



wwPDB EM Validation Summary Report ⓘ

May 5, 2026 – 10:26 PM JST

PDB ID : 9UFT / pdb_00009uft
EMDB ID : EMD-64122
Title : Ubiquinol Binding Site of Cytochrome bo3 from *Acinetobacter baumannii*
Authors : Li, J.; Zhu, J.P.
Deposited on : 2025-04-10
Resolution : 3.56 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 : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

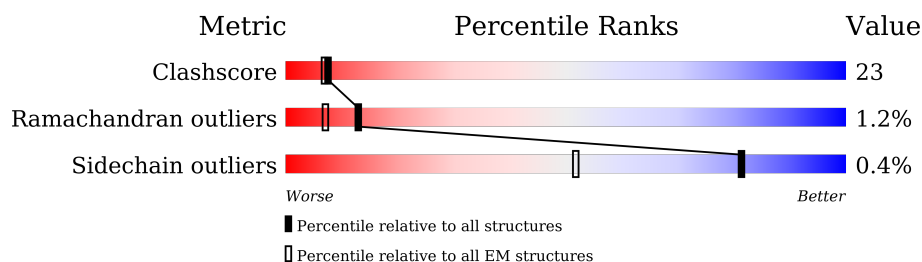
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	660	
2	B	277	
3	C	191	
4	D	97	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10290 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 bo(3) ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	660	Total	C	N	O	S	1	0
			5260	3547	816	861	36		

- Molecule 2 is a protein called Ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	277	Total	C	N	O	S	0	0
			2195	1421	368	396	10		

- Molecule 3 is a protein called Cytochrome bo(3) ubiquinol oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	191	Total	C	N	O	S	0	0
			1530	1030	233	261	6		

- Molecule 4 is a protein called Cytochrome bo(3) ubiquinol oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	97	Total	C	N	O	S	0	0
			761	509	119	124	9		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	13	GLY	-	expression tag	UNP V5VBE6
D	14	SER	-	expression tag	UNP V5VBE6
D	15	VAL	-	expression tag	UNP V5VBE6
D	16	LYS	-	expression tag	UNP V5VBE6
D	17	THR	-	expression tag	UNP V5VBE6
D	18	TYR	-	expression tag	UNP V5VBE6
D	19	MET	-	expression tag	UNP V5VBE6
D	20	THR	-	expression tag	UNP V5VBE6
D	26	ILE	VAL	conflict	UNP V5VBE6

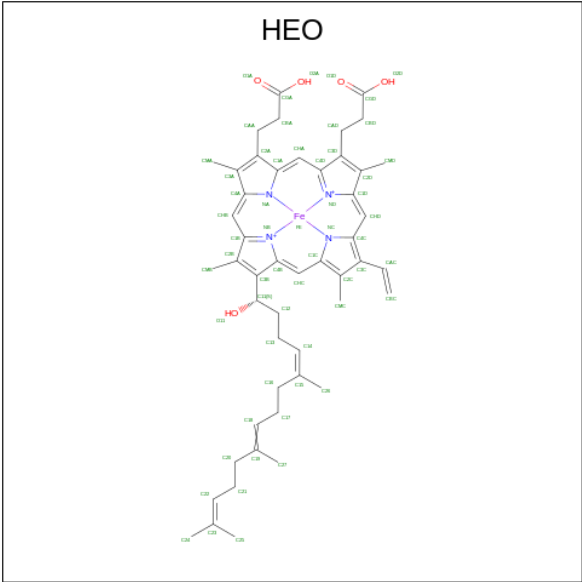
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Chain	Residue	Modelled	Actual	Comment	Reference
D	30	VAL	ILE	conflict	UNP V5VBE6
D	109	HIS	-	expression tag	UNP V5VBE6

- # HEM

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

- 

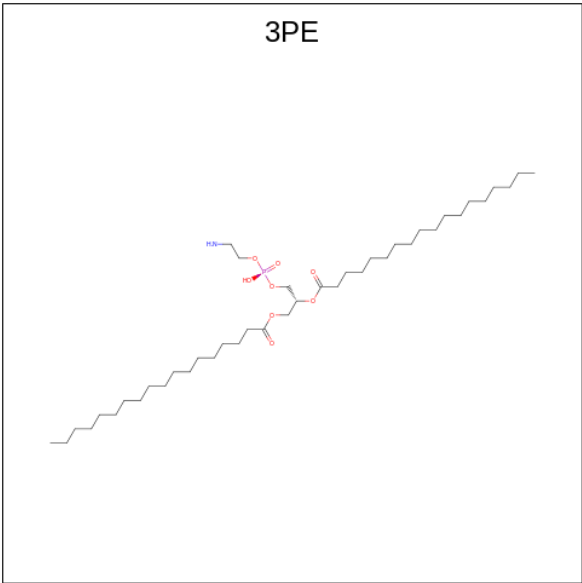


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Fe	N	O	0
			59	49	1	4	5	

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

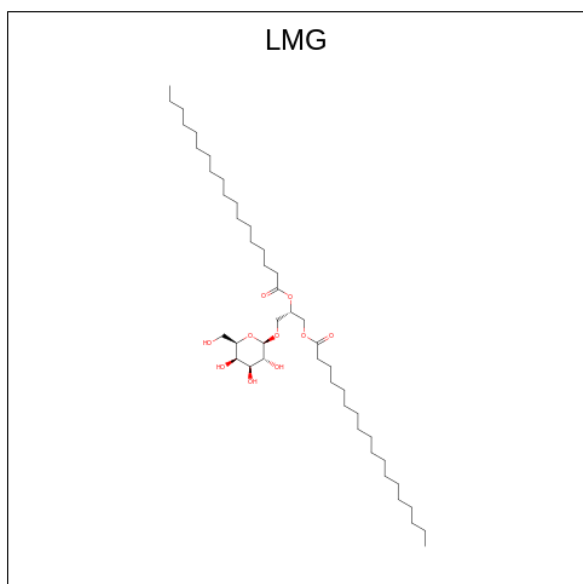
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Cu	0
			1	1	

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



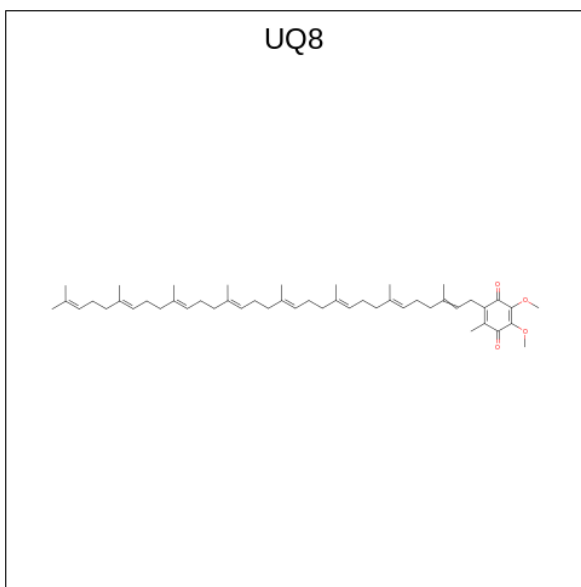
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
8	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
8	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
8	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	C	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 9 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			46	36	10	
9	A	1	Total	C	O	0
			40	30	10	
9	A	1	Total	C	O	0
			36	26	10	

- Molecule 10 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).

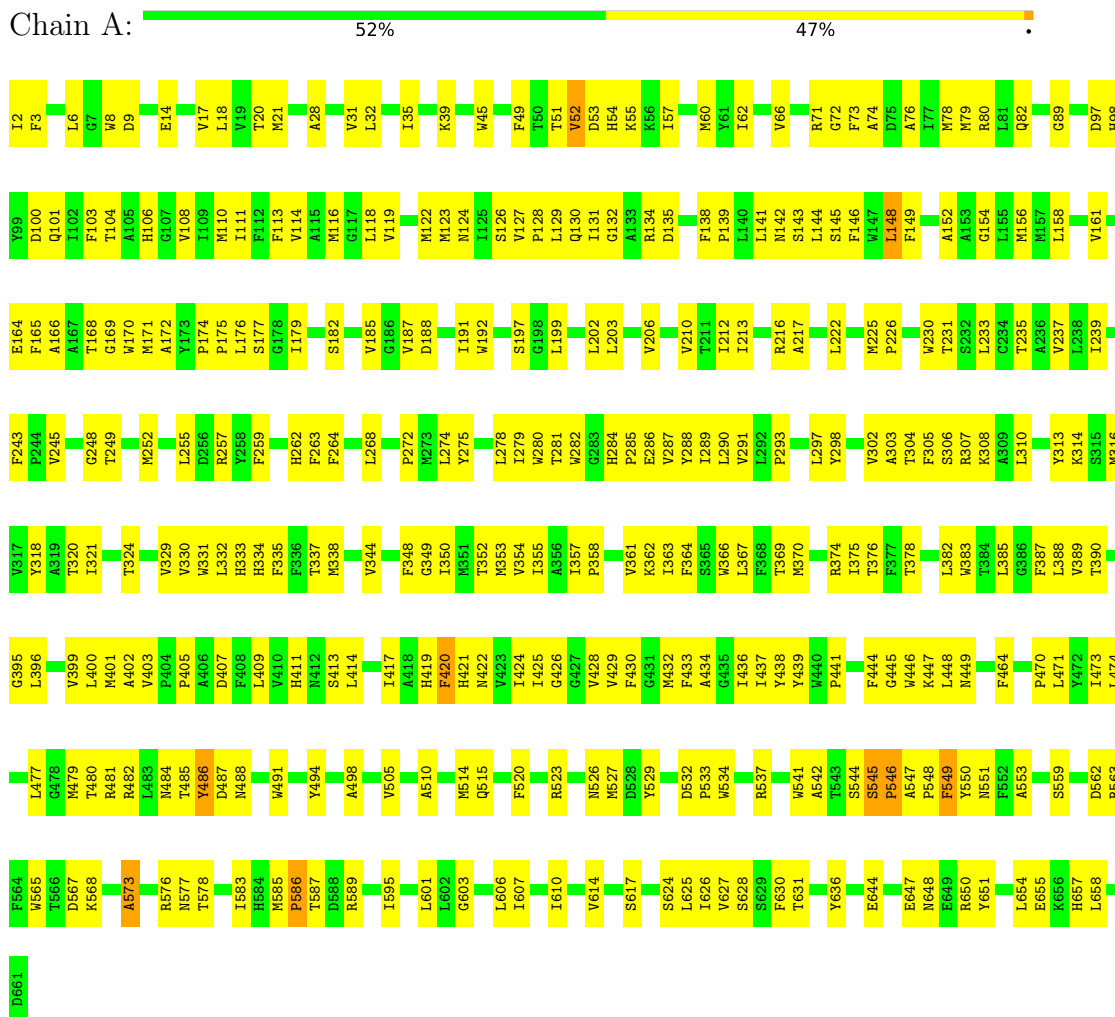


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	A	1	53	49	4	0

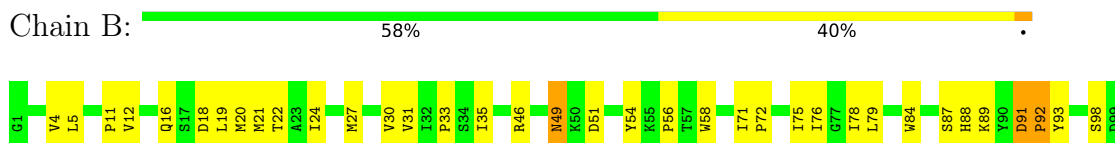
3 Residue-property plots

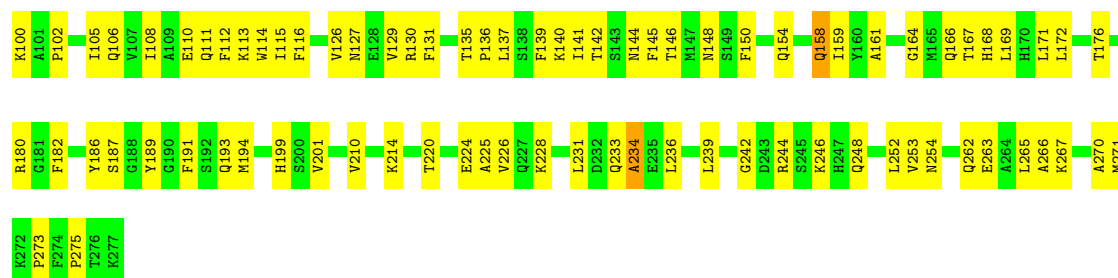
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 bo(3) ubiquinol oxidase subunit 1



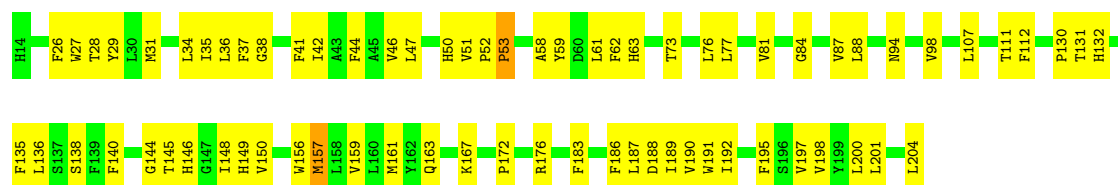
- Molecule 2: Ubiquinol oxidase subunit 2





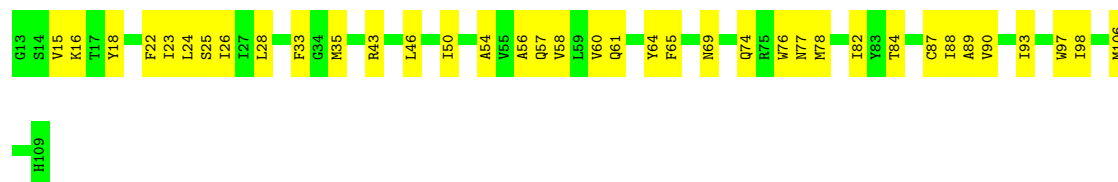
- Molecule 3: Cytochrome bo(3) ubiquinol oxidase subunit 3

Chain C: 63% 36%



- Molecule 4: Cytochrome bo(3) ubiquinol oxidase subunit 4

Chain D: 62% 38%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51625	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEO, HEM, LMG, 3PE, CU, UQ8

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	0.25	1/5442 (0.0%)	0.62	5/7420 (0.1%)
2	B	0.23	0/2256	0.68	1/3067 (0.0%)
3	C	0.20	0/1582	0.54	0/2161
4	D	0.17	0/778	0.50	0/1058
All	All	0.23	1/10058 (0.0%)	0.61	6/13706 (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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	PHE	CA-C	-5.11	1.45	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	92	PRO	CA-N-CD	-11.06	96.52	112.00
1	A	52	VAL	N-CA-C	-7.64	105.87	113.20
1	A	586	PRO	N-CD-CG	-6.00	94.20	103.20
1	A	419	HIS	CA-C-N	-5.83	110.94	121.14
1	A	419	HIS	C-N-CA	-5.83	110.94	121.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	SER	Peptide

5.2 Too-close contacts

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	5260	0	5258	289	0
2	B	2195	0	2179	106	0
3	C	1530	0	1511	77	0
4	D	761	0	800	33	0
5	A	43	0	30	7	0
6	A	59	0	56	14	0
7	A	1	0	0	0	0
8	A	171	0	247	17	0
8	C	95	0	147	16	0
9	A	122	0	154	9	0
10	A	53	0	74	4	0
All	All	10290	0	10456	477	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 23.

The worst 5 of 477 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)
3:C:34:LEU:HB3	4:D:84:THR:HG21	1.57	0.86
5:A:1001:HEM:HBC2	5:A:1001:HEM:HHD	1.62	0.81
1:A:52:VAL:HG22	1:A:139:PRO:HB2	1.63	0.79
3:C:46:VAL:O	3:C:50:HIS:HB2	1.82	0.78
1:A:274:LEU:HD21	3:C:46:VAL:HG22	1.68	0.75

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	659/660 (100%)	587 (89%)	65 (10%)	7 (1%)	11	43
2	B	275/277 (99%)	221 (80%)	48 (18%)	6 (2%)	5	30
3	C	189/191 (99%)	180 (95%)	8 (4%)	1 (0%)	24	57
4	D	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
All	All	1218/1225 (99%)	1075 (88%)	129 (11%)	14 (1%)	13	43

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	546	PRO
1	A	573	ALA
2	B	91	ASP
2	B	158	GLN

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	540/539 (100%)	538 (100%)	2 (0%)	84	80
2	B	231/231 (100%)	231 (100%)	0	100	100
3	C	168/168 (100%)	166 (99%)	2 (1%)	63	73
4	D	84/84 (100%)	84 (100%)	0	100	100
All	All	1023/1022 (100%)	1019 (100%)	4 (0%)	81	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	TRP
1	A	432	MET
3	C	26	PHE
3	C	157	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	262	GLN
3	C	96	ASN
4	D	109	HIS
4	D	69	ASN
4	D	74	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](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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
9	LMG	A	1009	-	40,40,55	0.81	0	48,48,63	1.35	6 (12%)
8	3PE	C	301	-	50,50,50	0.28	0	53,55,55	0.38	0
9	LMG	A	1008	-	46,46,55	0.89	3 (6%)	54,54,63	1.25	5 (9%)
6	HEO	A	1002	1	61,66,66	3.21	24 (39%)	46,102,102	2.24	14 (30%)
8	3PE	A	1004	-	50,50,50	0.27	0	53,55,55	0.41	0
5	HEM	A	1001	1	50,50,50	1.56	7 (14%)	66,82,82	1.68	13 (19%)
8	3PE	A	1005	-	41,41,50	0.30	0	44,46,55	0.34	0
8	3PE	A	1007	-	41,41,50	0.29	0	44,46,55	0.40	0
10	UQ8	A	1011	-	53,53,53	0.62	1 (1%)	64,67,67	0.85	4 (6%)
8	3PE	A	1006	-	35,35,50	0.31	0	38,40,55	0.36	0
8	3PE	C	302	-	43,43,50	0.29	0	46,48,55	0.32	0
9	LMG	A	1010	-	36,36,55	0.91	0	44,44,63	1.17	4 (9%)

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	LMG	A	1009	-	-	14/35/55/70	0/1/1/1
8	3PE	C	301	-	-	9/54/54/54	-
9	LMG	A	1008	-	-	18/41/61/70	0/1/1/1
6	HEO	A	1002	1	-	8/32/114/114	-
8	3PE	A	1004	-	-	11/54/54/54	-
5	HEM	A	1001	1	-	6/14/54/54	-
8	3PE	A	1005	-	-	9/45/45/54	-
8	3PE	A	1007	-	-	14/45/45/54	-
10	UQ8	A	1011	-	-	15/51/75/75	0/1/1/1
8	3PE	A	1006	-	-	8/39/39/54	-
8	3PE	C	302	-	-	10/47/47/54	-
9	LMG	A	1010	-	-	15/31/51/70	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	HEO	C3C-C4C	8.85	1.48	1.41
6	A	1002	HEO	C1A-C2A	7.86	1.49	1.39
6	A	1002	HEO	C1C-C2C	7.27	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	HEO	C4A-C3A	6.82	1.47	1.39
6	A	1002	HEO	C4B-NB	6.24	1.48	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	HEO	C2A-C1A-NA	8.18	115.97	109.34
6	A	1002	HEO	C1D-C2D-C3D	-5.08	104.38	108.61
6	A	1002	HEO	C13-C12-C11	-4.71	107.28	114.35
6	A	1002	HEO	C4B-C3B-C2B	-4.71	103.96	108.79
5	A	1001	HEM	CHC-C4B-NB	4.67	129.49	124.42

There are no chirality outliers.

5 of 137 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	HEO	C4D-C3D-CAD-CBD
8	A	1004	3PE	C1-O11-P-O13
8	A	1004	3PE	C1-O11-P-O14
8	A	1005	3PE	C11-O13-P-O12
8	A	1007	3PE	C1-O11-P-O14

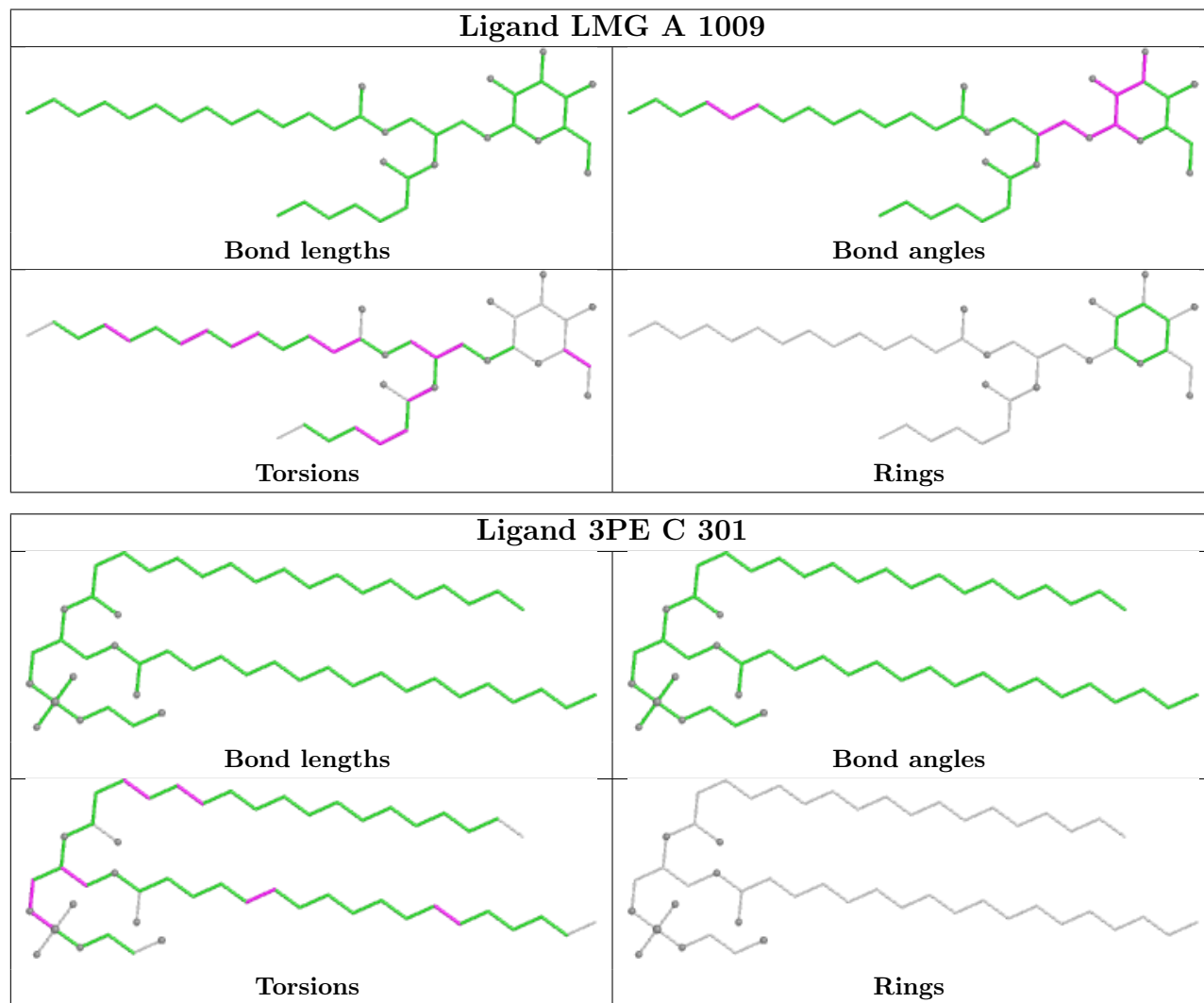
There are no ring outliers.

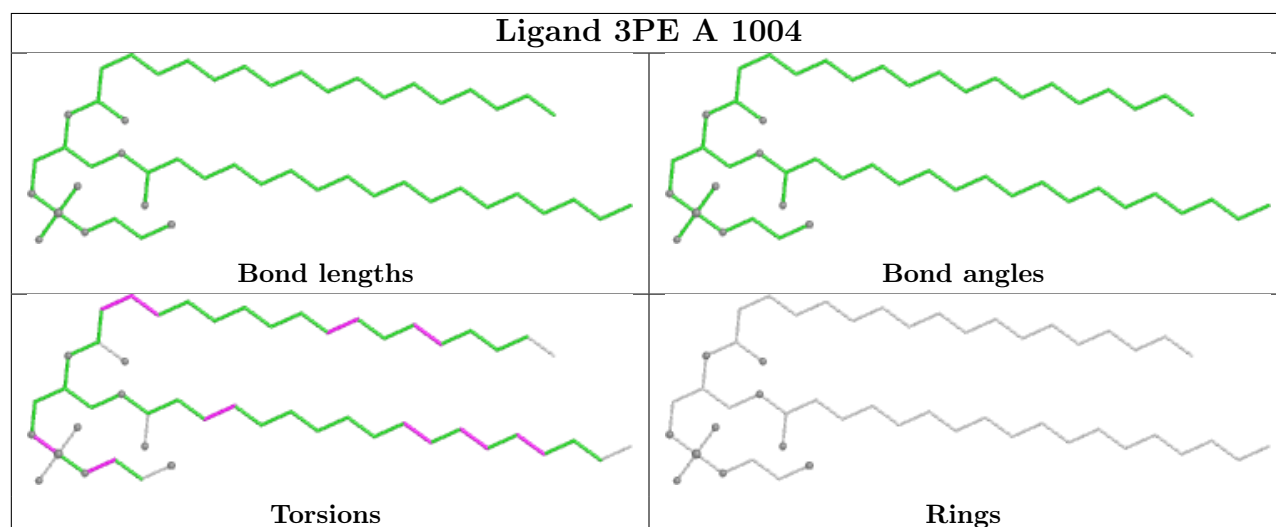
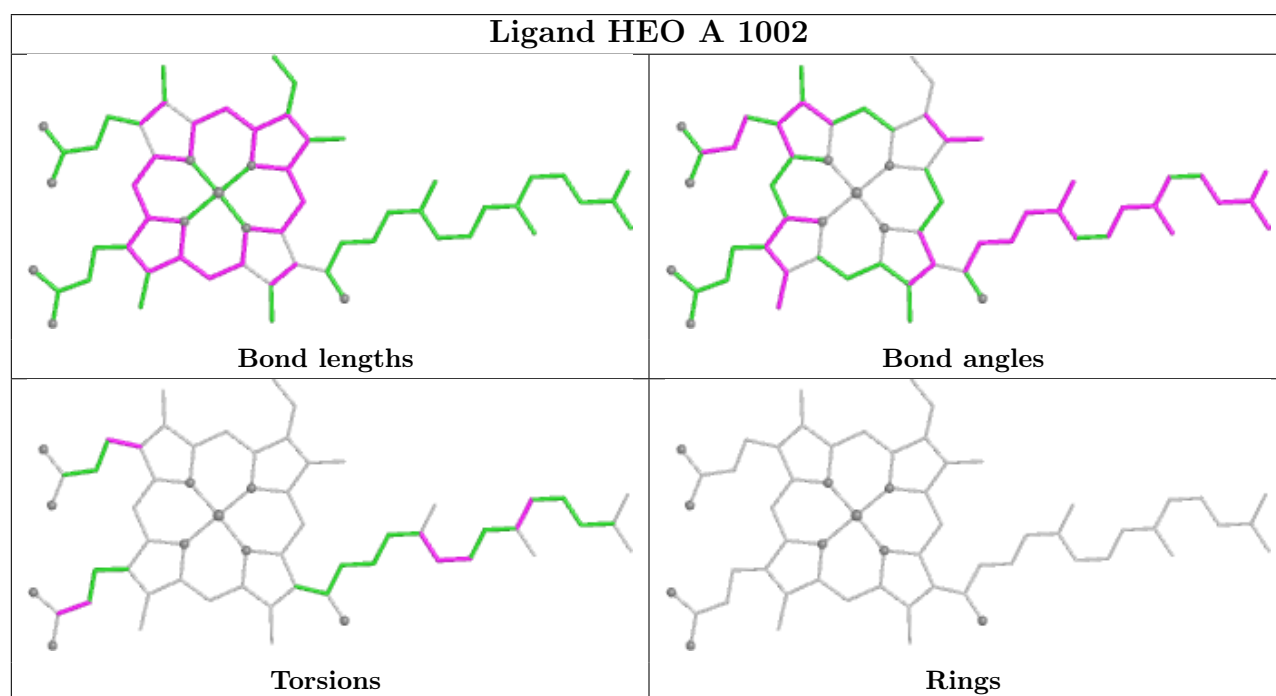
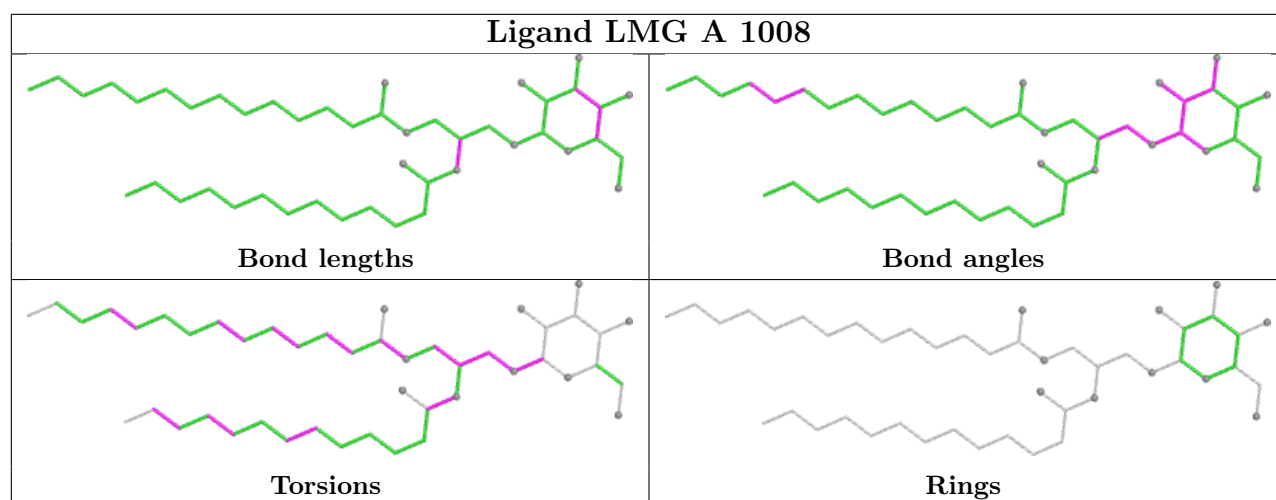
12 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1009	LMG	4	0
8	C	301	3PE	9	0
9	A	1008	LMG	4	0
6	A	1002	HEO	14	0
8	A	1004	3PE	6	0
5	A	1001	HEM	7	0
8	A	1005	3PE	4	0
8	A	1007	3PE	5	0
10	A	1011	UQ8	4	0
8	A	1006	3PE	4	0
8	C	302	3PE	7	0
9	A	1010	LMG	4	0

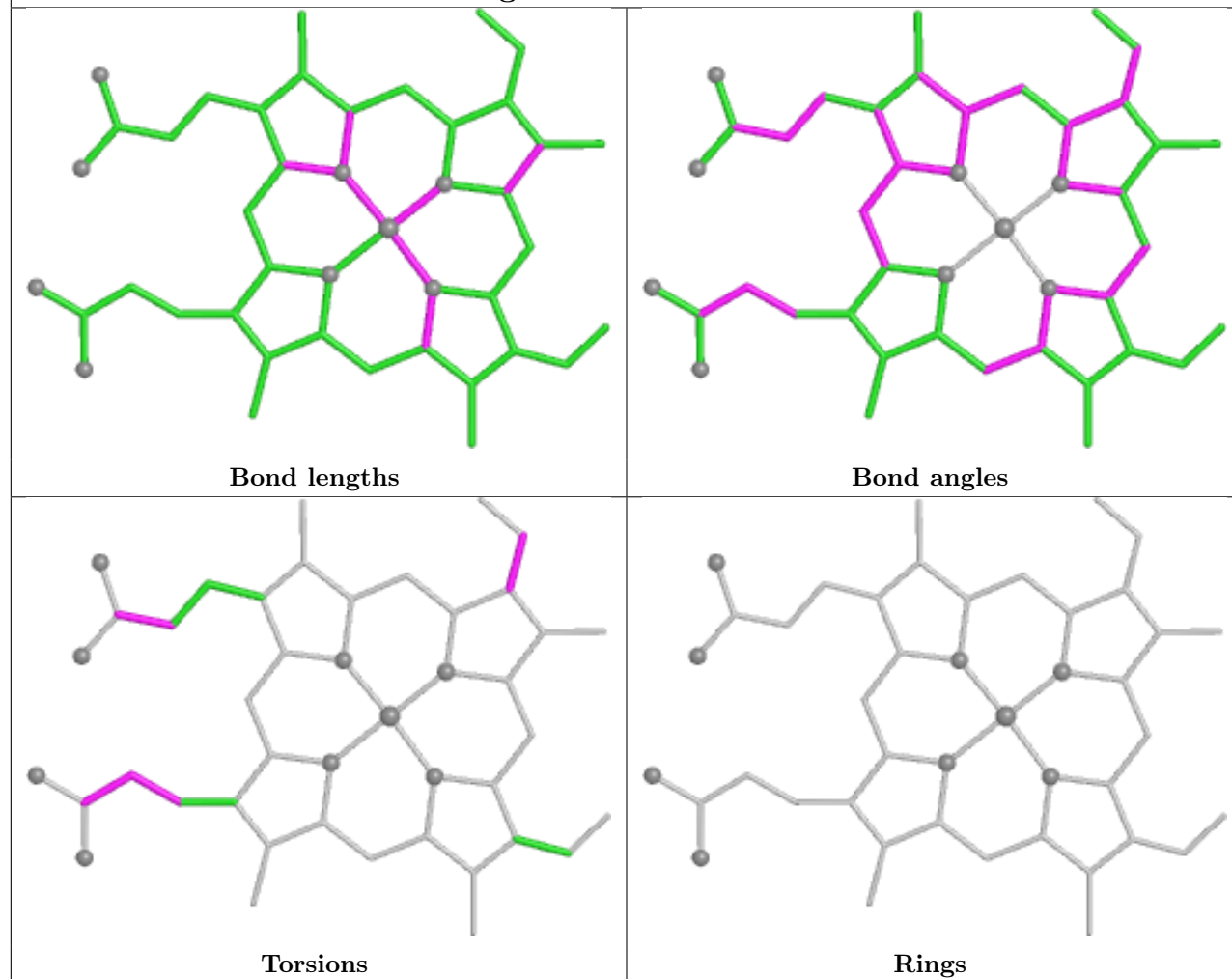
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

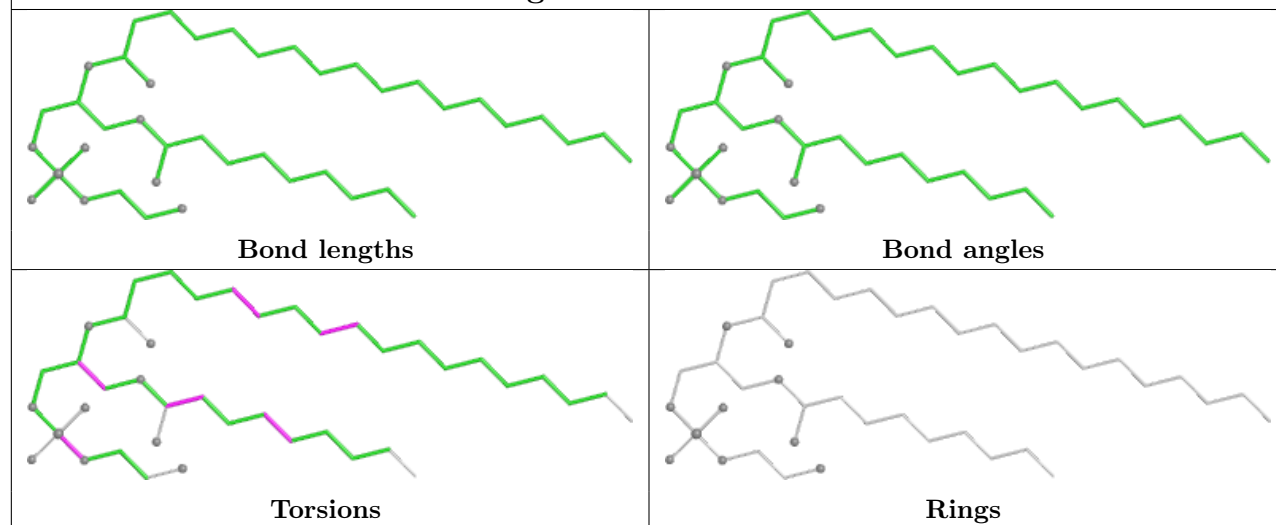


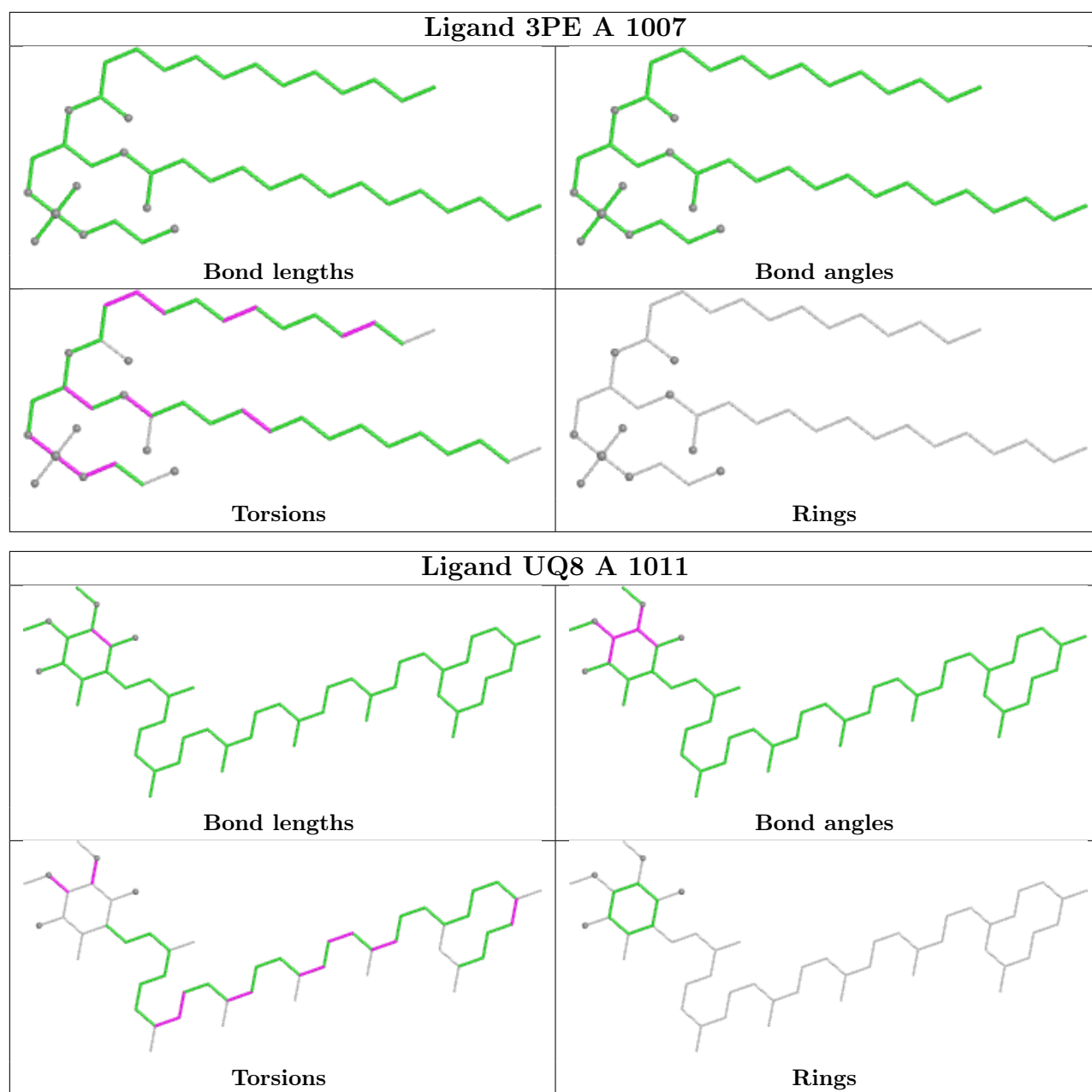


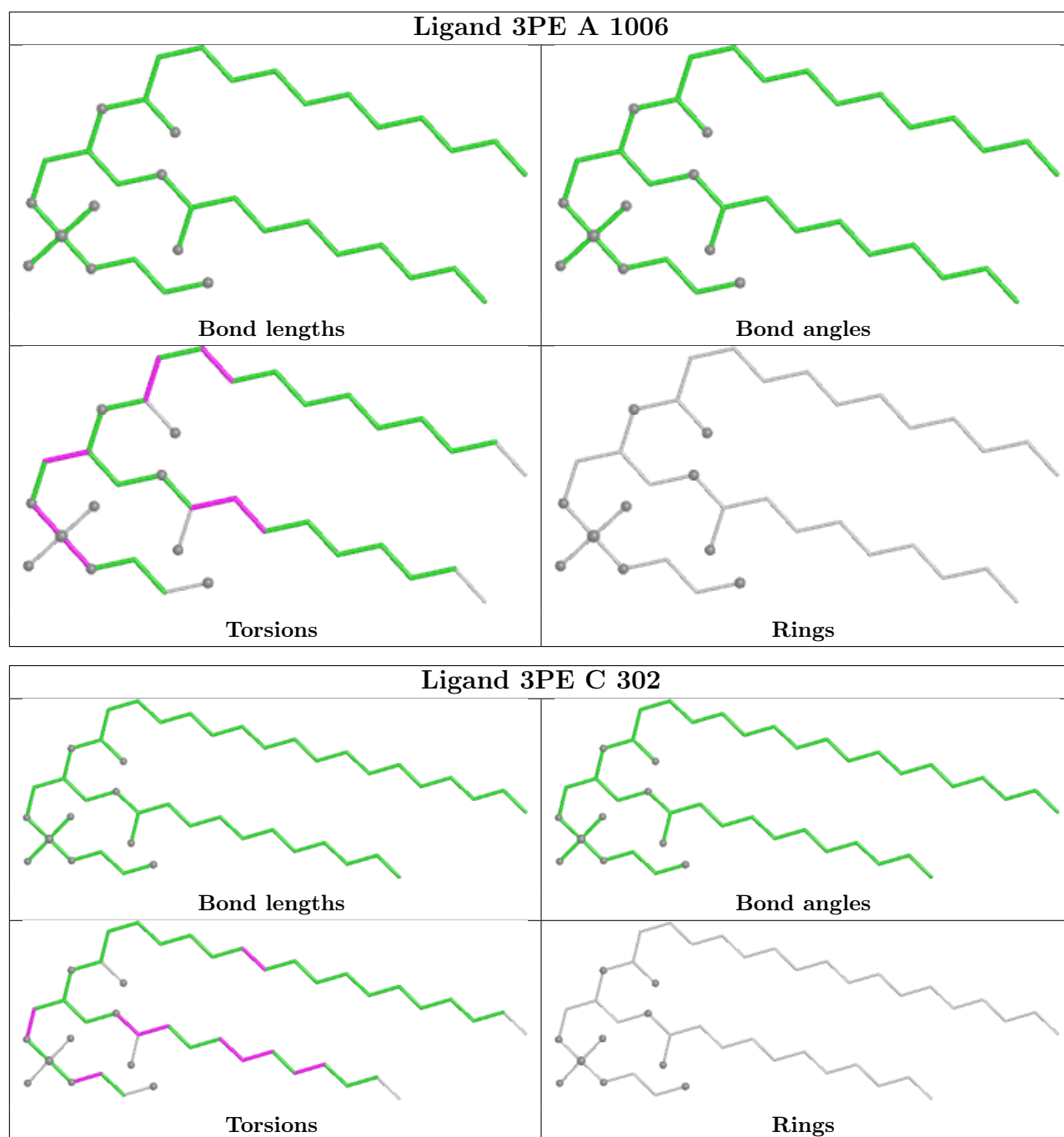
Ligand HEM A 1001

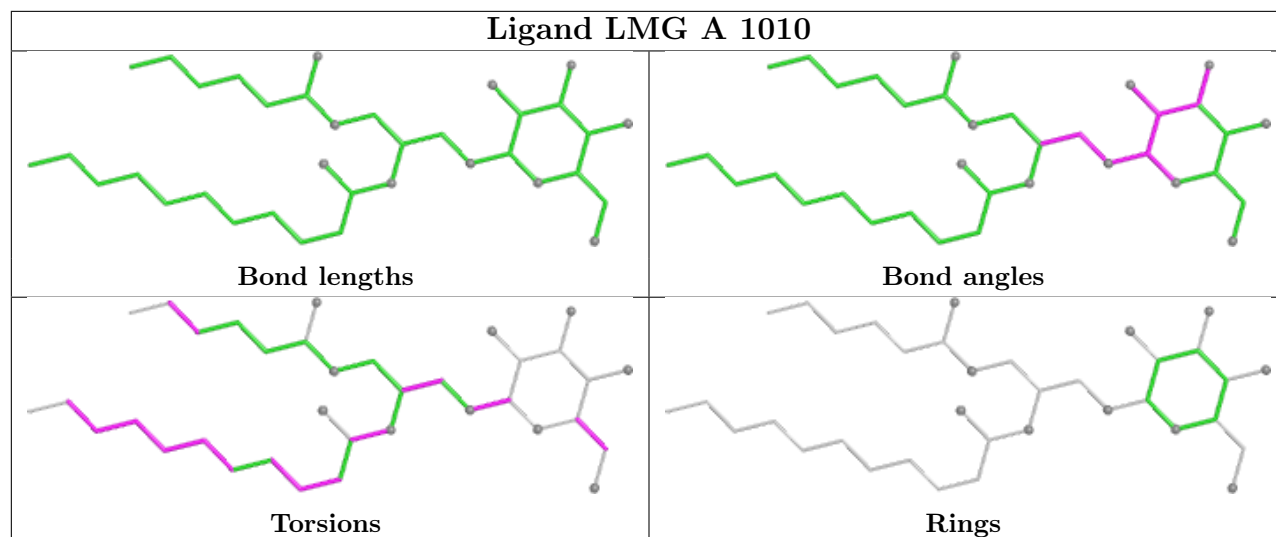


Ligand 3PE A 1005









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.