



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2025 – 10:10 PM JST

PDB ID : 8K9F
EMDB ID : EMD-36985
Title : Cryo-EM structure of the photosynthetic alternative complex III from *Chloroflexus aurantiacus* at 2.9 angstrom
Authors : Xu, X.
Deposited on : 2023-08-01
Resolution : 2.90 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

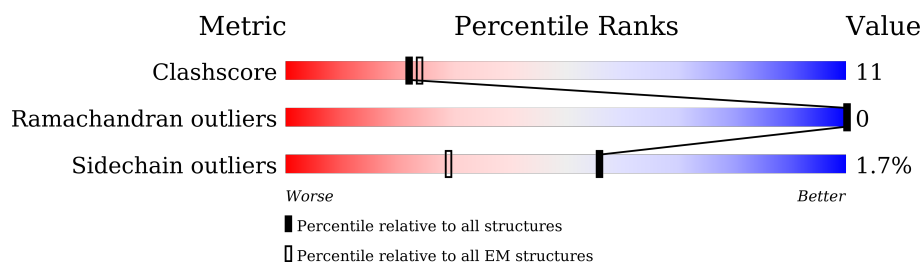
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	71% 28% .
2	B	1029	75% 17% 8%
3	C	486	71% 22% 8%
4	D	179	70% 26% ..
5	E	205	62% 17% 20%
6	F	411	77% 20% .
7	G	112	51% 21% 29%
8	I	37	84% 16%

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 19906 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
			1298	822	223	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		

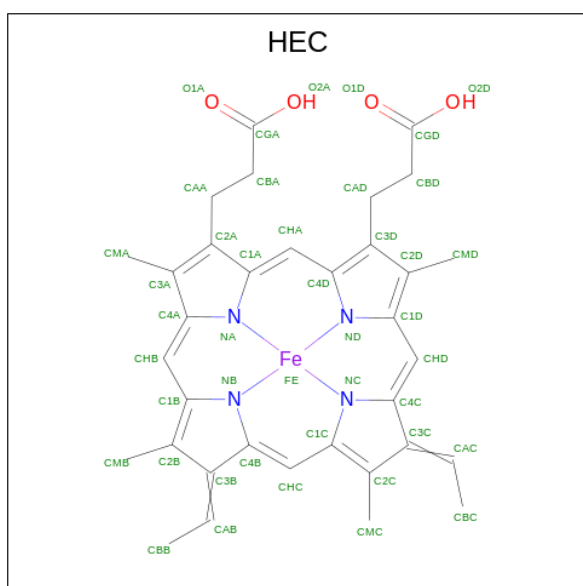
- Molecule 7 is a protein called hypothetical protein.

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.

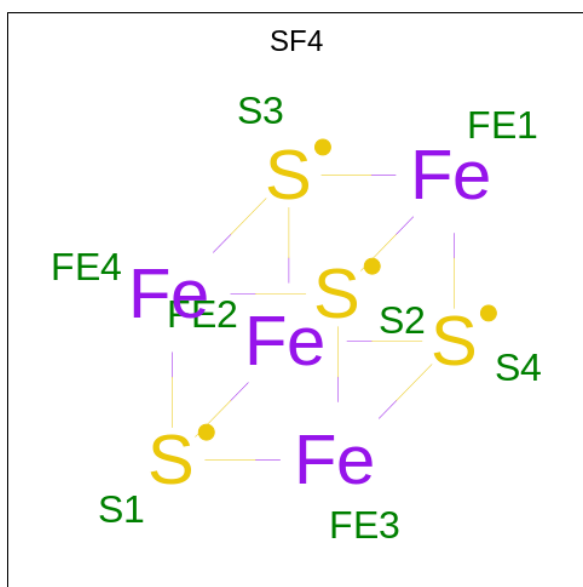
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			305	212	42	48	3		

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



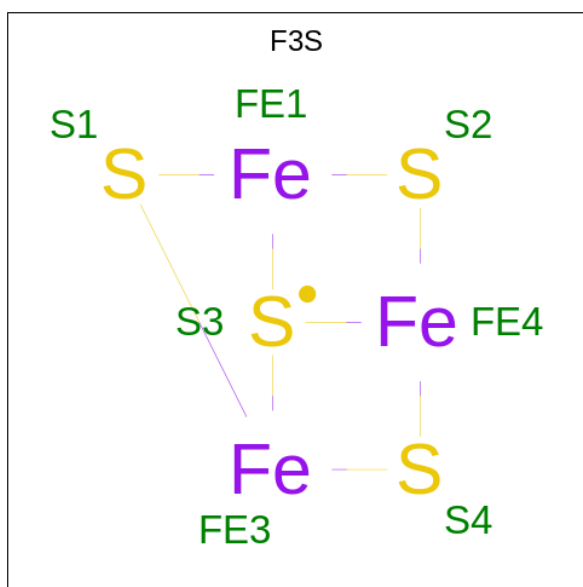
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- 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).

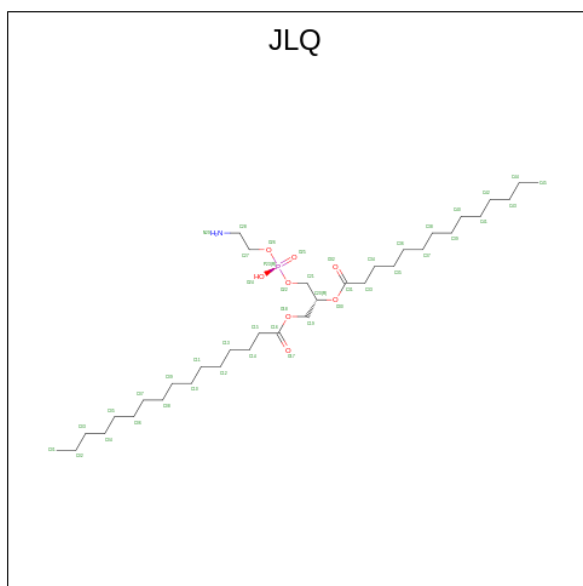


Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

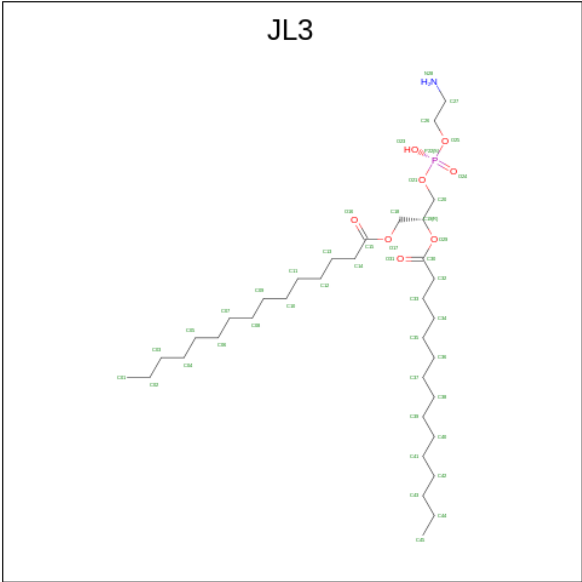
Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total	Mg	0
			1	1	

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



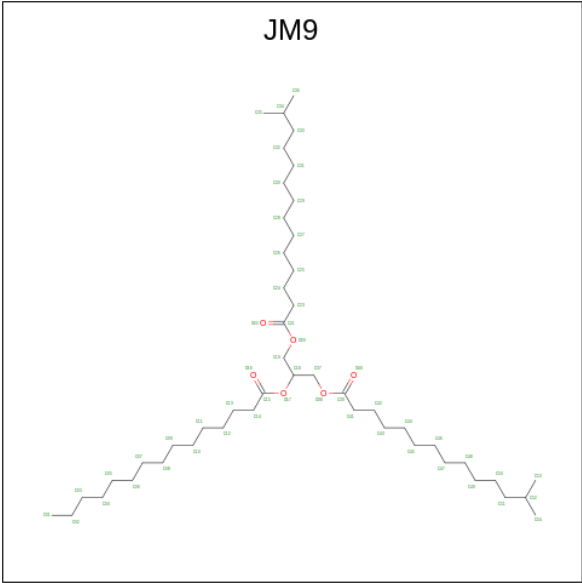
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			45	35	1	8	1	

- 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).

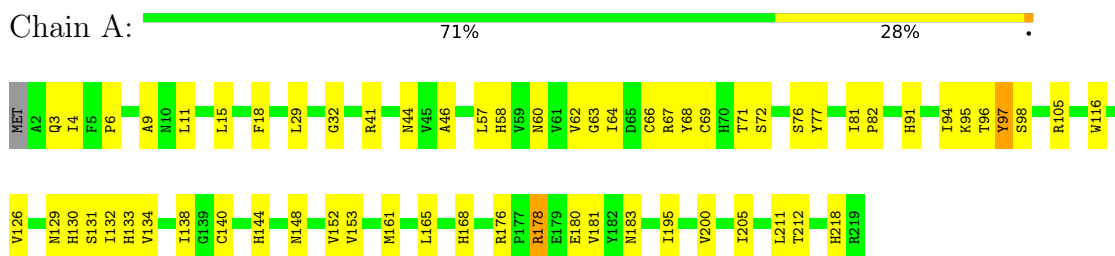


Mol	Chain	Residues	Atoms			AltConf
15	F	1	Total	C	O	0
			54	48	6	

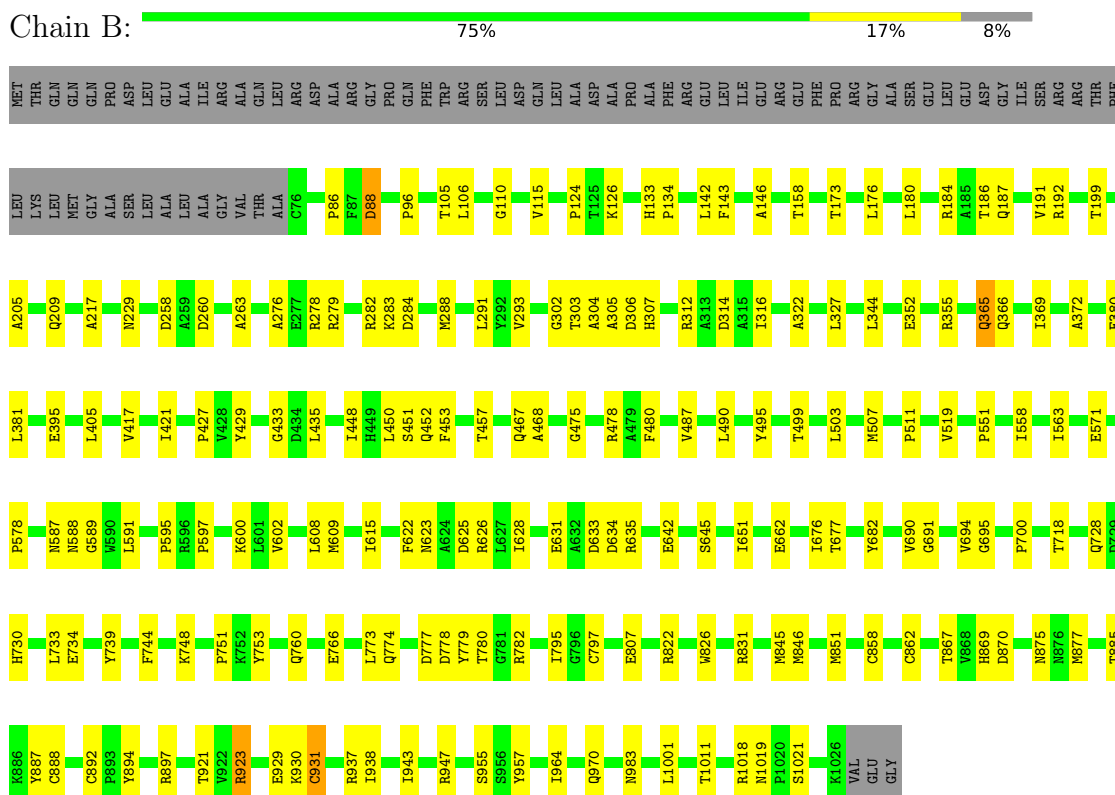
3 Residue-property plots [i](#)

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: Cytochrome c7-like domain-containing protein

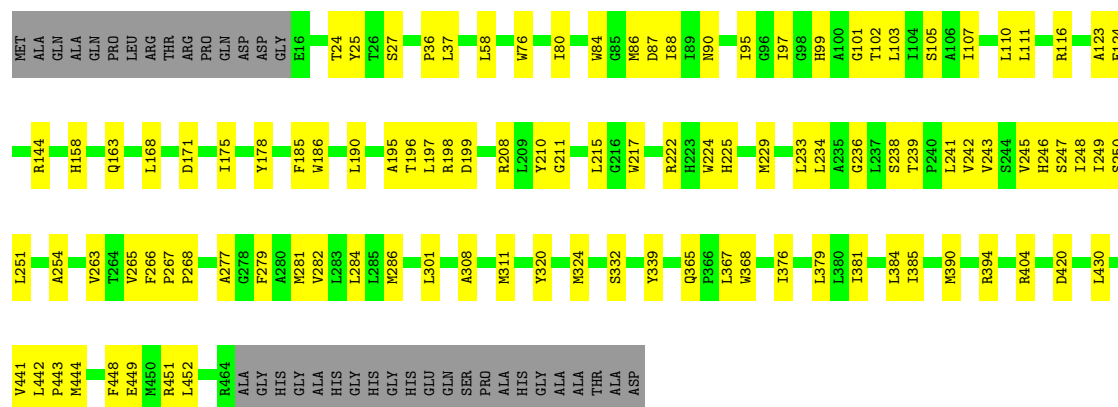


- Molecule 2: Fe-S-cluster-containing hydrogenase components 1-like protein



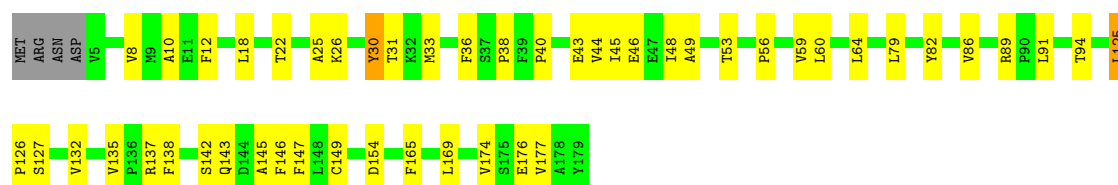
- Molecule 3: Polysulphide reductase NrfD





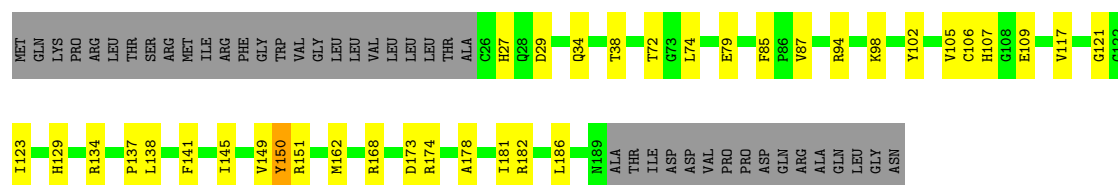
• Molecule 4: Quinol:cytochrome c oxidoreductase membrane protein

Chain D: 70% 26% ..



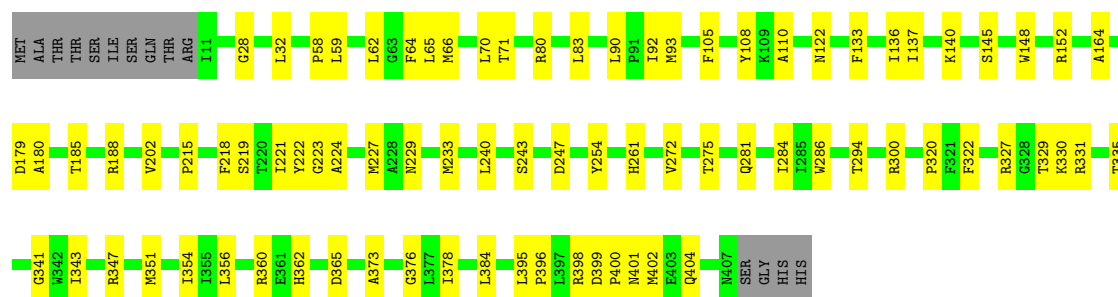
• Molecule 5: Cytochrome c domain-containing protein

Chain E: 62% 17% 20%



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

Chain F: 77% 20%

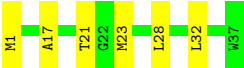
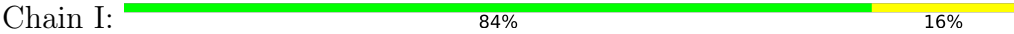


• Molecule 7: hypothetical protein

Chain G: 51% 21% 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	103633	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)	1000	Depositor
Maximum defocus (nm)	1800	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: SF4, JLQ, F3S, JM9, HEC, MG, JL3

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	0.48	0/1812	0.71	0/2472
2	B	0.39	0/7518	0.65	0/10249
3	C	0.41	0/3787	0.67	0/5179
4	D	0.41	0/1388	0.69	0/1895
5	E	0.42	0/1333	0.69	0/1810
6	F	0.40	0/3226	0.70	0/4408
7	G	0.34	0/635	0.71	0/865
8	I	0.38	0/318	0.69	0/436
All	All	0.41	0/20017	0.68	0/27314

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	1714	69	0
2	B	7350	0	7178	139	0
3	C	3655	0	3688	94	0
4	D	1350	0	1341	46	0
5	E	1298	0	1229	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	3128	0	3175	65	0
7	G	623	0	660	21	0
8	I	305	0	302	6	0
9	A	215	0	152	30	0
9	E	43	0	31	17	0
10	B	24	0	0	1	0
11	B	7	0	0	10	0
12	B	1	0	0	0	0
13	C	45	0	0	0	0
14	F	45	0	0	4	0
15	F	54	0	0	6	0
All	All	19906	0	19470	443	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 11.

The worst 5 of 443 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:66:CYS:CB	9:A:304:HEC:HAB	1.07	1.51
1:A:66:CYS:HB3	9:A:304:HEC:CAB	1.03	1.47
5:E:106:CYS:SG	9:E:301:HEC:CAC	2.18	1.31
4:D:26:LYS:HE2	4:D:48:ILE:HG22	1.29	1.08
1:A:66:CYS:SG	9:A:304:HEC:HAB	1.95	1.05

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	A	216/219 (99%)	202 (94%)	14 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	949/1029 (92%)	888 (94%)	61 (6%)	0	100	100
3	C	447/486 (92%)	425 (95%)	22 (5%)	0	100	100
4	D	173/179 (97%)	158 (91%)	15 (9%)	0	100	100
5	E	162/205 (79%)	149 (92%)	13 (8%)	0	100	100
6	F	395/411 (96%)	370 (94%)	25 (6%)	0	100	100
7	G	78/112 (70%)	72 (92%)	6 (8%)	0	100	100
8	I	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	2455/2678 (92%)	2297 (94%)	158 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	85
2	B	768/830 (92%)	756 (98%)	12 (2%)	58	84
3	C	382/405 (94%)	377 (99%)	5 (1%)	65	88
4	D	143/147 (97%)	137 (96%)	6 (4%)	25	59
5	E	136/171 (80%)	134 (98%)	2 (2%)	60	85
6	F	318/330 (96%)	312 (98%)	6 (2%)	52	81
7	G	69/95 (73%)	68 (99%)	1 (1%)	62	86
8	I	32/32 (100%)	32 (100%)	0	100	100
All	All	2046/2209 (93%)	2011 (98%)	35 (2%)	56	83

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	64	PHE
6	F	105	PHE

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Mol	Chain	Res	Type
6	F	261	HIS
2	B	923	ARG
2	B	887	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	229	ASN
6	F	332	ASN
6	F	401	ASN
6	F	362	HIS
3	C	90	ASN

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](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\# Z > 2$
10	SF4	B	1101	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SF4	B	1103	2	0,12,12	-	-	-		
11	F3S	B	1104	2	0,9,9	-	-	-		
9	HEC	A	303	1	32,50,50	2.73	9 (28%)	24,82,82	2.82	8 (33%)
9	HEC	A	302	1	32,50,50	2.50	9 (28%)	24,82,82	2.18	4 (16%)
9	HEC	E	301	5	32,50,50	2.43	7 (21%)	24,82,82	2.88	8 (33%)
9	HEC	A	304	1	32,50,50	2.54	8 (25%)	24,82,82	2.30	5 (20%)
9	HEC	A	305	1	32,50,50	2.41	8 (25%)	24,82,82	2.34	9 (37%)
15	JM9	F	502	-	53,53,53	1.23	8 (15%)	58,58,58	1.84	13 (22%)
9	HEC	A	301	1	32,50,50	2.45	3 (9%)	24,82,82	2.81	9 (37%)
10	SF4	B	1102	2	0,12,12	-	-	-		
14	JL3	F	501	-	44,44,44	0.99	5 (11%)	47,49,49	0.89	3 (6%)
13	JLQ	C	501	-	44,44,44	0.97	4 (9%)	47,49,49	1.20	5 (10%)

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
10	SF4	B	1101	2	-	-	0/6/5/5
10	SF4	B	1103	2	-	-	0/6/5/5
11	F3S	B	1104	2	-	-	0/3/3/3
9	HEC	A	303	1	-	1/10/54/54	-
9	HEC	A	302	1	-	8/10/54/54	-
9	HEC	E	301	5	-	5/10/54/54	-
9	HEC	A	304	1	-	2/10/54/54	-
9	HEC	A	305	1	-	5/10/54/54	-
15	JM9	F	502	-	-	28/56/56/56	-
9	HEC	A	301	1	-	6/10/54/54	-
10	SF4	B	1102	2	-	-	0/6/5/5
14	JL3	F	501	-	-	28/48/48/48	-
13	JLQ	C	501	-	-	29/48/48/48	-

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	303	HEC	C2B-C3B	-9.95	1.30	1.40
9	A	301	HEC	C2B-C3B	-8.61	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	304	HEC	C2B-C3B	-8.18	1.32	1.40
9	E	301	HEC	C2B-C3B	-8.14	1.32	1.40
9	A	304	HEC	C3C-C2C	-7.94	1.32	1.40

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	303	HEC	C1D-C2D-C3D	-8.71	100.94	107.00
9	A	302	HEC	CMC-C2C-C1C	-7.77	116.52	128.46
9	A	301	HEC	CMC-C2C-C3C	6.99	134.04	125.82
9	E	301	HEC	CMC-C2C-C1C	-6.58	118.35	128.46
9	E	301	HEC	CMC-C2C-C3C	6.10	132.99	125.82

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	301	HEC	C3D-CAD-CBD-CGD
9	A	302	HEC	C1A-C2A-CAA-CBA
9	A	302	HEC	C3A-C2A-CAA-CBA
9	A	302	HEC	C2A-CAA-CBA-CGA
9	A	302	HEC	C2D-C3D-CAD-CBD

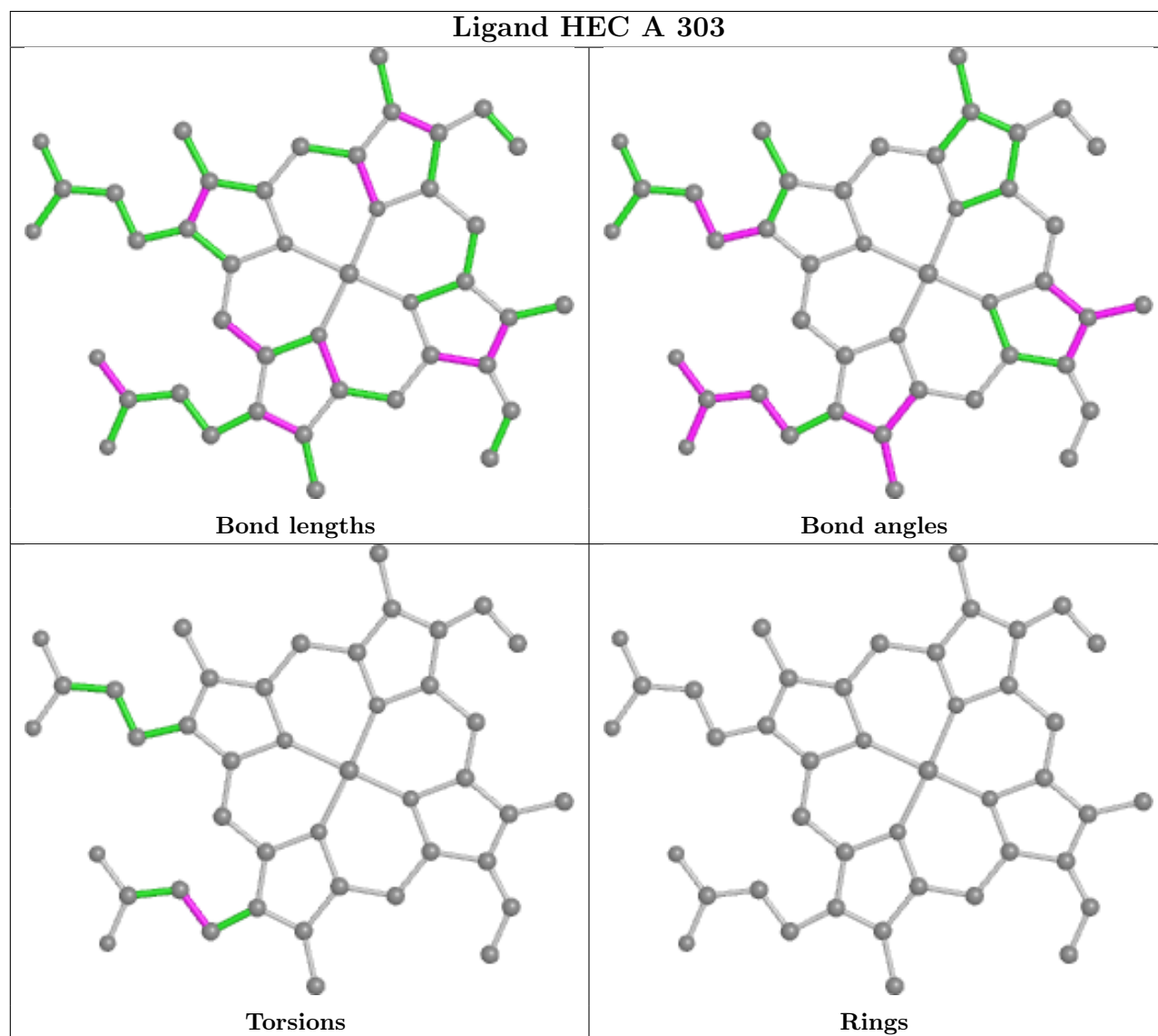
There are no ring outliers.

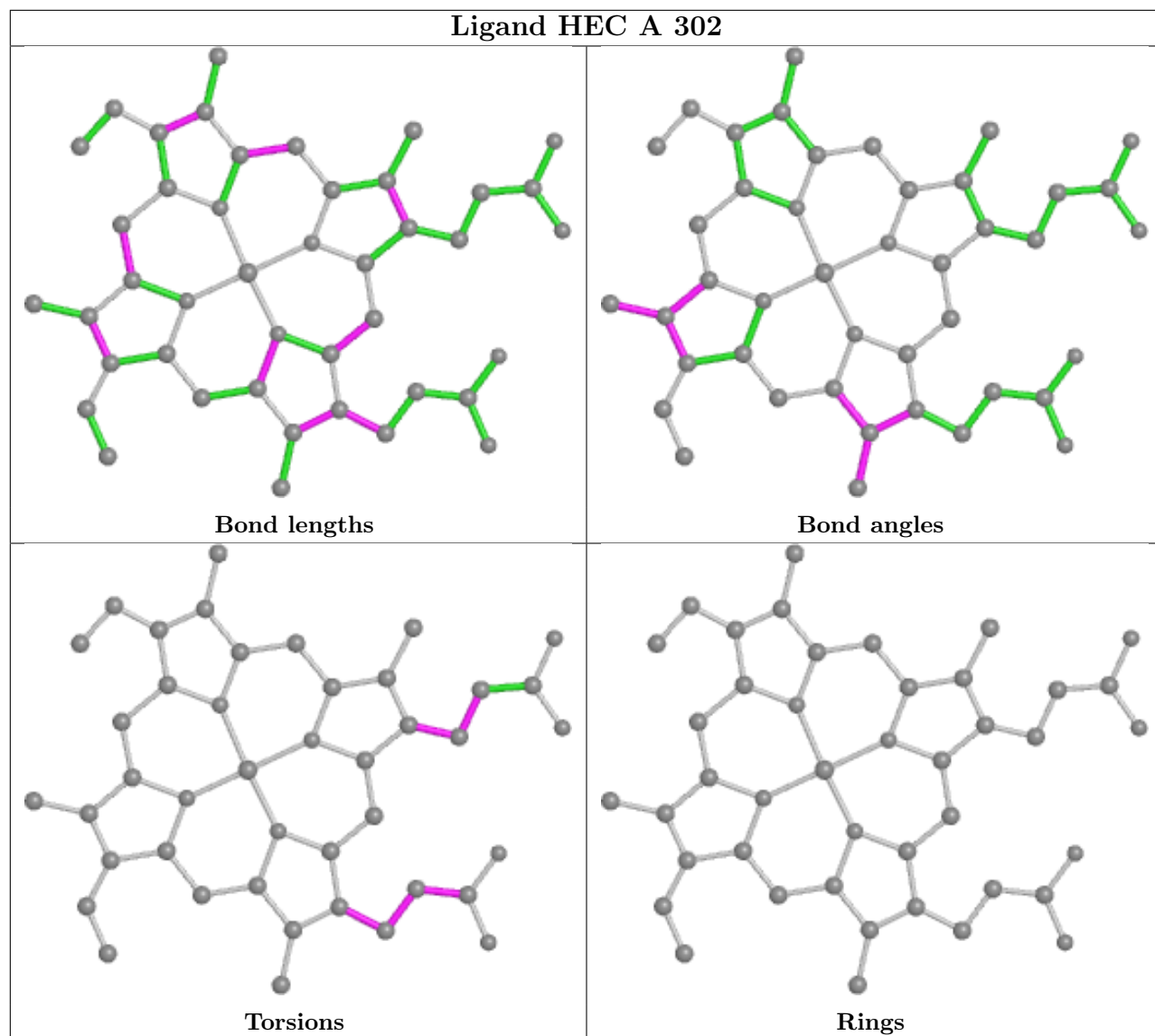
10 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1101	SF4	1	0
11	B	1104	F3S	10	0
9	A	303	HEC	2	0
9	A	302	HEC	7	0
9	E	301	HEC	17	0
9	A	304	HEC	10	0
9	A	305	HEC	7	0
15	F	502	JM9	6	0
9	A	301	HEC	5	0
14	F	501	JL3	4	0

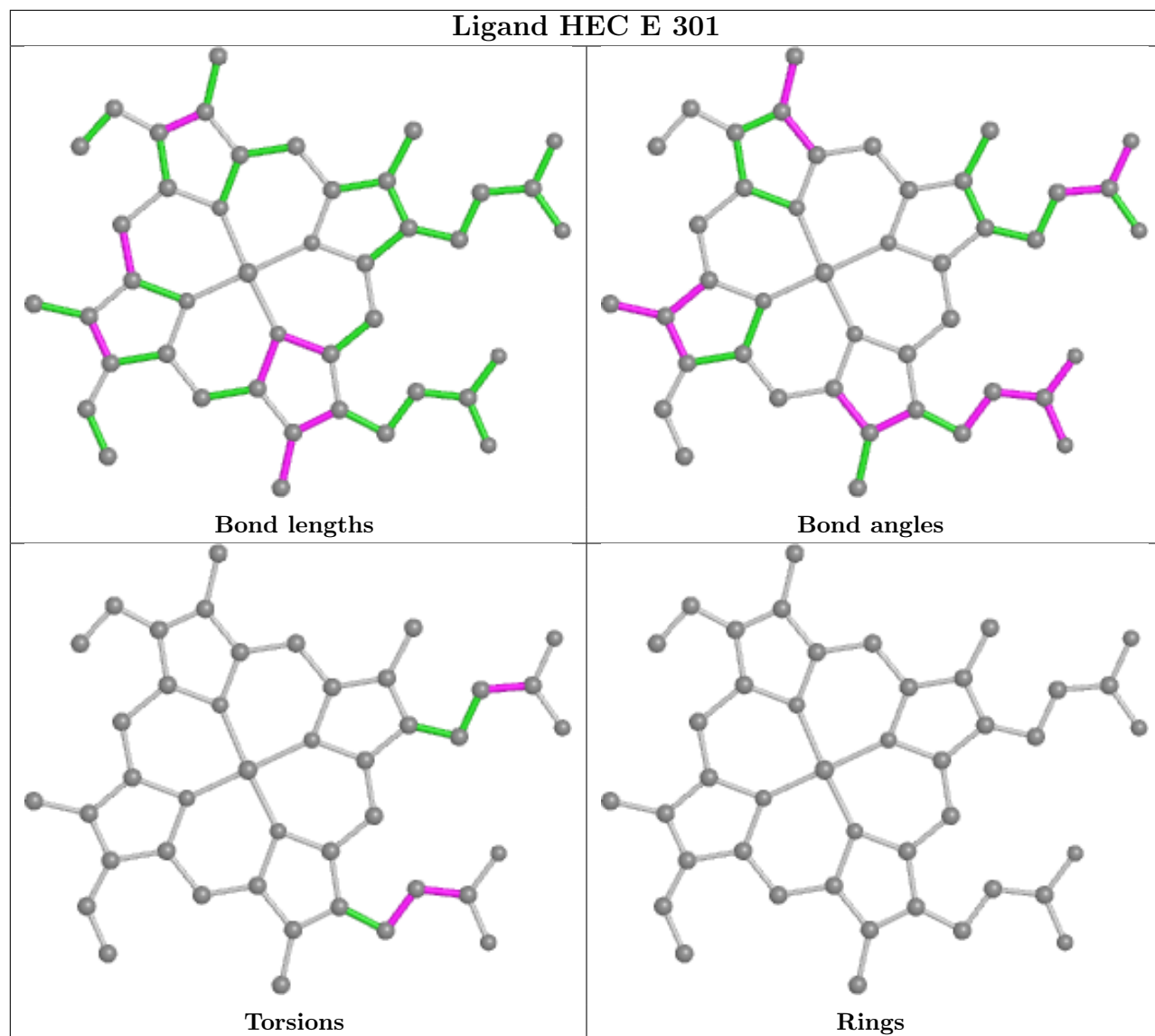
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

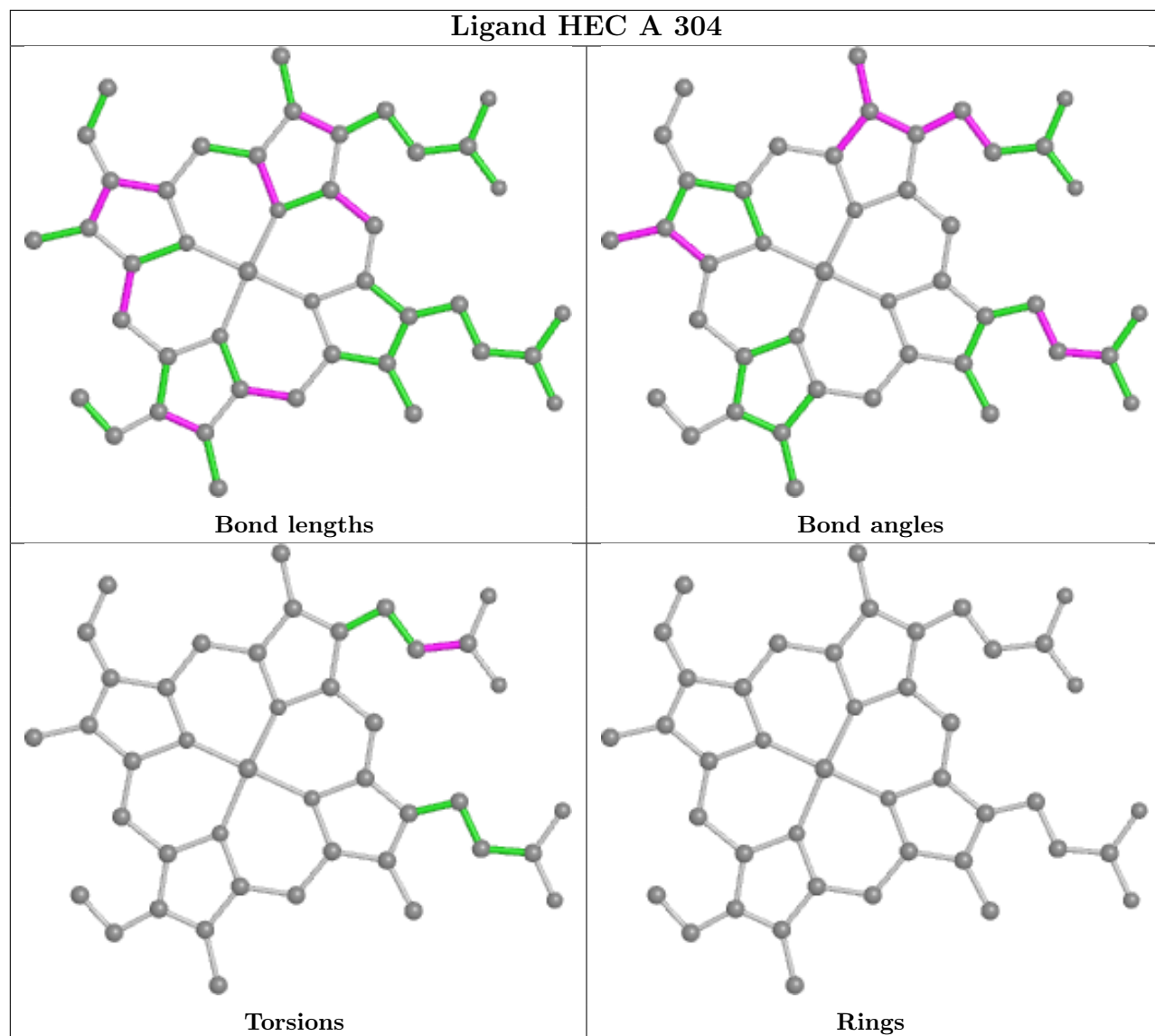
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

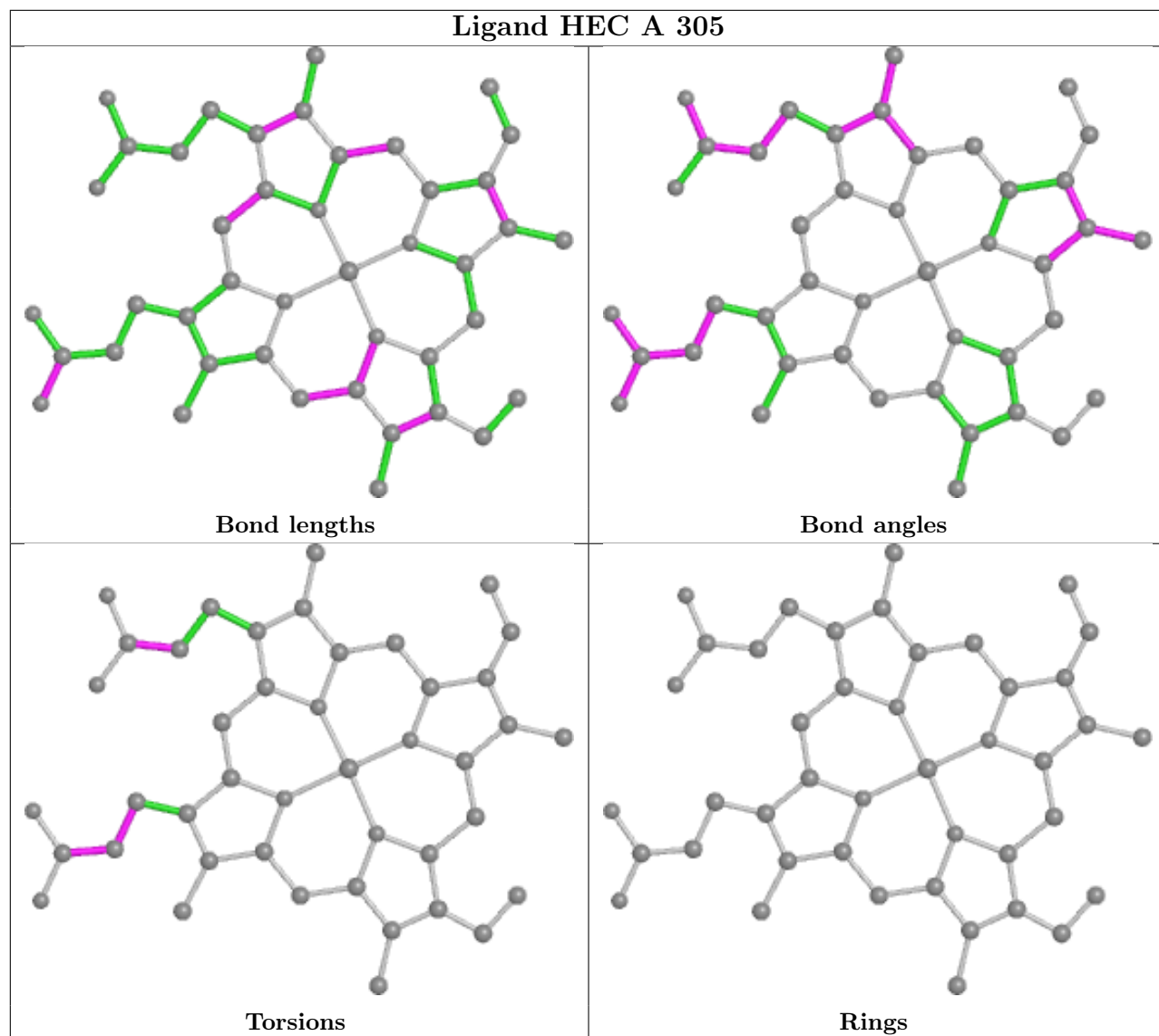


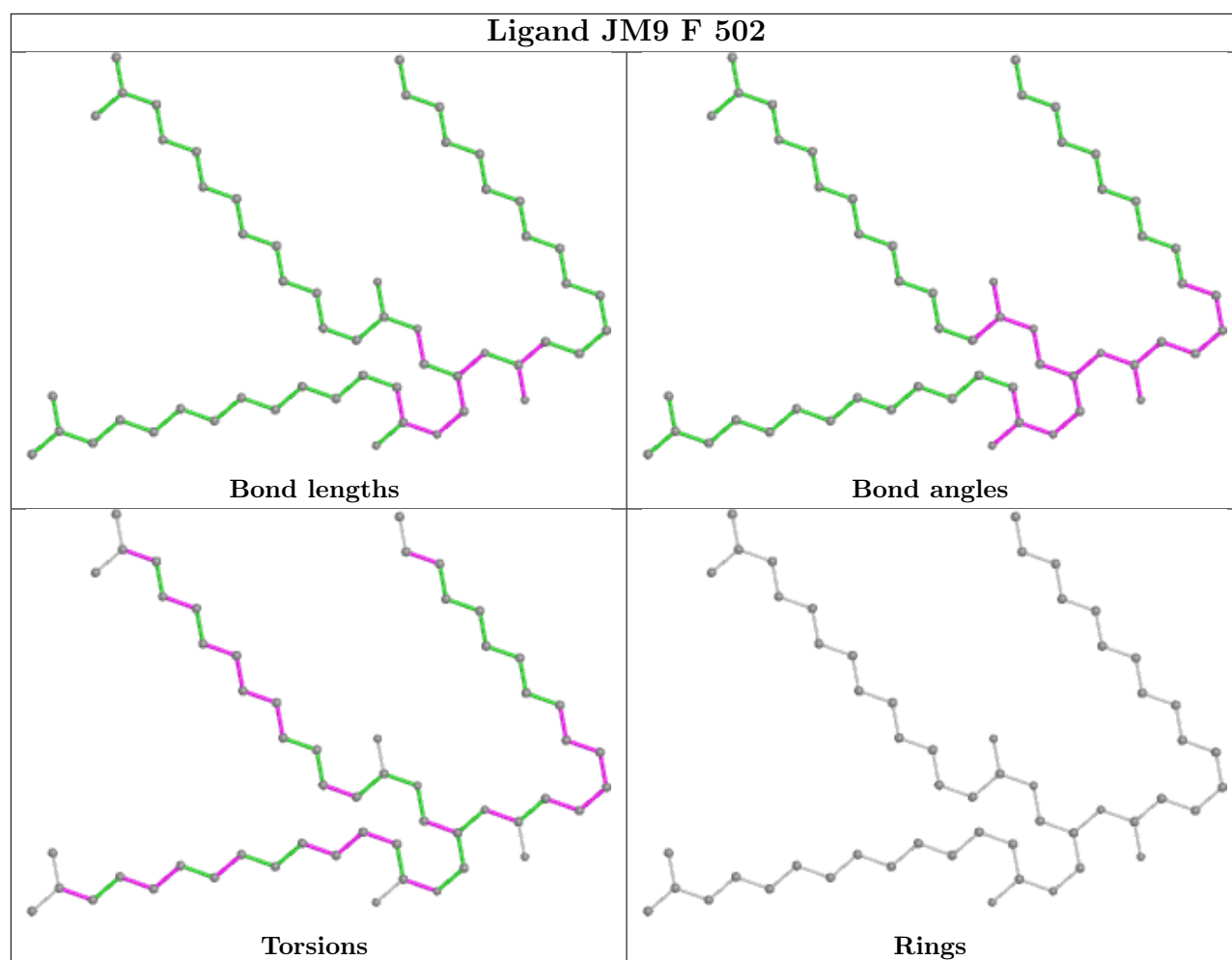


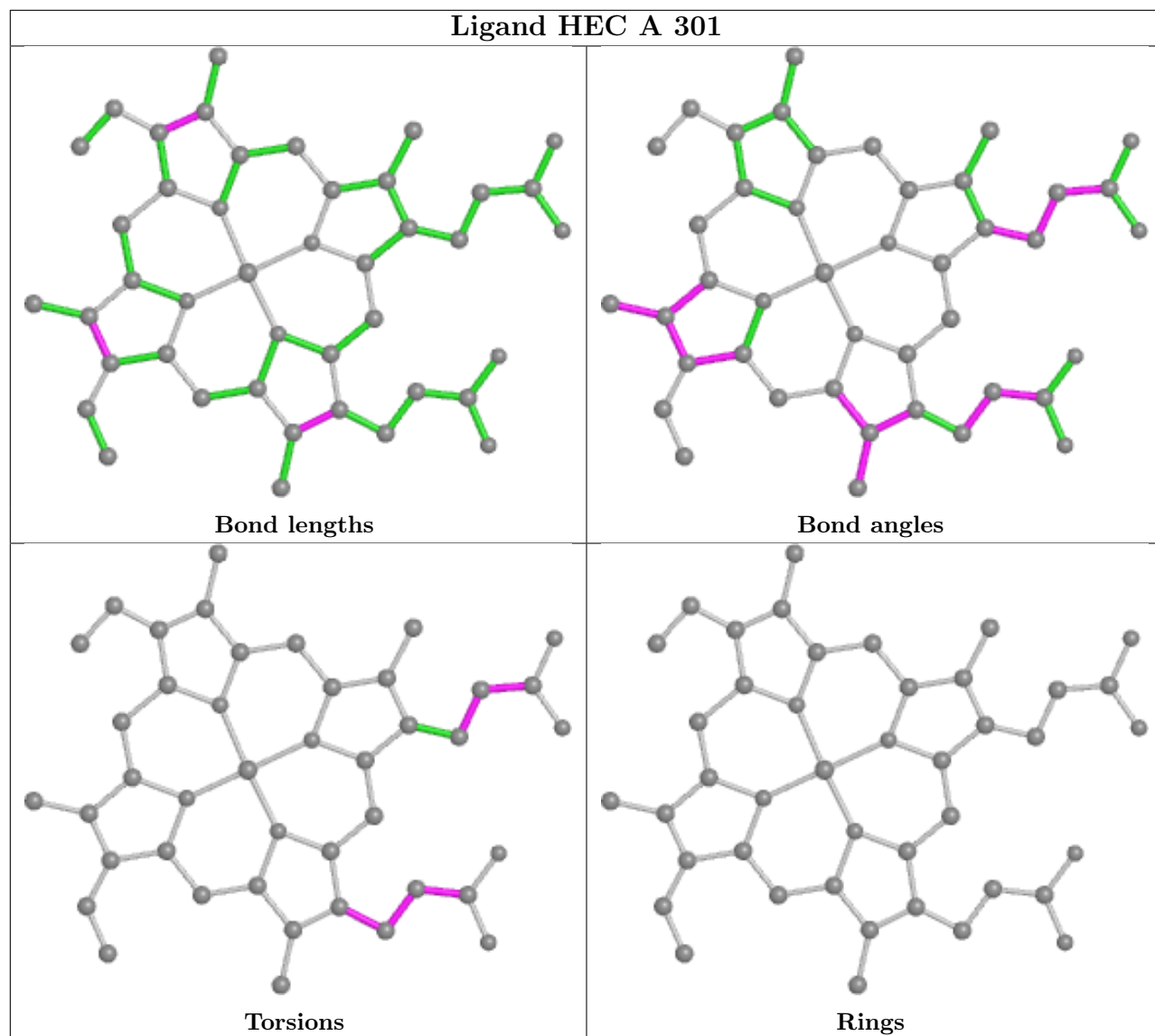
Ligand HEC E 301

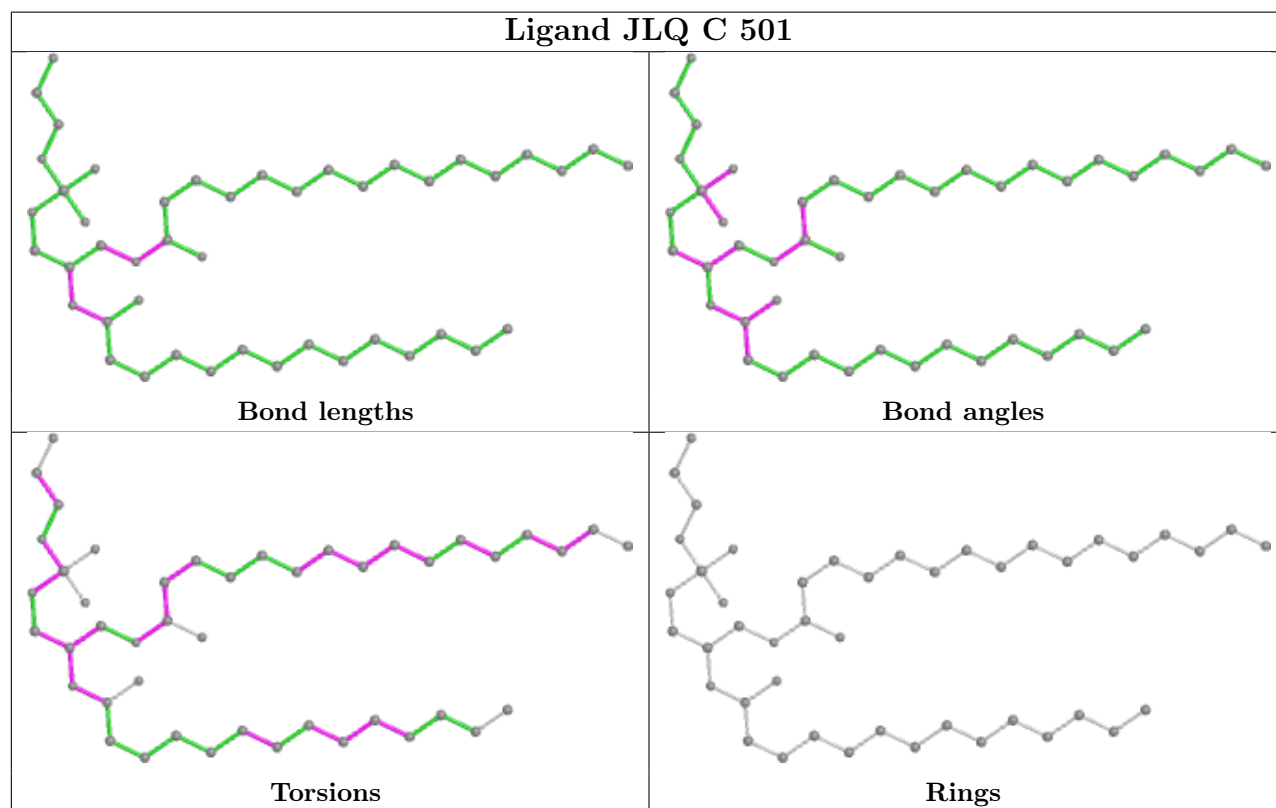
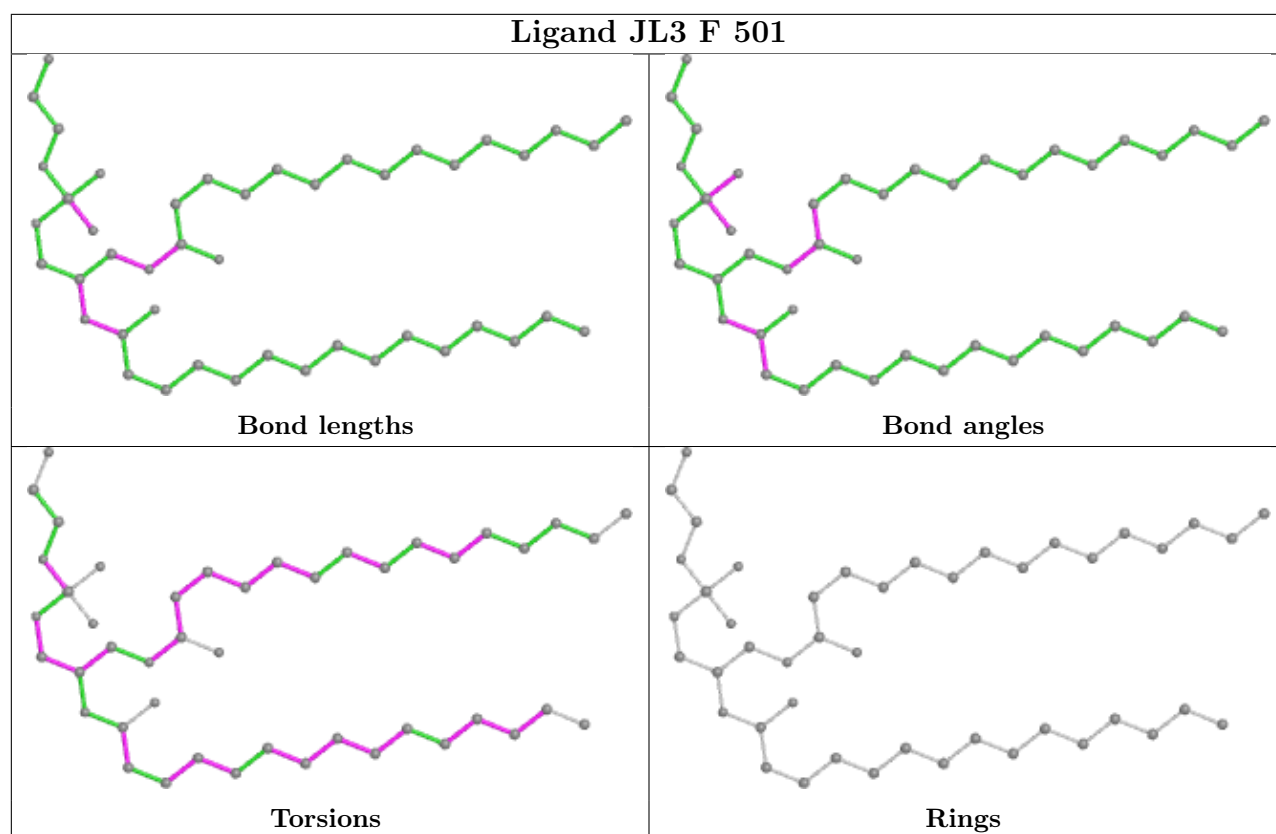












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.