



Full wwPDB EM Validation 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 Full wwPDB EM 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/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>.

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

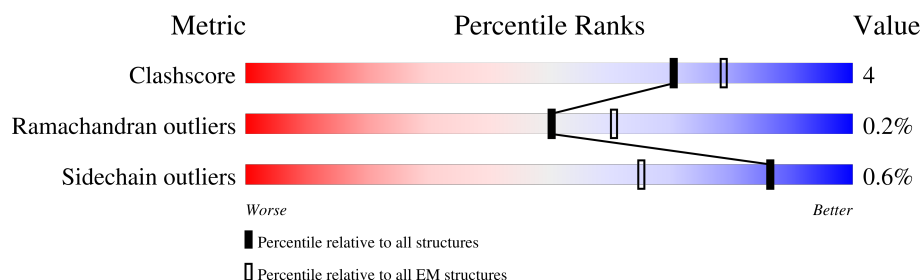
1 Overall quality at a glance

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 ≥ 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	
1	E	586	
1	H	586	
1	I	586	
1	L	586	
1	M	586	
1	P	586	
1	Q	586	
2	F	491	

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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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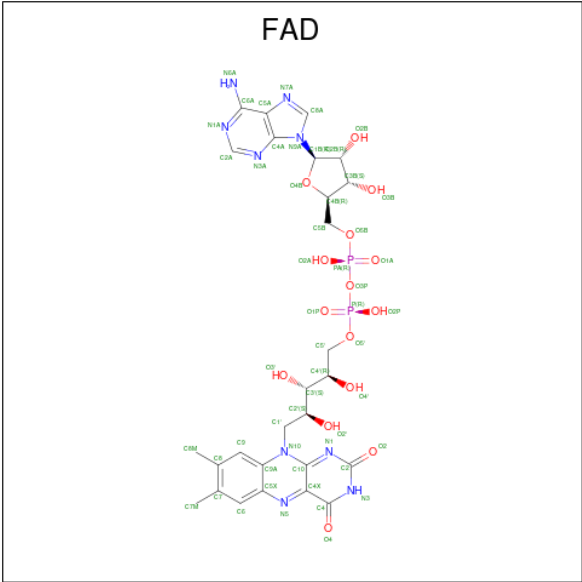
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		
2	J	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		
2	K	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		
2	N	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		
2	O	159	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: C₂₇H₃₃N₉O₁₅P₂).

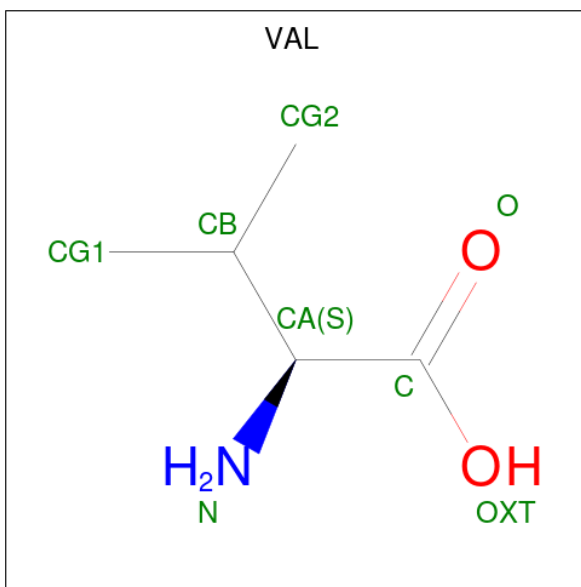


Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	E	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	H	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	I	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	L	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	M	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	P	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	Q	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



- Molecule 6 is VALINE (three-letter code: VAL) (formula: $\text{C}_5\text{H}_{11}\text{NO}_2$) (labeled as "Ligand of Interest" by depositor).

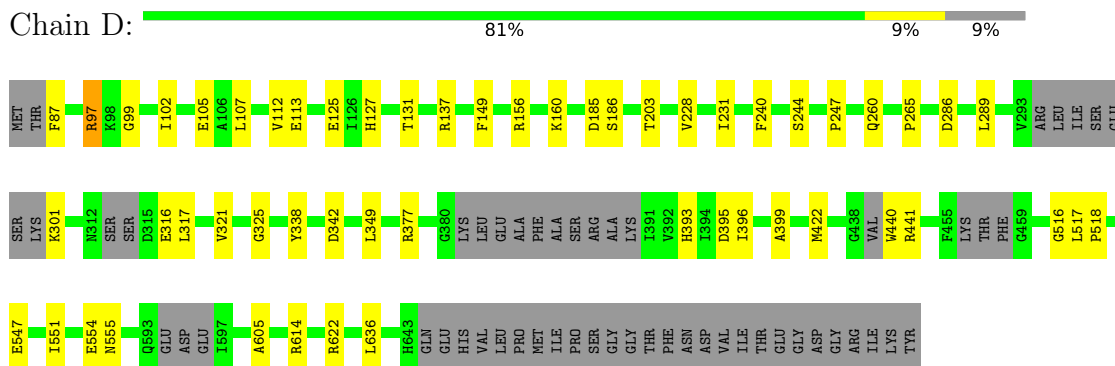


Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			8	5	1	2	
6	G	1	Total	C	N	O	0
			8	5	1	2	
6	J	1	Total	C	N	O	0
			8	5	1	2	
6	K	1	Total	C	N	O	0
			8	5	1	2	
6	N	1	Total	C	N	O	0
			8	5	1	2	
6	O	1	Total	C	N	O	0
			8	5	1	2	
6	R	1	Total	C	N	O	0
			8	5	1	2	
6	S	1	Total	C	N	O	0
			8	5	1	2	

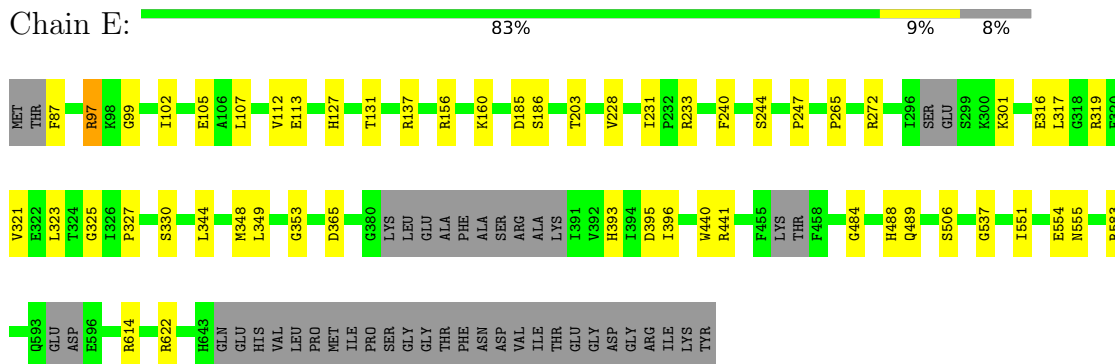
3 Residue-property plots [i](#)

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.

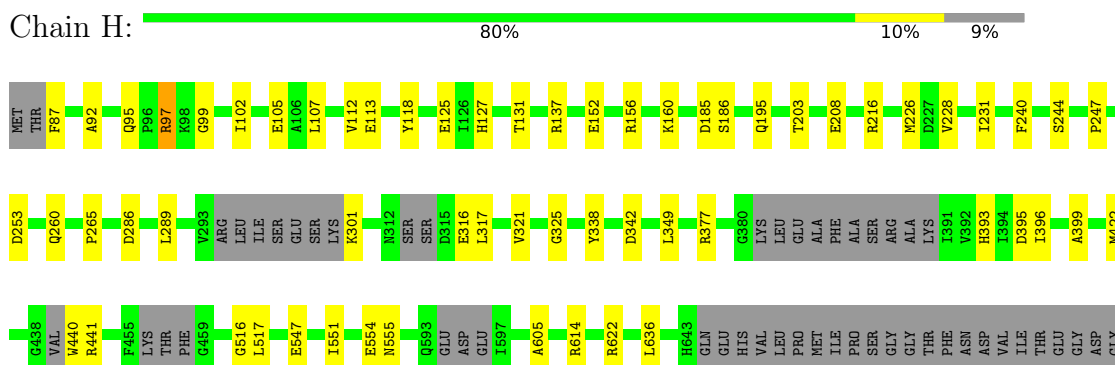
- Molecule 1: Acetolactate synthase, chloroplastic



- Molecule 1: Acetolactate synthase, chloroplastic

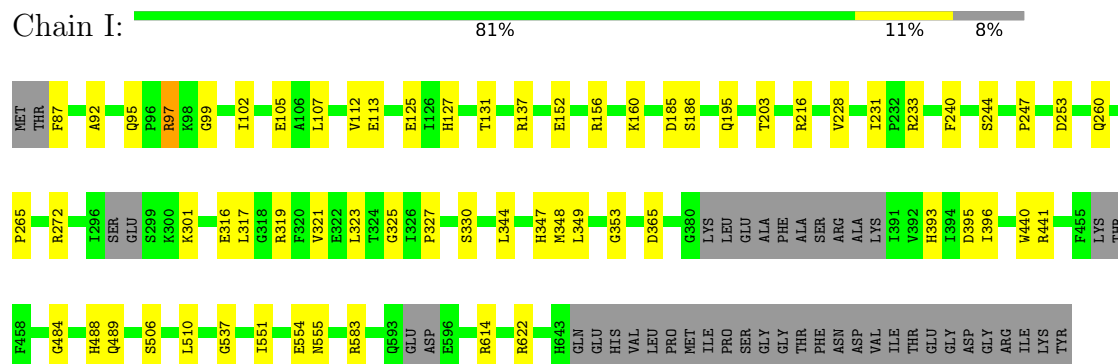


- Molecule 1: Acetolactate synthase, chloroplastic

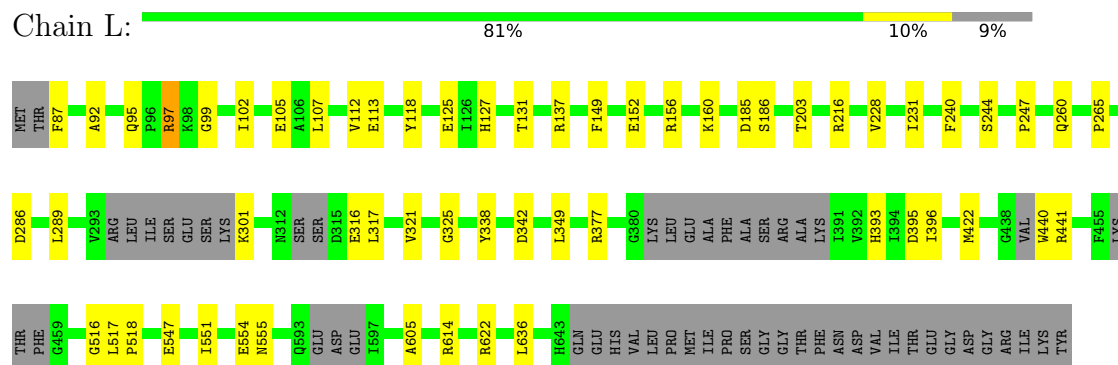


ARG
ILE
LYS
TYR

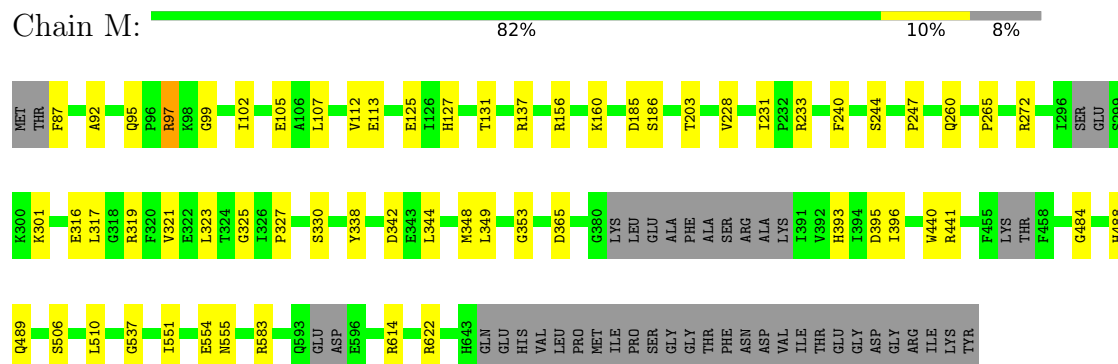
- Molecule 1: Acetolactate synthase, chloroplastic



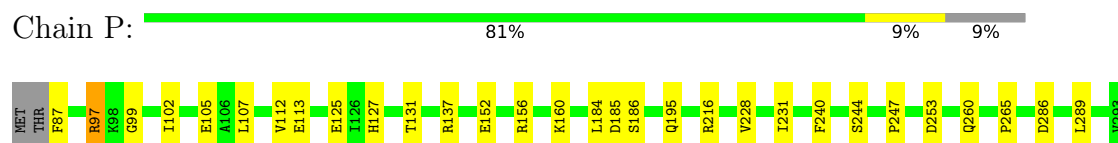
- Molecule 1: Acetolactate synthase, chloroplastic

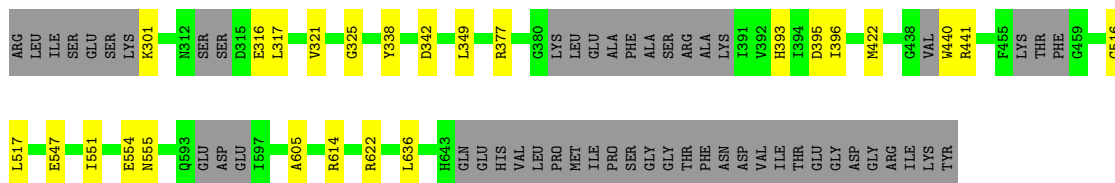


- Molecule 1: Acetolactate synthase, chloroplastic

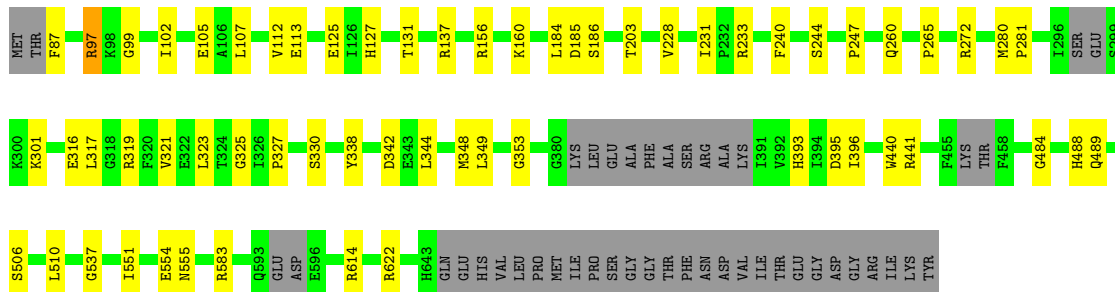
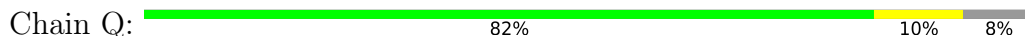


- Molecule 1: Acetolactate synthase, chloroplastic

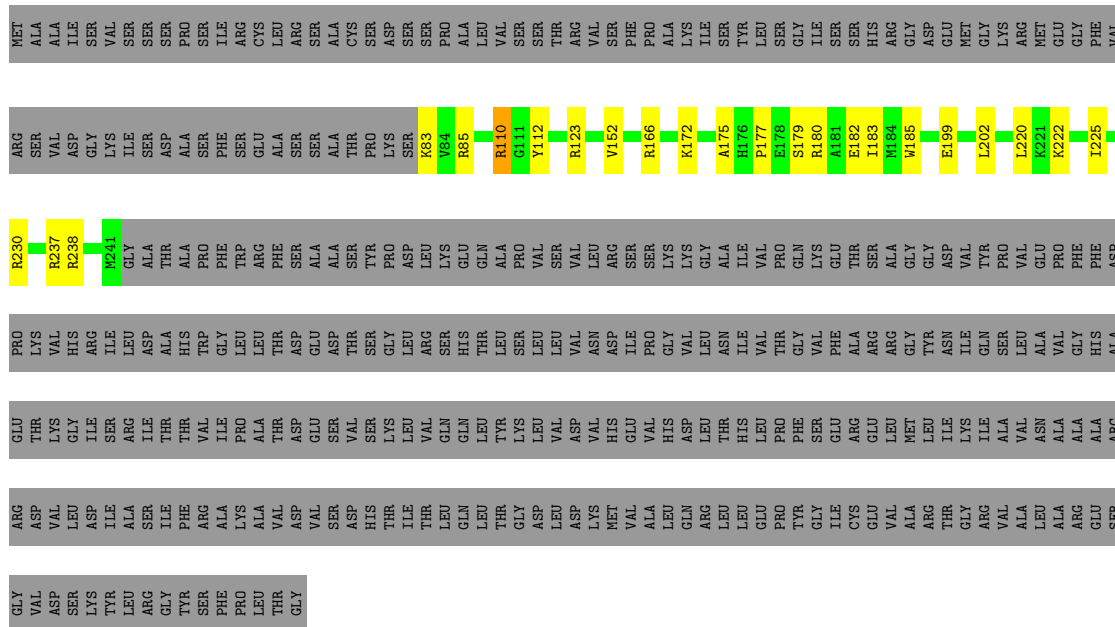




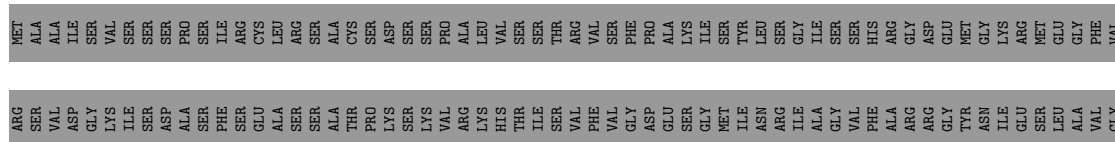
- Molecule 1: Acetolactate synthase, chloroplasic



- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic



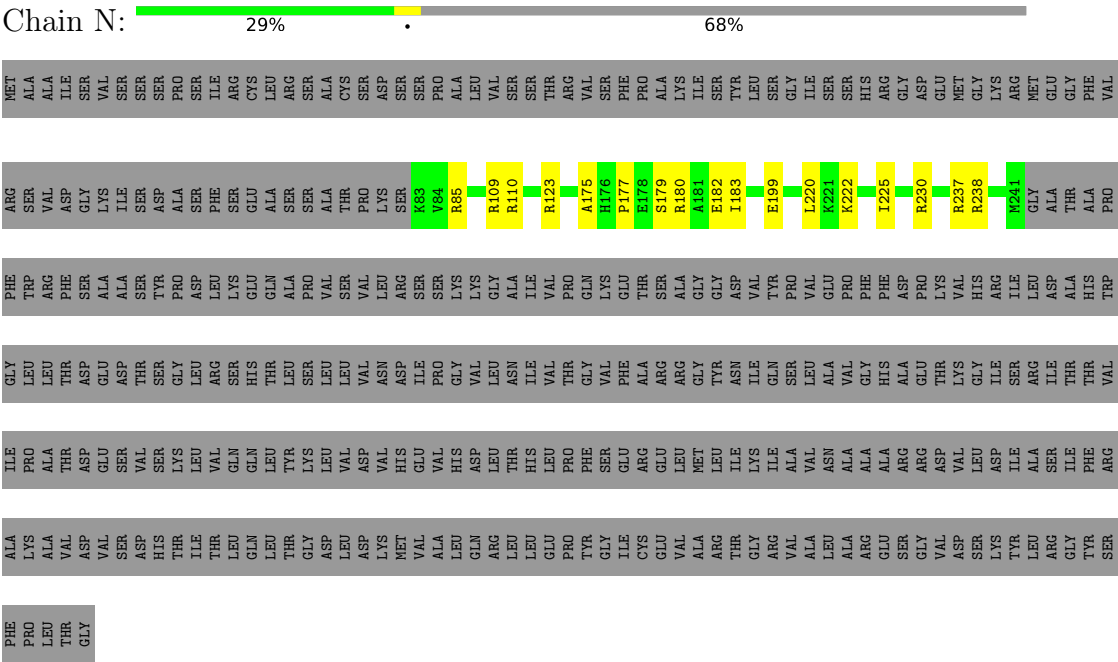
- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic



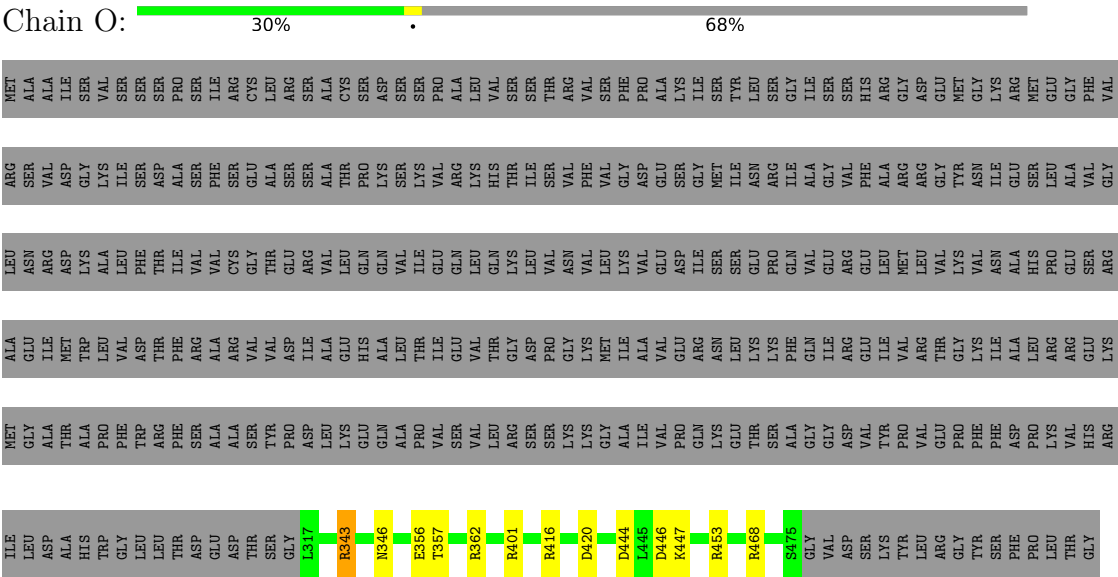




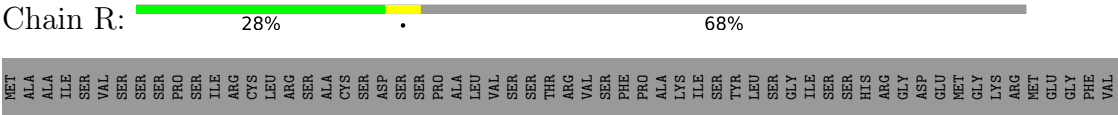
● Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

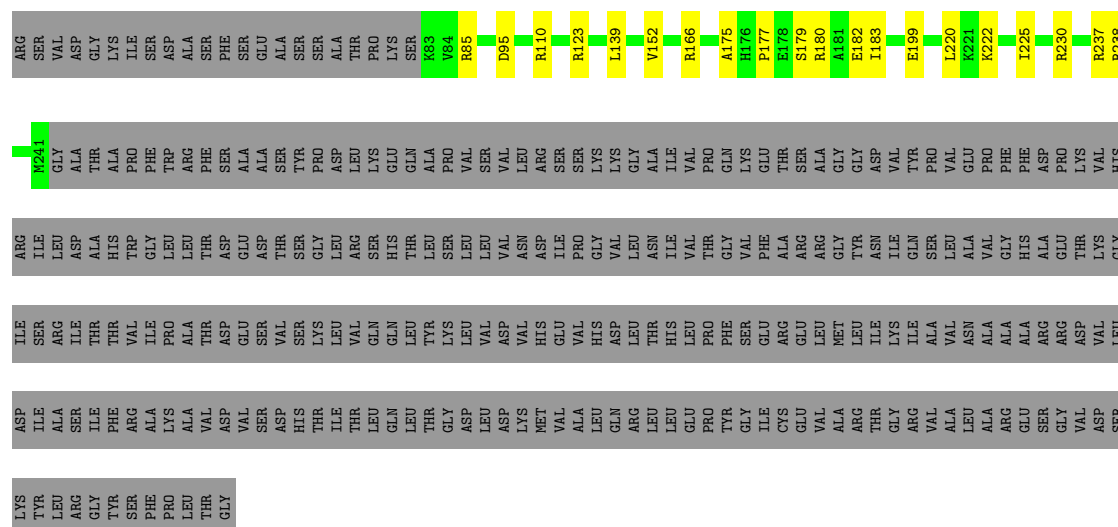


● Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

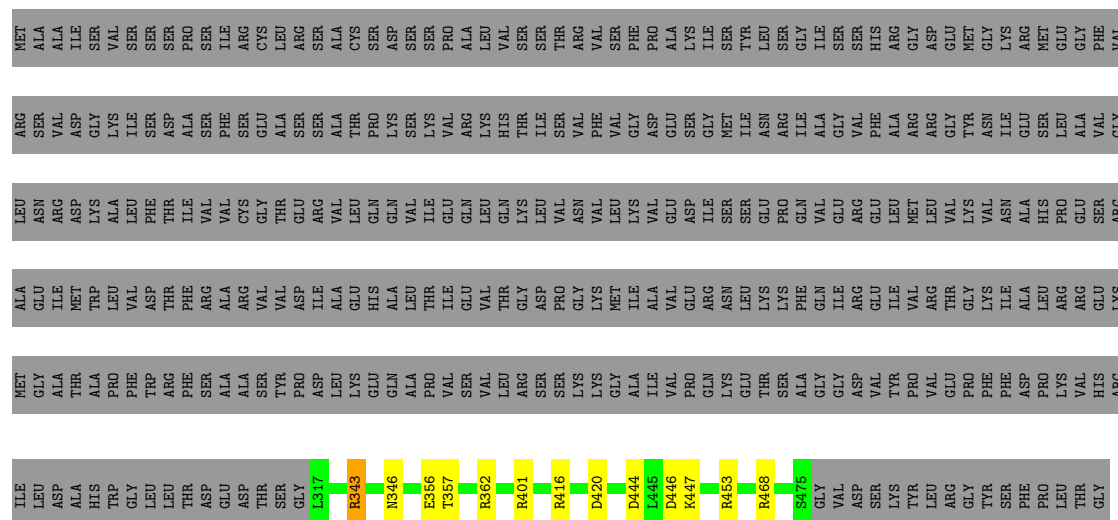


● Molecule 2: Acetolactate synthase small subunit 2, chloroplastic





- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic



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.

All (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
2	F	238	ARG	NE-CZ-NH2	7.81	124.20	120.30
2	J	237	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	N	237	ARG	NE-CZ-NH2	7.72	124.16	120.30
2	K	415	ARG	NE-CZ-NH2	7.71	124.16	120.30
2	J	238	ARG	NE-CZ-NH2	7.64	124.12	120.30
2	N	110	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	I	614	ARG	NE-CZ-NH1	7.05	123.83	120.30
2	R	238	ARG	NE-CZ-NH2	7.04	123.82	120.30
2	F	123	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	E	614	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	M	614	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	F	237	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	Q	614	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	N	238	ARG	NE-CZ-NH2	6.84	123.72	120.30
2	J	123	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	P	614	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	H	614	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	L	614	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	D	614	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	G	468	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	S	468	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	R	123	ARG	NE-CZ-NH1	6.05	123.32	120.30
2	K	468	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	S	453	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	O	468	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	F	166	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	R	110	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	O	343	ARG	NE-CZ-NH2	5.81	123.20	120.30
2	G	343	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	P	216	ARG	NE-CZ-NH2	5.79	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	343	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	Q	622	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	I	622	ARG	NE-CZ-NH1	5.69	123.14	120.30
2	J	85	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	E	622	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	N	123	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	O	453	ARG	NE-CZ-NH2	5.61	123.10	120.30
2	R	85	ARG	NE-CZ-NH2	5.60	123.10	120.30
2	O	362	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	M	622	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	P	622	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	K	453	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	L	622	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	G	362	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	S	362	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	622	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	N	85	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	N	109	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	I	216	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	M	583	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	R	166	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	L	216	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	I	583	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	J	166	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	K	362	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	H	622	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	P	377	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	Q	583	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	H	286	ASP	CB-CG-OD2	5.19	122.97	118.30
2	R	237	ARG	NE-CZ-NH1	-5.19	117.71	120.30
2	F	110	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	P	286	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	377	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	286	ASP	CB-CG-OD2	5.16	122.94	118.30
1	E	583	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	L	286	ASP	CB-CG-OD2	5.12	122.91	118.30
1	L	377	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	H	377	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	L	118	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	J	237	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	H	118	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (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
2	J	112	TYR	Sidechain
2	J	230	ARG	Sidechain
2	N	230	ARG	Sidechain
2	O	343	ARG	Sidechain
2	R	230	ARG	Sidechain
2	S	343	ARG	Sidechain

5.2 Too-close contacts [i](#)

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:H:113:GLU:OE1	1:H:160:LYS:NZ	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:GLU:OE1	1:D:160:LYS:NZ	2.20	0.74
1:I:113:GLU:OE1	1:I:160:LYS:NZ	2.20	0.74
1:M:113:GLU:OE1	1:M:160:LYS:NZ	2.20	0.73
2:G:356:GLU:HG3	2:G:357:THR:HG23	1.70	0.73
2:K:356:GLU:HG3	2:K:357:THR:HG23	1.70	0.73
2:O:416:ARG:NH1	2:O:420:ASP:OD1	2.23	0.72
2:S:356:GLU:HG3	2:S:357:THR:HG23	1.70	0.72
2:N:177:PRO:HA	2:N:180:ARG:HD2	1.72	0.71
2:O:356:GLU:HG3	2:O:357:THR:HG23	1.70	0.71
1:Q:156:ARG:NH2	1:Q:185:ASP:OD2	2.24	0.71
2:K:416:ARG:NH1	2:K:420:ASP:OD1	2.23	0.71
2:J:177:PRO:HA	2:J:180:ARG:HD2	1.72	0.70
2:R:177:PRO:HA	2:R:180:ARG:HD2	1.72	0.70
2:F:177:PRO:HA	2:F:180:ARG:HD2	1.72	0.69
1:M:156:ARG:NH2	1:M:185:ASP:OD2	2.24	0.69
1:D:156:ARG:NH2	1:D:185:ASP:OD2	2.24	0.69
2:S:416:ARG:NH1	2:S:420:ASP:OD1	2.23	0.69
1:I:156:ARG:NH2	1:I:185:ASP:OD2	2.24	0.68
2:G:416:ARG:NH1	2:G:420:ASP:OD1	2.23	0.68
1:H:156:ARG:NH2	1:H:185:ASP:OD2	2.24	0.68
1:E:156:ARG:NH2	1:E:185:ASP:OD2	2.24	0.68
2:N:180:ARG:NH2	2:N:199:GLU:O	2.27	0.67
2:R:180:ARG:NH2	2:R:199:GLU:O	2.27	0.67
2:F:180:ARG:NH2	2:F:199:GLU:O	2.27	0.66
2:J:180:ARG:NH2	2:J:199:GLU:O	2.27	0.66
1:P:156:ARG:NH2	1:P:185:ASP:OD2	2.24	0.65
2:F:175:ALA:O	2:F:180:ARG:NE	2.28	0.65
1:L:156:ARG:NH2	1:L:185:ASP:OD2	2.24	0.65
2:J:175:ALA:O	2:J:180:ARG:NE	2.28	0.64
6:R:501:VAL:N	2:S:346:ASN:OD1	2.31	0.63
2:N:175:ALA:O	2:N:180:ARG:NE	2.27	0.63
1:H:399:ALA:HA	2:K:379:GLN:NE2	2.14	0.63
6:F:501:VAL:N	2:G:346:ASN:OD1	2.32	0.62
2:R:175:ALA:O	2:R:180:ARG:NE	2.27	0.62
2:R:179:SER:HA	2:R:182:GLU:OE2	2.04	0.58
2:N:179:SER:HA	2:N:182:GLU:OE2	2.04	0.58
2:F:179:SER:HA	2:F:182:GLU:OE2	2.04	0.58
2:F:199:GLU:HG3	2:R:222:LYS:HE3	1.86	0.58
2:J:179:SER:HA	2:J:182:GLU:OE2	2.04	0.58
2:F:222:LYS:HE3	2:J:199:GLU:HG3	1.86	0.57
1:Q:327:PRO:HA	1:Q:344:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:PRO:HA	1:E:344:LEU:HB3	1.88	0.55
2:F:83:LYS:HE2	2:F:85:ARG:HD2	1.89	0.55
1:M:327:PRO:HA	1:M:344:LEU:HB3	1.88	0.55
1:M:87:PHE:CZ	1:M:105:GLU:HG3	2.42	0.55
1:Q:87:PHE:CZ	1:Q:105:GLU:HG3	2.42	0.55
1:L:87:PHE:CZ	1:L:105:GLU:HG3	2.42	0.54
1:E:87:PHE:CZ	1:E:105:GLU:HG3	2.42	0.54
1:I:327:PRO:HA	1:I:344:LEU:HB3	1.88	0.54
1:P:87:PHE:CZ	1:P:105:GLU:HG3	2.42	0.54
1:H:87:PHE:CZ	1:H:105:GLU:HG3	2.42	0.54
2:R:220:LEU:HB3	2:R:225:ILE:HD11	1.90	0.54
2:F:220:LEU:HB3	2:F:225:ILE:HD11	1.90	0.54
1:I:87:PHE:CZ	1:I:105:GLU:HG3	2.42	0.53
1:D:87:PHE:CZ	1:D:105:GLU:HG3	2.42	0.53
2:J:220:LEU:HB3	2:J:225:ILE:HD11	1.90	0.53
2:N:220:LEU:HB3	2:N:225:ILE:HD11	1.90	0.53
1:D:395:ASP:OD1	1:D:396:ILE:N	2.43	0.52
1:L:517:LEU:HD23	1:L:547:GLU:HB2	1.91	0.52
1:E:395:ASP:OD1	1:E:396:ILE:N	2.43	0.52
1:D:517:LEU:HD23	1:D:547:GLU:HB2	1.91	0.52
1:H:517:LEU:HD23	1:H:547:GLU:HB2	1.91	0.52
1:P:517:LEU:HD23	1:P:547:GLU:HB2	1.91	0.52
1:Q:395:ASP:OD1	1:Q:396:ILE:N	2.43	0.52
1:E:99:GLY:HA2	1:E:102:ILE:HD12	1.92	0.52
1:H:99:GLY:HA2	1:H:102:ILE:HD12	1.92	0.52
1:L:395:ASP:OD1	1:L:396:ILE:N	2.43	0.52
1:H:137:ARG:NH2	1:H:554:GLU:OE1	2.44	0.52
1:I:99:GLY:HA2	1:I:102:ILE:HD12	1.92	0.52
1:P:395:ASP:OD1	1:P:396:ILE:N	2.43	0.52
1:M:488:HIS:CE1	1:M:537:GLY:H	2.28	0.51
1:Q:137:ARG:NH2	1:Q:554:GLU:OE1	2.43	0.51
1:D:99:GLY:HA2	1:D:102:ILE:HD12	1.92	0.51
1:I:137:ARG:NH2	1:I:554:GLU:OE1	2.44	0.51
1:I:395:ASP:OD1	1:I:396:ILE:N	2.43	0.51
1:D:137:ARG:NH2	1:D:554:GLU:OE1	2.43	0.51
1:I:488:HIS:CE1	1:I:537:GLY:H	2.28	0.51
1:P:137:ARG:NH2	1:P:554:GLU:OE1	2.44	0.51
1:Q:99:GLY:HA2	1:Q:102:ILE:HD12	1.92	0.51
1:E:137:ARG:NH2	1:E:554:GLU:OE1	2.43	0.51
1:H:395:ASP:OD1	1:H:396:ILE:N	2.43	0.51
1:M:137:ARG:NH2	1:M:554:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:395:ASP:OD1	1:M:396:ILE:N	2.43	0.51
1:M:99:GLY:HA2	1:M:102:ILE:HD12	1.92	0.51
1:L:99:GLY:HA2	1:L:102:ILE:HD12	1.92	0.51
1:Q:488:HIS:CE1	1:Q:537:GLY:H	2.28	0.51
2:F:185:TRP:CH2	2:J:180:ARG:HD3	2.46	0.50
1:P:99:GLY:HA2	1:P:102:ILE:HD12	1.92	0.50
1:E:488:HIS:CE1	1:E:537:GLY:H	2.28	0.50
1:L:137:ARG:NH2	1:L:554:GLU:OE1	2.44	0.50
2:N:179:SER:HA	2:N:182:GLU:CD	2.32	0.50
1:E:316:GLU:OE1	1:E:316:GLU:N	2.45	0.49
1:E:330:SER:O	1:E:348:MET:HA	2.12	0.49
2:J:179:SER:HA	2:J:182:GLU:CD	2.32	0.49
2:R:179:SER:HA	2:R:182:GLU:CD	2.32	0.49
2:F:179:SER:HA	2:F:182:GLU:CD	2.32	0.49
1:H:338:TYR:OH	1:H:342:ASP:OD2	2.30	0.49
1:Q:330:SER:O	1:Q:348:MET:HA	2.12	0.49
2:N:177:PRO:O	2:N:180:ARG:HB2	2.13	0.49
2:R:177:PRO:O	2:R:180:ARG:HB2	2.13	0.49
1:I:330:SER:O	1:I:348:MET:HA	2.12	0.49
2:J:177:PRO:O	2:J:180:ARG:HB2	2.13	0.49
1:M:330:SER:O	1:M:348:MET:HA	2.12	0.49
2:S:446:ASP:OD2	2:S:447:LYS:N	2.46	0.48
2:F:177:PRO:O	2:F:180:ARG:HB2	2.13	0.48
2:G:446:ASP:OD2	2:G:447:LYS:N	2.46	0.48
1:Q:125:GLU:OE2	1:Q:260:GLN:NE2	2.30	0.48
1:Q:316:GLU:OE1	1:Q:316:GLU:N	2.45	0.48
1:D:125:GLU:OE2	1:D:260:GLN:NE2	2.30	0.48
1:D:316:GLU:OE1	1:D:316:GLU:N	2.45	0.48
1:I:125:GLU:OE2	1:I:260:GLN:NE2	2.31	0.48
1:L:338:TYR:OH	1:L:342:ASP:OD2	2.30	0.47
2:K:446:ASP:OD2	2:K:447:LYS:N	2.46	0.47
1:I:316:GLU:OE1	1:I:316:GLU:N	2.45	0.47
1:P:316:GLU:N	1:P:316:GLU:OE1	2.45	0.47
2:J:95:ASP:OD1	6:J:501:VAL:N	2.46	0.47
1:L:316:GLU:OE1	1:L:316:GLU:N	2.45	0.47
1:M:316:GLU:OE1	1:M:316:GLU:N	2.45	0.47
1:D:338:TYR:OH	1:D:342:ASP:OD2	2.30	0.47
1:M:125:GLU:OE2	1:M:260:GLN:NE2	2.30	0.47
2:G:416:ARG:HH21	2:G:416:ARG:HA	1.81	0.46
2:N:222:LYS:HE3	2:R:199:GLU:HG3	1.98	0.46
1:P:289:LEU:HD22	1:P:422:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:338:TYR:OH	1:P:342:ASP:OD2	2.30	0.46
1:H:289:LEU:HD22	1:H:422:MET:HG3	1.97	0.46
2:S:416:ARG:HH21	2:S:416:ARG:HA	1.81	0.46
2:J:220:LEU:HD23	2:J:220:LEU:HA	1.75	0.46
1:P:228:VAL:HG23	1:P:231:ILE:HD12	1.98	0.46
1:E:228:VAL:HG23	1:E:231:ILE:HD12	1.98	0.45
2:O:416:ARG:HA	2:O:416:ARG:HH21	1.81	0.45
1:Q:228:VAL:HG23	1:Q:231:ILE:HD12	1.99	0.45
1:I:228:VAL:HG23	1:I:231:ILE:HD12	1.99	0.45
2:O:446:ASP:OD2	2:O:447:LYS:N	2.47	0.45
1:Q:489:GLN:NE2	1:Q:506:SER:OG	2.43	0.45
1:D:127:HIS:O	1:D:131:THR:HG23	2.17	0.45
1:D:228:VAL:HG23	1:D:231:ILE:HD12	1.99	0.45
1:E:127:HIS:O	1:E:131:THR:HG23	2.17	0.45
1:I:127:HIS:O	1:I:131:THR:HG23	2.17	0.45
1:P:127:HIS:O	1:P:131:THR:HG23	2.17	0.45
1:D:289:LEU:HD22	1:D:422:MET:HG3	1.97	0.45
1:I:489:GLN:NE2	1:I:506:SER:OG	2.43	0.45
1:L:289:LEU:HD22	1:L:422:MET:HG3	1.97	0.45
1:L:127:HIS:O	1:L:131:THR:HG23	2.17	0.45
1:M:228:VAL:HG23	1:M:231:ILE:HD12	1.98	0.45
1:H:228:VAL:HG23	1:H:231:ILE:HD12	1.99	0.45
1:H:107:LEU:HB3	1:H:112:VAL:HG21	1.99	0.45
1:H:127:HIS:O	1:H:131:THR:HG23	2.17	0.45
1:Q:127:HIS:O	1:Q:131:THR:HG23	2.17	0.45
2:K:416:ARG:HA	2:K:416:ARG:HH21	1.81	0.44
1:L:107:LEU:HB3	1:L:112:VAL:HG21	1.99	0.44
1:E:107:LEU:HB3	1:E:112:VAL:HG21	1.99	0.44
1:H:125:GLU:OE2	1:H:260:GLN:NE2	2.30	0.44
1:M:107:LEU:HB3	1:M:112:VAL:HG21	1.99	0.44
1:M:489:GLN:NE2	1:M:506:SER:OG	2.43	0.44
1:L:228:VAL:HG23	1:L:231:ILE:HD12	1.98	0.44
1:M:127:HIS:O	1:M:131:THR:HG23	2.17	0.44
1:E:349:LEU:C	1:E:353:GLY:HA3	2.38	0.44
2:F:220:LEU:HD23	2:F:220:LEU:HA	1.75	0.44
1:H:316:GLU:OE1	1:H:316:GLU:N	2.45	0.44
1:Q:349:LEU:C	1:Q:353:GLY:HA3	2.38	0.44
1:M:349:LEU:C	1:M:353:GLY:HA3	2.38	0.44
1:M:338:TYR:OH	1:M:342:ASP:OD2	2.30	0.43
1:I:107:LEU:HB3	1:I:112:VAL:HG21	1.99	0.43
1:Q:107:LEU:HB3	1:Q:112:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:SER:O	1:H:247:PRO:HG2	2.19	0.43
1:I:349:LEU:C	1:I:353:GLY:HA3	2.38	0.43
1:P:107:LEU:HB3	1:P:112:VAL:HG21	1.99	0.43
1:D:107:LEU:HB3	1:D:112:VAL:HG21	1.99	0.43
2:F:179:SER:O	2:F:183:ILE:HG12	2.19	0.43
1:H:152:GLU:OE1	1:H:156:ARG:NE	2.44	0.43
1:P:317:LEU:O	1:P:321:VAL:HG23	2.19	0.43
1:Q:338:TYR:OH	1:Q:342:ASP:OD2	2.30	0.43
2:R:179:SER:O	2:R:183:ILE:HG12	2.19	0.43
1:Q:280:MET:HA	1:Q:281:PRO:HD3	1.94	0.43
1:E:393:HIS:CE1	1:E:395:ASP:HB2	2.54	0.43
1:H:399:ALA:HA	2:K:379:GLN:HE21	1.84	0.43
1:L:152:GLU:OE1	1:L:156:ARG:NE	2.44	0.43
1:M:186:SER:O	1:M:247:PRO:HG2	2.19	0.43
1:M:317:LEU:O	1:M:321:VAL:HG23	2.19	0.43
1:P:393:HIS:CE1	1:P:395:ASP:HB2	2.54	0.43
1:Q:186:SER:O	1:Q:247:PRO:HG2	2.19	0.43
1:H:393:HIS:CE1	1:H:395:ASP:HB2	2.54	0.43
1:L:605:ALA:HB2	1:L:636:LEU:HD23	2.01	0.43
1:Q:317:LEU:O	1:Q:321:VAL:HG23	2.19	0.43
1:E:186:SER:O	1:E:247:PRO:HG2	2.19	0.43
1:H:317:LEU:O	1:H:321:VAL:HG23	2.19	0.43
1:H:605:ALA:HB2	1:H:636:LEU:HD23	2.01	0.43
1:L:317:LEU:O	1:L:321:VAL:HG23	2.19	0.43
1:M:393:HIS:CE1	1:M:395:ASP:HB2	2.54	0.43
1:Q:393:HIS:CE1	1:Q:395:ASP:HB2	2.54	0.43
1:I:240:PHE:CE1	1:I:244:SER:HB3	2.54	0.43
1:P:186:SER:O	1:P:247:PRO:HG2	2.19	0.43
1:L:393:HIS:CE1	1:L:395:ASP:HB2	2.54	0.42
1:L:97:ARG:NH1	1:L:265:PRO:HG3	2.35	0.42
1:L:301:LYS:HA	1:L:440:TRP:CD1	2.55	0.42
2:N:179:SER:O	2:N:183:ILE:HG12	2.19	0.42
1:P:97:ARG:NH1	1:P:265:PRO:HG3	2.34	0.42
1:D:399:ALA:HA	2:G:379:GLN:NE2	2.34	0.42
2:J:179:SER:O	2:J:183:ILE:HG12	2.19	0.42
1:L:186:SER:O	1:L:247:PRO:HG2	2.19	0.42
1:M:240:PHE:CE1	1:M:244:SER:HB3	2.54	0.42
1:P:301:LYS:HA	1:P:440:TRP:CD1	2.55	0.42
1:E:240:PHE:CE1	1:E:244:SER:HB3	2.54	0.42
1:E:317:LEU:O	1:E:321:VAL:HG23	2.19	0.42
1:H:97:ARG:NH1	1:H:265:PRO:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:301:LYS:HA	1:I:440:TRP:CD1	2.54	0.42
1:I:317:LEU:O	1:I:321:VAL:HG23	2.19	0.42
1:L:240:PHE:CE1	1:L:244:SER:HB3	2.54	0.42
1:D:186:SER:O	1:D:247:PRO:HG2	2.19	0.42
1:E:325:GLY:O	1:E:441:ARG:HD3	2.20	0.42
1:I:186:SER:O	1:I:247:PRO:HG2	2.19	0.42
1:Q:240:PHE:CE1	1:Q:244:SER:HB3	2.54	0.42
1:I:97:ARG:NH1	1:I:265:PRO:HG3	2.35	0.42
1:Q:97:ARG:NH1	1:Q:265:PRO:HG3	2.35	0.42
1:Q:325:GLY:O	1:Q:441:ARG:HD3	2.20	0.42
1:H:325:GLY:O	1:H:441:ARG:HD3	2.20	0.42
1:I:152:GLU:OE1	1:I:156:ARG:NE	2.44	0.42
1:L:325:GLY:O	1:L:441:ARG:HD3	2.20	0.42
1:P:240:PHE:CE1	1:P:244:SER:HB3	2.54	0.42
1:Q:301:LYS:HA	1:Q:440:TRP:CD1	2.54	0.42
1:D:301:LYS:HA	1:D:440:TRP:CD1	2.55	0.42
1:D:317:LEU:O	1:D:321:VAL:HG23	2.19	0.42
1:E:551:ILE:O	1:E:555:ASN:N	2.53	0.42
1:H:301:LYS:HA	1:H:440:TRP:CD1	2.54	0.42
1:M:301:LYS:HA	1:M:440:TRP:CD1	2.54	0.42
1:P:605:ALA:HB2	1:P:636:LEU:HD23	2.01	0.42
1:D:97:ARG:NH1	1:D:265:PRO:HG3	2.34	0.42
1:D:393:HIS:CE1	1:D:395:ASP:HB2	2.54	0.42
1:I:325:GLY:O	1:I:441:ARG:HD3	2.20	0.42
1:I:393:HIS:CE1	1:I:395:ASP:HB2	2.54	0.42
1:D:605:ALA:HB2	1:D:636:LEU:HD23	2.01	0.42
1:H:349:LEU:HD23	1:H:349:LEU:H	1.85	0.42
1:P:325:GLY:O	1:P:441:ARG:HD3	2.20	0.42
1:I:551:ILE:O	1:I:555:ASN:N	2.53	0.41
1:D:240:PHE:CE1	1:D:244:SER:HB3	2.54	0.41
1:E:301:LYS:HA	1:E:440:TRP:CD1	2.54	0.41
1:D:325:GLY:O	1:D:441:ARG:HD3	2.20	0.41
2:S:416:ARG:HA	2:S:416:ARG:NH2	2.36	0.41
1:L:551:ILE:O	1:L:555:ASN:N	2.53	0.41
1:M:97:ARG:NH1	1:M:265:PRO:HG3	2.34	0.41
1:M:325:GLY:O	1:M:441:ARG:HD3	2.20	0.41
2:O:416:ARG:HA	2:O:416:ARG:NH2	2.36	0.41
1:Q:319:ARG:NH2	1:Q:323:LEU:HG	2.35	0.41
1:H:240:PHE:CE1	1:H:244:SER:HB3	2.54	0.41
1:H:551:ILE:O	1:H:555:ASN:N	2.53	0.41
1:L:349:LEU:HD23	1:L:349:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:510:LEU:HD12	1:M:510:LEU:HA	1.86	0.41
1:M:551:ILE:O	1:M:555:ASN:N	2.53	0.41
1:Q:184:LEU:HD23	1:Q:184:LEU:HA	1.87	0.41
1:D:349:LEU:H	1:D:349:LEU:HD23	1.86	0.41
1:D:551:ILE:O	1:D:555:ASN:N	2.53	0.41
1:Q:551:ILE:O	1:Q:555:ASN:N	2.53	0.41
2:R:95:ASP:OD1	6:R:501:VAL:N	2.53	0.41
1:E:319:ARG:NH2	1:E:323:LEU:HG	2.35	0.41
1:Q:510:LEU:HD12	1:Q:510:LEU:HA	1.86	0.41
1:M:233:ARG:NH2	1:M:272:ARG:HD2	2.35	0.41
1:M:301:LYS:H	1:M:365:ASP:CG	2.24	0.41
1:M:319:ARG:NH2	1:M:323:LEU:HG	2.35	0.41
1:P:551:ILE:O	1:P:555:ASN:N	2.53	0.41
1:E:97:ARG:NH1	1:E:265:PRO:HG3	2.35	0.41
1:E:233:ARG:NH2	1:E:272:ARG:HD2	2.36	0.41
1:I:319:ARG:NH2	1:I:323:LEU:HG	2.35	0.41
2:K:416:ARG:HA	2:K:416:ARG:NH2	2.36	0.41
1:L:125:GLU:OE2	1:L:260:GLN:NE2	2.30	0.41
1:M:321:VAL:O	1:M:325:GLY:N	2.38	0.41
2:O:401:ARG:NE	2:O:401:ARG:HA	2.36	0.41
1:P:195:GLN:NE2	1:P:253:ASP:OD1	2.52	0.41
2:S:401:ARG:NE	2:S:401:ARG:HA	2.36	0.41
1:E:349:LEU:HD23	1:E:349:LEU:H	1.86	0.41
2:G:401:ARG:NE	2:G:401:ARG:HA	2.36	0.41
1:I:195:GLN:NE2	1:I:253:ASP:OD1	2.52	0.41
1:I:233:ARG:NH2	1:I:272:ARG:HD2	2.36	0.41
1:P:152:GLU:OE1	1:P:156:ARG:NE	2.44	0.41
1:E:489:GLN:NE2	1:E:506:SER:OG	2.43	0.40
1:I:92:ALA:HB3	1:I:95:GLN:HB2	2.04	0.40
1:I:347:HIS:HB3	1:I:348:MET:H	1.80	0.40
1:I:510:LEU:HA	1:I:510:LEU:HD12	1.86	0.40
2:J:172:LYS:HA	2:J:202:LEU:O	2.22	0.40
1:P:125:GLU:OE2	1:P:260:GLN:NE2	2.30	0.40
1:P:349:LEU:H	1:P:349:LEU:HD23	1.85	0.40
1:H:92:ALA:HB3	1:H:95:GLN:HB2	2.04	0.40
1:I:349:LEU:HD23	1:I:349:LEU:H	1.86	0.40
1:L:149:PHE:CB	1:L:518:PRO:HB2	2.51	0.40
2:F:172:LYS:HA	2:F:202:LEU:O	2.21	0.40
2:G:416:ARG:HA	2:G:416:ARG:NH2	2.36	0.40
1:L:92:ALA:HB3	1:L:95:GLN:HB2	2.04	0.40
1:M:92:ALA:HB3	1:M:95:GLN:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:184:LEU:HD23	1:P:184:LEU:HA	1.87	0.40
1:D:149:PHE:CB	1:D:518:PRO:HB2	2.51	0.40
1:I:301:LYS:H	1:I:365:ASP:CG	2.24	0.40
1:E:301:LYS:H	1:E:365:ASP:CG	2.24	0.40
1:H:195:GLN:NE2	1:H:253:ASP:OD1	2.52	0.40
1:Q:233:ARG:NH2	1:Q:272:ARG:HD2	2.36	0.40

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
2	R	157/491 (32%)	154 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	E	484	GLY
1	I	484	GLY
1	M	484	GLY
1	Q	484	GLY

5.3.2 Protein sidechains [i](#)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	97	ARG
1	D	203	THR
1	E	97	ARG
1	E	203	THR
2	F	152	VAL
2	G	444	ASP
1	H	97	ARG
1	H	203	THR
1	H	208	GLU
1	H	226	MET
1	I	97	ARG
1	I	203	THR
2	K	444	ASP
1	L	97	ARG
1	L	203	THR
1	M	97	ARG
1	M	203	THR
2	O	444	ASP
1	P	97	ARG
1	Q	97	ARG
1	Q	203	THR
2	R	139	LEU
2	R	152	VAL
2	S	444	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	393	HIS

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Mol	Chain	Res	Type
1	D	582	ASN
1	E	128	GLN
1	E	393	HIS
1	H	393	HIS
1	L	393	HIS
1	M	393	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
5	H	703	TPP	C6-C5	3.09	1.52	1.50
4	E	702	FAD	C5'-C4'	3.08	1.56	1.51
4	Q	702	FAD	C5'-C4'	3.07	1.56	1.51
4	I	702	FAD	C5'-C4'	3.02	1.56	1.51
5	L	703	TPP	C6-C5	2.99	1.52	1.50
4	M	702	FAD	C5'-C4'	2.99	1.56	1.51
5	P	703	TPP	C6-C5	2.95	1.52	1.50
5	L	703	TPP	C5'-C4'	-2.79	1.38	1.42
5	P	703	TPP	C5'-C4'	-2.77	1.38	1.42
5	D	703	TPP	C5'-C4'	-2.75	1.38	1.42
5	H	703	TPP	C5'-C4'	-2.71	1.38	1.42
6	G	501	VAL	CA-N	2.55	1.55	1.47
5	E	703	TPP	C5'-C4'	-2.52	1.38	1.42
6	G	501	VAL	OXT-C	-2.51	1.22	1.30
6	O	501	VAL	CA-N	2.50	1.54	1.47
5	I	703	TPP	C5'-C4'	-2.49	1.38	1.42
6	O	501	VAL	OXT-C	-2.49	1.22	1.30
4	I	702	FAD	C1'-C2'	2.49	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	703	TPP	C5'-C4'	-2.48	1.38	1.42
6	S	501	VAL	OXT-C	-2.47	1.22	1.30
6	K	501	VAL	OXT-C	-2.47	1.22	1.30
6	R	501	VAL	OXT-C	-2.47	1.22	1.30
4	E	702	FAD	C1'-C2'	2.46	1.56	1.52
4	M	702	FAD	C1'-C2'	2.45	1.56	1.52
6	S	501	VAL	CA-N	2.45	1.54	1.47
5	Q	703	TPP	C5'-C4'	-2.45	1.38	1.42
4	L	702	FAD	C5'-C4'	2.44	1.55	1.51
4	P	702	FAD	C5'-C4'	2.44	1.55	1.51
5	I	703	TPP	C4'-N3'	-2.43	1.31	1.35
5	Q	703	TPP	C4'-N3'	-2.42	1.31	1.35
6	K	501	VAL	CA-N	2.42	1.54	1.47
6	J	501	VAL	OXT-C	-2.41	1.22	1.30
4	Q	702	FAD	C1'-C2'	2.41	1.56	1.52
6	N	501	VAL	OXT-C	-2.41	1.22	1.30
4	H	702	FAD	C5'-C4'	2.39	1.55	1.51
5	E	703	TPP	C4'-N3'	-2.38	1.31	1.35
6	F	501	VAL	OXT-C	-2.37	1.22	1.30
4	D	702	FAD	C5'-C4'	2.37	1.55	1.51
5	P	703	TPP	C4'-N3'	-2.37	1.31	1.35
5	H	703	TPP	C4'-N3'	-2.37	1.31	1.35
4	M	702	FAD	O4B-C1B	2.37	1.44	1.41
5	M	703	TPP	C4'-N3'	-2.36	1.31	1.35
4	Q	702	FAD	O4B-C1B	2.34	1.44	1.41
4	E	702	FAD	O4B-C1B	2.32	1.44	1.41
4	I	702	FAD	O4B-C1B	2.32	1.44	1.41
5	L	703	TPP	C4'-N3'	-2.32	1.31	1.35
5	D	703	TPP	C4'-N3'	-2.32	1.31	1.35
6	R	501	VAL	CA-N	2.12	1.53	1.47
6	J	501	VAL	CA-N	2.12	1.53	1.47
6	N	501	VAL	CA-N	2.11	1.53	1.47
4	H	702	FAD	C4X-N5	2.08	1.34	1.30
4	L	702	FAD	C4X-N5	2.05	1.34	1.30
4	P	702	FAD	C4X-N5	2.04	1.34	1.30
4	P	702	FAD	C5A-C4A	-2.04	1.35	1.40
4	D	702	FAD	C4X-N5	2.03	1.34	1.30
4	H	702	FAD	C5A-C4A	-2.02	1.35	1.40
4	M	702	FAD	C4X-N5	2.01	1.34	1.30

All (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
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
4	M	702	FAD	C4X-C10-N10	6.43	125.89	116.48
4	E	702	FAD	C4X-C10-N10	6.42	125.88	116.48
4	I	702	FAD	C4X-C10-N10	6.39	125.83	116.48
4	M	702	FAD	C9A-N10-C10	-6.10	111.26	120.77
4	Q	702	FAD	C9A-N10-C10	-6.09	111.28	120.77
4	E	702	FAD	C9A-N10-C10	-6.09	111.29	120.77
4	I	702	FAD	C9A-N10-C10	-6.06	111.33	120.77
5	L	703	TPP	C6-C5-C4	-5.89	122.71	127.43
5	D	703	TPP	C6-C5-C4	-5.88	122.71	127.43
5	H	703	TPP	C6-C5-C4	-5.85	122.74	127.43
5	P	703	TPP	C6-C5-C4	-5.83	122.75	127.43
4	L	702	FAD	C9A-N10-C10	-5.82	111.70	120.77
4	P	702	FAD	C9A-N10-C10	-5.80	111.73	120.77
4	H	702	FAD	C9A-N10-C10	-5.80	111.74	120.77
4	D	702	FAD	C9A-N10-C10	-5.77	111.78	120.77
5	E	703	TPP	C6-C5-C4	-4.76	123.61	127.43
5	Q	703	TPP	C6-C5-C4	-4.75	123.62	127.43
5	M	703	TPP	C6-C5-C4	-4.74	123.62	127.43
5	I	703	TPP	C6-C5-C4	-4.71	123.65	127.43
4	H	702	FAD	C4A-C5A-N7A	4.51	114.10	109.40
4	D	702	FAD	C4A-C5A-N7A	4.50	114.09	109.40
4	P	702	FAD	C4A-C5A-N7A	4.45	114.04	109.40
4	L	702	FAD	C4A-C5A-N7A	4.40	113.98	109.40
4	H	702	FAD	P-O3P-PA	-4.24	118.26	132.83
4	P	702	FAD	P-O3P-PA	-4.24	118.29	132.83
4	D	702	FAD	P-O3P-PA	-4.24	118.29	132.83
5	P	703	TPP	CM4-C4-N3	4.23	127.92	122.53
4	L	702	FAD	P-O3P-PA	-4.21	118.37	132.83
5	D	703	TPP	CM4-C4-N3	4.18	127.86	122.53
4	Q	702	FAD	C4A-C5A-N7A	4.18	113.75	109.40
5	H	703	TPP	CM4-C4-N3	4.15	127.83	122.53
4	M	702	FAD	C4A-C5A-N7A	4.15	113.72	109.40
5	L	703	TPP	CM4-C4-N3	4.15	127.82	122.53
4	E	702	FAD	C4A-C5A-N7A	4.12	113.69	109.40
4	I	702	FAD	C4A-C5A-N7A	4.10	113.67	109.40
4	D	702	FAD	C10-N1-C2	4.08	125.06	116.90
4	H	702	FAD	C10-N1-C2	4.07	125.04	116.90
4	P	702	FAD	C10-N1-C2	4.06	125.02	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	702	FAD	C10-N1-C2	4.02	124.95	116.90
5	H	703	TPP	PA-O3A-PB	-4.00	119.10	132.83
5	L	703	TPP	PA-O3A-PB	-3.99	119.15	132.83
5	D	703	TPP	PA-O3A-PB	-3.98	119.16	132.83
5	P	703	TPP	PA-O3A-PB	-3.98	119.16	132.83
4	M	702	FAD	P-O3P-PA	-3.86	119.59	132.83
4	E	702	FAD	P-O3P-PA	-3.84	119.65	132.83
4	Q	702	FAD	P-O3P-PA	-3.84	119.65	132.83
4	I	702	FAD	P-O3P-PA	-3.84	119.66	132.83
4	M	702	FAD	C10-N1-C2	3.73	124.36	116.90
4	I	702	FAD	C10-N1-C2	3.73	124.36	116.90
4	Q	702	FAD	C10-N1-C2	3.71	124.31	116.90
4	E	702	FAD	C10-N1-C2	3.69	124.28	116.90
5	Q	703	TPP	CM4-C4-N3	3.56	127.08	122.53
5	E	703	TPP	CM4-C4-N3	3.55	127.06	122.53
5	H	703	TPP	O2B-PB-O3A	3.51	116.40	104.64
5	L	703	TPP	O2B-PB-O3A	3.51	116.40	104.64
5	I	703	TPP	CM4-C4-N3	3.51	127.00	122.53
5	P	703	TPP	O2B-PB-O3A	3.50	116.39	104.64
5	D	703	TPP	O2B-PB-O3A	3.50	116.38	104.64
5	M	703	TPP	CM4-C4-N3	3.49	126.99	122.53
5	M	703	TPP	C7'-N3-C2	-3.41	119.18	125.35
5	Q	703	TPP	C7'-N3-C2	-3.37	119.25	125.35
5	I	703	TPP	C7'-N3-C2	-3.36	119.28	125.35
5	E	703	TPP	C7'-N3-C2	-3.36	119.29	125.35
5	D	703	TPP	C7'-N3-C2	-3.22	119.53	125.35
5	H	703	TPP	C7'-N3-C2	-3.20	119.56	125.35
5	P	703	TPP	C7'-N3-C2	-3.20	119.58	125.35
5	L	703	TPP	C7'-N3-C2	-3.18	119.60	125.35
4	H	702	FAD	C10-C4X-N5	-3.11	118.26	124.86
4	L	702	FAD	C10-C4X-N5	-3.10	118.28	124.86
4	D	702	FAD	C10-C4X-N5	-3.08	118.31	124.86
4	L	702	FAD	O4B-C1B-C2B	-3.08	102.43	106.93
4	P	702	FAD	C10-C4X-N5	-3.05	118.39	124.86
4	P	702	FAD	O4B-C1B-C2B	-3.04	102.49	106.93
4	L	702	FAD	C4-C4X-N5	3.04	122.55	118.23
4	M	702	FAD	C10-C4X-N5	-3.03	118.43	124.86
4	E	702	FAD	O4B-C1B-C2B	-3.03	102.50	106.93
4	D	702	FAD	O4B-C1B-C2B	-3.02	102.51	106.93
4	I	702	FAD	O4B-C1B-C2B	-3.02	102.51	106.93
4	Q	702	FAD	O4B-C1B-C2B	-3.02	102.51	106.93
4	M	702	FAD	O4B-C1B-C2B	-3.02	102.51	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	702	FAD	O4B-C1B-C2B	-3.02	102.52	106.93
4	D	702	FAD	C4-C4X-N5	3.01	122.52	118.23
4	H	702	FAD	C4-C4X-N5	3.01	122.52	118.23
4	D	702	FAD	C4X-C10-N1	-3.01	117.74	124.73
4	I	702	FAD	C10-C4X-N5	-3.01	118.47	124.86
4	E	702	FAD	C10-C4X-N5	-3.01	118.47	124.86
4	Q	702	FAD	C10-C4X-N5	-3.01	118.48	124.86
4	H	702	FAD	C4X-C10-N1	-3.00	117.76	124.73
4	P	702	FAD	C4X-C10-N1	-2.99	117.78	124.73
4	L	702	FAD	C4X-C10-N1	-2.98	117.82	124.73
4	M	702	FAD	C1'-N10-C9A	2.94	125.42	120.51
4	P	702	FAD	C4-C4X-N5	2.94	122.41	118.23
4	I	702	FAD	C1'-N10-C9A	2.94	125.41	120.51
4	Q	702	FAD	C1'-N10-C9A	2.93	125.40	120.51
4	E	702	FAD	C1'-N10-C9A	2.91	125.37	120.51
5	D	703	TPP	N4'-C4'-N3'	-2.85	113.00	117.03
4	M	702	FAD	C4X-C10-N1	-2.85	118.11	124.73
5	E	703	TPP	N4'-C4'-N3'	-2.85	113.00	117.03
4	I	702	FAD	C4X-C10-N1	-2.84	118.14	124.73
5	I	703	TPP	N4'-C4'-N3'	-2.83	113.03	117.03
5	P	703	TPP	N4'-C4'-N3'	-2.83	113.03	117.03
4	Q	702	FAD	C4X-C10-N1	-2.83	118.17	124.73
5	L	703	TPP	N4'-C4'-N3'	-2.82	113.05	117.03
4	E	702	FAD	C4X-C10-N1	-2.82	118.19	124.73
5	M	703	TPP	N4'-C4'-N3'	-2.81	113.06	117.03
4	M	702	FAD	C4-C4X-N5	2.80	122.22	118.23
5	H	703	TPP	N4'-C4'-N3'	-2.80	113.08	117.03
5	Q	703	TPP	N4'-C4'-N3'	-2.79	113.09	117.03
4	I	702	FAD	C4-C4X-N5	2.78	122.19	118.23
4	E	702	FAD	C4-C4X-N5	2.78	122.19	118.23
4	Q	702	FAD	C4-C4X-N5	2.78	122.18	118.23
5	I	703	TPP	PA-O3A-PB	-2.73	123.46	132.83
5	E	703	TPP	PA-O3A-PB	-2.72	123.50	132.83
5	M	703	TPP	PA-O3A-PB	-2.71	123.53	132.83
5	Q	703	TPP	PA-O3A-PB	-2.71	123.54	132.83
4	I	702	FAD	N6A-C6A-N1A	-2.60	113.18	118.57
4	L	702	FAD	C5X-C9A-N10	2.59	120.63	117.95
4	Q	702	FAD	N6A-C6A-N1A	-2.58	113.21	118.57
4	M	702	FAD	N6A-C6A-N1A	-2.58	113.22	118.57
4	P	702	FAD	C5X-C9A-N10	2.56	120.59	117.95
4	E	702	FAD	N6A-C6A-N1A	-2.56	113.27	118.57
4	H	702	FAD	C5X-C9A-N10	2.54	120.57	117.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	FAD	C5X-C9A-N10	2.50	120.53	117.95
4	M	702	FAD	C5X-C9A-N10	2.46	120.49	117.95
4	Q	702	FAD	C5X-C9A-N10	2.45	120.48	117.95
4	L	702	FAD	C1'-N10-C9A	2.42	124.55	120.51
4	I	702	FAD	C5A-C6A-N6A	2.41	124.02	120.35
4	Q	702	FAD	C5A-C6A-N6A	2.41	124.02	120.35
4	E	702	FAD	C5X-C9A-N10	2.41	120.44	117.95
5	I	703	TPP	O3B-PB-O3A	2.40	112.69	104.64
4	I	702	FAD	C5X-C9A-N10	2.40	120.43	117.95
4	H	702	FAD	C1'-N10-C9A	2.39	124.50	120.51
4	M	702	FAD	C5A-C6A-N6A	2.39	123.98	120.35
5	Q	703	TPP	O3B-PB-O3A	2.38	112.62	104.64
5	E	703	TPP	O3B-PB-O3A	2.37	112.60	104.64
5	M	703	TPP	O3B-PB-O3A	2.37	112.59	104.64
4	D	702	FAD	C1'-N10-C9A	2.37	124.46	120.51
4	P	702	FAD	C1'-N10-C9A	2.37	124.46	120.51
4	E	702	FAD	C5A-C6A-N6A	2.37	123.95	120.35
5	P	703	TPP	C5'-C4'-N3'	2.35	124.94	121.24
5	D	703	TPP	C5'-C4'-N3'	2.34	124.92	121.24
5	L	703	TPP	C5'-C4'-N3'	2.33	124.90	121.24
5	H	703	TPP	C5'-C4'-N3'	2.31	124.87	121.24
4	D	702	FAD	N6A-C6A-N1A	-2.29	113.83	118.57
4	P	702	FAD	N6A-C6A-N1A	-2.28	113.84	118.57
4	L	702	FAD	N6A-C6A-N1A	-2.28	113.85	118.57
4	H	702	FAD	N6A-C6A-N1A	-2.27	113.85	118.57
4	L	702	FAD	C2A-N1A-C6A	-2.11	115.14	118.75
4	P	702	FAD	C2A-N1A-C6A	-2.08	115.19	118.75
4	D	702	FAD	C2A-N1A-C6A	-2.08	115.20	118.75
4	H	702	FAD	C2A-N1A-C6A	-2.04	115.27	118.75
4	Q	702	FAD	C2A-N1A-C6A	-2.03	115.28	118.75
4	P	702	FAD	O5B-C5B-C4B	2.03	115.97	108.99
4	M	702	FAD	C2A-N1A-C6A	-2.02	115.29	118.75
5	D	703	TPP	C2'-N3'-C4'	-2.02	114.93	118.08
4	L	702	FAD	O5B-C5B-C4B	2.02	115.95	108.99
4	I	702	FAD	C2A-N1A-C6A	-2.02	115.30	118.75
5	P	703	TPP	CM4-C4-C5	-2.02	123.19	127.60
5	H	703	TPP	C2'-N3'-C4'	-2.02	114.94	118.08
5	P	703	TPP	C2'-N3'-C4'	-2.01	114.95	118.08
4	H	702	FAD	O5B-C5B-C4B	2.01	115.90	108.99
4	D	702	FAD	O5B-C5B-C4B	2.01	115.90	108.99
5	L	703	TPP	C2'-N3'-C4'	-2.01	114.96	118.08

There are no chirality outliers.

All (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
4	H	702	FAD	C4B-C5B-O5B-PA
4	H	702	FAD	N10-C1'-C2'-O2'
4	H	702	FAD	N10-C1'-C2'-C3'
4	H	702	FAD	C5'-O5'-P-O1P
4	H	702	FAD	C5'-O5'-P-O3P
4	L	702	FAD	C4B-C5B-O5B-PA
4	L	702	FAD	N10-C1'-C2'-O2'
4	L	702	FAD	N10-C1'-C2'-C3'
4	L	702	FAD	C5'-O5'-P-O1P
4	L	702	FAD	C5'-O5'-P-O3P
4	P	702	FAD	C4B-C5B-O5B-PA
4	P	702	FAD	N10-C1'-C2'-O2'
4	P	702	FAD	N10-C1'-C2'-C3'
4	P	702	FAD	C5'-O5'-P-O1P
4	P	702	FAD	C5'-O5'-P-O3P
5	E	703	TPP	C4-C5-C6-C7
5	I	703	TPP	C4-C5-C6-C7
5	M	703	TPP	C4-C5-C6-C7
5	Q	703	TPP	C4-C5-C6-C7
4	E	702	FAD	PA-O3P-P-O5'
4	I	702	FAD	PA-O3P-P-O5'
4	M	702	FAD	PA-O3P-P-O5'
4	Q	702	FAD	PA-O3P-P-O5'
5	D	703	TPP	PB-O3A-PA-O7
5	E	703	TPP	PB-O3A-PA-O7
5	H	703	TPP	PB-O3A-PA-O7
5	I	703	TPP	PB-O3A-PA-O7
5	L	703	TPP	PB-O3A-PA-O7
5	M	703	TPP	PB-O3A-PA-O7
5	P	703	TPP	PB-O3A-PA-O7
5	Q	703	TPP	PB-O3A-PA-O7
6	F	501	VAL	OXT-C-CA-CB
4	E	702	FAD	C4'-C5'-O5'-P
4	I	702	FAD	C4'-C5'-O5'-P
4	M	702	FAD	C4'-C5'-O5'-P
4	Q	702	FAD	C4'-C5'-O5'-P
6	F	501	VAL	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
6	N	501	VAL	OXT-C-CA-CB
4	E	702	FAD	C4B-C5B-O5B-PA
4	I	702	FAD	C4B-C5B-O5B-PA
4	M	702	FAD	C4B-C5B-O5B-PA
4	Q	702	FAD	C4B-C5B-O5B-PA
6	N	501	VAL	OXT-C-CA-N
6	O	501	VAL	OXT-C-CA-N
4	M	702	FAD	PA-O3P-P-O2P
6	F	501	VAL	C-CA-CB-CG2
6	J	501	VAL	C-CA-CB-CG2
6	N	501	VAL	C-CA-CB-CG2
4	E	702	FAD	C5'-O5'-P-O1P
4	I	702	FAD	C5'-O5'-P-O1P
4	M	702	FAD	C5'-O5'-P-O1P
4	Q	702	FAD	C5'-O5'-P-O1P
4	D	702	FAD	O4B-C4B-C5B-O5B
4	E	702	FAD	O4B-C4B-C5B-O5B
4	H	702	FAD	O4B-C4B-C5B-O5B
4	I	702	FAD	O4B-C4B-C5B-O5B
4	L	702	FAD	O4B-C4B-C5B-O5B
4	M	702	FAD	O4B-C4B-C5B-O5B
4	P	702	FAD	O4B-C4B-C5B-O5B
4	Q	702	FAD	O4B-C4B-C5B-O5B
5	D	703	TPP	C4-C5-C6-C7
5	H	703	TPP	C4-C5-C6-C7
5	L	703	TPP	C4-C5-C6-C7
5	P	703	TPP	C4-C5-C6-C7

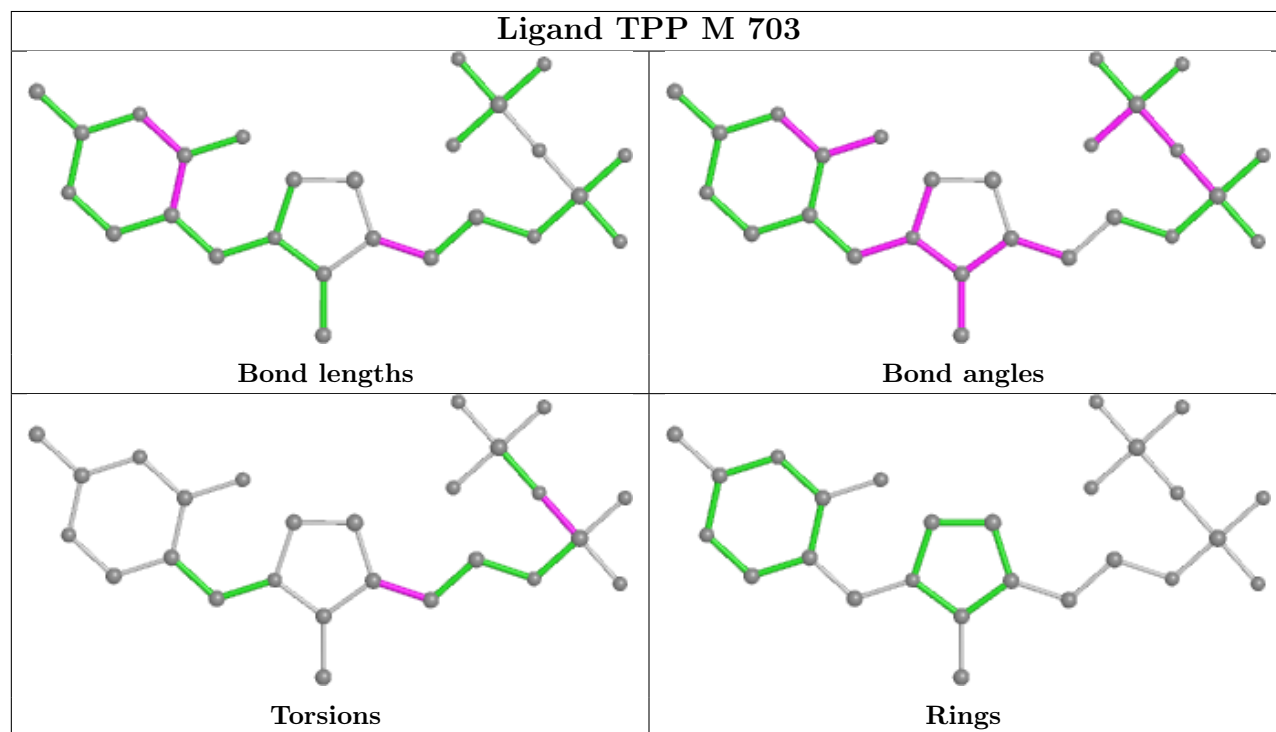
There are no ring outliers.

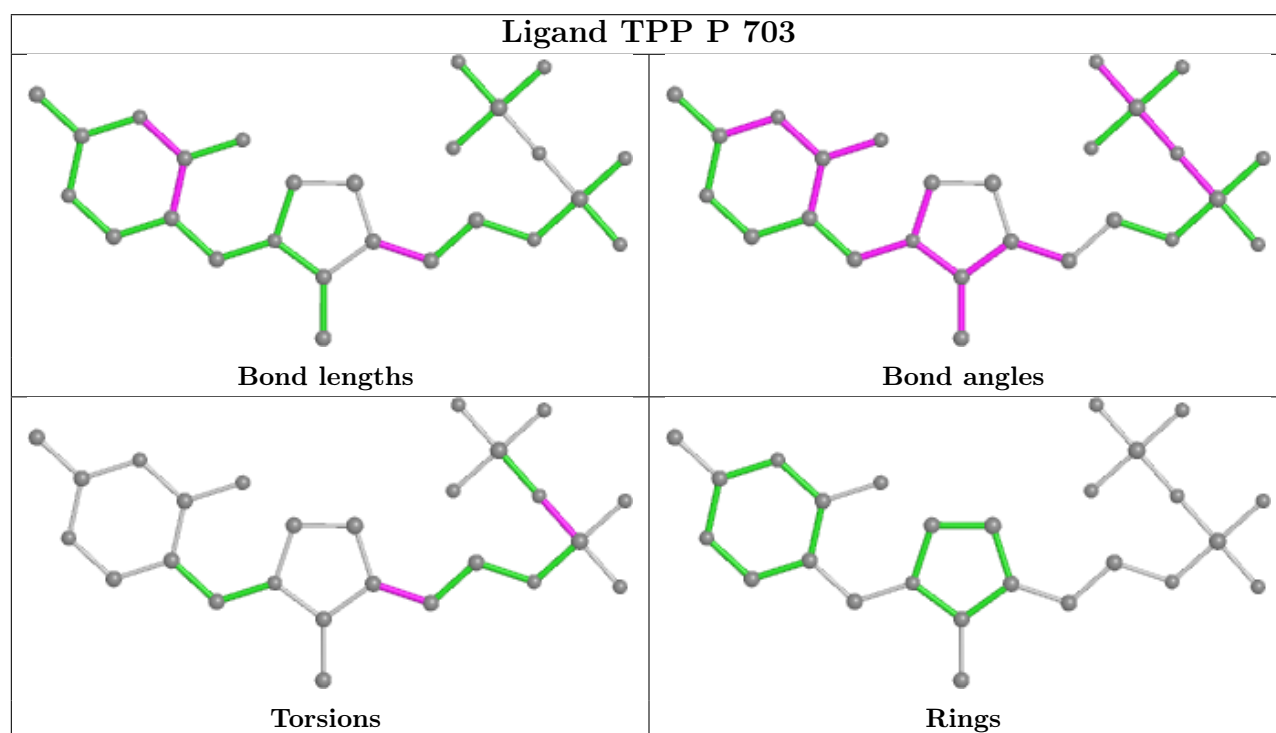
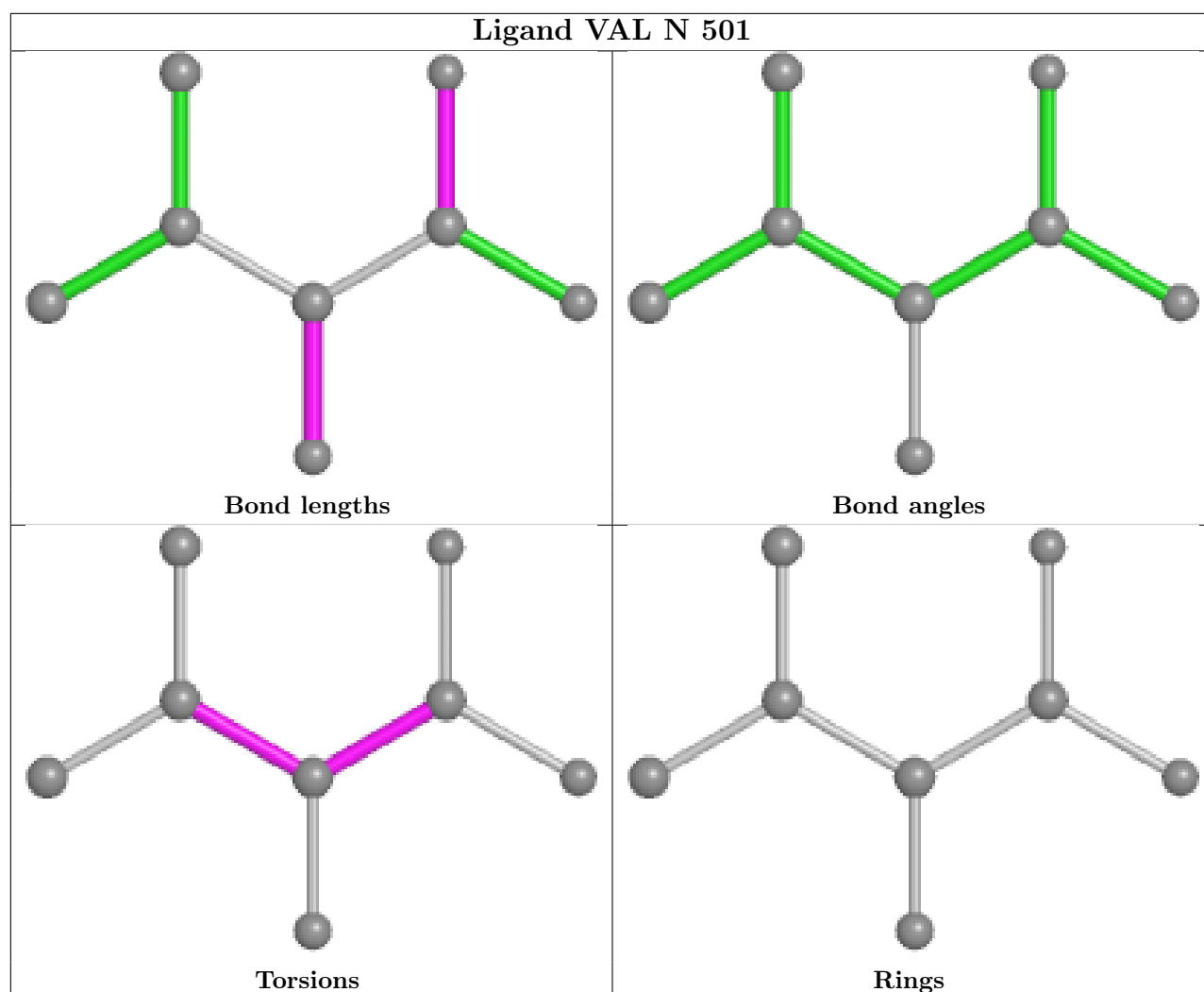
4 monomers are involved in 5 short contacts:

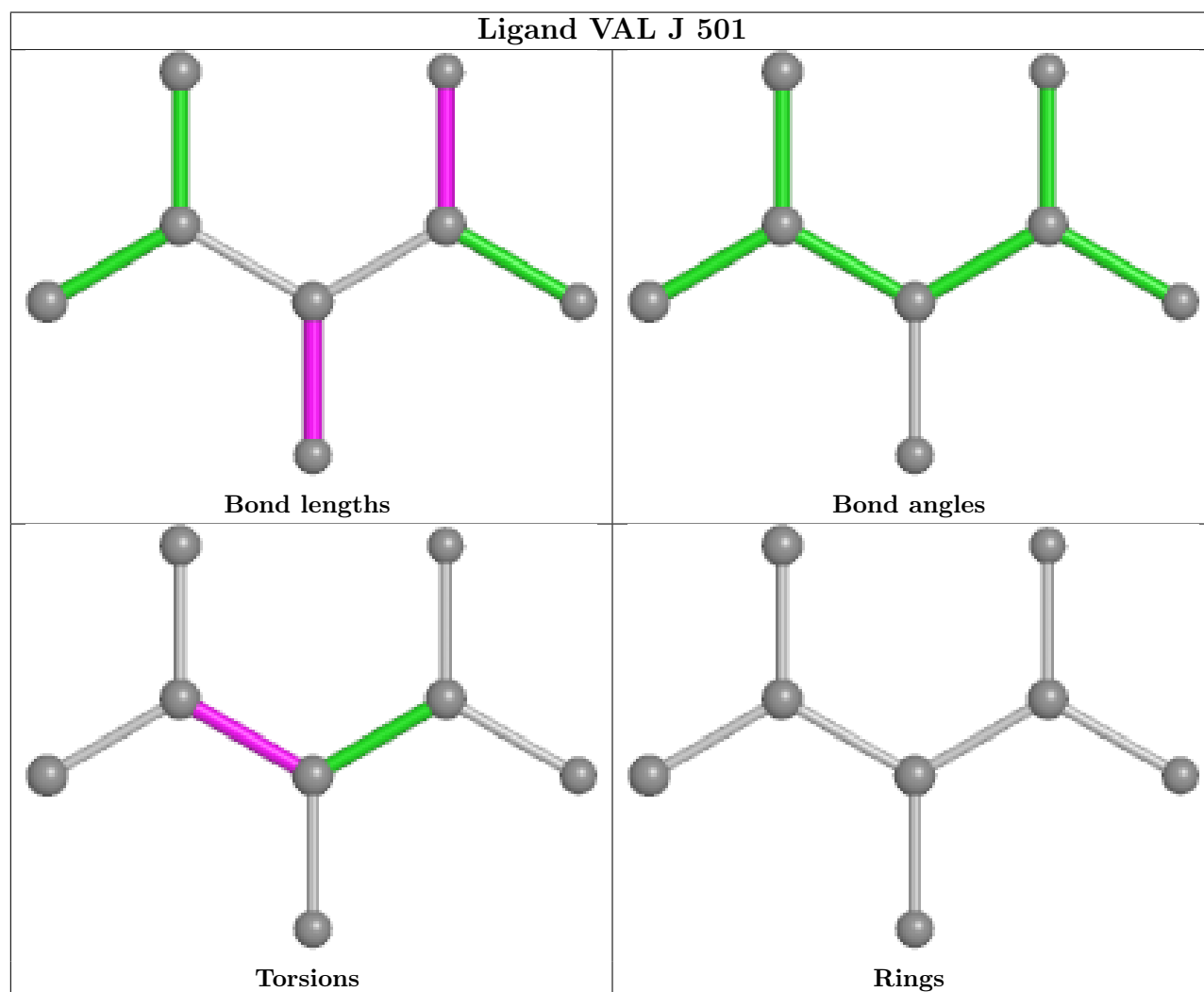
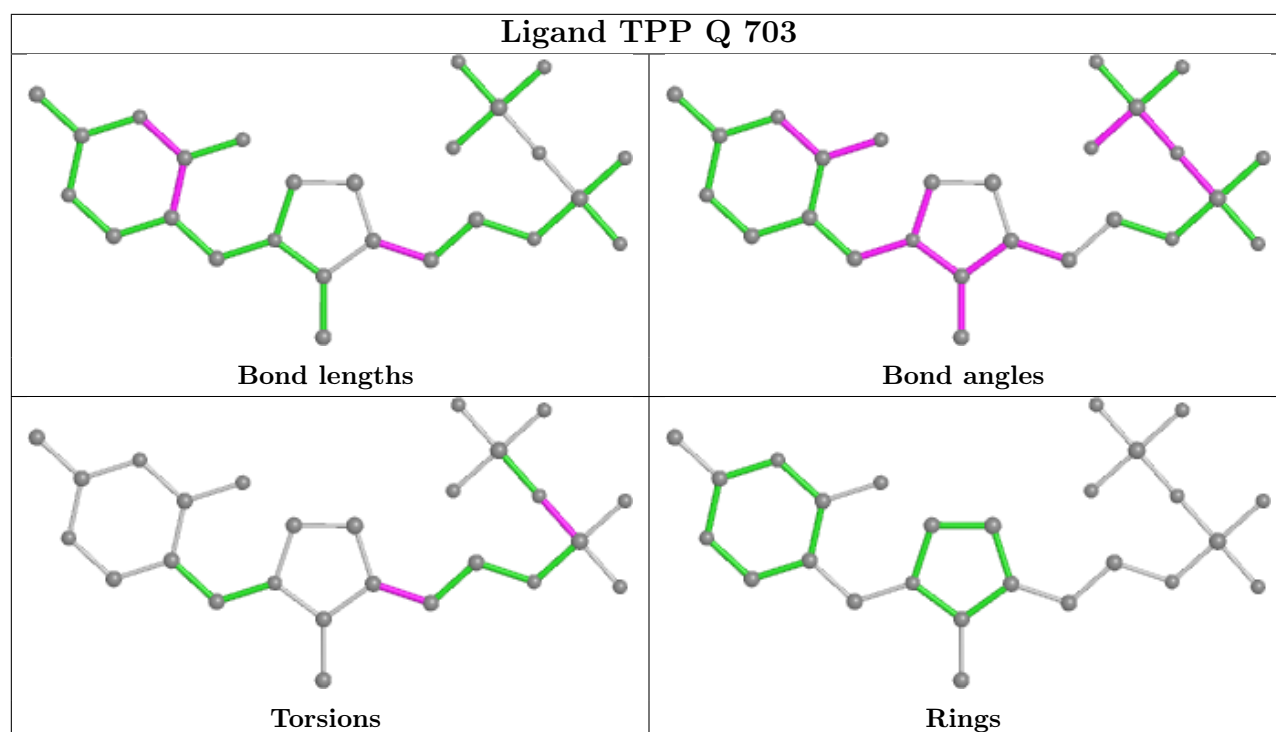
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	501	VAL	1	0
6	J	501	VAL	1	0
6	F	501	VAL	1	0
6	R	501	VAL	2	0

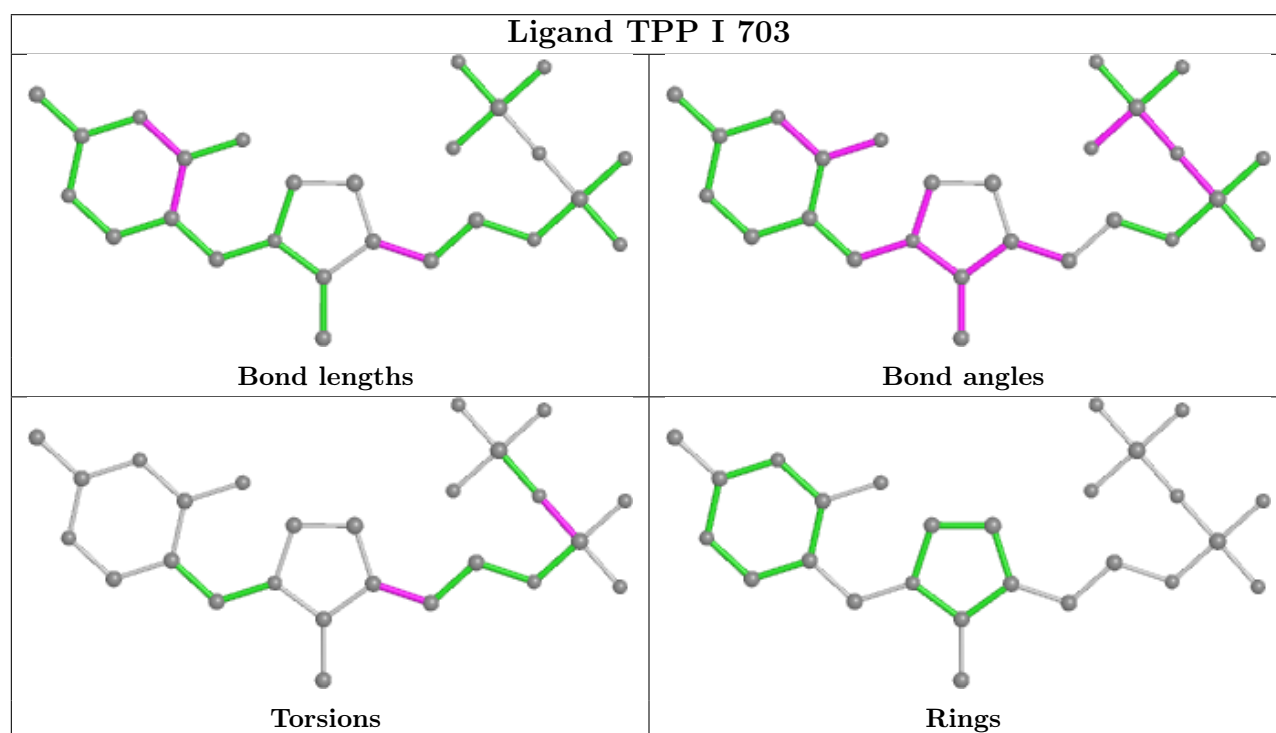
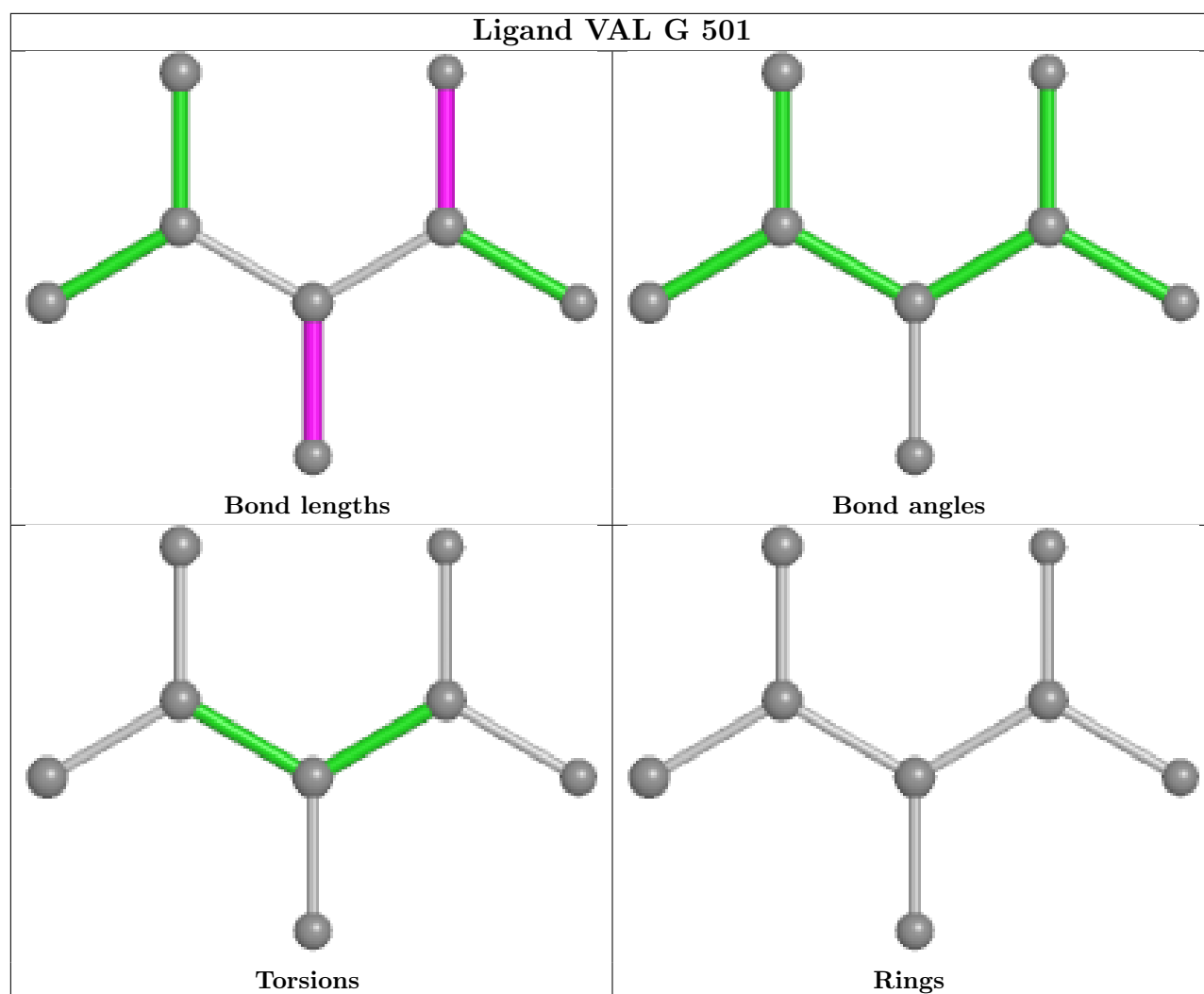
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

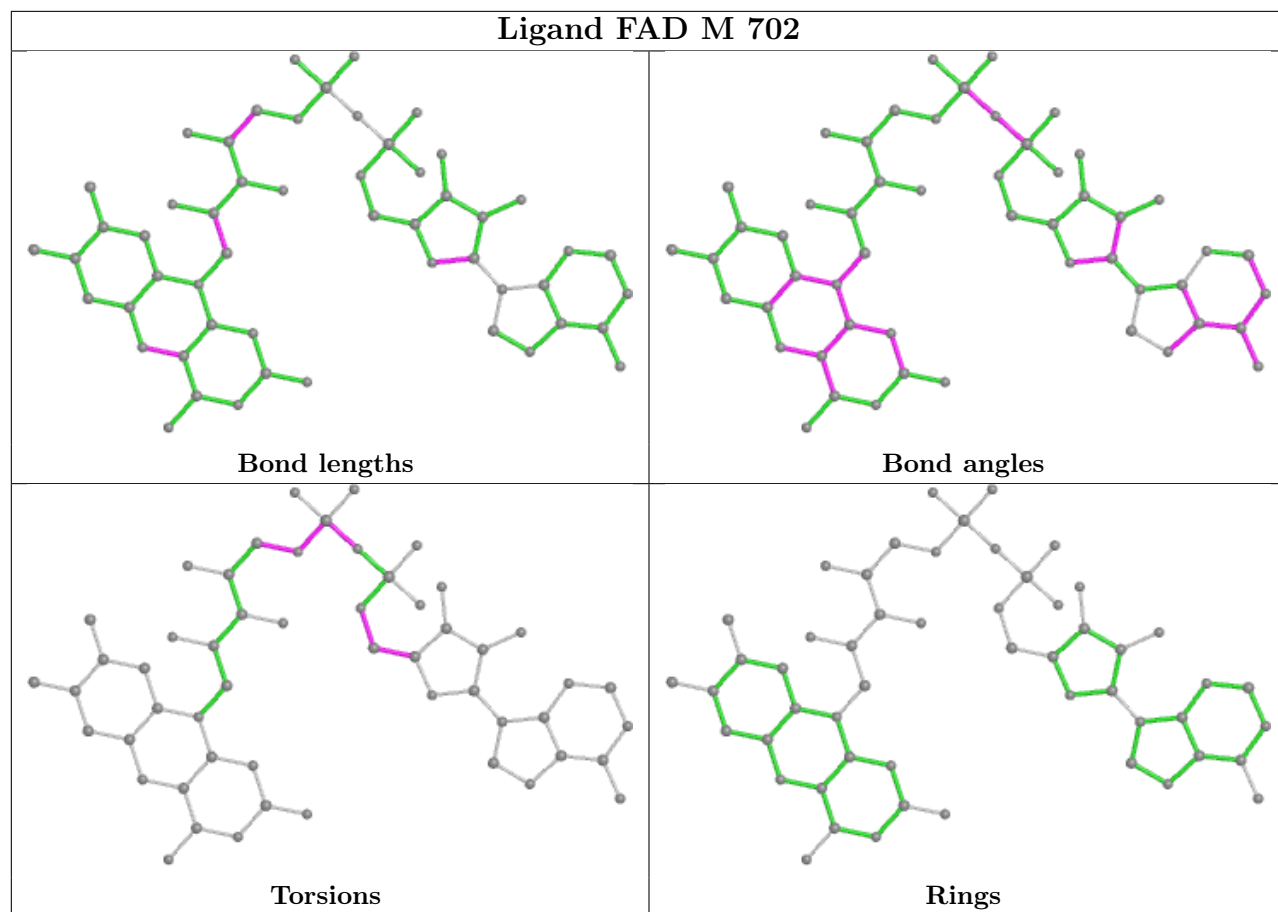
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

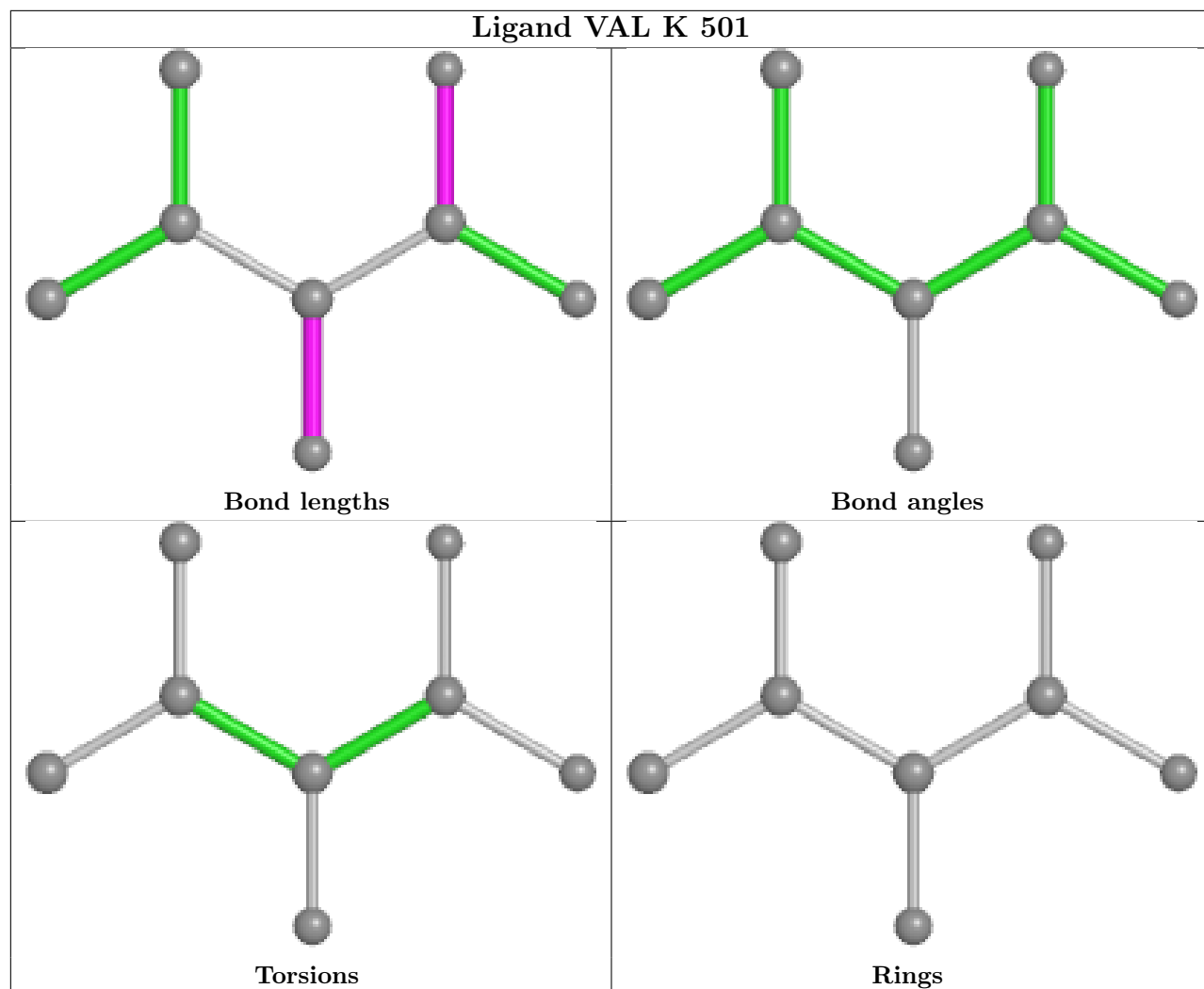


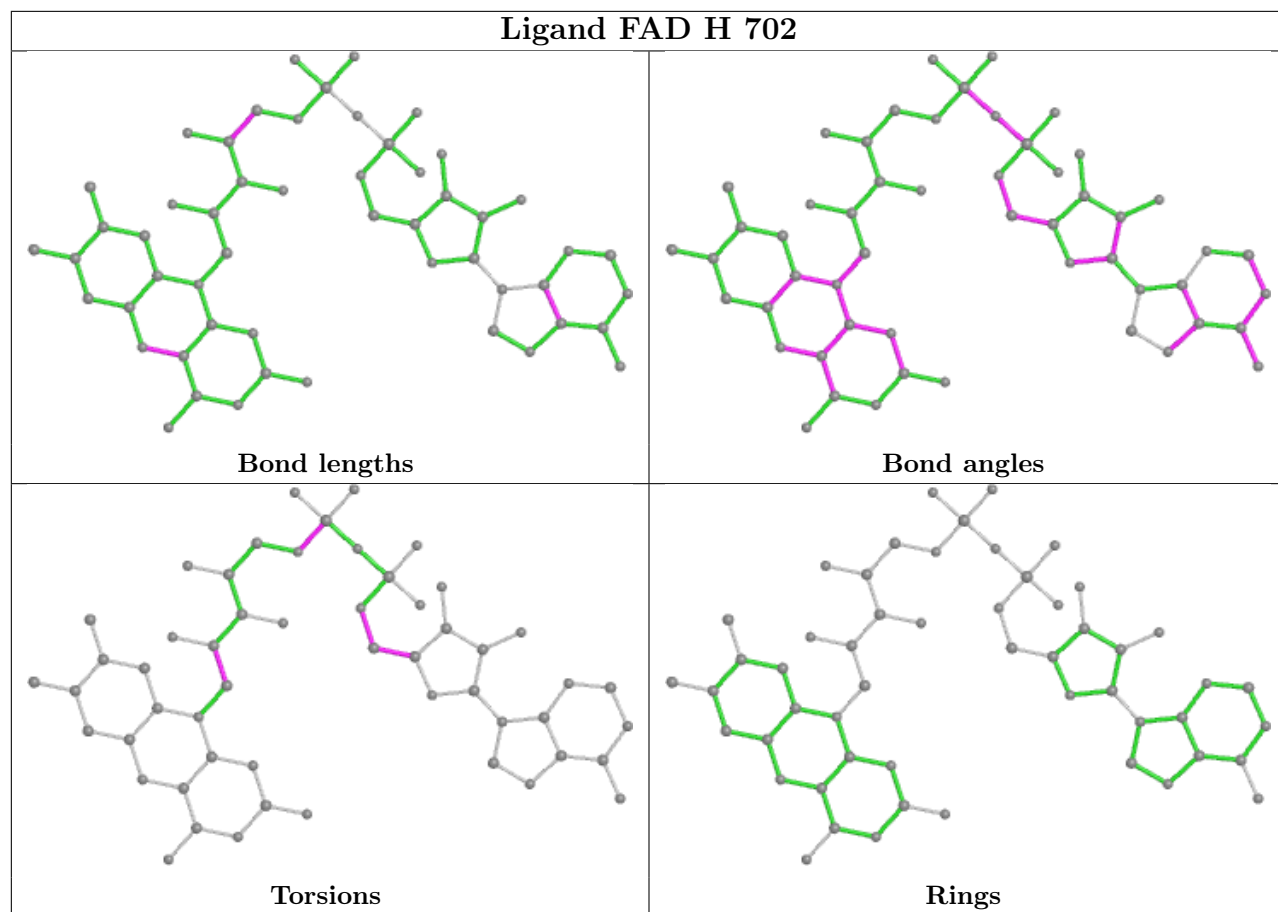


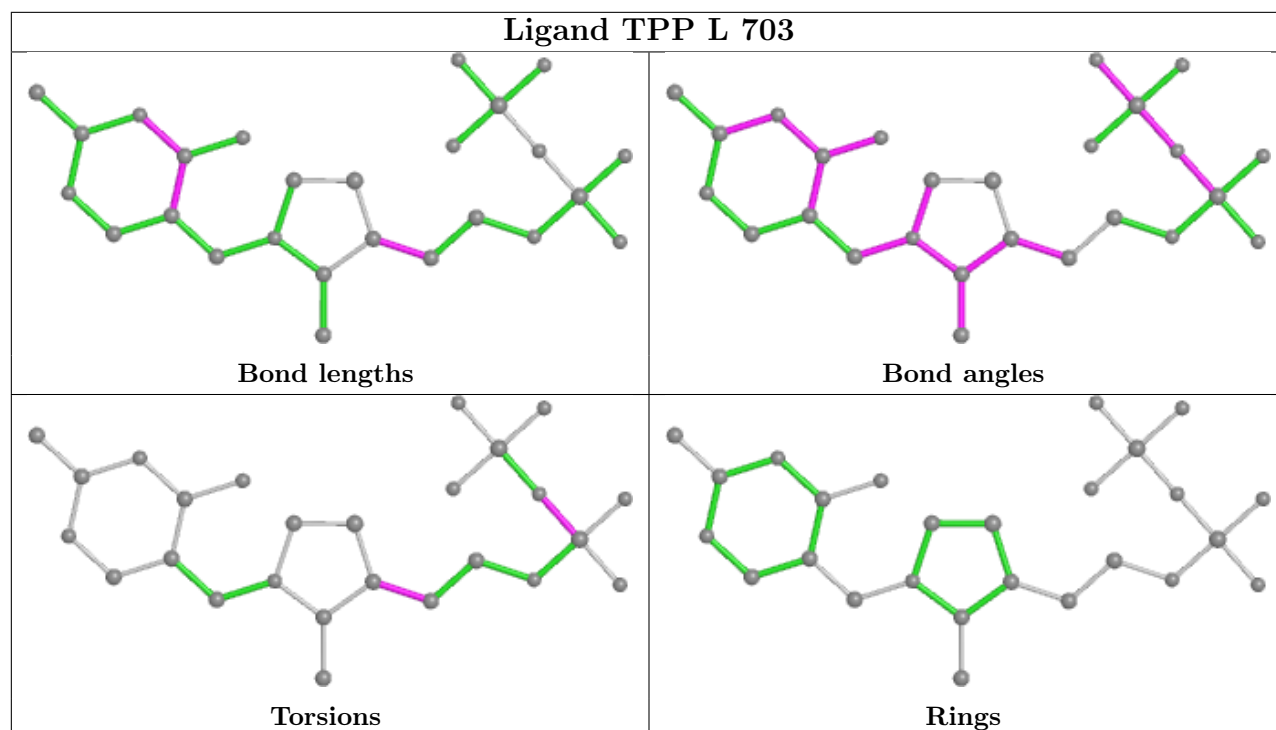
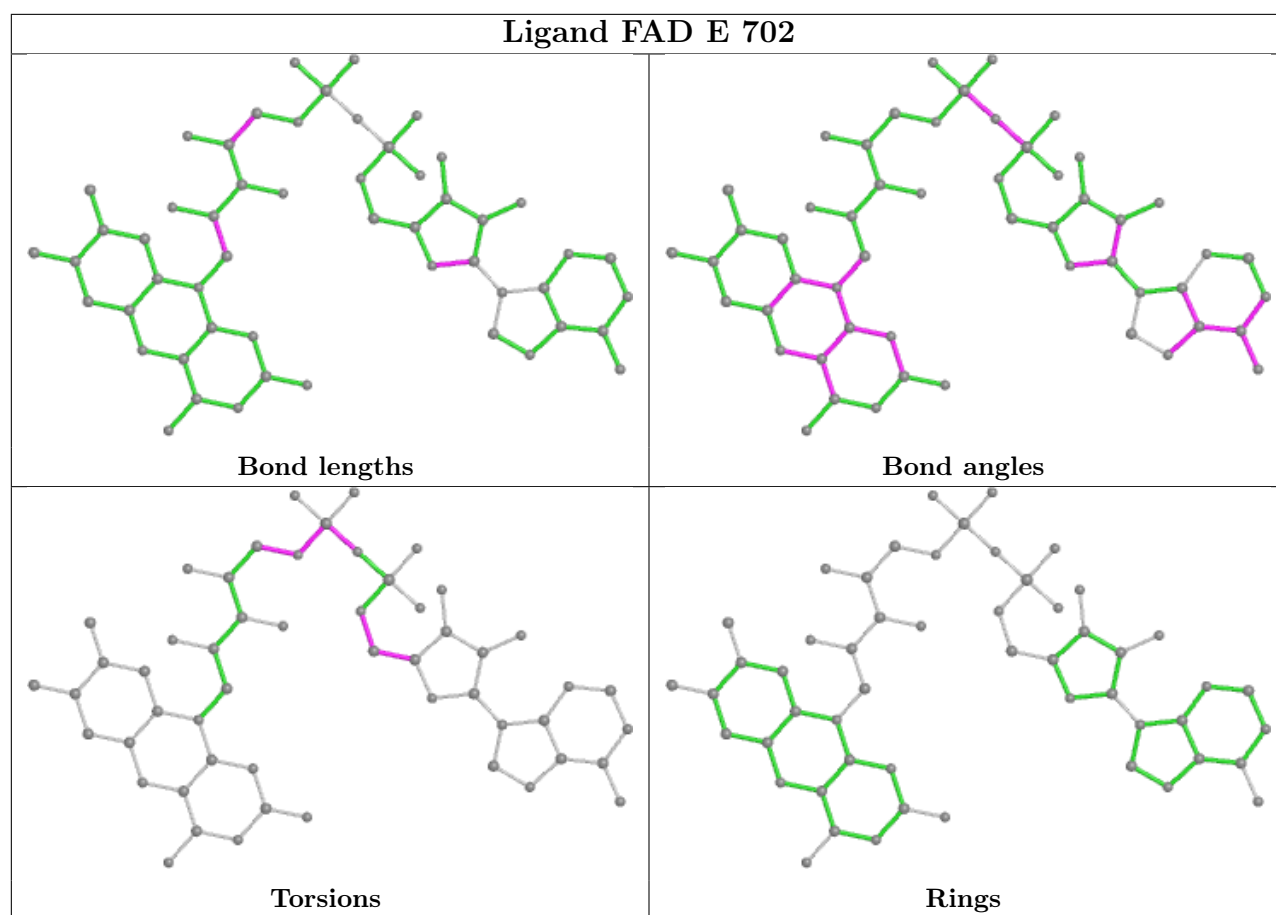


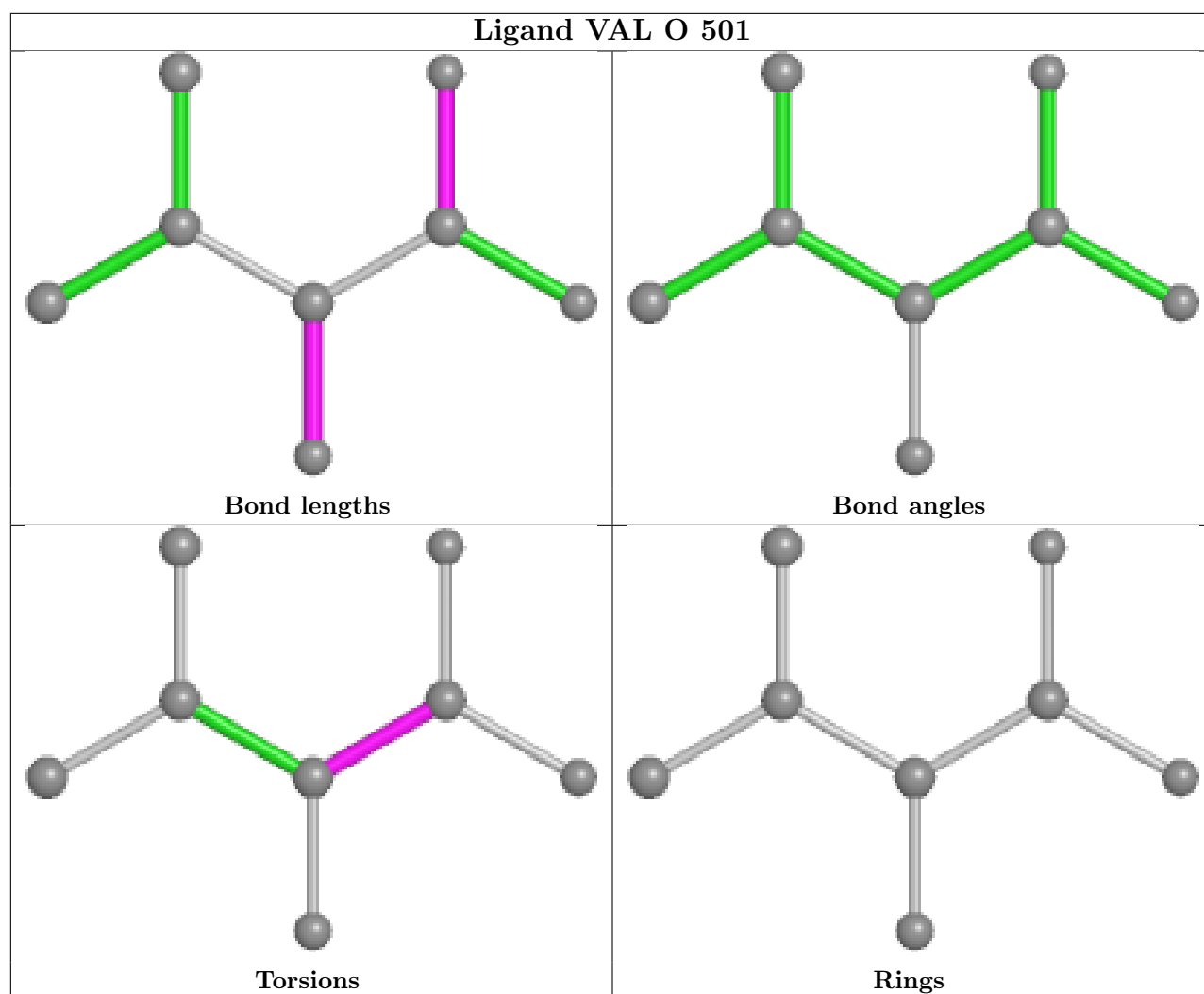


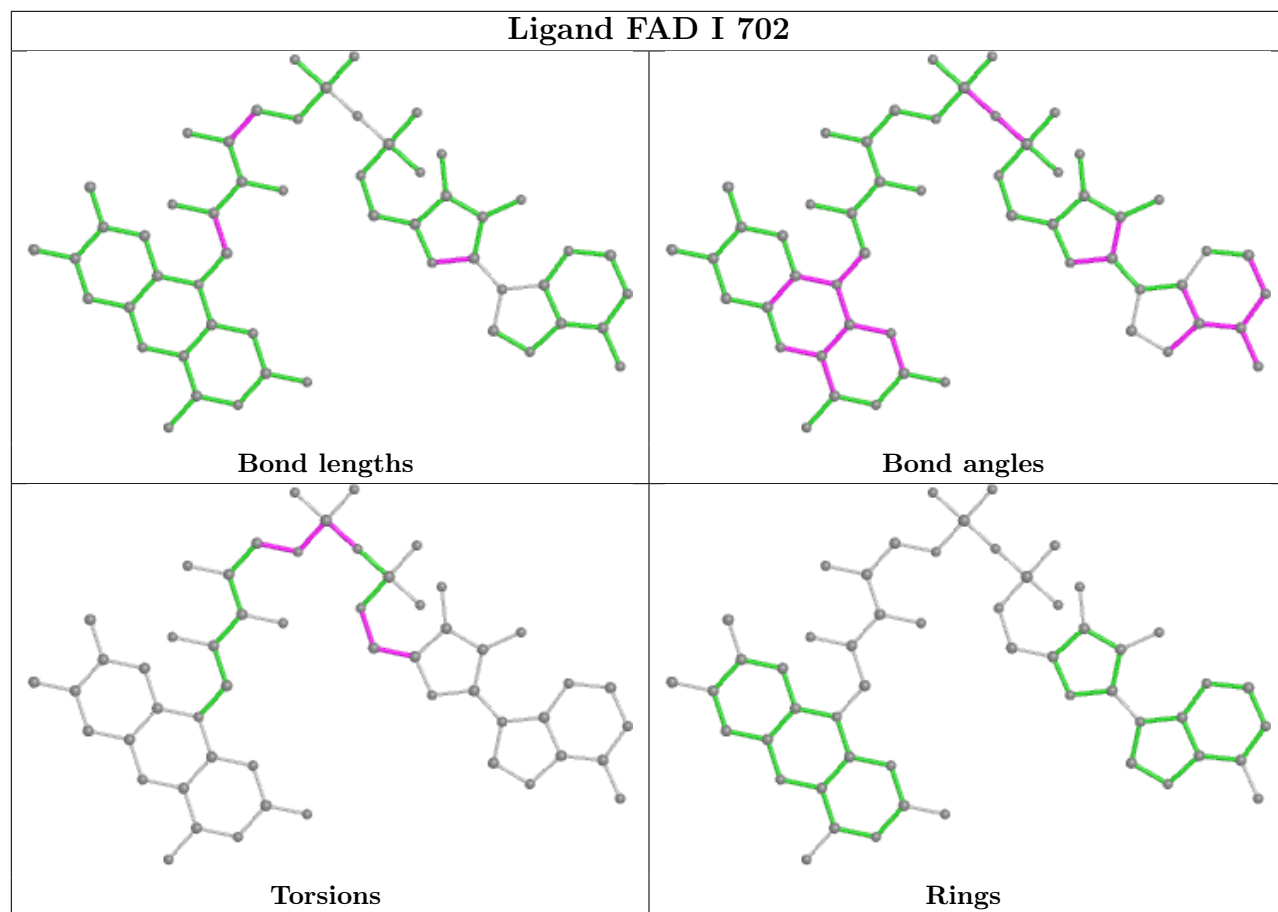




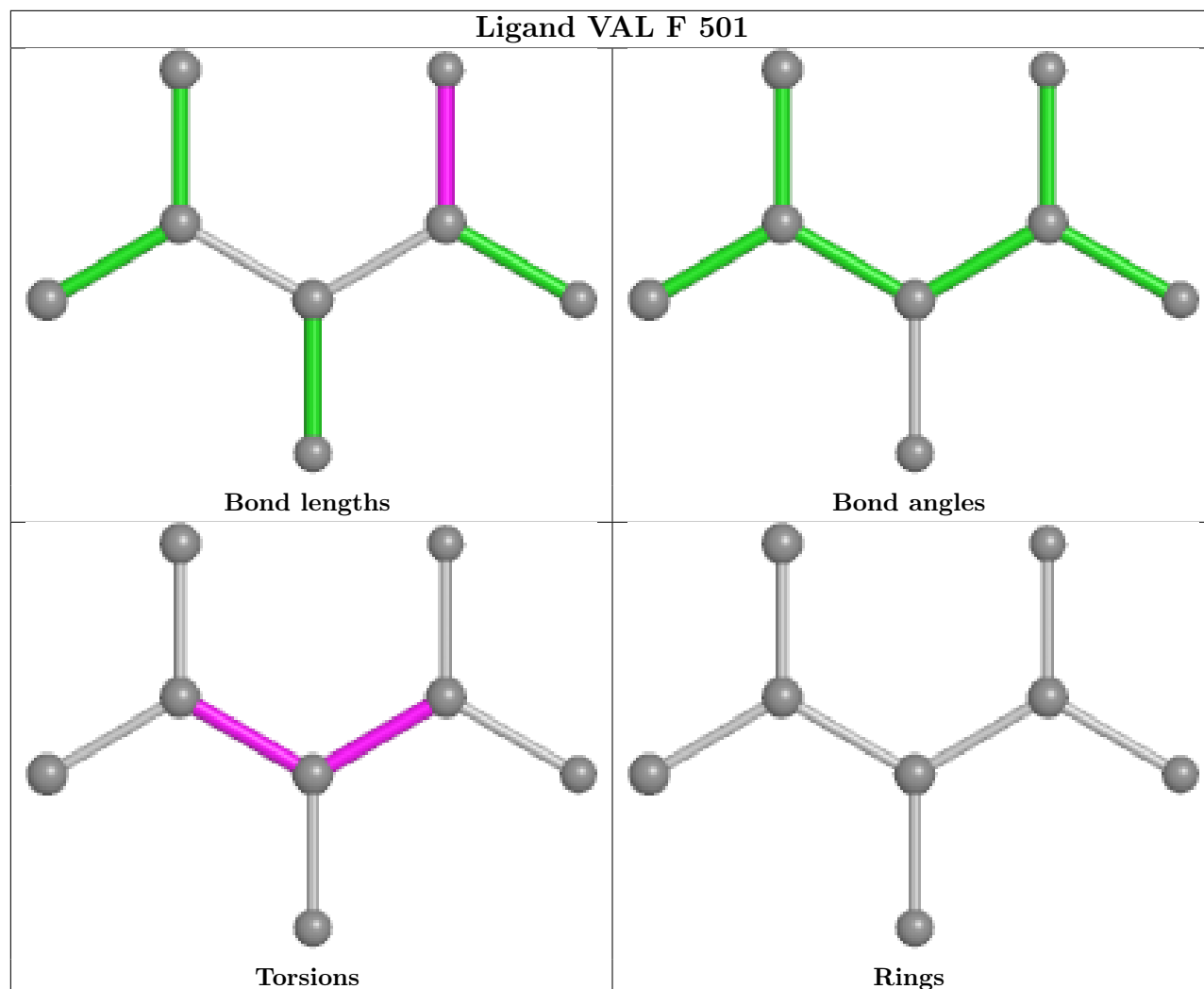




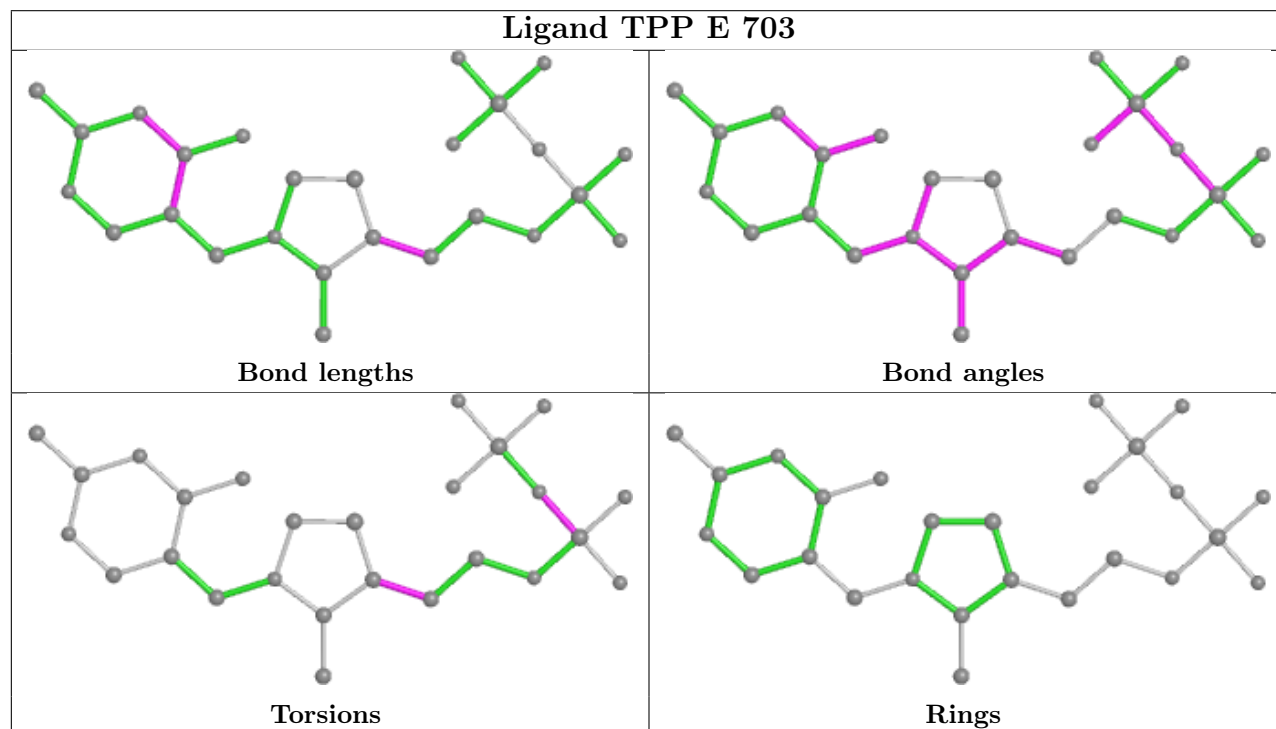


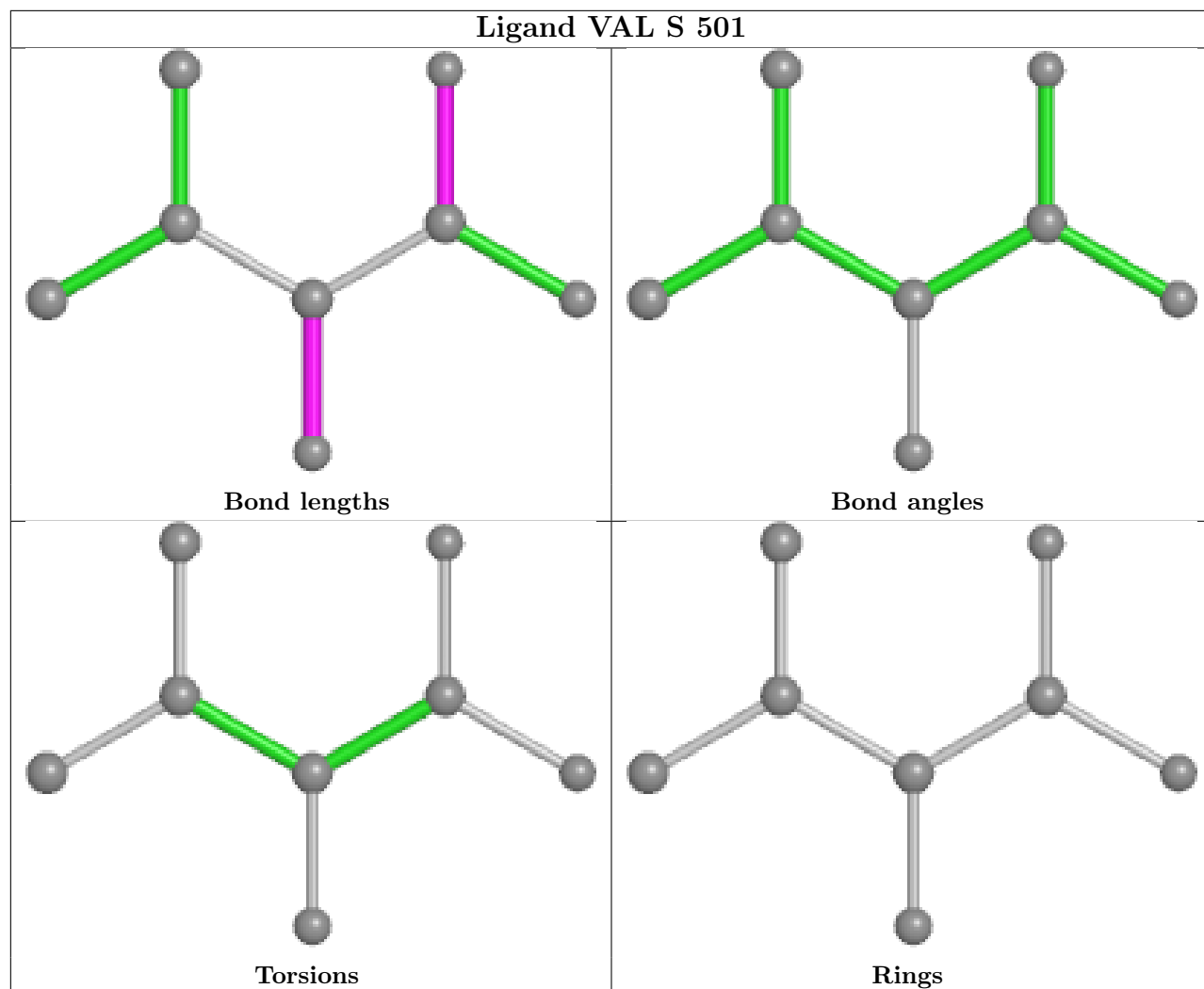


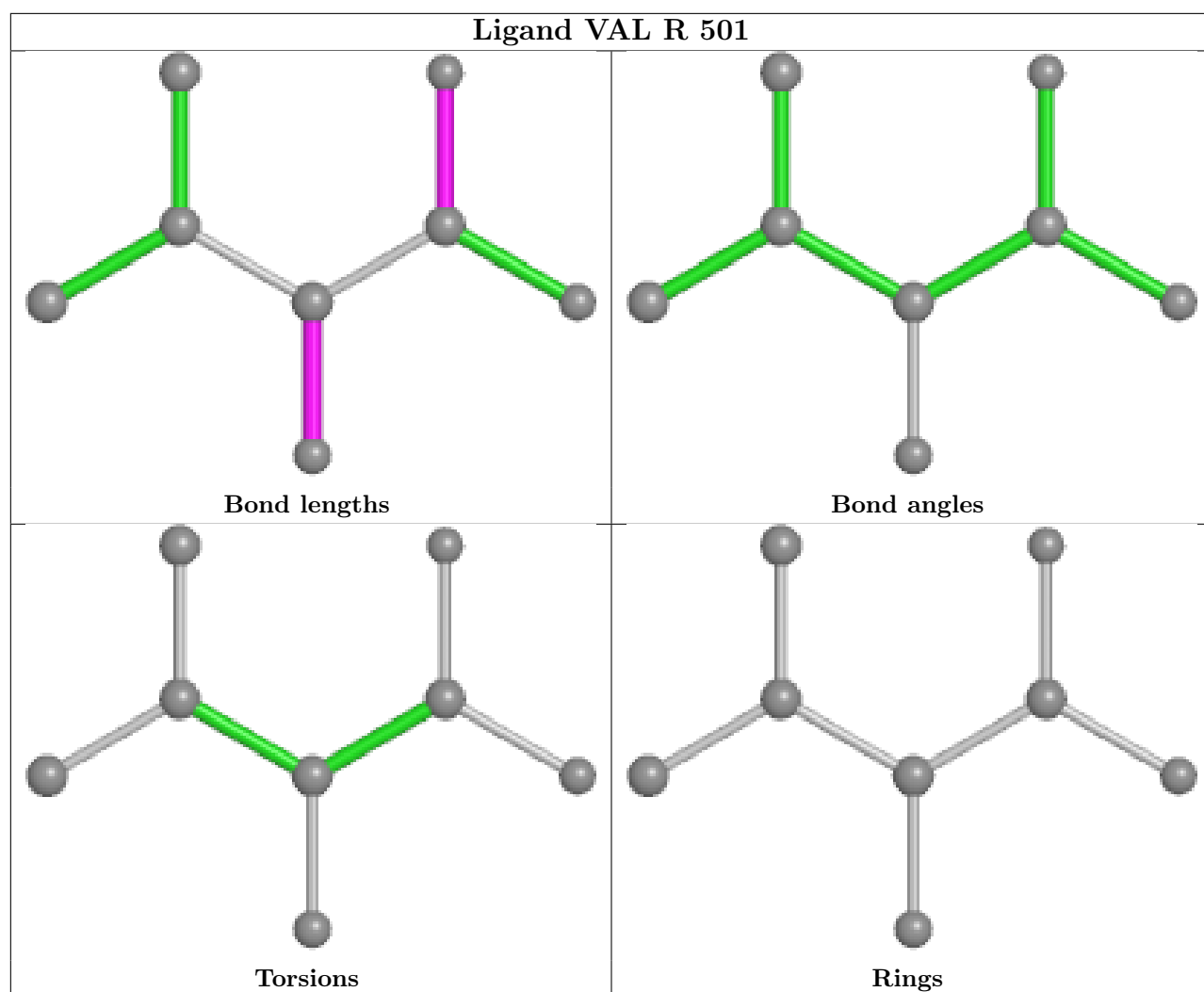
Ligand VAL F 501

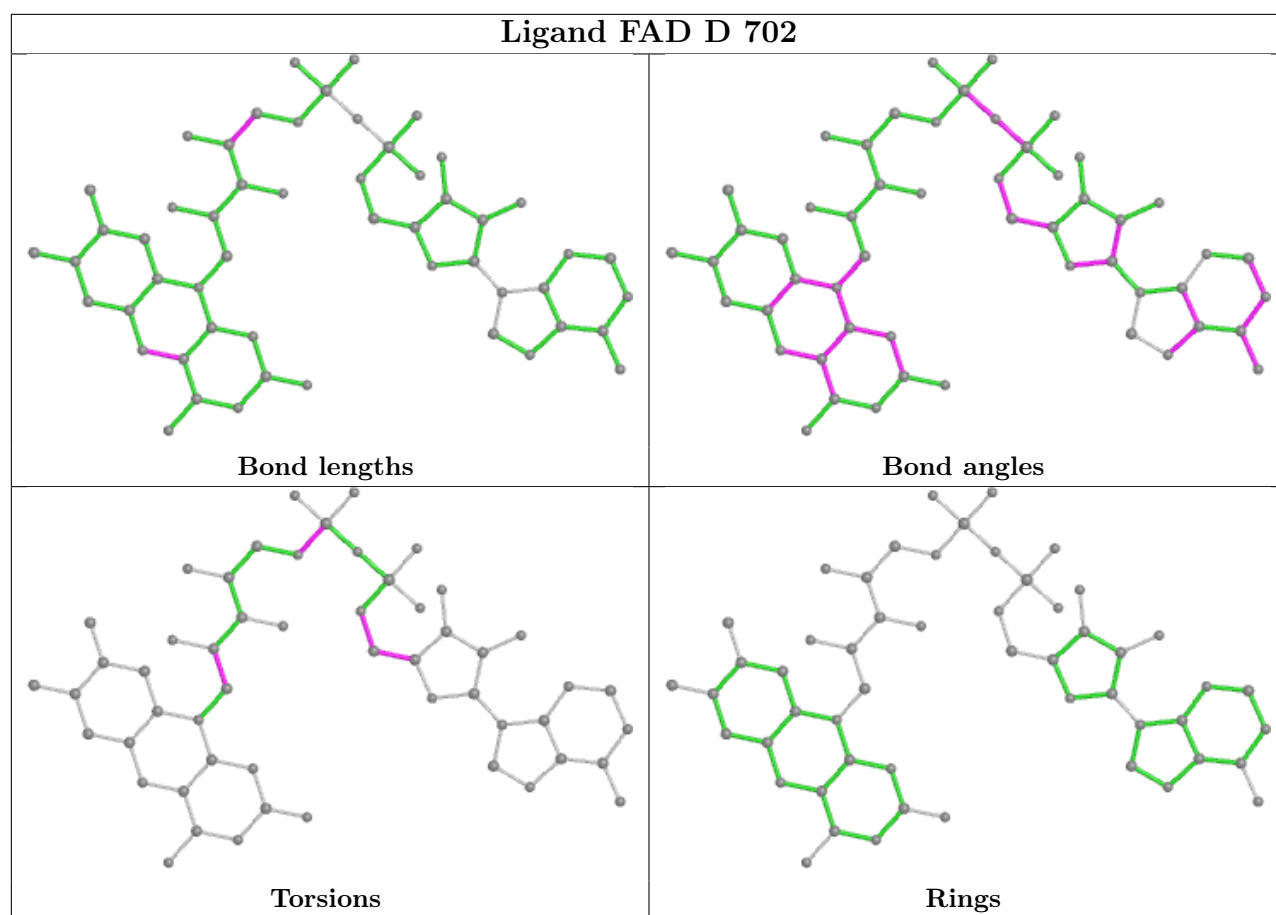


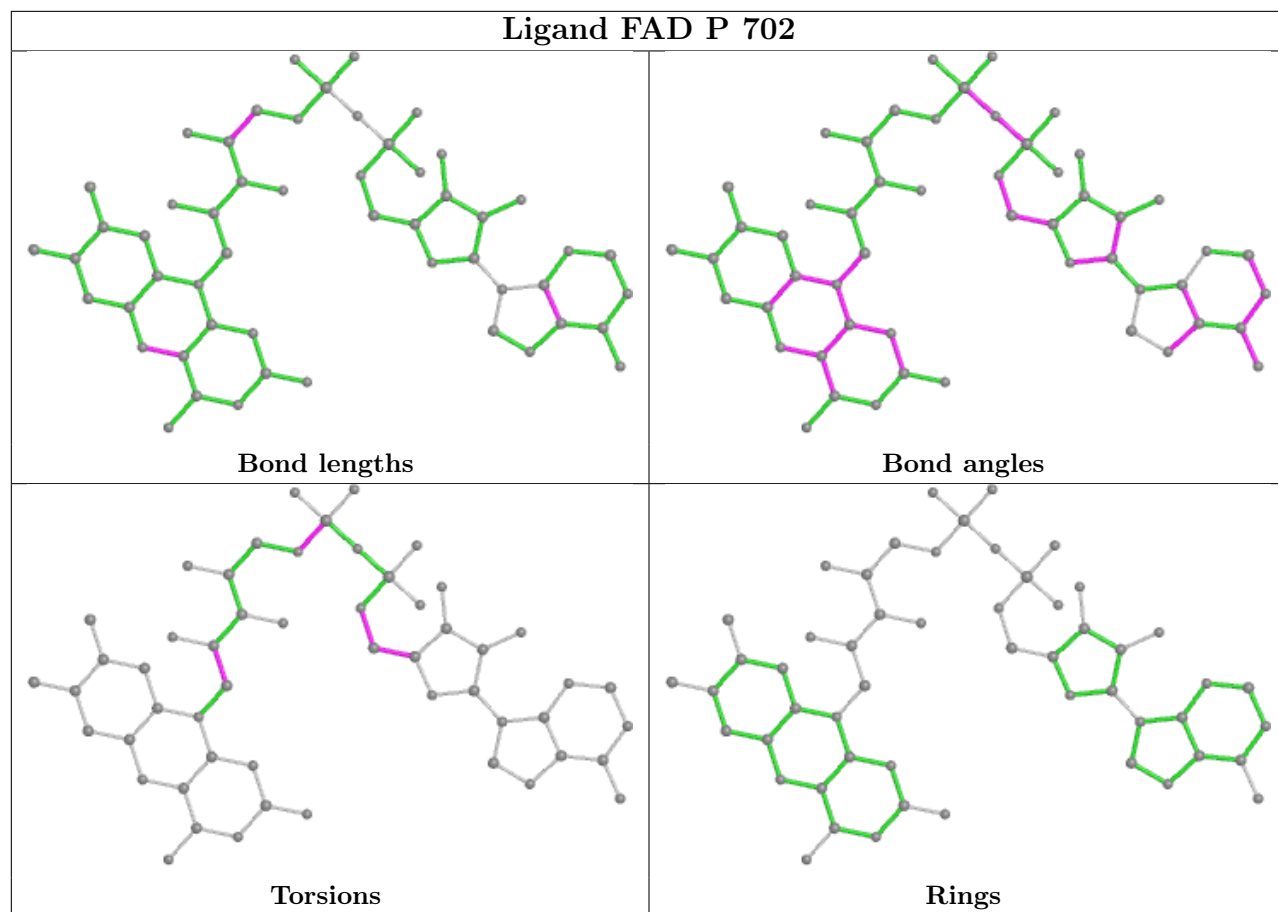
Ligand TPP E 703



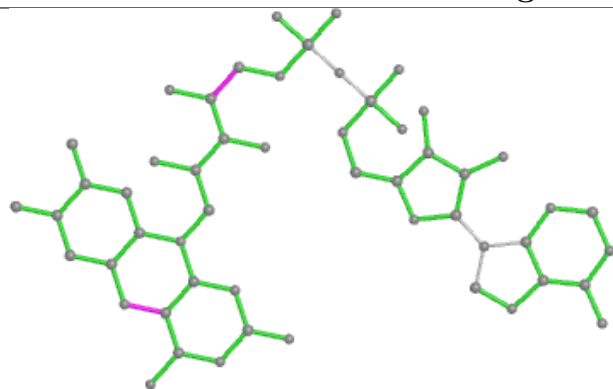




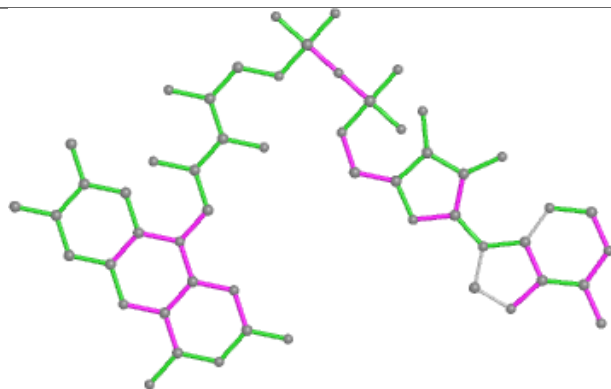




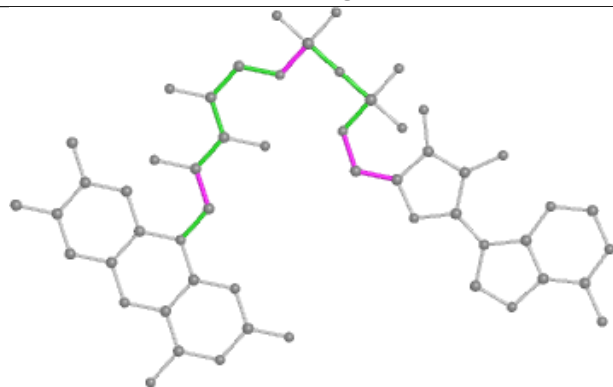
Ligand FAD L 702



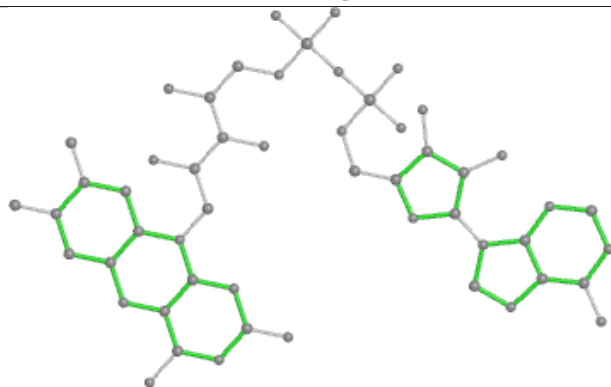
Bond lengths



Bond angles

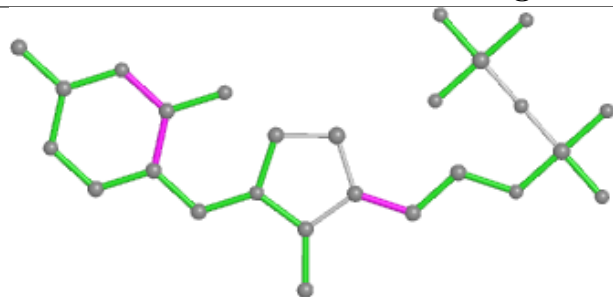


Torsions

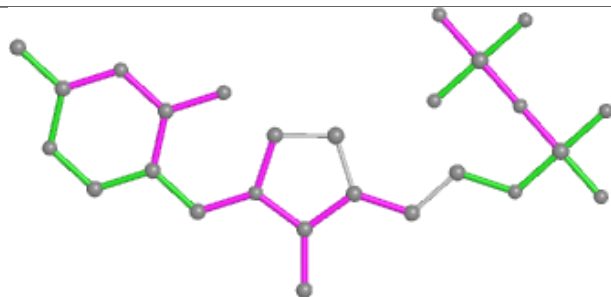


Rings

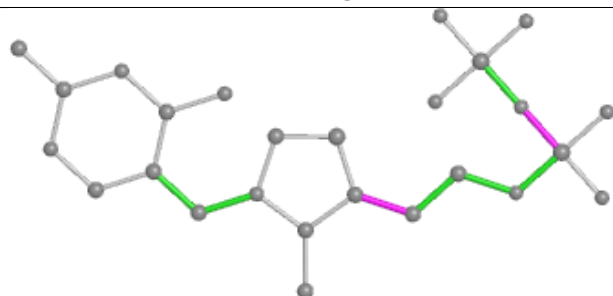
Ligand TPP H 703



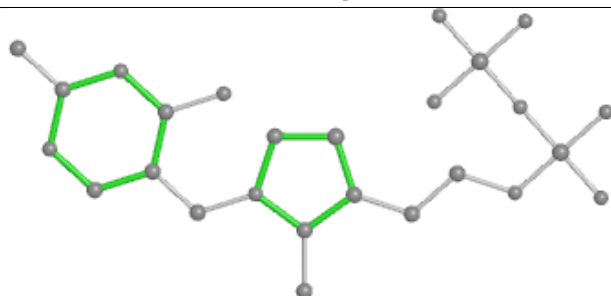
Bond lengths



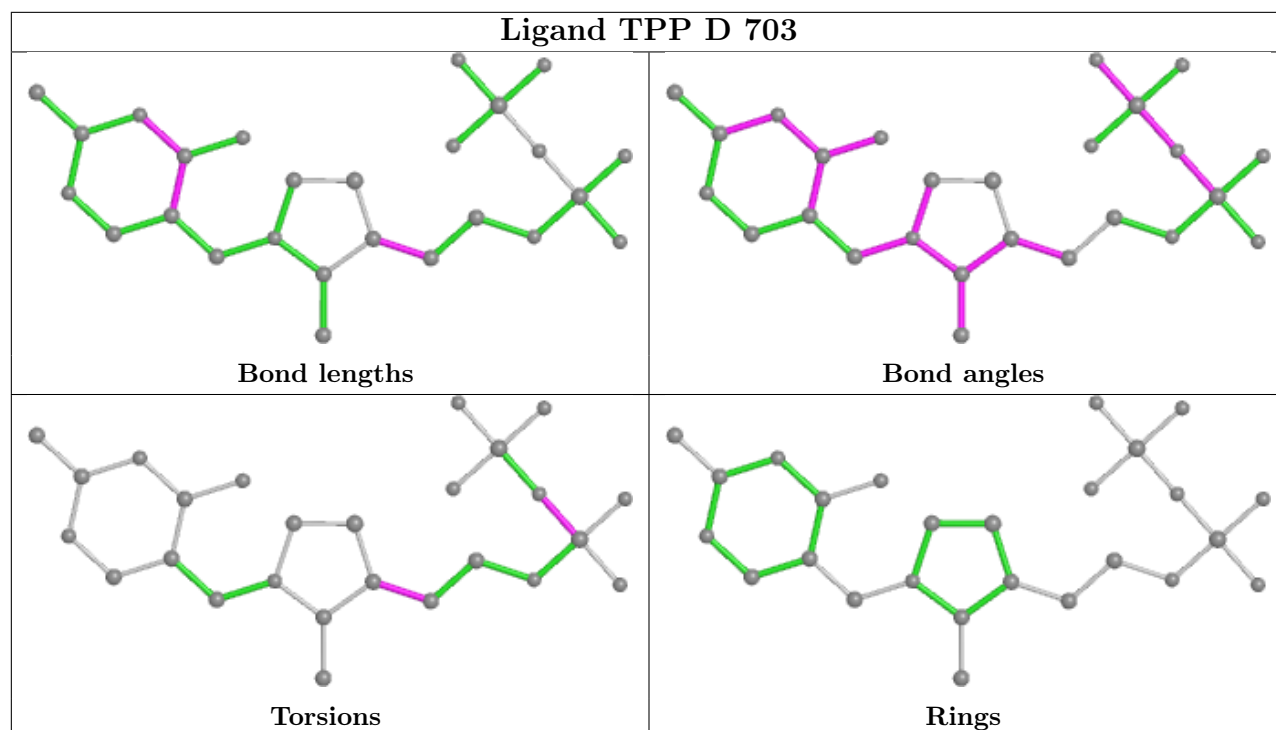
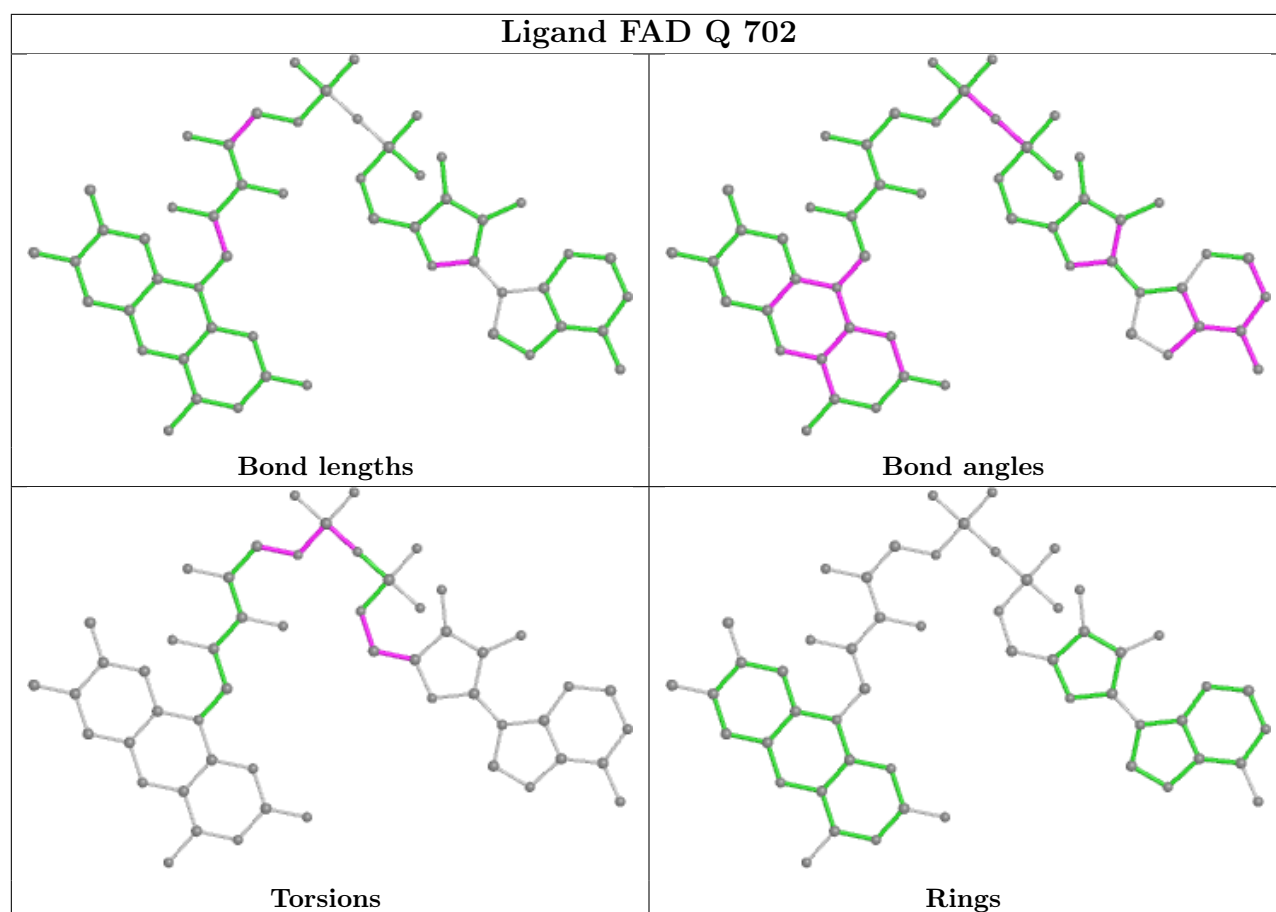
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.