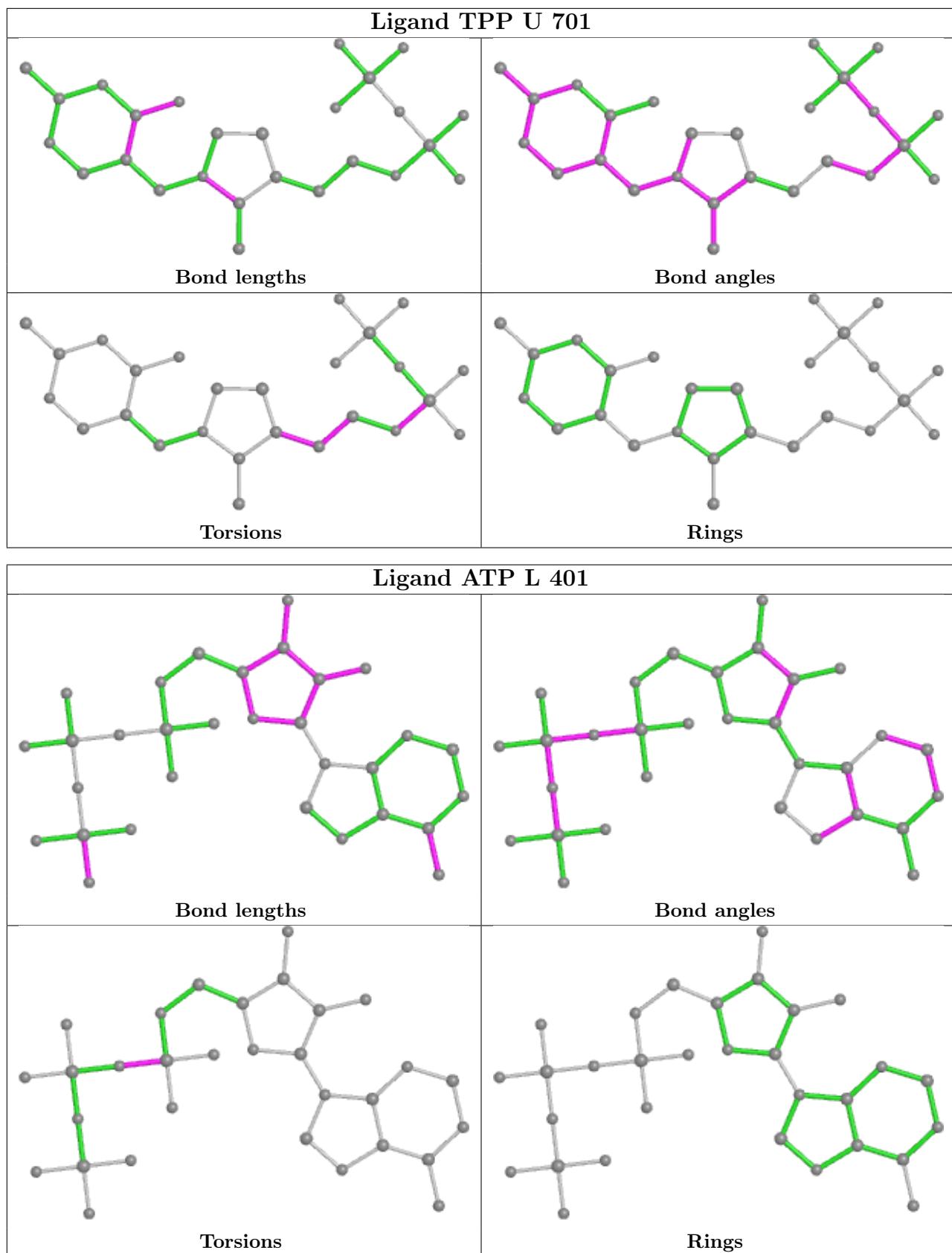
There are no ring outliers.

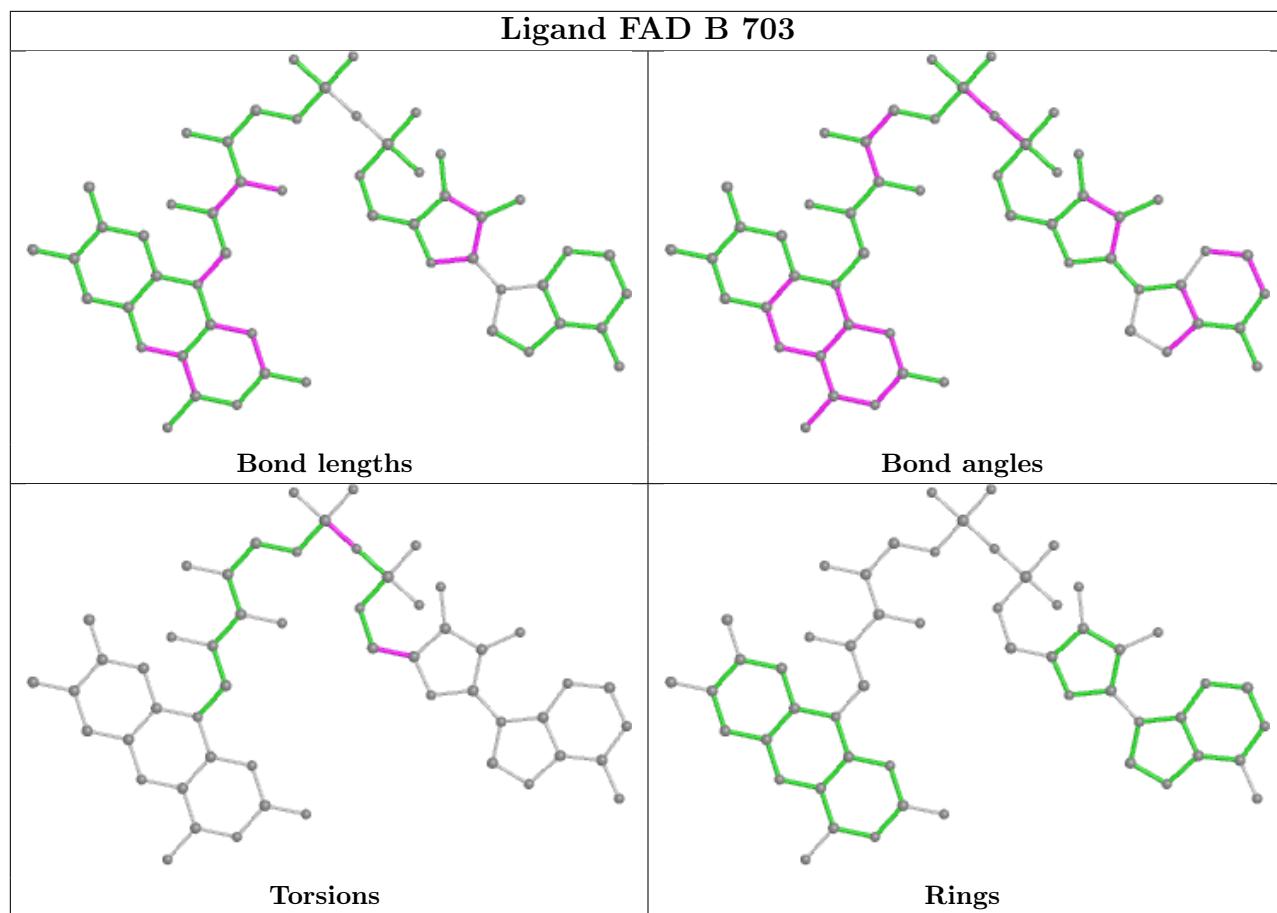
No monomer is involved in short contacts.

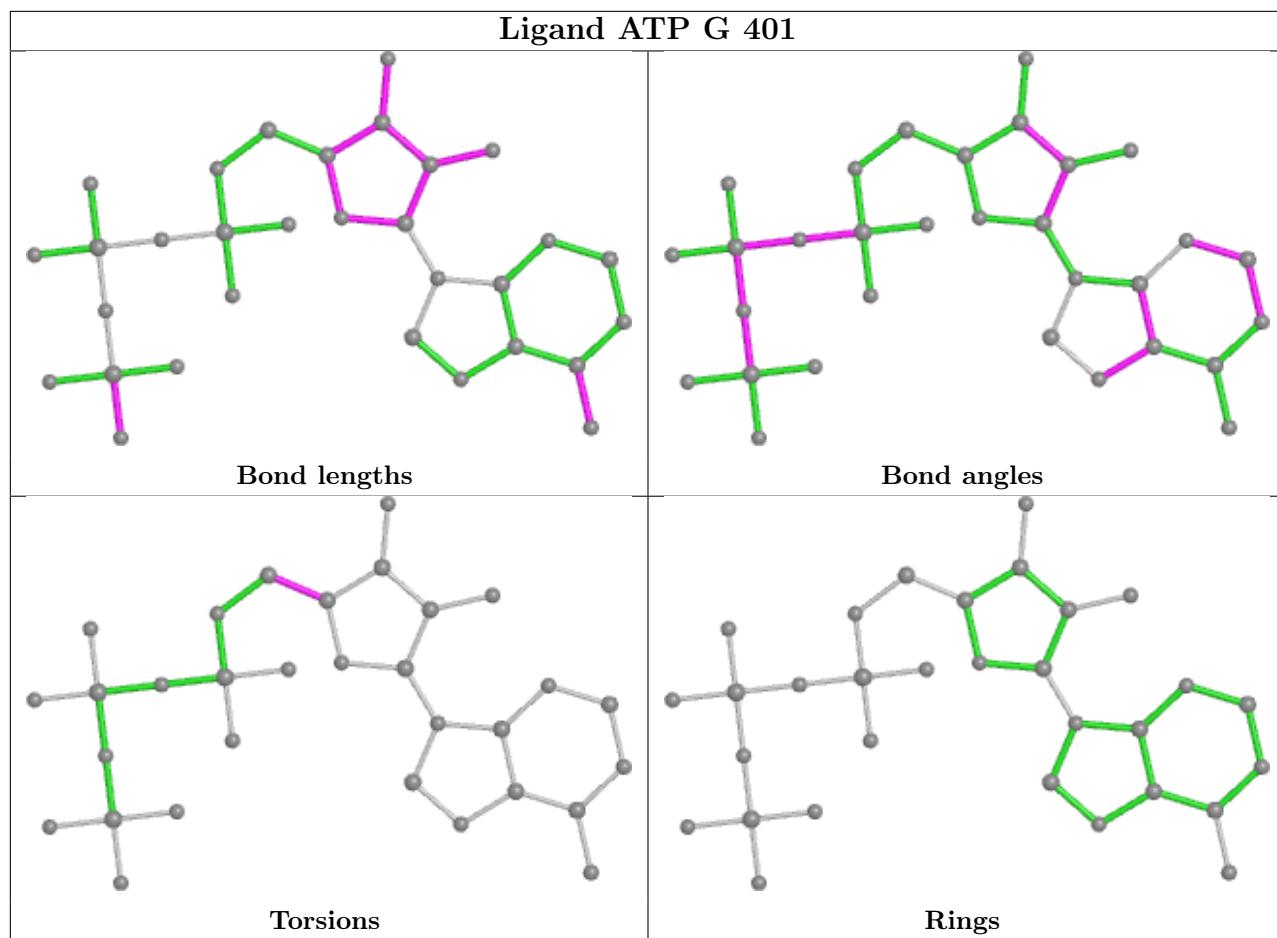
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

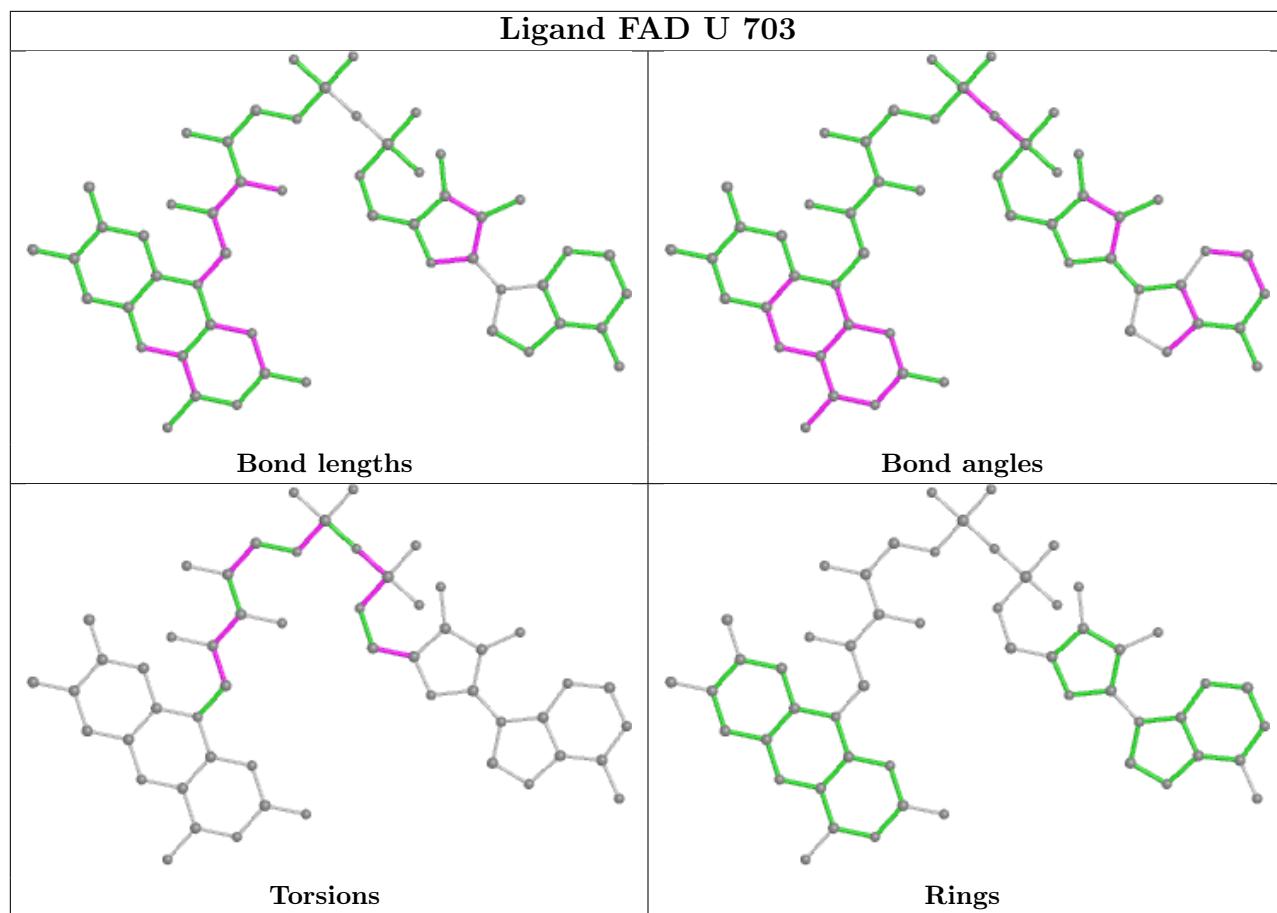
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

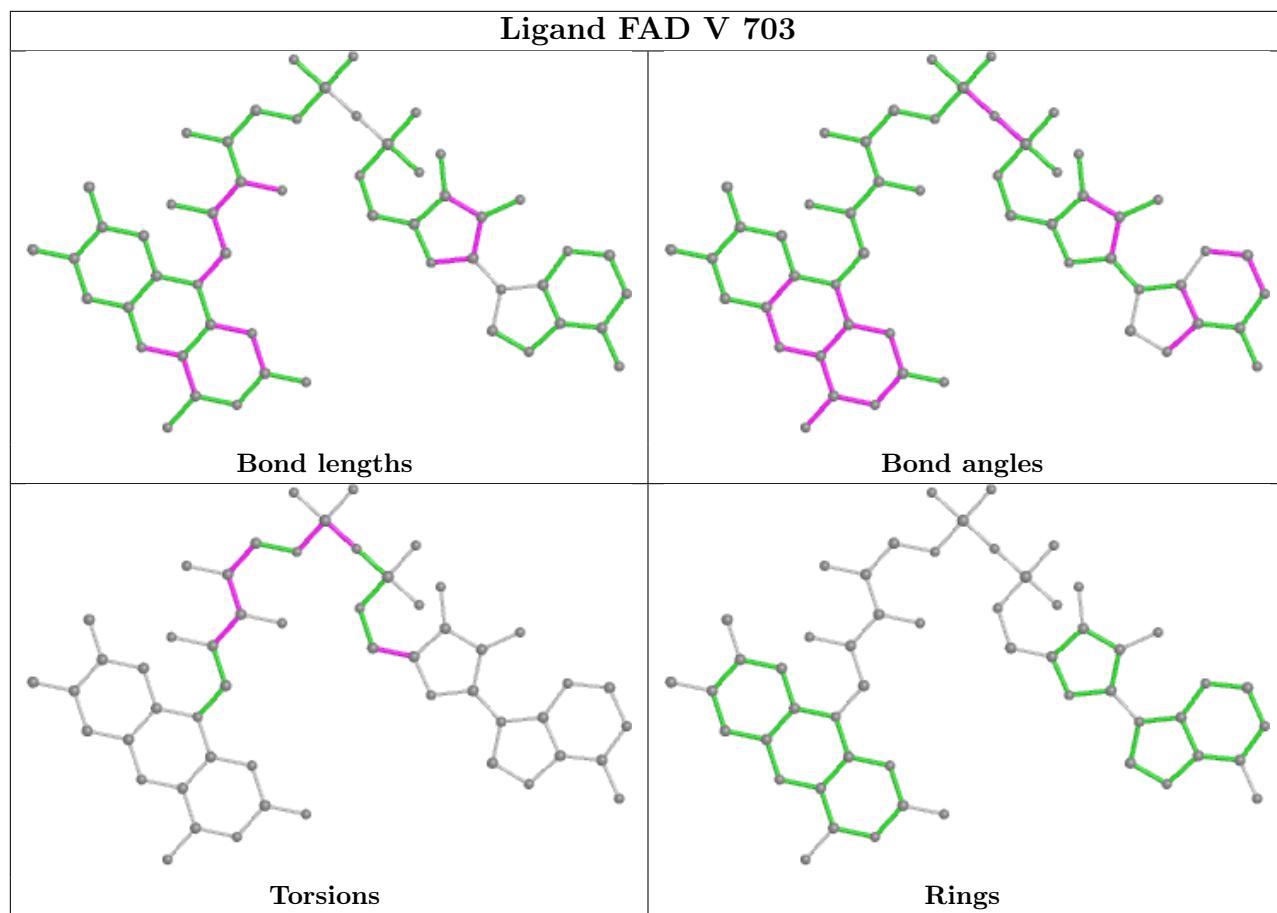


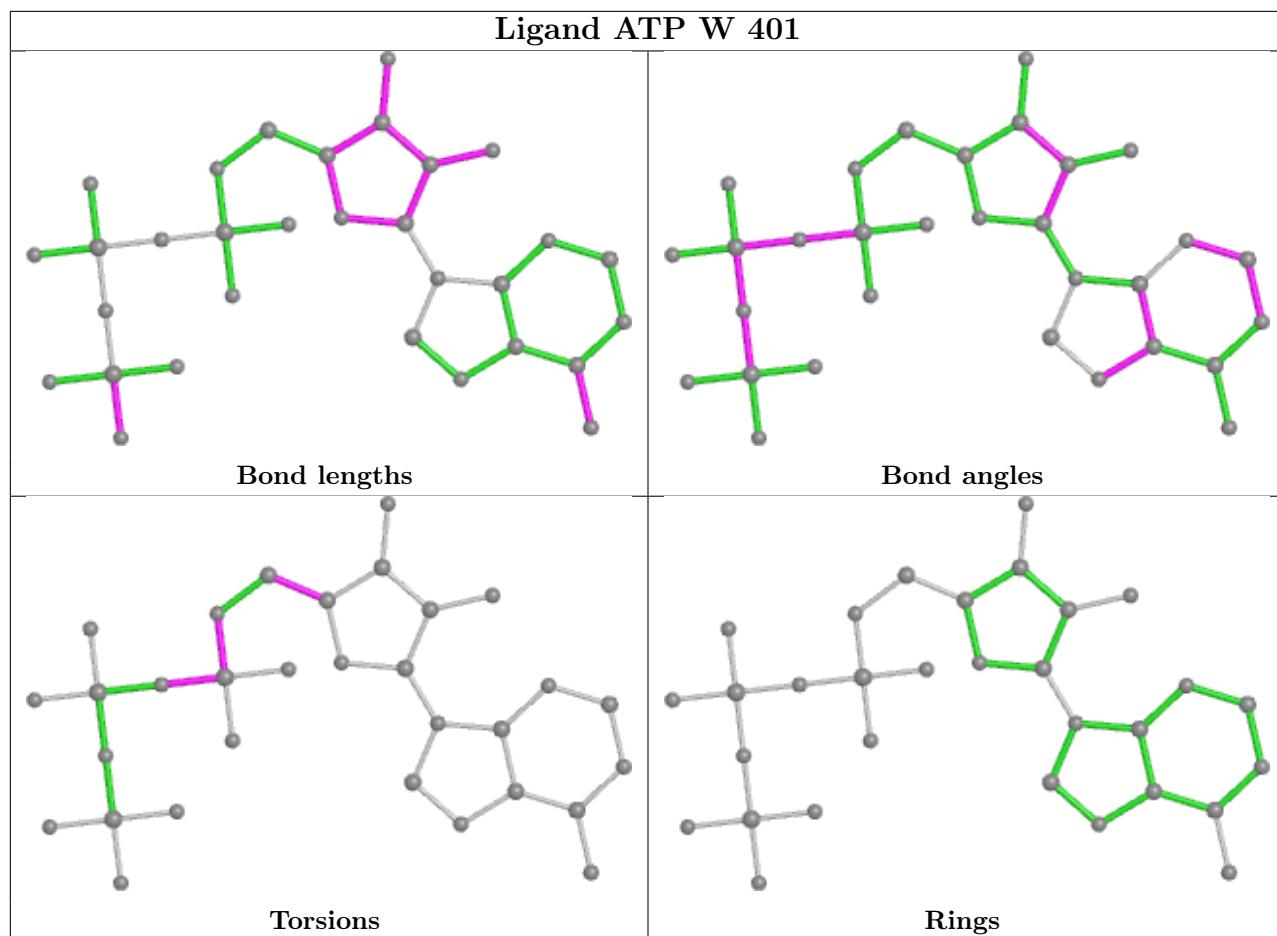


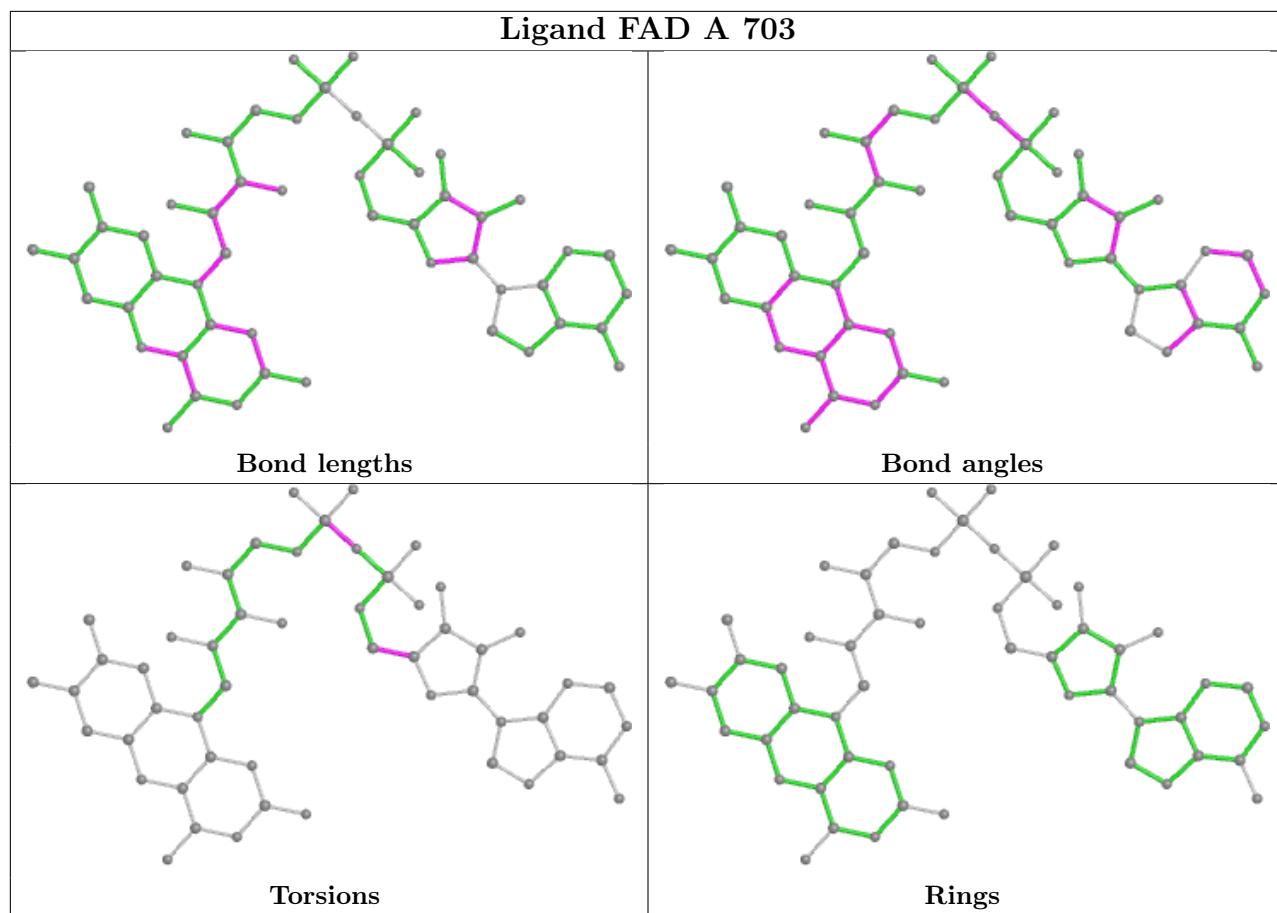


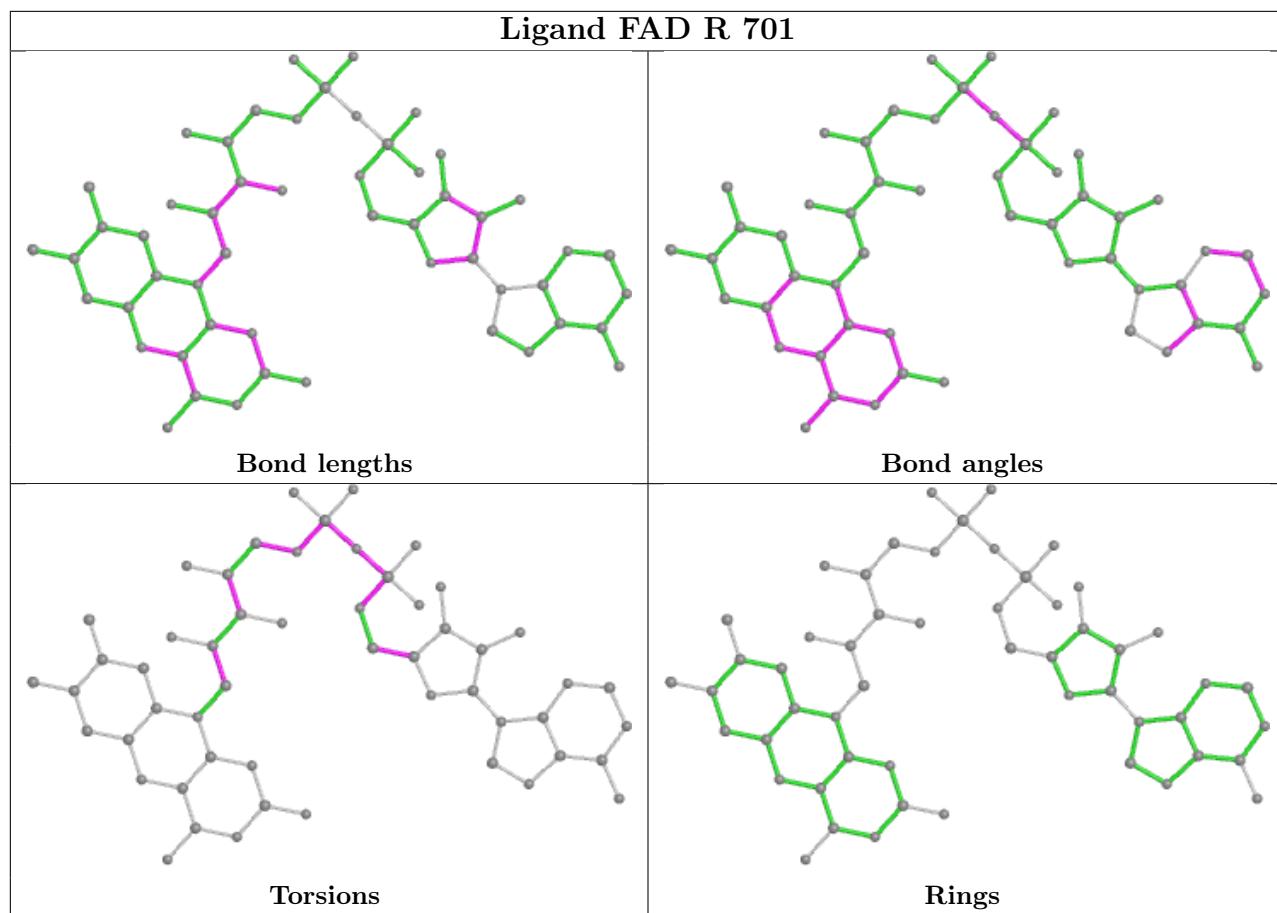


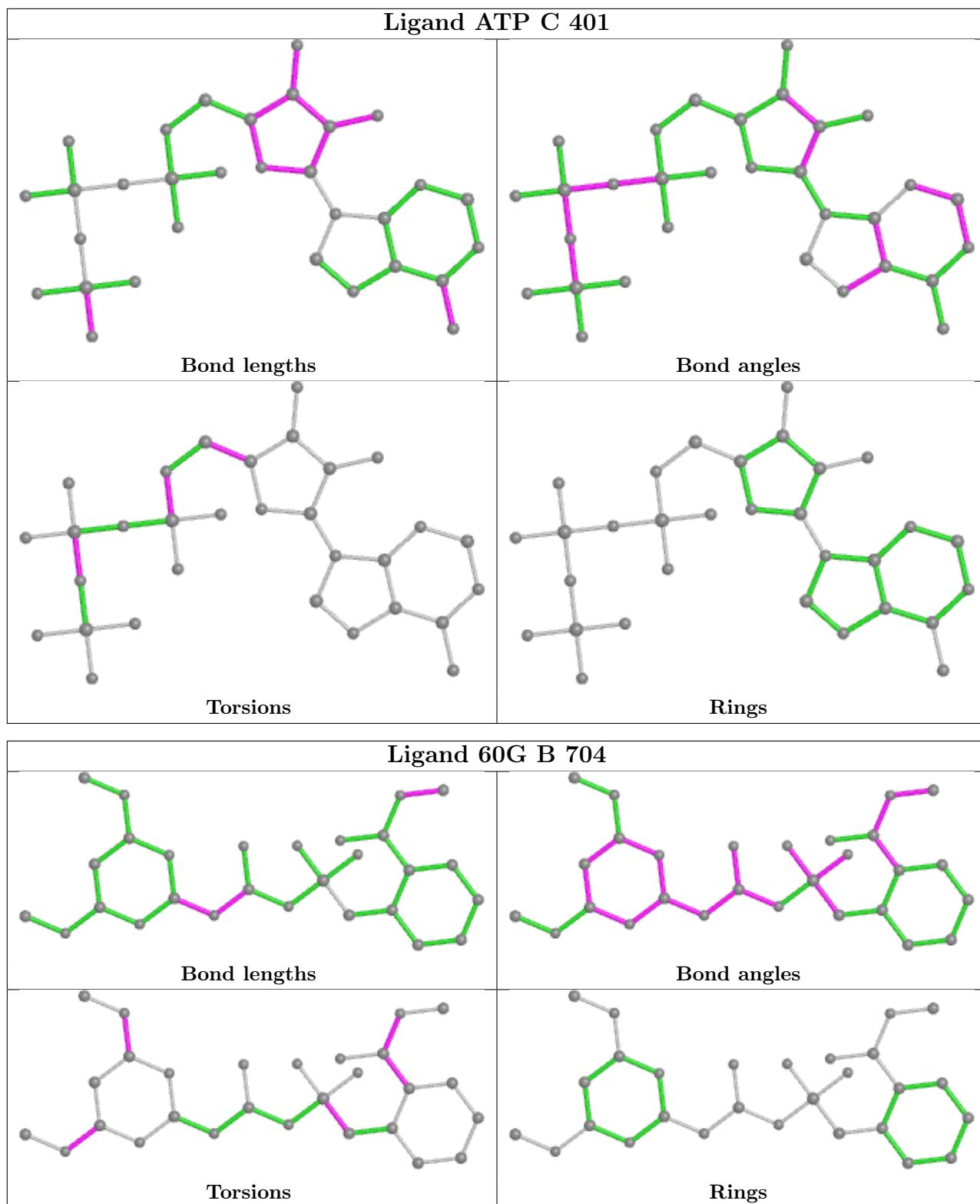


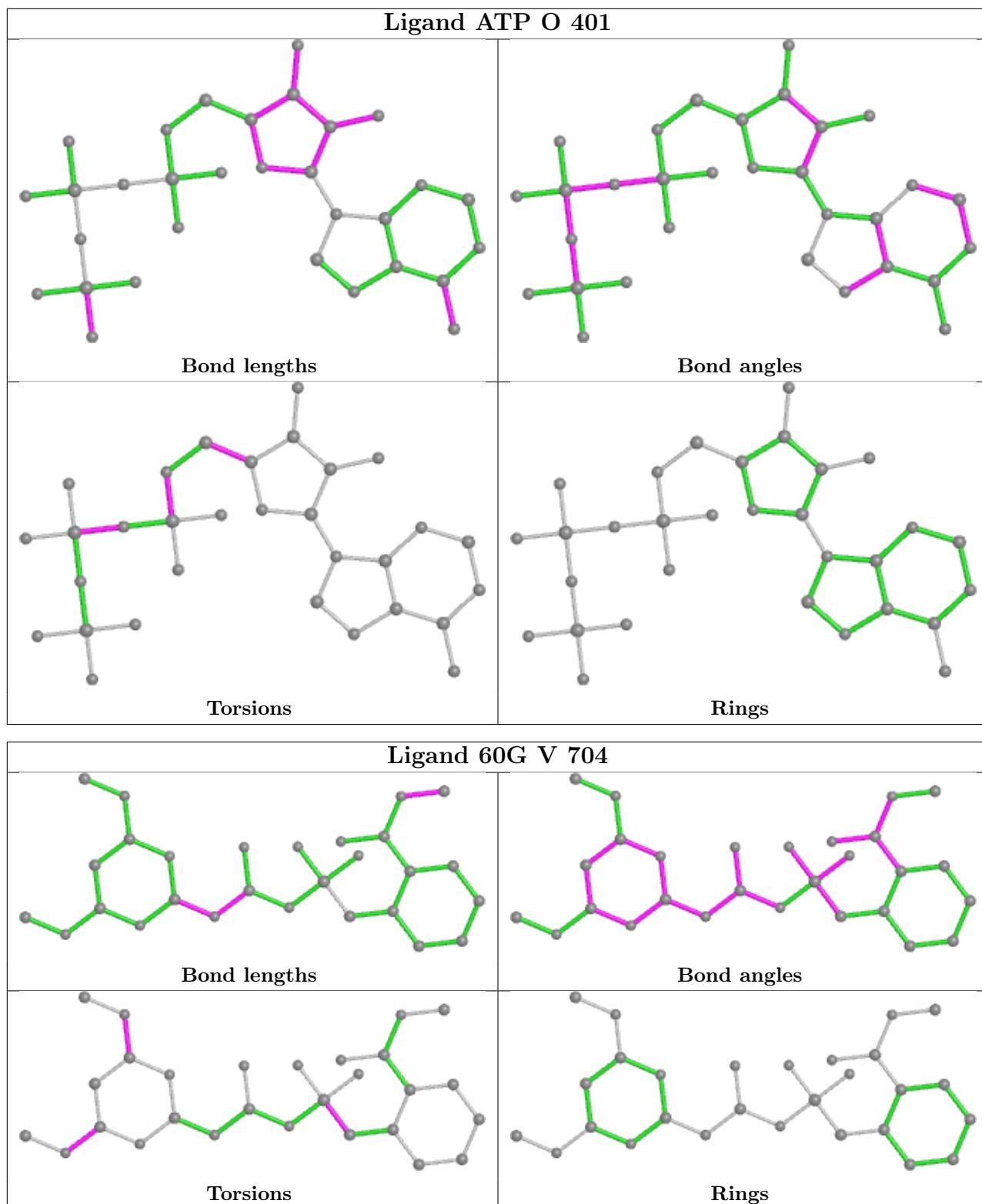


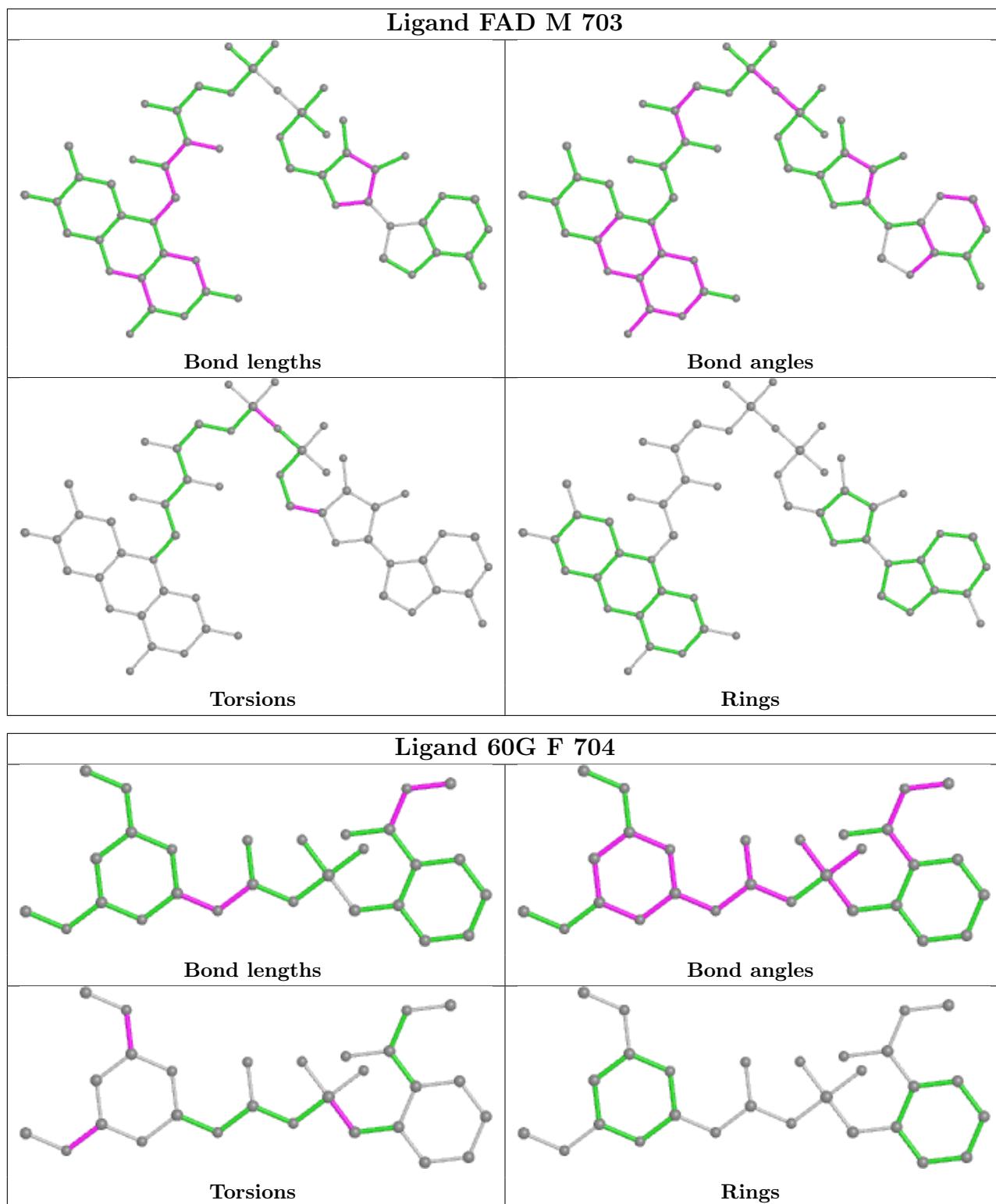


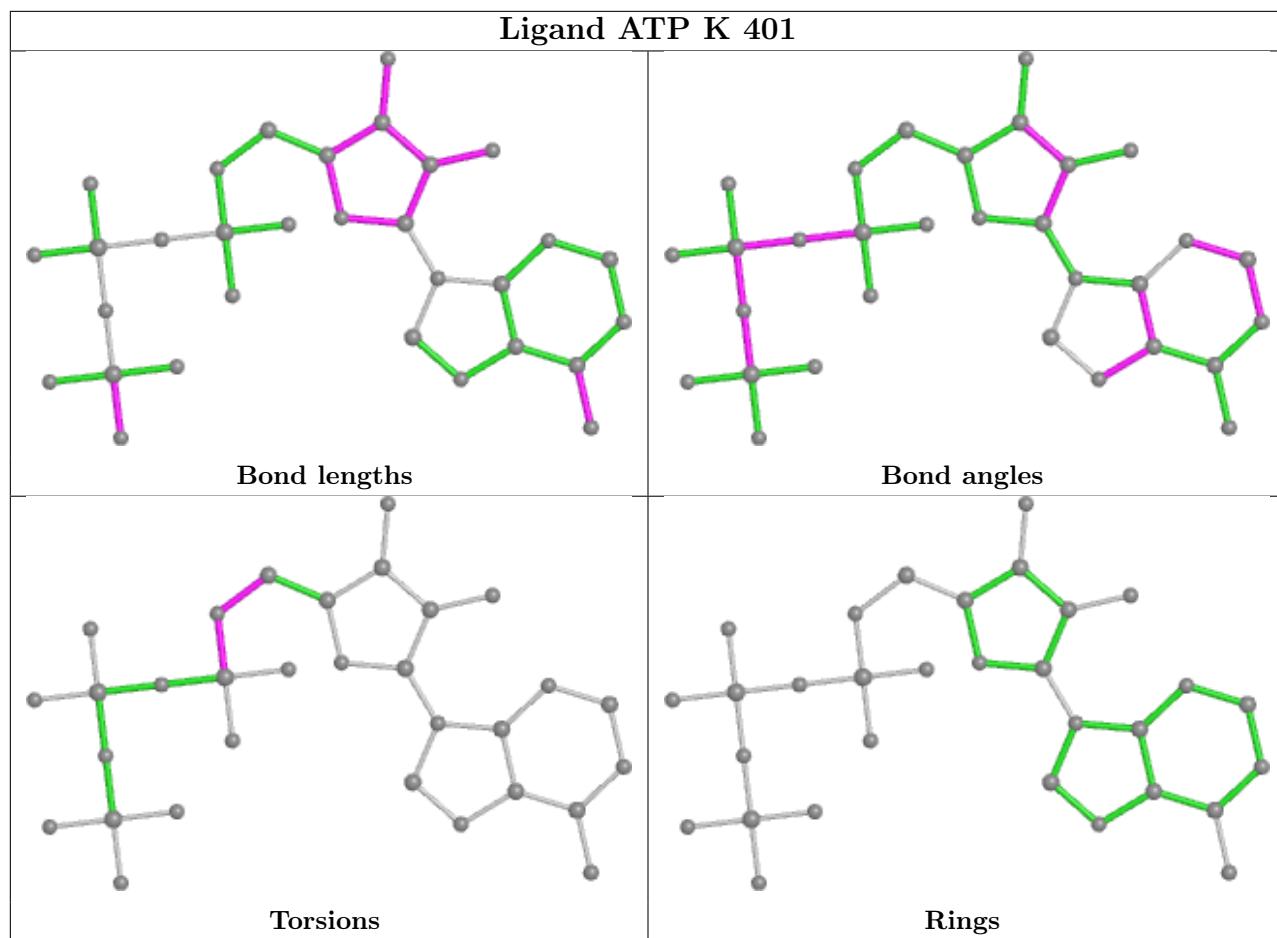


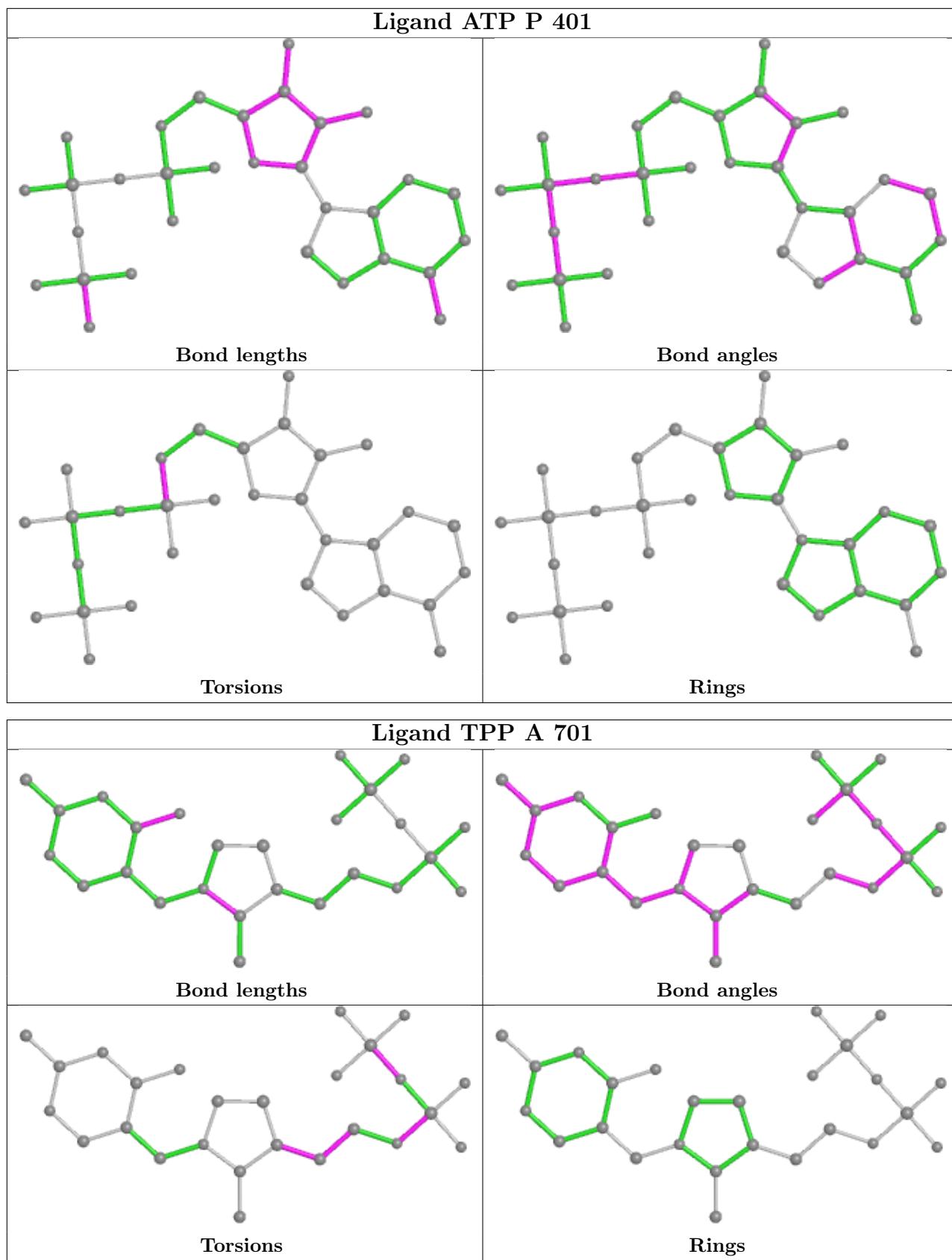


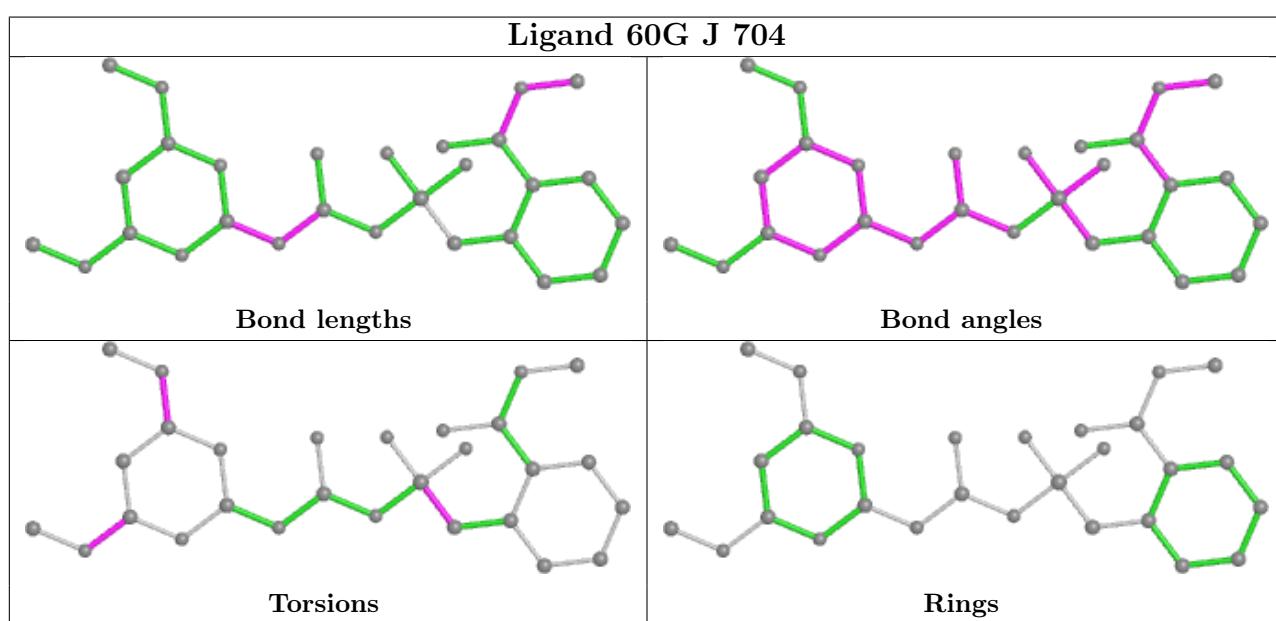
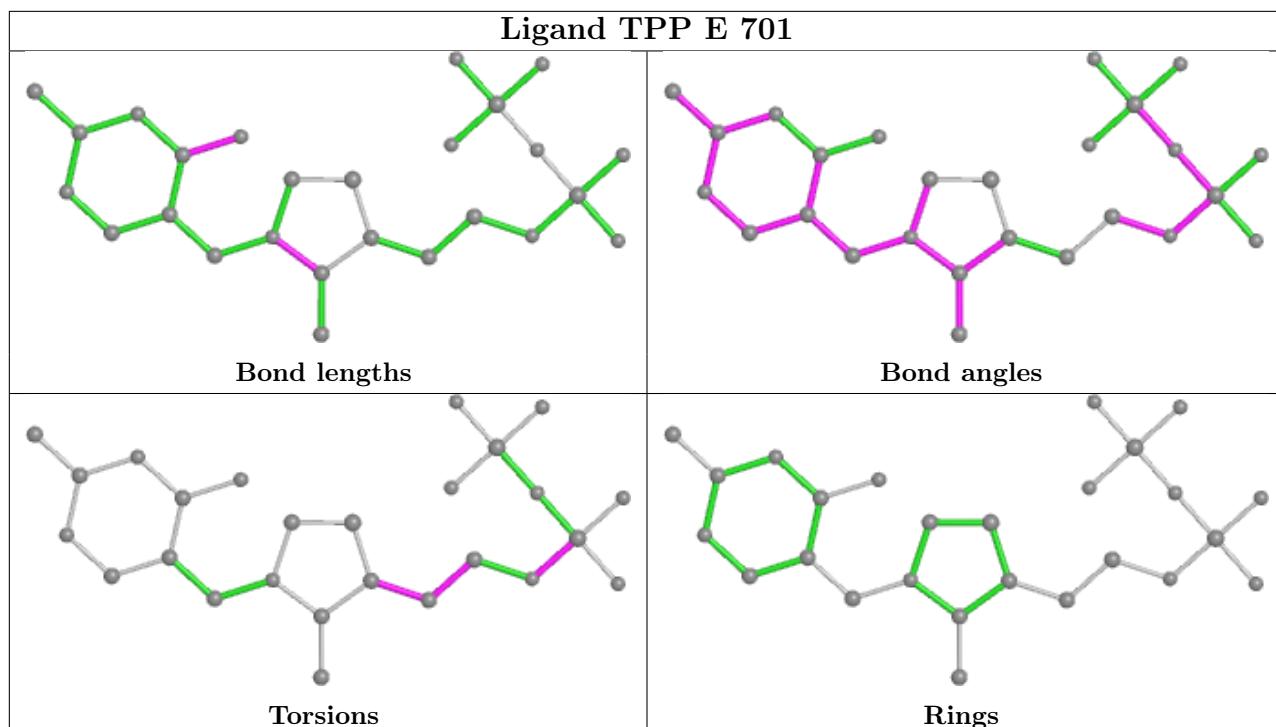


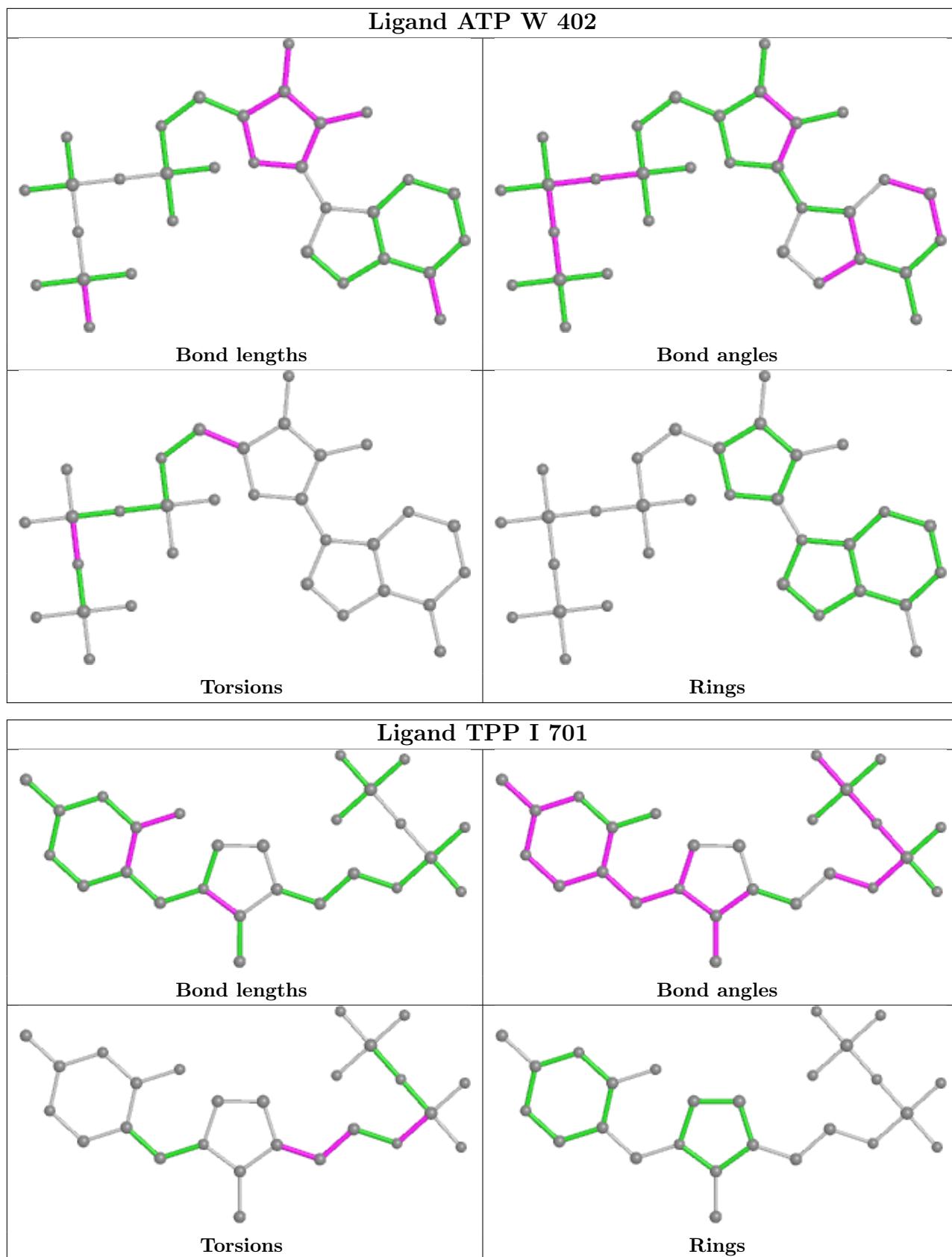


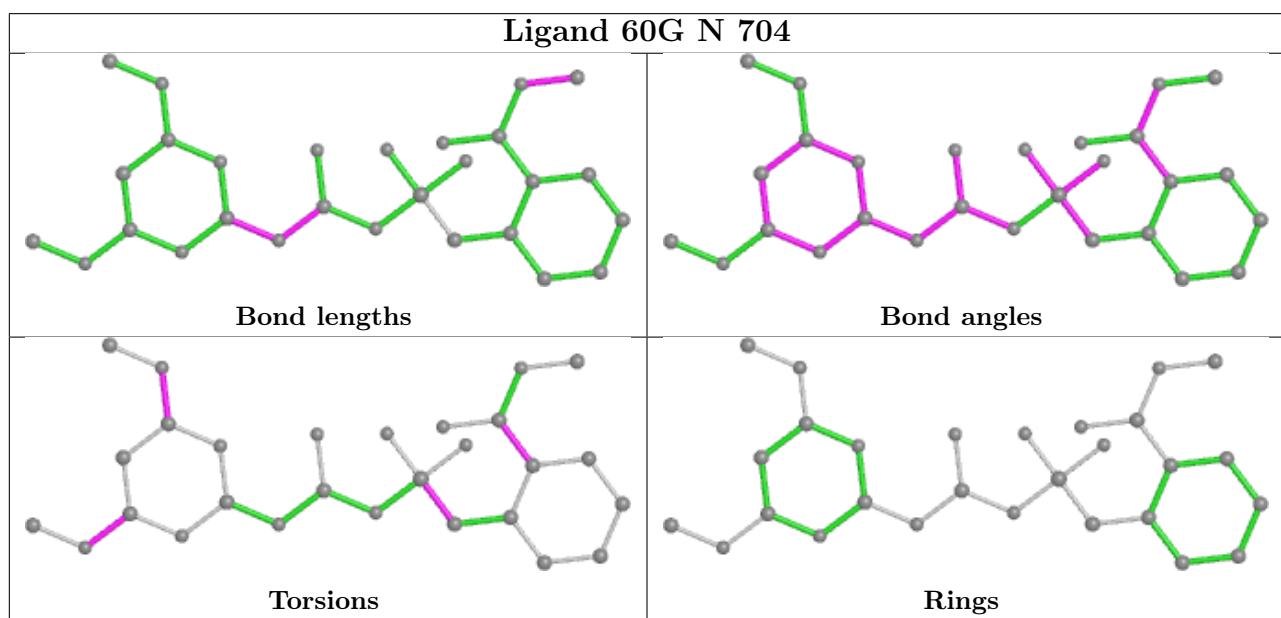
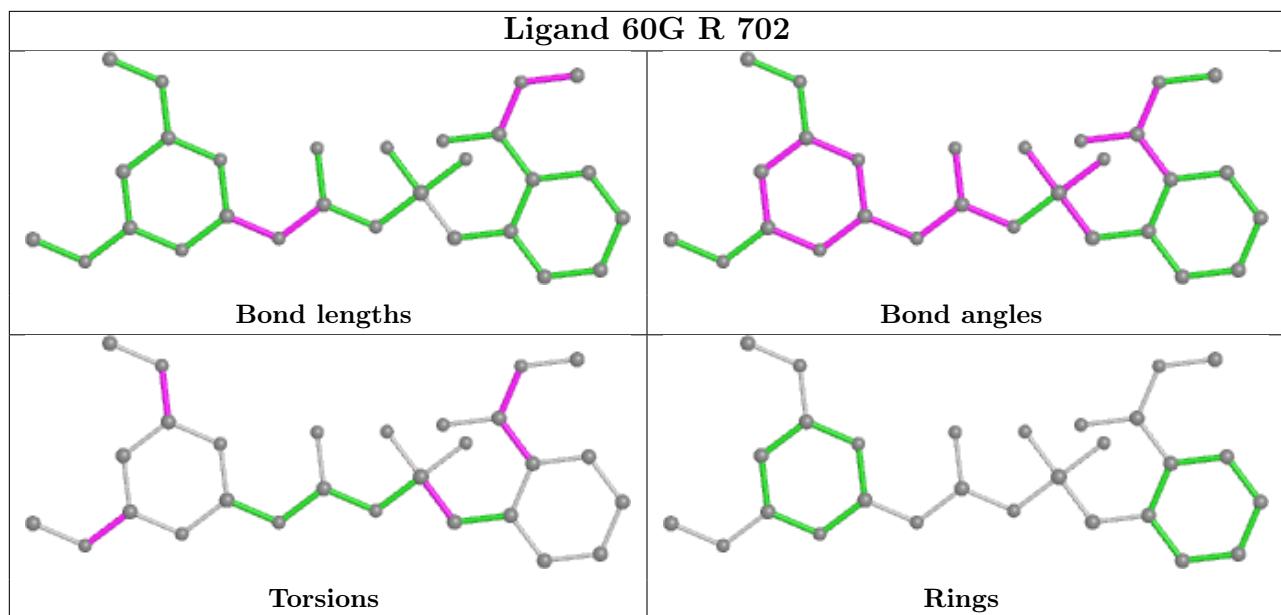


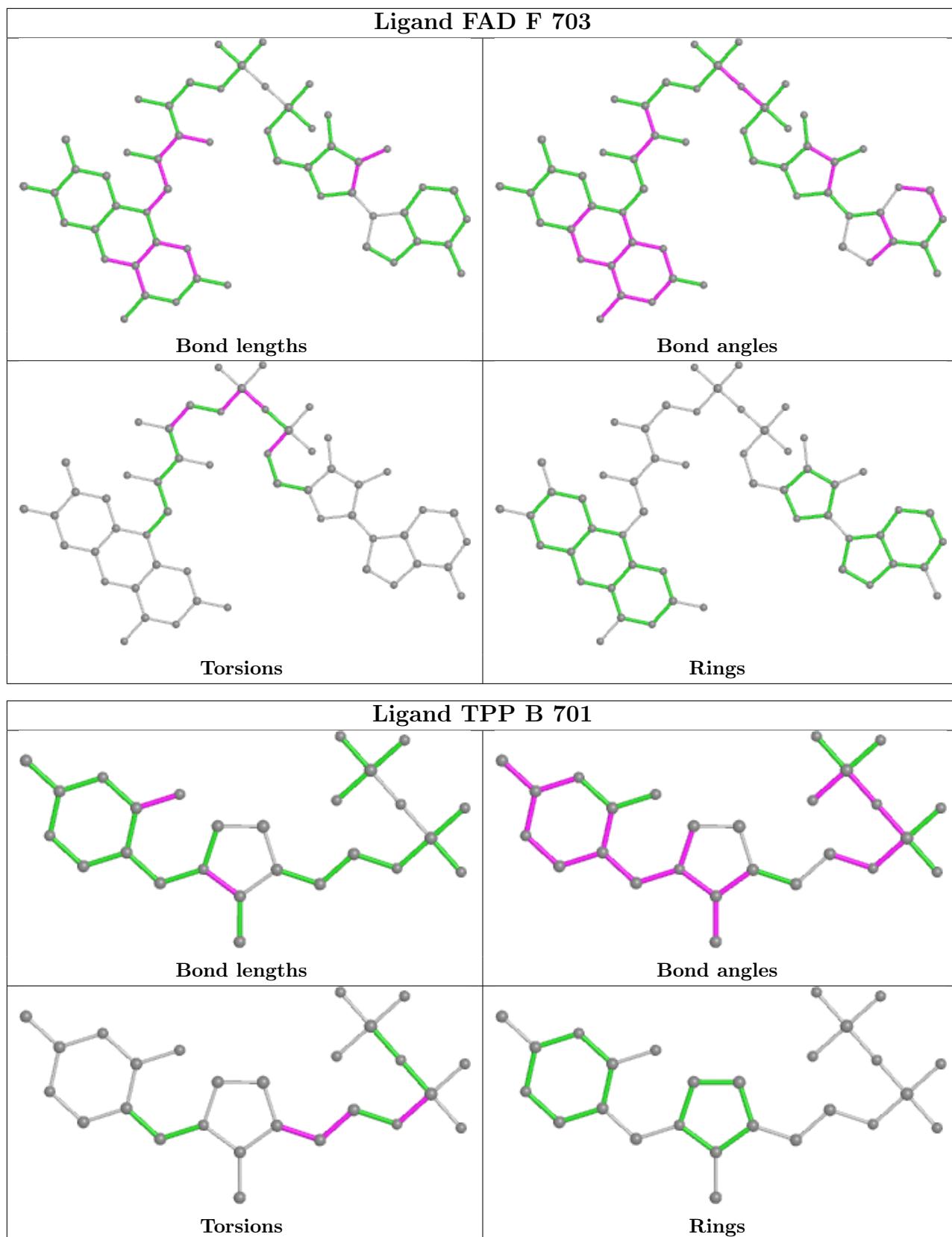


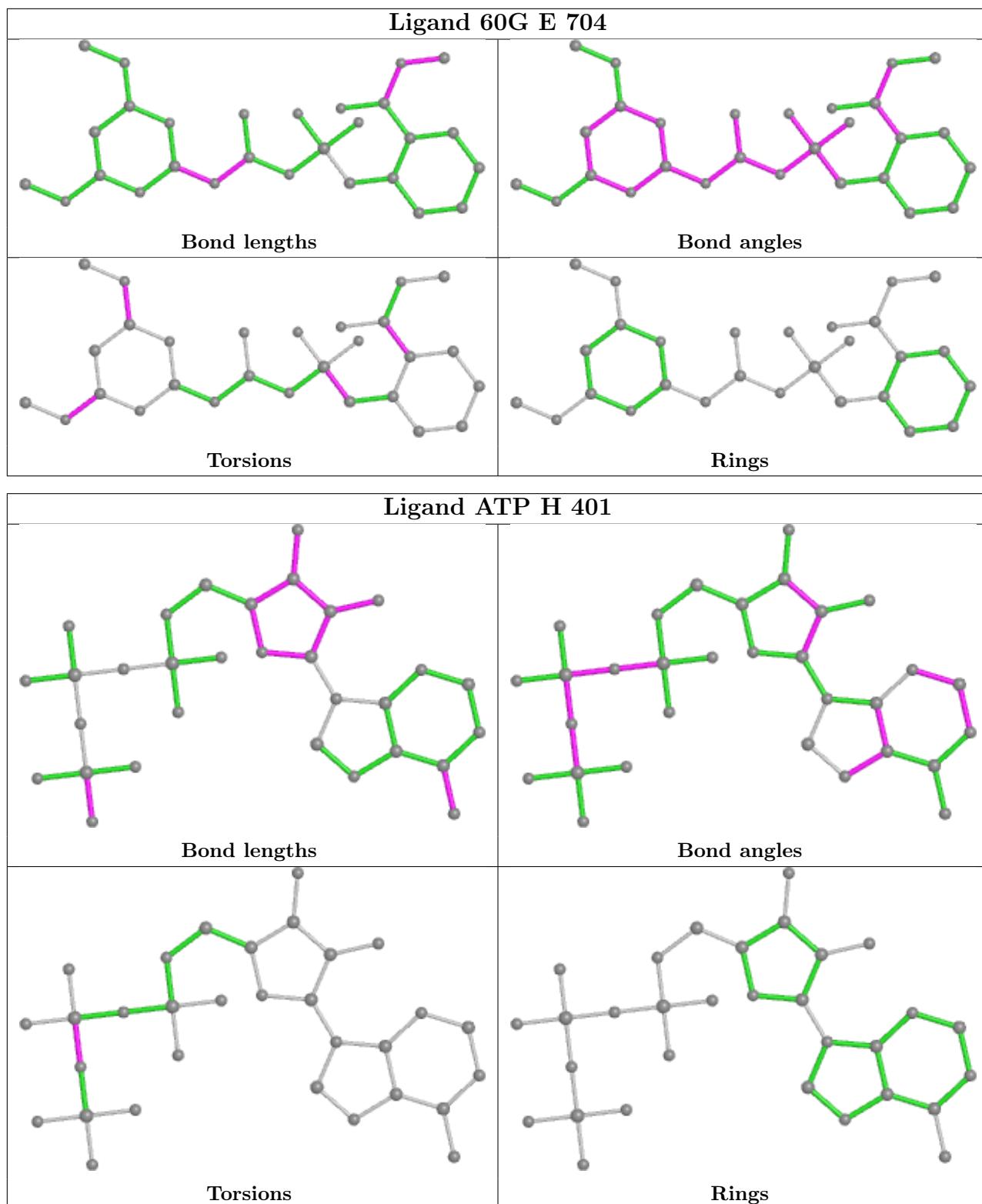


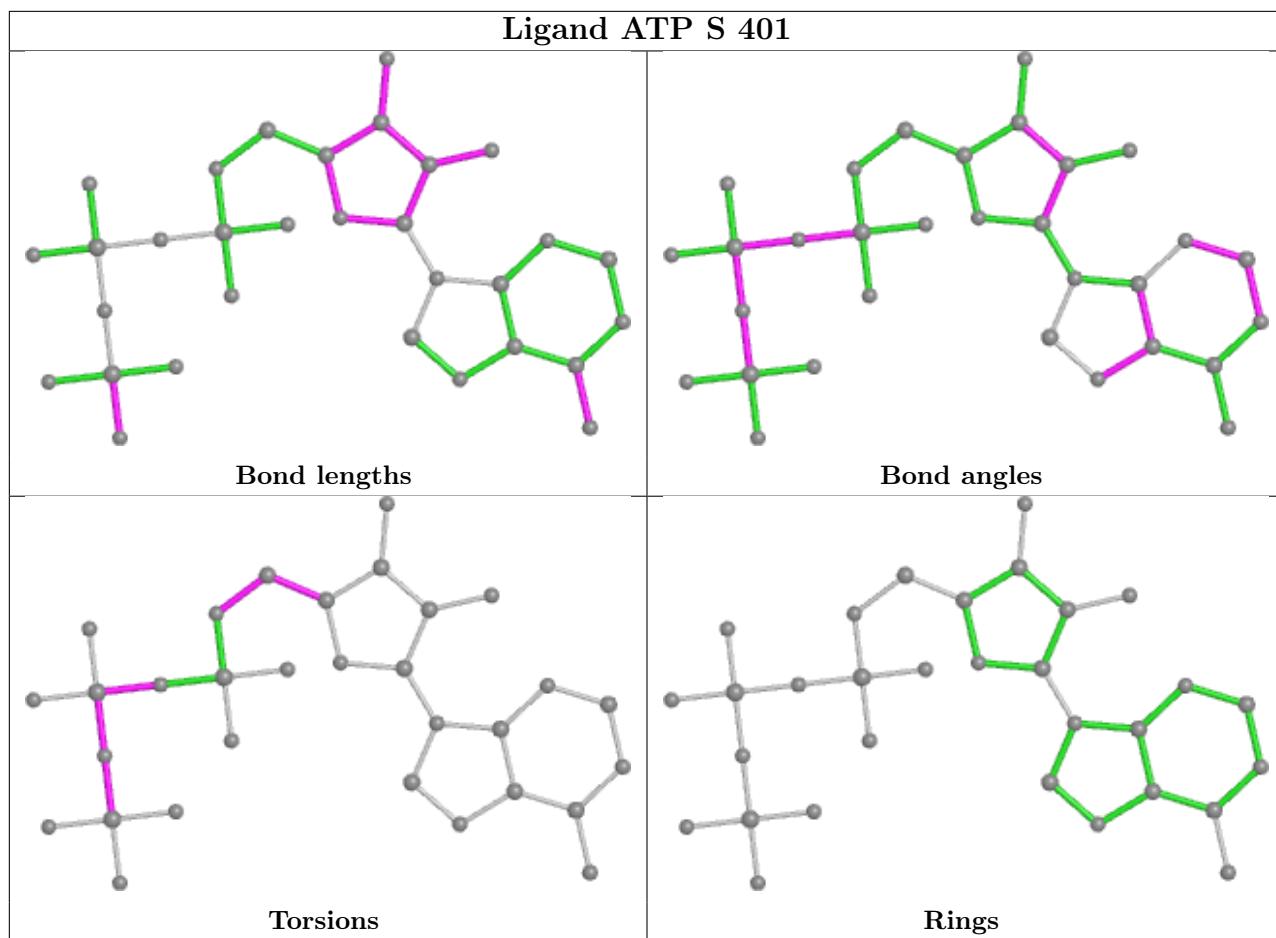


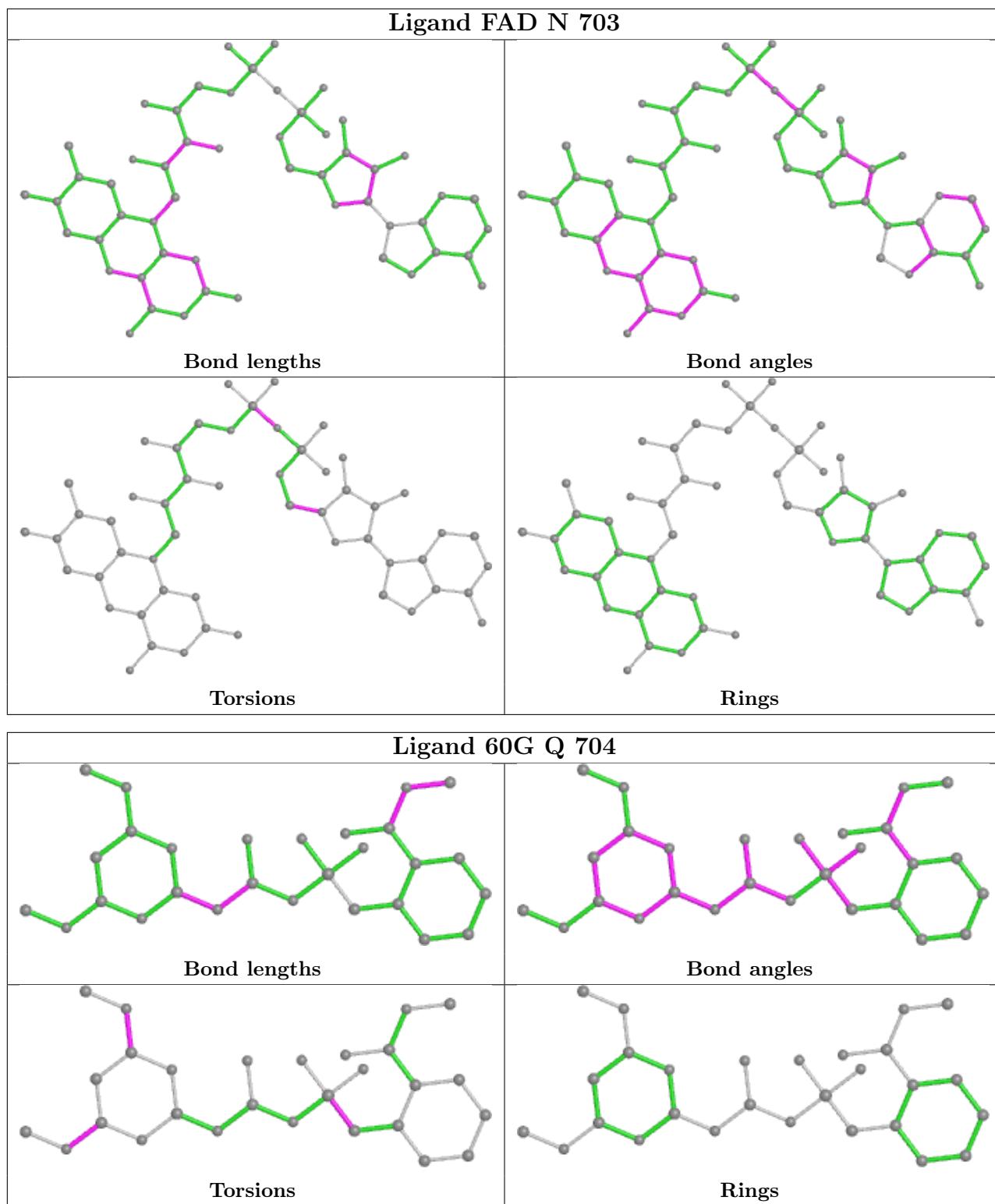


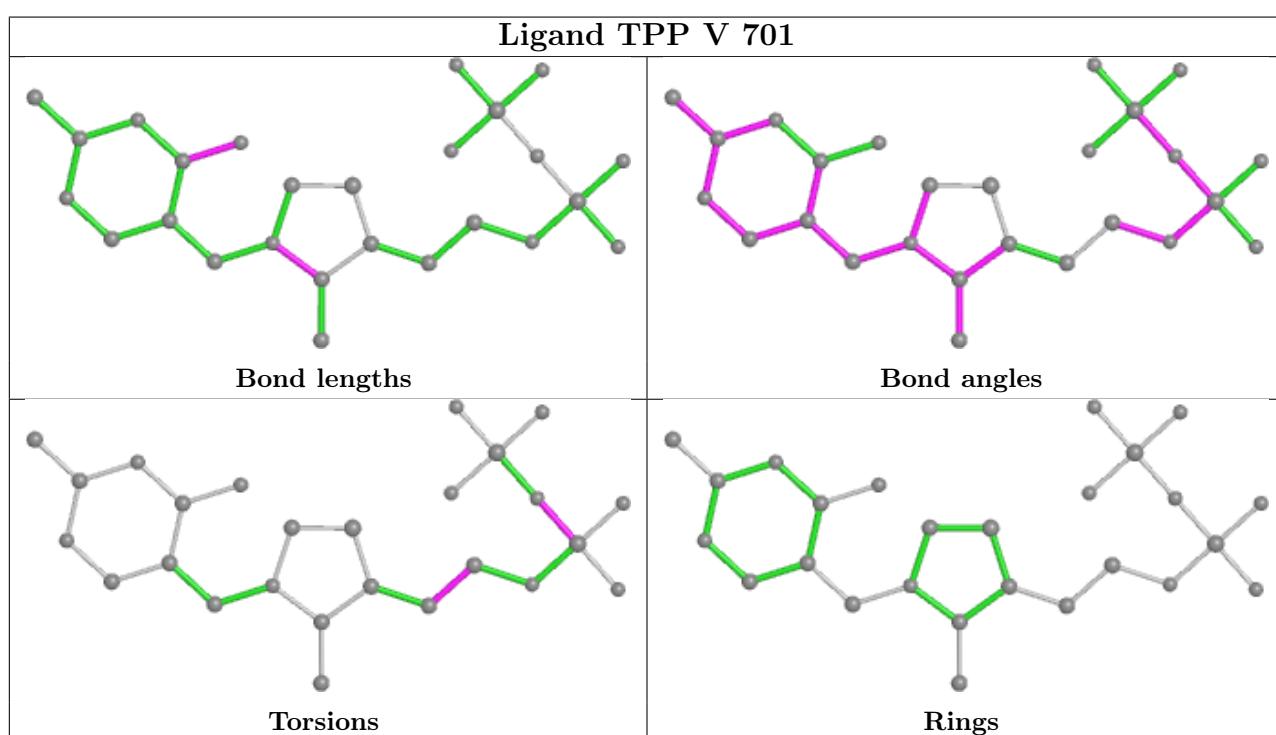
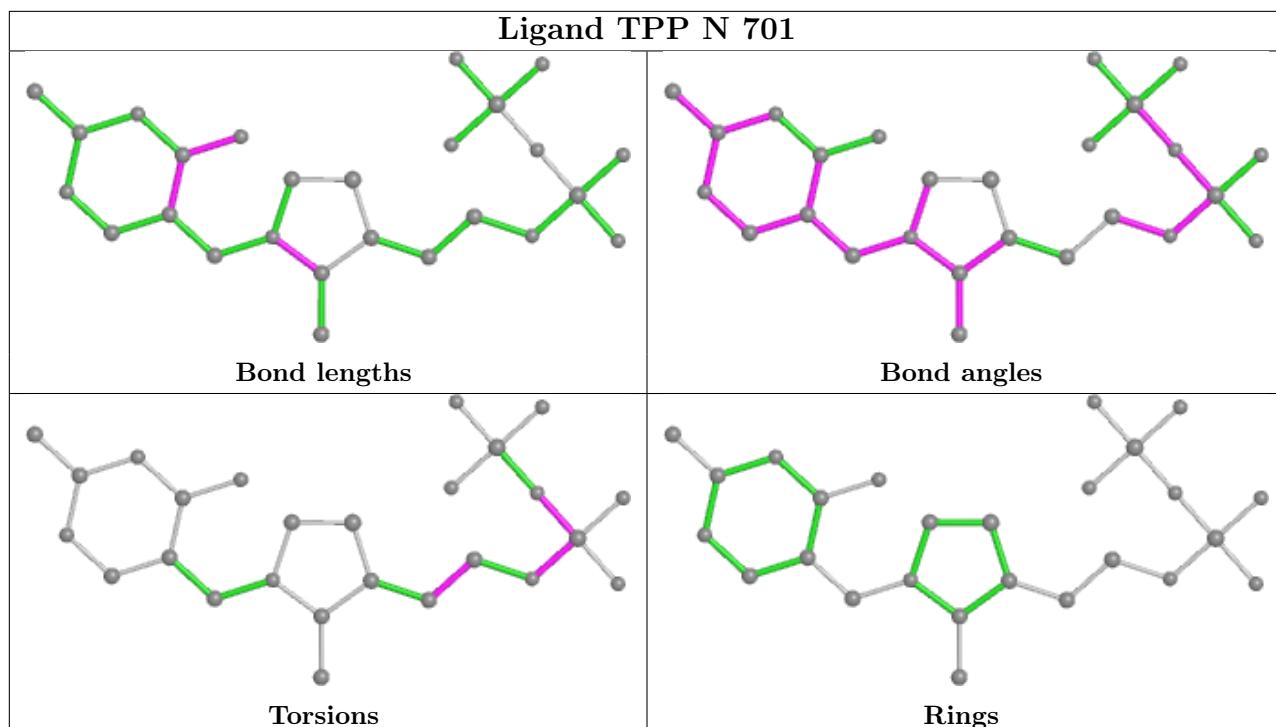


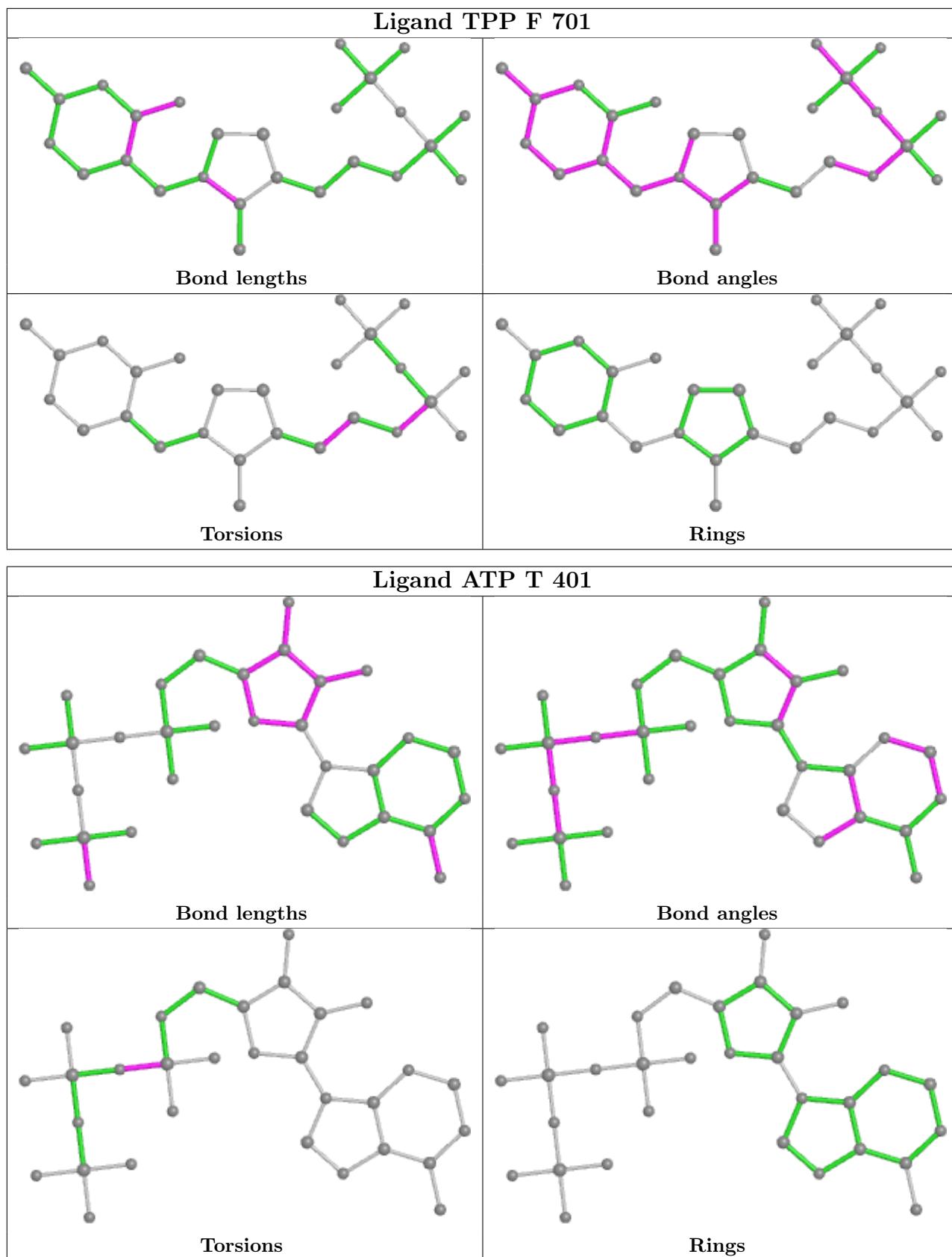


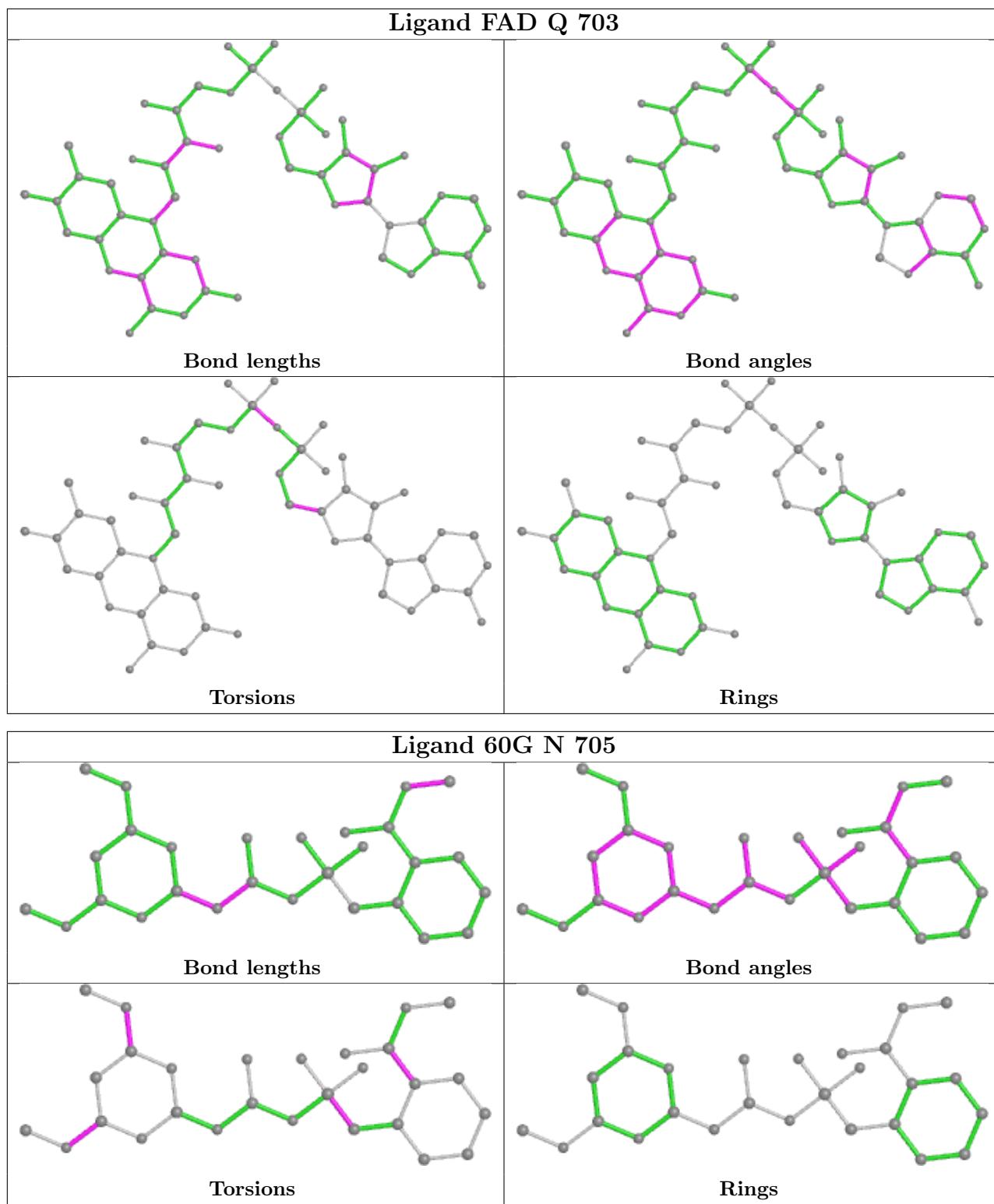


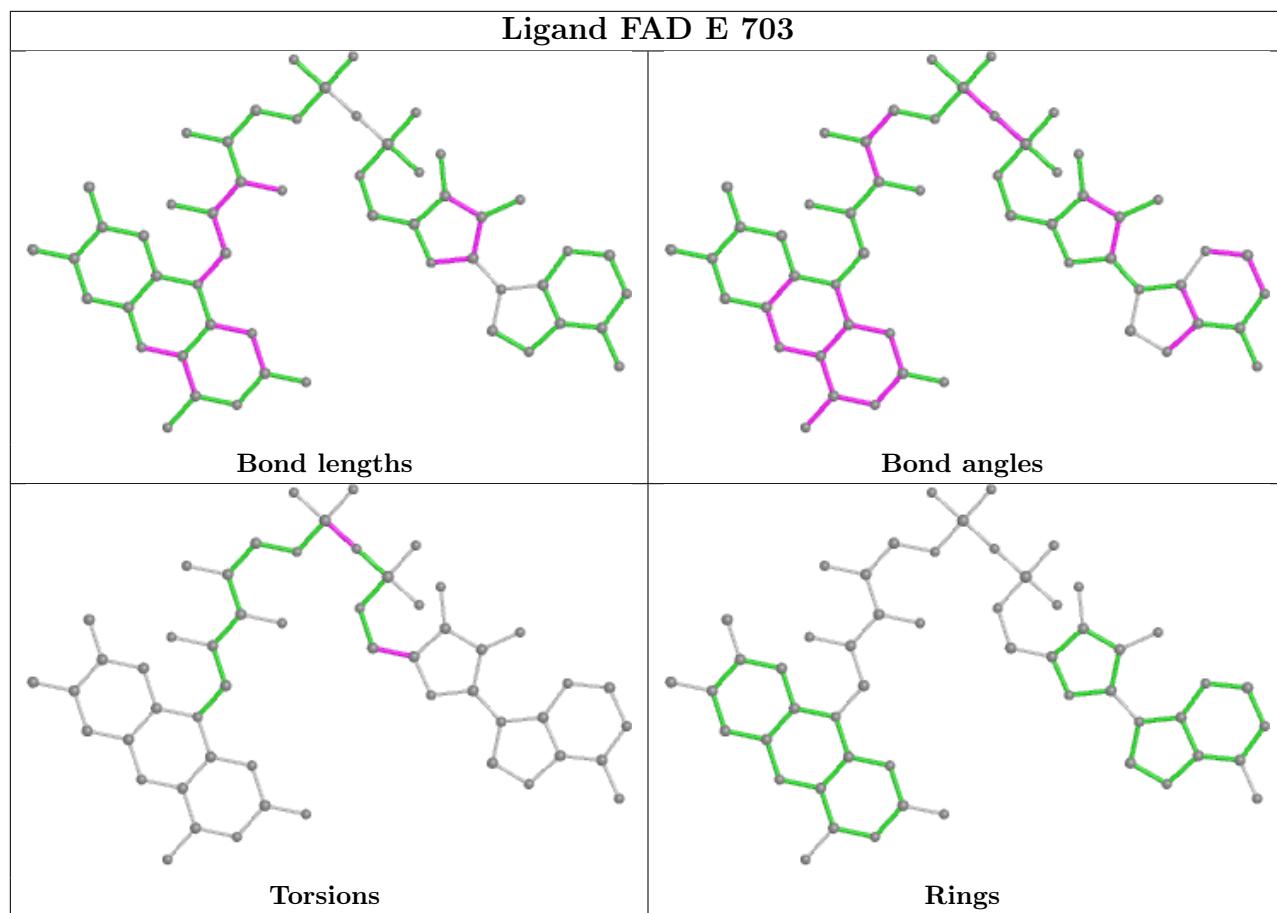


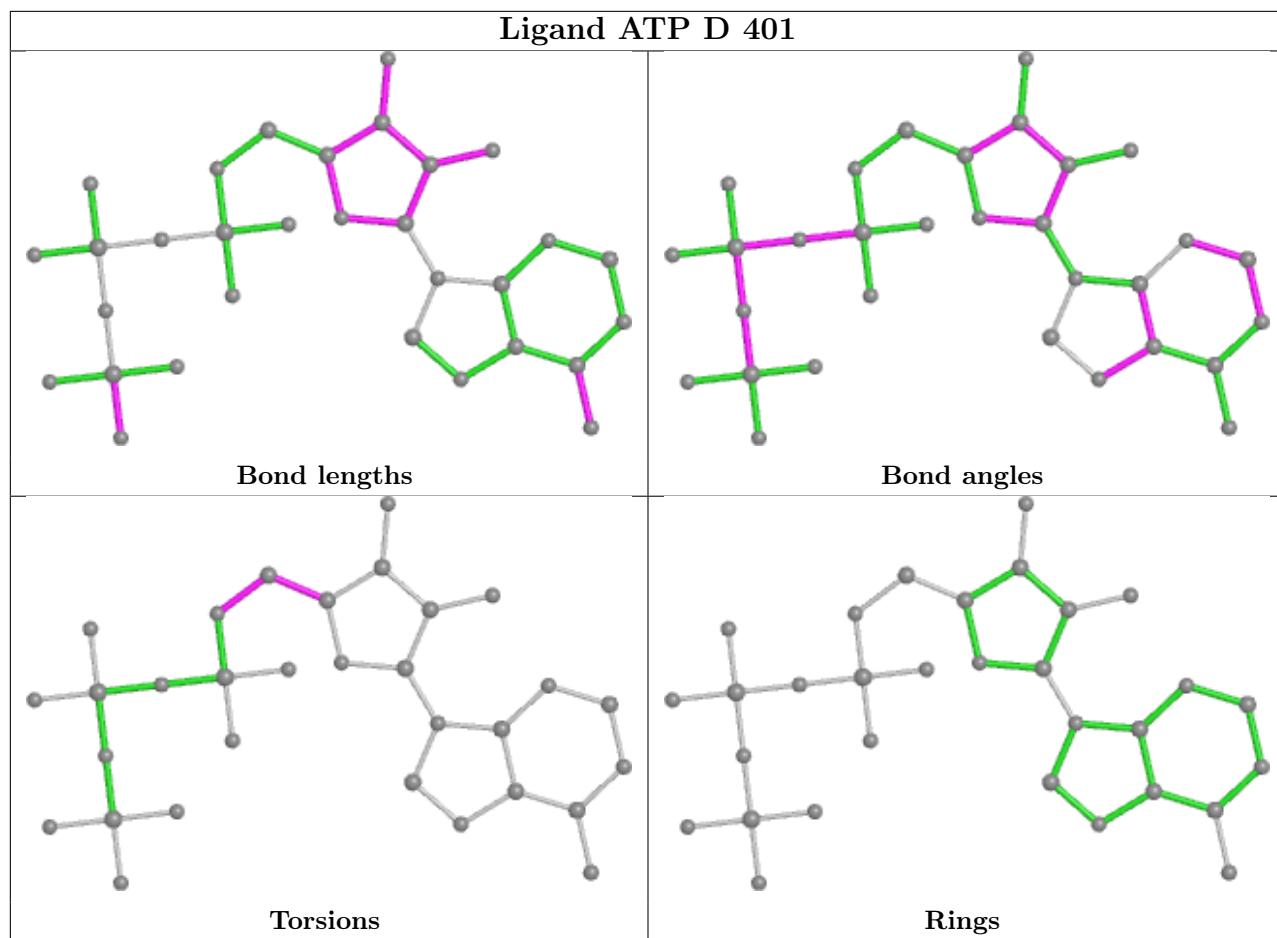


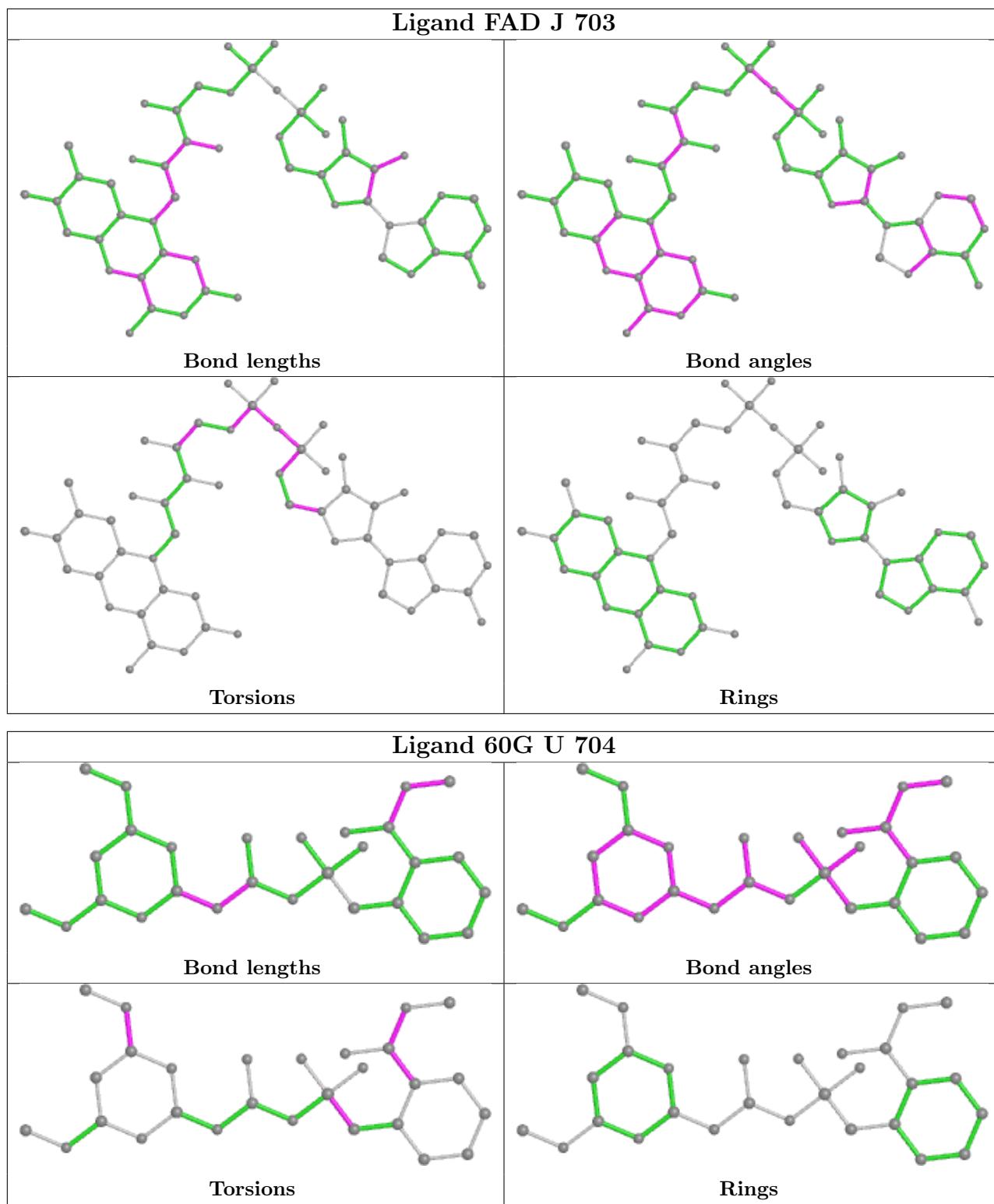


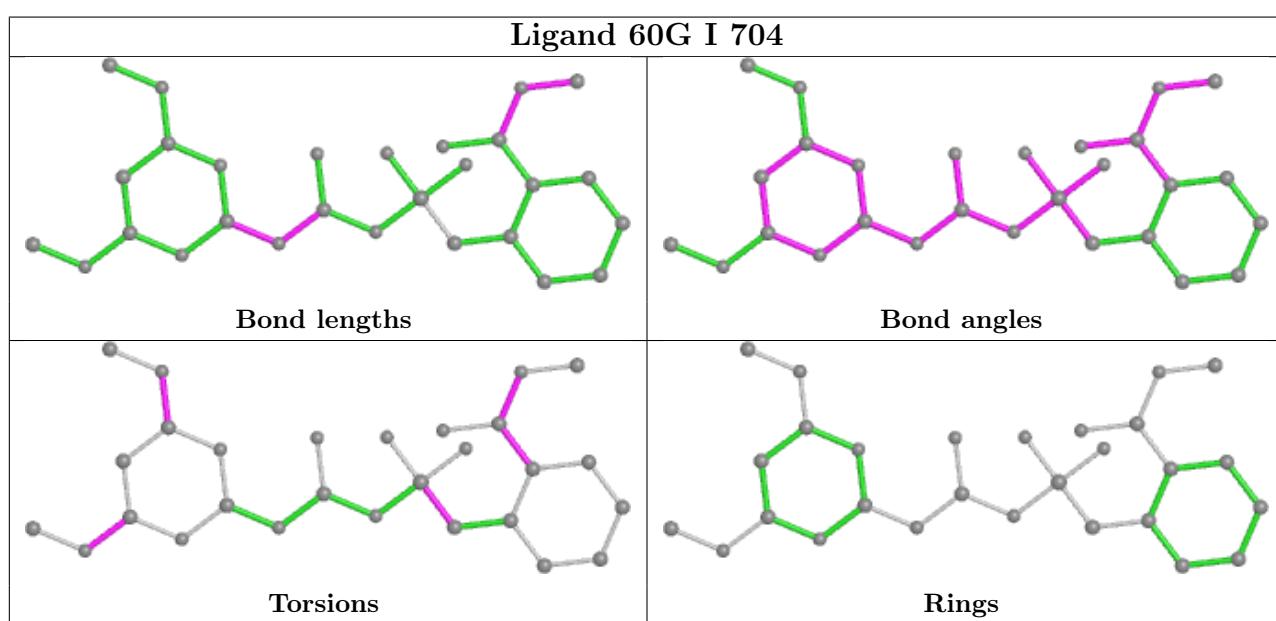
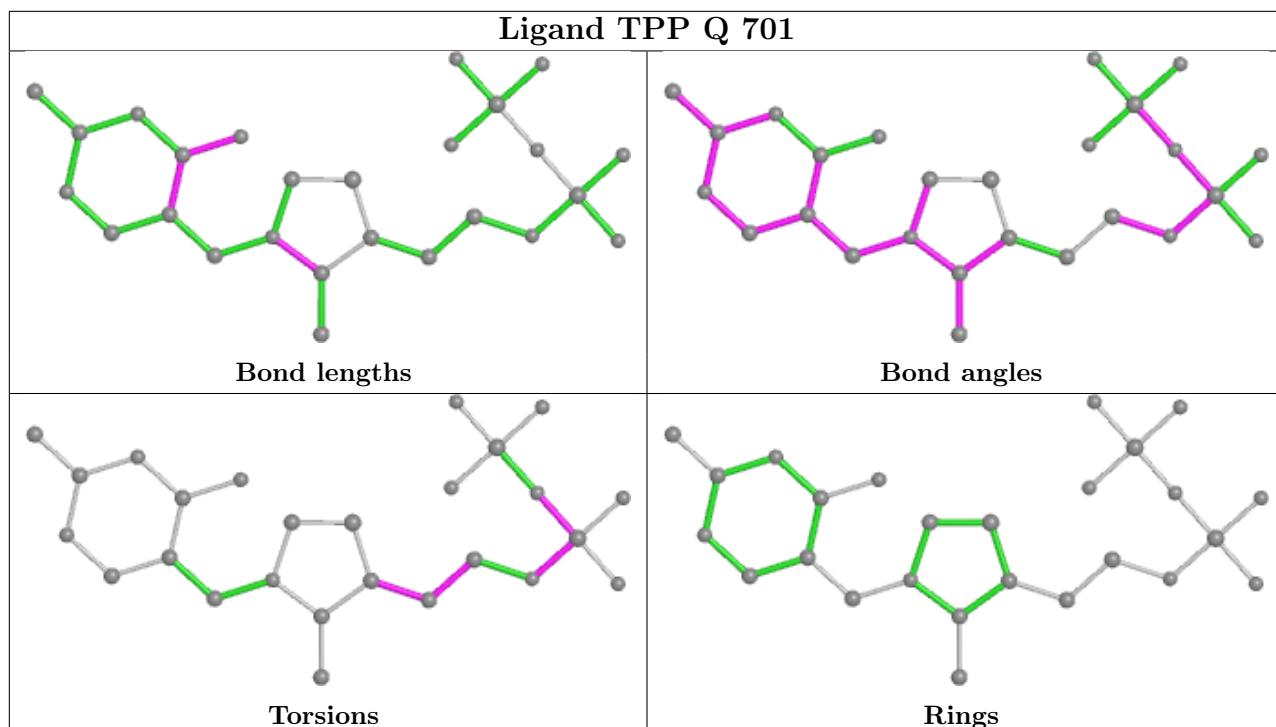


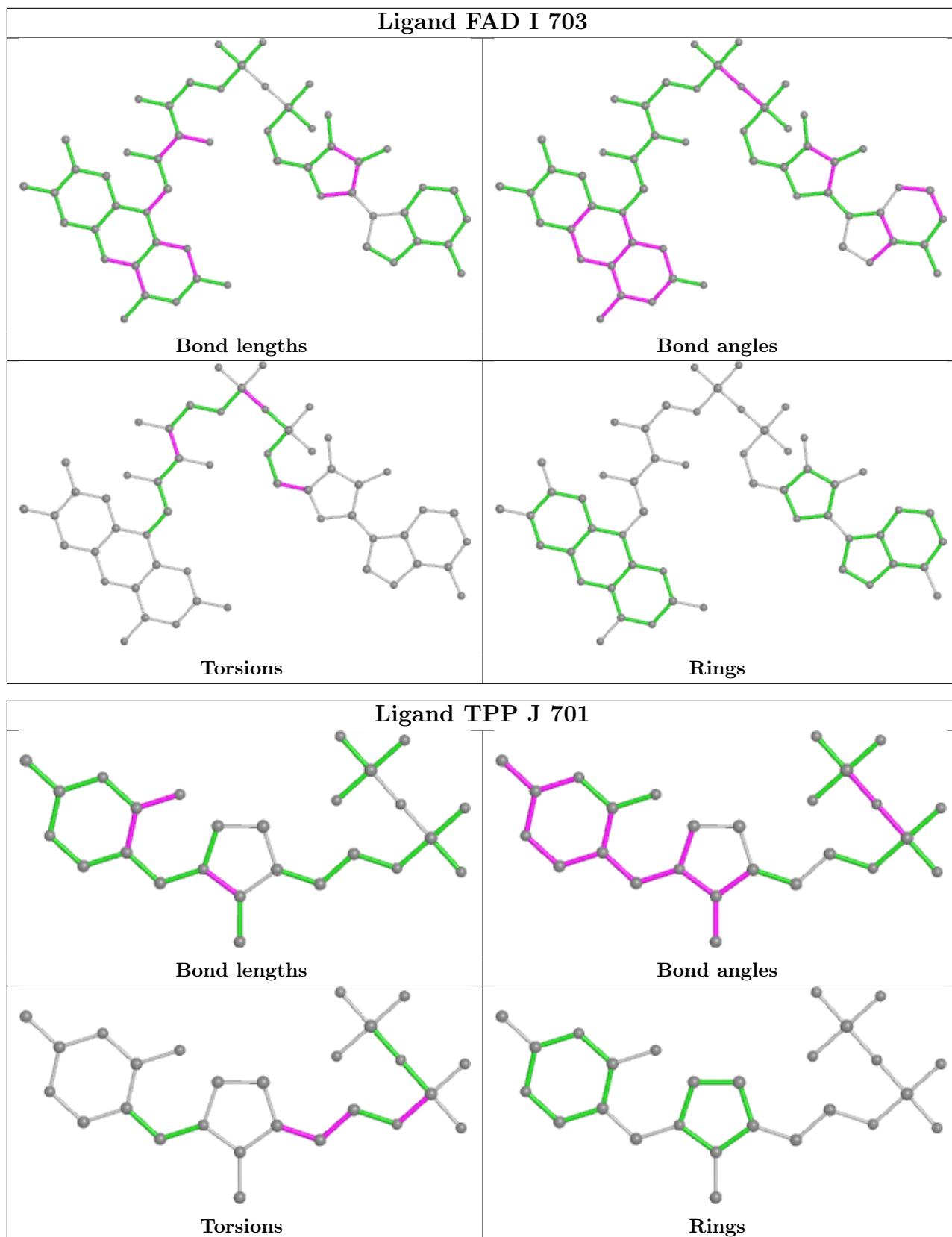












4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data [\(i\)](#)

5.1 Protein, DNA and RNA chains [\(i\)](#)

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

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

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

5.3 Carbohydrates [\(i\)](#)

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

5.4 Ligands [\(i\)](#)

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

5.5 Other polymers [\(i\)](#)

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