



wwPDB EM Model Validation Summary Report ⓘ

May 19, 2020 – 10:27 AM EDT

PDB ID : 6LUM
EMDB ID : EMD-0981
Title : Structure of Mycobacterium smegmatis succinate dehydrogenase 2
Authors : Gao, Y.; Gong, H.; Zhou, X.; Xiao, Y.; Wang, W.; Ji, W.; Wang, Q.; Rao, Z.
Deposited on : 2020-01-29
Resolution : 2.84 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

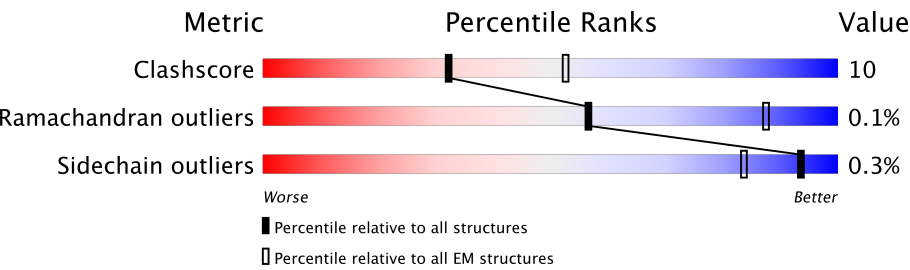
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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	C	138	<div><div>72%17%12%</div></div>
1	G	138	<div><div>72%17%11%</div></div>
1	M	138	<div><div>72%17%11%</div></div>
2	D	166	<div><div>69%19%12%</div></div>
2	H	166	<div><div>60%12%28%</div></div>
2	N	166	<div><div>59%11%30%</div></div>
3	E	32	<div><div>88%9%. </div></div>
3	I	32	<div><div>84%13%. </div></div>
3	O	32	<div><div>78%19%. </div></div>

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Mol	Chain	Length	Quality of chain
4	A	584	 71%21%8%
4	J	584	 70%21%9%
4	P	584	 67%25%8%
5	B	261	 72%19%9%
5	K	261	 73%21%5%
5	Q	261	 67%24%9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	F3S	Q	303	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 26191 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 Succinate dehydrogenase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	122	Total	C	N	O	S	0	0
			978	649	170	154	5		
1	G	123	Total	C	N	O	S	0	0
			989	658	171	155	5		
1	M	123	Total	C	N	O	S	0	0
			990	660	171	154	5		

- Molecule 2 is a protein called Succinate dehydrogenase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	146	Total	C	N	O	S	0	0
			1193	793	202	191	7		
2	H	120	Total	C	N	O	S	0	0
			991	669	159	157	6		
2	N	116	Total	C	N	O	S	0	0
			961	650	152	153	6		

- Molecule 3 is a protein called Succinate dehydrogenase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	31	Total	C	N	O	S	0	0
			256	179	35	41	1		
3	I	31	Total	C	N	O	S	0	0
			256	179	35	41	1		
3	O	31	Total	C	N	O	S	0	0
			256	179	35	41	1		

- Molecule 4 is a protein called Succinate dehydrogenase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	539	Total	C	N	O	S	0	0
			4129	2575	748	782	24		

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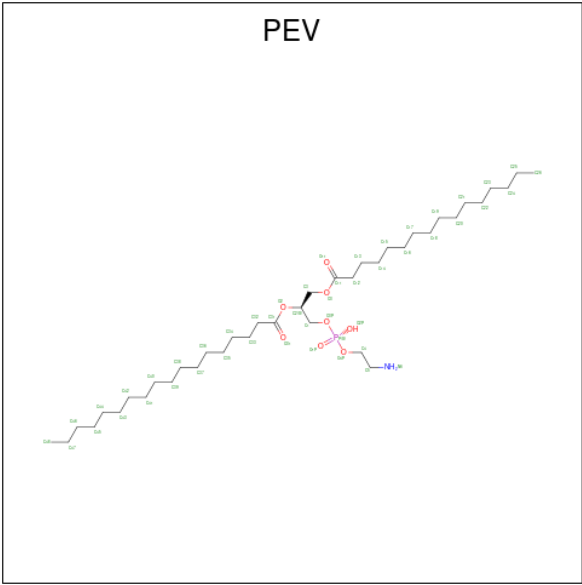
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	534	Total	C	N	O	S	0	0
			4109	2565	741	779	24		
4	P	539	Total	C	N	O	S	0	0
			4025	2513	722	767	23		

- Molecule 5 is a protein called Succinate dehydrogenase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	238	Total	C	N	O	S	0	0
			1873	1182	335	338	18		
5	K	247	Total	C	N	O	S	0	0
			1938	1225	344	351	18		
5	Q	238	Total	C	N	O	S	0	0
			1849	1170	330	331	18		

- Molecule 6 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C₃₉H₇₈NO₈P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			85	65	2	16	2	
6	C	1	Total	C	N	O	P	0
			85	65	2	16	2	
6	G	1	Total	C	N	O	P	0
			44	34	1	8	1	

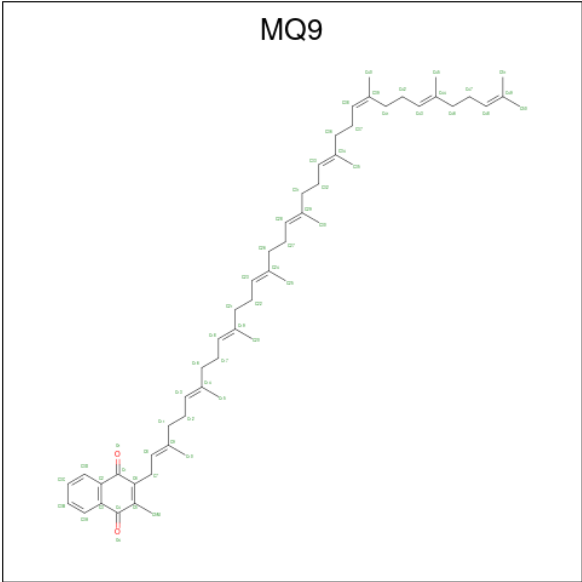
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Mol	Chain	Residues	Atoms					AltConf
6	K	1	Total 41	C 31	N 1	O 8	P 1	0
6	O	1	Total 44	C 34	N 1	O 8	P 1	0
6	Q	1	Total 41	C 31	N 1	O 8	P 1	0

- # HEM

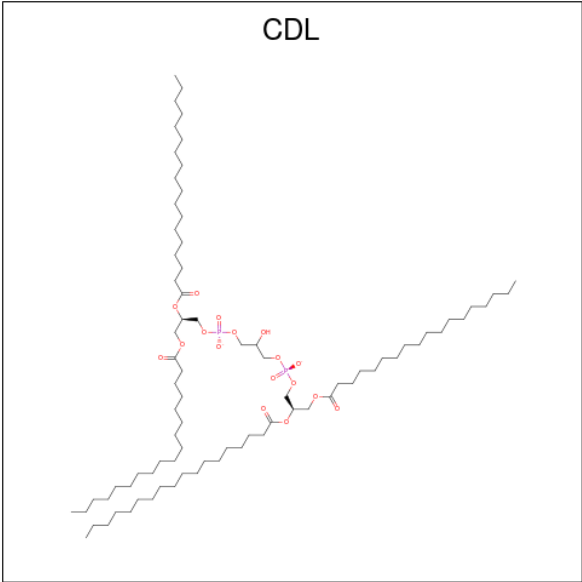
Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total 86	C 68	Fe 2	N 8	O 8	0
7	D	1	Total 86	C 68	Fe 2	N 8	O 8	0
7	H	1	Total 86	C 68	Fe 2	N 8	O 8	0
7	H	1	Total 86	C 68	Fe 2	N 8	O 8	0
7	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
7	N	1	Total 43	C 34	Fe 1	N 4	O 4	0

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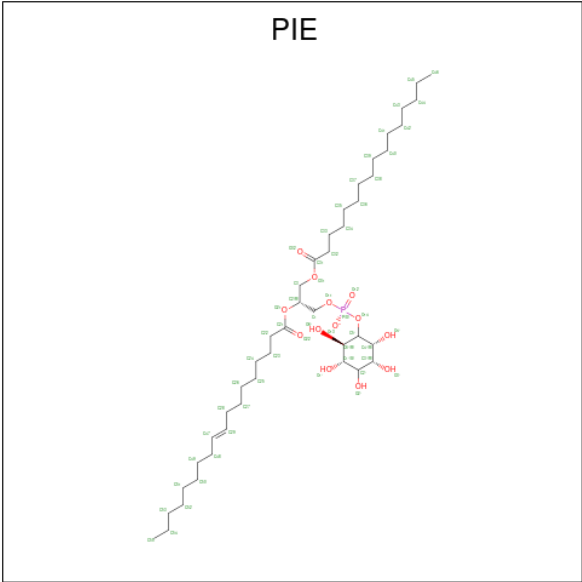
Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C	O	0
			47	43	4	
8	D	1	Total	C	O	0
			47	43	4	
8	H	1	Total	C	O	0
			47	43	4	
8	H	1	Total	C	O	0
			47	43	4	
8	N	1	Total	C	O	0
			47	43	4	
8	N	1	Total	C	O	0
			47	43	4	

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by author).



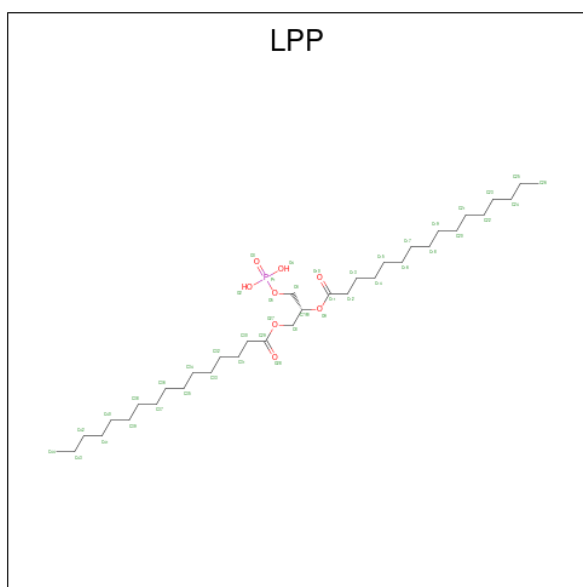
Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	O	P	0
			84	65	17	2	
9	H	1	Total	C	O	P	0
			84	65	17	2	
9	N	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOINOSITOL (three-letter code: PIE) (formula: $C_{43}H_{80}O_{13}P$) (labeled as "Ligand of Interest" by author).



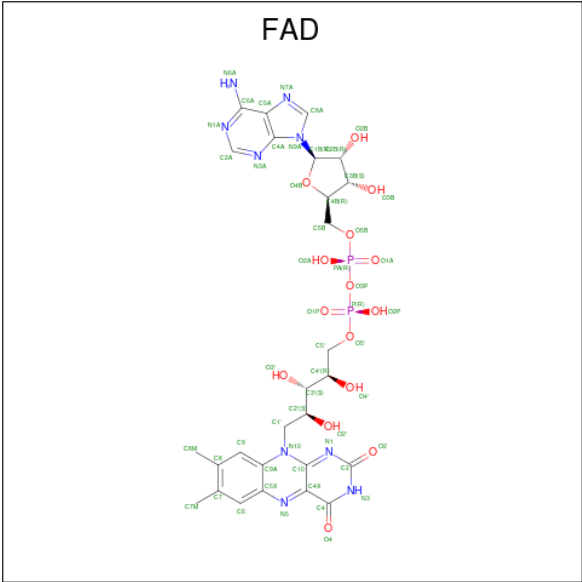
Mol	Chain	Residues	Atoms				AltConf
10	D	1	Total	C	O	P	0
			48	34	13	1	
10	I	1	Total	C	O	P	0
			48	34	13	1	
10	M	1	Total	C	O	P	0
			48	34	13	1	

- Molecule 11 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$).



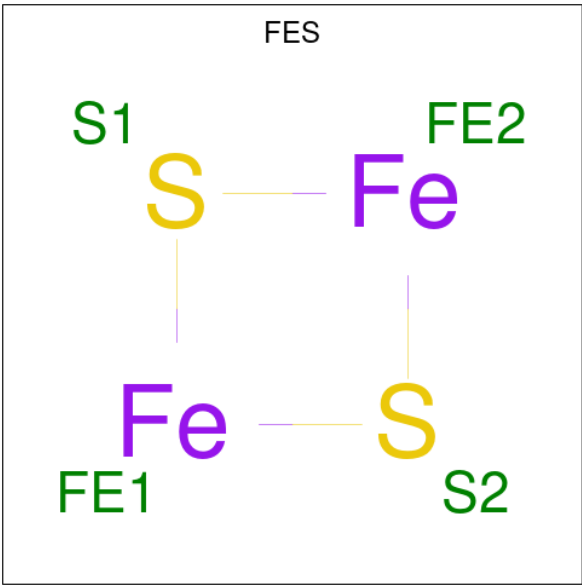
Mol	Chain	Residues	Atoms				AltConf
11	E	1	Total	C	O	P	0
			44	35	8	1	
11	N	1	Total	C	O	P	0
			44	35	8	1	
11	O	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 12 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
12	J	1	Total	C	N	O	P	0
			53	27	9	15	2	
12	P	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



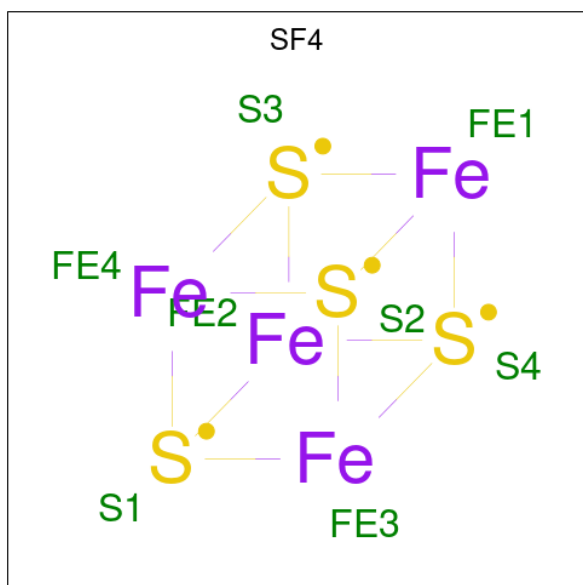
Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	Fe	S	0
			4	2	2	

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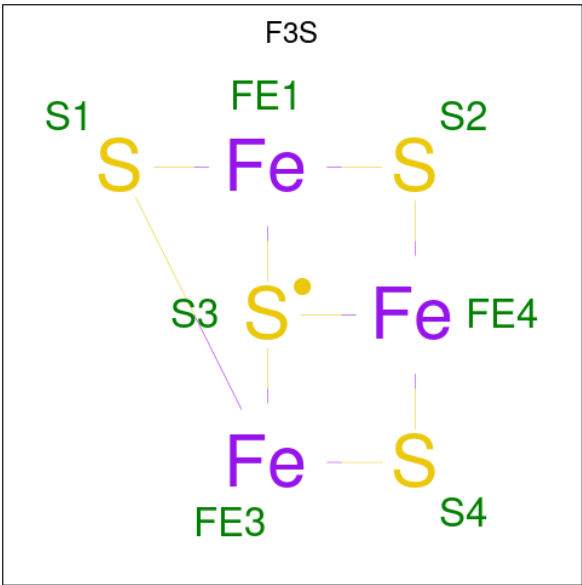
Mol	Chain	Residues	Atoms			AltConf
13	K	1	Total	Fe	S	0
			4	2	2	
13	Q	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	Fe	S	0
			8	4	4	
14	K	1	Total	Fe	S	0
			8	4	4	
14	Q	1	Total	Fe	S	0
			8	4	4	

- Molecule 15 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



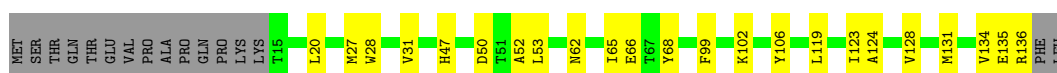
Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	Fe	S	0
			7	3	4	
15	K	1	Total	Fe	S	0
			7	3	4	
15	Q	1	Total	Fe	S	0
			7	3	4	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Succinate dehydrogenase subunit C

Chain C: 



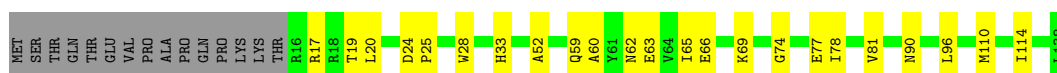
- Molecule 1: Succinate dehydrogenase subunit C

Chain G: 



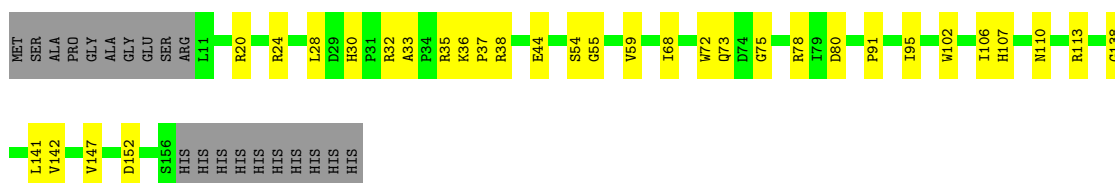
- Molecule 1: Succinate dehydrogenase subunit C

Chain M: 



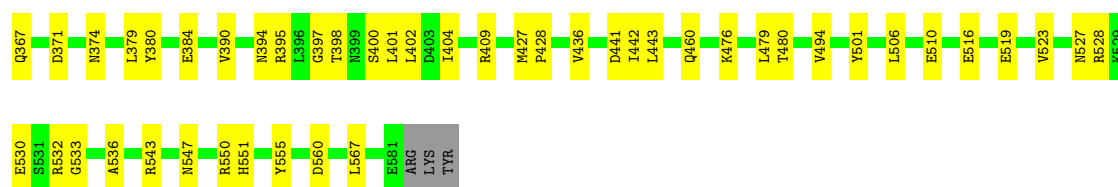
- Molecule 2: Succinate dehydrogenase subunit D

Chain D: 



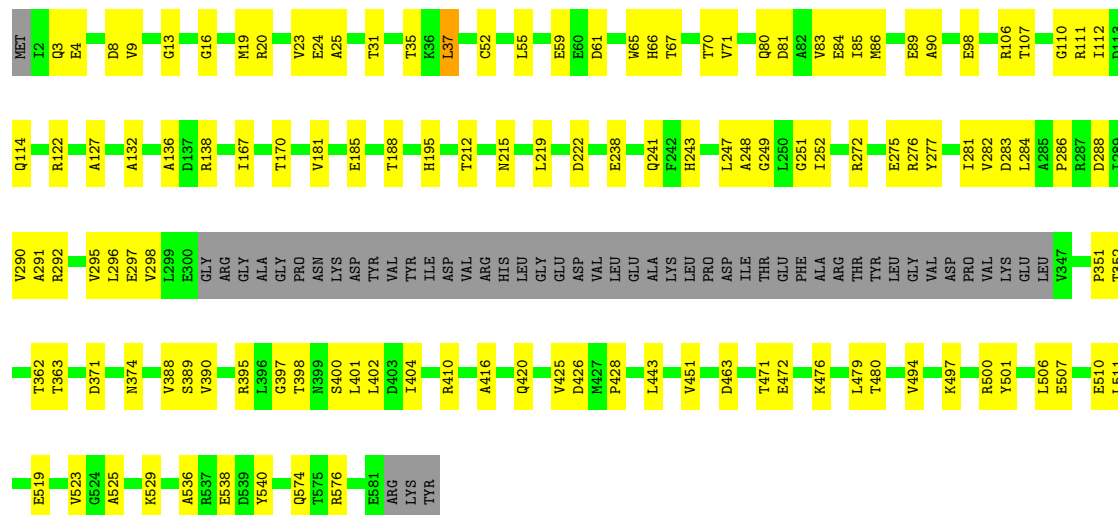
- Molecule 2: Succinate dehydrogenase subunit D

Chain H: 



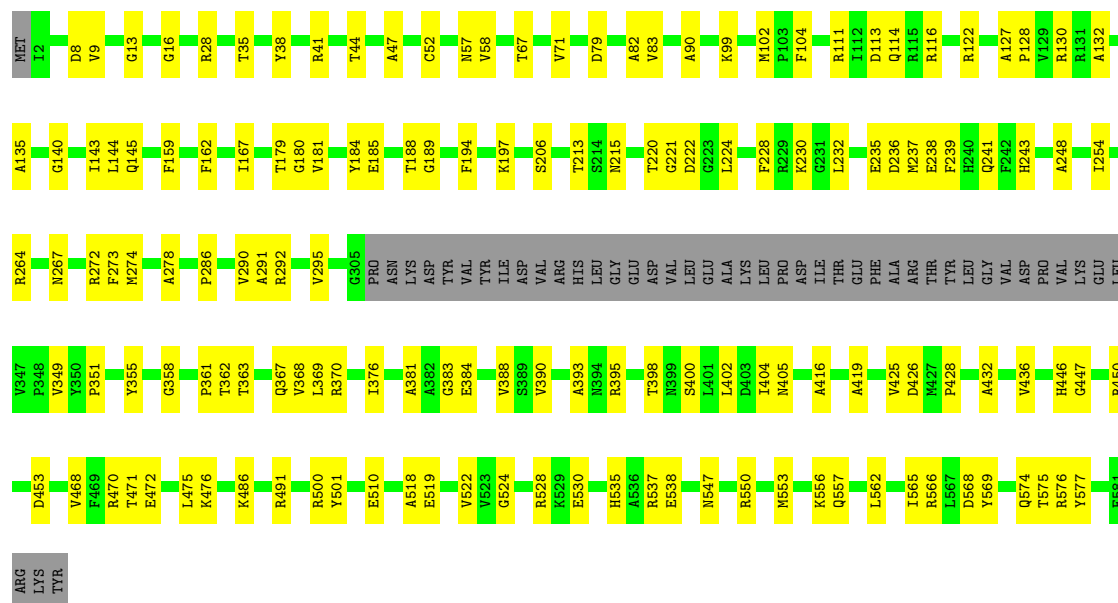
- Molecule 4: Succinate dehydrogenase subunit A

Chain J: 70% 21% 9%



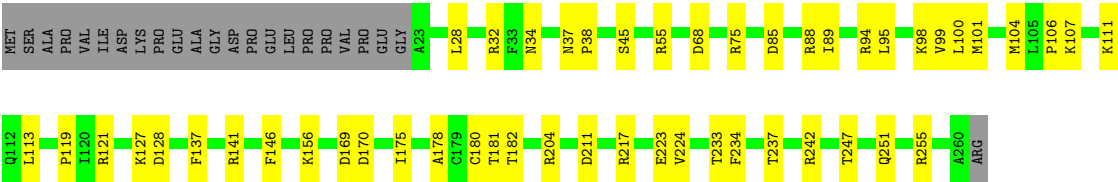
- Molecule 4: Succinate dehydrogenase subunit A

Chain P: 67% 25% 8%



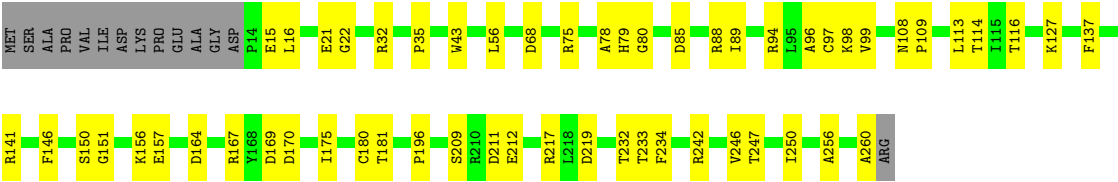
- Molecule 5: Succinate dehydrogenase subunit B

Chain B: 72% 19% 9%



• Molecule 5: Succinate dehydrogenase subunit B

Chain K: 73% 21% 5%



• Molecule 5: Succinate dehydrogenase subunit B

Chain Q: 67% 24% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	461385	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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
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: CDL, SF4, PIE, LPP, F3S, FES, MQ9, HEM, PEV, FAD

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	C	0.53	0/1003	0.51	0/1363
1	G	0.48	0/1015	0.50	0/1379
1	M	0.44	0/1016	0.51	0/1380
2	D	0.55	0/1234	0.48	0/1680
2	H	0.54	0/1025	0.50	0/1394
2	N	0.50	0/994	0.48	0/1352
3	E	0.47	0/262	0.48	0/359
3	I	0.47	0/262	0.48	0/359
3	O	0.47	0/262	0.48	0/359
4	A	0.46	0/4209	0.53	2/5704 (0.0%)
4	J	0.41	1/4189 (0.0%)	0.52	0/5677
4	P	0.31	0/4102	0.50	0/5573
5	B	0.61	0/1916	0.56	0/2605
5	K	0.57	0/1985	0.55	0/2702
5	Q	0.46	0/1891	0.52	0/2573
All	All	0.47	1/25365 (0.0%)	0.52	2/34459 (0.0%)

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
5	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	37	LEU	C-N	-5.79	1.20	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	GLY	C-N-CA	-5.96	106.79	121.70
4	A	106	ARG	C-N-CA	5.22	134.76	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	K	80	GLY	Peptide

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	C	978	0	1020	20	0
1	G	989	0	1029	19	0
1	M	990	0	1032	17	0
2	D	1193	0	1184	24	0
2	H	991	0	985	15	0
2	N	961	0	950	13	0
3	E	256	0	271	10	0
3	I	256	0	271	4	0
3	O	256	0	271	8	0
4	A	4129	0	4015	87	0
4	J	4109	0	4003	83	0
4	P	4025	0	3853	102	0
5	B	1873	0	1855	32	0
5	K	1938	0	1918	42	0
5	Q	1849	0	1826	42	0
6	C	85	0	116	0	0
6	G	44	0	61	6	0
6	K	41	0	55	2	0
6	O	44	0	61	0	0
6	Q	41	0	55	0	0
7	D	86	0	60	6	0
7	H	86	0	60	11	0
7	M	43	0	30	3	0
7	N	43	0	30	3	0
8	D	47	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	47	0	44	3	0
8	N	47	0	44	3	0
9	D	84	0	115	3	0
9	H	84	0	115	3	0
9	N	84	0	115	6	0
10	D	48	0	56	3	0
10	I	48	0	56	2	0
10	M	48	0	55	1	0
11	E	44	0	67	3	0
11	N	44	0	67	1	0
11	O	44	0	67	1	0
12	A	53	0	29	4	0
12	J	53	0	29	5	0
12	P	53	0	29	3	0
13	B	4	0	0	0	0
13	K	4	0	0	0	0
13	Q	4	0	0	0	0
14	B	8	0	0	0	0
14	K	8	0	0	0	0
14	Q	8	0	0	1	0
15	B	7	0	0	1	0
15	K	7	0	0	1	0
15	Q	7	0	0	2	0
All	All	26191	0	25943	529	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 10.

The worst 5 of 529 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:C:53:LEU:HD11	3:E:1:MET:CE	1.46	1.44
5:B:233:THR:O	15:B:303:F3S:S4	2.06	1.14
5:K:233:THR:O	15:K:303:F3S:S4	2.06	1.14
4:A:35:THR:HG22	4:A:37:LEU:H	1.16	1.08
5:Q:233:THR:O	15:Q:303:F3S:S4	2.12	1.07

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	C	120/138 (87%)	113 (94%)	7 (6%)	0	100	100
1	G	121/138 (88%)	117 (97%)	4 (3%)	0	100	100
1	M	121/138 (88%)	116 (96%)	5 (4%)	0	100	100
2	D	144/166 (87%)	138 (96%)	6 (4%)	0	100	100
2	H	118/166 (71%)	113 (96%)	5 (4%)	0	100	100
2	N	114/166 (69%)	111 (97%)	3 (3%)	0	100	100
3	E	29/32 (91%)	29 (100%)	0	0	100	100
3	I	29/32 (91%)	29 (100%)	0	0	100	100
3	O	29/32 (91%)	29 (100%)	0	0	100	100
4	A	535/584 (92%)	480 (90%)	54 (10%)	1 (0%)	49	79
4	J	530/584 (91%)	464 (88%)	65 (12%)	1 (0%)	49	79
4	P	535/584 (92%)	482 (90%)	53 (10%)	0	100	100
5	B	236/261 (90%)	199 (84%)	36 (15%)	1 (0%)	36	67
5	K	245/261 (94%)	200 (82%)	44 (18%)	1 (0%)	36	67
5	Q	236/261 (90%)	198 (84%)	38 (16%)	0	100	100
All	All	3142/3543 (89%)	2818 (90%)	320 (10%)	4 (0%)	56	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	248	ALA
4	A	248	ALA
5	B	101	MET
5	K	96	ALA

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	C	101/116 (87%)	101 (100%)	0	100	100
1	G	102/116 (88%)	102 (100%)	0	100	100
1	M	102/116 (88%)	102 (100%)	0	100	100
2	D	120/137 (88%)	120 (100%)	0	100	100
2	H	100/137 (73%)	100 (100%)	0	100	100
2	N	97/137 (71%)	97 (100%)	0	100	100
3	E	27/28 (96%)	27 (100%)	0	100	100
3	I	27/28 (96%)	27 (100%)	0	100	100
3	O	27/28 (96%)	27 (100%)	0	100	100
4	A	421/467 (90%)	421 (100%)	0	100	100
4	J	422/467 (90%)	422 (100%)	0	100	100
4	P	400/467 (86%)	400 (100%)	0	100	100
5	B	205/225 (91%)	202 (98%)	3 (2%)	67	89
5	K	213/225 (95%)	212 (100%)	1 (0%)	90	96
5	Q	199/225 (88%)	196 (98%)	3 (2%)	67	89
All	All	2563/2919 (88%)	2556 (100%)	7 (0%)	93	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	75	ARG
5	Q	217	ARG
5	Q	75	ARG
5	B	111	LYS
5	Q	204	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	460	GLN
5	K	245	GLN
4	P	557	GLN
4	J	477	GLN
1	M	33	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

39 ligands are modelled in this entry.

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	$\# Z > 2$
14	SF4	Q	302	5	0,12,12	0.00	-	-		
6	PEV	K	304	-	40,40,48	0.97	3 (7%)	43,45,53	0.95	2 (4%)
6	PEV	Q	304	-	40,40,48	0.99	3 (7%)	43,45,53	0.93	2 (4%)
8	MQ9	N	203	-	24,24,59	3.80	12 (50%)	30,33,75	2.84	12 (40%)
10	PIE	M	202	-	48,48,57	0.95	4 (8%)	58,60,69	1.02	4 (6%)
13	FES	Q	301	5	0,4,4	0.00	-	-		
15	F3S	Q	303	5	0,9,9	0.00	-	-		
12	FAD	A	601	-	51,58,58	1.29	5 (9%)	60,89,89	2.24	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CDL	D	205	-	83,83,99	1.35	10 (12%)	89,95,111	1.01	4 (4%)
9	CDL	H	205	-	83,83,99	1.36	10 (12%)	89,95,111	0.97	4 (4%)
8	MQ9	H	204	-	24,24,59	3.88	14 (58%)	30,33,75	3.16	12 (40%)
7	HEM	H	201	-	27,50,50	1.83	4 (14%)	17,82,82	1.90	7 (41%)
6	PEV	G	201	-	43,43,48	0.97	3 (6%)	46,48,53	0.92	2 (4%)
12	FAD	P	601	-	51,58,58	1.23	4 (7%)	60,89,89	2.24	7 (11%)
7	HEM	M	201	2	27,50,50	1.86	4 (14%)	17,82,82	1.67	4 (23%)
15	F3S	K	303	5	0,9,9	0.00	-	-	-	-
12	FAD	J	601	-	51,58,58	1.27	4 (7%)	60,89,89	2.25	8 (13%)
10	PIE	I	101	-	48,48,57	0.95	4 (8%)	58,60,69	0.99	3 (5%)
8	MQ9	D	203	-	25,25,59	3.91	14 (56%)	31,34,75	3.13	11 (35%)
6	PEV	O	102	-	43,43,48	0.98	3 (6%)	46,48,53	0.95	2 (4%)
6	PEV	C	202	-	43,43,48	0.98	3 (6%)	46,48,53	0.95	2 (4%)
7	HEM	N	201	1	27,50,50	1.94	7 (25%)	17,82,82	2.11	8 (47%)
11	LPP	O	101	-	43,43,43	1.08	3 (6%)	47,48,48	0.88	2 (4%)
13	FES	K	301	5	0,4,4	0.00	-	-	-	-
11	LPP	E	101	-	43,43,43	1.08	3 (6%)	47,48,48	0.90	2 (4%)
13	FES	B	301	5	0,4,4	0.00	-	-	-	-
8	MQ9	N	202	-	25,25,59	3.89	14 (56%)	31,34,75	3.05	10 (32%)
14	SF4	K	302	5	0,12,12	0.00	-	-	-	-
7	HEM	D	202	1	27,50,50	1.96	7 (25%)	17,82,82	2.06	8 (47%)
7	HEM	D	201	2	27,50,50	1.88	4 (14%)	17,82,82	1.74	3 (17%)
6	PEV	C	201	-	40,40,48	0.98	4 (10%)	43,45,53	0.89	2 (4%)
15	F3S	B	303	5	0,9,9	0.00	-	-	-	-
11	LPP	N	204	-	43,43,43	1.08	3 (6%)	47,48,48	0.93	2 (4%)
14	SF4	B	302	5	0,12,12	0.00	-	-	-	-
7	HEM	H	202	2	27,50,50	1.89	4 (14%)	17,82,82	1.74	5 (29%)
10	PIE	D	206	-	48,48,57	0.94	4 (8%)	58,60,69	0.91	2 (3%)
8	MQ9	D	204	-	24,24,59	3.89	12 (50%)	30,33,75	2.39	9 (30%)
8	MQ9	H	203	-	25,25,59	3.81	12 (48%)	31,34,75	3.22	12 (38%)
9	CDL	N	205	-	83,83,99	1.35	10 (12%)	89,95,111	0.99	4 (4%)

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
14	SF4	Q	302	5	-	-	0/6/5/5
6	PEV	K	304	-	-	23/44/44/52	-
6	PEV	Q	304	-	-	26/44/44/52	-
8	MQ9	N	203	-	-	9/11/31/73	0/2/2/2
10	PIE	M	202	-	-	22/43/67/76	0/1/1/1
13	FES	Q	301	5	-	-	0/1/1/1
12	FAD	A	601	-	-	8/30/50/50	0/6/6/6
9	CDL	D	205	-	-	51/94/94/110	-
9	CDL	H	205	-	-	54/94/94/110	-
8	MQ9	H	204	-	-	7/11/31/73	0/2/2/2
7	HEM	H	201	-	-	2/6/54/54	-
6	PEV	G	201	-	-	22/47/47/52	-
12	FAD	P	601	-	-	12/30/50/50	0/6/6/6
7	HEM	M	201	2	-	0/6/54/54	-
14	SF4	K	302	5	-	-	0/6/5/5
15	F3S	K	303	5	-	-	0/3/3/3
10	PIE	I	101	-	-	24/43/67/76	0/1/1/1
8	MQ9	D	203	-	-	7/13/33/73	0/2/2/2
6	PEV	O	102	-	-	27/47/47/52	-
6	PEV	C	202	-	-	23/47/47/52	-
7	HEM	N	201	1	-	3/6/54/54	-
11	LPP	O	101	-	-	28/45/45/45	-
13	FES	K	301	5	-	-	0/1/1/1
11	LPP	E	101	-	-	26/45/45/45	-
13	FES	B	301	5	-	-	0/1/1/1
8	MQ9	N	202	-	-	6/13/33/73	0/2/2/2
15	F3S	Q	303	5	-	-	0/3/3/3
7	HEM	D	202	1	-	3/6/54/54	-
7	HEM	D	201	2	-	0/6/54/54	-
6	PEV	C	201	-	-	24/44/44/52	-
15	F3S	B	303	5	-	-	0/3/3/3
12	FAD	J	601	-	-	20/30/50/50	0/6/6/6
11	LPP	N	204	-	-	24/45/45/45	-
14	SF4	B	302	5	-	-	0/6/5/5
7	HEM	H	202	2	-	0/6/54/54	-
10	PIE	D	206	-	-	20/43/67/76	0/1/1/1
8	MQ9	D	204	-	-	6/11/31/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MQ9	H	203	-	-	9/13/33/73	0/2/2/2
9	CDL	N	205	-	-	64/94/94/110	-

The worst 5 of 191 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	204	MQ9	C8-C9	9.27	1.55	1.33
8	D	203	MQ9	C13-C14	9.22	1.55	1.33
8	N	202	MQ9	C13-C14	9.19	1.55	1.33
8	D	203	MQ9	C8-C9	8.97	1.54	1.33
8	H	204	MQ9	C8-C9	8.94	1.54	1.33

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	601	FAD	C4-N3-C2	13.04	126.15	115.14
12	J	601	FAD	C4-N3-C2	13.01	126.12	115.14
12	A	601	FAD	C4-N3-C2	13.00	126.12	115.14
8	H	204	MQ9	C7-C8-C9	-10.83	108.75	126.79
8	H	203	MQ9	C7-C8-C9	-8.63	112.42	126.79

There are no chirality outliers.

5 of 550 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Q	304	PEV	C1-O3P-P-O1P
6	Q	304	PEV	C1-O3P-P-O2P
6	Q	304	PEV	C1-O3P-P-O4P
6	Q	304	PEV	C4-O4P-P-O3P
6	Q	304	PEV	O4P-C4-C5-N6

There are no ring outliers.

30 monomers are involved in 77 short contacts:

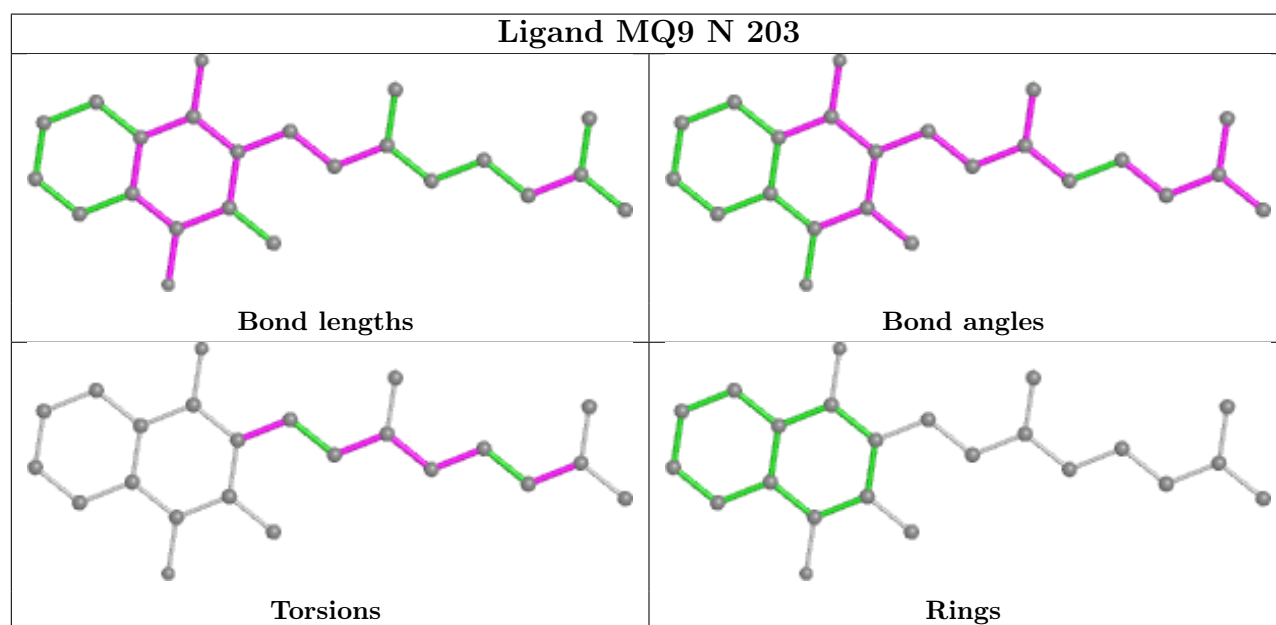
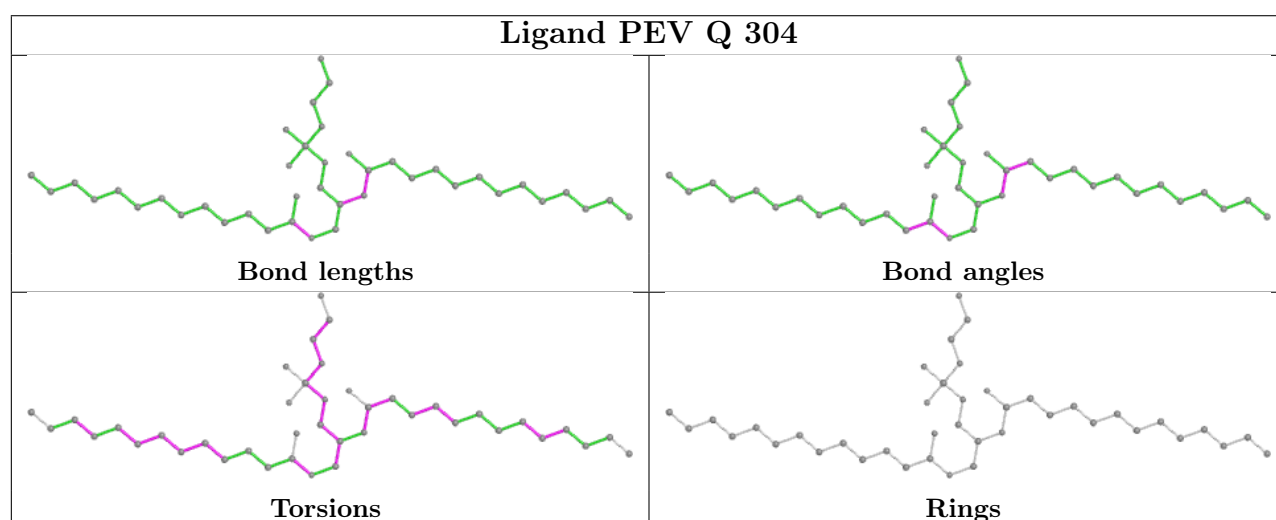
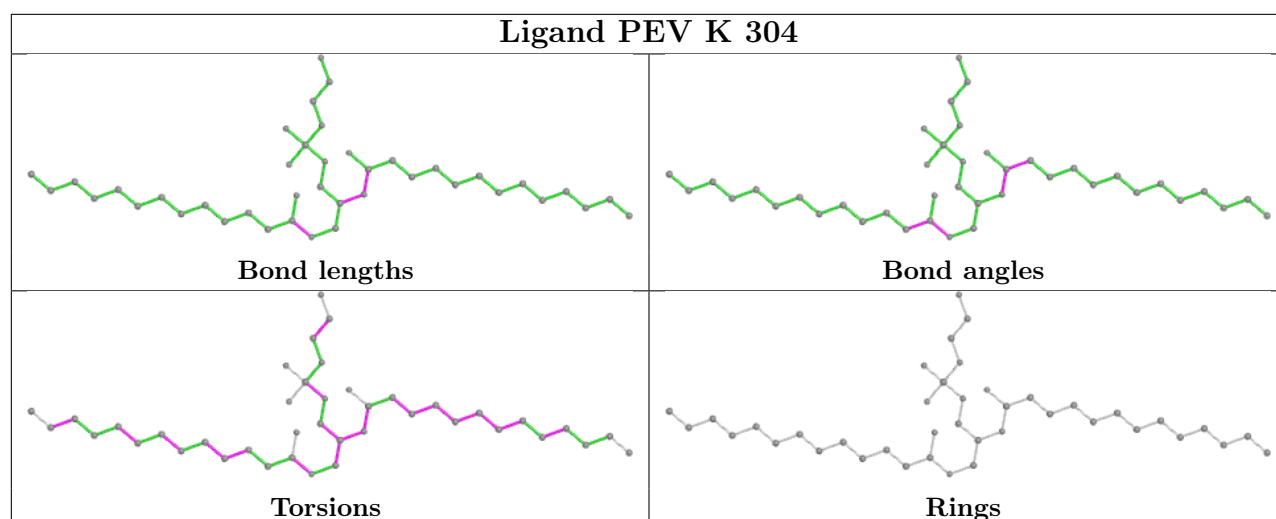
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Q	302	SF4	1	0
6	K	304	PEV	2	0
8	N	203	MQ9	2	0
10	M	202	PIE	1	0
12	A	601	FAD	4	0

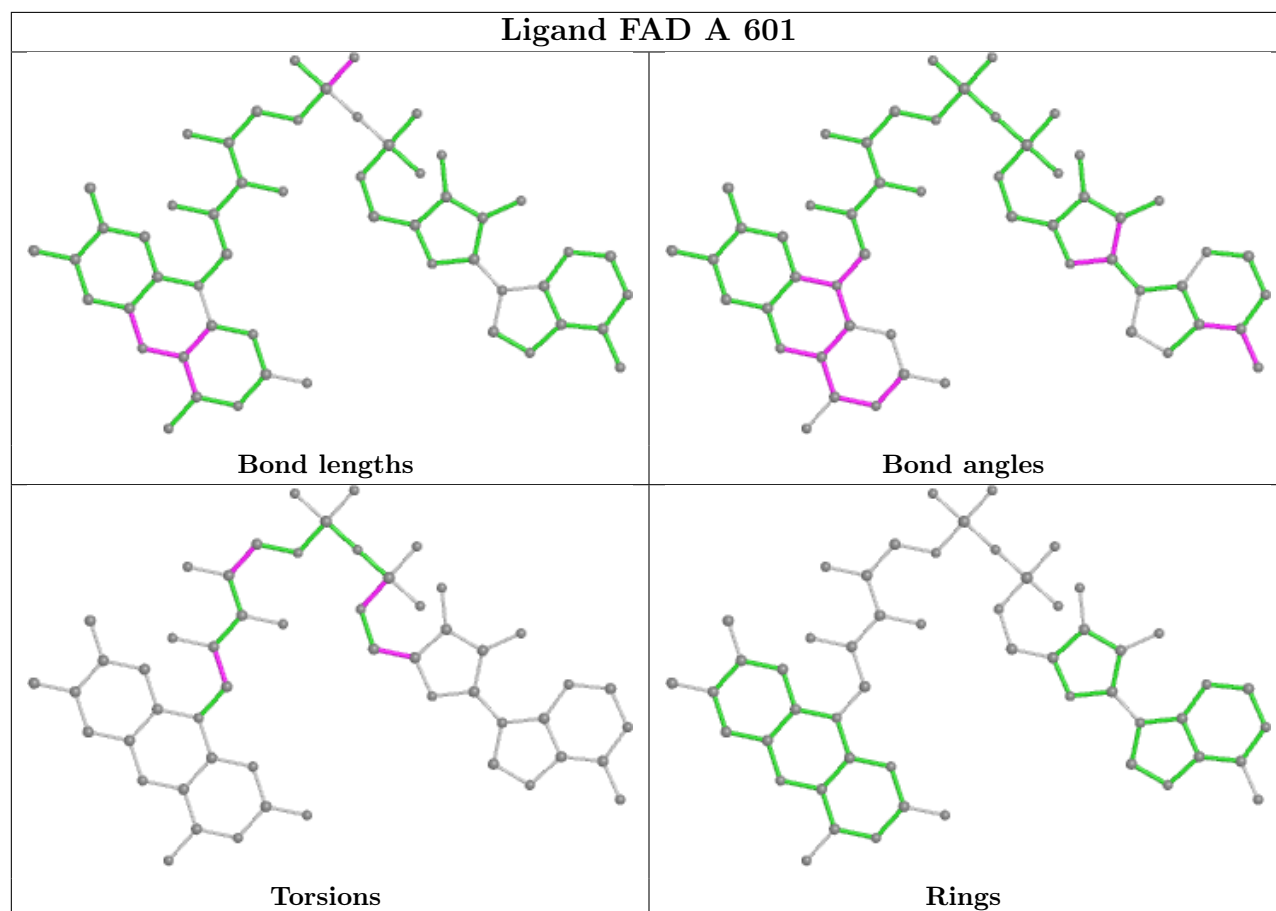
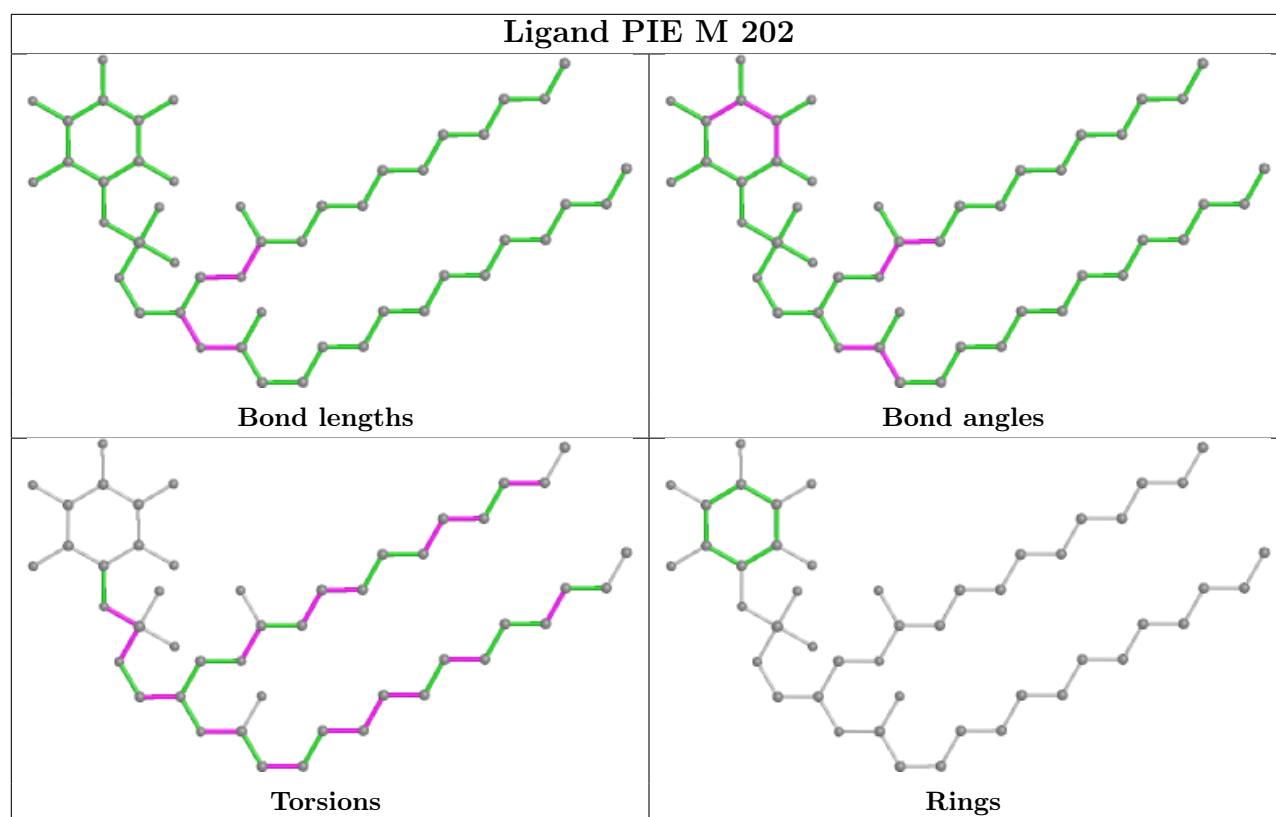
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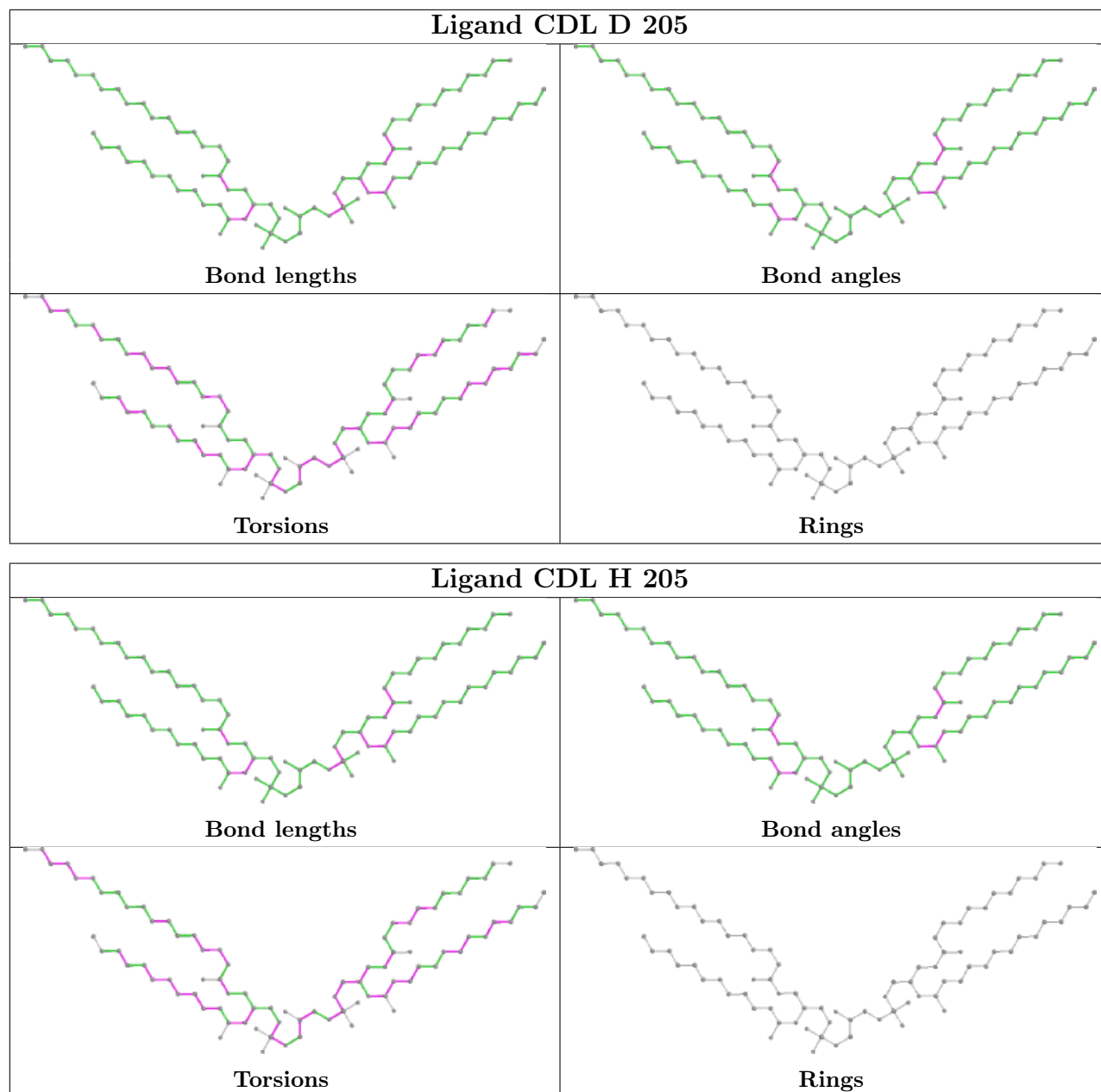
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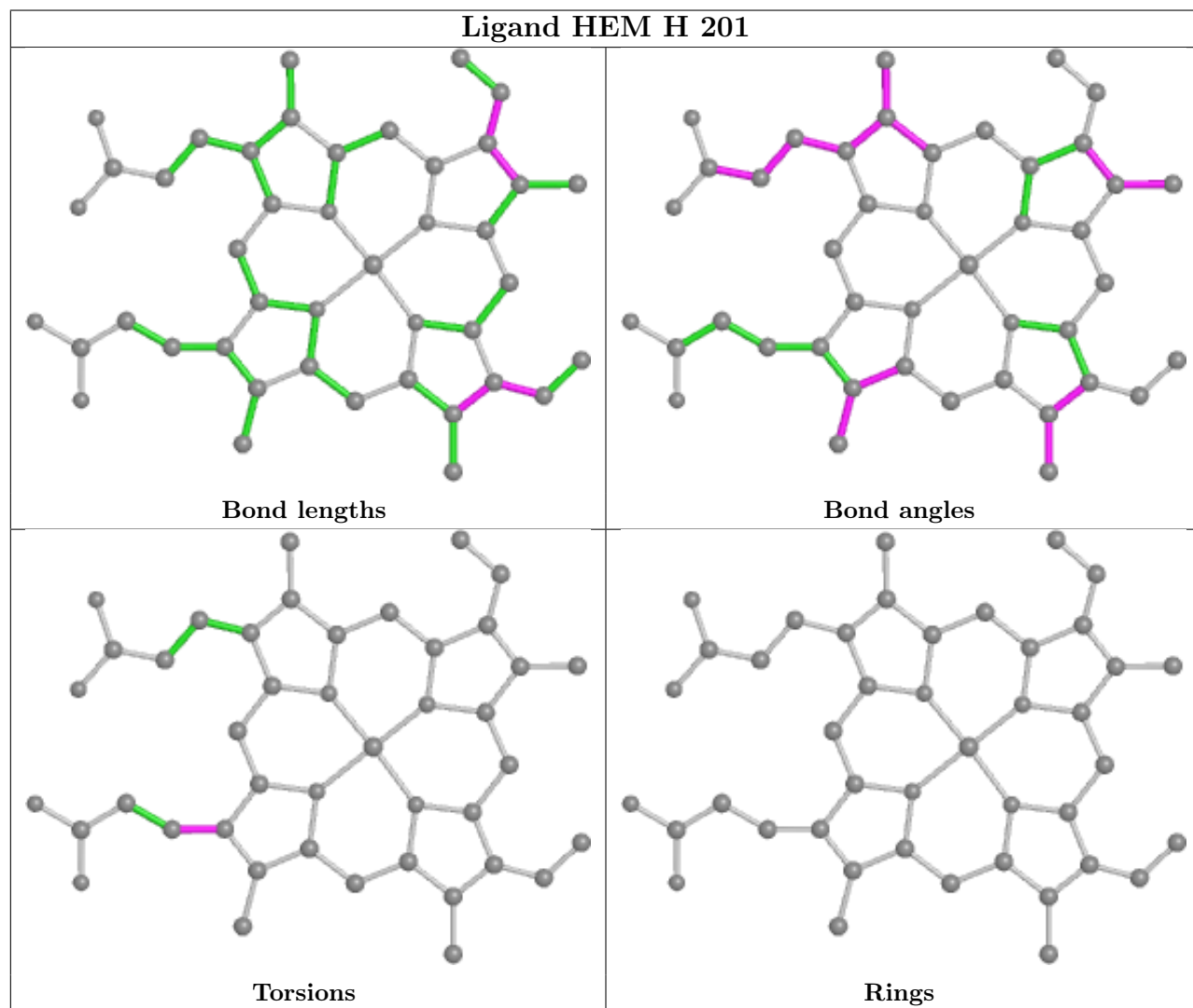
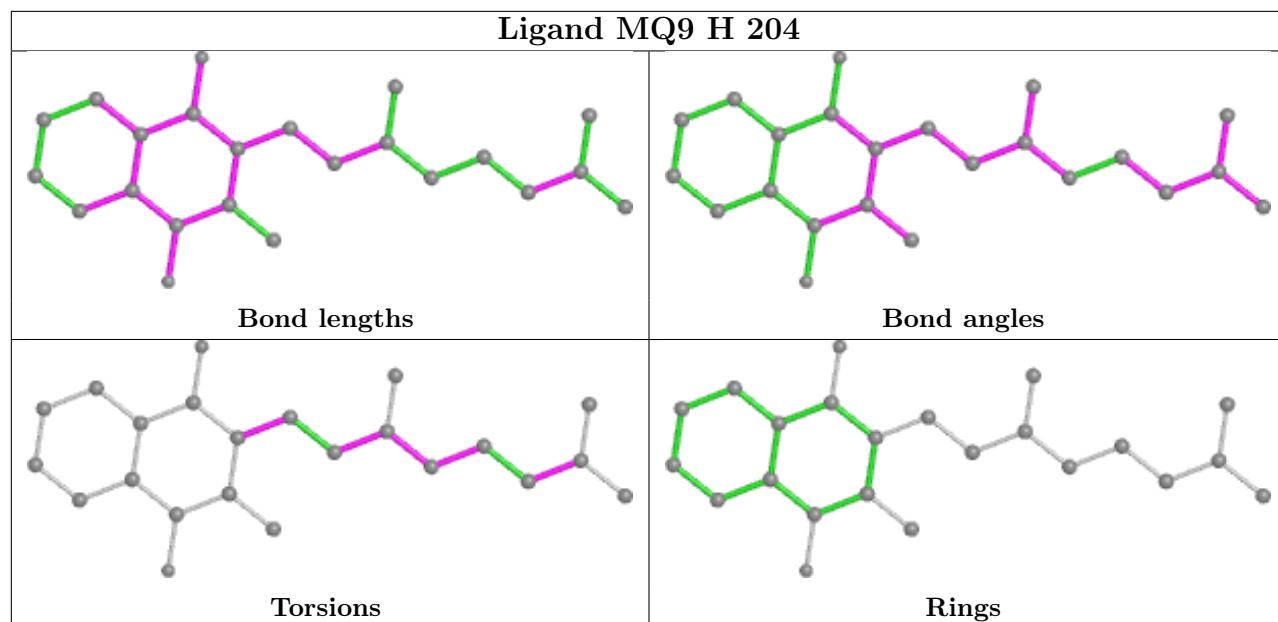
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	205	CDL	3	0
9	H	205	CDL	3	0
8	H	204	MQ9	1	0
7	H	201	HEM	8	0
6	G	201	PEV	6	0
12	P	601	FAD	3	0
7	M	201	HEM	3	0
15	K	303	F3S	1	0
10	I	101	PIE	2	0
8	D	203	MQ9	1	0
7	N	201	HEM	3	0
11	O	101	LPP	1	0
11	E	101	LPP	3	0
8	N	202	MQ9	1	0
15	Q	303	F3S	2	0
7	D	202	HEM	3	0
7	D	201	HEM	3	0
15	B	303	F3S	1	0
12	J	601	FAD	5	0
11	N	204	LPP	1	0
7	H	202	HEM	5	0
10	D	206	PIE	3	0
8	D	204	MQ9	2	0
8	H	203	MQ9	2	0
9	N	205	CDL	6	0

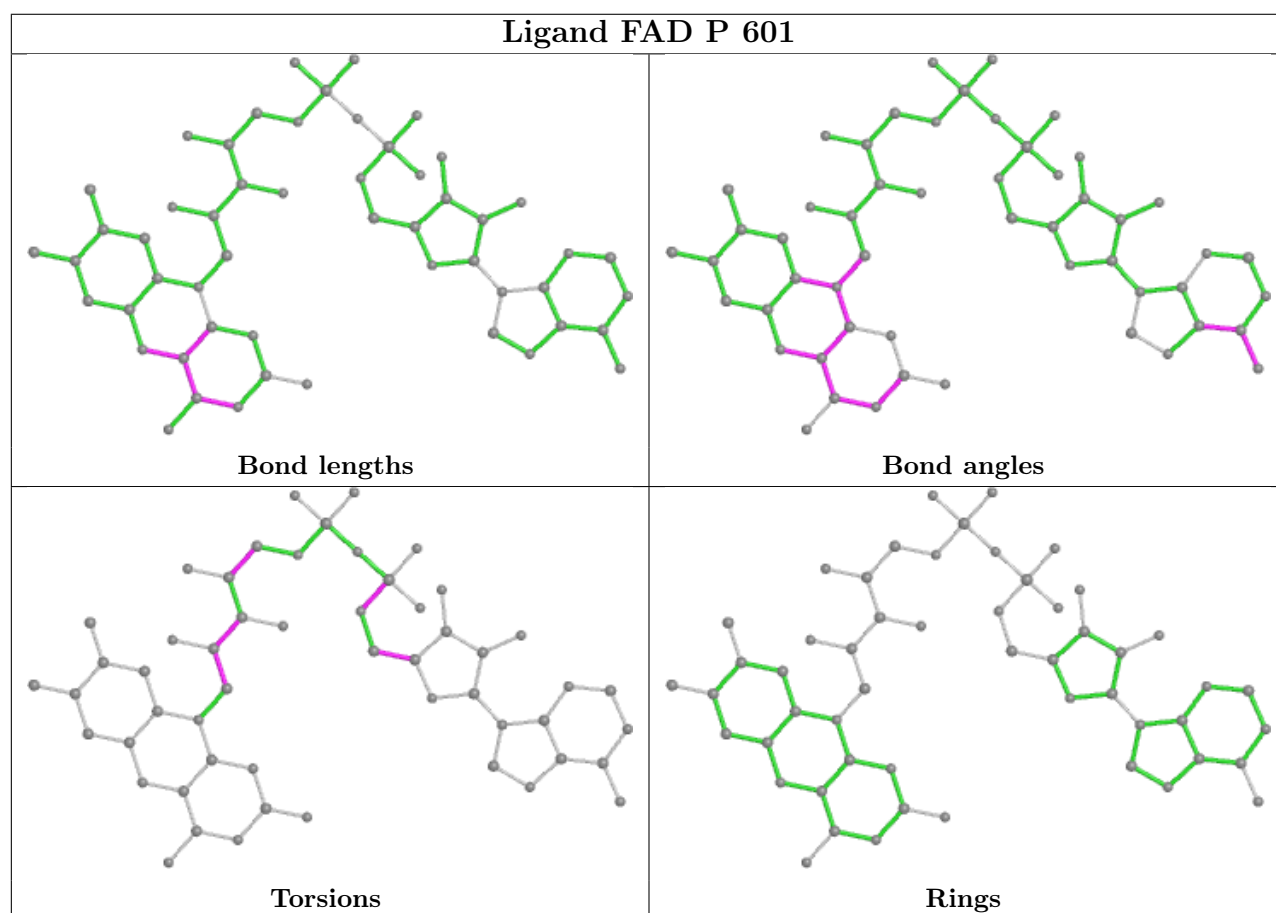
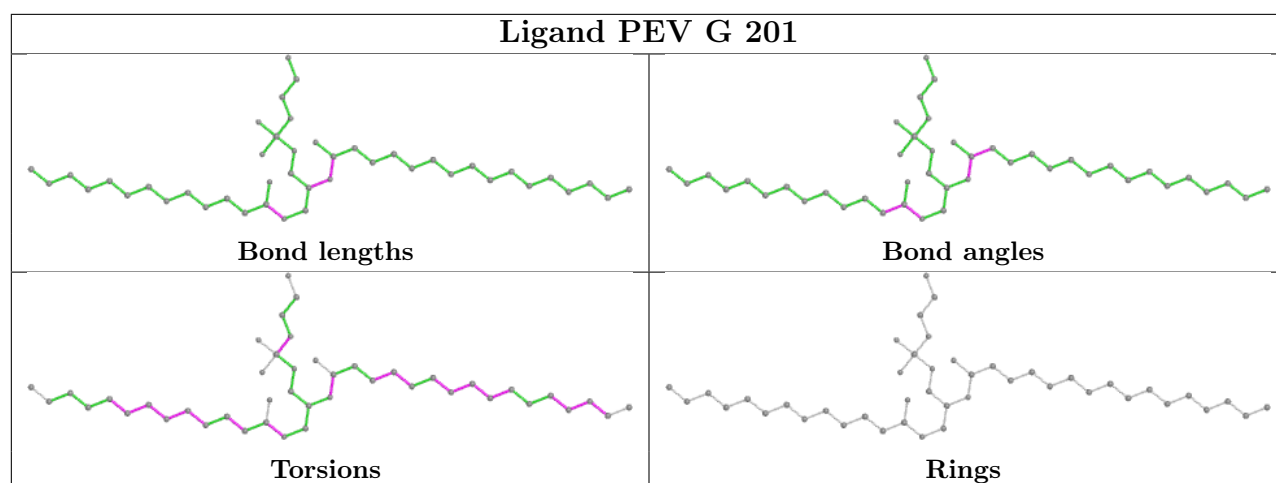
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

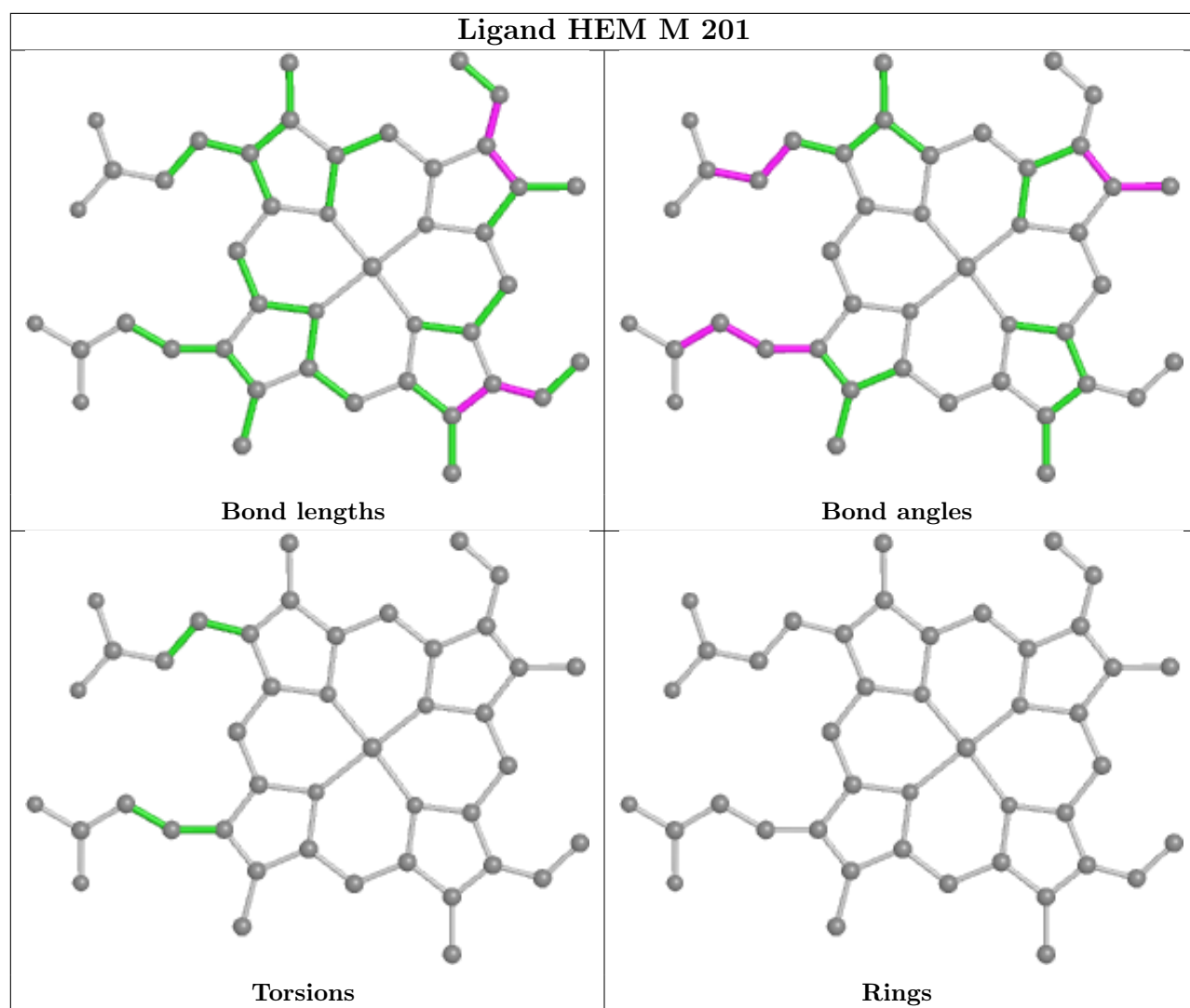


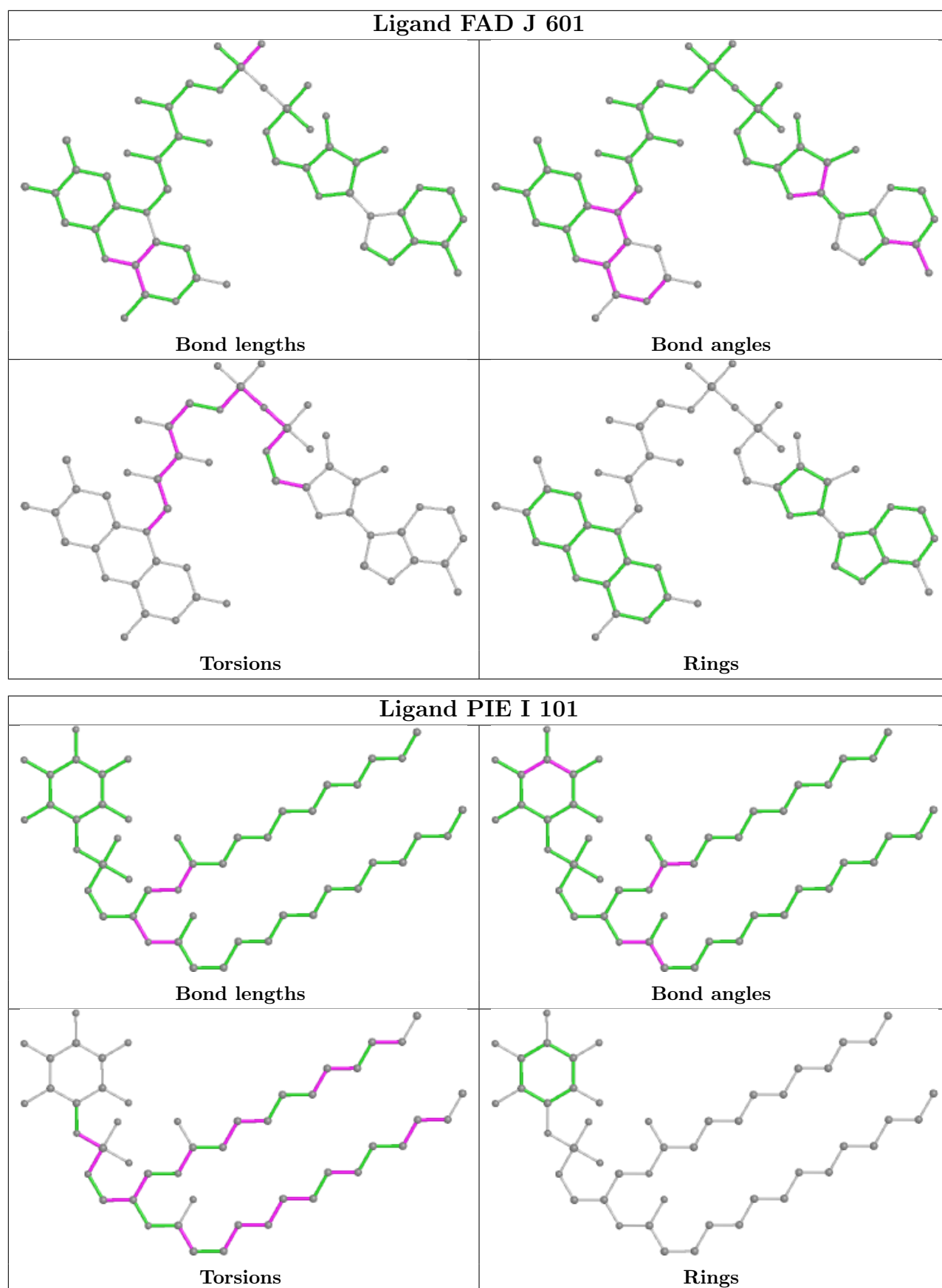


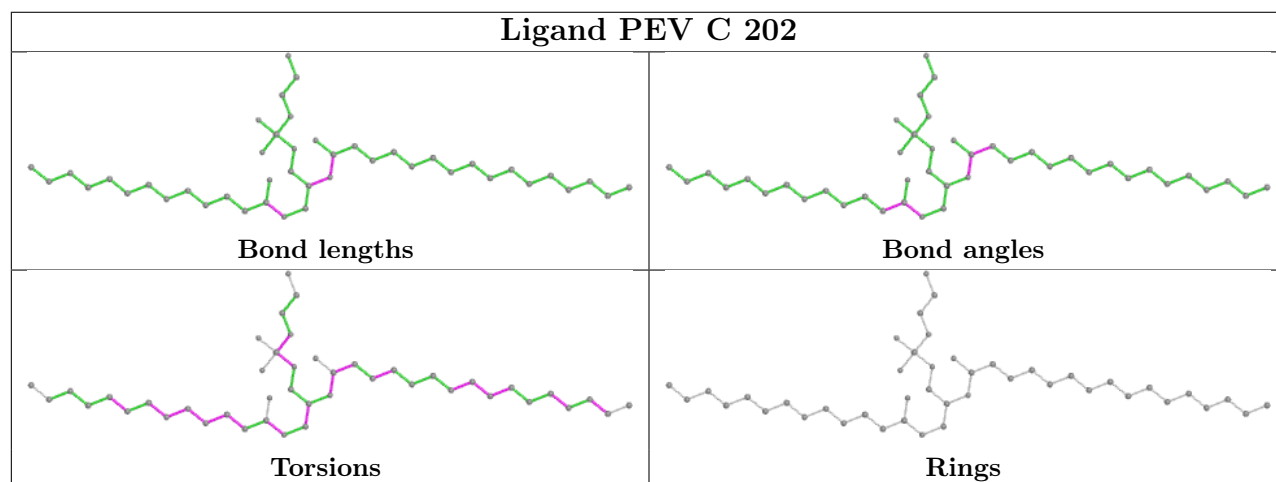
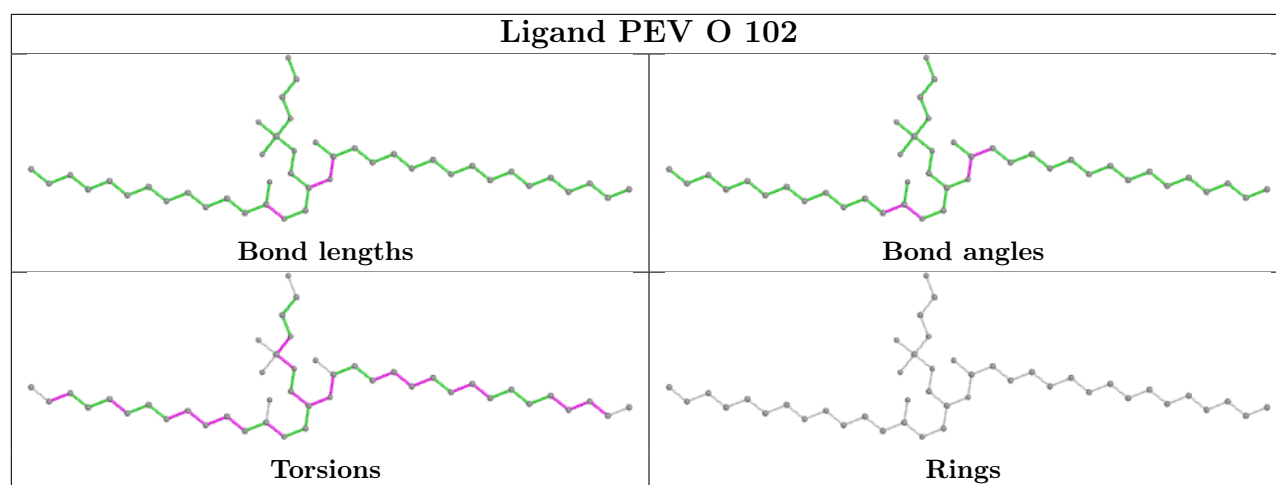
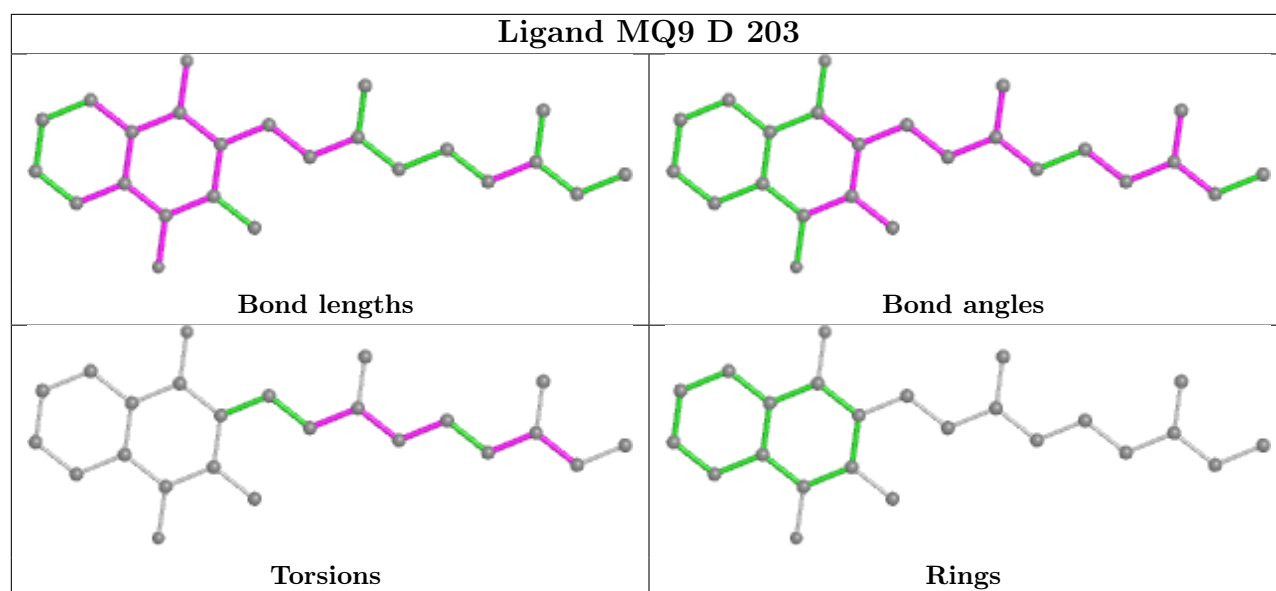


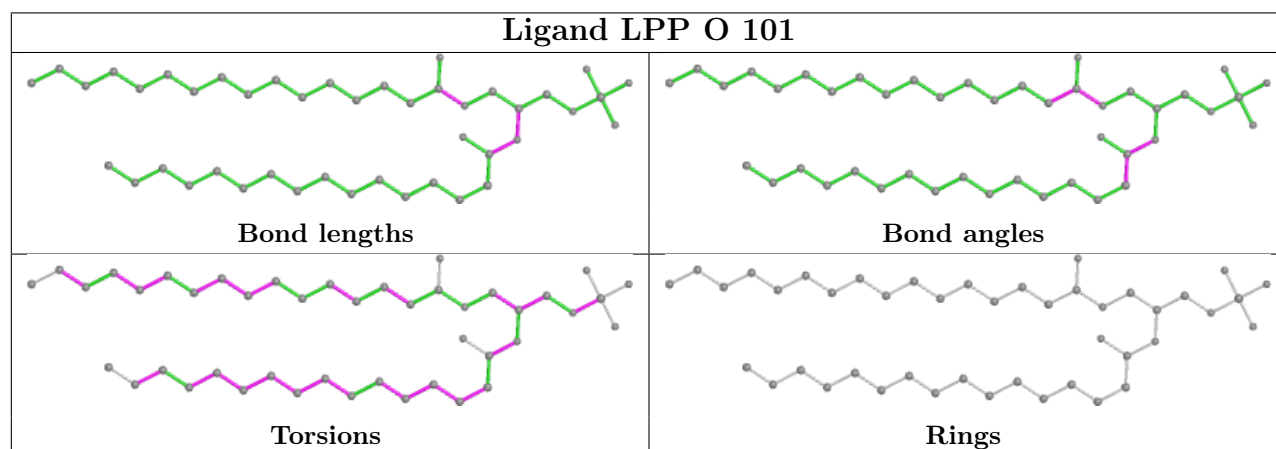
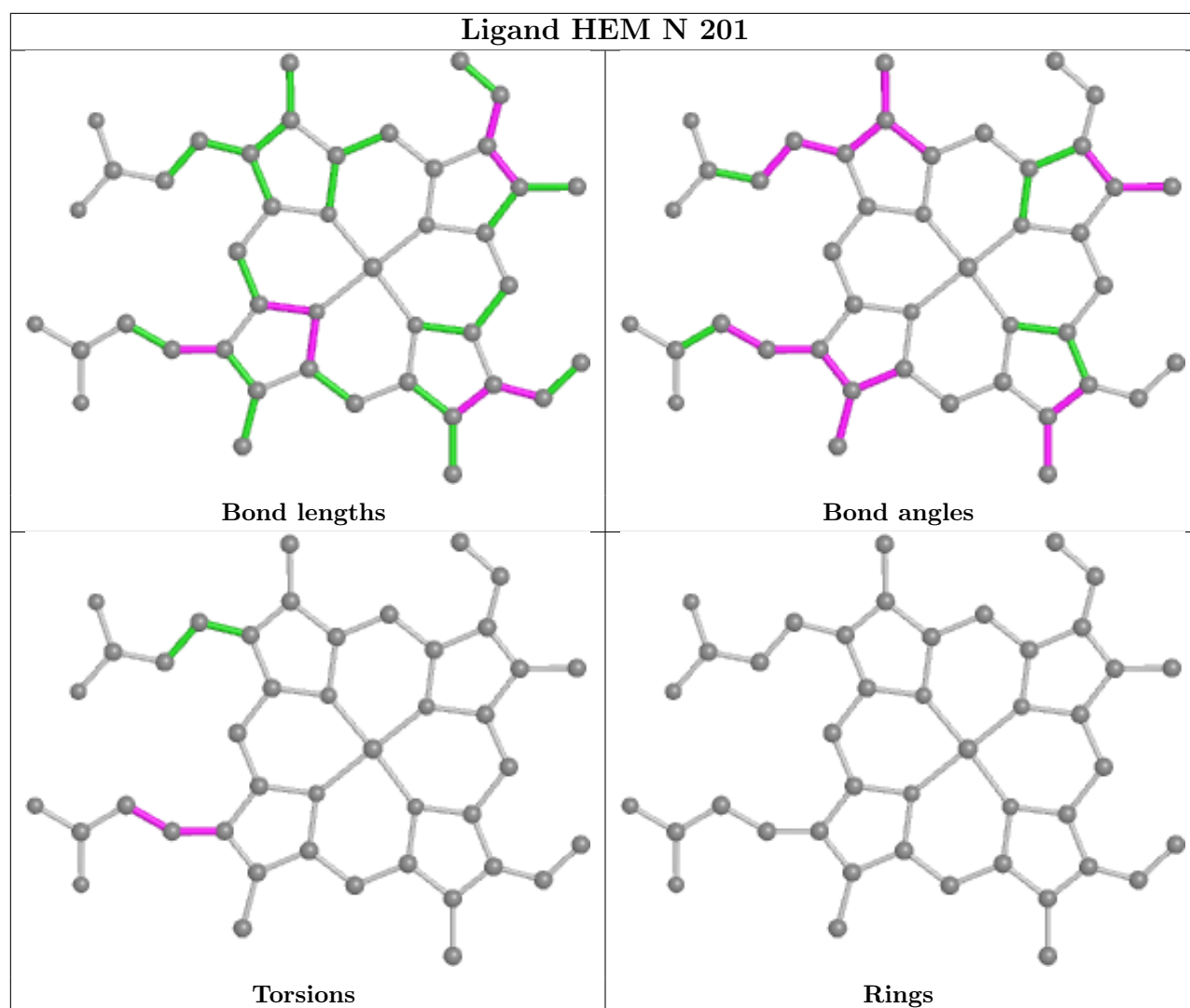




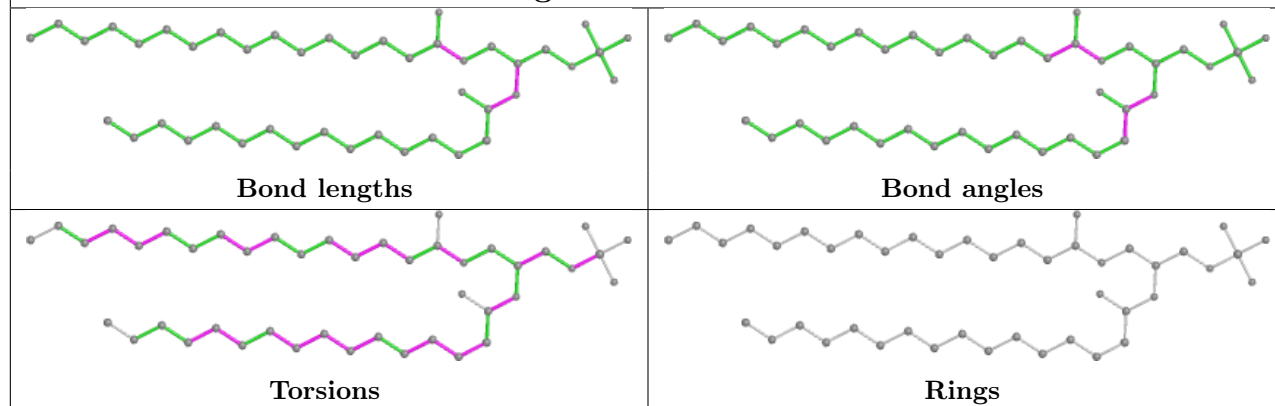




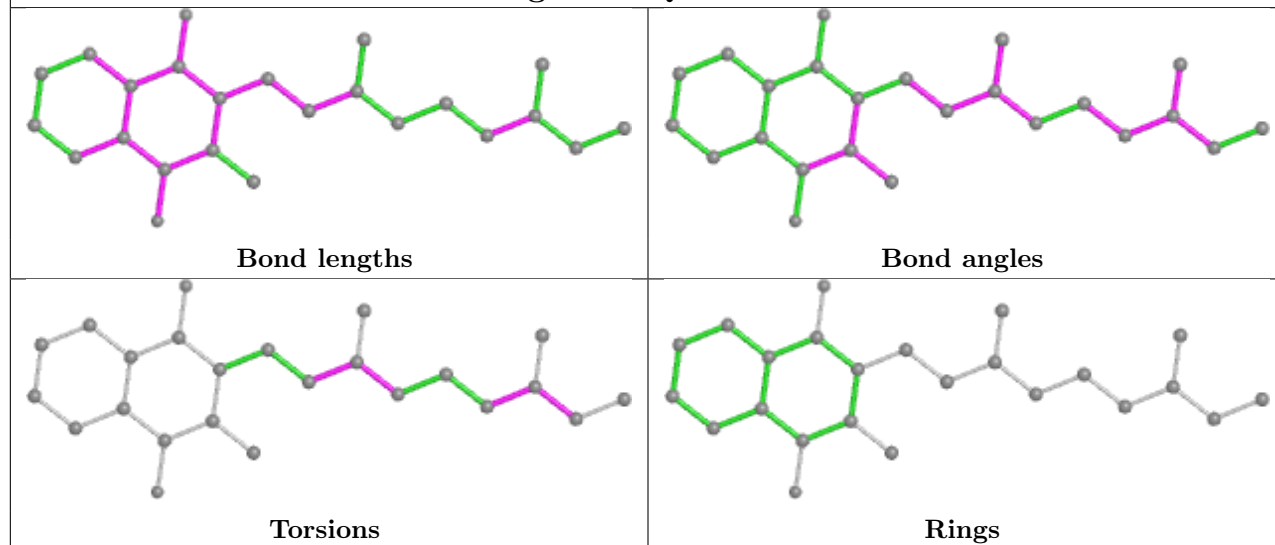


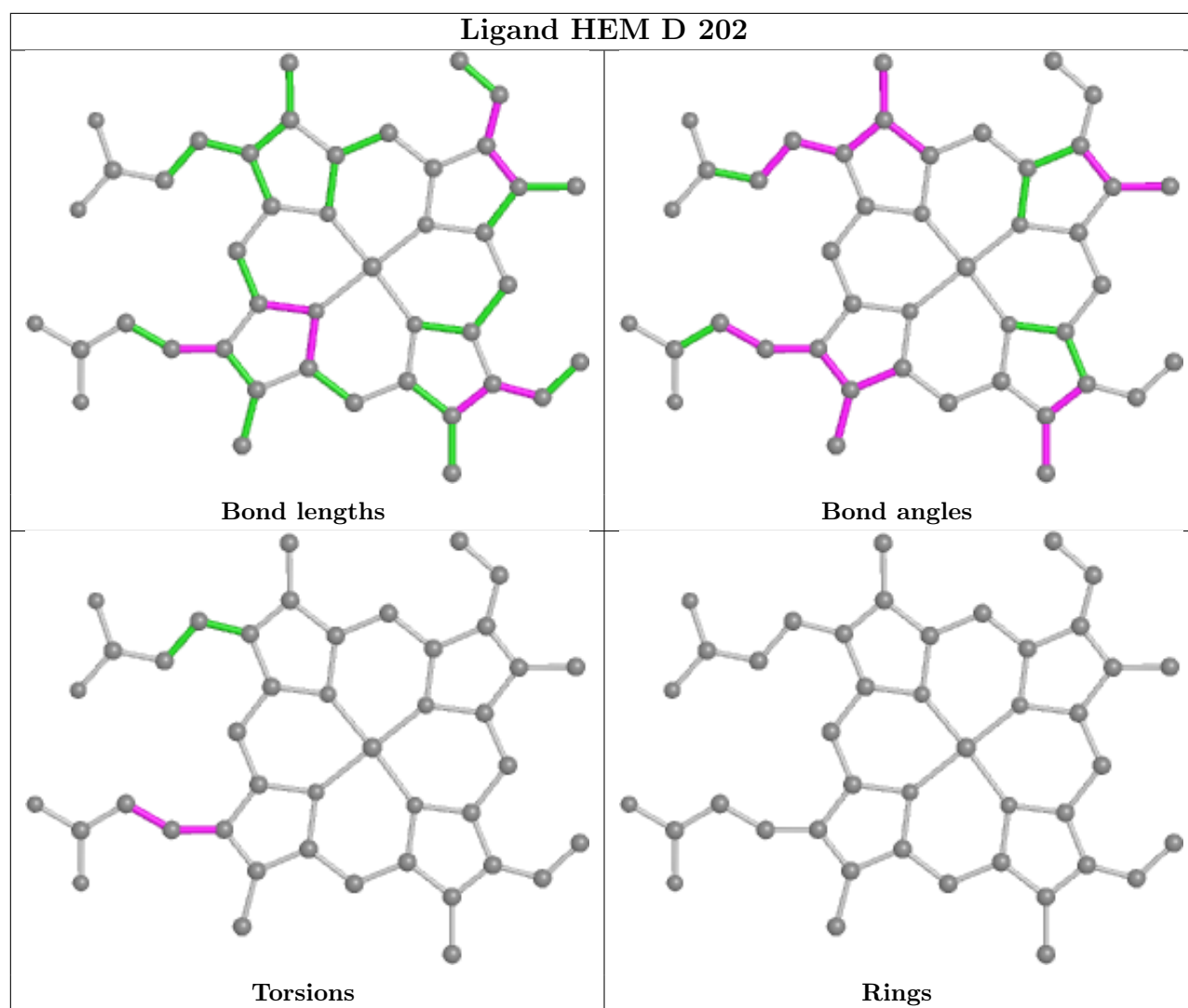


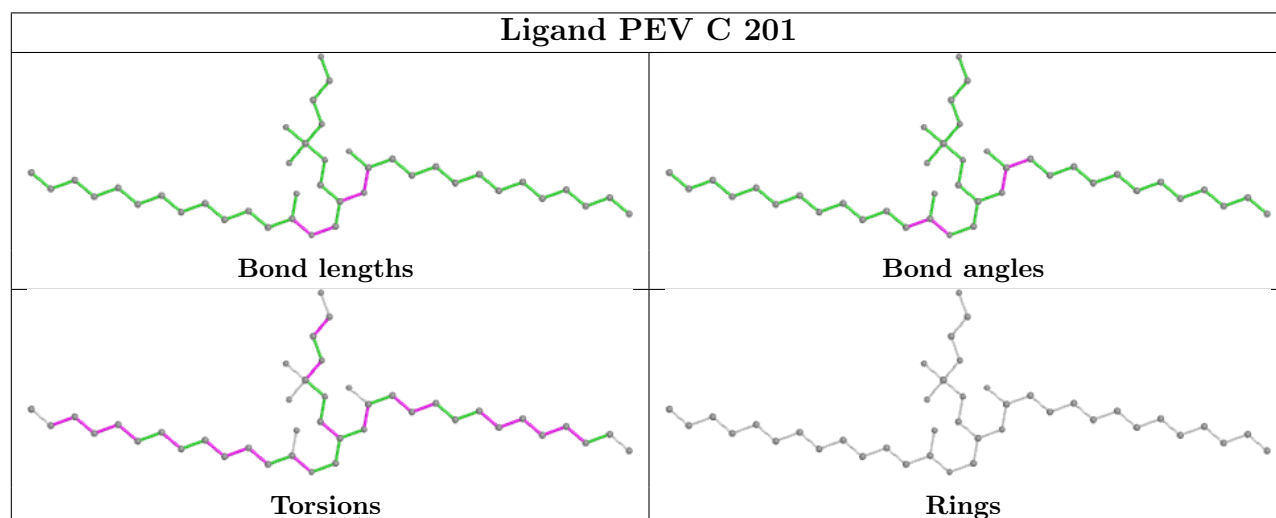
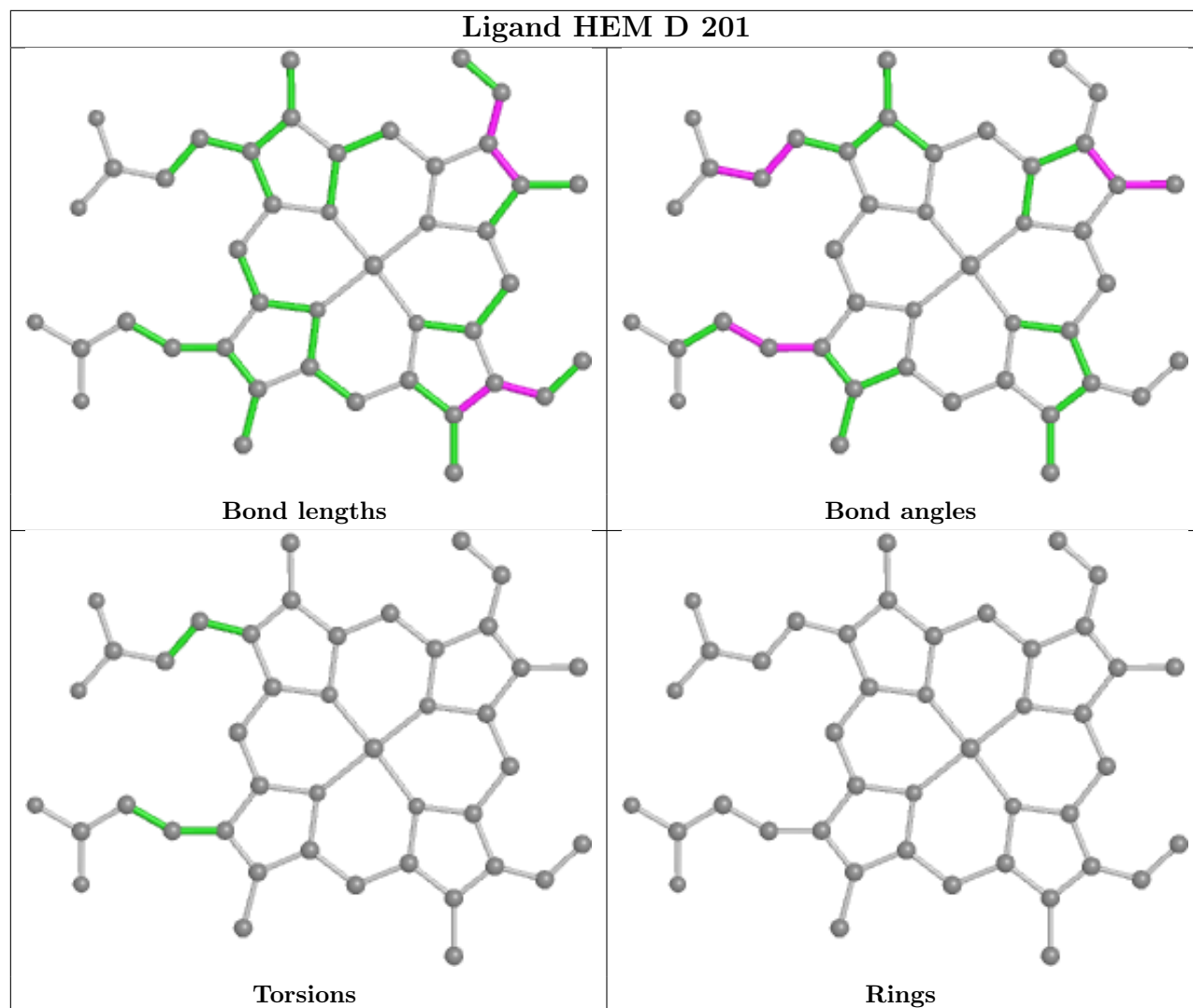
Ligand LPP E 101

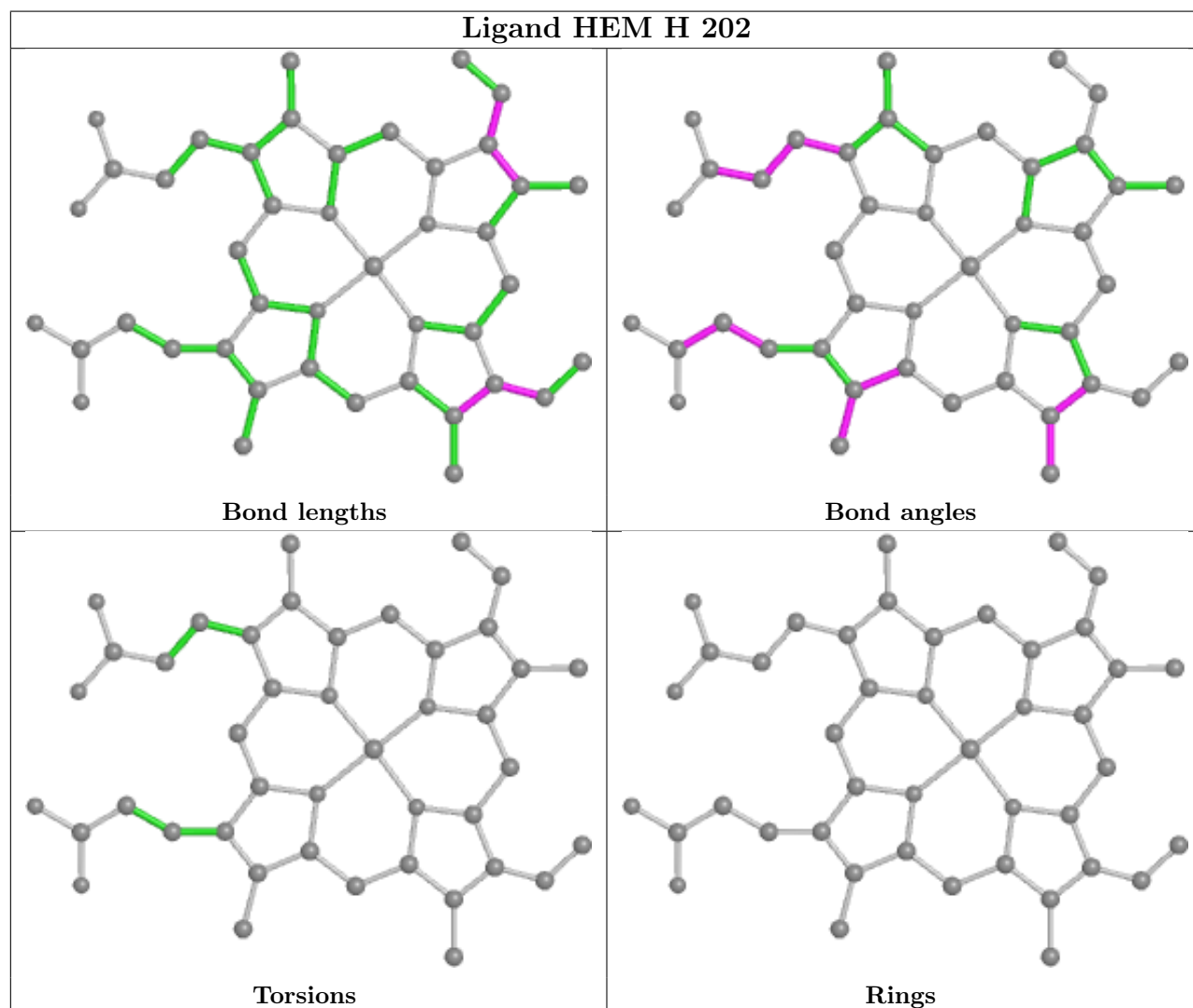
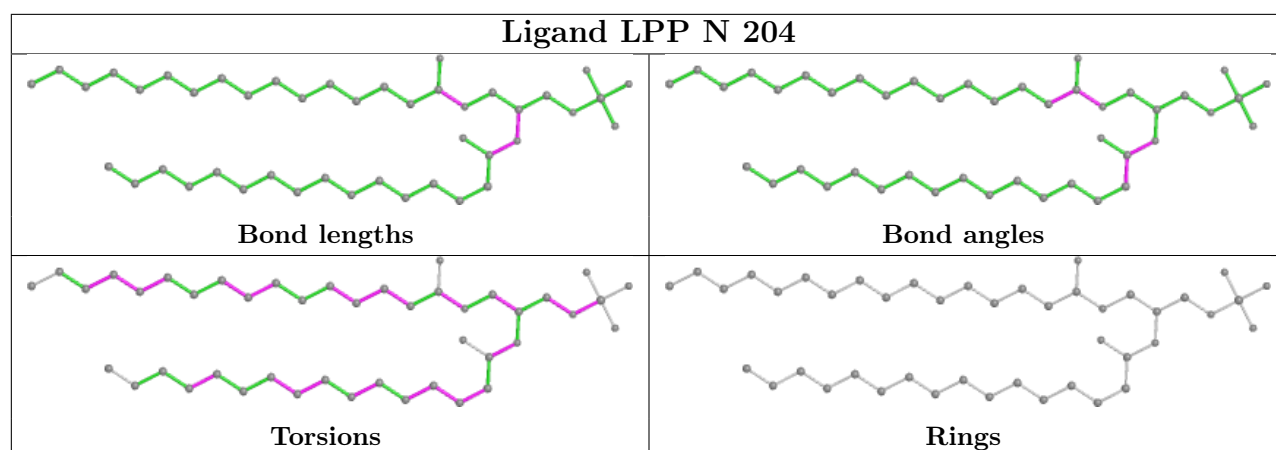


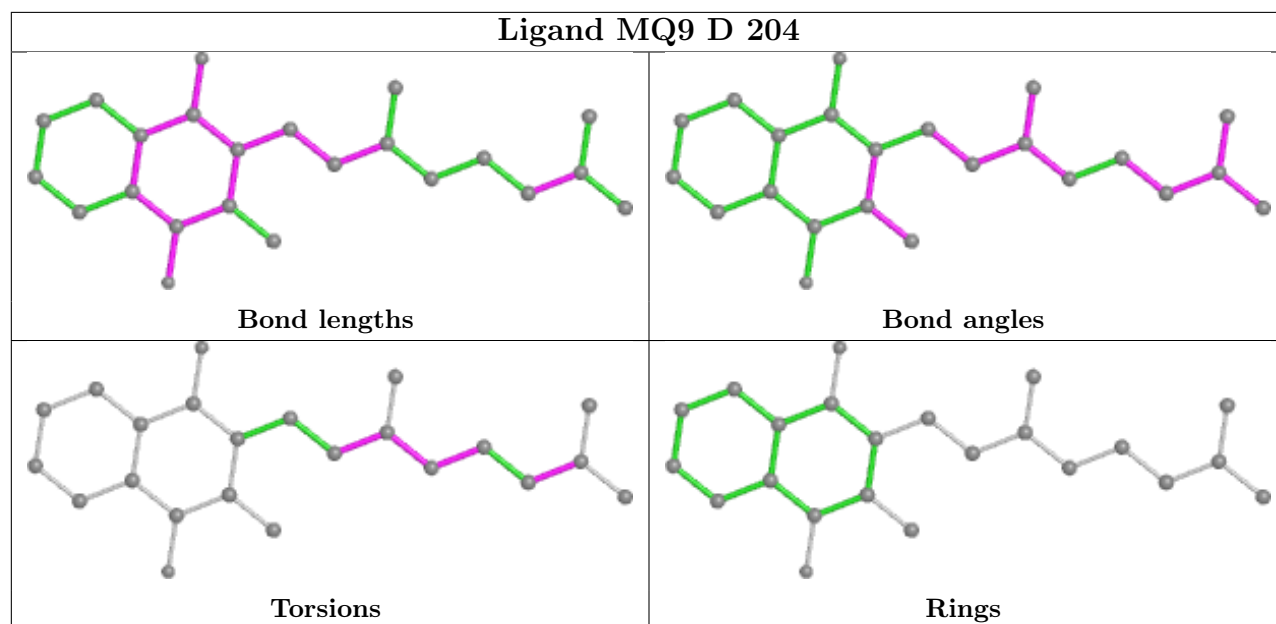
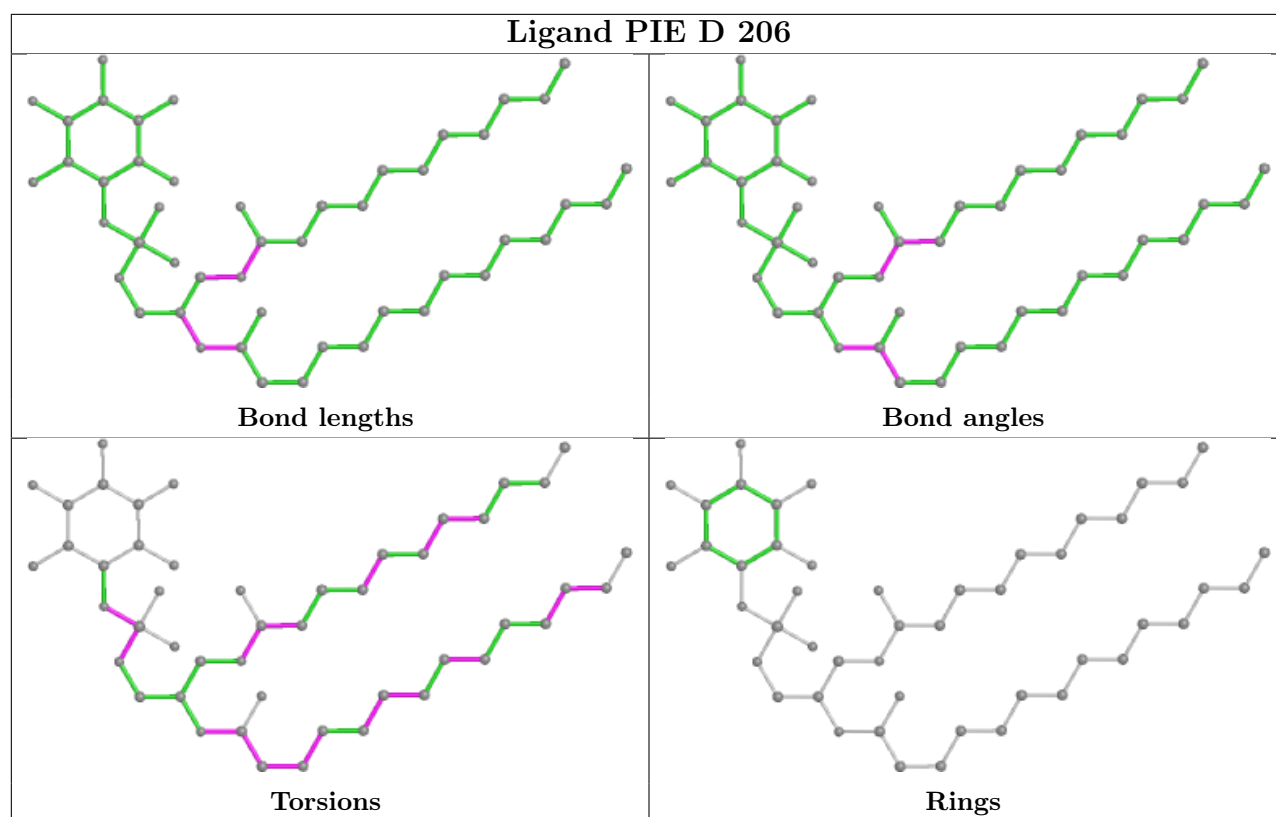
Ligand MQ9 N 202

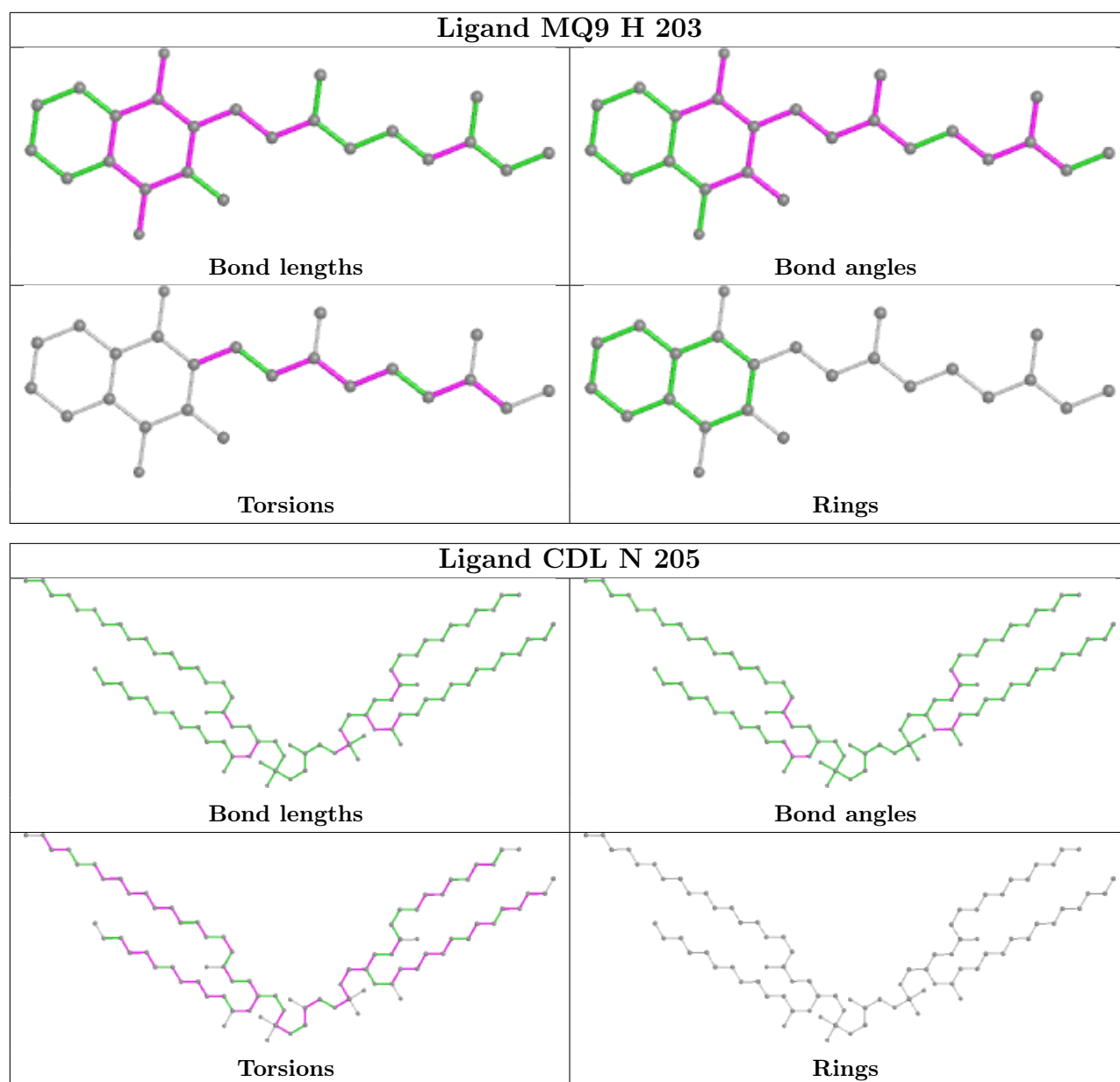












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.