



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2025 – 10:12 PM JST

PDB ID : 8K9E
EMDB ID : EMD-36984
Title : Cryo-EM structure of the photosynthetic alternative complex III from *Chloroflexus aurantiacus* at 3.3 angstrom
Authors : Xu, X.
Deposited on : 2023-08-01
Resolution : 3.33 Å(reported)

This is a wwPDB EM Validation Summary 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	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.41.2

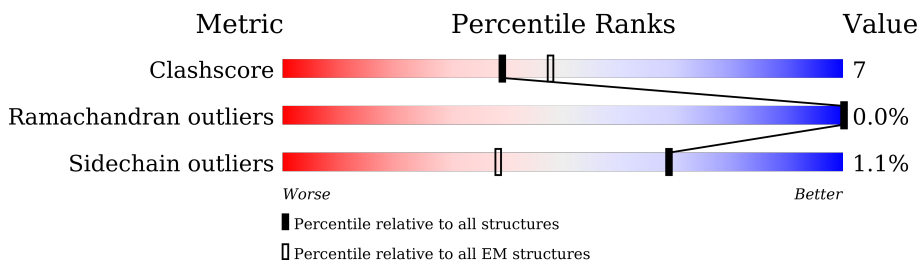
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	219	83% 15% .
2	B	1029	81% 11% 8%
3	C	486	78% 14% 8%
4	D	179	79% 18% .
5	E	205	68% 12% 20%
6	F	411	82% 15% .
7	G	112	66% 5% 29%
8	I	37	84% 16%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 19954 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 Cytochrome c7-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1763	1129	306	313	15		

- Molecule 2 is a protein called Fe-S-cluster-containing hydrogenase components 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	951	Total	C	N	O	S	0	0
			7350	4622	1303	1395	30		

- Molecule 3 is a protein called Polysulphide reductase NrfD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3655	2476	576	586	17		

- Molecule 4 is a protein called Quinol:cytochrome c oxidoreductase membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1350	884	215	245	6		

- Molecule 5 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	164	Total	C	N	O	S	0	0
			1292	819	220	246	7		

- Molecule 6 is a protein called Quinol:cytochrome c oxidoreductase quinone-binding subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	397	Total	C	N	O	S	0	0
			3128	2091	506	514	17		

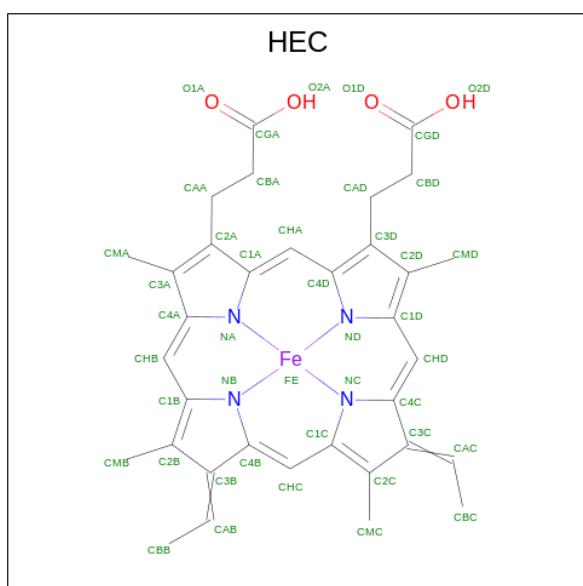
- Molecule 7 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	80	Total	C	N	O	S	0	0
			623	404	108	107	4		

- Molecule 8 is a protein called unknown.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			305	212	42	48	3		

- Molecule 9 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



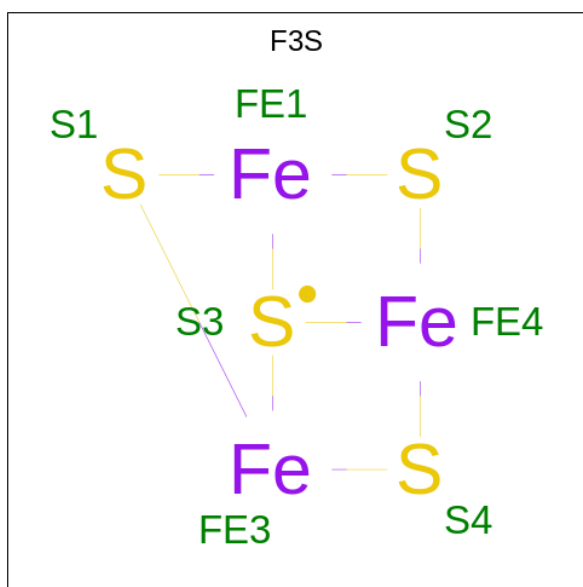
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



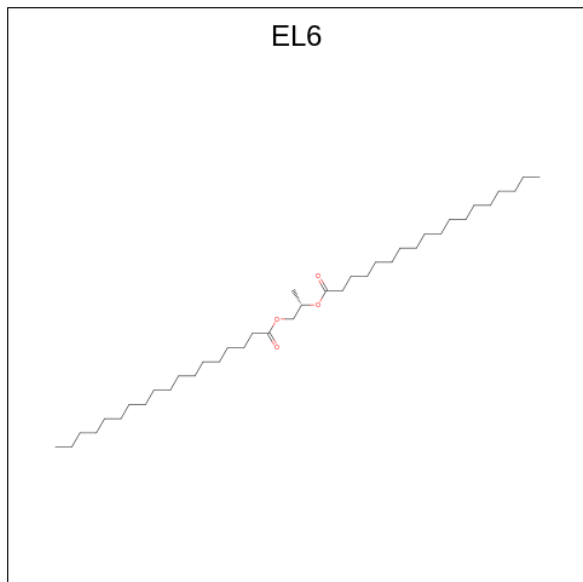
Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



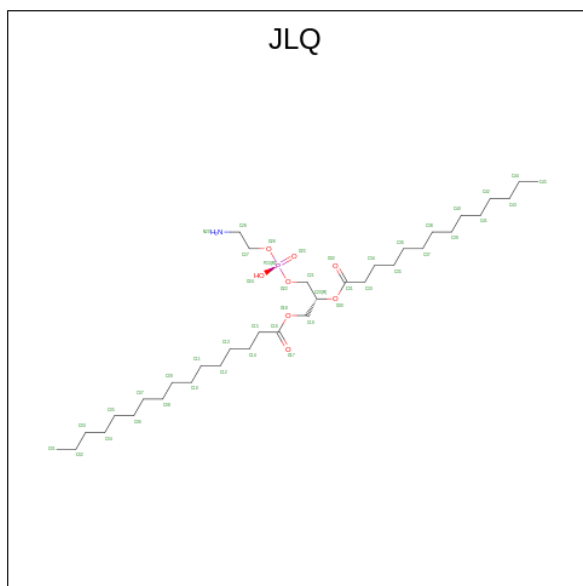
Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 12 is [(2S)-2-octadecanoyloxypropyl] octadecanoate (three-letter code: EL6) (formula: C₃₉H₇₆O₄).



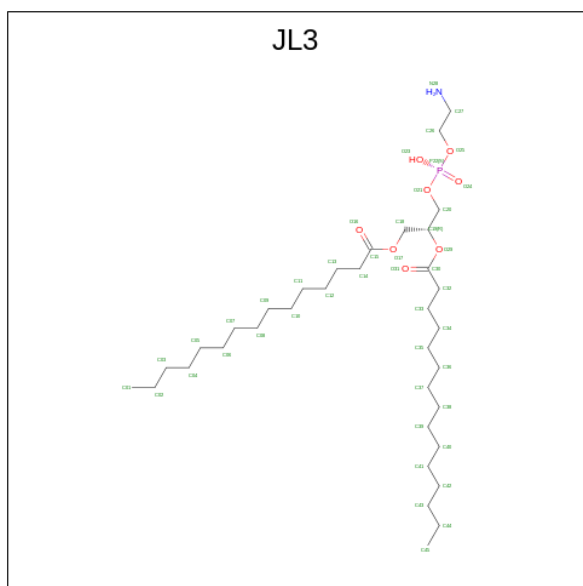
Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	C	O	0
			27	23	4	
12	E	1	Total	C	O	0
			28	24	4	

- Molecule 13 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-tetradecanoyloxy-propyl] hexadecanoate (three-letter code: JLQ) (formula: C₃₅H₇₀NO₈P).



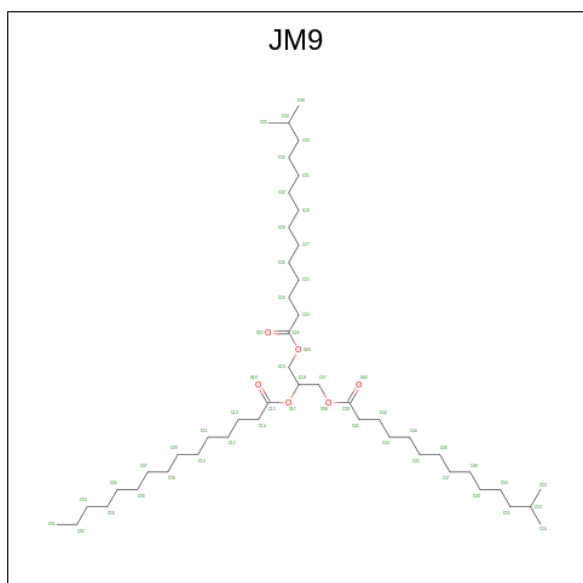
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 14 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-pentadecanoyloxy-propyl] pentadecanoate (three-letter code: JL3) (formula: C₃₅H₇₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 15 is 1,3-bis(13-methyltetradecanoyloxy)propan-2-yl pentadecanoate (three-letter code: JM9) (formula: C₄₈H₉₂O₆).




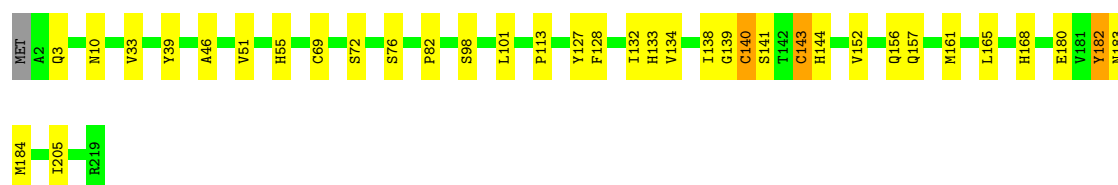
Mol	Chain	Residues	Atoms			AltConf
15	F	1	Total	C	O	0
			54	48	6	

3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

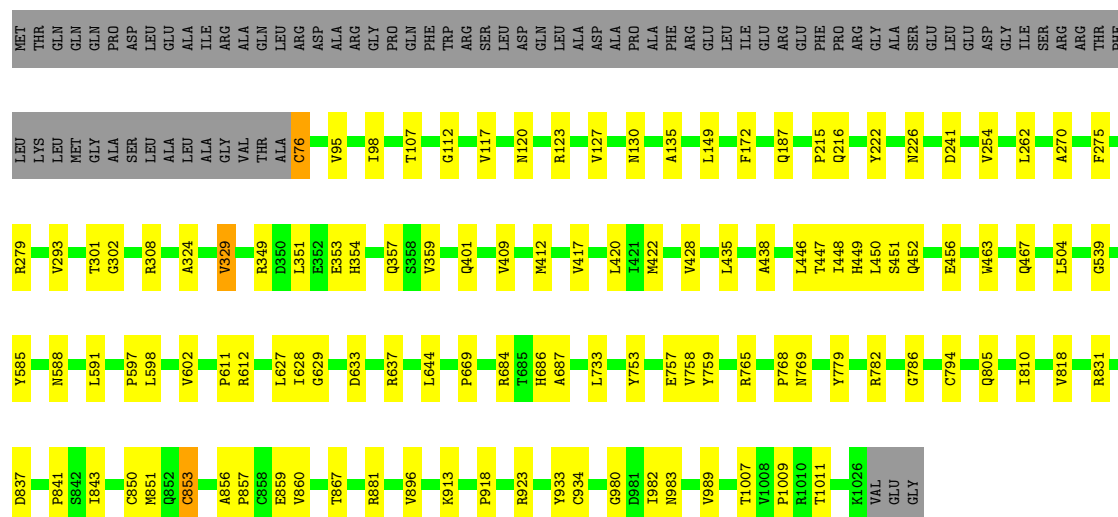
- Molecule 1: Cytochrome c7-like domain-containing protein

Chain A: 




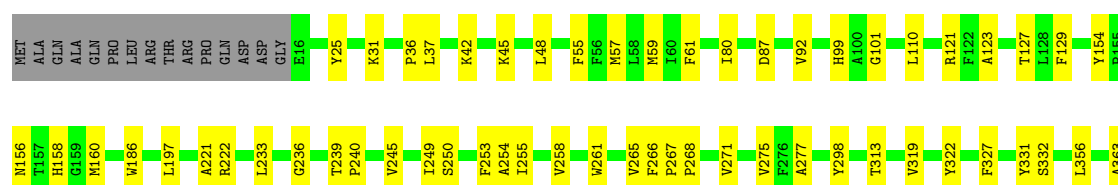
- Molecule 2: Fe-S-cluster-containing hydrogenase components 1-like protein

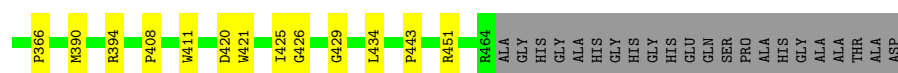
Chain B: 



- Molecule 3: Polysulphide reductase NrfD

Chain C: 





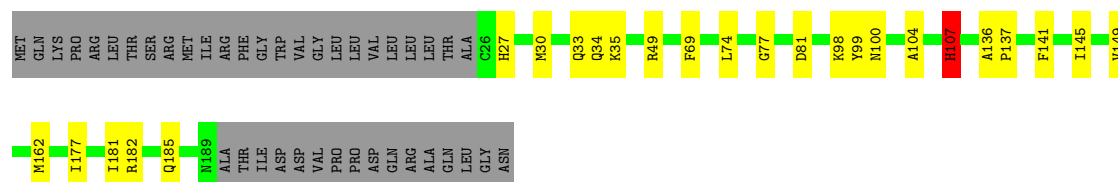
- Molecule 4: Quinol:cytochrome c oxidoreductase membrane protein

Chain D: 79% 18%



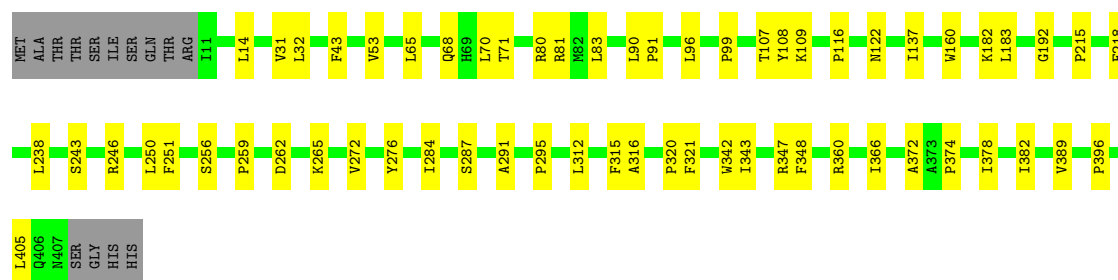
- Molecule 5: Cytochrome c domain-containing protein

Chain E: 68% 12% 20%



- Molecule 6: Quinol:cytochrome c oxidoreductase quinone-binding subunit 2

Chain F: 82% 15%



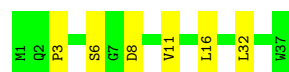
- Molecule 7: Uncharacterized protein

Chain G: 66% 5% 29%



- Molecule 8: unknown

Chain I: 84% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	425867	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, HEC, JL3, SF4, EL6, JM9, JLQ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/1812	0.56	0/2472
2	B	0.59	0/7518	0.65	0/10249
3	C	0.48	0/3787	0.56	0/5179
4	D	0.39	0/1388	0.58	0/1895
5	E	0.41	0/1327	0.57	0/1803
6	F	0.58	0/3226	0.65	0/4408
7	G	0.37	0/635	0.59	0/865
8	I	0.65	0/318	0.77	0/436
All	All	0.53	0/20011	0.61	0/27307

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	1763	0	1713	50	0
2	B	7350	0	7179	74	0
3	C	3655	0	3688	50	0
4	D	1350	0	1341	26	0
5	E	1292	0	1216	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	3128	0	3175	54	0
7	G	623	0	660	3	0
8	I	305	0	302	7	0
9	A	215	0	153	27	0
9	E	43	0	30	6	0
10	B	24	0	0	2	0
11	B	7	0	0	0	0
12	B	27	0	0	1	0
12	E	28	0	0	0	0
13	C	45	0	0	10	0
14	F	45	0	0	2	0
15	F	54	0	0	17	0
All	All	19954	0	19457	272	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 7.

The worst 5 of 272 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:A:140:CYS:SG	9:A:303:HEC:CAB	2.02	1.45
2:B:76:CYS:SG	12:B:1105:EL6:C1	2.16	1.32
1:A:140:CYS:SG	9:A:303:HEC:CBB	1.14	1.23
6:F:272:VAL:HG23	15:F:502:JM9:C31	1.70	1.19
6:F:272:VAL:CG2	15:F:502:JM9:C31	2.23	1.16

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	A	216/219 (99%)	200 (93%)	16 (7%)	0	100	100
2	B	949/1029 (92%)	911 (96%)	38 (4%)	0	100	100
3	C	447/486 (92%)	434 (97%)	13 (3%)	0	100	100
4	D	173/179 (97%)	160 (92%)	13 (8%)	0	100	100
5	E	162/205 (79%)	155 (96%)	6 (4%)	1 (1%)	22	53
6	F	395/411 (96%)	379 (96%)	16 (4%)	0	100	100
7	G	78/112 (70%)	73 (94%)	5 (6%)	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	2455/2678 (92%)	2346 (96%)	108 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	107	HIS

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	A	198/199 (100%)	195 (98%)	3 (2%)	60	77
2	B	768/830 (92%)	758 (99%)	10 (1%)	65	79
3	C	382/405 (94%)	382 (100%)	0	100	100
4	D	143/147 (97%)	140 (98%)	3 (2%)	48	70
5	E	135/171 (79%)	132 (98%)	3 (2%)	47	70
6	F	318/330 (96%)	316 (99%)	2 (1%)	84	90
7	G	69/95 (73%)	68 (99%)	1 (1%)	62	78
8	I	32/32 (100%)	32 (100%)	0	100	100
All	All	2045/2209 (93%)	2023 (99%)	22 (1%)	69	82

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	143	GLN
5	E	69	PHE
5	E	27	HIS
5	E	107	HIS
2	B	504	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
2	B	120	ASN
2	B	869	HIS
4	D	143	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
9	HEC	A	304	1	32,50,50	2.51	5 (15%)	24,82,82	1.41	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	EL6	B	1105	-	26,26,42	1.19	4 (15%)	28,28,44	1.49	4 (14%)
11	F3S	B	1104	2	0,9,9	-	-	-	-	-
12	EL6	E	302	-	27,27,42	1.17	4 (14%)	29,29,44	1.47	3 (10%)
9	HEC	A	303	1	32,50,50	2.56	4 (12%)	24,82,82	1.24	1 (4%)
9	HEC	E	301	5	32,50,50	2.52	5 (15%)	24,82,82	1.52	4 (16%)
9	HEC	A	302	1	32,50,50	2.52	5 (15%)	24,82,82	1.44	3 (12%)
9	HEC	A	305	1	32,50,50	2.53	5 (15%)	24,82,82	1.45	4 (16%)
10	SF4	B	1101	2	0,12,12	-	-	-	-	-
10	SF4	B	1102	2	0,12,12	-	-	-	-	-
10	SF4	B	1103	2	0,12,12	-	-	-	-	-
14	JL3	F	501	-	44,44,44	0.97	4 (9%)	47,49,49	1.06	4 (8%)
15	JM9	F	502	-	53,53,53	0.98	4 (7%)	58,58,58	0.76	3 (5%)
9	HEC	A	301	1	32,50,50	2.53	5 (15%)	24,82,82	1.56	6 (25%)
13	JLQ	C	501	-	44,44,44	0.96	3 (6%)	47,49,49	1.22	6 (12%)

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
9	HEC	A	304	1	-	2/10/54/54	-
12	EL6	B	1105	-	-	9/27/27/43	-
11	F3S	B	1104	2	-	-	0/3/3/3
12	EL6	E	302	-	-	10/28/28/43	-
9	HEC	A	303	1	-	2/10/54/54	-
9	HEC	E	301	5	-	1/10/54/54	-
9	HEC	A	302	1	-	1/10/54/54	-
9	HEC	A	305	1	-	1/10/54/54	-
10	SF4	B	1101	2	-	-	0/6/5/5
10	SF4	B	1102	2	-	-	0/6/5/5
14	JL3	F	501	-	-	18/48/48/48	-
15	JM9	F	502	-	-	21/56/56/56	-
10	SF4	B	1103	2	-	-	0/6/5/5
9	HEC	A	301	1	-	0/10/54/54	-
13	JLQ	C	501	-	-	19/48/48/48	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	303	HEC	C2B-C3B	-8.15	1.32	1.40
9	A	301	HEC	C3C-C2C	-8.10	1.32	1.40
9	A	303	HEC	C3C-C2C	-7.94	1.32	1.40
9	A	304	HEC	C3C-C2C	-7.94	1.32	1.40
9	A	305	HEC	C3C-C2C	-7.88	1.32	1.40

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1105	EL6	O21-C21-C22	4.50	121.19	111.50
13	C	501	JLQ	O30-C31-C33	4.41	121.01	111.50
12	E	302	EL6	O21-C21-C22	4.30	120.76	111.50
14	F	501	JL3	O29-C30-C32	3.89	119.89	111.50
9	E	301	HEC	CMC-C2C-C1C	-3.51	123.07	128.46

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	1105	EL6	C1-C2-C3-O31
12	B	1105	EL6	O21-C2-C3-O31
13	C	501	JLQ	O18-C19-C20-O30
13	C	501	JLQ	O32-C31-O30-C20
13	C	501	JLQ	C33-C31-O30-C20

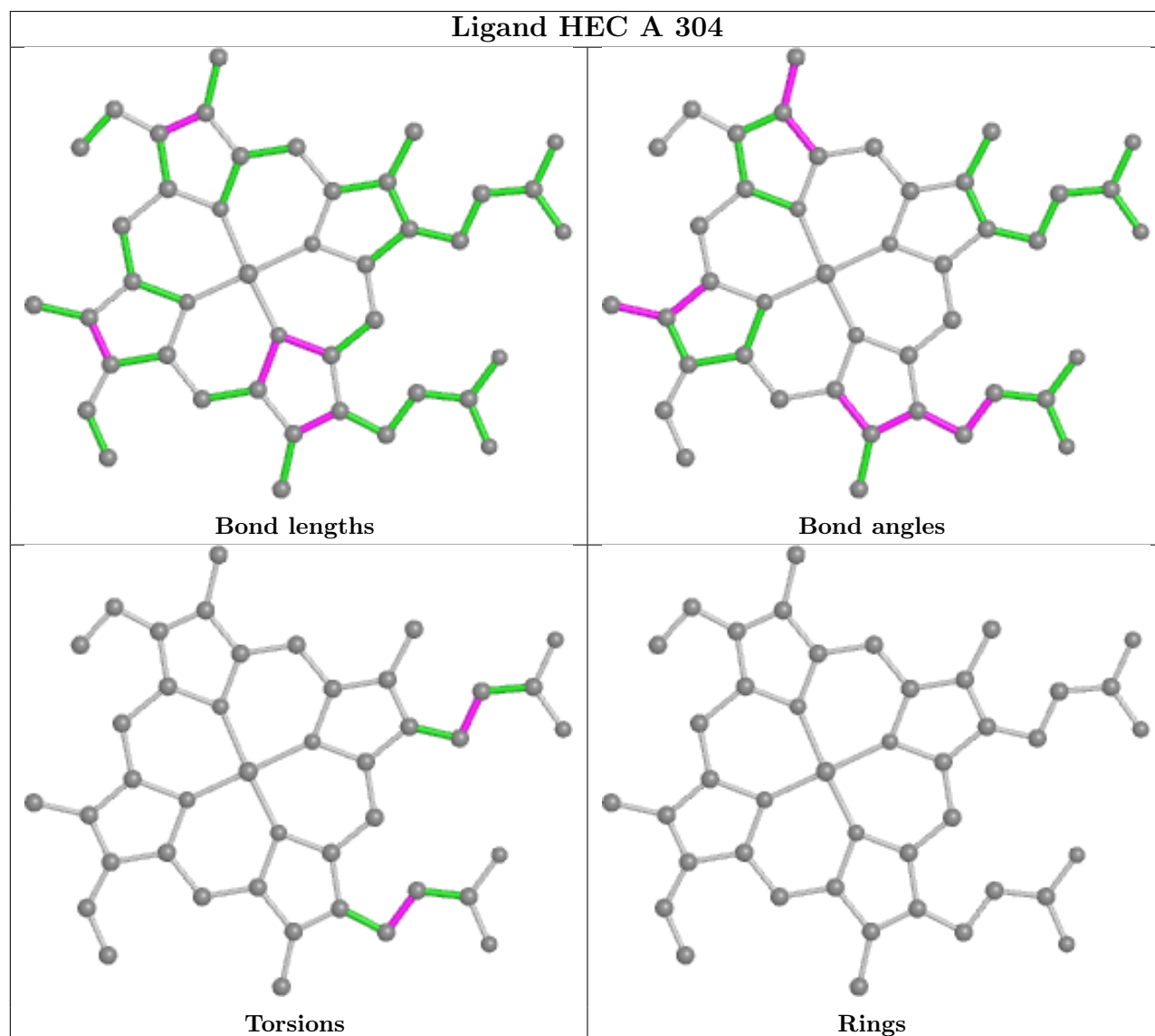
There are no ring outliers.

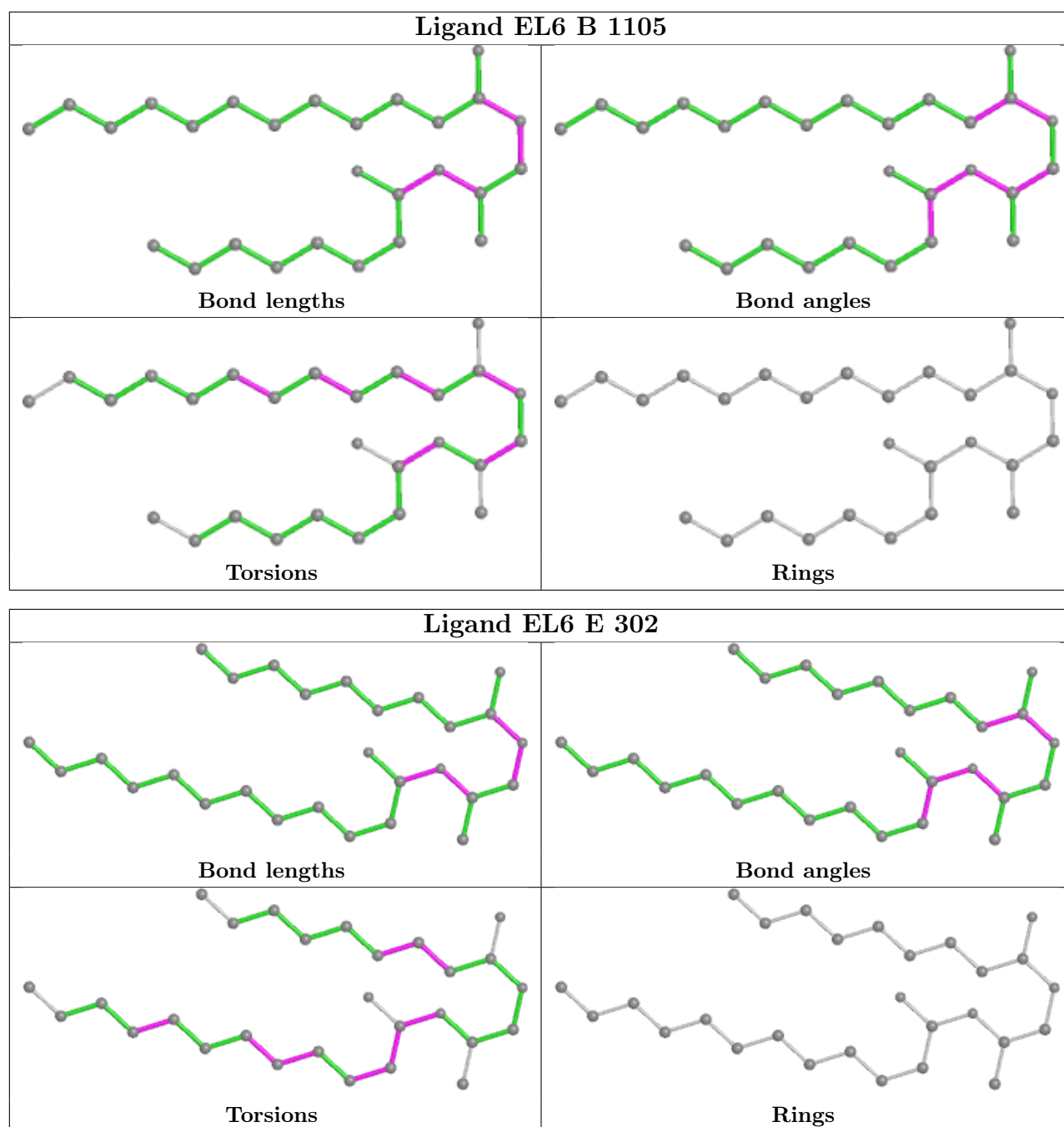
11 monomers are involved in 65 short contacts:

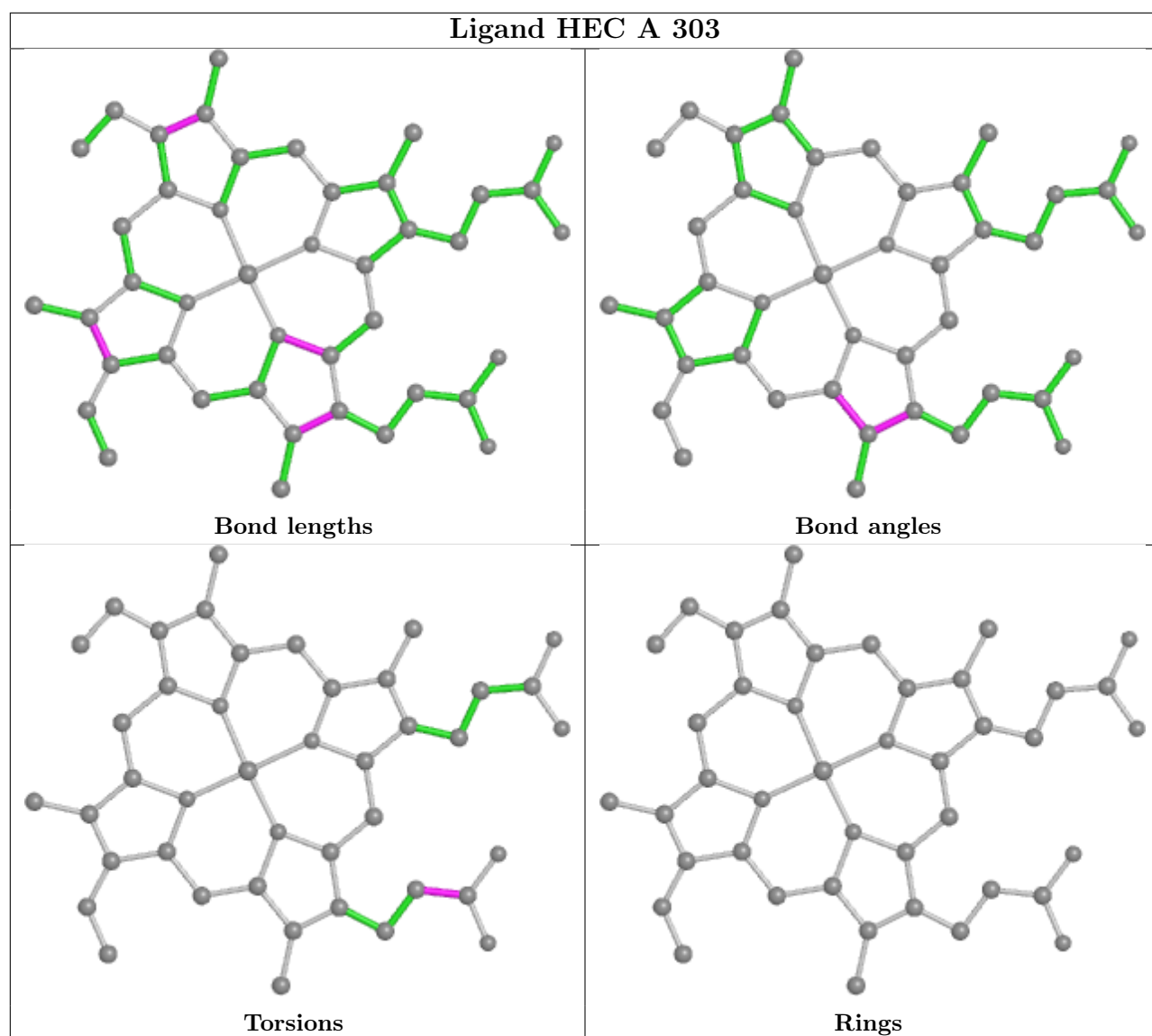
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	304	HEC	2	0
12	B	1105	EL6	1	0
9	A	303	HEC	12	0
9	E	301	HEC	6	0
9	A	302	HEC	3	0
10	B	1101	SF4	1	0
10	B	1102	SF4	1	0
14	F	501	JL3	2	0
15	F	502	JM9	17	0
9	A	301	HEC	10	0
13	C	501	JLQ	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

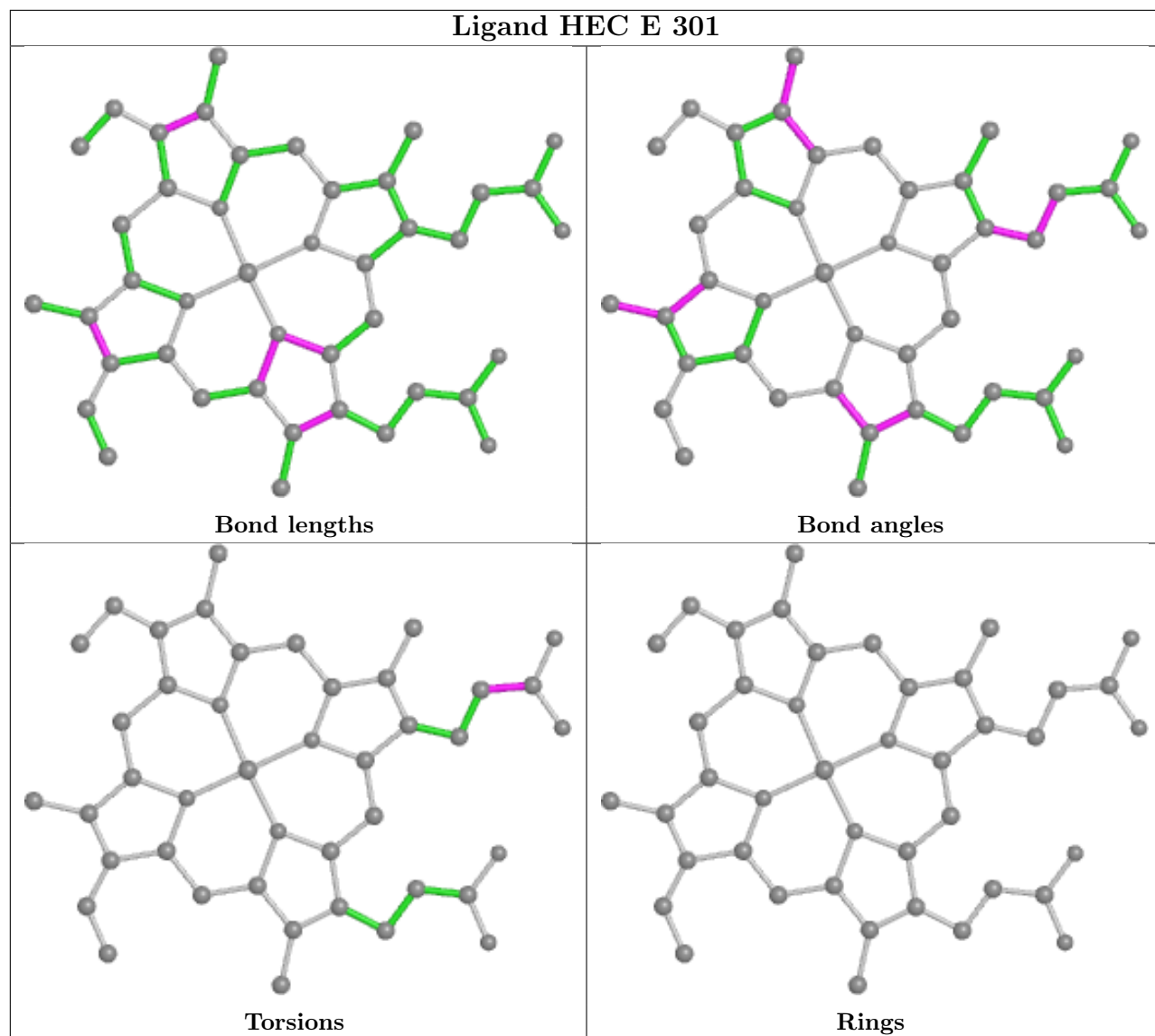
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

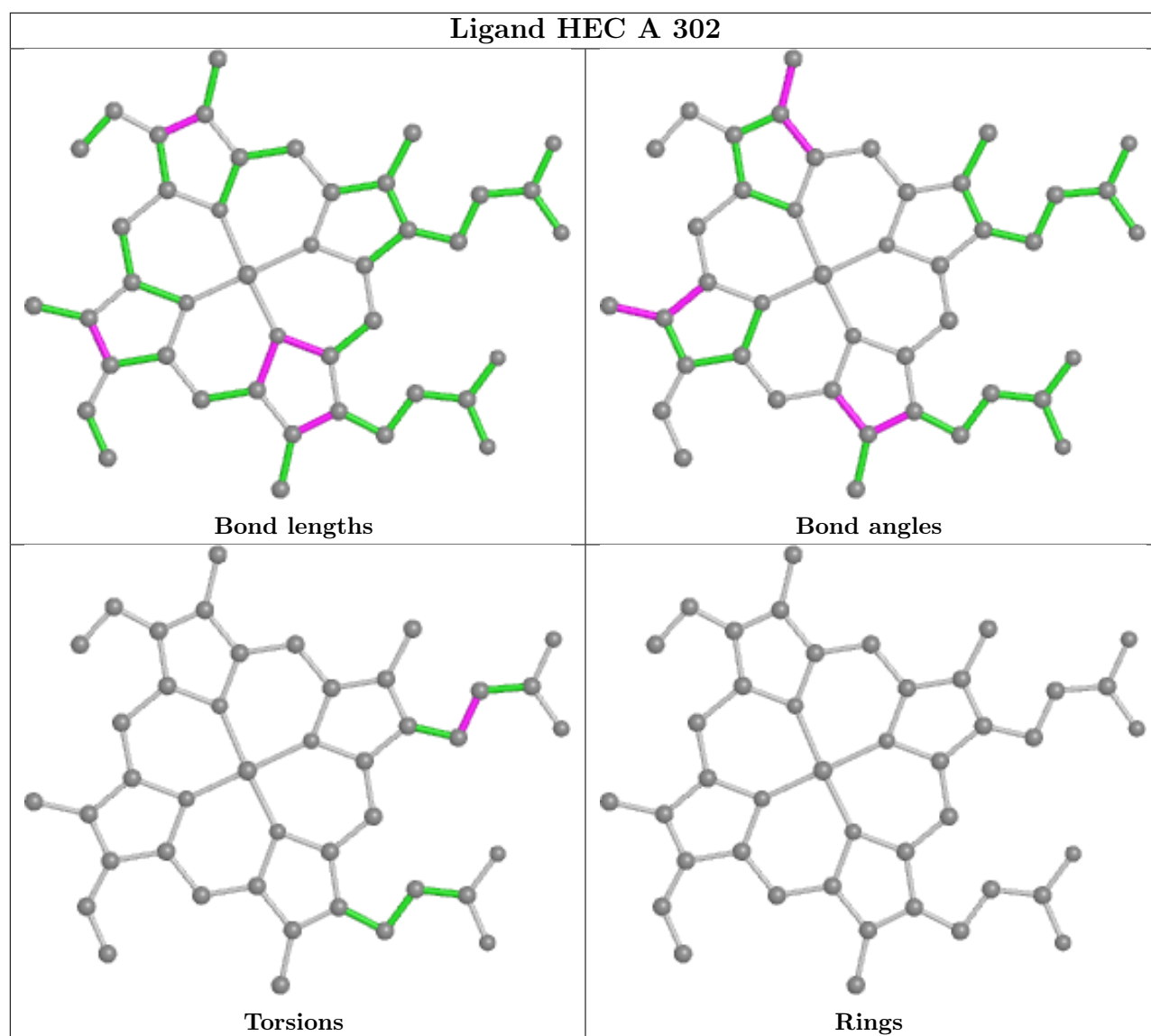


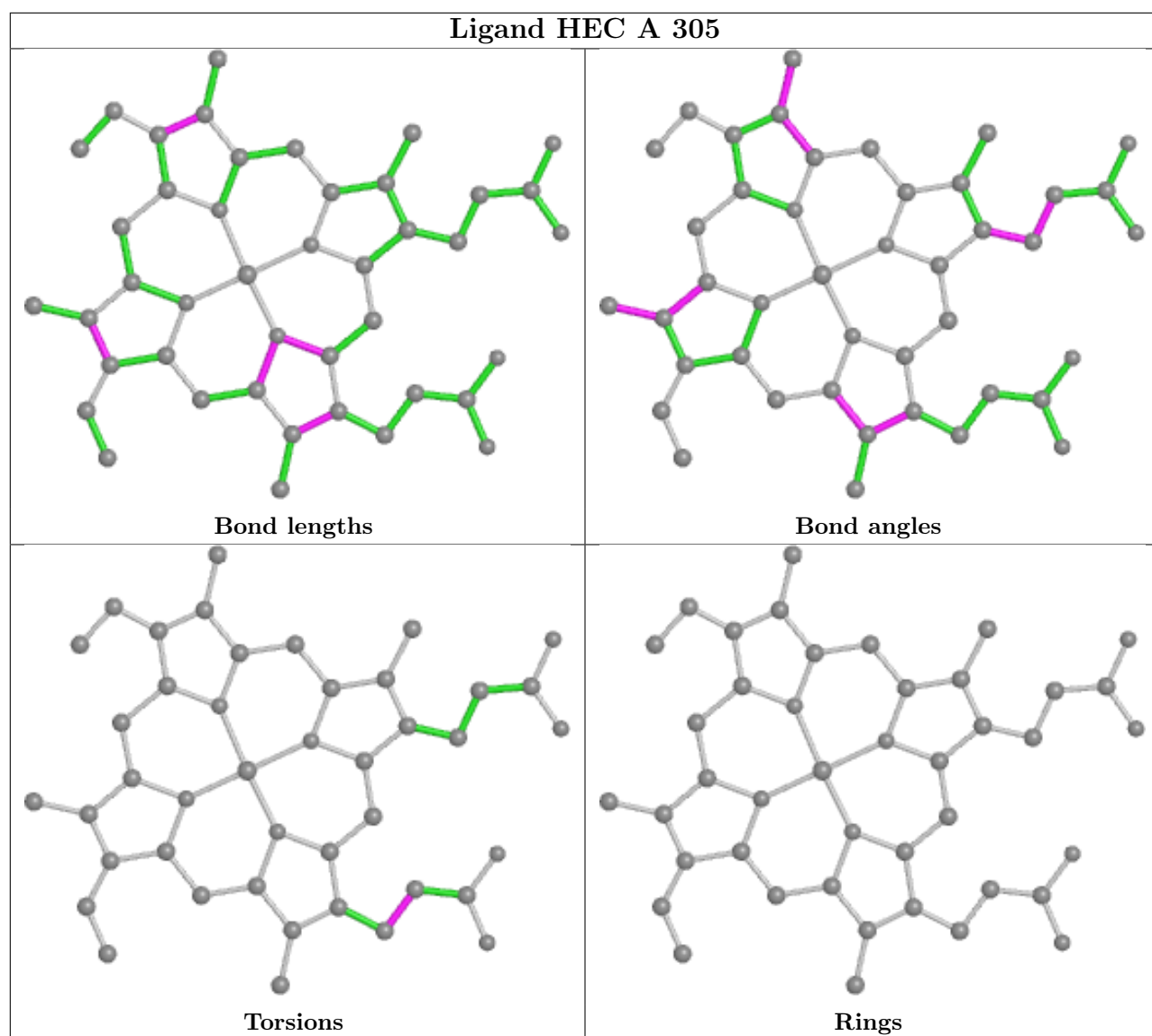


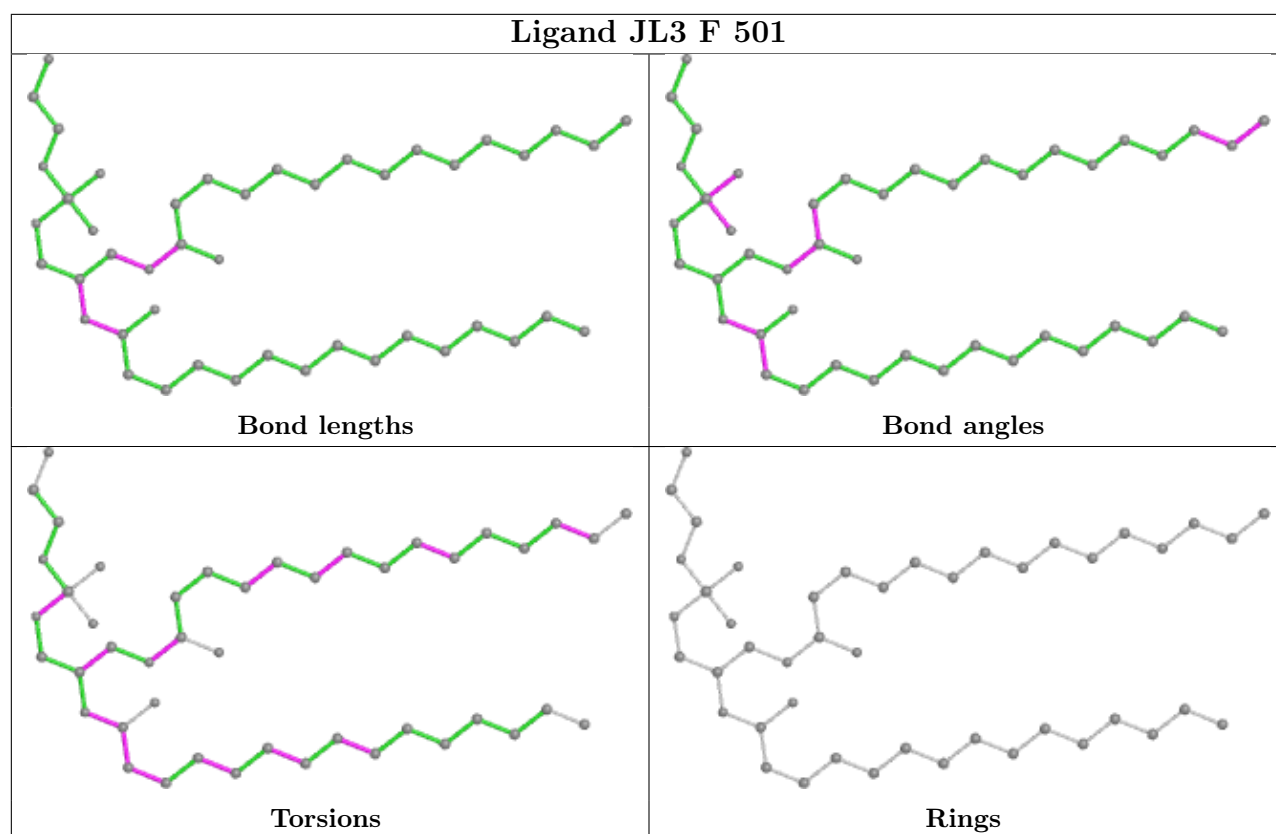


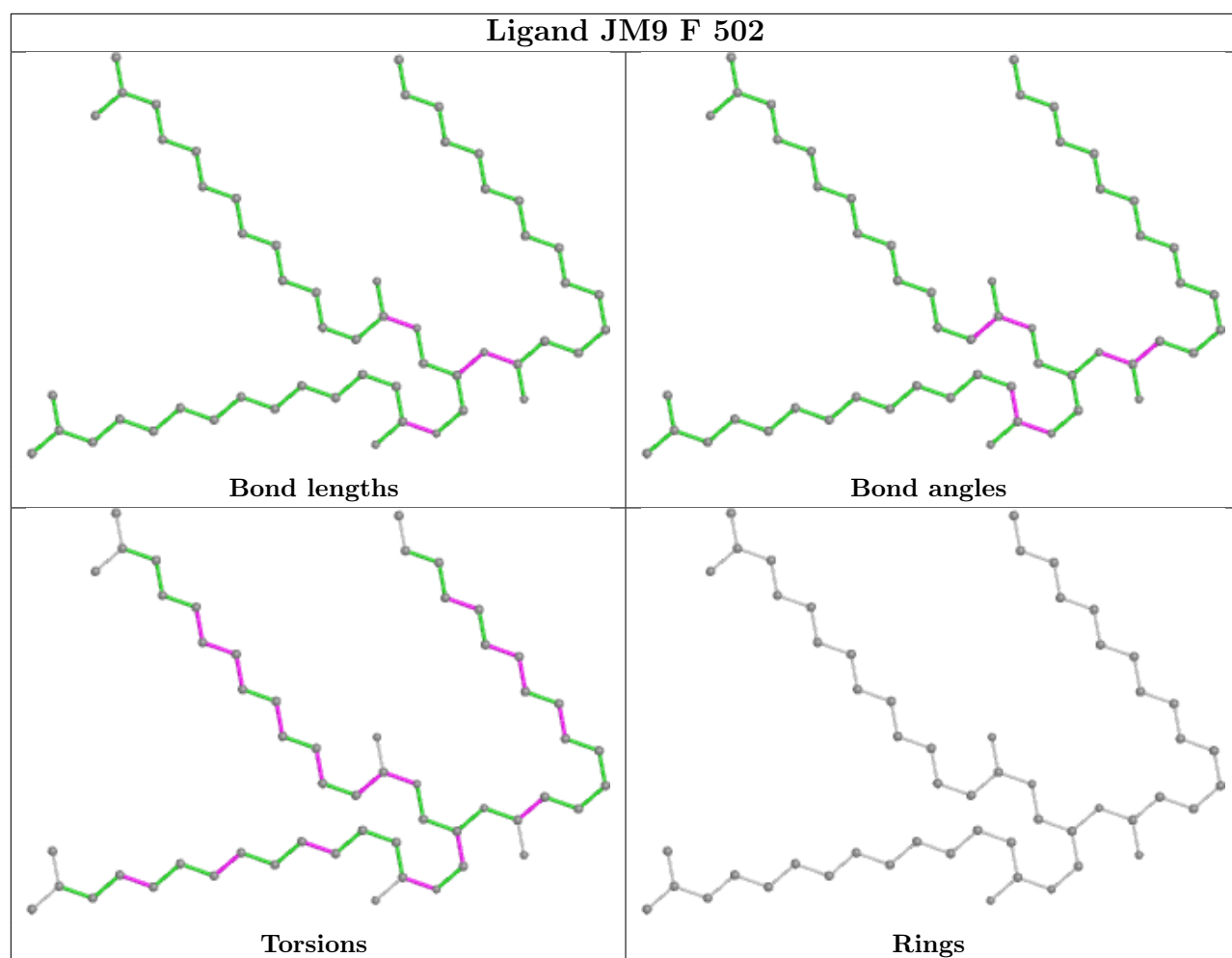
Ligand HEC E 301

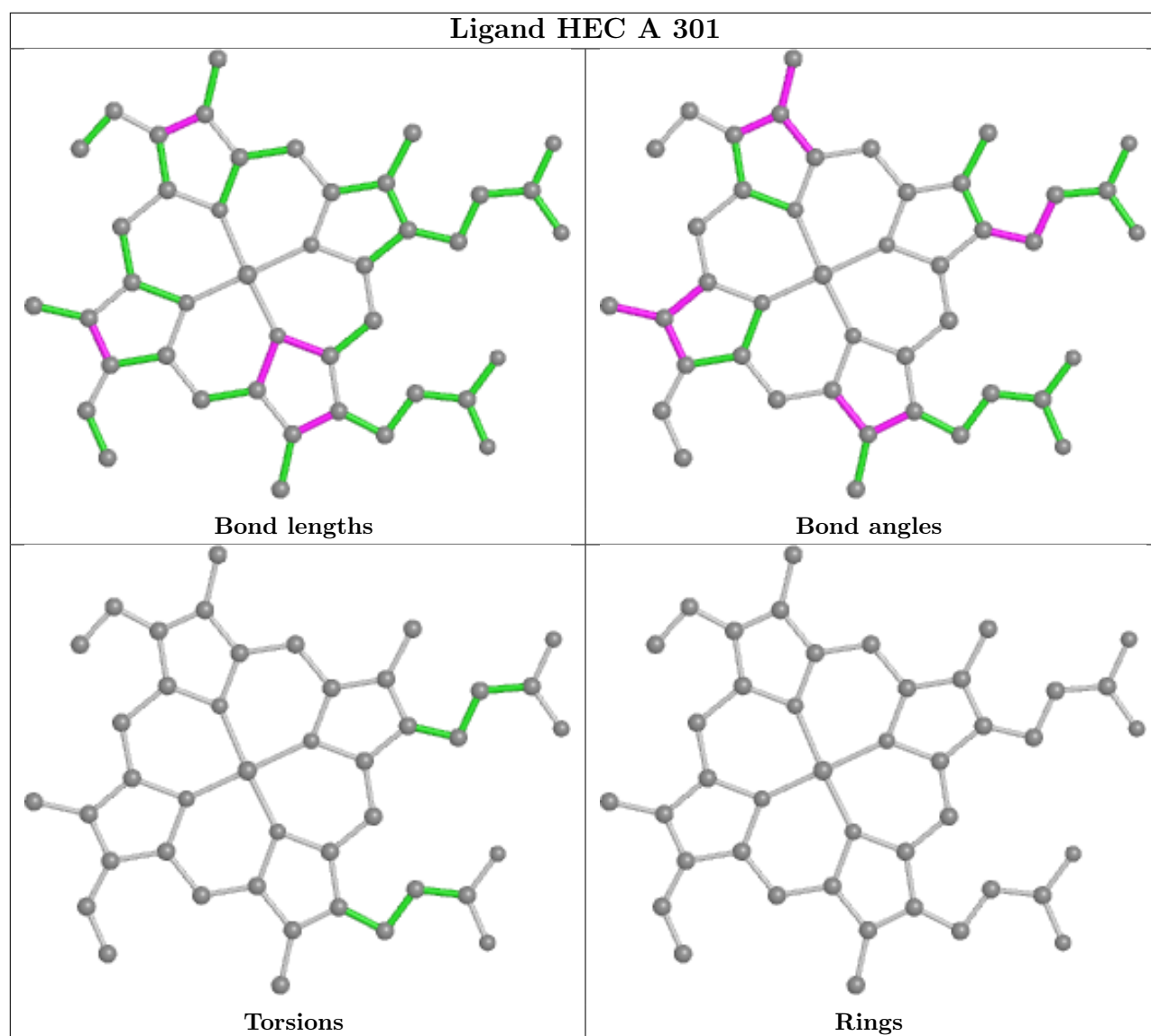


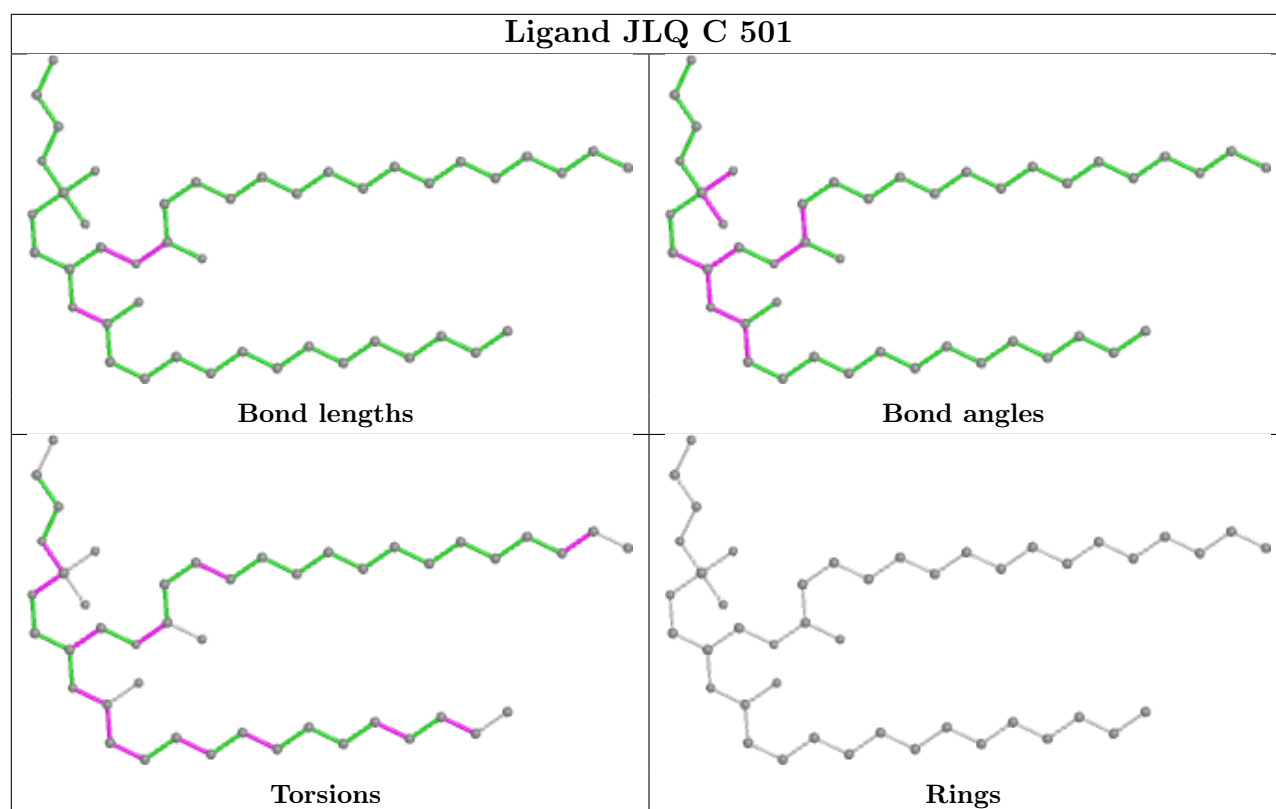












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.