



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2025 – 10:10 PM JST

PDB ID : 8X2J
EMDB ID : EMD-38012
Title : Cryo-EM structure of the photosynthetic alternative complex III with a quinone inhibitor HQNO from *Chloroflexus aurantiacus*
Authors : Xu, X.
Deposited on : 2023-11-09
Resolution : 2.70 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

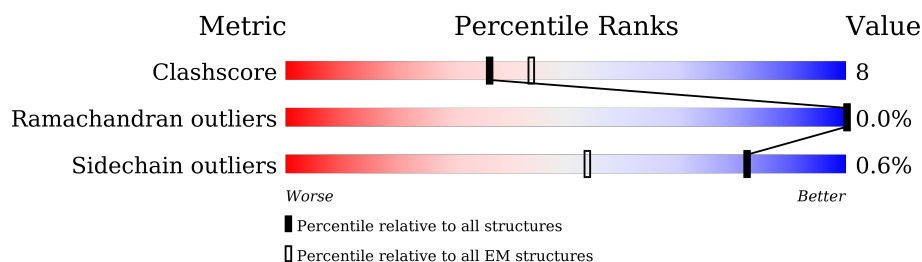
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	
2	B	1029	
3	C	486	
4	D	179	
5	E	205	
6	F	411	
7	G	112	
8	I	37	

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
11	F3S	B	1104	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 19918 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		

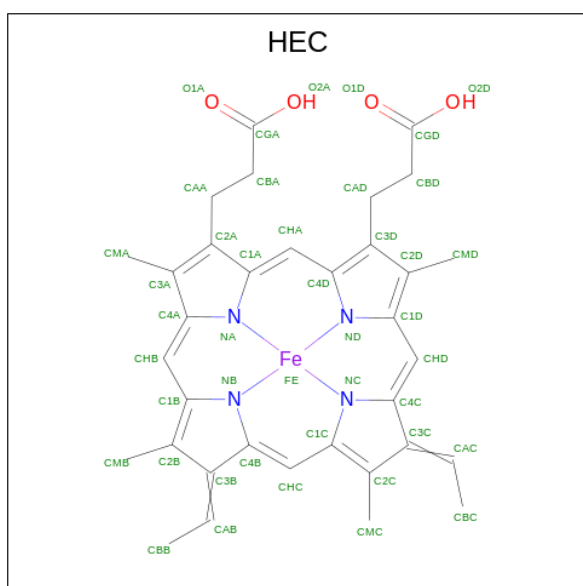
- Molecule 7 is a protein called Uncharacterized protein.

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.

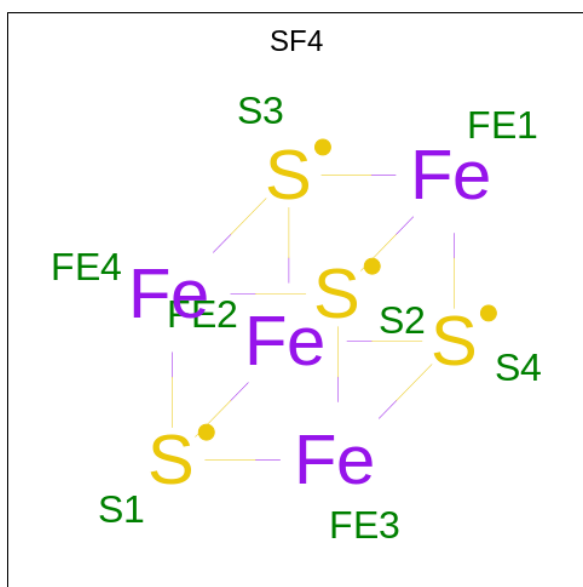
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			305	212	42	48	3		

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



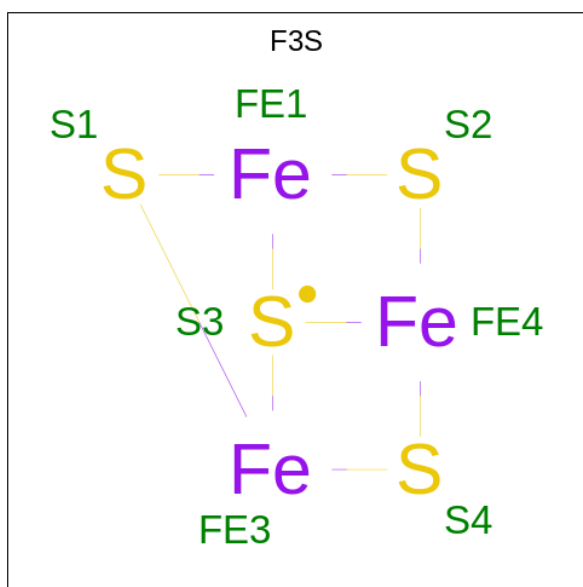
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



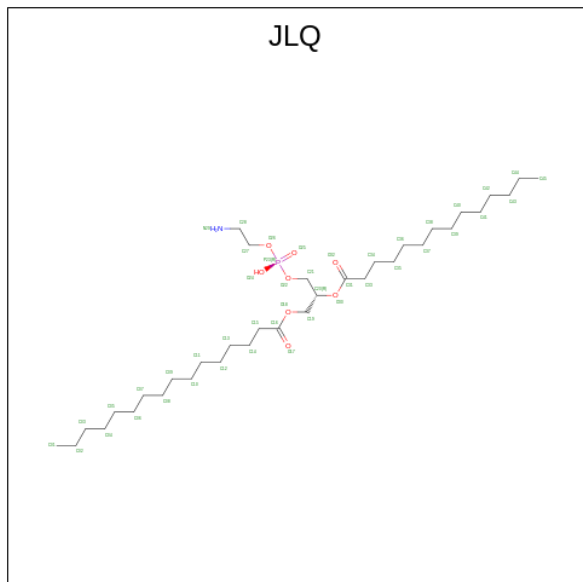
Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	

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



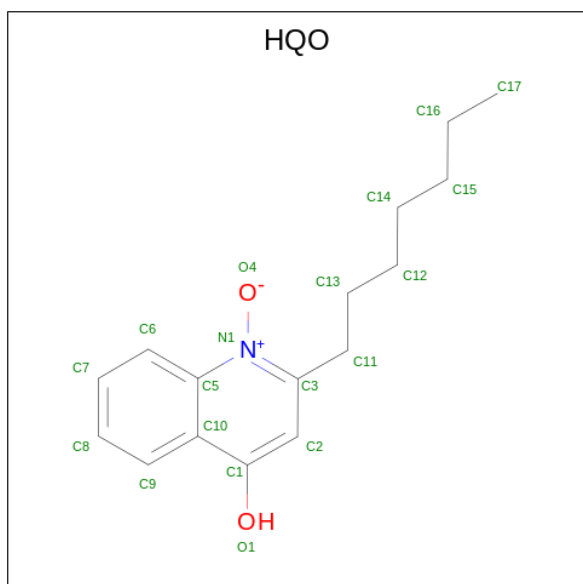
Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 12 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-tetradecanoyloxy-propyl] hexadecanoate (three-letter code: JLQ) (formula: $C_{35}H_{70}NO_8P$).



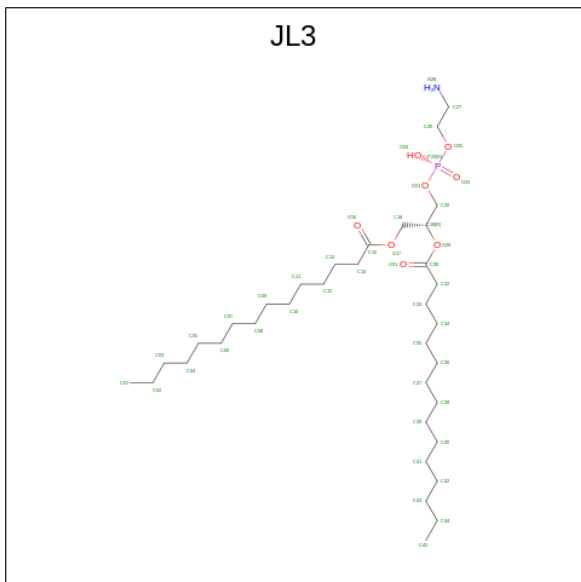
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	C	1	45	35	1	8	1	0

- Molecule 13 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: $C_{16}H_{21}NO_2$).



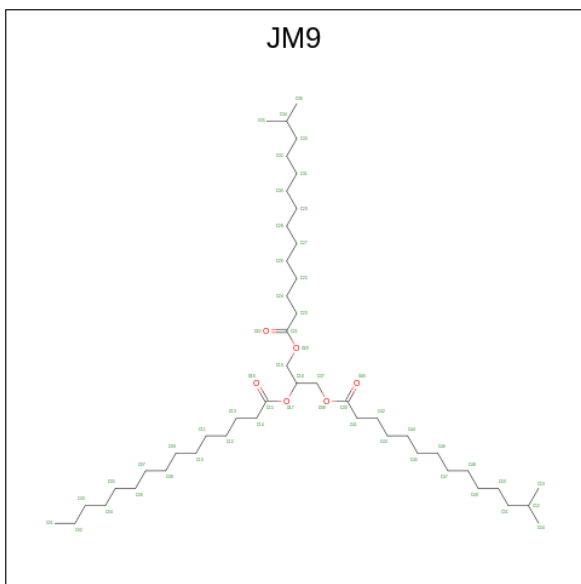
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	C	1	19	16	1	2	0

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




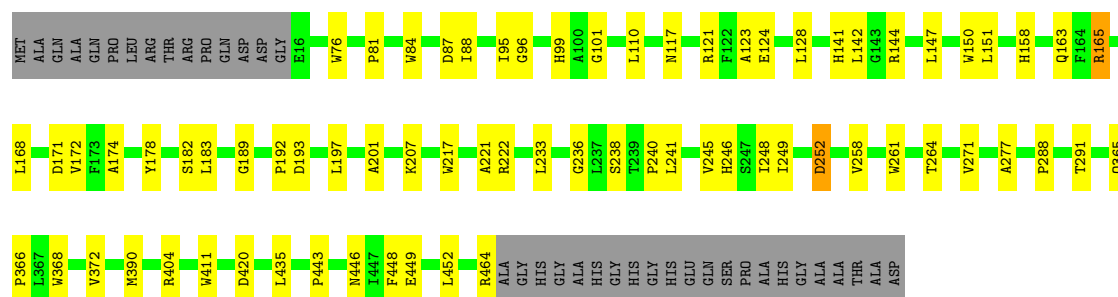
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	N	O	P	0
			45	35	1	8	1	

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




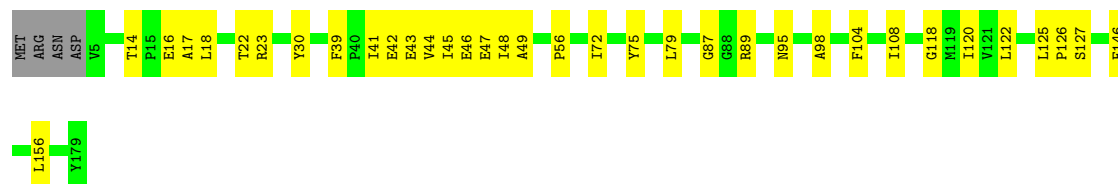
Mol	Chain	Residues	Atoms			AltConf
15	C	1	Total	C	O	0
			54	48	6	

Chain C:  78% 14% 8%



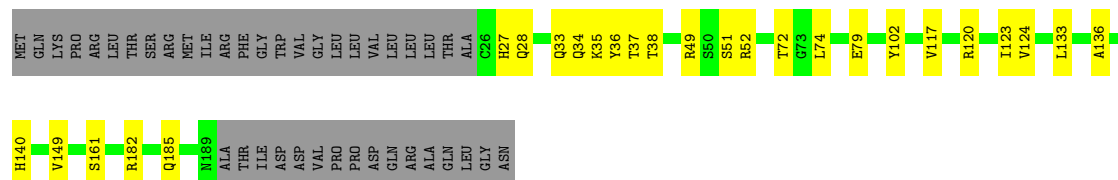
- Molecule 4: Quinol:cytochrome c oxidoreductase membrane protein

Chain D:  78% 20% .




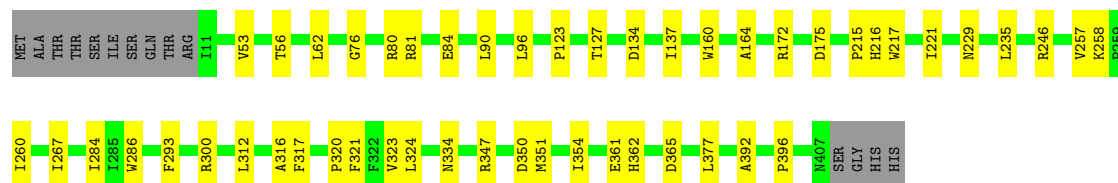
- Molecule 5: Cytochrome c domain-containing protein

Chain E:  67% 13% 20%



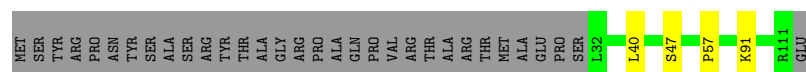
- Molecule 6: Quinol:cytochrome c oxidoreductase quinone-binding subunit 2

Chain F:  84% 12% .



- Molecule 7: Uncharacterized protein

Chain G:  68% 29%



- Molecule 8: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160264	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)	1000	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: JM9, SF4, HEC, F3S, HQO, JL3, 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	0.34	0/1812	0.55	0/2472
2	B	0.32	0/7518	0.58	0/10249
3	C	0.31	0/3787	0.55	1/5179 (0.0%)
4	D	0.35	0/1388	0.54	0/1895
5	E	0.29	0/1327	0.54	0/1803
6	F	0.31	0/3226	0.58	0/4408
7	G	0.26	0/635	0.62	0/865
8	I	0.29	0/318	0.54	0/436
All	All	0.32	0/20011	0.57	1/27307 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	252	ASP	CB-CG-OD2	5.27	123.05	118.30

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	34	0
2	B	7350	0	7178	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3655	0	3686	56	0
4	D	1350	0	1341	33	0
5	E	1292	0	1216	26	0
6	F	3128	0	3175	28	0
7	G	623	0	660	4	0
8	I	305	0	302	5	0
9	A	215	0	150	12	0
9	E	43	0	30	2	0
10	B	24	0	0	1	0
11	B	7	0	0	5	0
12	C	45	0	0	0	0
13	C	19	0	20	1	0
14	C	45	0	0	0	0
15	C	54	0	0	0	0
All	All	19918	0	19471	297	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 8.

The worst 5 of 297 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)
2:B:888:CYS:SG	11:B:1104:F3S:FE1	1.42	1.09
4:D:156:LEU:HD12	4:D:156:LEU:O	1.65	0.95
3:C:171:ASP:OD1	3:C:248:ILE:HG22	1.80	0.81
5:E:124:VAL:O	5:E:124:VAL:HG13	1.82	0.80
2:B:620:LEU:HD13	2:B:647:VAL:HG21	1.66	0.78

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%)	206 (95%)	10 (5%)	0	100	100
2	B	949/1029 (92%)	892 (94%)	56 (6%)	1 (0%)	48	73
3	C	447/486 (92%)	432 (97%)	15 (3%)	0	100	100
4	D	173/179 (97%)	160 (92%)	13 (8%)	0	100	100
5	E	162/205 (79%)	155 (96%)	7 (4%)	0	100	100
6	F	395/411 (96%)	380 (96%)	15 (4%)	0	100	100
7	G	78/112 (70%)	75 (96%)	3 (4%)	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	2455/2678 (92%)	2334 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	886	LYS

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	83
2	B	768/830 (92%)	763 (99%)	5 (1%)	81	93
3	C	382/405 (94%)	379 (99%)	3 (1%)	79	91
4	D	143/147 (97%)	142 (99%)	1 (1%)	81	93
5	E	135/171 (79%)	135 (100%)	0	100	100
6	F	318/330 (96%)	317 (100%)	1 (0%)	91	97
7	G	69/95 (73%)	69 (100%)	0	100	100
8	I	32/32 (100%)	32 (100%)	0	100	100
All	All	2045/2209 (93%)	2032 (99%)	13 (1%)	82	94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	930	LYS
3	C	141	HIS
6	F	361	GLU
3	C	464	ARG
4	D	95	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	588	ASN
2	B	880	ASN
3	C	141	HIS
3	C	246	HIS
3	C	365	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](#)

14 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	303	1	32,50,50	2.41	5 (15%)	24,82,82	1.45	4 (16%)
9	HEC	A	301	1	32,50,50	2.39	7 (21%)	24,82,82	1.89	7 (29%)
10	SF4	B	1102	2	0,12,12	-	-	-	-	-
10	SF4	B	1103	2	0,12,12	-	-	-	-	-
10	SF4	B	1101	2	0,12,12	-	-	-	-	-
15	JM9	C	504	-	53,53,53	0.97	4 (7%)	58,58,58	0.89	3 (5%)
11	F3S	B	1104	2	0,9,9	-	-	-	-	-
13	HQO	C	502	-	20,20,20	2.84	3 (15%)	18,26,26	1.25	2 (11%)
9	HEC	A	305	1	32,50,50	2.39	5 (15%)	24,82,82	1.46	4 (16%)
9	HEC	A	304	1	32,50,50	2.38	5 (15%)	24,82,82	1.77	7 (29%)
12	JLQ	C	501	-	44,44,44	0.99	4 (9%)	47,49,49	1.10	3 (6%)
9	HEC	E	301	5	32,50,50	2.44	5 (15%)	24,82,82	1.38	4 (16%)
14	JL3	C	503	-	44,44,44	0.96	3 (6%)	47,49,49	1.12	5 (10%)
9	HEC	A	302	1	32,50,50	2.49	6 (18%)	24,82,82	1.79	7 (29%)

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	303	1	-	2/10/54/54	-
9	HEC	A	301	1	-	0/10/54/54	-
10	SF4	B	1102	2	-	-	0/6/5/5
10	SF4	B	1103	2	-	-	0/6/5/5
10	SF4	B	1101	2	-	-	0/6/5/5
15	JM9	C	504	-	-	28/56/56/56	-
13	HQO	C	502	-	-	3/7/7/7	0/2/2/2
11	F3S	B	1104	2	-	-	0/3/3/3
9	HEC	A	305	1	-	0/10/54/54	-
9	HEC	A	304	1	-	2/10/54/54	-
12	JLQ	C	501	-	-	33/48/48/48	-
9	HEC	E	301	5	-	4/10/54/54	-
14	JL3	C	503	-	-	25/48/48/48	-
9	HEC	A	302	1	-	4/10/54/54	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HQO	O4-N1	-11.68	1.23	1.38
9	A	302	HEC	C2B-C3B	-8.25	1.32	1.40
9	A	303	HEC	C3C-C2C	-7.72	1.32	1.40
9	E	301	HEC	C2B-C3B	-7.43	1.33	1.40
9	A	305	HEC	C2B-C3B	-7.37	1.33	1.40

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	JLQ	O30-C31-C33	5.28	122.88	111.50
14	C	503	JL3	O29-C30-C32	4.29	120.74	111.50
9	A	301	HEC	CMC-C2C-C1C	-4.18	122.05	128.46
9	A	301	HEC	CMC-C2C-C3C	4.12	130.66	125.82
15	C	504	JM9	O17-C15-C14	3.74	119.56	111.50

There are no chirality outliers.

5 of 101 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	302	HEC	C2D-C3D-CAD-CBD
9	A	302	HEC	C4D-C3D-CAD-CBD
12	C	501	JLQ	C21-O22-P23-O24
12	C	501	JLQ	C21-O22-P23-O25
12	C	501	JLQ	C27-O26-P23-O25

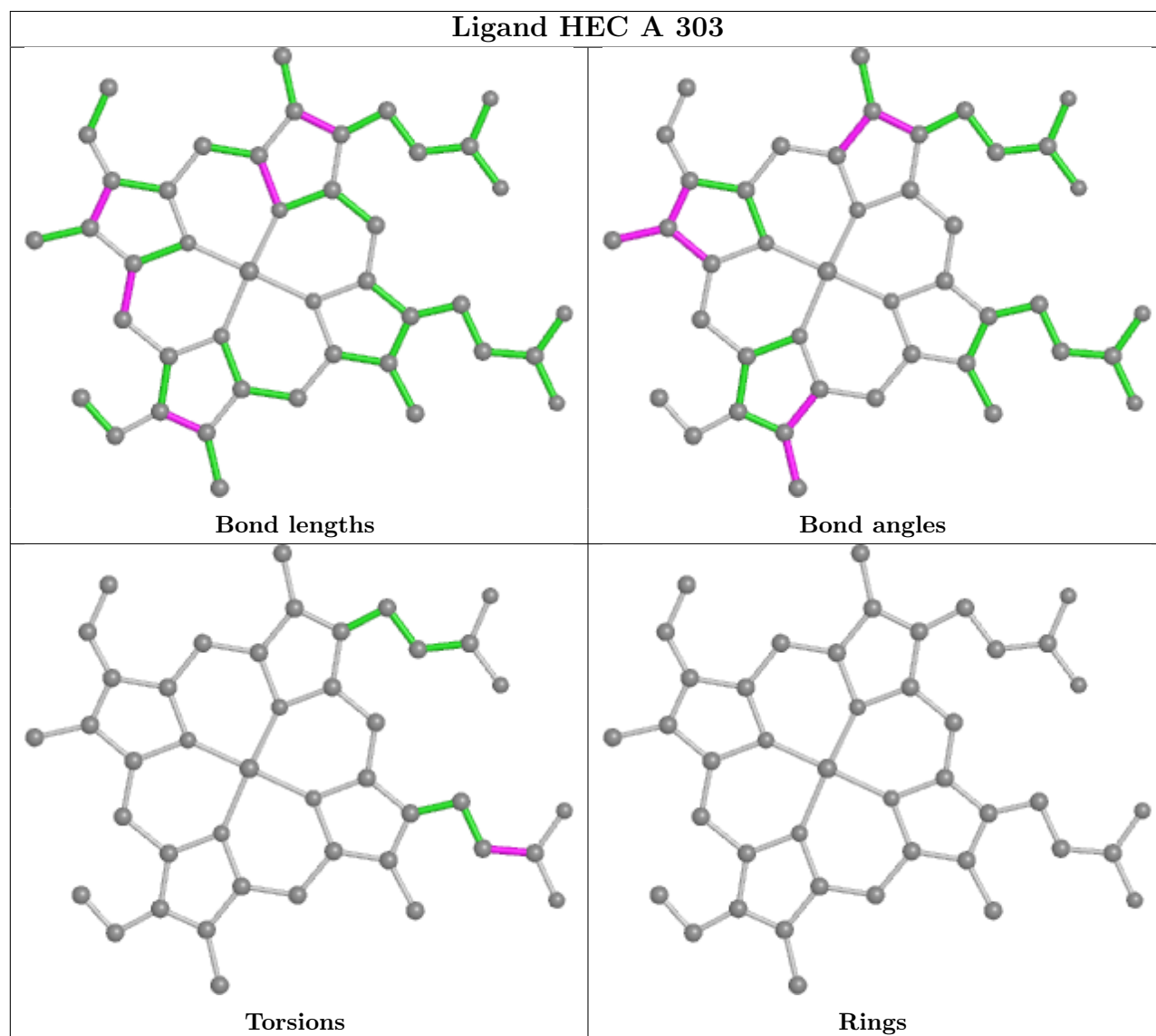
There are no ring outliers.

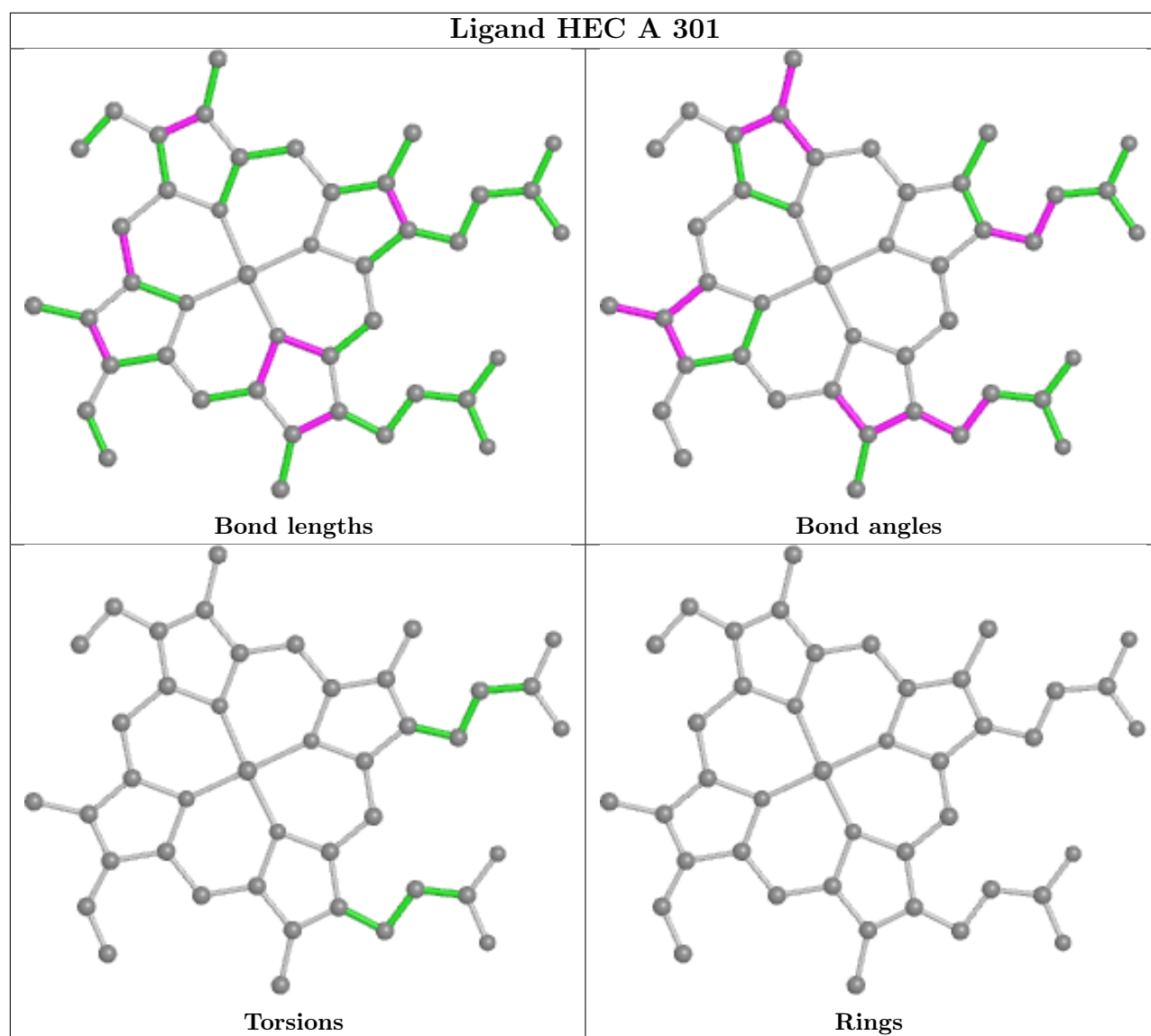
9 monomers are involved in 21 short contacts:

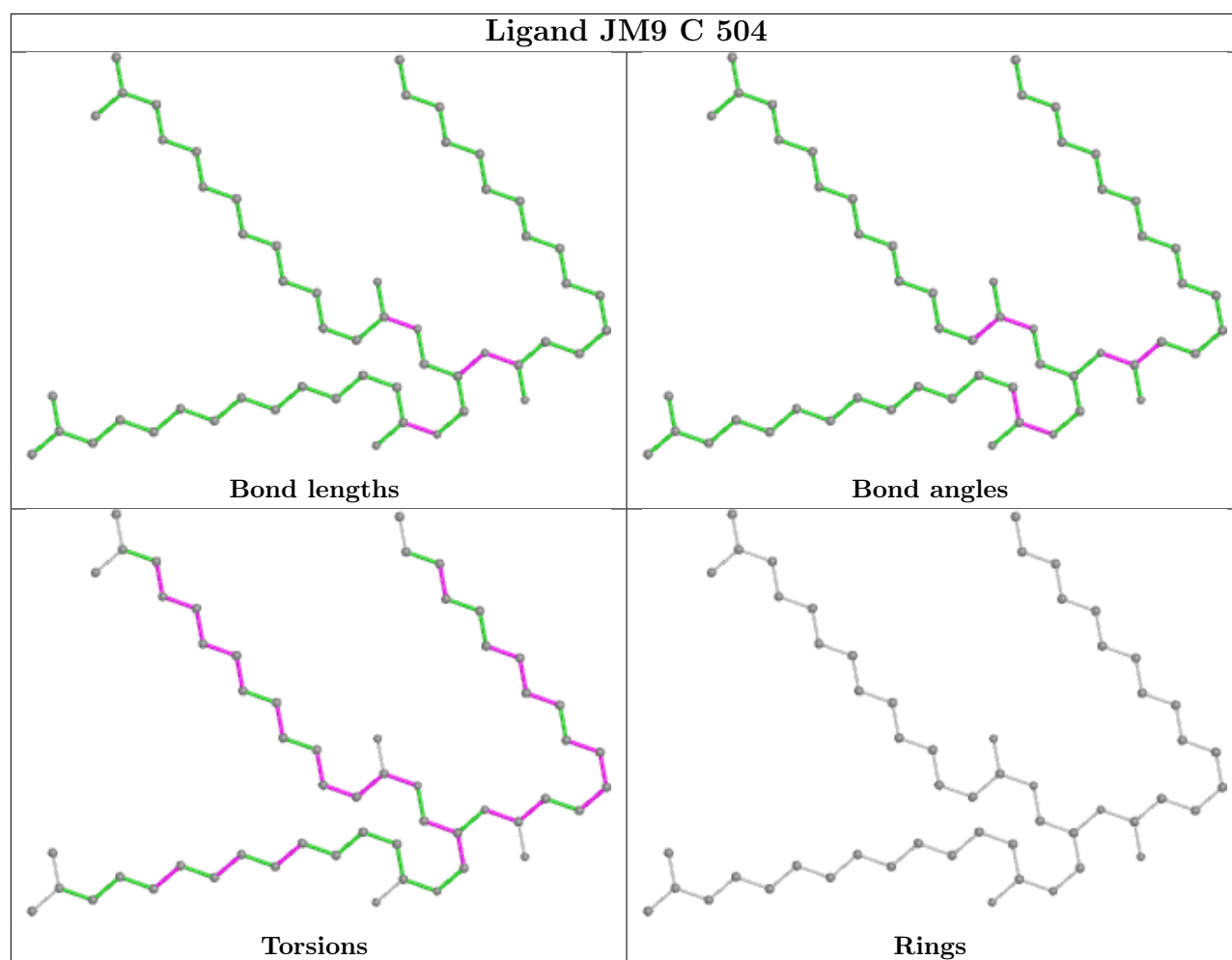
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	303	HEC	1	0
9	A	301	HEC	5	0
10	B	1103	SF4	1	0
11	B	1104	F3S	5	0
13	C	502	HQO	1	0
9	A	305	HEC	2	0
9	A	304	HEC	1	0
9	E	301	HEC	2	0
9	A	302	HEC	3	0

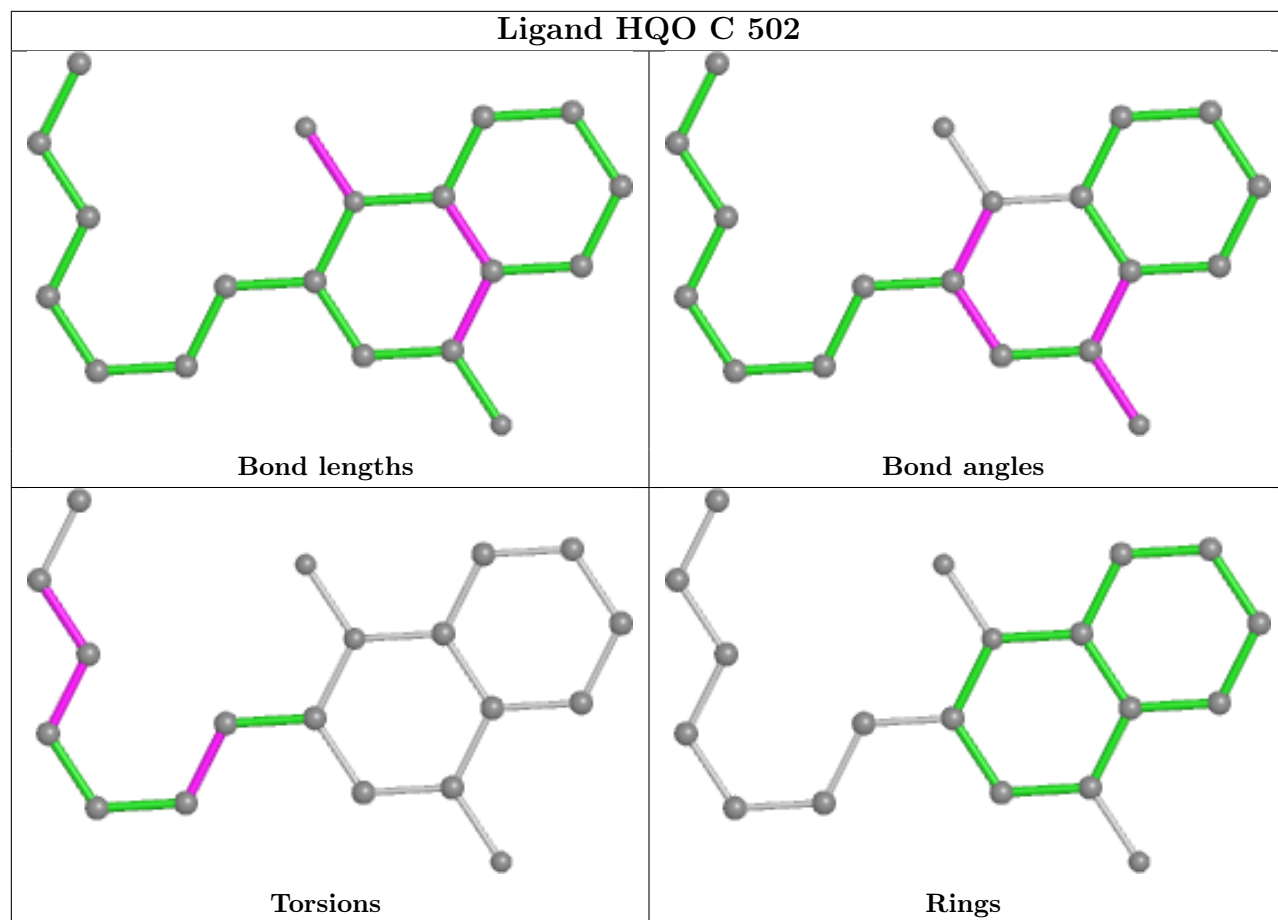
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

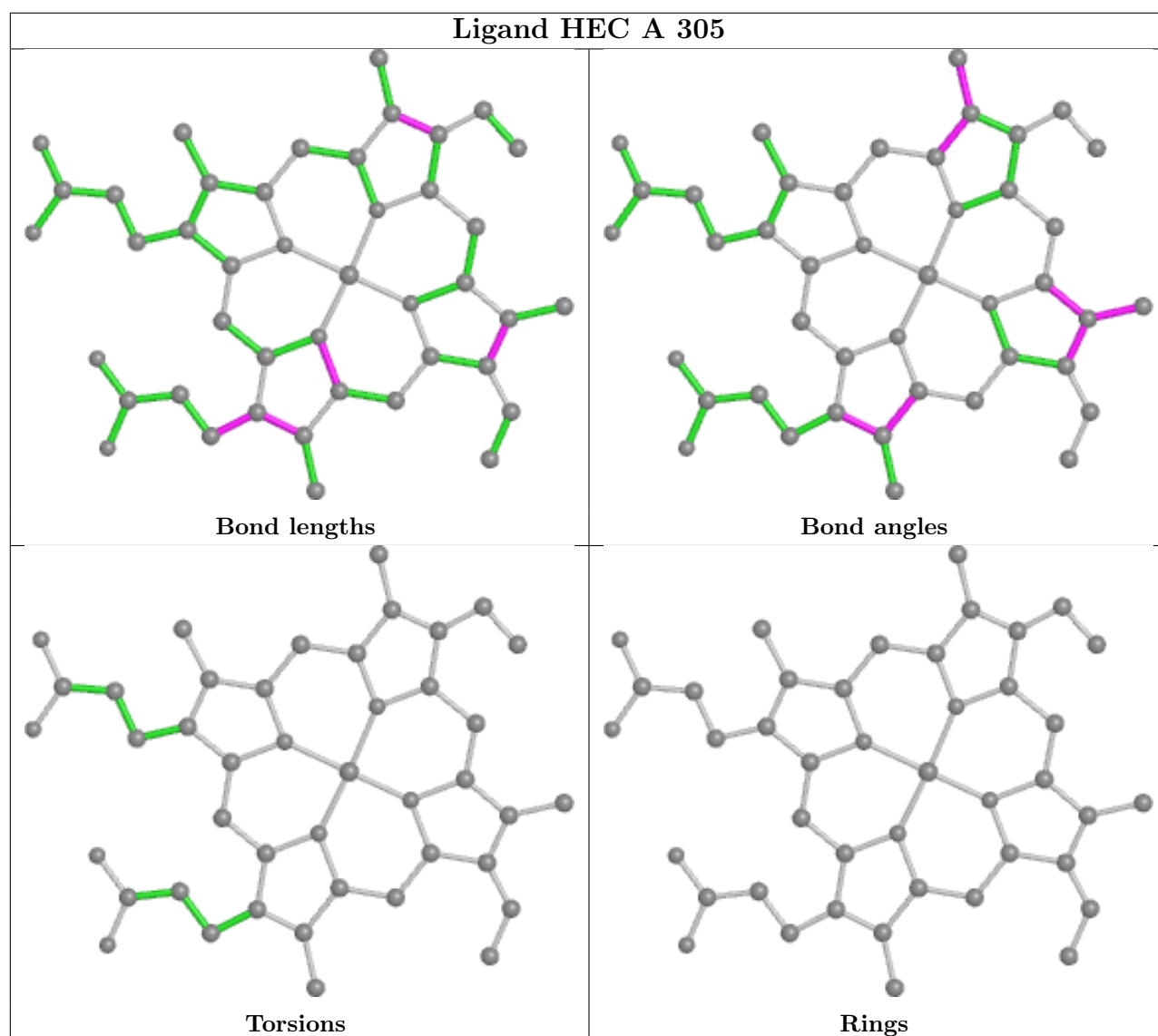
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

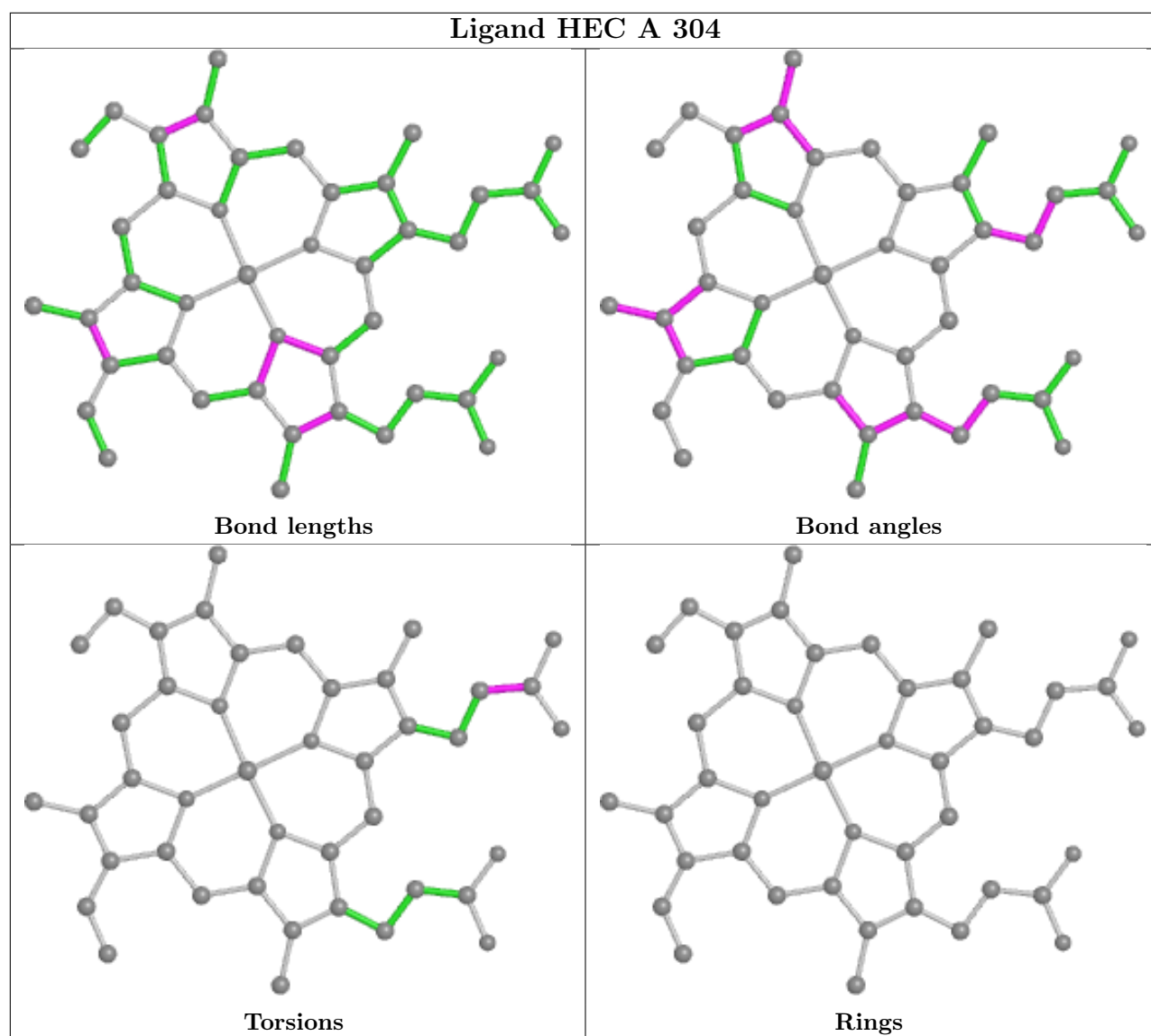


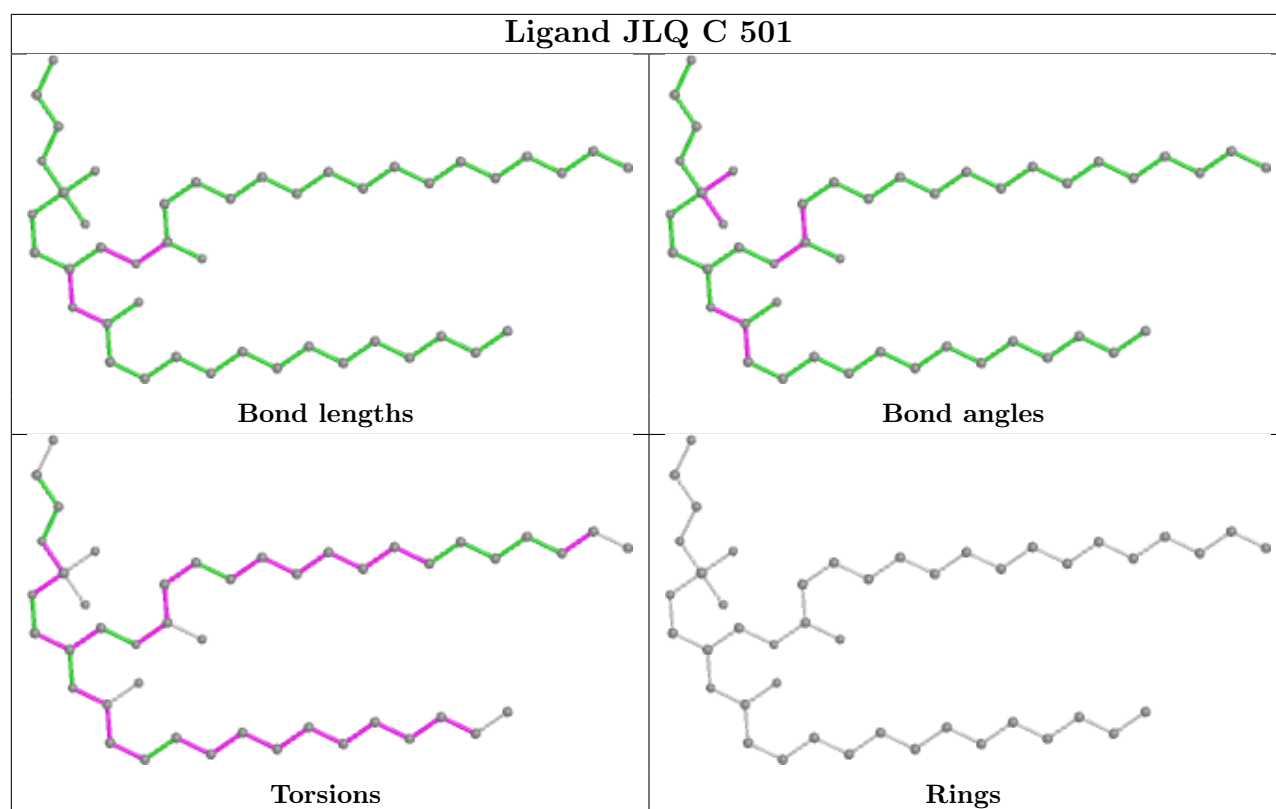


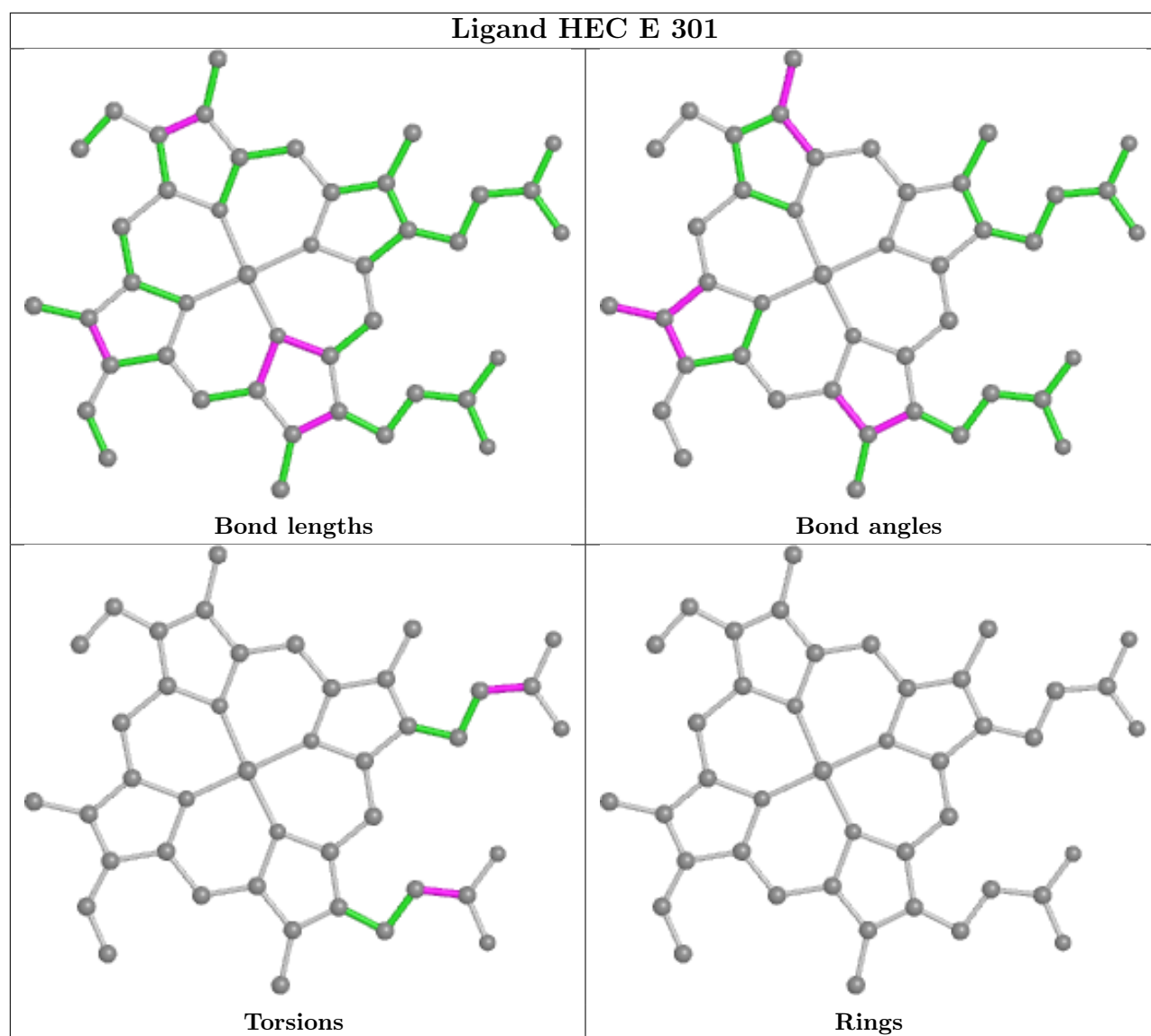


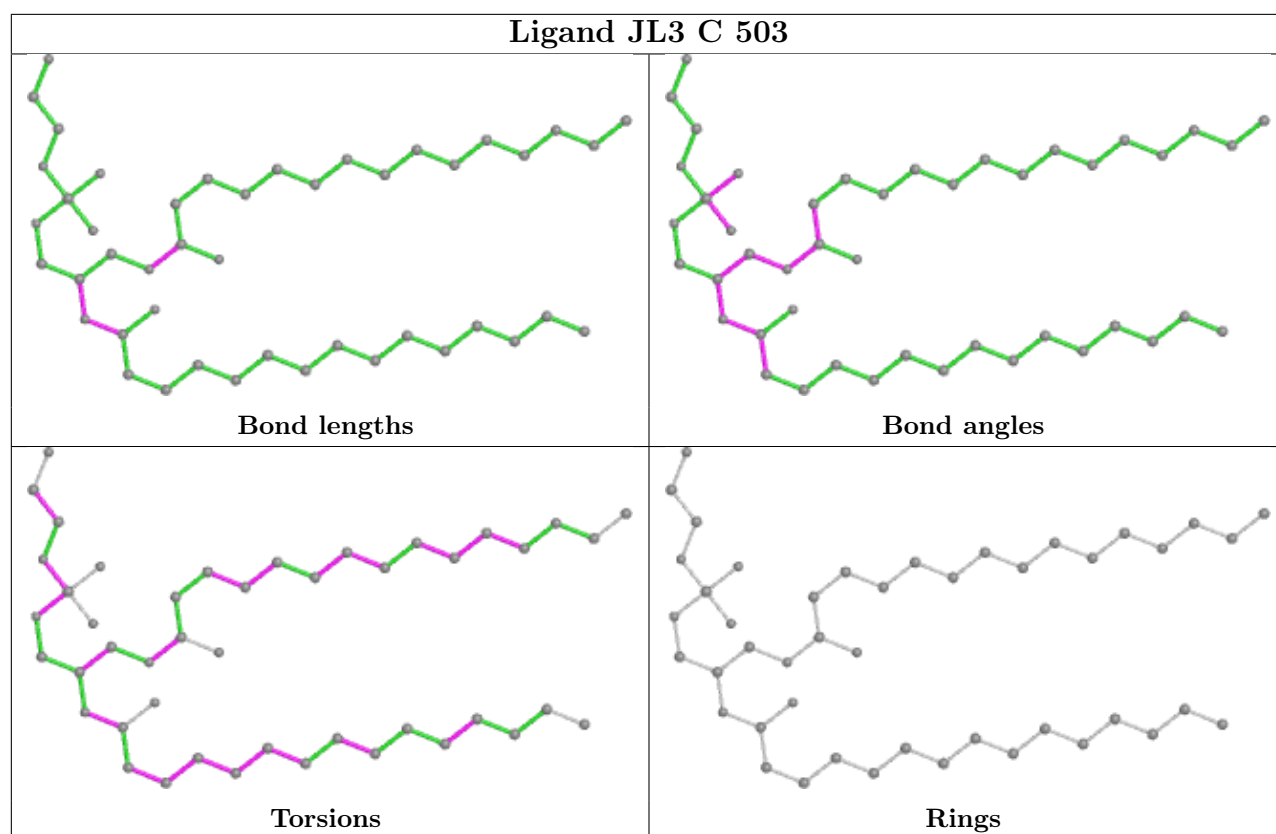


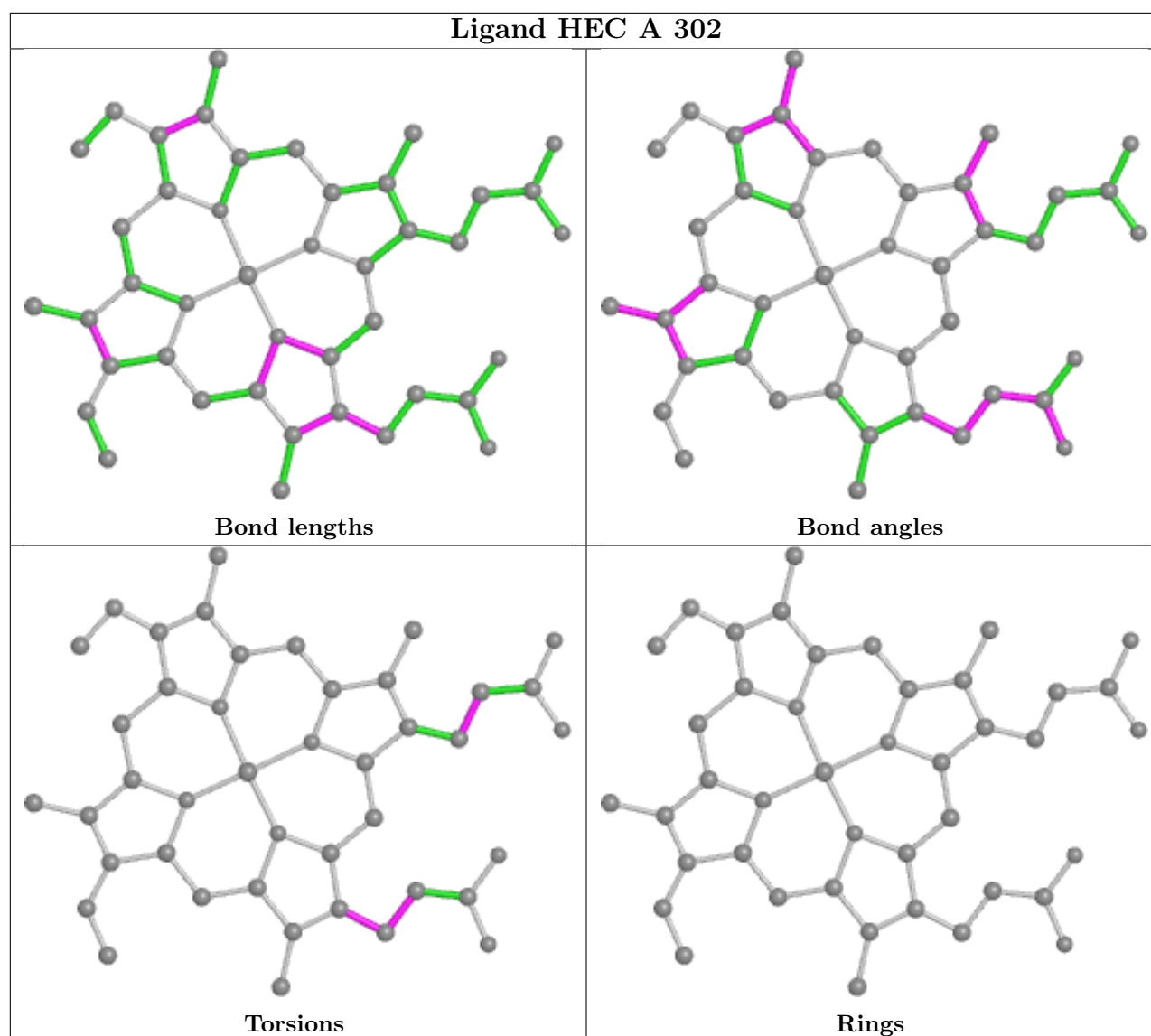












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.