



## wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 09:49 AM EST

PDB ID : 6VZ8  
EMDB ID : EMD-21487  
Title : Arabidopsis thaliana acetohydroxyacid synthase complex with valine bound  
Authors : Guddat, L.W.; Low, Y.S.  
Deposited on : 2020-02-27  
Resolution : 3.45 Å(reported)  
Based on initial models : 5K6Q, 2PC6

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

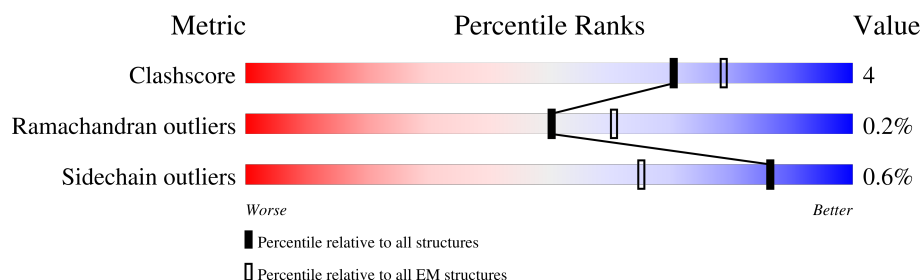
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.45 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	D	586	<div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	E	586	<div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	H	586	<div> <div>80%</div> <div>10%</div> <div>9%</div> </div>
1	I	586	<div> <div>81%</div> <div>11%</div> <div>8%</div> </div>
1	L	586	<div> <div>81%</div> <div>10%</div> <div>9%</div> </div>
1	M	586	<div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
1	P	586	<div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	Q	586	<div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
2	F	491	<div> <div>28%</div> <div>.</div> <div>68%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	491	 30% . 68%
2	J	491	 28% . 68%
2	K	491	 30% . 68%
2	N	491	 29% . 68%
2	O	491	 30% . 68%
2	R	491	 28% . 68%
2	S	491	 30% . 68%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 42132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	531	Total	C	N	O	S	0	0
			3910	2490	675	725	20		
1	E	541	Total	C	N	O	S	0	0
			3953	2514	684	736	19		
1	H	531	Total	C	N	O	S	0	0
			3910	2490	675	725	20		
1	I	541	Total	C	N	O	S	0	0
			3953	2514	684	736	19		
1	L	531	Total	C	N	O	S	0	0
			3910	2490	675	725	20		
1	M	541	Total	C	N	O	S	0	0
			3953	2514	684	736	19		
1	P	531	Total	C	N	O	S	0	0
			3910	2490	675	725	20		
1	Q	541	Total	C	N	O	S	0	0
			3953	2514	684	736	19		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	85	MET	-	initiating methionine	UNP P17597
E	85	MET	-	initiating methionine	UNP P17597
H	85	MET	-	initiating methionine	UNP P17597
I	85	MET	-	initiating methionine	UNP P17597
L	85	MET	-	initiating methionine	UNP P17597
M	85	MET	-	initiating methionine	UNP P17597
P	85	MET	-	initiating methionine	UNP P17597
Q	85	MET	-	initiating methionine	UNP P17597

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		

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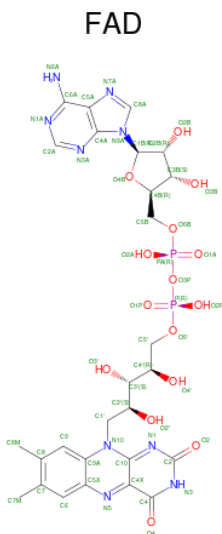
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		
2	J	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		
2	K	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		
2	N	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		
2	O	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		
2	R	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		
2	S	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		

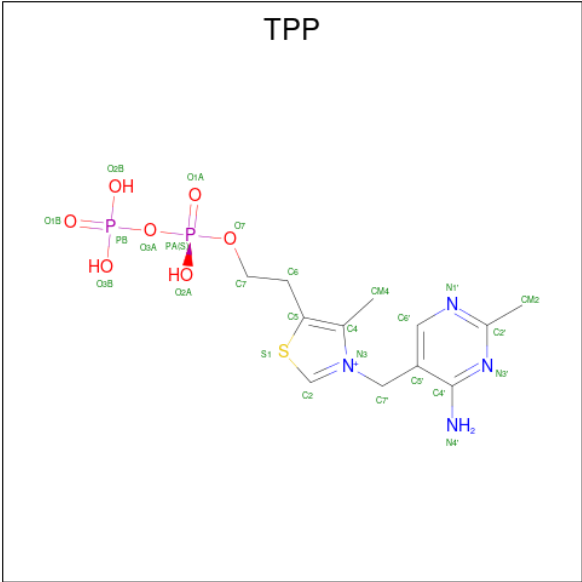
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	H	1	Total	Mg	0
			1	1	
3	I	1	Total	Mg	0
			1	1	
3	L	1	Total	Mg	0
			1	1	
3	M	1	Total	Mg	0
			1	1	
3	P	1	Total	Mg	0
			1	1	
3	Q	1	Total	Mg	0
			1	1	

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).

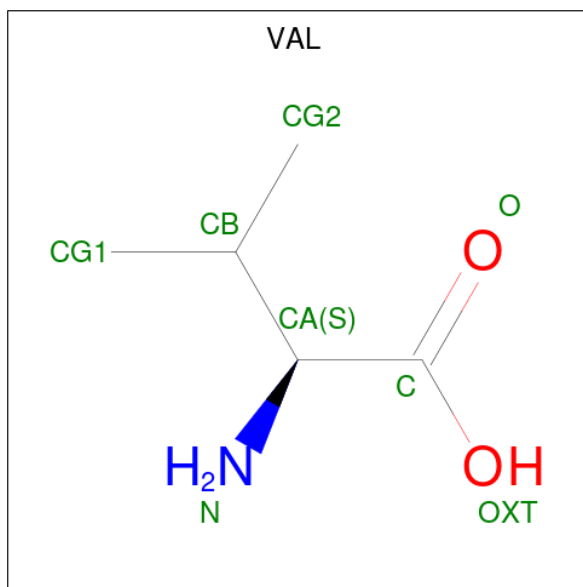


- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $\text{C}_{12}\text{H}_{19}\text{N}_4\text{O}_7\text{P}_2\text{S}$ ).



Mol	Chain	Residues	Atoms						AltConf
5	D	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
5	E	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
5	H	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
5	I	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
5	L	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
5	M	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
5	P	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
5	Q	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	

- Molecule 6 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



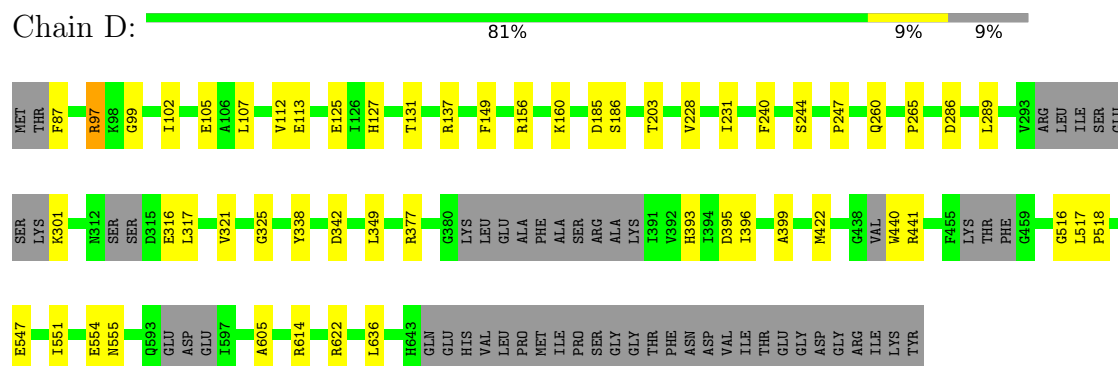
Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			8	5	1	2	
6	G	1	Total	C	N	O	0
			8	5	1	2	
6	J	1	Total	C	N	O	0
			8	5	1	2	
6	K	1	Total	C	N	O	0
			8	5	1	2	
6	N	1	Total	C	N	O	0
			8	5	1	2	
6	O	1	Total	C	N	O	0
			8	5	1	2	
6	R	1	Total	C	N	O	0
			8	5	1	2	
6	S	1	Total	C	N	O	0
			8	5	1	2	



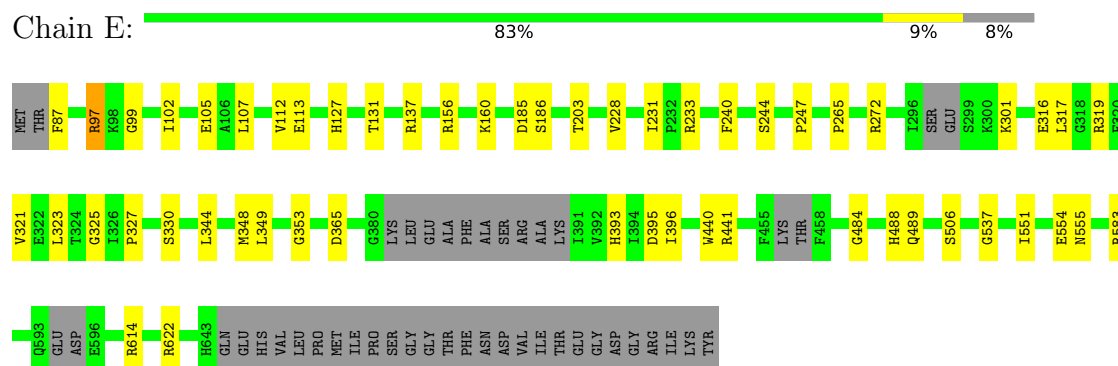
### 3 Residue-property plots [i](#)

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. 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. 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.

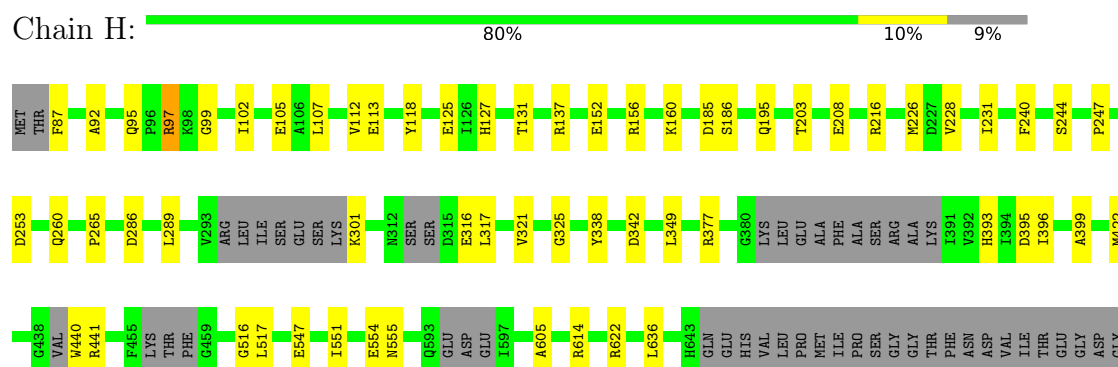
- Molecule 1: Acetolactate synthase, chloroplastic



- Molecule 1: Acetolactate synthase, chloroplastic

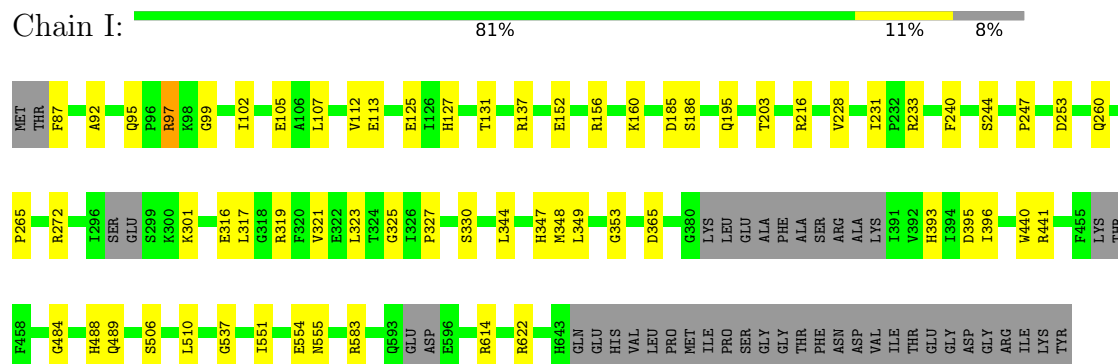


- Molecule 1: Acetolactate synthase, chloroplastic

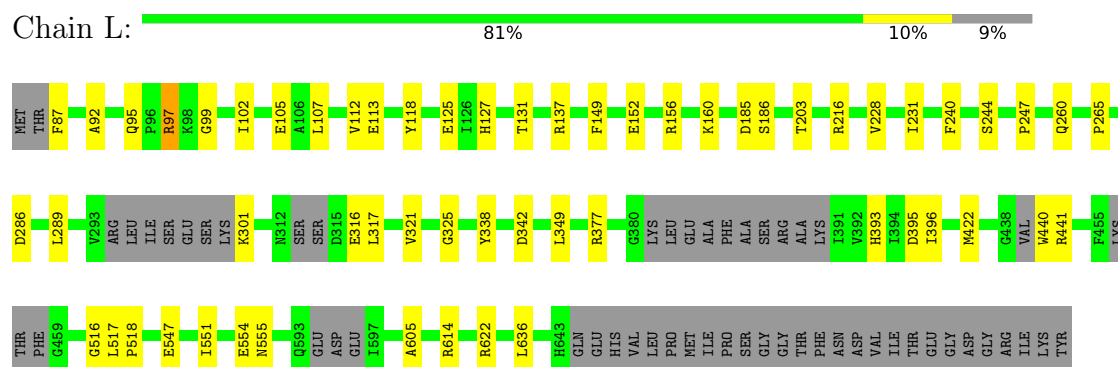


ARG  
ILE  
LYS  
TYR

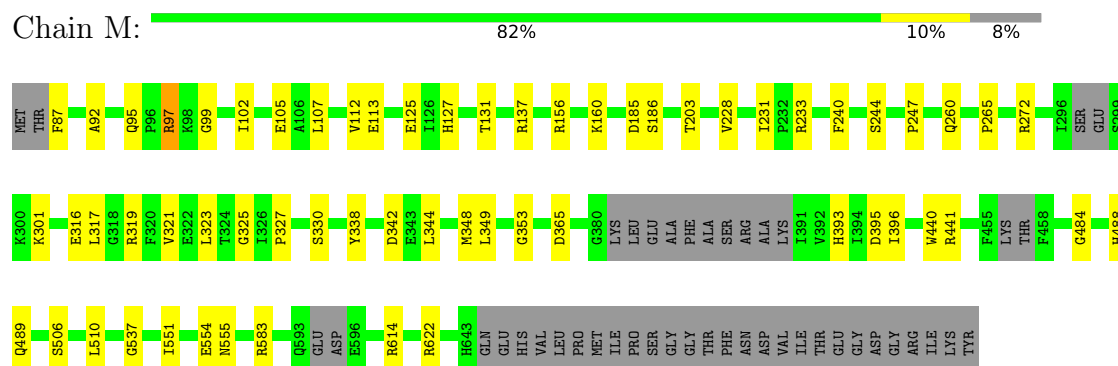
- Molecule 1: Acetolactate synthase, chloroplastic



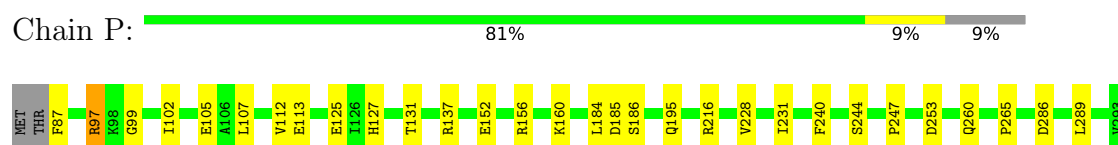
- Molecule 1: Acetolactate synthase, chloroplastic




- Molecule 1: Acetolactate synthase, chloroplastic

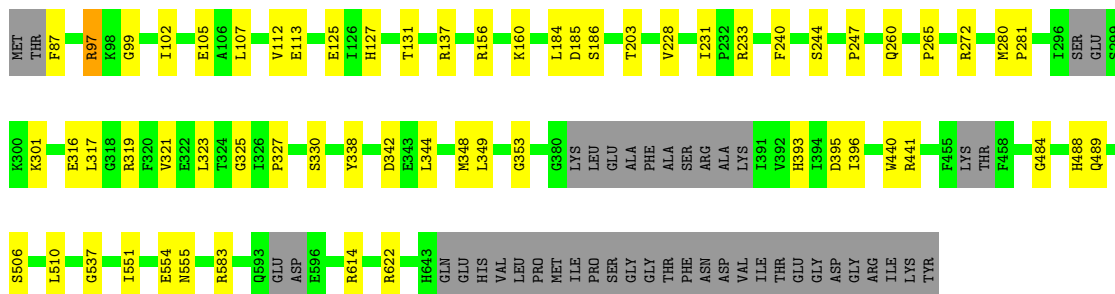


- Molecule 1: Acetolactate synthase, chloroplastic



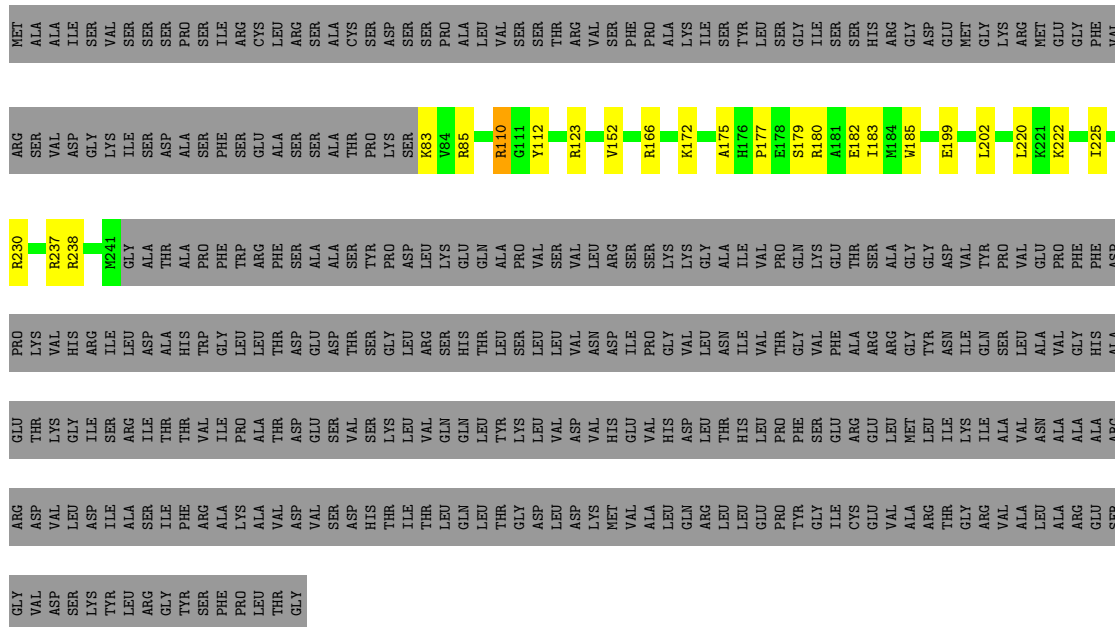
- Molecule 1: Acetolactate synthase, chloroplasic

Chain Q:  82% 10% 8%



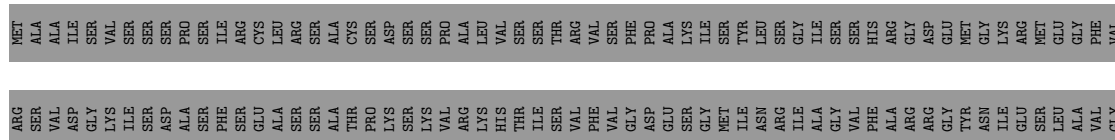
- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

Chain F:  28% 1% 68%



- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

Chain G:  30% 68%



Ile	Met	Ala	Leu
Asp	Gly	Glu	Arg
Ala	Thr	Tyr	Asn
His	Ala	Met	Lys
Trp	Pro	Val	Ala
Gly	Phe	Val	Leu
Leu	Trp	Asp	Phe
Leu	Phe	Thr	Ile
Thr	Abs	Thr	Ile
Asp	Ser	Arg	Val
Glu	Ala	Ala	Val
Asp	Ala	Arg	Cys
Ser	Ser	Val	Gly
Ser	Tyr	Val	Thr
Gly	Pro	Asp	Glu
L317	Asp	Ile	Arg
R343	Leu	Ala	Val
N346	Lys	Glu	Leu
E356	Gln	His	Gln
T357	Ala	Leu	Val
R362	Pro	Thr	Ile
Q379	Val	Ile	Glu
R401	Ser	Glu	Gln
R416	Val	Val	Gln
D420	Leu	Thr	Lys
D444	Arg	Gly	Lys
L445	Ser	Pro	Val
K447	Ser	Gly	Asn
R468	Glu	Leu	Ser
S475	Thr	Lys	Glu
Gly	Ser	Lys	Pro
Val	Ala	Phe	Gln
Asp	Gly	Ile	Val
Ser	Asp	Arg	Arg
Lys	Val	Glu	Glu
Tyr	Tyr	Ile	Leu
Leu	Pro	Val	Met
Arg	Val	Arg	Leu
Gly	Glu	Thr	Val
Tyr	Phe	Gly	Lys
Ser	Phe	Ile	Asn
Phe	Asp	Ala	Ala
Pro	Pro	Leu	His
Leu	Lys	Arg	Pro
Thr	Val	Arg	Glu
Gly	His	Glu	Ser

- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

Chain J:  28% . 68%

ASP	VAL	LYS	VAL	LYS	VAL	R237	ARG	MET
SER	LEU	GLY	HIS	GLY	HIS	R238	SER	ALA
LYS	ASP	ILE	ARG	ASP	ARG	R239	VAL	ALA
TYR	ILE	SER	ILE	SER	ILE	R241	ASP	ILE
ARG	ASP	ARG	LEU	ASP	LEU	GLY	GLY	VAL
GLY	THR	ILE	ALA	THR	ALA	ALA	ILE	SER
TYR	PHE	THR	HIS	THR	HIS	ALA	SER	SER
SER	ARG	VAL	TRP	PRO	TRP	ALA	ASP	PRO
PHE	ALA	ILE	GLY	GLY	GLY	THR	ALA	SER
PRO	LYS	PRO	LEU	LEU	LEU	ARG	THR	SER
LEU	ALA	ALA	THR	THR	THR	PHE	PHE	ILE
LEU	VAL	THR	ASP	THR	ASP	GLY	SER	ARG
THR	ASP	ASP	GLY	GLY	GLY	ALA	GLU	CYS
GLY	VAL	GLY	GLY	GLY	GLY	ALA	ALA	LEU
	SER	SER	ASP	ASP	ASP	ALA	LYS	ARG
	ASP	VAL	THR	VAL	THR	SER	SER	SER
	HIS	SER	SER	SER	TYR	ALA	ALA	ALA
	THR	LYS	GLY	GLY	PRO	THR	THR	CYS
	ILE	LEU	LEU	LEU	ASP	PRO	PRO	SER
	THR	VAL	ARG	ARG	LEU	LEU	LYS	ASP
	LEU	GLN	SER	SER	LEU	LEU	SER	SER
	LEU	GLN	HIS	GLY	GLY	GLN	R483	SER
	THR	TYR	THR	LEU	ALA	ALA	R484	PRO
	ASP	LYS	SER	LEU	VAL	PRO	R85	ALA
	GLY	VAL	LEU	LEU	VAL	VAL	D95	LEU
	LEU	VAL	LEU	VAL	SER	SER	SER	SER
	ASP	VAL	VAL	VAL	VAL	VAL	R110	THR
	LYS	VAL	ASN	ASN	ASN	LEU	G113	ARG
	MET	HIS	ASP	ASP	ILE	ARG	Y112	VAL
	VAL	GLY	ILE	ILE	PRO	SER	R123	SER
	ALA	VAL	PRO	GLY	GLY	LYS	LYS	PHE
	LEU	HIS	VAL	VAL	VAL	LYS	V138	PRO
	GLN	ASP	VAL	ASP	VAL	GLY	V138	ALA
	ARG	LEU	LEU	LEU	LEU	ALA	R166	LYS
	LEU	THR	ASN	THR	ASN	ILE	R166	ILE
	LEU	HIS	ILE	ILE	ILE	VAL	K172	SER
	GLY	LEU	VAL	VAL	VAL	VAL	K172	TYR
	PRO	PRO	THR	THR	THR	GLN	A175	LEU
	TYR	PHE	GLY	GLY	GLY	PRO	A175	SER
	GLY	SER	VAL	VAL	VAL	LYS	H176	ILE
	ILE	GLY	PHE	PHE	PHE	THR	P177	GLY
	ILE	ARG	GLY	ARG	ALA	GLY	E178	ILE
	CYS	ARG	ALA	ARG	ARG	SER	S179	SER
	GLY	GLY	ARG	ARG	ALA	ALA	R180	SER
	VAL	LEU	LEU	LEU	LEU	GLY	A181	HIS
	ALA	MET	GLY	GLY	GLY	TYR	E182	ARG
	ARG	LEU	ASN	THR	ASN	ASP	I183	GLY
	THR	ILE	GLY	ILE	ILE	VAL	I183	GLY
	GLY	LYS	ILE	ILE	ILE	VAL	E199	ASP
	GLY	ILE	GLN	GLN	GLN	TYR	E199	GLY
	VAL	ALA	SER	SER	SER	PRO	L202	MET
	ALA	VAL	LEU	VAL	VAL	VAL	L202	GLY
	LEU	ASN	ALA	ASN	ALA	GLY	L220	LYS
	ALA	ALA	VAL	VAL	VAL	PRO	L220	ARG
	ARG	ALA	GLY	ALA	GLY	PHE	L225	GLY
	GLY	ALA	HIS	HIS	HIS	ASP	L225	GLY
	SER	ARG	ALA	ALA	ALA	PRO	R230	PHE
	GLY	ASP	THR	THR	THR	VAL	R230	VAL
	VAL	ARG	GLY	ARG	GLY	THR	R230	THR

- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

Chain K:  30% . 68%

[illegible]





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	290516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	D	0.54	0/3988	0.74	4/5427 (0.1%)
1	E	0.53	0/4033	0.75	3/5495 (0.1%)
1	H	0.54	0/3988	0.74	5/5427 (0.1%)
1	I	0.54	0/4033	0.75	4/5495 (0.1%)
1	L	0.54	0/3988	0.75	6/5427 (0.1%)
1	M	0.53	0/4033	0.75	3/5495 (0.1%)
1	P	0.54	0/3988	0.75	5/5427 (0.1%)
1	Q	0.54	0/4033	0.75	3/5495 (0.1%)
2	F	0.56	0/1279	0.94	6/1719 (0.3%)
2	G	0.54	0/1243	0.89	3/1687 (0.2%)
2	J	0.57	0/1279	1.00	8/1719 (0.5%)
2	K	0.55	0/1243	0.90	4/1687 (0.2%)
2	N	0.57	0/1279	0.93	6/1719 (0.3%)
2	O	0.54	0/1243	0.92	4/1687 (0.2%)
2	R	0.57	0/1279	0.95	8/1719 (0.5%)
2	S	0.55	0/1243	0.89	4/1687 (0.2%)
All	All	0.54	0/42172	0.79	76/57312 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
2	F	0	3
2	G	0	1
2	J	0	2
2	N	0	1
2	O	0	1
2	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	S	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	138	VAL	CA-CB-CG1	11.83	128.64	110.90
2	R	110	ARG	NE-CZ-NH1	10.59	125.60	120.30
2	F	110	ARG	NE-CZ-NH1	10.12	125.36	120.30
2	J	110	ARG	NE-CZ-NH1	9.19	124.89	120.30
2	R	237	ARG	NE-CZ-NH2	8.13	124.36	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	110	ARG	Sidechain
2	F	112	TYR	Sidechain
2	F	230	ARG	Sidechain
2	G	343	ARG	Sidechain
1	H	216	ARG	Sidechain

## 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	D	3910	0	3810	26	0
1	E	3953	0	3817	27	0
1	H	3910	0	3810	29	0
1	I	3953	0	3817	33	0
1	L	3910	0	3810	27	0
1	M	3953	0	3817	31	0
1	P	3910	0	3810	27	0
1	Q	3953	0	3817	30	0
2	F	1266	0	1338	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1228	0	1283	8	0
2	J	1266	0	1338	13	0
2	K	1228	0	1283	7	0
2	N	1266	0	1338	9	0
2	O	1228	0	1283	7	0
2	R	1266	0	1338	11	0
2	S	1228	0	1283	7	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
4	D	53	0	31	0	0
4	E	53	0	31	0	0
4	H	53	0	31	0	0
4	I	53	0	31	0	0
4	L	53	0	31	0	0
4	M	53	0	31	0	0
4	P	53	0	31	0	0
4	Q	53	0	31	0	0
5	D	26	0	16	0	0
5	E	26	0	16	0	0
5	H	26	0	16	0	0
5	I	26	0	16	0	0
5	L	26	0	16	0	0
5	M	26	0	16	0	0
5	P	26	0	16	0	0
5	Q	26	0	16	0	0
6	F	8	0	8	1	0
6	G	8	0	8	0	0
6	J	8	0	8	1	0
6	K	8	0	8	0	0
6	N	8	0	8	1	0
6	O	8	0	8	0	0
6	R	8	0	8	2	0
6	S	8	0	8	0	0
All	All	42132	0	41432	299	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 4.

The worst 5 of 299 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:113:GLU:OE1	1:E:160:LYS:NZ	2.20	0.75
1:L:113:GLU:OE1	1:L:160:LYS:NZ	2.20	0.75
6:N:501:VAL:N	2:O:346:ASN:OD1	2.20	0.74
1:P:113:GLU:OE1	1:P:160:LYS:NZ	2.20	0.74
1:Q:113:GLU:OE1	1:Q:160:LYS:NZ	2.20	0.74

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	D	517/586 (88%)	499 (96%)	17 (3%)	1 (0%)	47	80
1	E	531/586 (91%)	512 (96%)	18 (3%)	1 (0%)	47	80
1	H	517/586 (88%)	499 (96%)	17 (3%)	1 (0%)	47	80
1	I	531/586 (91%)	511 (96%)	19 (4%)	1 (0%)	47	80
1	L	517/586 (88%)	498 (96%)	18 (4%)	1 (0%)	47	80
1	M	531/586 (91%)	512 (96%)	18 (3%)	1 (0%)	47	80
1	P	517/586 (88%)	497 (96%)	19 (4%)	1 (0%)	47	80
1	Q	531/586 (91%)	512 (96%)	18 (3%)	1 (0%)	47	80
2	F	157/491 (32%)	150 (96%)	7 (4%)	0	100	100
2	G	157/491 (32%)	153 (98%)	4 (2%)	0	100	100
2	J	157/491 (32%)	153 (98%)	3 (2%)	1 (1%)	25	62
2	K	157/491 (32%)	151 (96%)	6 (4%)	0	100	100
2	N	157/491 (32%)	151 (96%)	6 (4%)	0	100	100
2	O	157/491 (32%)	154 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	157/491 (32%)	154 (98%)	3 (2%)	0	100	100
2	S	157/491 (32%)	152 (97%)	5 (3%)	0	100	100
All	All	5448/8616 (63%)	5258 (96%)	181 (3%)	9 (0%)	50	80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	123	ARG
1	D	516	GLY
1	H	516	GLY
1	L	516	GLY
1	P	516	GLY

### 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 PDB entries followed by that with respect to all EM entries.

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	D	396/483 (82%)	394 (100%)	2 (0%)	88	95
1	E	395/483 (82%)	393 (100%)	2 (0%)	88	95
1	H	396/483 (82%)	392 (99%)	4 (1%)	76	89
1	I	395/483 (82%)	393 (100%)	2 (0%)	88	95
1	L	396/483 (82%)	394 (100%)	2 (0%)	88	95
1	M	395/483 (82%)	393 (100%)	2 (0%)	88	95
1	P	396/483 (82%)	395 (100%)	1 (0%)	92	98
1	Q	395/483 (82%)	393 (100%)	2 (0%)	88	95
2	F	139/418 (33%)	138 (99%)	1 (1%)	84	93
2	G	136/418 (32%)	135 (99%)	1 (1%)	84	93
2	J	139/418 (33%)	139 (100%)	0	100	100
2	K	136/418 (32%)	135 (99%)	1 (1%)	84	93
2	N	139/418 (33%)	139 (100%)	0	100	100
2	O	136/418 (32%)	135 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	139/418 (33%)	137 (99%)	2 (1%)	67	85
2	S	136/418 (32%)	135 (99%)	1 (1%)	84	93
All	All	4264/7208 (59%)	4240 (99%)	24 (1%)	86	95

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	203	THR
2	O	444	ASP
1	M	203	THR
1	P	97	ARG
1	H	97	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	393	HIS
1	H	393	HIS
1	M	393	HIS
1	L	393	HIS
1	E	128	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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$
5	TPP	M	703	3	22,27,27	1.28	3 (13%)	29,40,40	1.71	6 (20%)
6	VAL	N	501	-	5,7,7	1.48	2 (40%)	7,9,9	0.76	0
5	TPP	P	703	3	22,27,27	1.15	3 (13%)	29,40,40	2.08	9 (31%)
5	TPP	Q	703	3	22,27,27	1.30	3 (13%)	29,40,40	1.71	6 (20%)
6	VAL	J	501	-	5,7,7	1.49	2 (40%)	7,9,9	0.73	0
6	VAL	G	501	-	5,7,7	1.63	2 (40%)	7,9,9	0.63	0
5	TPP	I	703	3	22,27,27	1.29	3 (13%)	29,40,40	1.71	6 (20%)
4	FAD	M	702	-	53,58,58	1.09	4 (7%)	68,89,89	1.79	14 (20%)
6	VAL	K	501	-	5,7,7	1.58	2 (40%)	7,9,9	0.67	0
4	FAD	H	702	-	53,58,58	1.02	3 (5%)	68,89,89	1.84	14 (20%)
4	FAD	E	702	-	53,58,58	1.09	3 (5%)	68,89,89	1.78	13 (19%)
5	TPP	L	703	3	22,27,27	1.16	3 (13%)	29,40,40	2.08	8 (27%)
6	VAL	O	501	-	5,7,7	1.61	2 (40%)	7,9,9	0.55	0
4	FAD	I	702	-	53,58,58	1.08	3 (5%)	68,89,89	1.78	14 (20%)
6	VAL	F	501	-	5,7,7	1.44	1 (20%)	7,9,9	0.74	0
5	TPP	E	703	3	22,27,27	1.29	3 (13%)	29,40,40	1.71	6 (20%)
6	VAL	S	501	-	5,7,7	1.59	2 (40%)	7,9,9	0.67	0
6	VAL	R	501	-	5,7,7	1.50	2 (40%)	7,9,9	0.82	0
4	FAD	D	702	-	53,58,58	1.01	2 (3%)	68,89,89	1.83	14 (20%)
4	FAD	P	702	-	53,58,58	1.02	3 (5%)	68,89,89	1.83	14 (20%)
4	FAD	L	702	-	53,58,58	1.02	2 (3%)	68,89,89	1.83	14 (20%)
5	TPP	H	703	3	22,27,27	1.17	3 (13%)	29,40,40	2.08	8 (27%)
4	FAD	Q	702	-	53,58,58	1.08	3 (5%)	68,89,89	1.78	14 (20%)
5	TPP	D	703	3	22,27,27	1.17	3 (13%)	29,40,40	2.09	8 (27%)

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
5	TPP	M	703	3	-	2/16/17/17	0/2/2/2
6	VAL	N	501	-	-	3/8/8/8	-
5	TPP	P	703	3	-	2/16/17/17	0/2/2/2
5	TPP	Q	703	3	-	2/16/17/17	0/2/2/2
6	VAL	J	501	-	-	1/8/8/8	-
6	VAL	G	501	-	-	0/8/8/8	-
5	TPP	I	703	3	-	2/16/17/17	0/2/2/2
4	FAD	M	702	-	-	6/30/50/50	0/6/6/6
6	VAL	K	501	-	-	0/8/8/8	-
4	FAD	H	702	-	-	6/30/50/50	0/6/6/6
4	FAD	E	702	-	-	5/30/50/50	0/6/6/6
5	TPP	L	703	3	-	2/16/17/17	0/2/2/2
6	VAL	O	501	-	-	1/8/8/8	-
4	FAD	I	702	-	-	5/30/50/50	0/6/6/6
6	VAL	F	501	-	-	3/8/8/8	-
5	TPP	E	703	3	-	2/16/17/17	0/2/2/2
6	VAL	S	501	-	-	0/8/8/8	-
6	VAL	R	501	-	-	0/8/8/8	-
4	FAD	D	702	-	-	6/30/50/50	0/6/6/6
4	FAD	P	702	-	-	6/30/50/50	0/6/6/6
4	FAD	L	702	-	-	6/30/50/50	0/6/6/6
5	TPP	H	703	3	-	2/16/17/17	0/2/2/2
4	FAD	Q	702	-	-	5/30/50/50	0/6/6/6
5	TPP	D	703	3	-	2/16/17/17	0/2/2/2

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	703	TPP	C6-C5	4.15	1.52	1.50
5	E	703	TPP	C6-C5	4.01	1.52	1.50
5	M	703	TPP	C6-C5	4.00	1.52	1.50
5	I	703	TPP	C6-C5	3.98	1.52	1.50
5	D	703	TPP	C6-C5	3.16	1.52	1.50

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	702	FAD	C4X-C10-N10	6.56	126.07	116.48
4	P	702	FAD	C4X-C10-N10	6.54	126.05	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	702	FAD	C4X-C10-N10	6.53	126.04	116.48
4	D	702	FAD	C4X-C10-N10	6.53	126.03	116.48
4	Q	702	FAD	C4X-C10-N10	6.44	125.91	116.48

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	702	FAD	C4B-C5B-O5B-PA
4	D	702	FAD	N10-C1'-C2'-O2'
4	D	702	FAD	N10-C1'-C2'-C3'
4	D	702	FAD	C5'-O5'-P-O1P
4	D	702	FAD	C5'-O5'-P-O3P

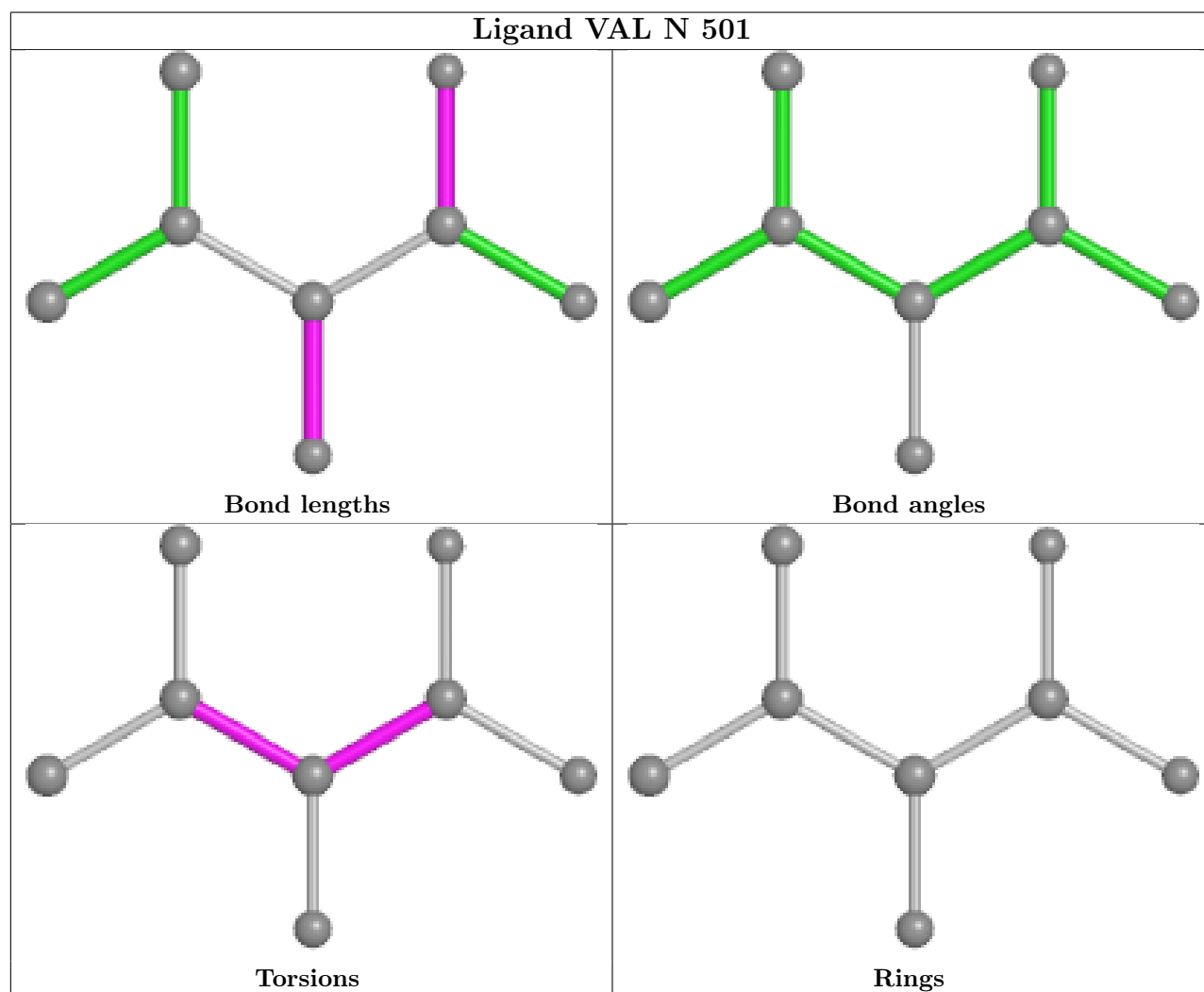
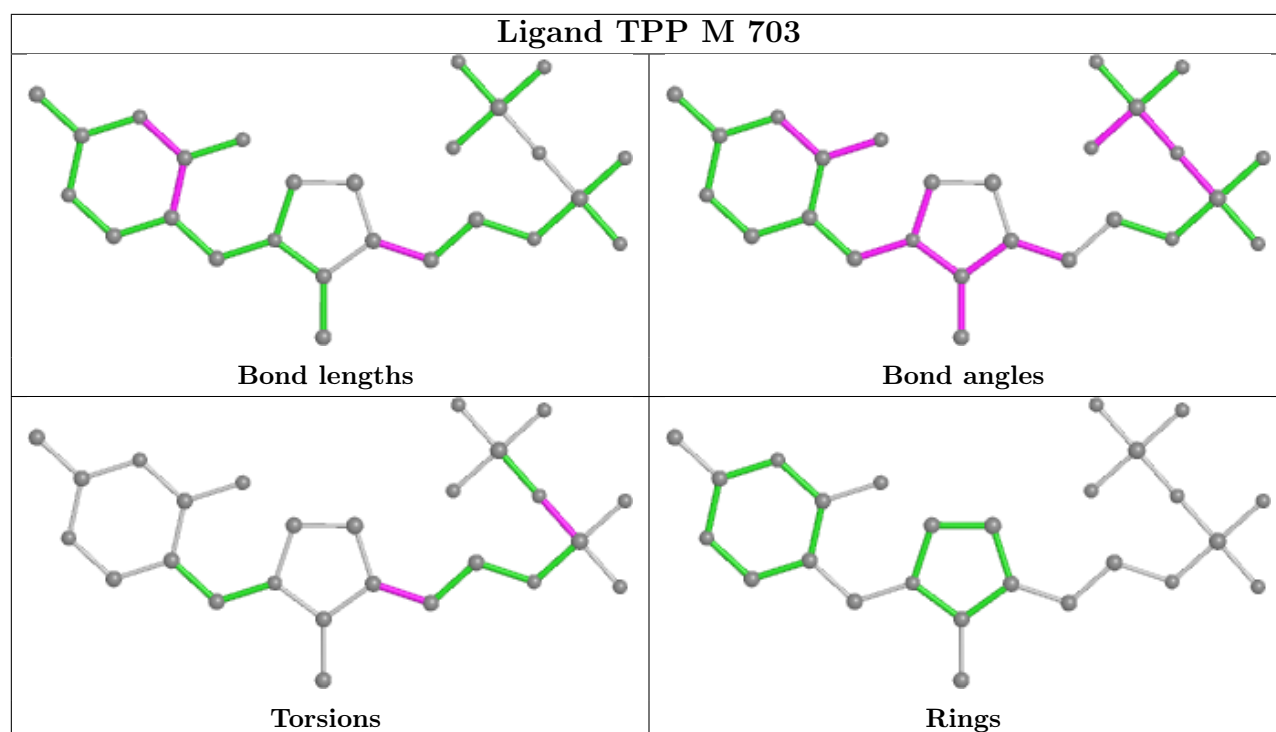
There are no ring outliers.

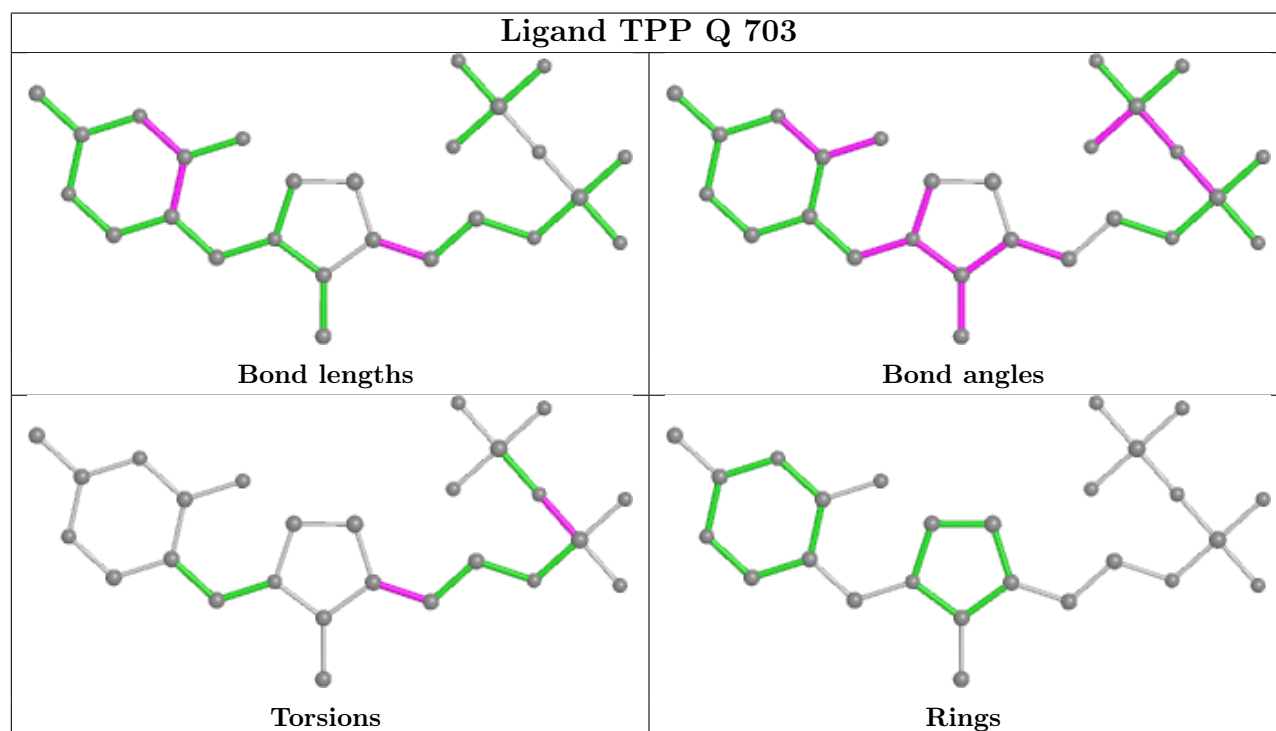
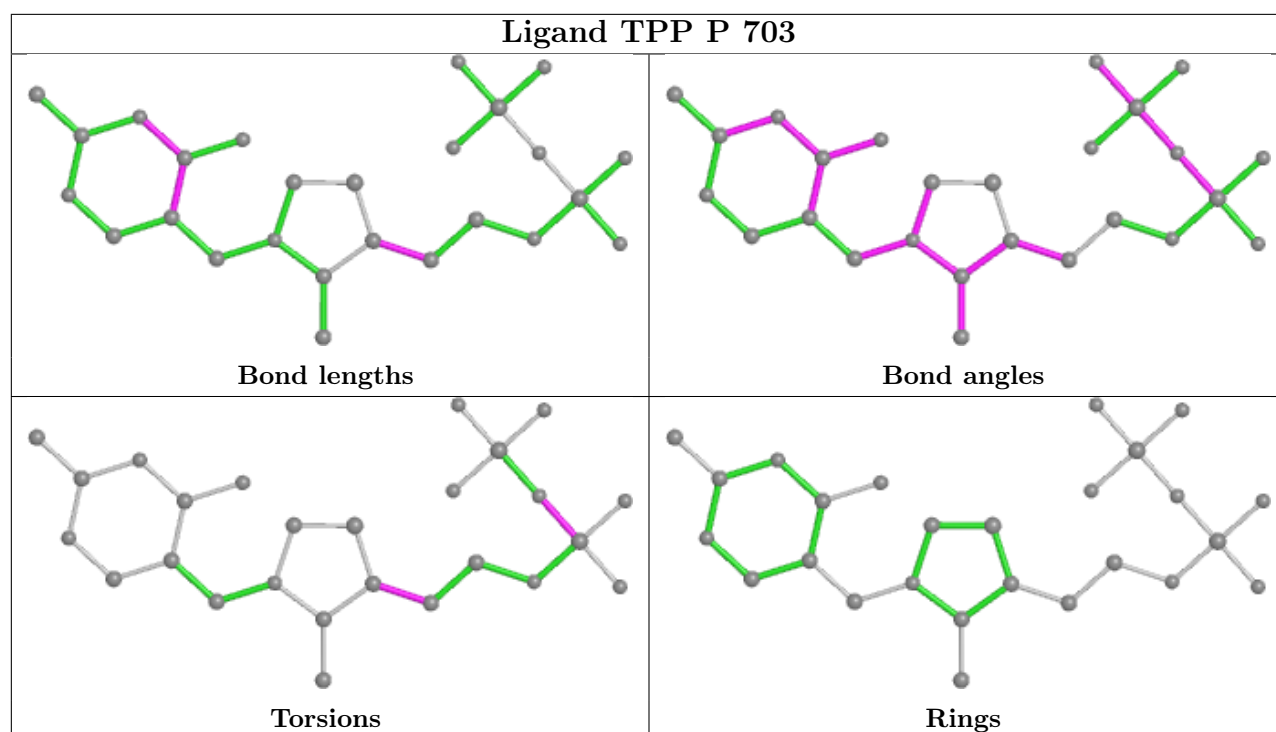
4 monomers are involved in 5 short contacts:

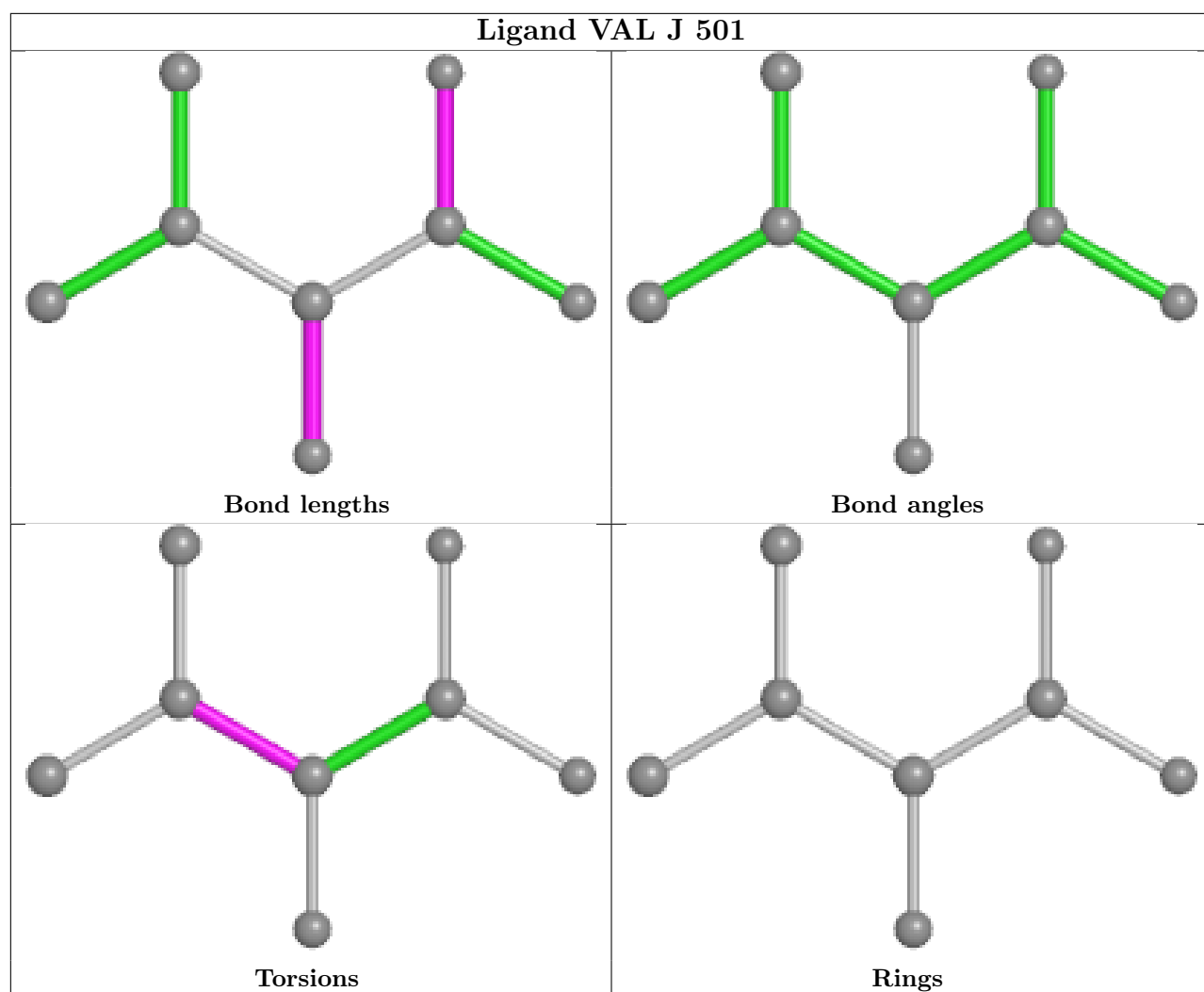
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	501	VAL	1	0
6	J	501	VAL	1	0
6	F	501	VAL	1	0
6	R	501	VAL	2	0

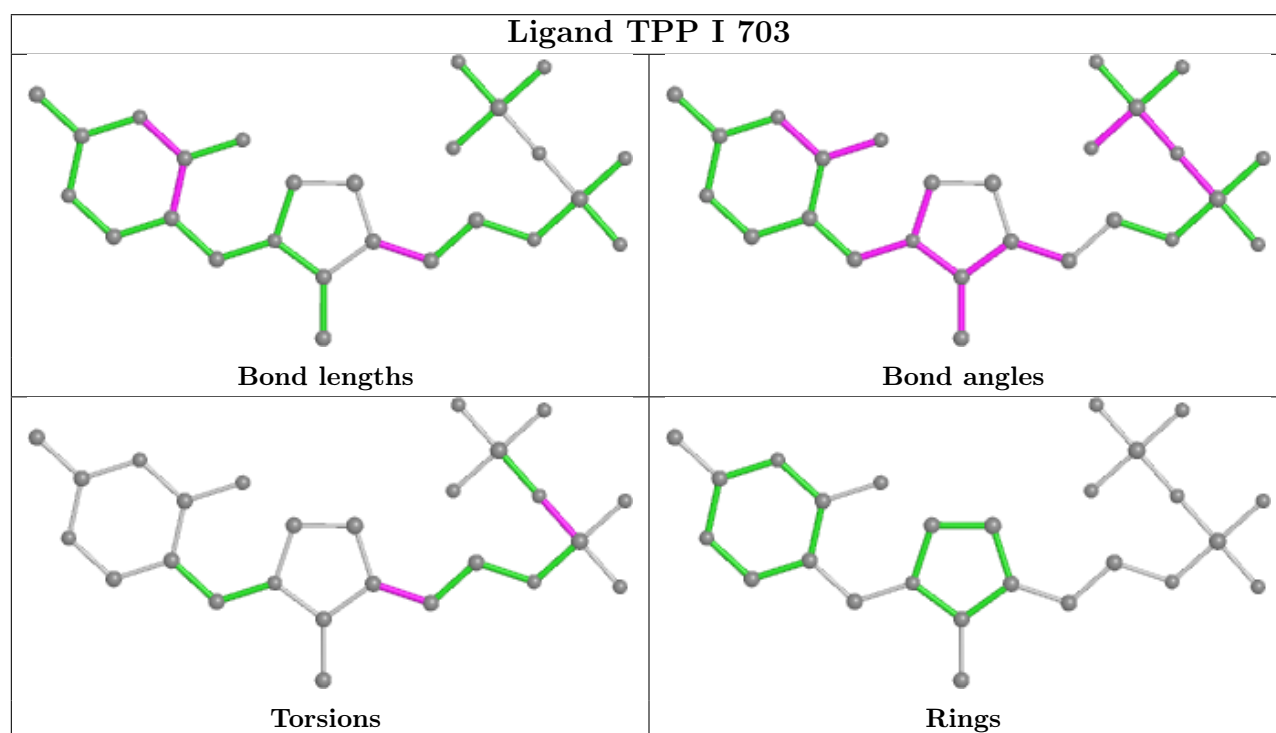
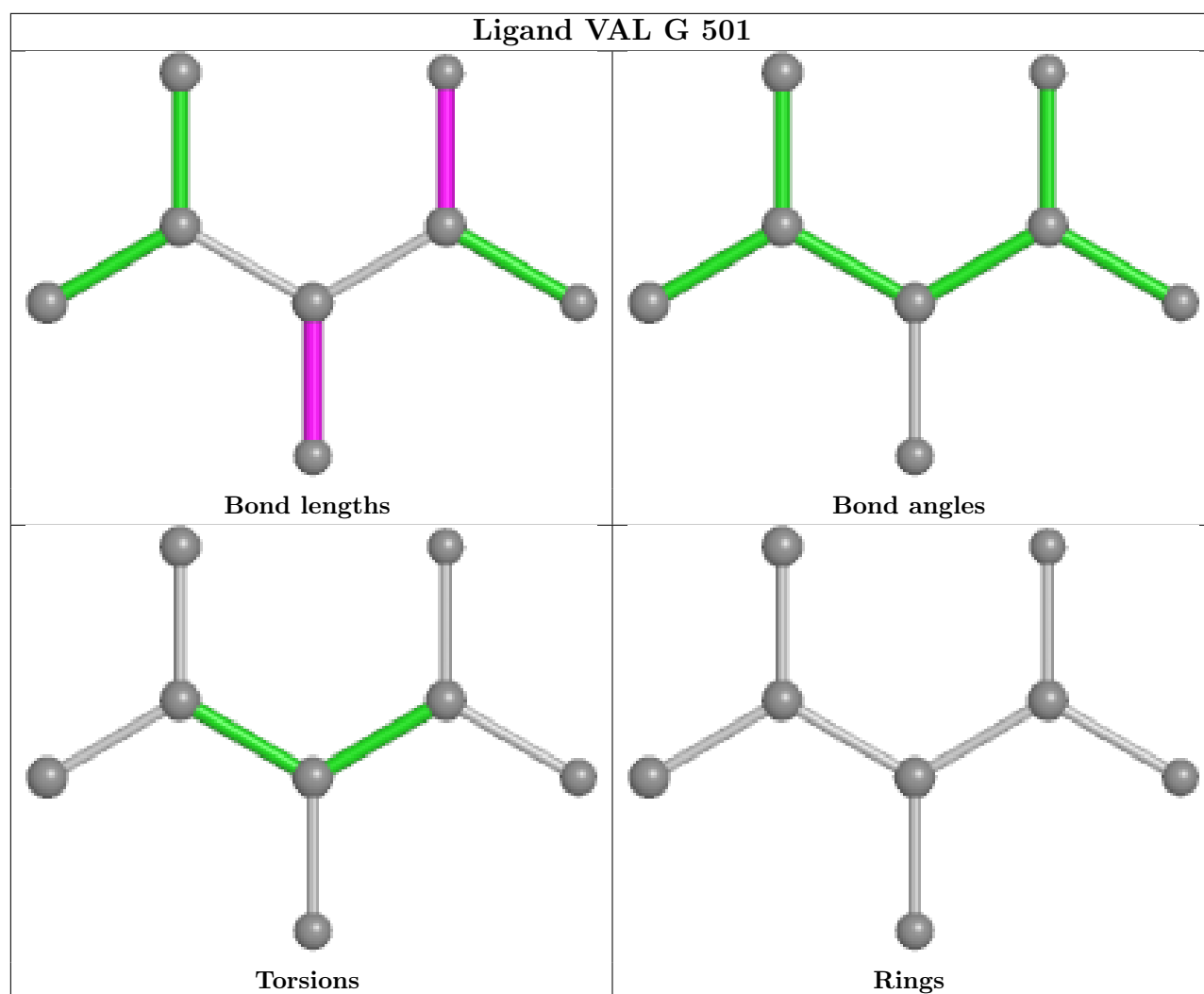
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

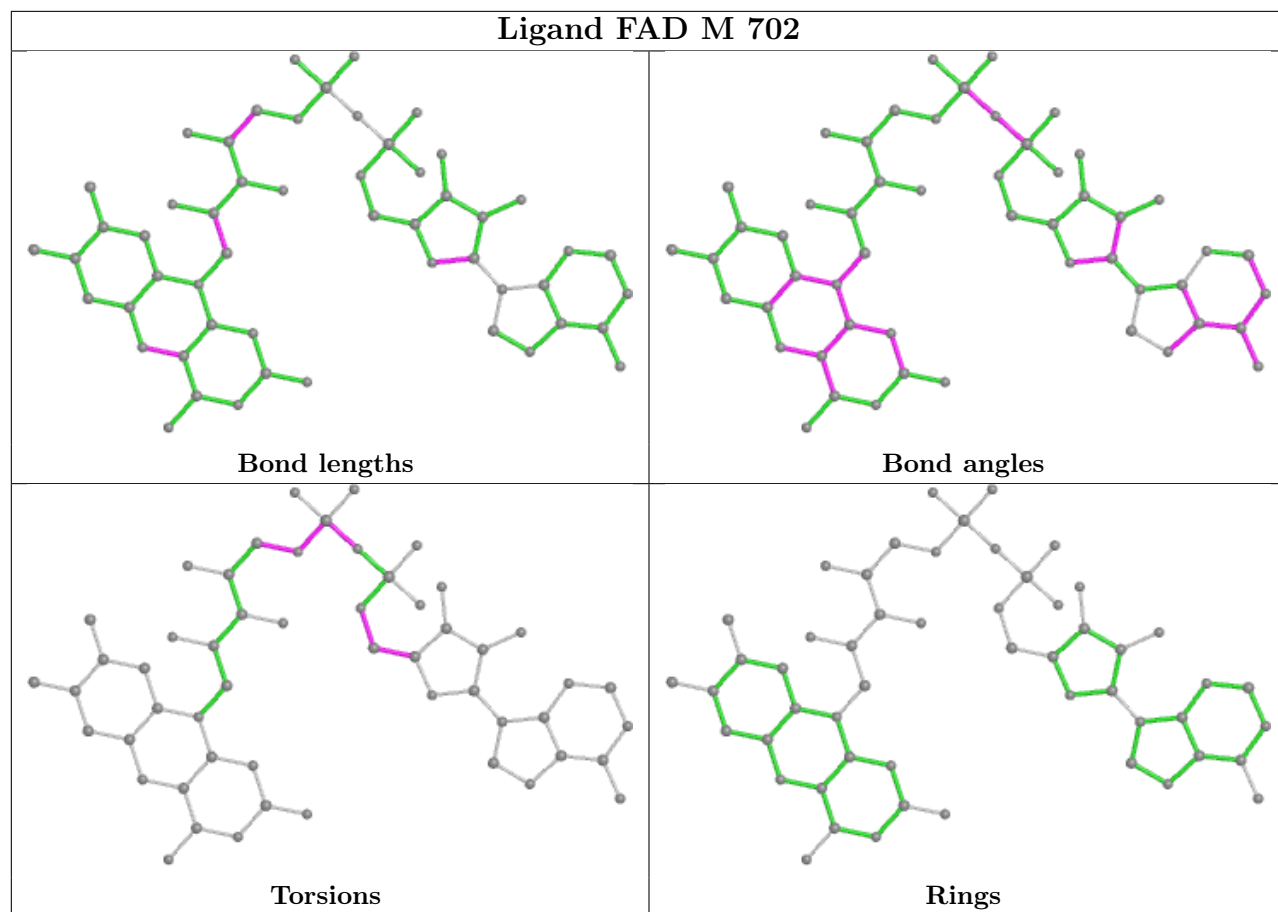


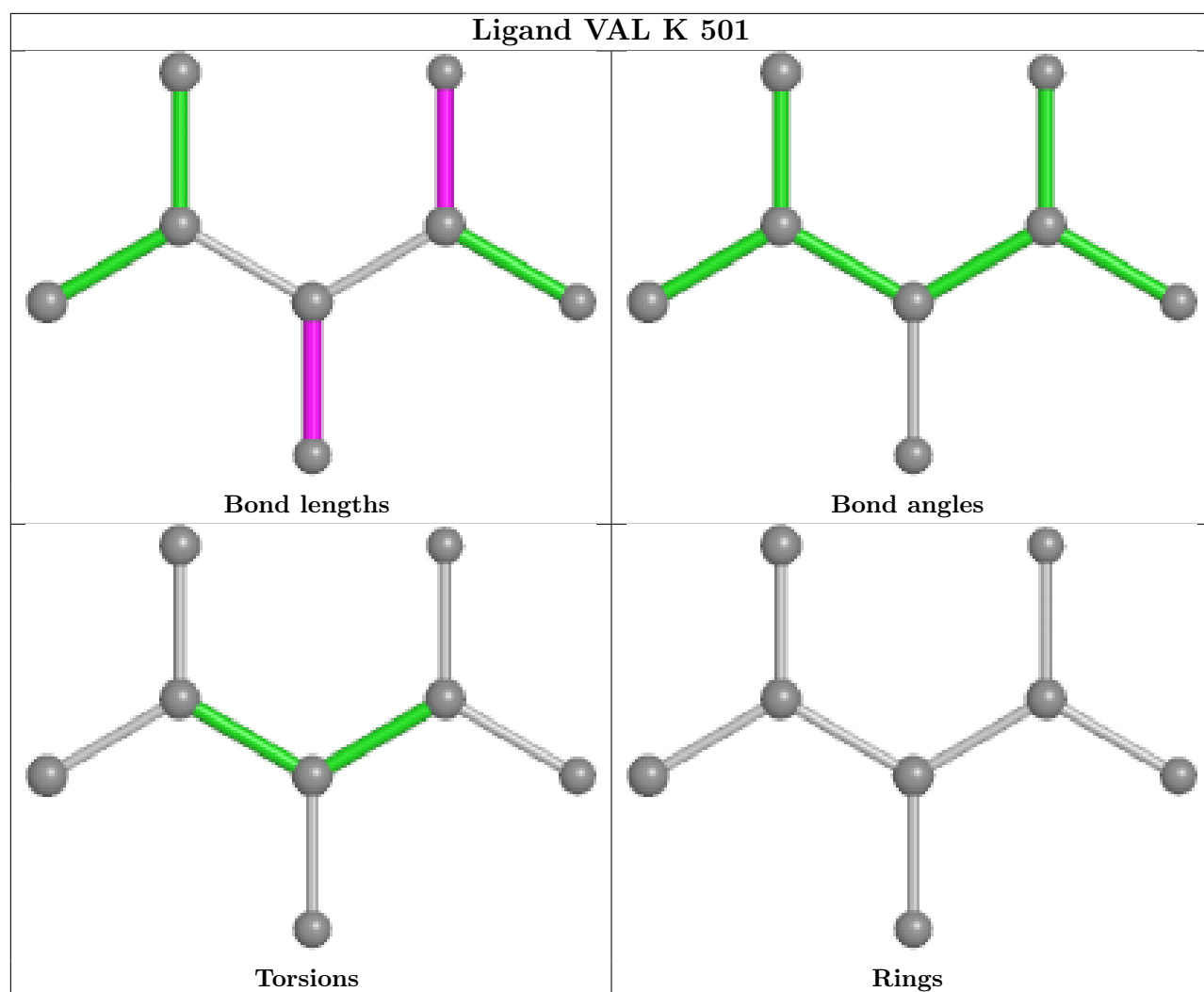


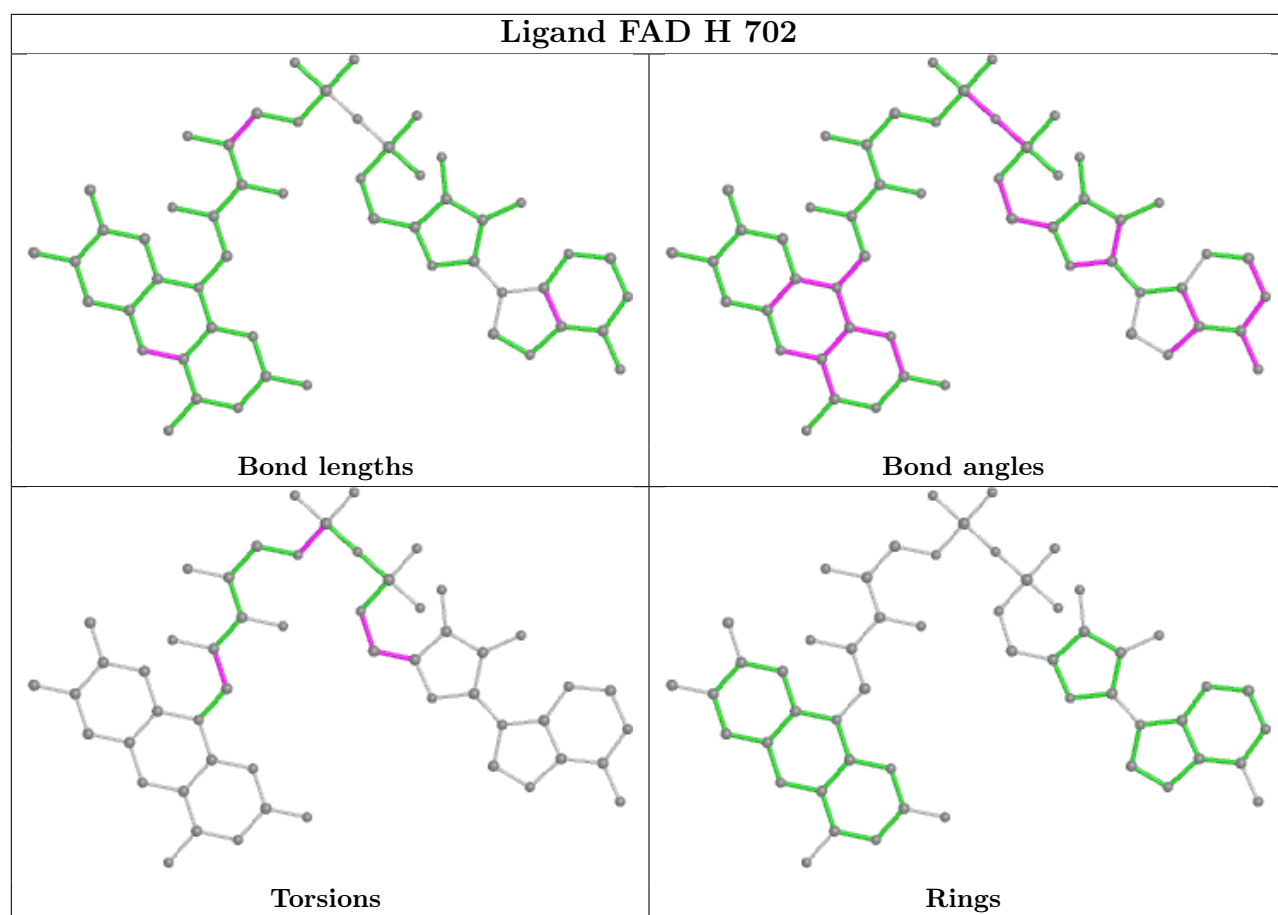


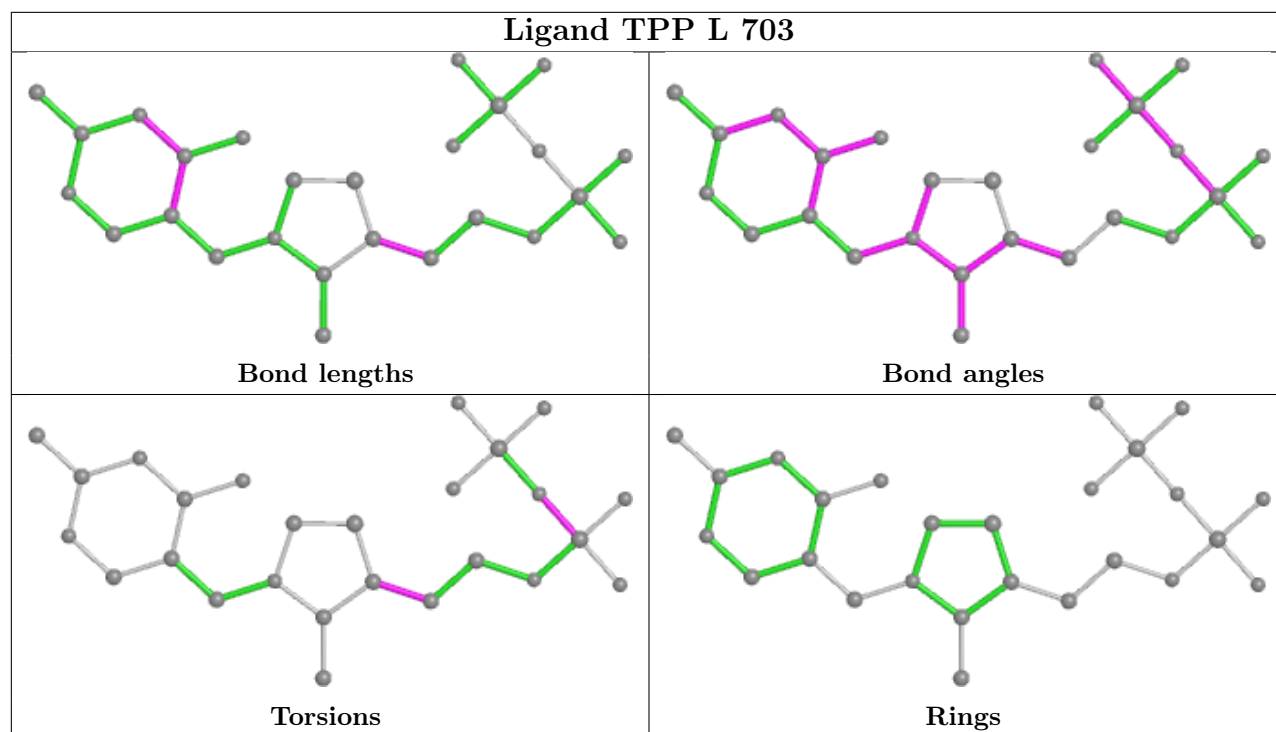
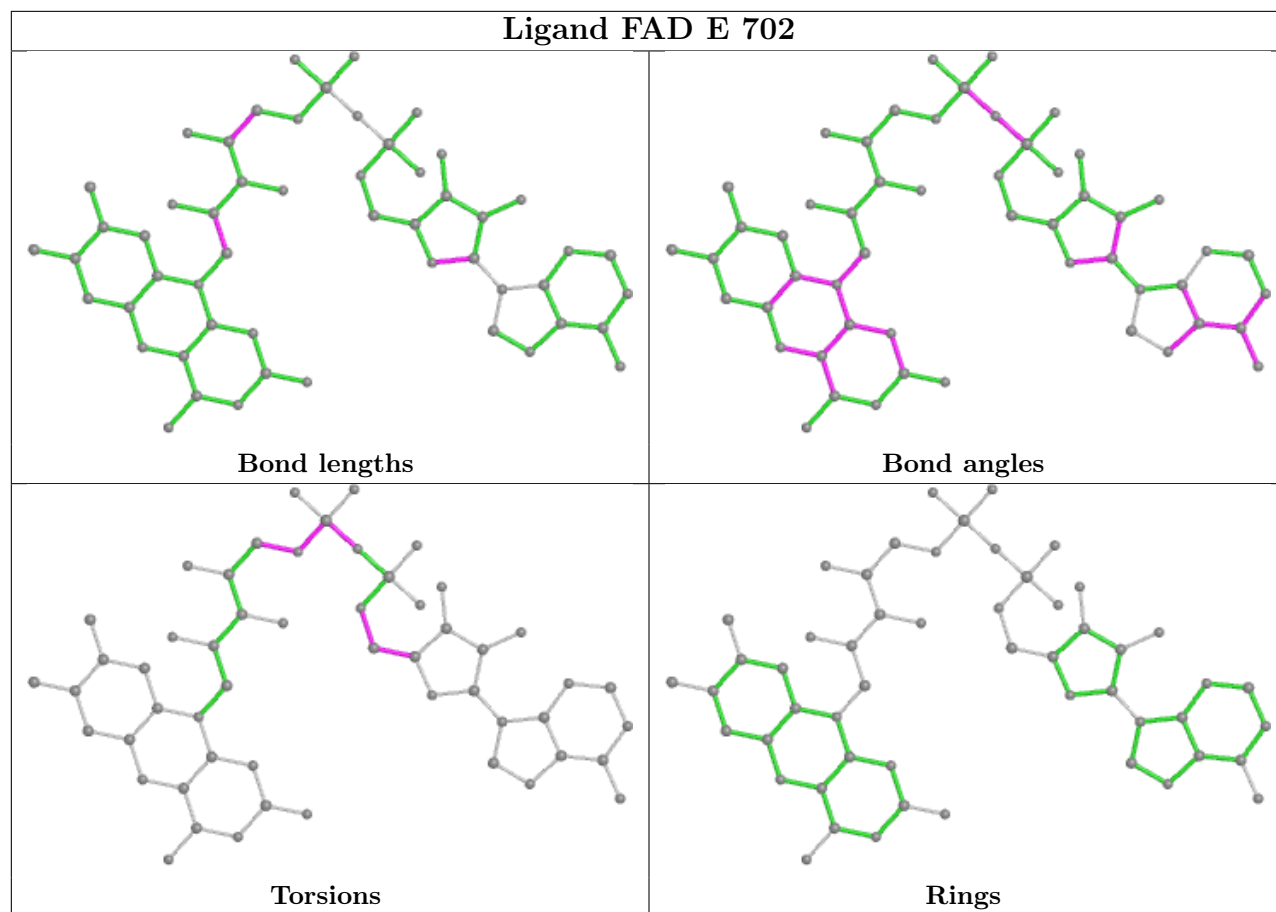




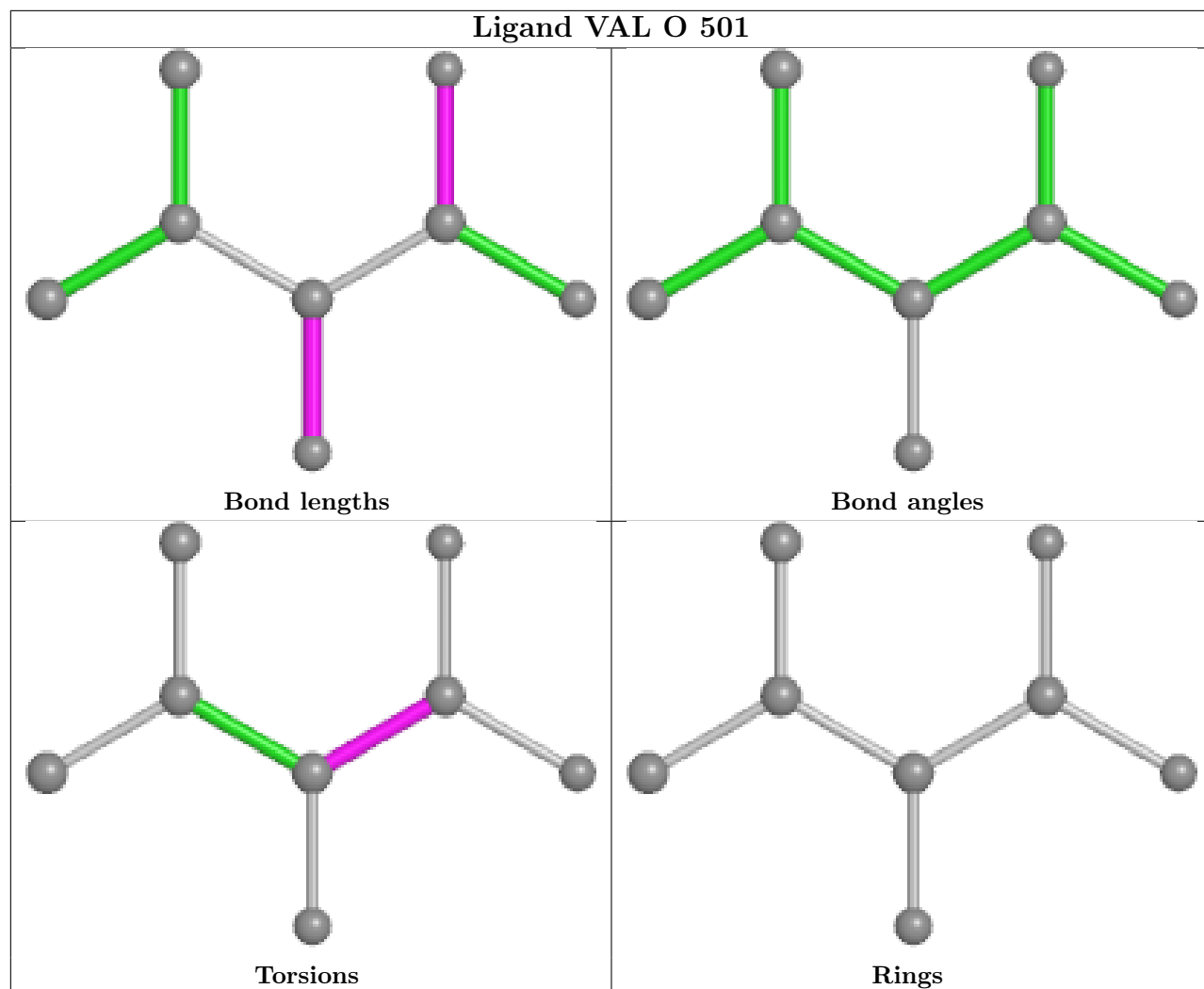




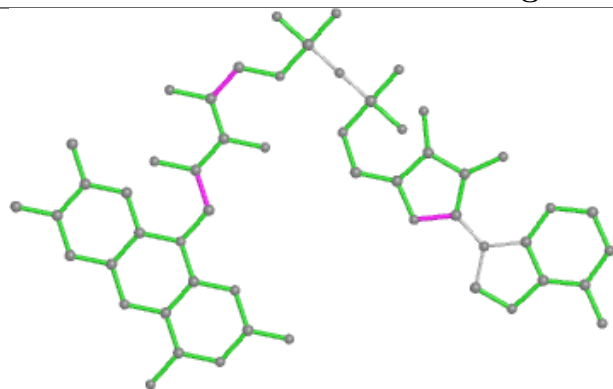




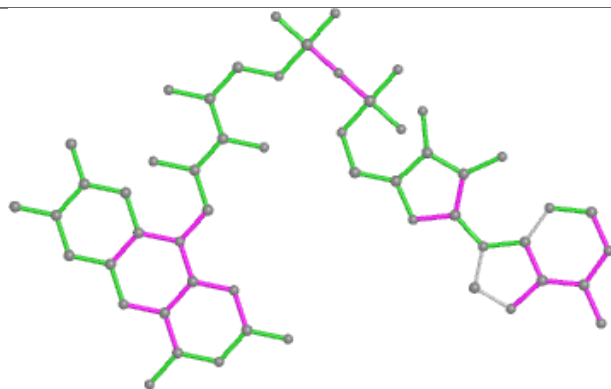




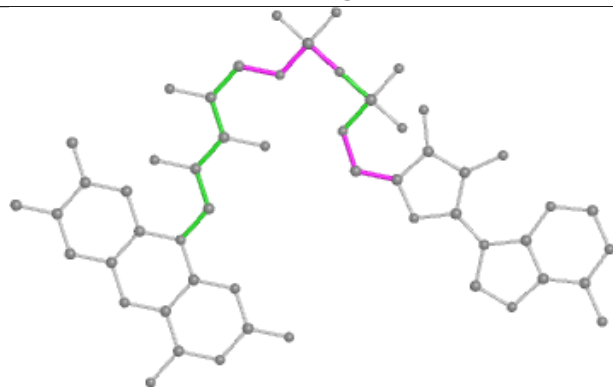
## Ligand FAD I 702



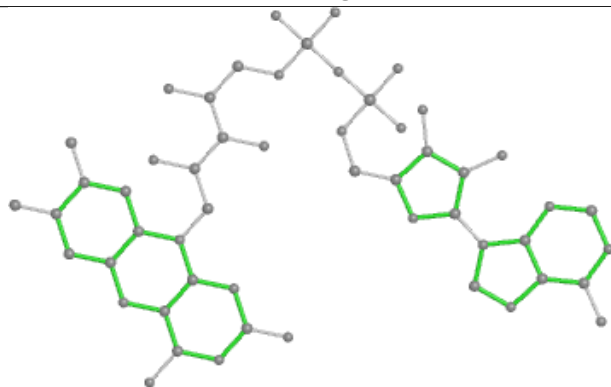
Bond lengths



Bond angles

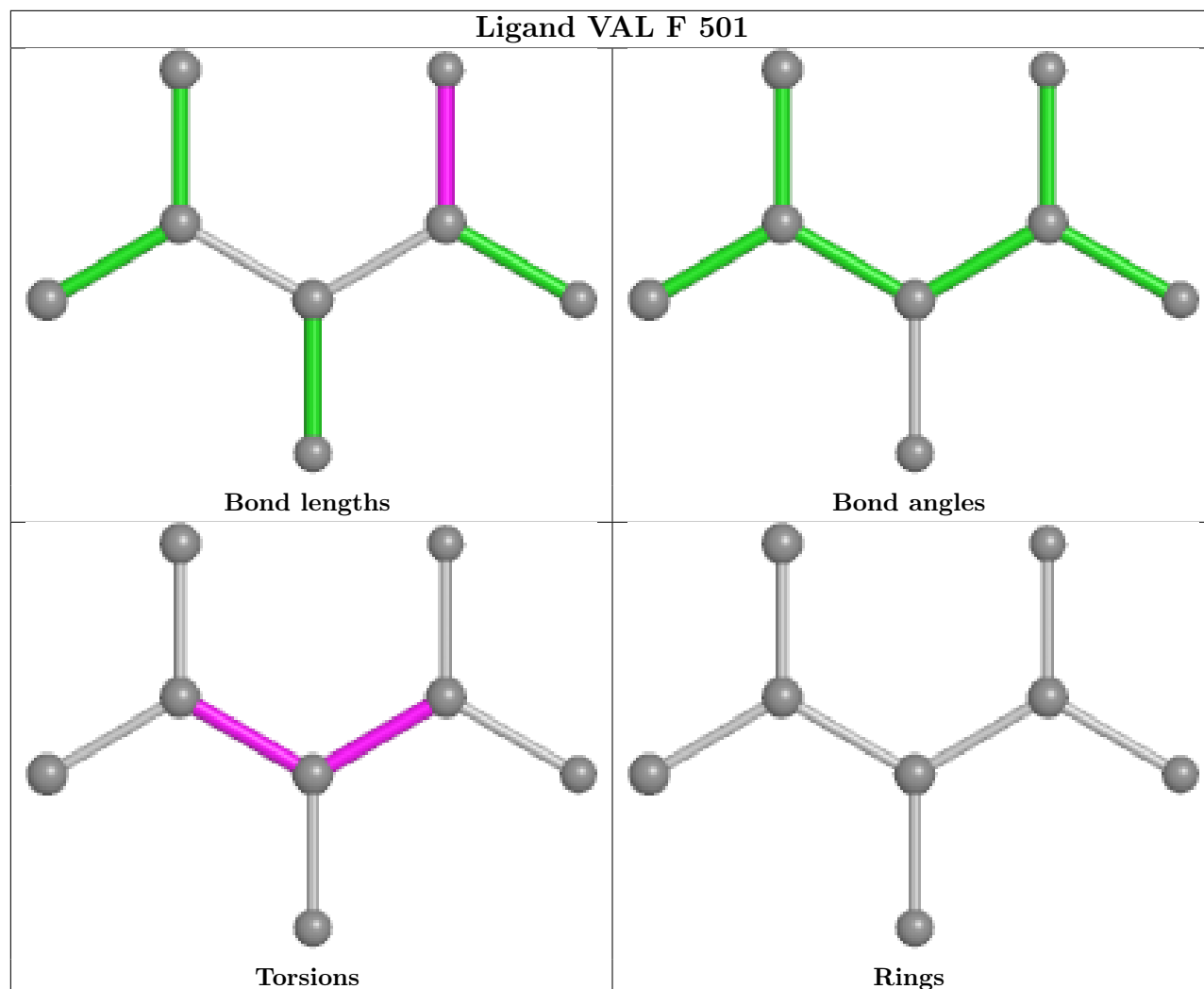


Torsions

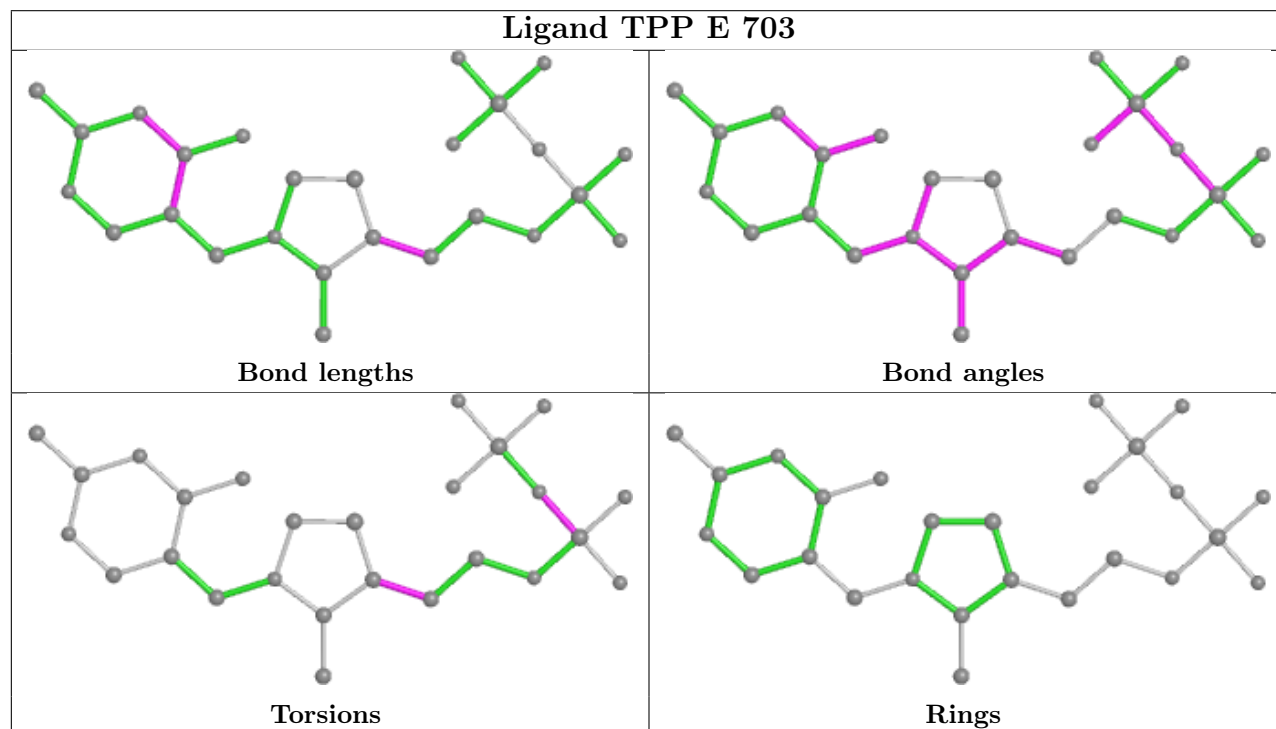


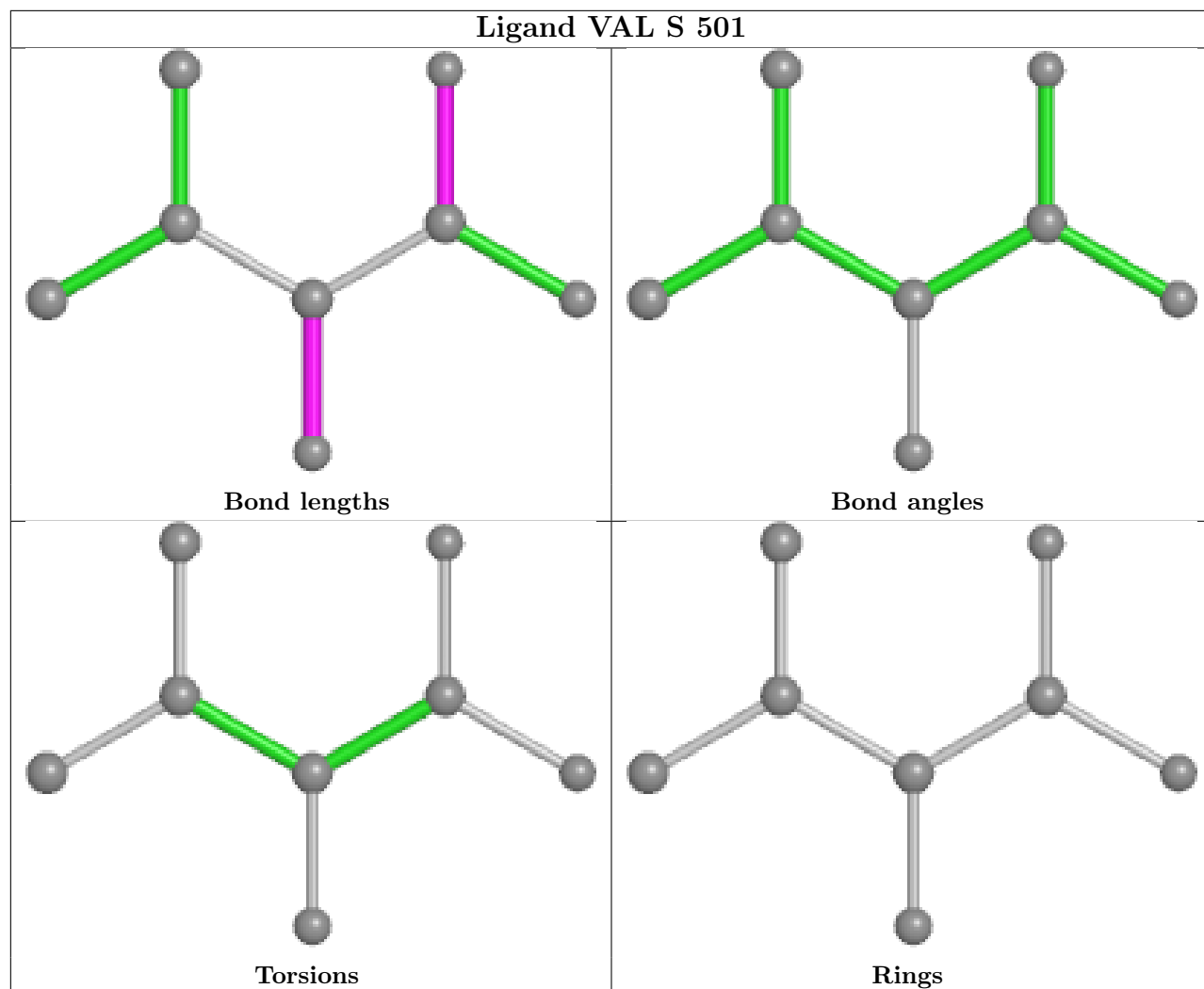
Rings

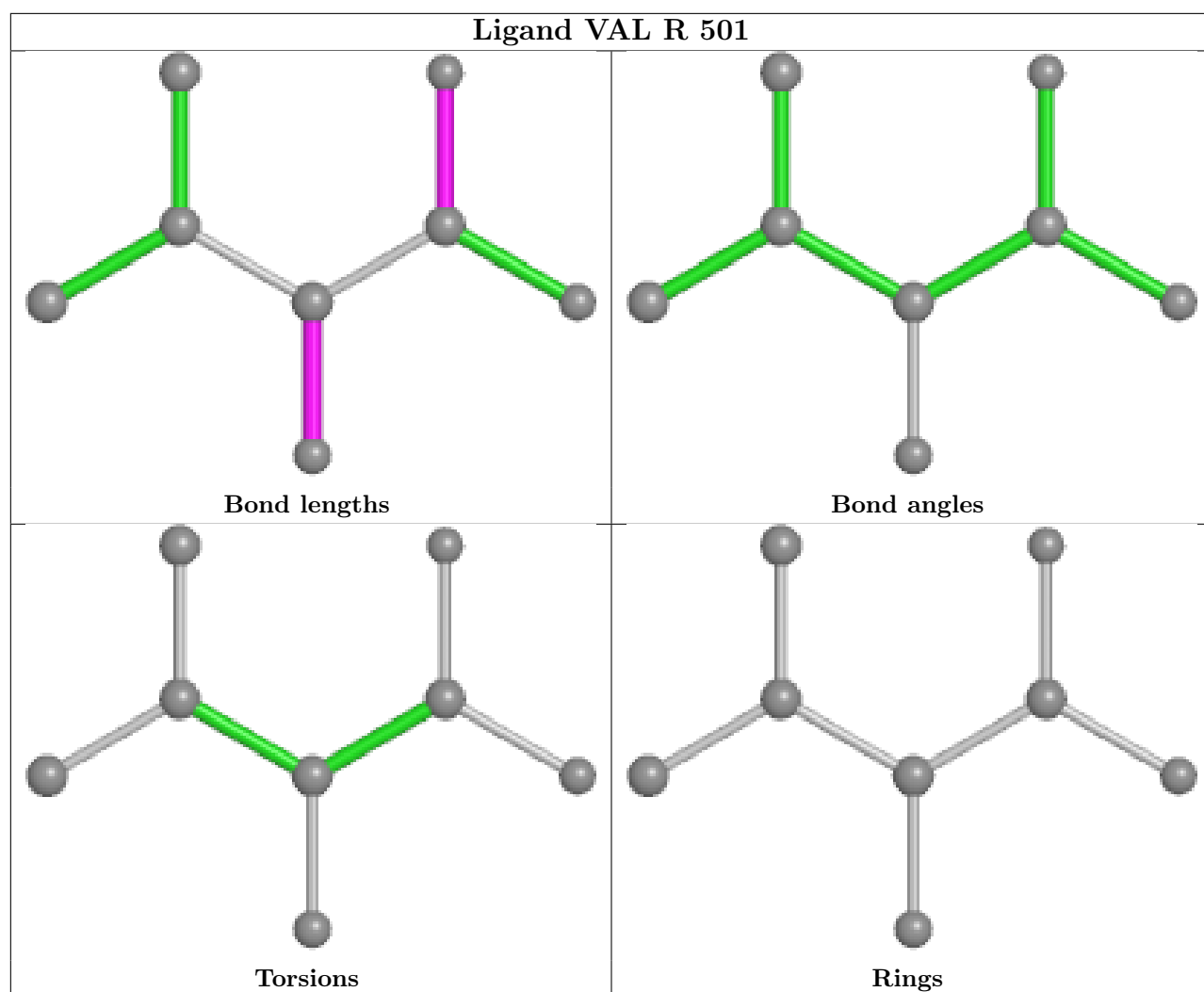
## Ligand VAL F 501

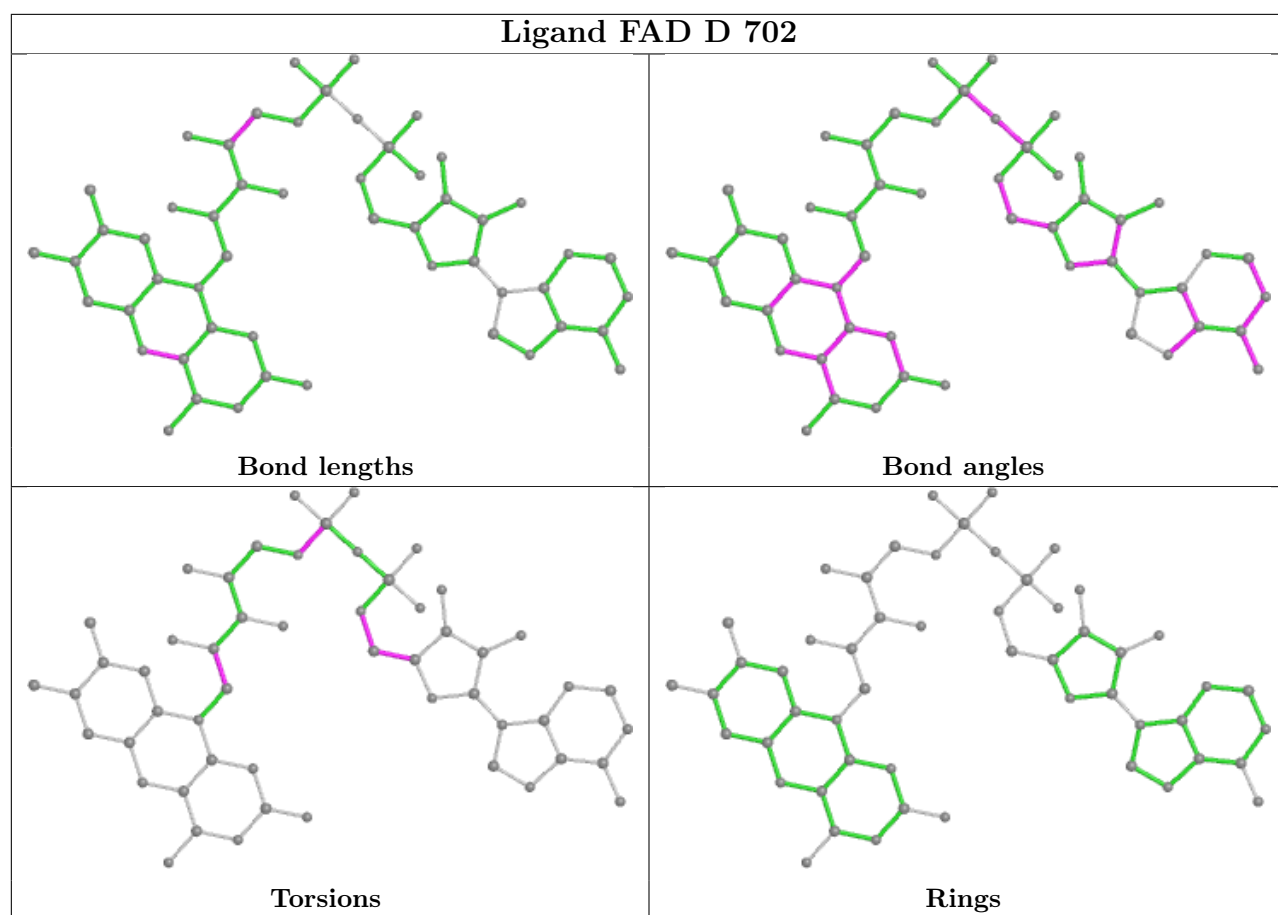


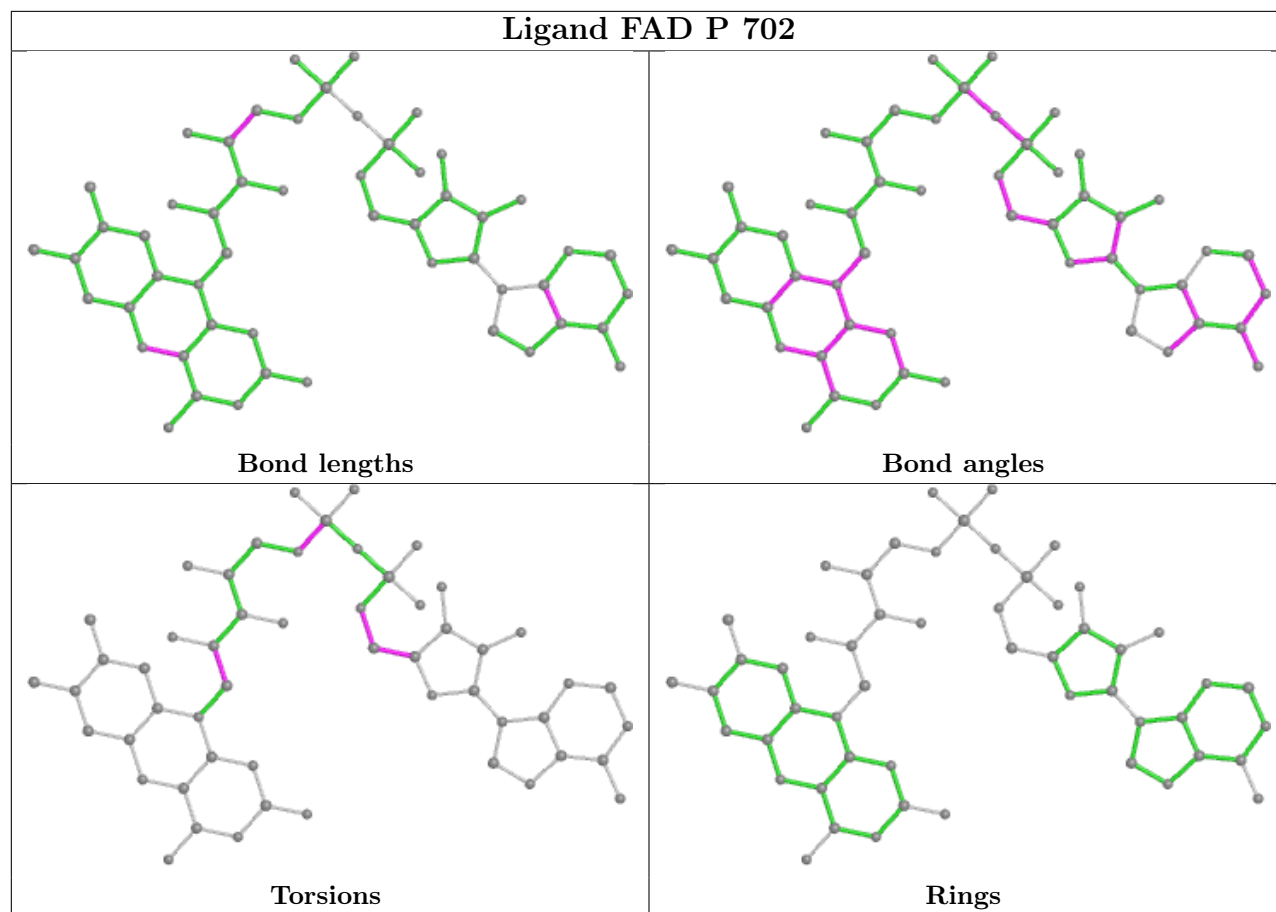
## Ligand TPP E 703



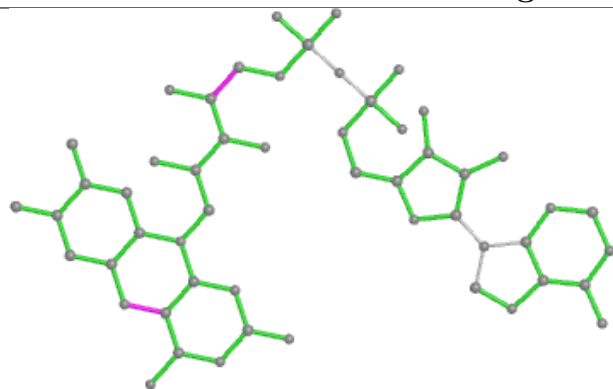




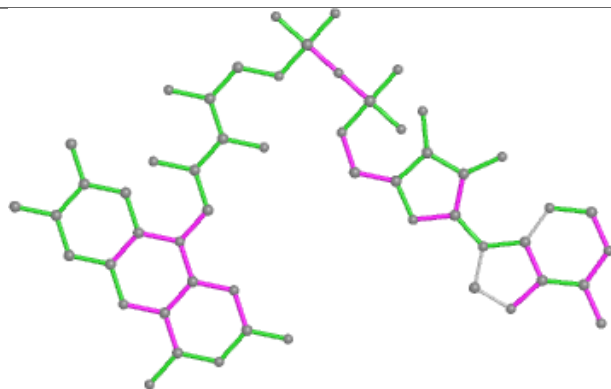




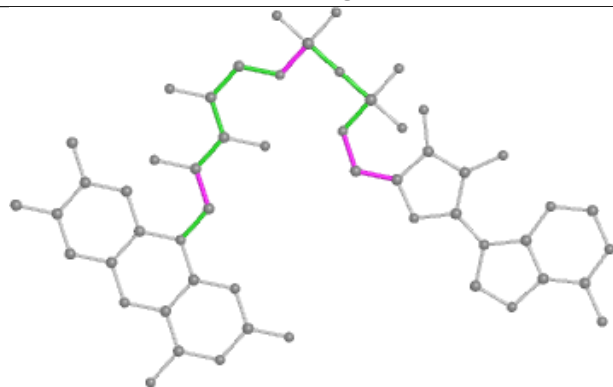
## Ligand FAD L 702



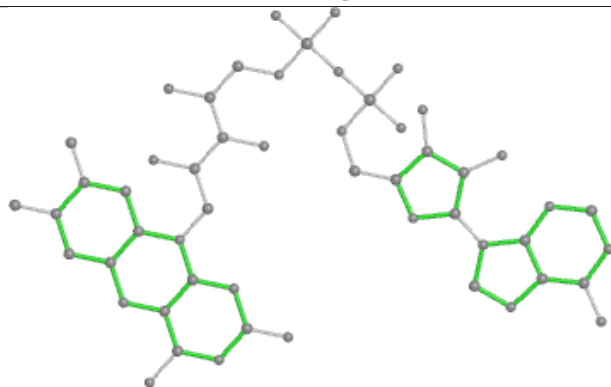
Bond lengths



Bond angles

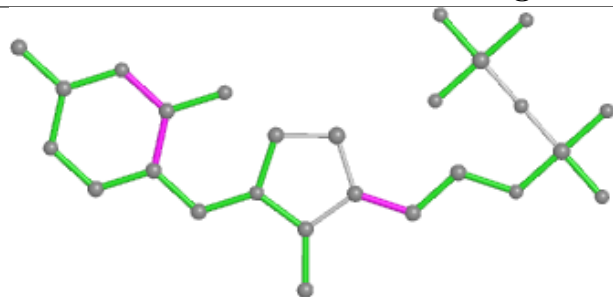


Torsions

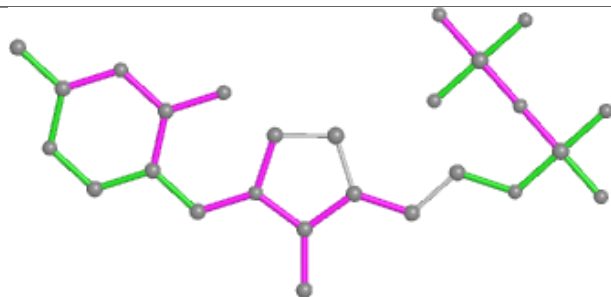


Rings

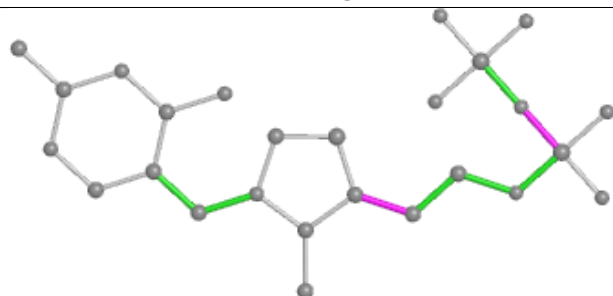
## Ligand TPP H 703



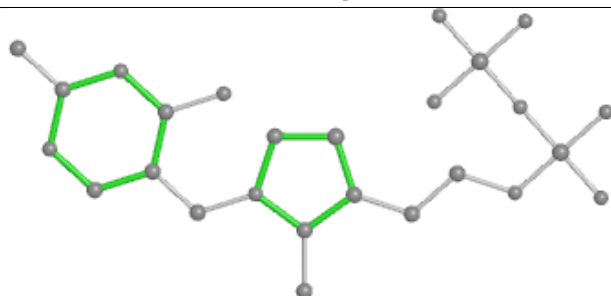
Bond lengths



Bond angles

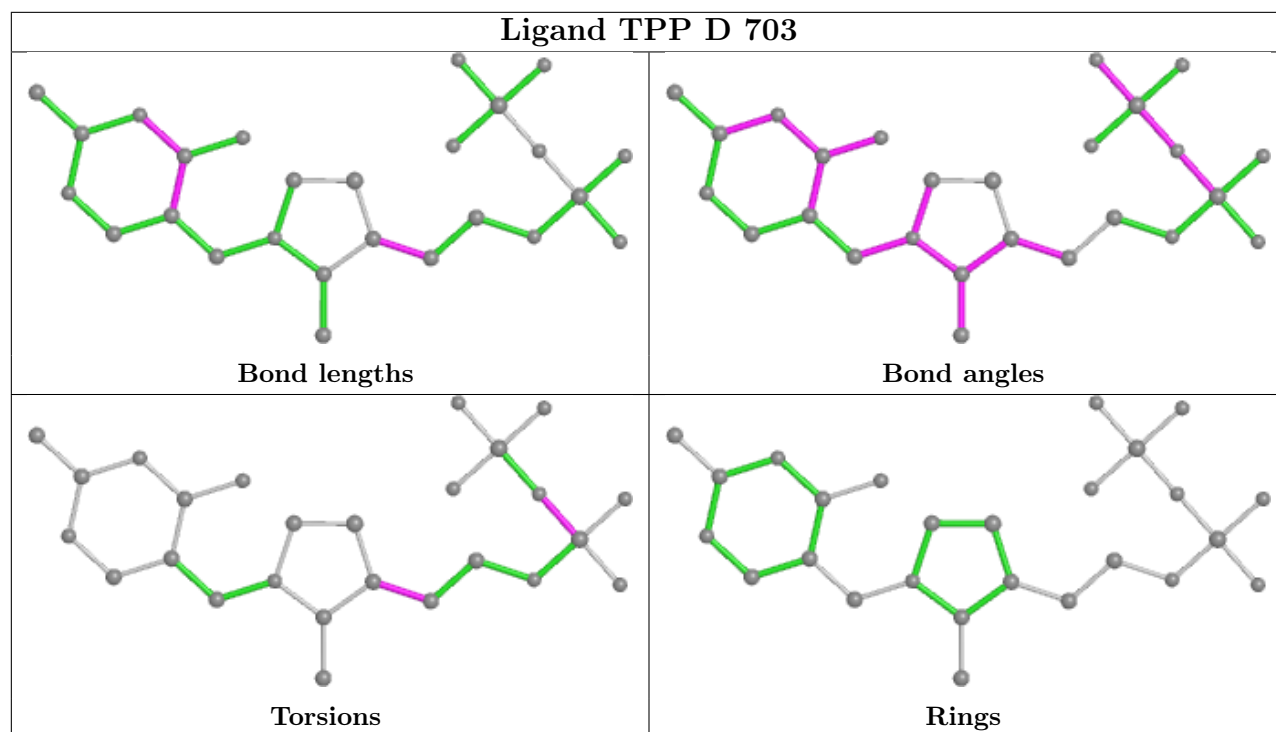
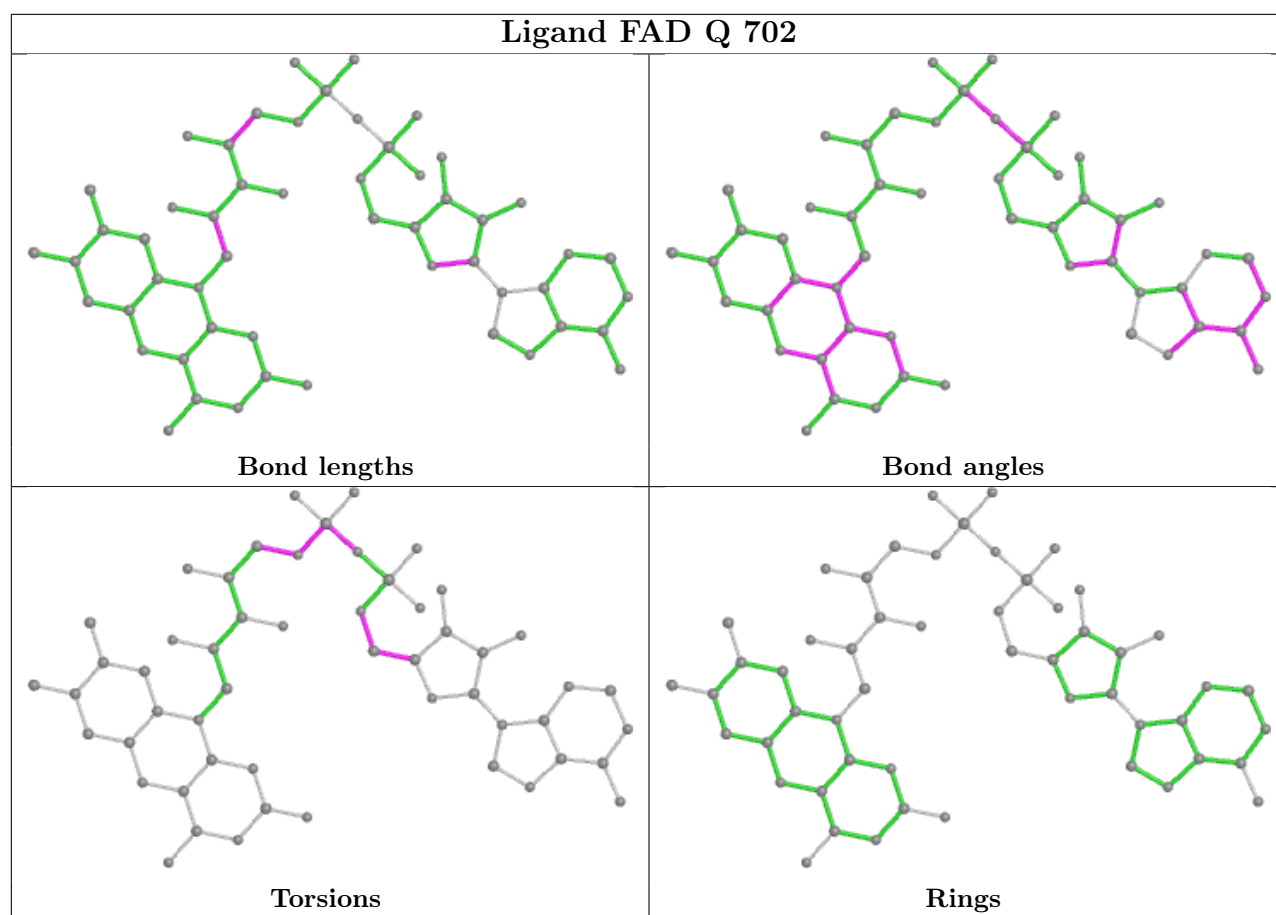


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.