



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:06 AM UTC

PDB ID : 9ETZ / pdb_00009etz
EMDB ID : EMD-19963
Title : III2IV respiratory supercomplex from *Saccharomyces cerevisiae*
Authors : Moe, A.; Brzezinski, P.
Deposited on : 2024-03-27
Resolution : 2.40 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:

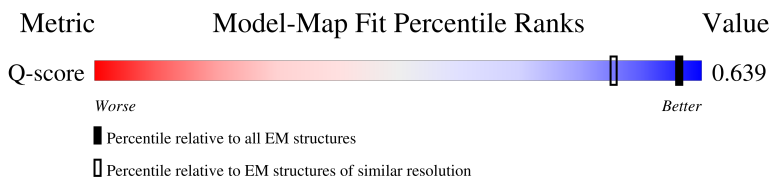
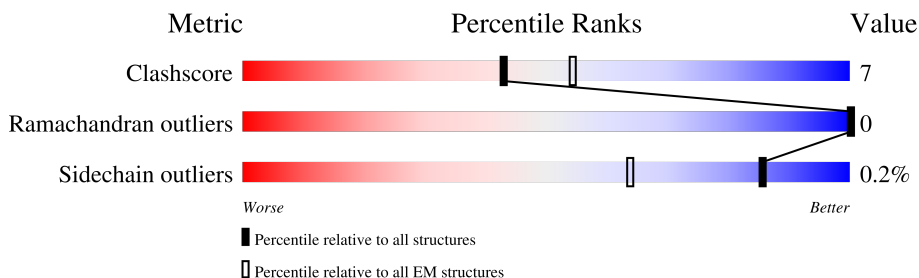
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 2.40 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.



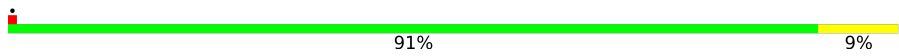

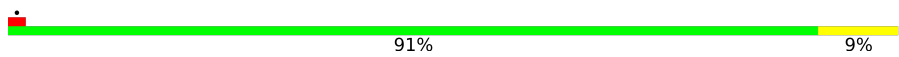
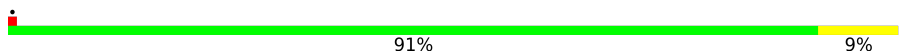




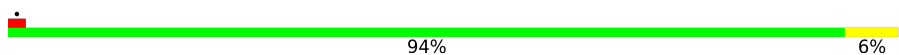

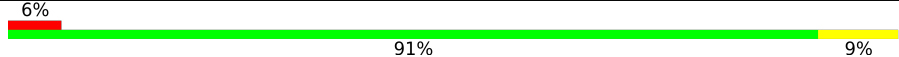

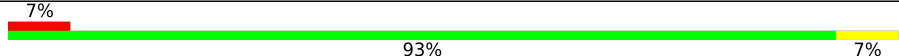
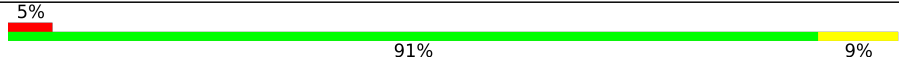
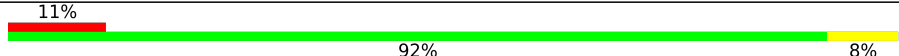
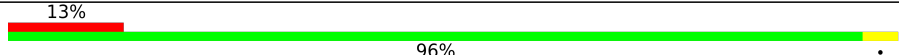
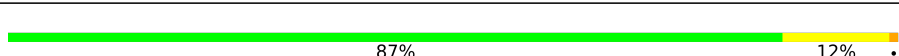
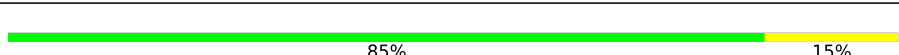
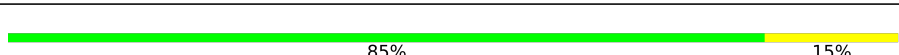
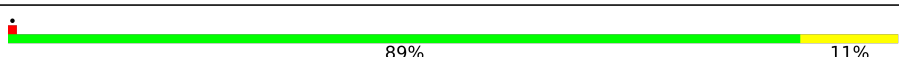
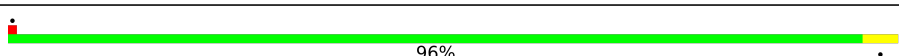

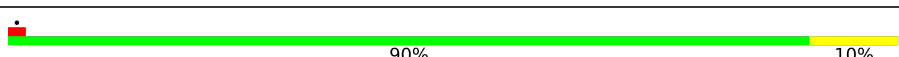

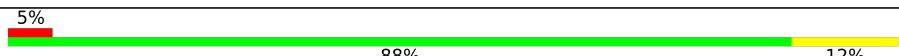
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	 86% 14%
1	L	431	 89% 11%
2	B	352	 93% 7%
2	M	352	 92% 8%




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Mol	Chain	Length	Quality of chain
3	C	385	
3	N	385	
4	D	247	
4	O	247	
5	E	185	
5	P	185	
6	F	75	
6	Q	75	
7	G	126	
7	R	126	
8	H	93	
8	S	93	
9	I	57	
9	T	57	
10	J	76	
10	U	76	
11	a	534	
12	b	236	
13	c	269	
14	d	120	
15	f	102	
16	g	59	
17	h	51	
18	i	55	
19	j	75	

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Mol	Chain	Length	Quality of chain
20	k	113	 89% 11%
21	l	45	 82% 18%
22	e	133	 86% 14%

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 48795 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	L	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
3	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		
4	O	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	185	1411	893	242	266	10	0	0
5	P	185	1411	893	242	266	10	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	75	633	396	109	126	2	0	0
6	Q	75	633	396	109	126	2	0	0

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	126	1019	653	173	191	2	0	0
7	R	126	1019	653	173	191	2	0	0

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	93	773	510	131	130	2	0	0
8	S	93	773	510	131	130	2	0	0

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	57	465	310	77	78	0	0
9	T	57	465	310	77	78	0	0

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	76	599	391	98	108	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	U	76	599	391	98	108	2	0	0

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	a	534	4162	2778	649	713	22	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	b	236	1889	1242	286	351	10	0	0

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	c	269	2146	1430	344	357	15	0	0

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	d	120	906	571	150	180	5	0	0

- Molecule 15 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	f	102	851	545	137	168	1	0	0

- Molecule 16 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	g	59	484	328	83	73	0	0

- Molecule 17 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	h	51	409	278	66	64	1	0	0

- Molecule 18 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	i	55	456	300	79	74	3	0	0

- Molecule 19 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	j	75	627	403	107	112	5	0	0

- Molecule 20 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	k	113	928	605	160	160	3	0	0

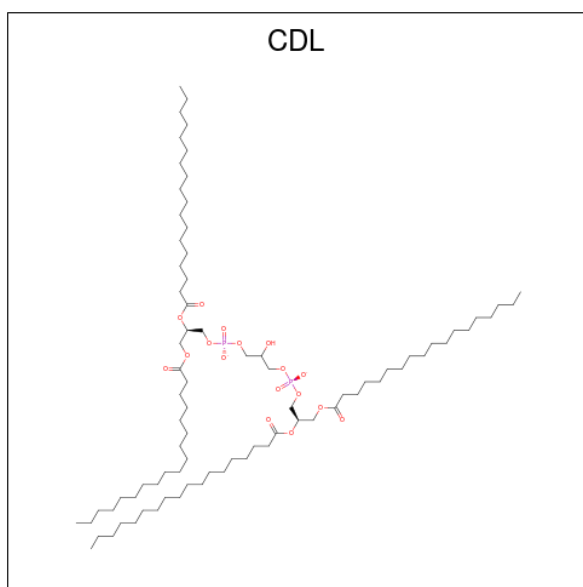
- Molecule 21 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	l	45	361	238	63	59	1	0	0

- Molecule 22 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

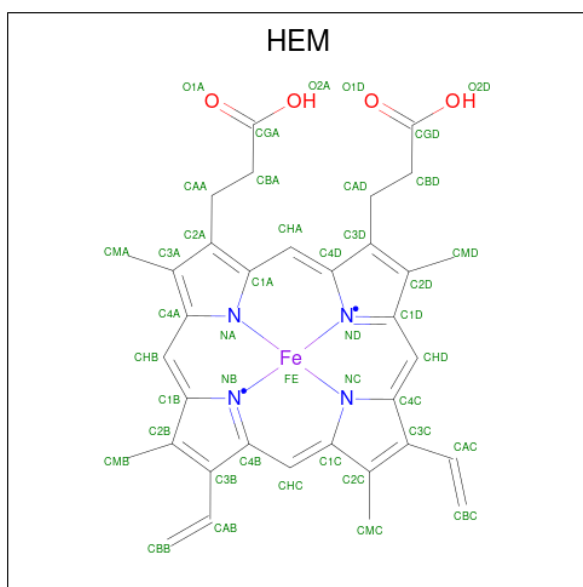
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	e	133	1049	663	184	198	4	0	0

- Molecule 23 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



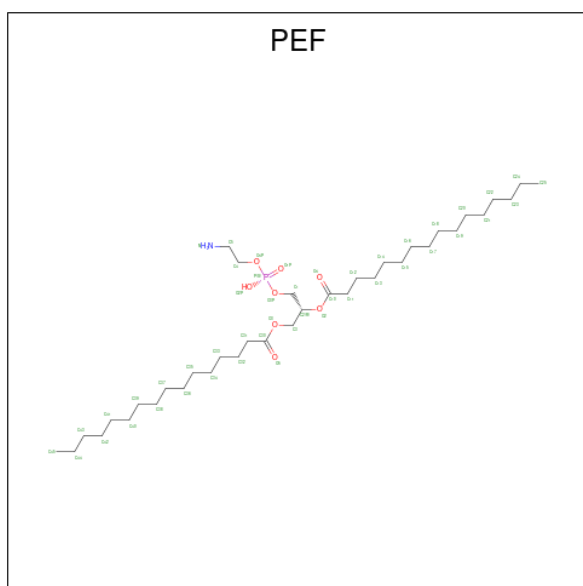
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	A	1	77	58	17	2	0
23	A	1	54	35	17	2	0
23	E	1	53	34	17	2	0
23	H	1	66	47	17	2	0
23	H	1	71	52	17	2	0
23	L	1	55	36	17	2	0
23	L	1	67	48	17	2	0
23	N	1	53	34	17	2	0
23	P	1	48	29	17	2	0
23	S	1	75	56	17	2	0
23	c	1	86	67	17	2	0

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 25 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



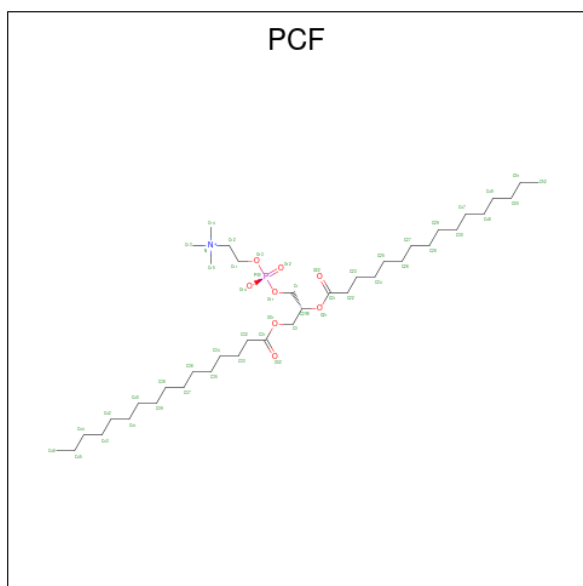
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	C	1	Total 44	C 34	N 1	O 8	P 1	0
25	C	1	Total 47	C 37	N 1	O 8	P 1	0
25	C	1	Total 40	C 30	N 1	O 8	P 1	0
25	E	1	Total 42	C 32	N 1	O 8	P 1	0
25	G	1	Total 32	C 22	N 1	O 8	P 1	0
25	H	1	Total 34	C 24	N 1	O 8	P 1	0
25	J	1	Total 26	C 16	N 1	O 8	P 1	0
25	J	1	Total 29	C 19	N 1	O 8	P 1	0
25	N	1	Total 40	C 30	N 1	O 8	P 1	0
25	N	1	Total 43	C 33	N 1	O 8	P 1	0
25	N	1	Total 32	C 22	N 1	O 8	P 1	0
25	P	1	Total 43	C 33	N 1	O 8	P 1	0
25	P	1	Total 39	C 29	N 1	O 8	P 1	0
25	S	1	Total 36	C 26	N 1	O 8	P 1	0
25	U	1	Total 37	C 27	N 1	O 8	P 1	0
25	a	1	Total 40	C 30	N 1	O 8	P 1	0
25	a	1	Total 40	C 30	N 1	O 8	P 1	0
25	a	1	Total 47	C 37	N 1	O 8	P 1	0
25	a	1	Total 30	C 20	N 1	O 8	P 1	0
25	b	1	Total 40	C 30	N 1	O 8	P 1	0
25	b	1	Total 47	C 37	N 1	O 8	P 1	0
25	c	1	Total 47	C 37	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	c	1	Total 47	C 37	N 1	O 8	P 1	0
25	h	1	Total 47	C 37	N 1	O 8	P 1	0
25	l	1	Total 47	C 37	N 1	O 8	P 1	0
25	e	1	Total 47	C 37	N 1	O 8	P 1	0

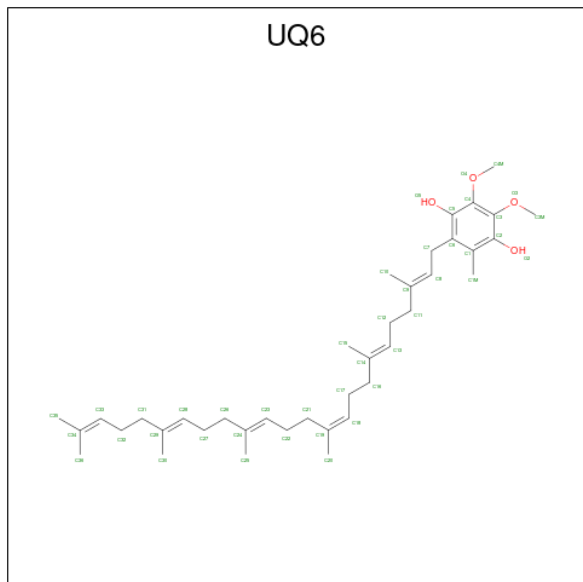
- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
26	C	1	Total 39	C 29	N 1	O 8	P 1	0
26	H	1	Total 32	C 22	N 1	O 8	P 1	0
26	I	1	Total 30	C 20	N 1	O 8	P 1	0
26	N	1	Total 50	C 40	N 1	O 8	P 1	0
26	T	1	Total 47	C 37	N 1	O 8	P 1	0
26	e	1	Total 50	C 40	N 1	O 8	P 1	0

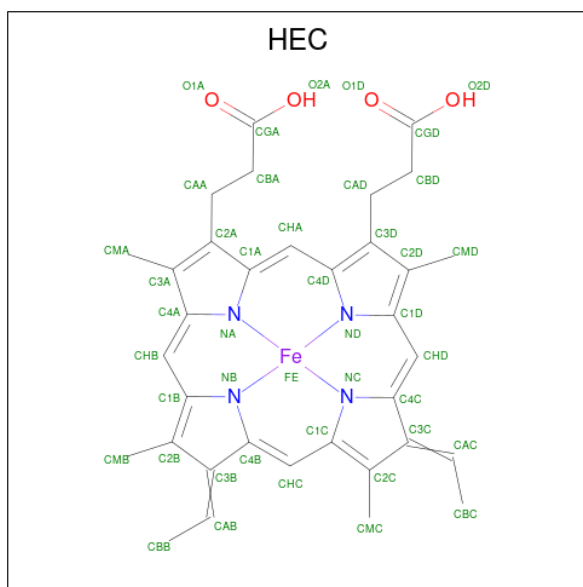
- Molecule 27 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA

ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$).



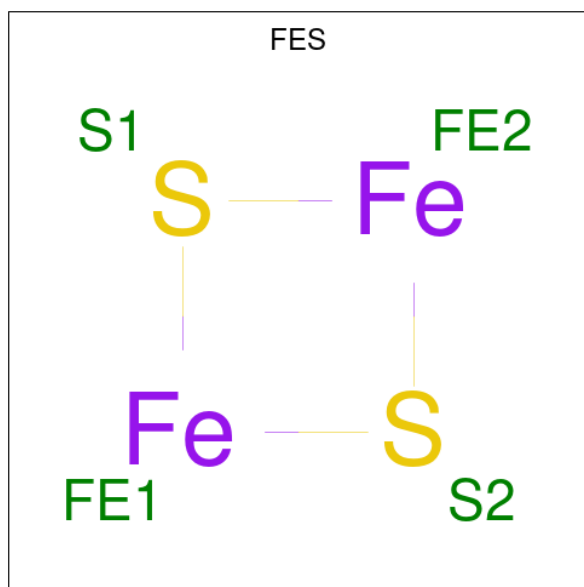
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	C	O	0
			43	39	4	
27	N	1	Total	C	O	0
			43	39	4	

- Molecule 28 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms				AltConf	
28	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

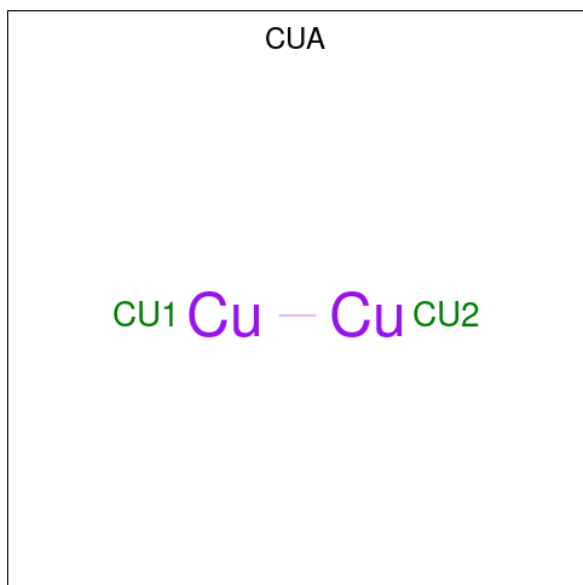


Mol	Chain	Residues	Atoms			AltConf
29	E	1	Total	Fe	S	0
			4	2	2	
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total	Cu	0
			1	1	

- Molecule 31 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms	AltConf
34	b	1	Total Cu 2 2	0

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
35	d	1	Total Zn 1 1	0

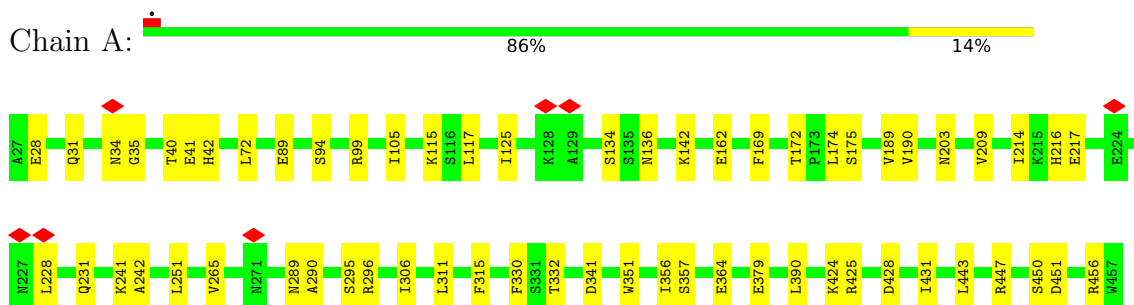
- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	a	11	Total O 11 11	0

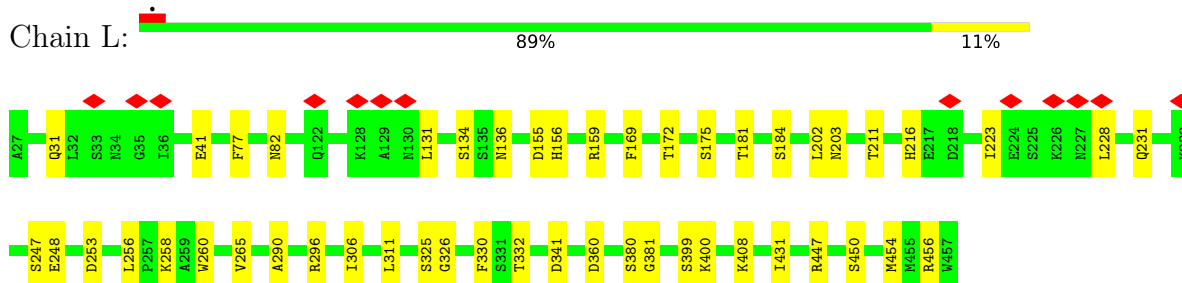
3 Residue-property plots

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

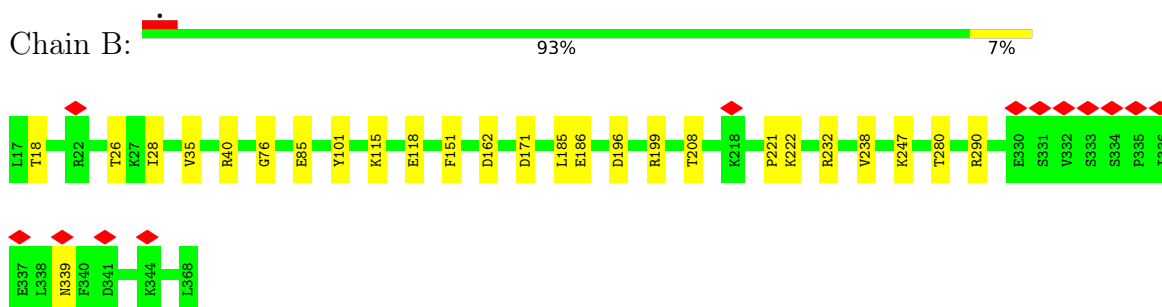
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

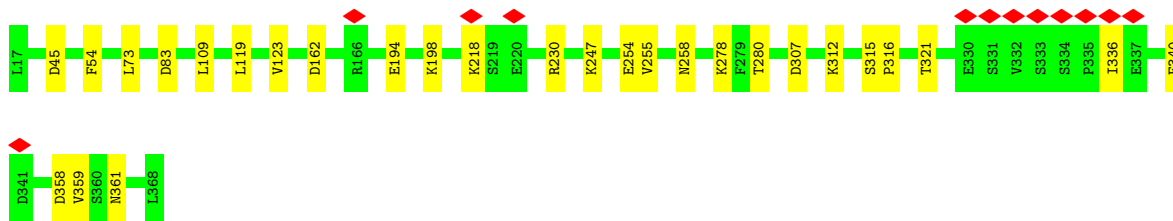


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

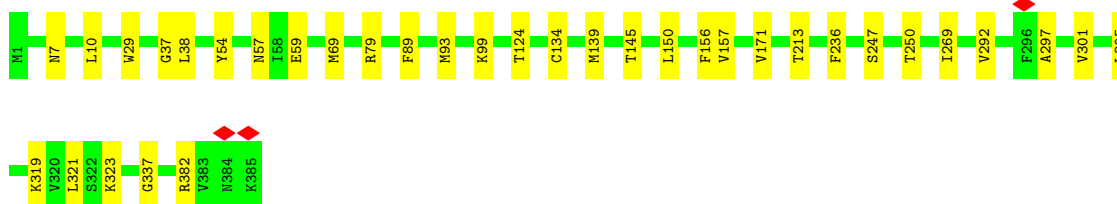
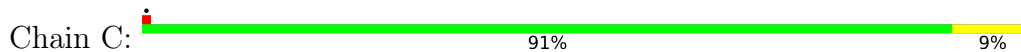


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

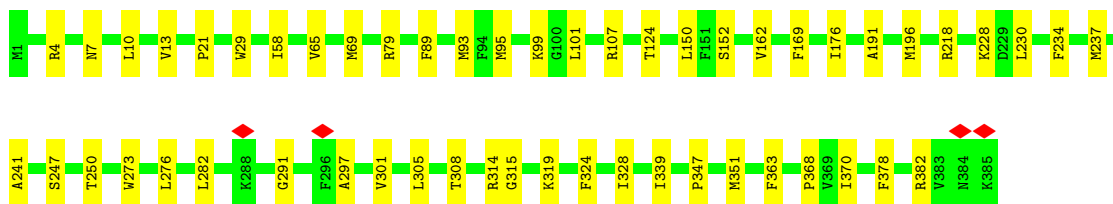
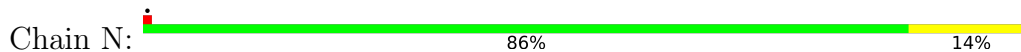




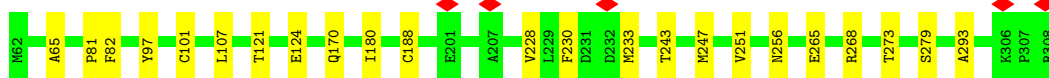
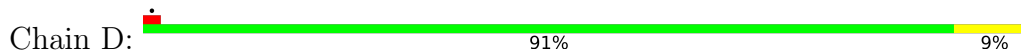
• Molecule 3: Cytochrome b



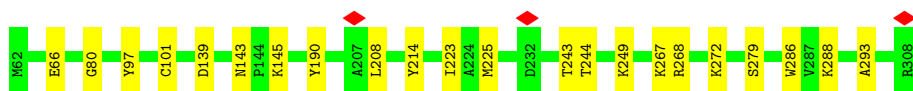
• Molecule 3: Cytochrome b



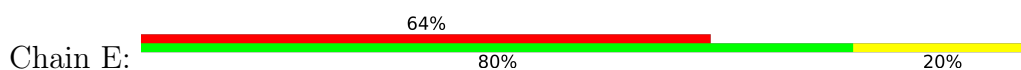
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

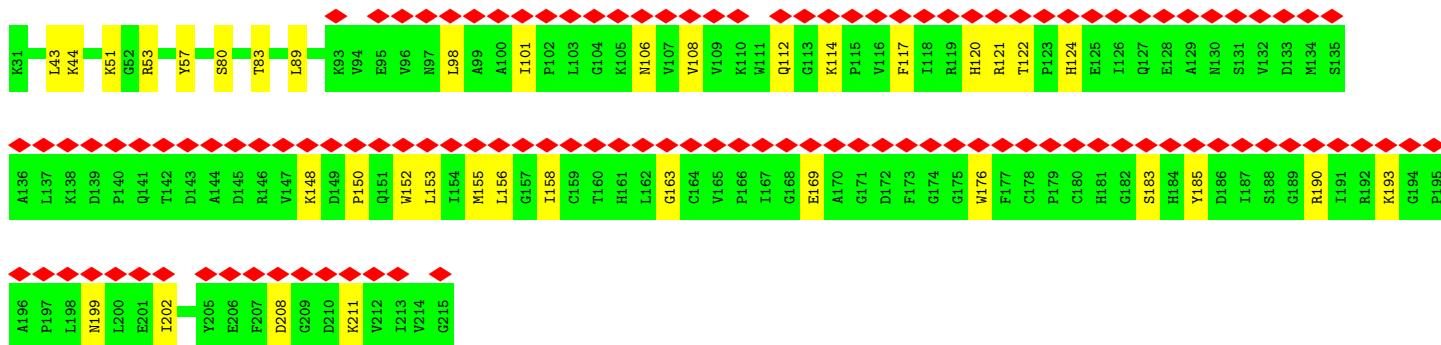


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

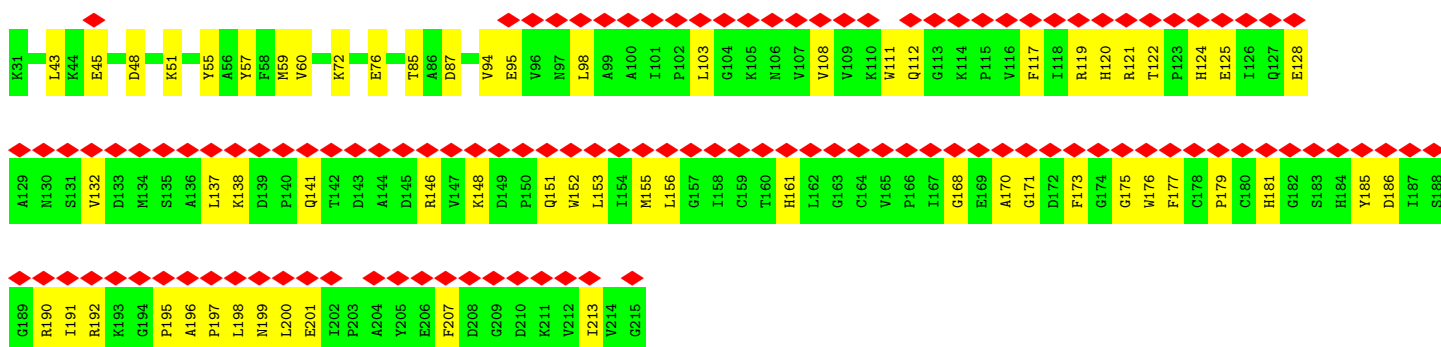


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

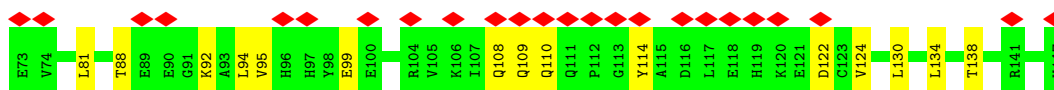
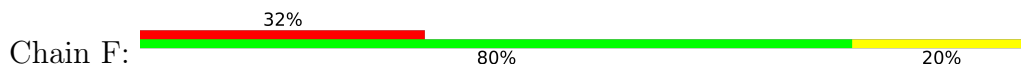




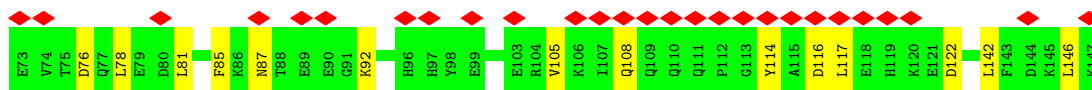
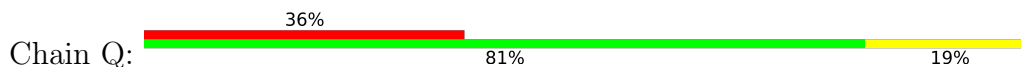
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



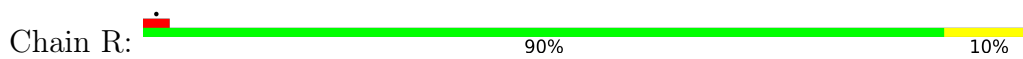
• Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



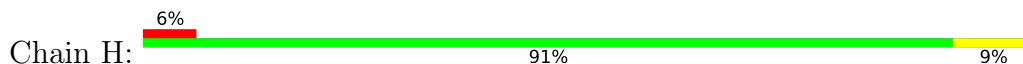
• Molecule 7: Cytochrome b-c1 complex subunit 7, mitochondrial



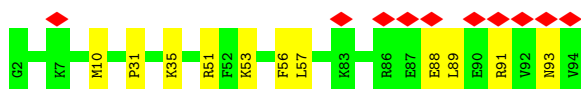
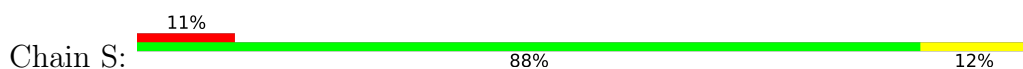
• Molecule 7: Cytochrome b-c1 complex subunit 7, mitochondrial



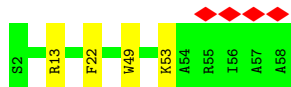
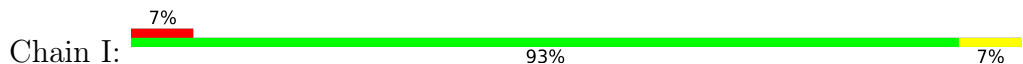
- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial



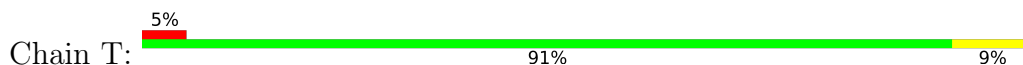
- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial



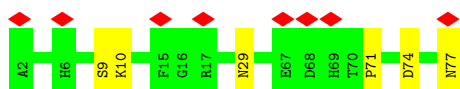
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



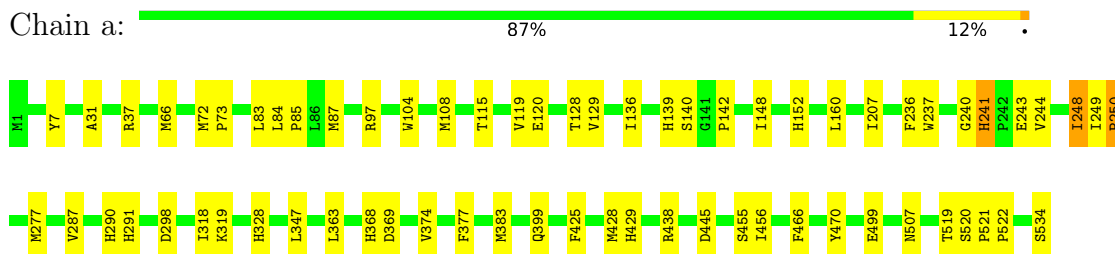
- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



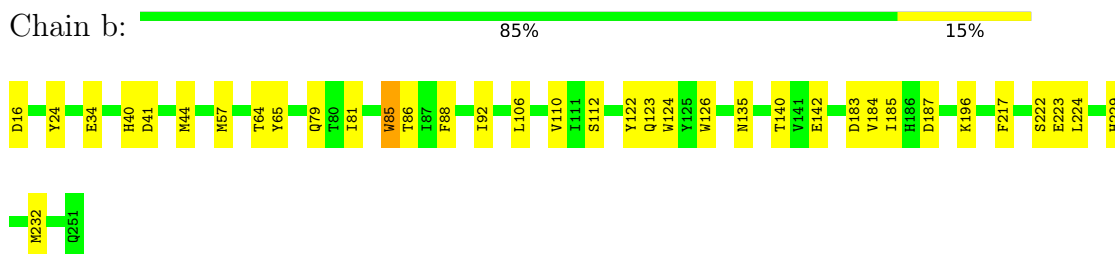
- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



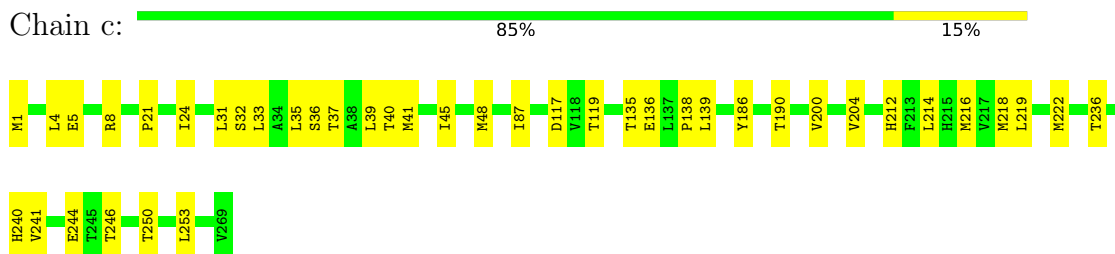
- Molecule 11: Cytochrome c oxidase subunit 1



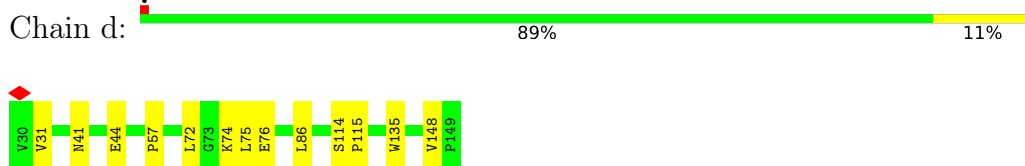
- Molecule 12: Cytochrome c oxidase subunit 2



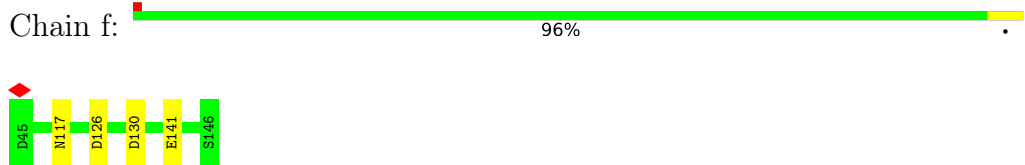
- Molecule 13: Cytochrome c oxidase subunit 3



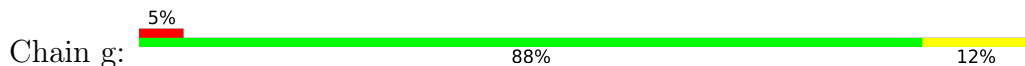
- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial



- Molecule 15: Cytochrome c oxidase subunit 6, mitochondrial



- Molecule 16: Cytochrome c oxidase subunit 7, mitochondrial





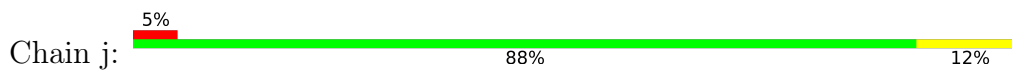
- Molecule 17: Cytochrome c oxidase subunit 8, mitochondrial



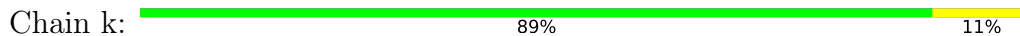
- Molecule 18: Cytochrome c oxidase subunit 9, mitochondrial



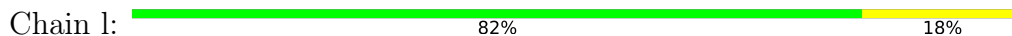
- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial



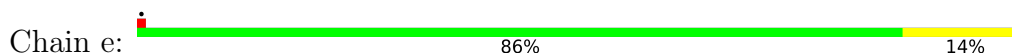
- Molecule 20: Cytochrome c oxidase subunit 13, mitochondrial



- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



- Molecule 22: Cytochrome c oxidase subunit 5A, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196457	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.990	Depositor
Minimum map value	-0.993	Depositor
Average map value	0.027	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.55	Depositor
Map size (\AA)	512.9184, 511.22562, 512.9184	wwPDB
Map dimensions	606, 604, 606	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8464, 0.8464, 0.8464	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: CDL, ZN, CU, HEM, PCF, CA, MG, HEC, HEA, FES, PEF, CUA, UQ6

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	0.17	0/3406	0.30	0/4615
1	L	0.17	0/3406	0.28	0/4615
2	B	0.16	0/2781	0.27	0/3764
2	M	0.17	0/2781	0.30	0/3764
3	C	0.17	0/3192	0.29	0/4354
3	N	0.17	0/3192	0.29	0/4354
4	D	0.16	0/2012	0.29	0/2740
4	O	0.16	0/2012	0.27	0/2740
5	E	0.14	0/1444	0.32	0/1957
5	P	0.13	0/1444	0.33	0/1957
6	F	0.11	0/647	0.22	0/870
6	Q	0.12	0/647	0.24	0/870
7	G	0.16	0/1040	0.28	0/1408
7	R	0.16	0/1040	0.28	0/1408
8	H	0.16	0/804	0.26	0/1088
8	S	0.14	0/804	0.22	0/1088
9	I	0.15	0/479	0.24	0/646
9	T	0.14	0/479	0.21	0/646
10	J	0.13	0/619	0.27	0/841
10	U	0.13	0/619	0.27	0/841
11	a	0.49	4/4290 (0.1%)	0.55	4/5857 (0.1%)
12	b	0.39	0/1941	0.49	0/2653
13	c	0.28	0/2218	0.36	0/3036
14	d	0.27	0/924	0.40	0/1258
15	f	0.32	0/868	0.35	0/1174
16	g	0.30	0/500	0.41	0/681
17	h	0.31	0/424	0.37	0/569
18	i	0.29	0/468	0.31	0/626
19	j	0.37	0/649	0.48	0/880
20	k	0.21	0/962	0.30	0/1310
21	l	0.27	0/372	0.32	0/502
22	e	0.30	0/1074	0.36	0/1451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.25	4/47538 (0.0%)	0.34	4/64563 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	287	VAL	C-O	-8.12	1.14	1.24
11	a	250	PRO	C-O	-7.97	1.14	1.24
11	a	237	TRP	C-O	-5.84	1.16	1.24
11	a	248	ILE	C-O	-5.51	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	290	HIS	N-CA-C	-8.17	102.87	113.17
11	a	290	HIS	CB-CA-C	5.52	119.31	110.09
11	a	291	HIS	N-CA-C	-5.42	106.04	113.30
11	a	241	HIS	CA-CB-CG	-5.10	108.70	113.80

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	3345	0	3323	53	0
1	L	3345	0	3323	35	0
2	B	2735	0	2774	20	0
2	M	2735	0	2774	16	0
3	C	3090	0	3129	52	0
3	N	3090	0	3129	49	0
4	D	1951	0	1877	16	0
4	O	1951	0	1877	27	0
5	E	1411	0	1386	43	0
5	P	1411	0	1386	57	0
6	F	633	0	587	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	633	0	587	13	0
7	G	1019	0	1034	17	0
7	R	1019	0	1034	10	0
8	H	773	0	736	9	0
8	S	773	0	736	11	0
9	I	465	0	459	4	0
9	T	465	0	459	4	0
10	J	599	0	594	6	0
10	U	599	0	594	3	0
11	a	4162	0	4191	66	0
12	b	1889	0	1866	37	0
13	c	2146	0	2135	30	0
14	d	906	0	901	14	0
15	f	851	0	822	5	0
16	g	484	0	517	5	0
17	h	409	0	408	4	0
18	i	456	0	469	18	0
19	j	627	0	577	14	0
20	k	928	0	906	14	0
21	l	361	0	363	10	0
22	e	1049	0	1030	20	0
23	A	131	0	150	4	0
23	E	53	0	50	2	0
23	H	137	0	165	4	0
23	L	122	0	135	6	0
23	N	53	0	50	4	0
23	P	48	0	40	1	0
23	S	75	0	97	2	0
23	c	86	0	122	3	0
24	C	86	0	60	4	0
24	N	86	0	60	4	0
25	C	131	0	190	7	0
25	E	42	0	60	2	0
25	G	32	0	37	1	0
25	H	34	0	41	0	0
25	J	55	0	56	1	0
25	N	115	0	152	4	0
25	P	82	0	113	5	0
25	S	36	0	48	3	0
25	U	37	0	50	2	0
25	a	157	0	215	8	0
25	b	87	0	129	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	c	94	0	146	7	0
25	e	47	0	73	2	0
25	h	47	0	73	1	0
25	l	47	0	73	4	0
26	C	39	0	55	1	0
26	H	32	0	38	1	0
26	I	30	0	34	2	0
26	N	50	0	80	3	0
26	T	47	0	71	4	0
26	e	50	0	80	1	0
27	C	43	0	58	2	0
27	N	43	0	58	1	0
28	D	43	0	32	4	0
28	O	43	0	32	5	0
29	E	4	0	0	0	0
29	P	4	0	0	0	0
30	a	1	0	0	0	0
31	a	120	0	108	3	0
32	a	1	0	0	0	0
33	a	1	0	0	0	0
34	b	2	0	0	0	0
35	d	1	0	0	0	0
36	a	11	0	0	1	0
All	All	48795	0	49014	646	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 646 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:N:89:PHE:CE2	3:N:124:THR:HG21	1.59	1.38
3:N:69:MET:SD	3:N:79:ARG:HD3	1.66	1.34
3:C:89:PHE:CE2	3:C:124:THR:HG21	1.62	1.33
5:P:155:MET:SD	5:P:200:LEU:HD13	1.89	1.12
5:E:122:THR:CG2	5:E:124:HIS:ND1	2.13	1.11

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	429/431 (100%)	417 (97%)	12 (3%)	0	100	100
1	L	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
2	B	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
2	M	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	C	383/385 (100%)	374 (98%)	9 (2%)	0	100	100
3	N	383/385 (100%)	372 (97%)	11 (3%)	0	100	100
4	D	245/247 (99%)	241 (98%)	4 (2%)	0	100	100
4	O	245/247 (99%)	239 (98%)	6 (2%)	0	100	100
5	E	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
5	P	183/185 (99%)	164 (90%)	19 (10%)	0	100	100
6	F	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	Q	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
7	G	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
7	R	124/126 (98%)	124 (100%)	0	0	100	100
8	H	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
8	S	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
9	I	55/57 (96%)	55 (100%)	0	0	100	100
9	T	55/57 (96%)	55 (100%)	0	0	100	100
10	J	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
10	U	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
11	a	532/534 (100%)	512 (96%)	20 (4%)	0	100	100
12	b	234/236 (99%)	223 (95%)	11 (5%)	0	100	100
13	c	267/269 (99%)	259 (97%)	8 (3%)	0	100	100
14	d	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
15	f	100/102 (98%)	98 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	g	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
17	h	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
18	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
19	j	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
20	k	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
21	l	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
22	e	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
All	All	5782/5846 (99%)	5599 (97%)	183 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	370/370 (100%)	370 (100%)	0	100	100
1	L	370/370 (100%)	370 (100%)	0	100	100
2	B	301/301 (100%)	301 (100%)	0	100	100
2	M	301/301 (100%)	299 (99%)	2 (1%)	76	88
3	C	338/338 (100%)	338 (100%)	0	100	100
3	N	338/338 (100%)	338 (100%)	0	100	100
4	D	205/205 (100%)	205 (100%)	0	100	100
4	O	205/205 (100%)	205 (100%)	0	100	100
5	E	151/151 (100%)	150 (99%)	1 (1%)	76	88
5	P	151/151 (100%)	151 (100%)	0	100	100
6	F	68/68 (100%)	68 (100%)	0	100	100
6	Q	68/68 (100%)	68 (100%)	0	100	100
7	G	110/110 (100%)	110 (100%)	0	100	100
7	R	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	77/77 (100%)	77 (100%)	0	100	100
8	S	77/77 (100%)	77 (100%)	0	100	100
9	I	47/47 (100%)	47 (100%)	0	100	100
9	T	47/47 (100%)	47 (100%)	0	100	100
10	J	65/65 (100%)	65 (100%)	0	100	100
10	U	65/65 (100%)	65 (100%)	0	100	100
11	a	447/447 (100%)	444 (99%)	3 (1%)	76	88
12	b	209/209 (100%)	207 (99%)	2 (1%)	68	84
13	c	228/228 (100%)	228 (100%)	0	100	100
14	d	101/101 (100%)	101 (100%)	0	100	100
15	f	91/91 (100%)	91 (100%)	0	100	100
16	g	50/50 (100%)	50 (100%)	0	100	100
17	h	41/41 (100%)	41 (100%)	0	100	100
18	i	46/46 (100%)	46 (100%)	0	100	100
19	j	67/67 (100%)	66 (98%)	1 (2%)	57	77
20	k	99/99 (100%)	98 (99%)	1 (1%)	68	84
21	l	36/36 (100%)	36 (100%)	0	100	100
22	e	110/110 (100%)	110 (100%)	0	100	100
All	All	4989/4989 (100%)	4979 (100%)	10 (0%)	85	94

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	b	106	LEU
19	j	44	ASP
20	k	65	LEU
11	a	139	HIS
11	a	244	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	136	GLN
11	a	62	HIS
2	M	170	GLN

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Mol	Chain	Res	Type
5	P	46	ASN
11	a	404	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 60 ligands modelled in this entry, 4 are monoatomic - leaving 56 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	$\# Z > 2$
29	FES	P	302	5	0,4,4	-	-	-		
25	PEF	C	404	-	46,46,46	0.91	4 (8%)	49,51,51	1.14	2 (4%)
31	HEA	a	603	11	67,67,67	1.18	7 (10%)	81,103,103	1.61	14 (17%)
25	PEF	N	405	-	42,42,46	0.94	3 (7%)	45,47,51	1.11	2 (4%)
25	PEF	U	101	-	36,36,46	1.02	3 (8%)	39,41,51	1.16	3 (7%)
23	CDL	A	501	-	76,76,99	0.38	0	82,88,111	0.28	0
23	CDL	S	101	-	74,74,99	0.38	0	80,86,111	0.22	0
23	CDL	L	502	-	66,66,99	0.39	0	72,78,111	0.24	0
25	PEF	a	608	-	46,46,46	0.95	3 (6%)	49,51,51	1.13	2 (4%)
27	UQ6	N	407	-	43,43,43	0.33	0	54,55,55	0.59	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	HEC	O	401	4	46,50,50	1.83	5 (10%)	58,82,82	1.83	5 (8%)
25	PEF	E	302	-	41,41,46	0.95	4 (9%)	44,46,51	1.14	2 (4%)
26	PCF	e	202	-	49,49,49	1.12	3 (6%)	55,57,57	1.05	4 (7%)
25	PEF	P	301	-	42,42,46	0.94	4 (9%)	45,47,51	1.15	2 (4%)
25	PEF	N	408	-	31,31,46	1.10	4 (12%)	34,36,51	1.15	2 (5%)
25	PEF	J	102	-	28,28,46	1.15	4 (14%)	31,33,51	1.22	2 (6%)
25	PEF	a	601	-	39,39,46	0.96	4 (10%)	42,44,51	1.21	3 (7%)
25	PEF	h	101	-	46,46,46	0.90	3 (6%)	49,51,51	1.28	3 (6%)
25	PEF	H	103	-	33,33,46	1.08	3 (9%)	36,38,51	1.06	2 (5%)
26	PCF	T	101	-	46,46,49	1.14	3 (6%)	52,54,57	1.07	3 (5%)
23	CDL	c	303	-	85,85,99	0.40	0	91,97,111	0.25	0
25	PEF	S	102	-	35,35,46	1.04	4 (11%)	38,40,51	1.12	2 (5%)
23	CDL	A	502	-	53,53,99	0.44	0	59,65,111	0.26	0
26	PCF	I	101	-	29,29,49	1.40	4 (13%)	35,37,57	1.09	2 (5%)
24	HEM	N	402	3	50,50,50	1.37	7 (14%)	67,82,82	1.02	3 (4%)
29	FES	E	301	5	0,4,4	-	-	-	-	-
25	PEF	c	301	-	46,46,46	0.92	3 (6%)	49,51,51	1.24	4 (8%)
25	PEF	N	404	-	39,39,46	0.97	4 (10%)	42,44,51	1.22	2 (4%)
27	UQ6	C	406	-	43,43,43	0.34	0	54,55,55	1.15	4 (7%)
25	PEF	l	101	-	46,46,46	0.90	3 (6%)	49,51,51	1.14	2 (4%)
25	PEF	b	302	-	39,39,46	0.99	4 (10%)	42,44,51	1.20	2 (4%)
23	CDL	L	501	-	54,54,99	0.44	0	60,66,111	0.27	0
23	CDL	E	303	-	52,52,99	0.44	0	58,64,111	0.30	0
23	CDL	H	101	-	65,65,99	0.42	0	71,77,111	0.27	0
25	PEF	a	607	-	39,39,46	0.97	3 (7%)	42,44,51	1.12	2 (4%)
25	PEF	e	201	-	46,46,46	0.91	4 (8%)	49,51,51	1.09	2 (4%)
26	PCF	C	405	-	38,38,49	1.23	4 (10%)	44,46,57	1.15	2 (4%)
28	HEC	D	401	4	46,50,50	1.84	4 (8%)	58,82,82	1.79	7 (12%)
25	PEF	b	303	-	46,46,46	0.89	4 (8%)	49,51,51	1.12	2 (4%)
24	HEM	C	401	3	50,50,50	1.48	9 (18%)	67,82,82	1.44	11 (16%)
25	PEF	c	302	-	46,46,46	0.90	3 (6%)	49,51,51	1.16	2 (4%)
23	CDL	N	403	-	52,52,99	0.45	0	58,64,111	0.28	0
23	CDL	H	102	-	70,70,99	0.40	0	76,82,111	0.24	0
26	PCF	N	406	-	49,49,49	1.10	3 (6%)	55,57,57	1.06	2 (3%)
25	PEF	G	201	-	31,31,46	1.09	4 (12%)	34,36,51	1.21	2 (5%)
25	PEF	C	407	-	39,39,46	0.98	4 (10%)	42,44,51	1.13	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	HEA	a	604	11	67,67,67	2.45	24 (35%)	81,103,103	2.48	32 (39%)
24	HEM	N	401	3	50,50,50	1.44	9 (18%)	67,82,82	1.31	8 (11%)
25	PEF	P	303	-	38,38,46	0.98	4 (10%)	41,43,51	1.04	2 (4%)
25	PEF	C	403	-	43,43,46	0.92	4 (9%)	46,48,51	1.16	2 (4%)
34	CUA	b	301	12	0,1,1	-	-	-	-	-
23	CDL	P	304	-	47,47,99	0.45	0	53,59,111	0.31	0
25	PEF	a	609	-	29,29,46	1.13	4 (13%)	32,34,51	1.23	2 (6%)
25	PEF	J	101	-	25,25,46	1.21	4 (16%)	28,30,51	1.19	2 (7%)
26	PCF	H	104	-	31,31,49	1.34	3 (9%)	37,39,57	1.15	3 (8%)
24	HEM	C	402	3	50,50,50	1.38	7 (14%)	67,82,82	1.06	4 (5%)

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
29	FES	P	302	5	-	-	0/1/1/1
25	PEF	C	404	-	-	23/50/50/50	-
31	HEA	a	603	11	-	18/36/76/76	-
25	PEF	N	405	-	-	14/46/46/50	-
25	PEF	U	101	-	-	15/40/40/50	-
23	CDL	A	501	-	-	44/87/87/110	-
23	CDL	S	101	-	-	47/85/85/110	-
23	CDL	L	502	-	-	40/77/77/110	-
25	PEF	a	608	-	-	24/50/50/50	-
27	UQ6	N	407	-	-	11/39/39/39	0/1/1/1
28	HEC	O	401	4	-	4/14/54/54	-
25	PEF	E	302	-	-	13/45/45/50	-
26	PCF	e	202	-	-	19/53/53/53	-
25	PEF	P	301	-	-	21/46/46/50	-
25	PEF	N	408	-	-	14/35/35/50	-
25	PEF	J	102	-	-	9/32/32/50	-
25	PEF	a	601	-	-	18/43/43/50	-
25	PEF	h	101	-	-	25/50/50/50	-
25	PEF	H	103	-	-	14/37/37/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PCF	T	101	-	-	23/50/50/53	-
23	CDL	c	303	-	-	62/96/96/110	-
25	PEF	S	102	-	-	15/39/39/50	-
23	CDL	A	502	-	-	27/64/64/110	-
26	PCF	I	101	-	-	8/33/33/53	-
24	HEM	N	402	3	-	1/14/54/54	-
29	FES	E	301	5	-	-	0/1/1/1
25	PEF	c	301	-	-	17/50/50/50	-
25	PEF	N	404	-	-	18/43/43/50	-
27	UQ6	C	406	-	-	5/39/39/39	0/1/1/1
25	PEF	l	101	-	-	19/50/50/50	-
25	PEF	b	302	-	-	19/43/43/50	-
23	CDL	L	501	-	-	42/64/64/110	-
23	CDL	E	303	-	-	24/63/63/110	-
23	CDL	H	101	-	-	40/76/76/110	-
25	PEF	a	607	-	-	18/43/43/50	-
25	PEF	e	201	-	-	23/50/50/50	-
26	PCF	C	405	-	-	14/42/42/53	-
28	HEC	D	401	4	-	5/14/54/54	-
25	PEF	b	303	-	-	25/50/50/50	-
24	HEM	C	401	3	-	2/14/54/54	-
25	PEF	c	302	-	-	21/50/50/50	-
23	CDL	N	403	-	-	31/63/63/110	-
23	CDL	H	102	-	-	33/81/81/110	-
26	PCF	N	406	-	-	23/53/53/53	-
25	PEF	G	201	-	-	18/35/35/50	-
25	PEF	C	407	-	-	21/43/43/50	-
31	HEA	a	604	11	-	3/36/76/76	-
24	HEM	N	401	3	-	2/14/54/54	-
25	PEF	P	303	-	-	22/42/42/50	-
25	PEF	C	403	-	-	15/47/47/50	-
23	CDL	P	304	-	-	25/58/58/110	-
25	PEF	a	609	-	-	15/33/33/50	-
25	PEF	J	101	-	-	7/29/29/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PCF	H	104	-	-	12/35/35/53	-
24	HEM	C	402	3	-	4/14/54/54	-

The worst 5 of 187 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	604	HEA	FE-NB	6.50	2.14	1.94
28	D	401	HEC	CAC-C3C	6.32	1.55	1.35
28	O	401	HEC	CAB-C3B	6.27	1.55	1.35
28	D	401	HEC	CAB-C3B	6.16	1.55	1.35
28	O	401	HEC	CAC-C3C	6.13	1.54	1.35

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	O	401	HEC	CBC-CAC-C3C	-8.85	109.75	127.43
28	D	401	HEC	CBB-CAB-C3B	-7.59	112.26	127.43
28	O	401	HEC	CBB-CAB-C3B	-6.12	115.20	127.43
28	D	401	HEC	CBC-CAC-C3C	-6.06	115.32	127.43
31	a	604	HEA	C2B-C1B-NB	6.01	116.85	109.90

There are no chirality outliers.

5 of 1032 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	501	CDL	CA3-OA5-PA1-OA2
23	A	501	CDL	CA3-OA5-PA1-OA3
23	A	501	CDL	CA3-OA5-PA1-OA4
23	A	501	CDL	CA3-CA4-OA6-CA5
23	A	501	CDL	OA6-CA4-CA6-OA8

There are no ring outliers.

49 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	404	PEF	1	0
31	a	603	HEA	3	0
25	U	101	PEF	2	0
23	A	501	CDL	2	0
23	S	101	CDL	2	0

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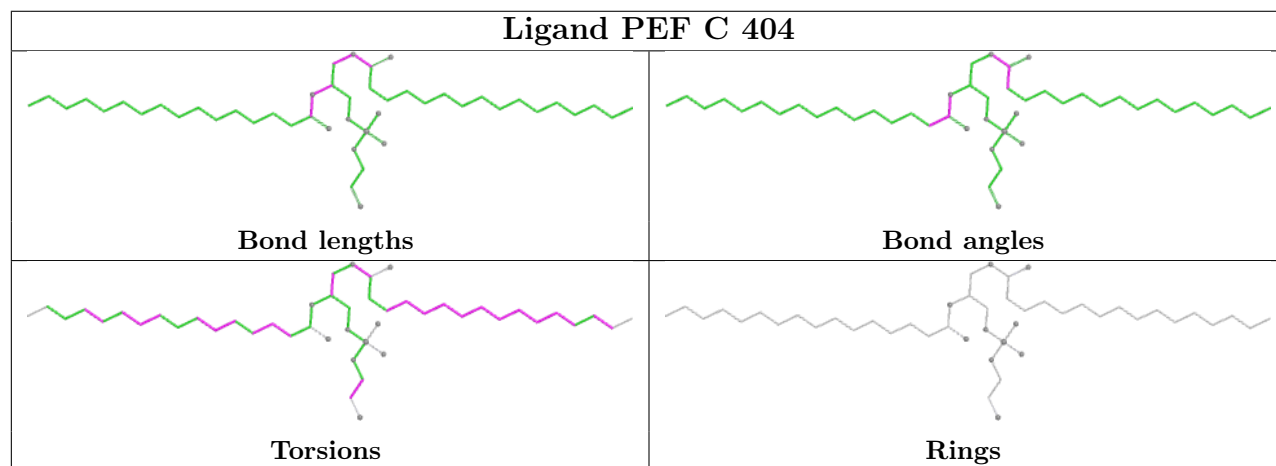
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	502	CDL	4	0
25	a	608	PEF	2	0
27	N	407	UQ6	1	0
28	O	401	HEC	5	0
25	E	302	PEF	2	0
26	e	202	PCF	1	0
25	P	301	PEF	3	0
25	N	408	PEF	2	0
25	J	102	PEF	1	0
25	a	601	PEF	2	0
25	h	101	PEF	1	0
26	T	101	PCF	4	0
23	c	303	CDL	3	0
25	S	102	PEF	3	0
23	A	502	CDL	2	0
26	I	101	PCF	2	0
24	N	402	HEM	1	0
25	c	301	PEF	1	0
25	N	404	PEF	2	0
27	C	406	UQ6	2	0
25	l	101	PEF	4	0
25	b	302	PEF	2	0
23	L	501	CDL	3	0
23	E	303	CDL	2	0
23	H	101	CDL	3	0
25	a	607	PEF	3	0
25	e	201	PEF	2	0
26	C	405	PCF	1	0
28	D	401	HEC	4	0
25	b	303	PEF	1	0
24	C	401	HEM	2	0
25	c	302	PEF	6	0
23	N	403	CDL	4	0
23	H	102	CDL	1	0
26	N	406	PCF	3	0
25	G	201	PEF	1	0
25	C	407	PEF	2	0
24	N	401	HEM	3	0
25	P	303	PEF	2	0
25	C	403	PEF	4	0
23	P	304	CDL	1	0
25	a	609	PEF	1	0

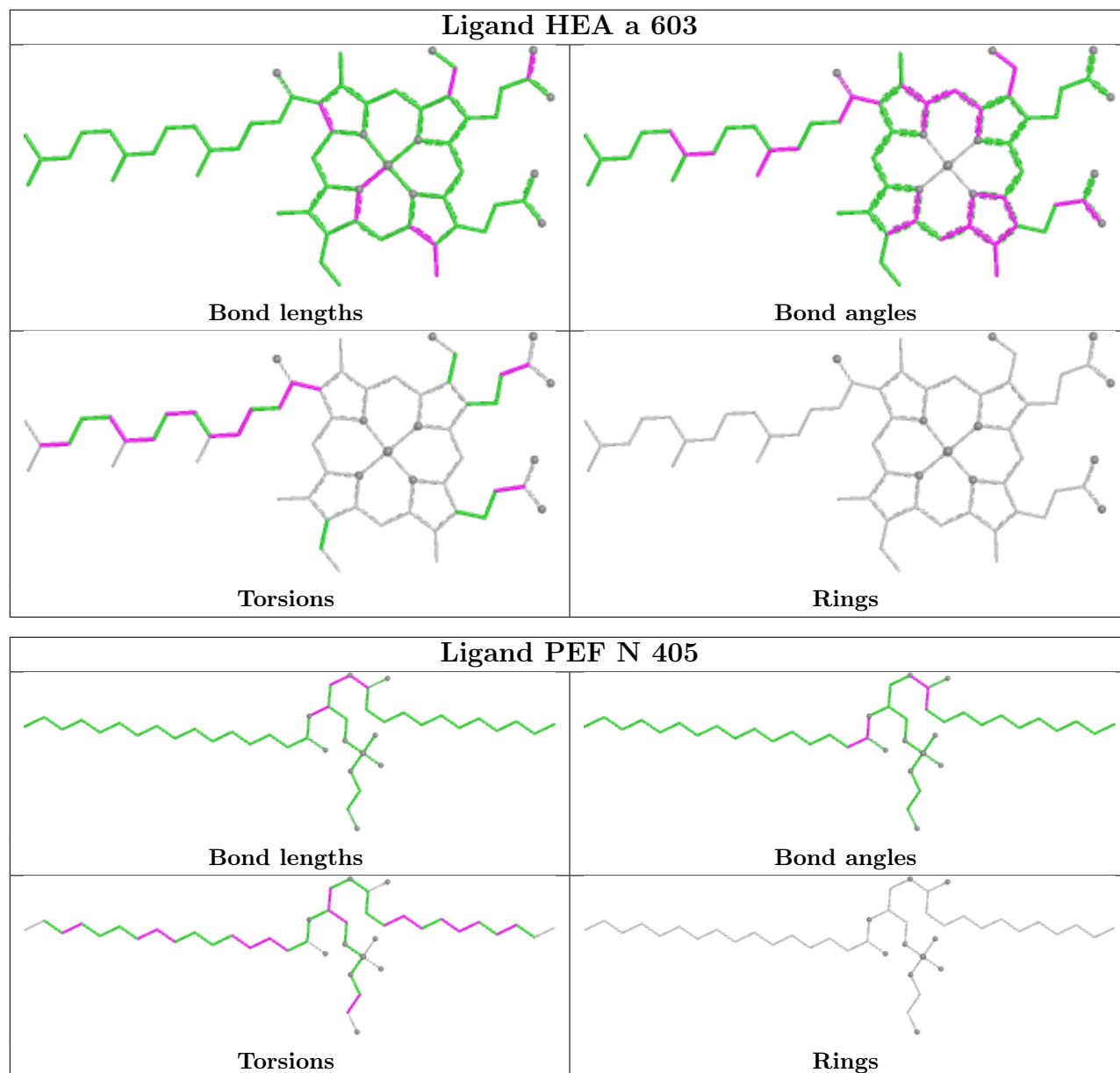
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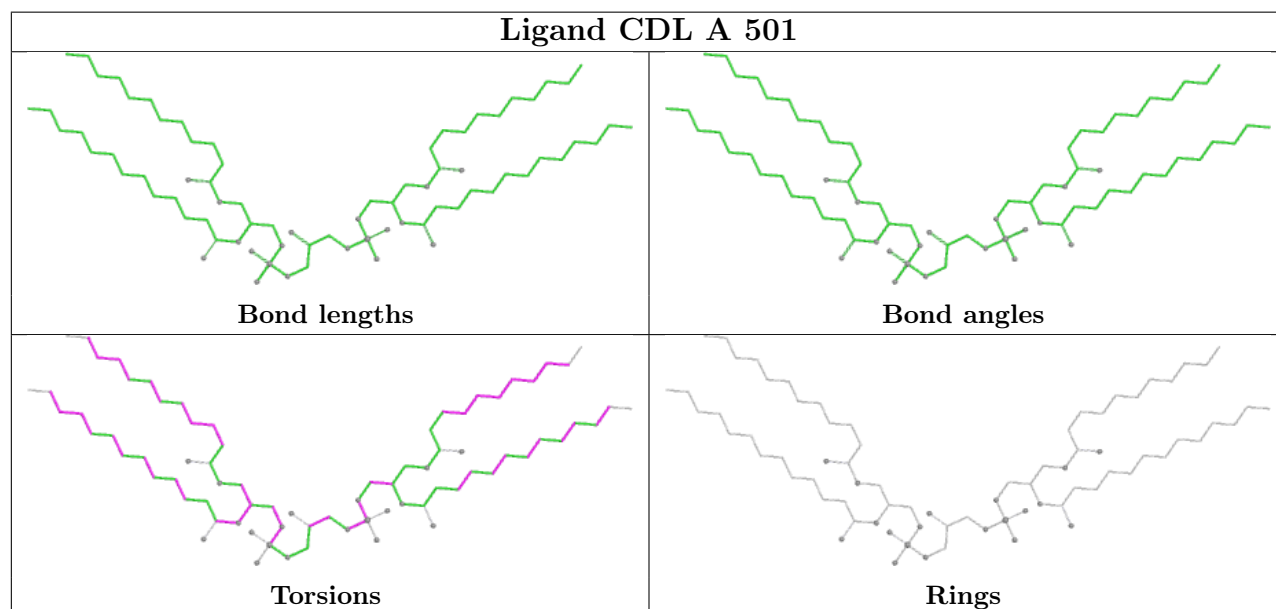
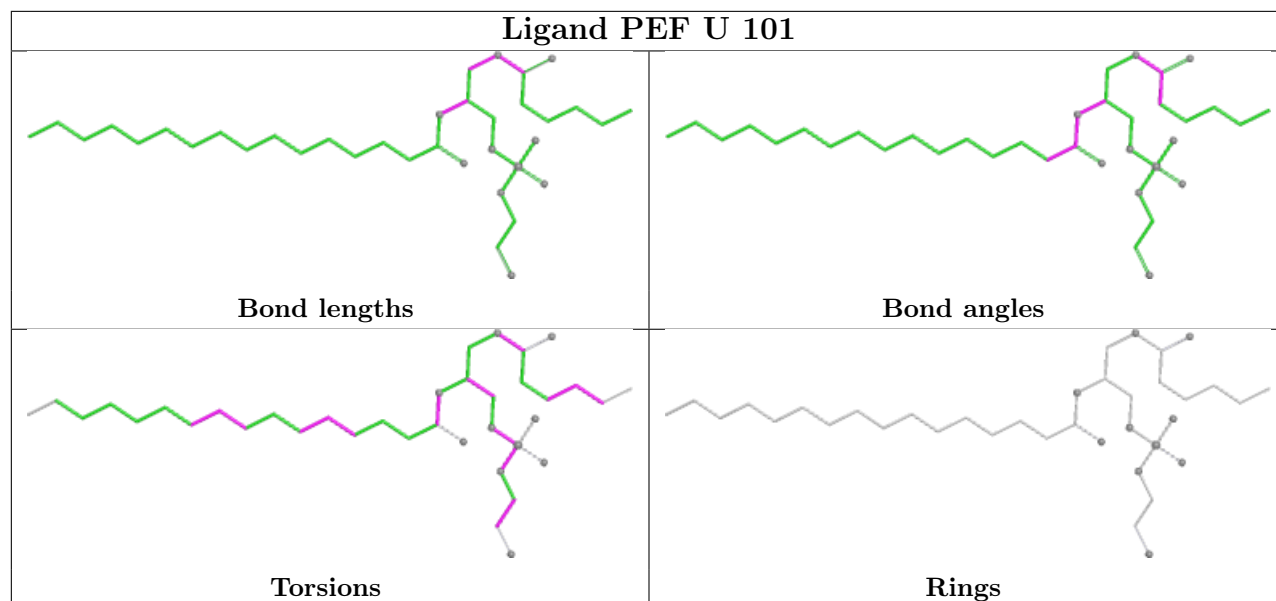
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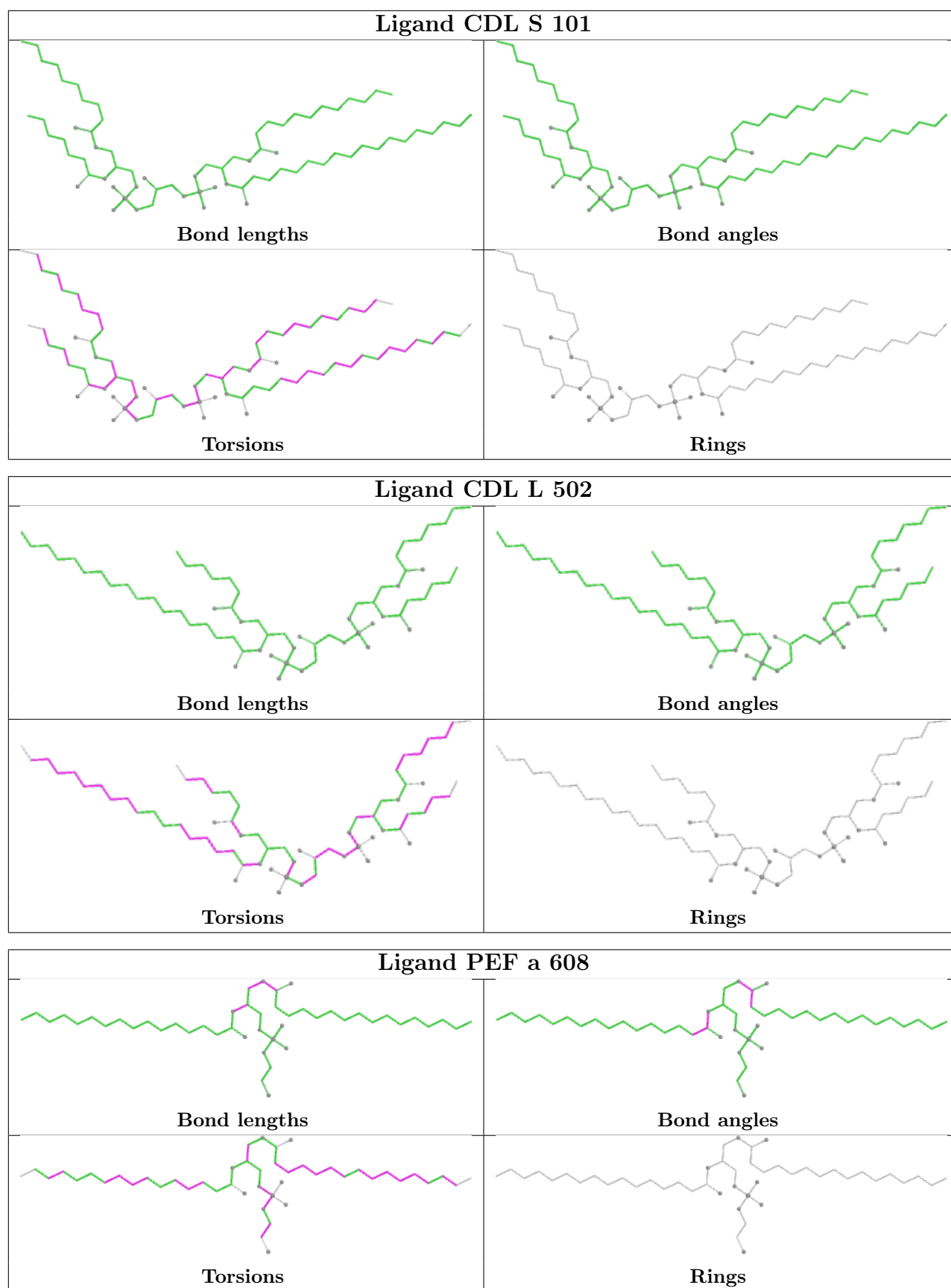
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	H	104	PCF	1	0
24	C	402	HEM	2	0

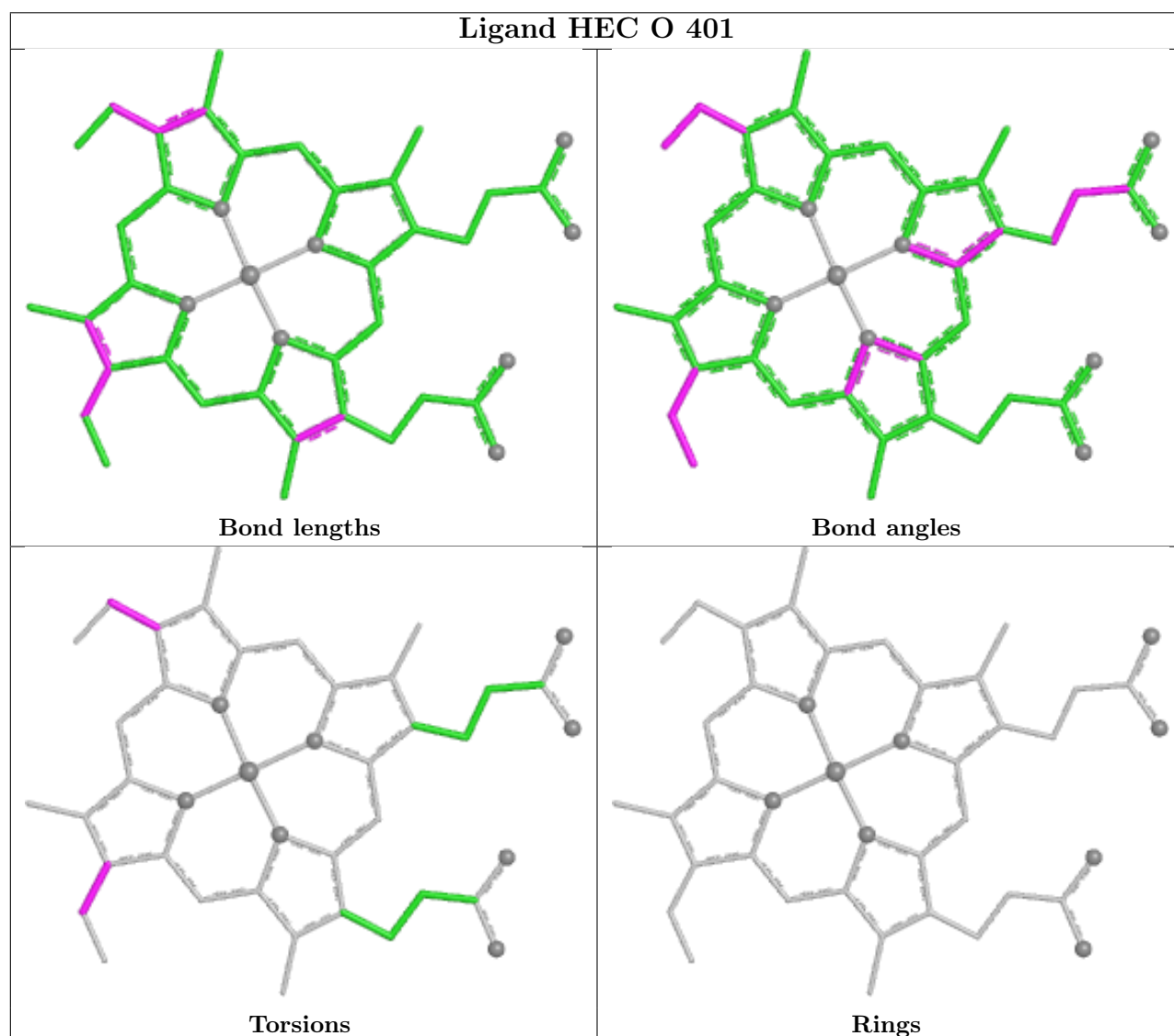
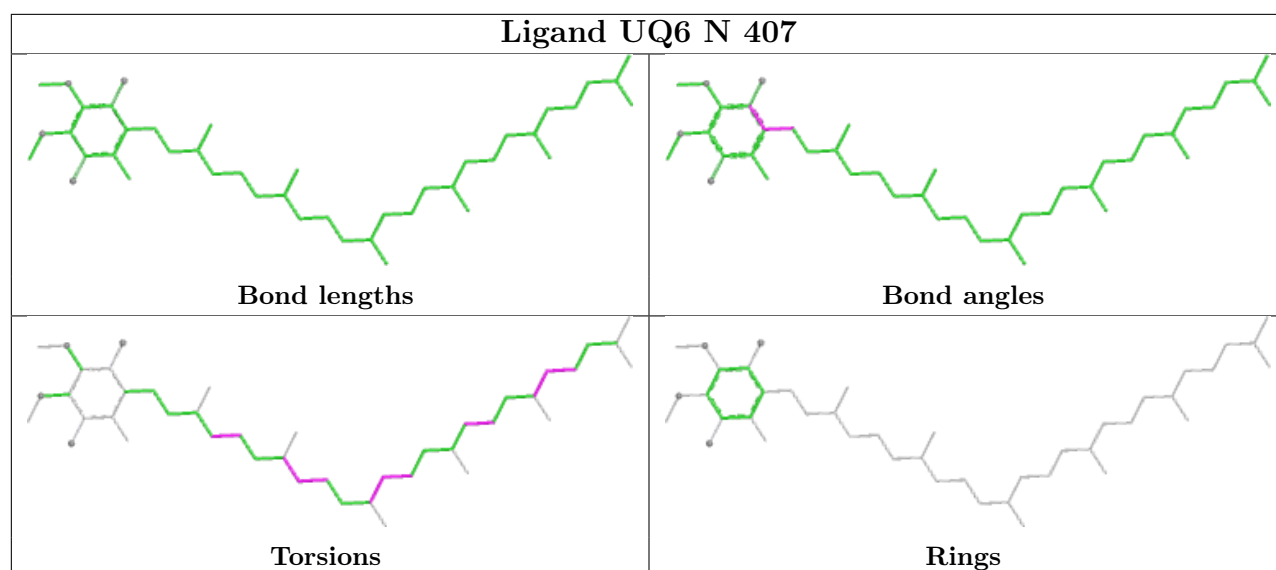
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

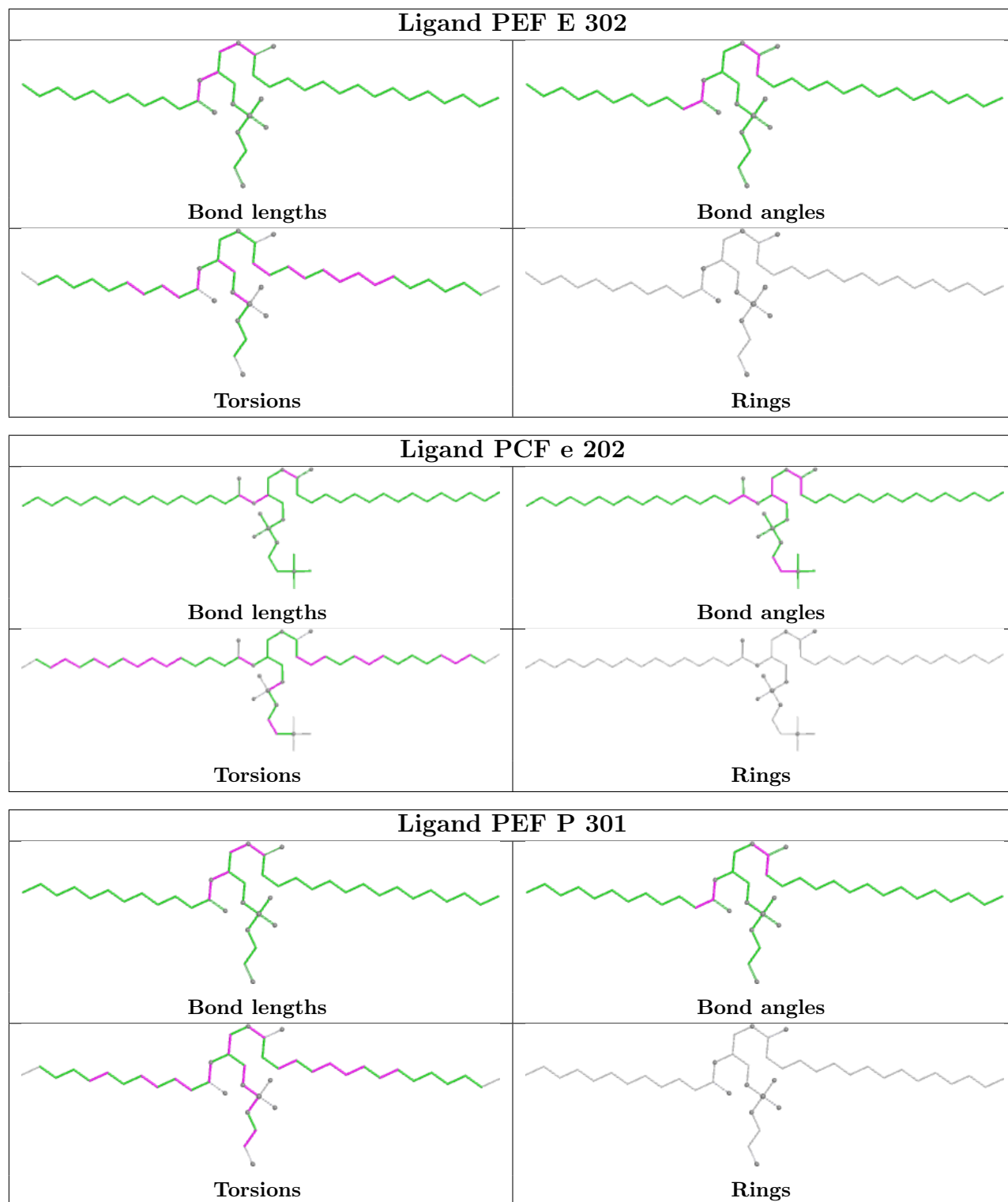


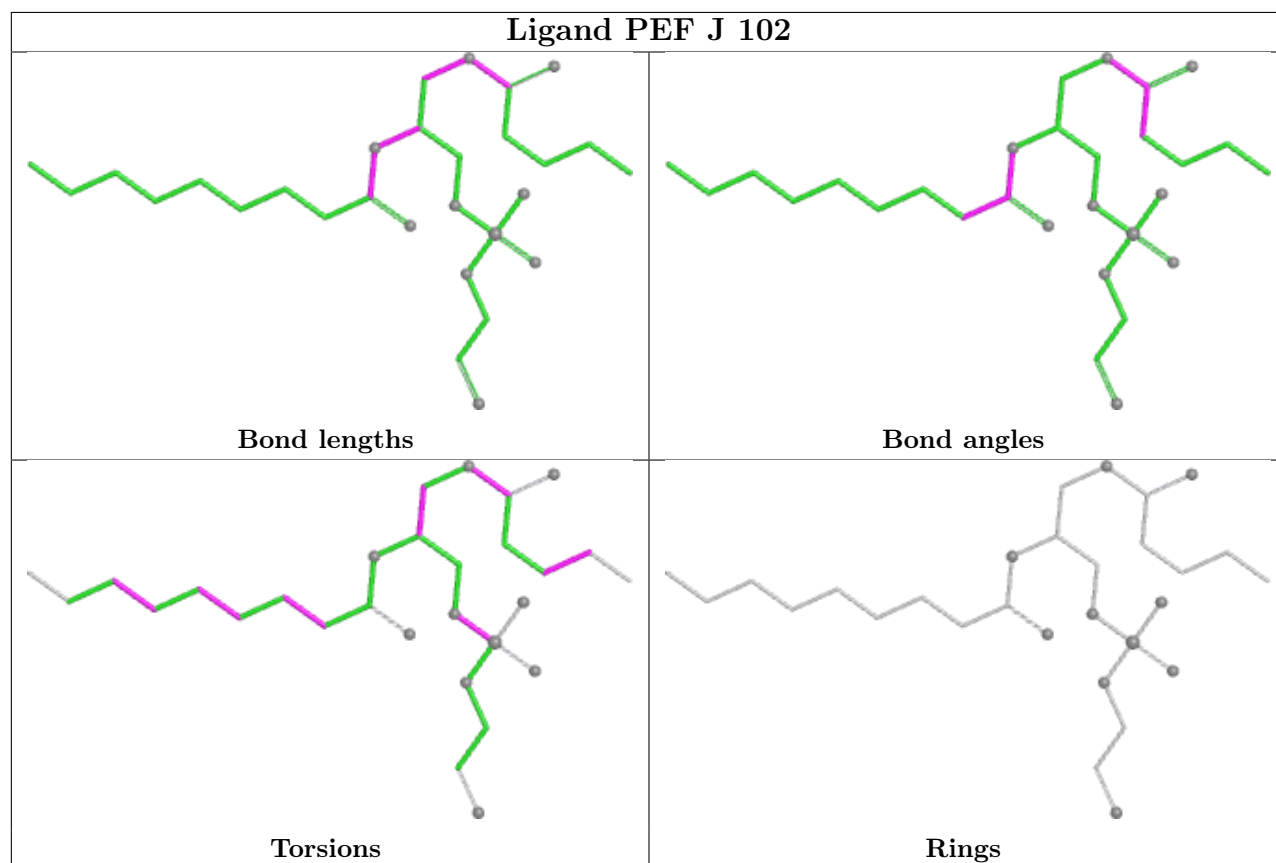
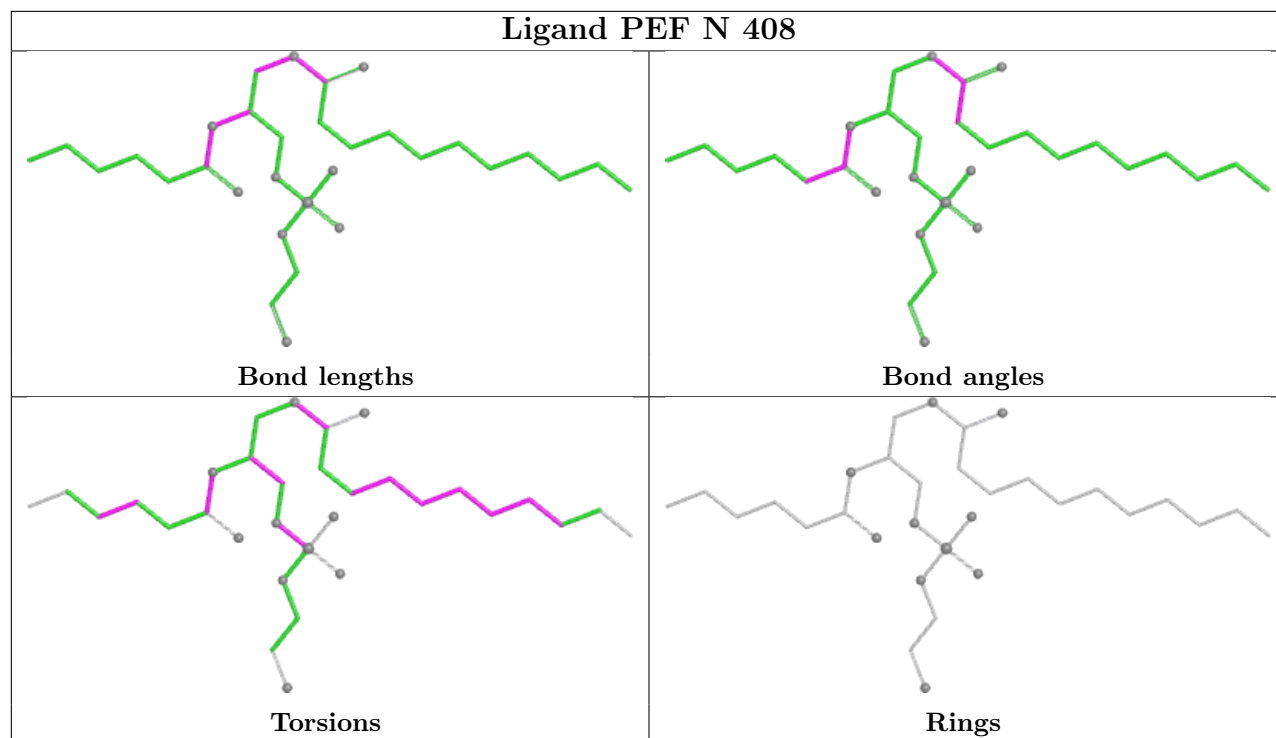


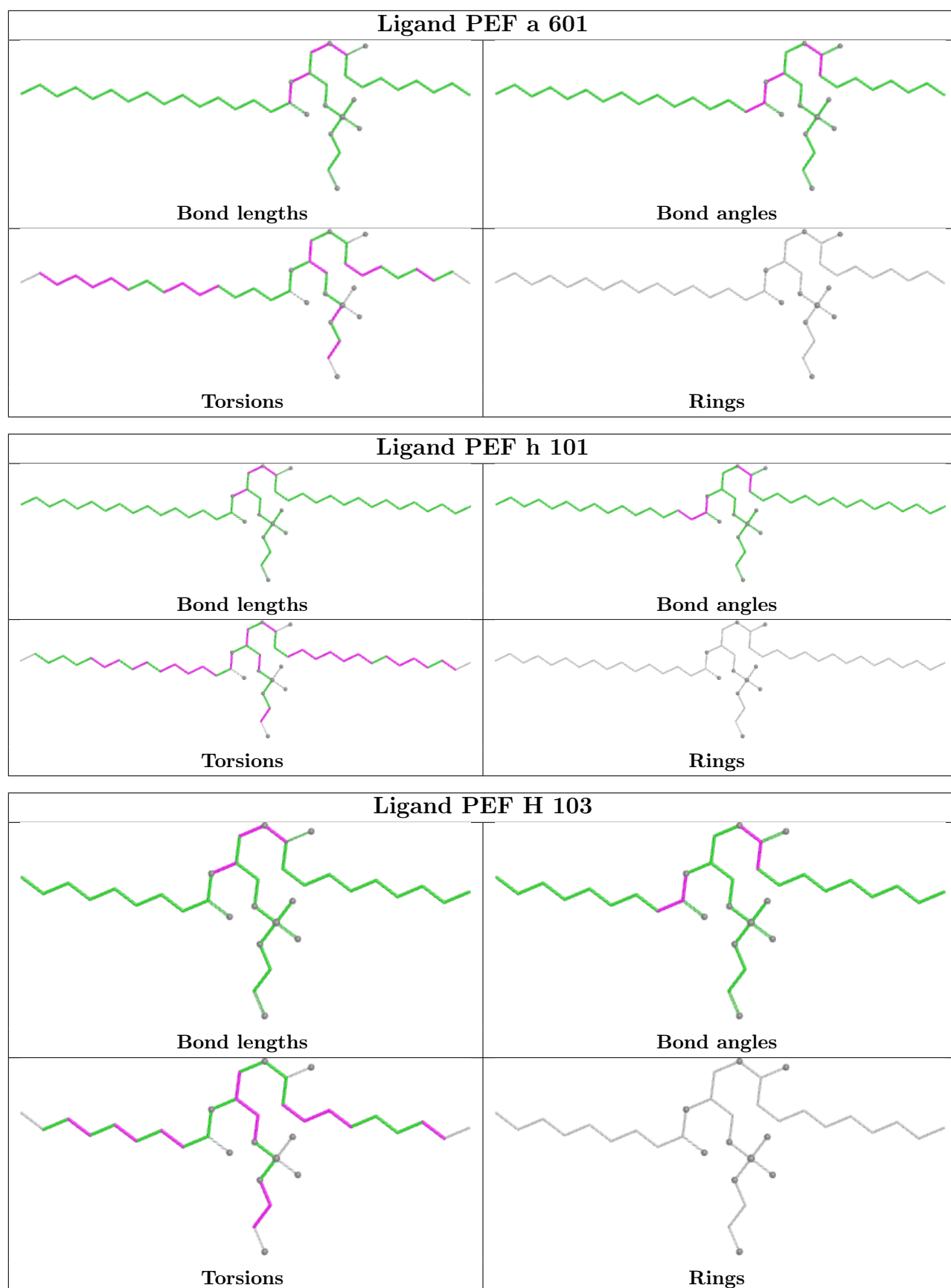


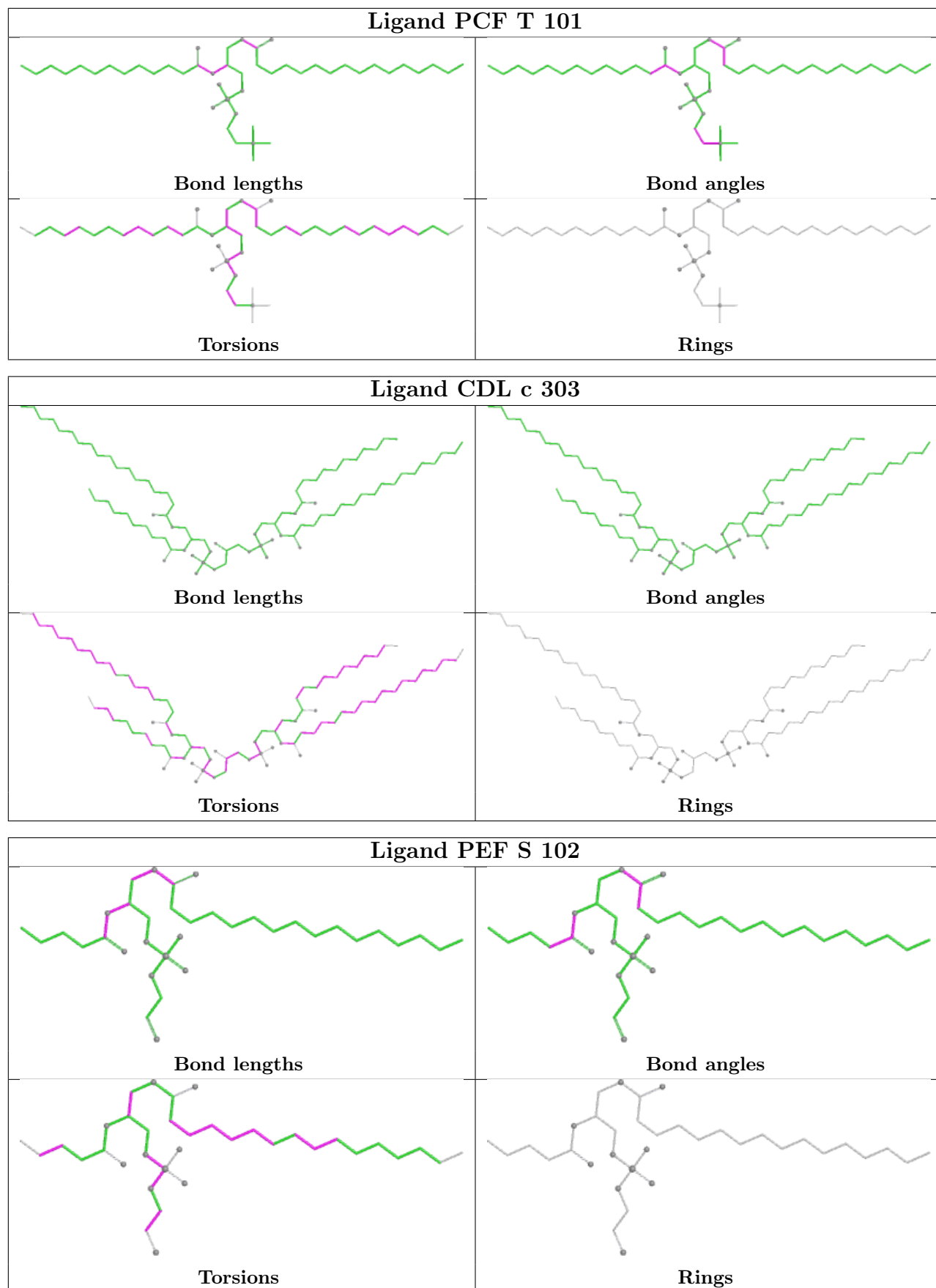


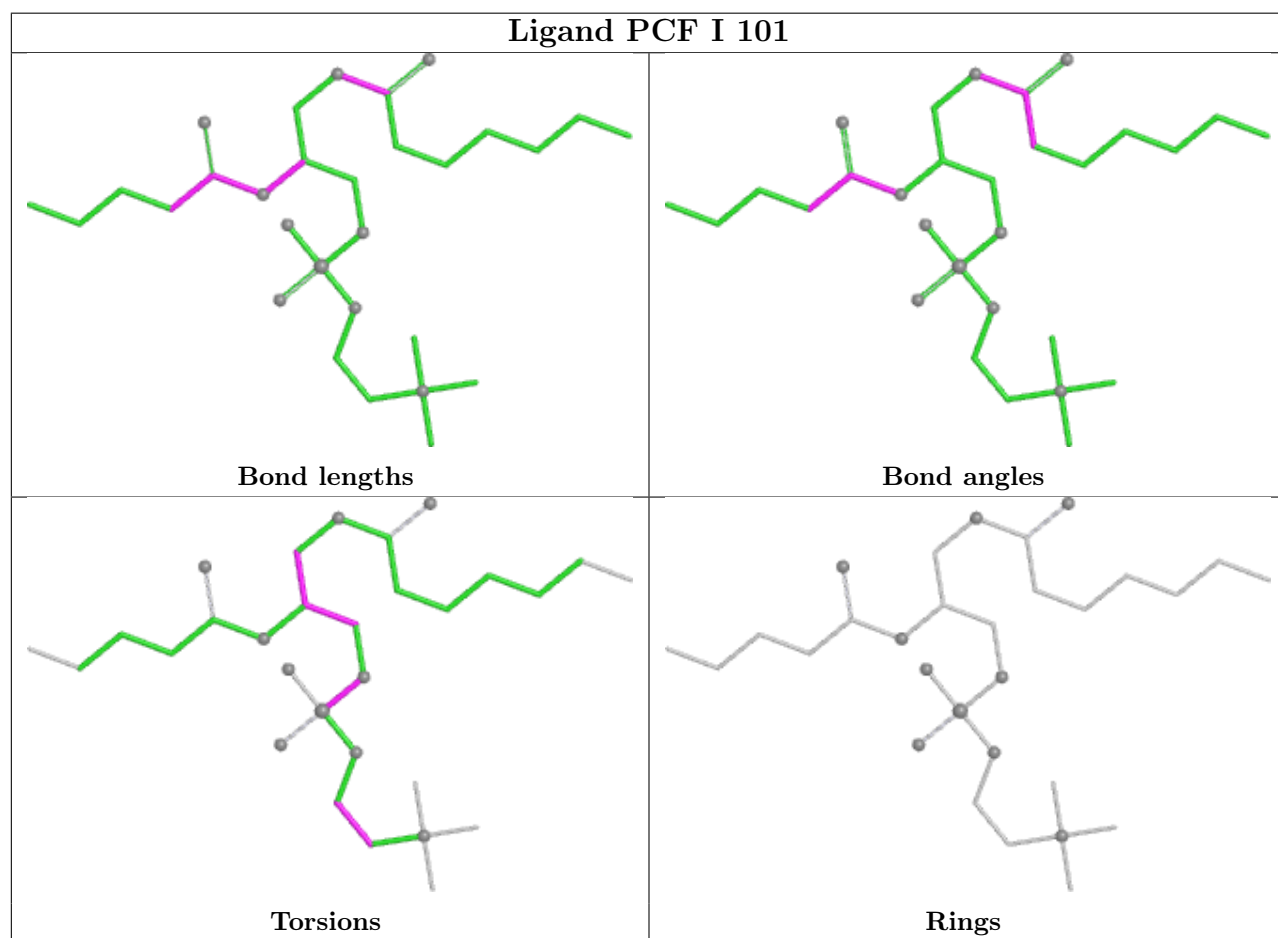
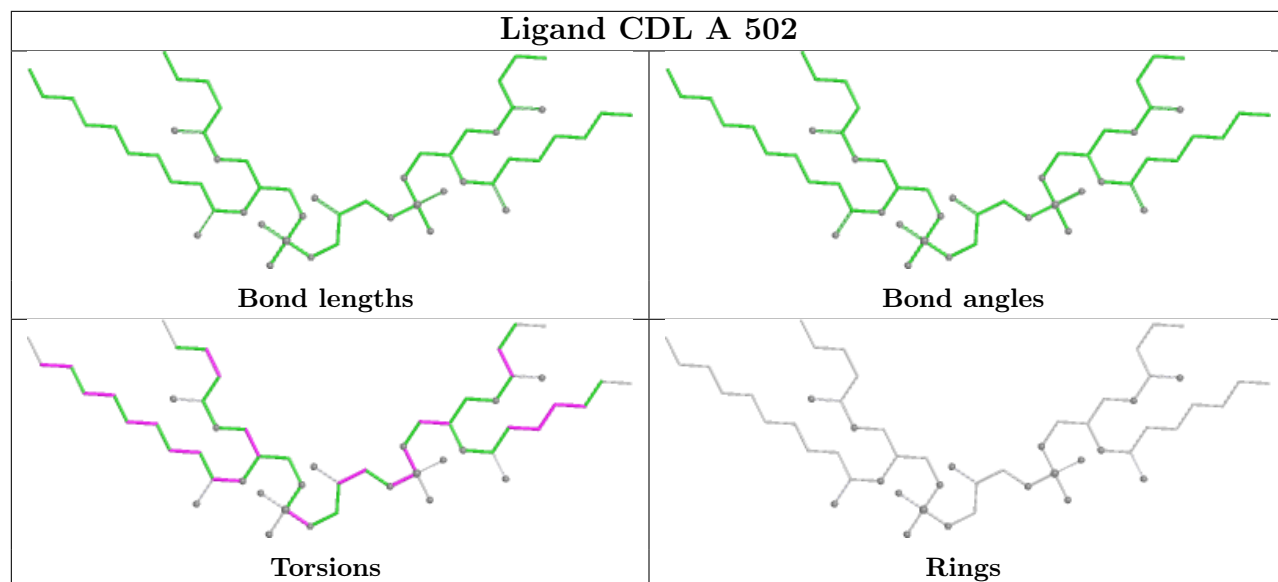


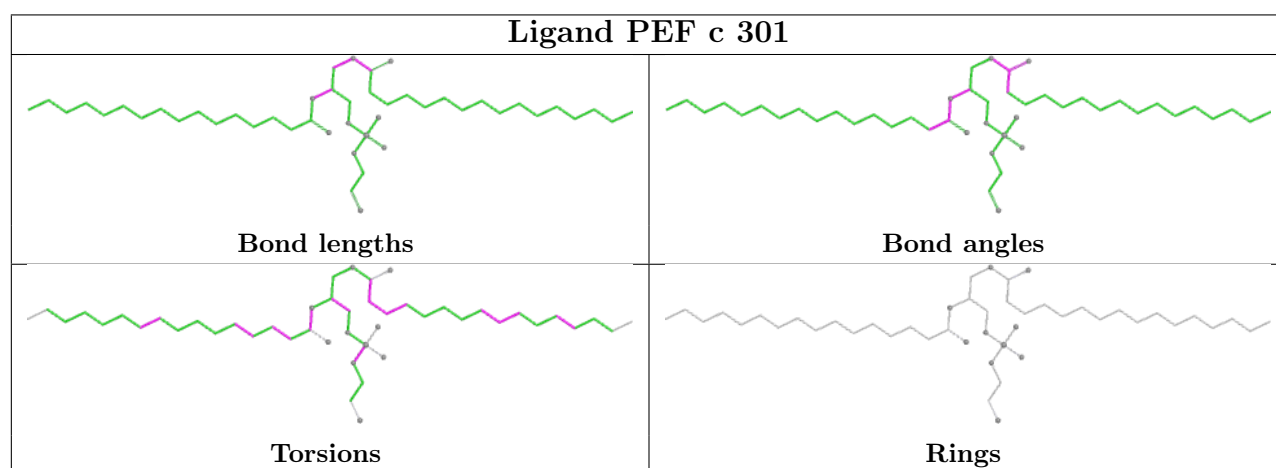
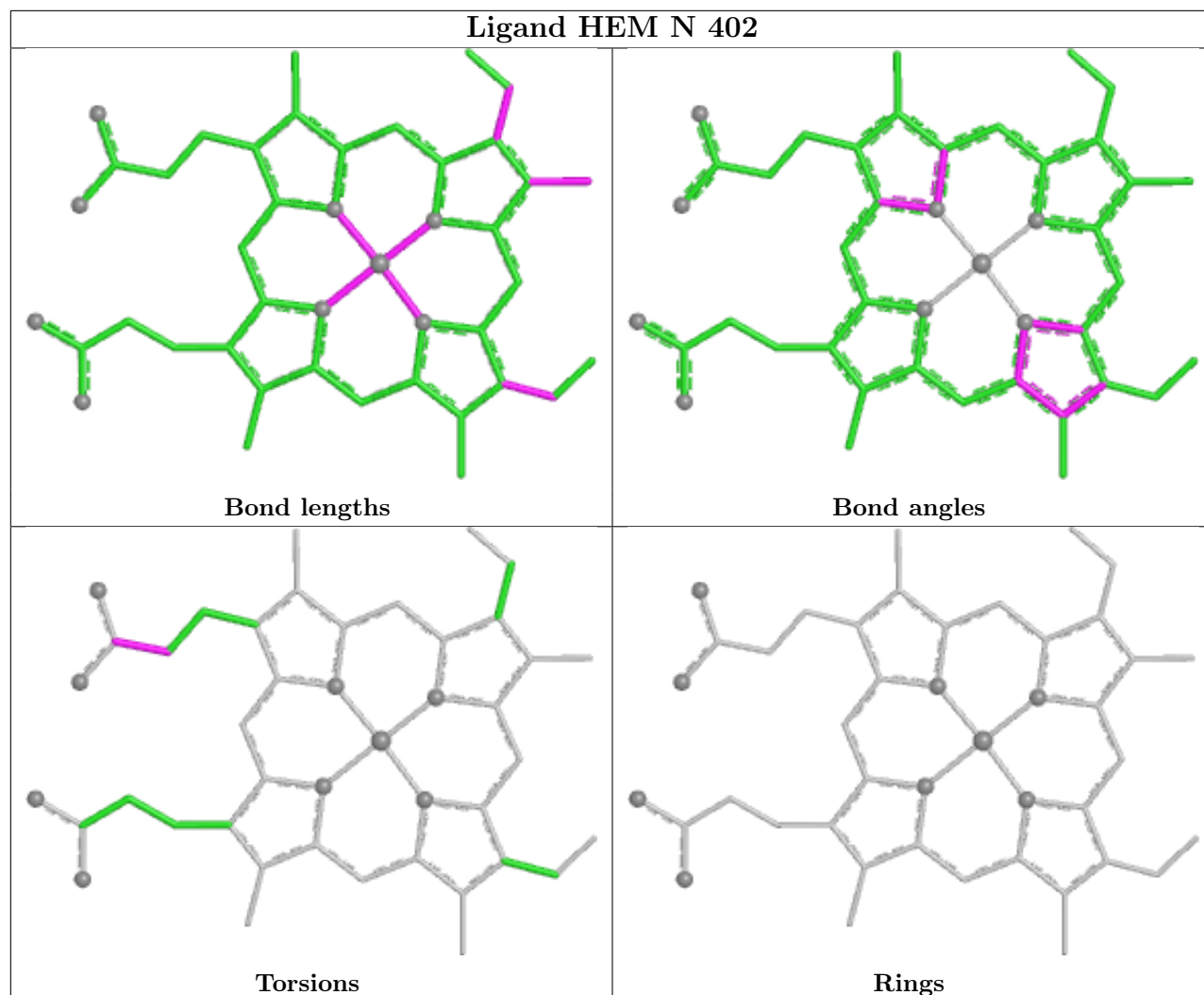


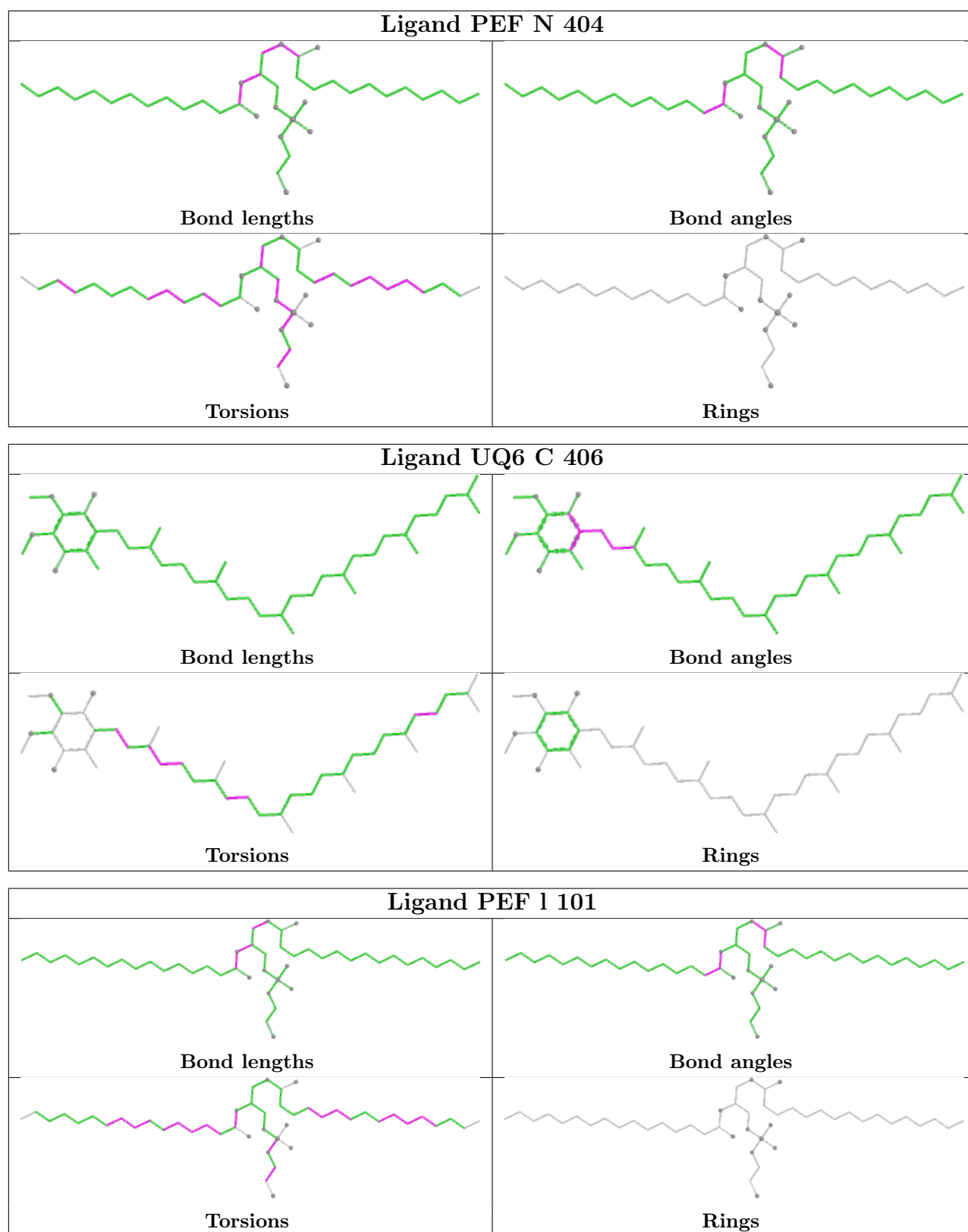


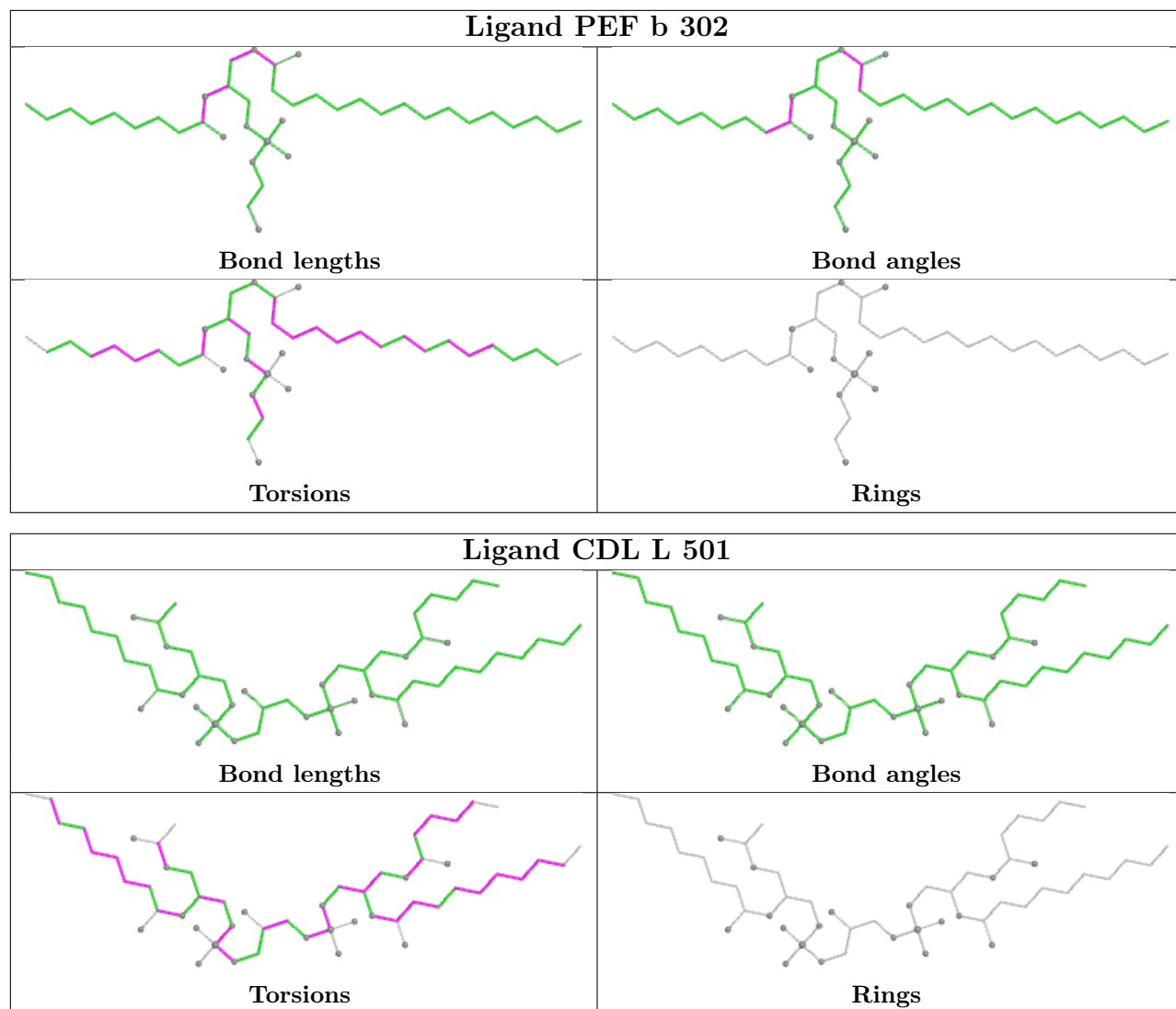


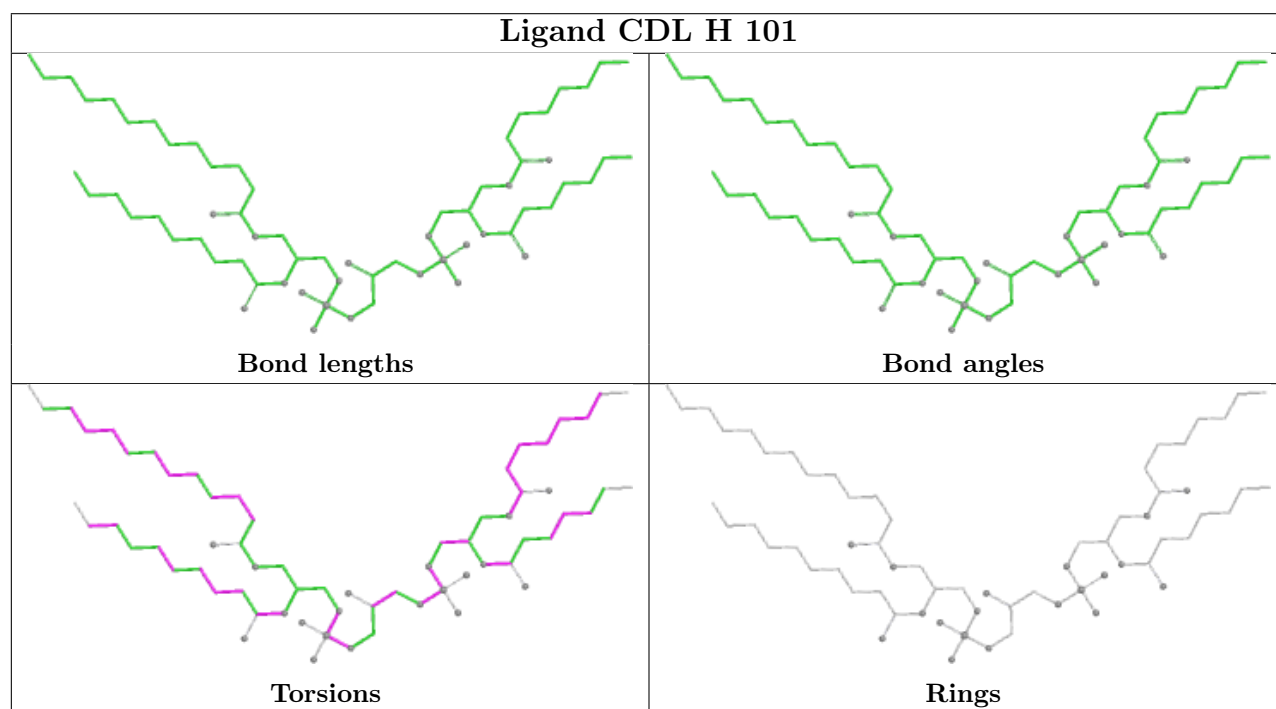
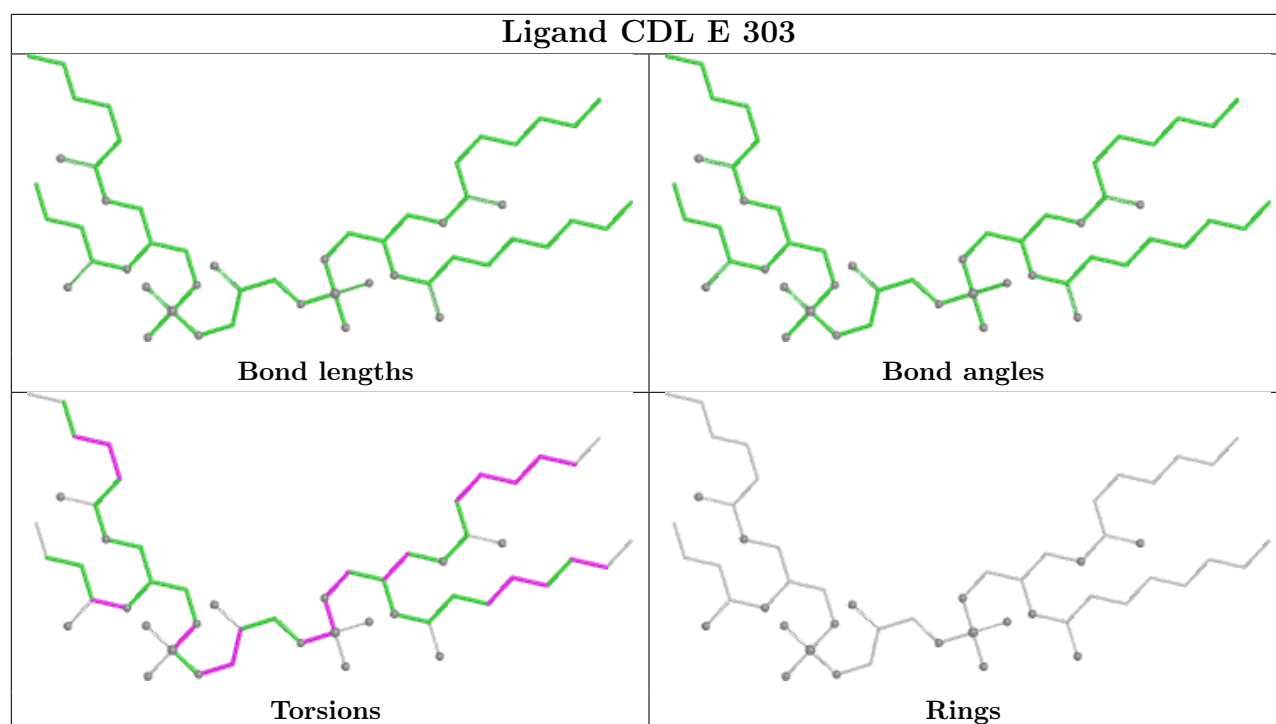


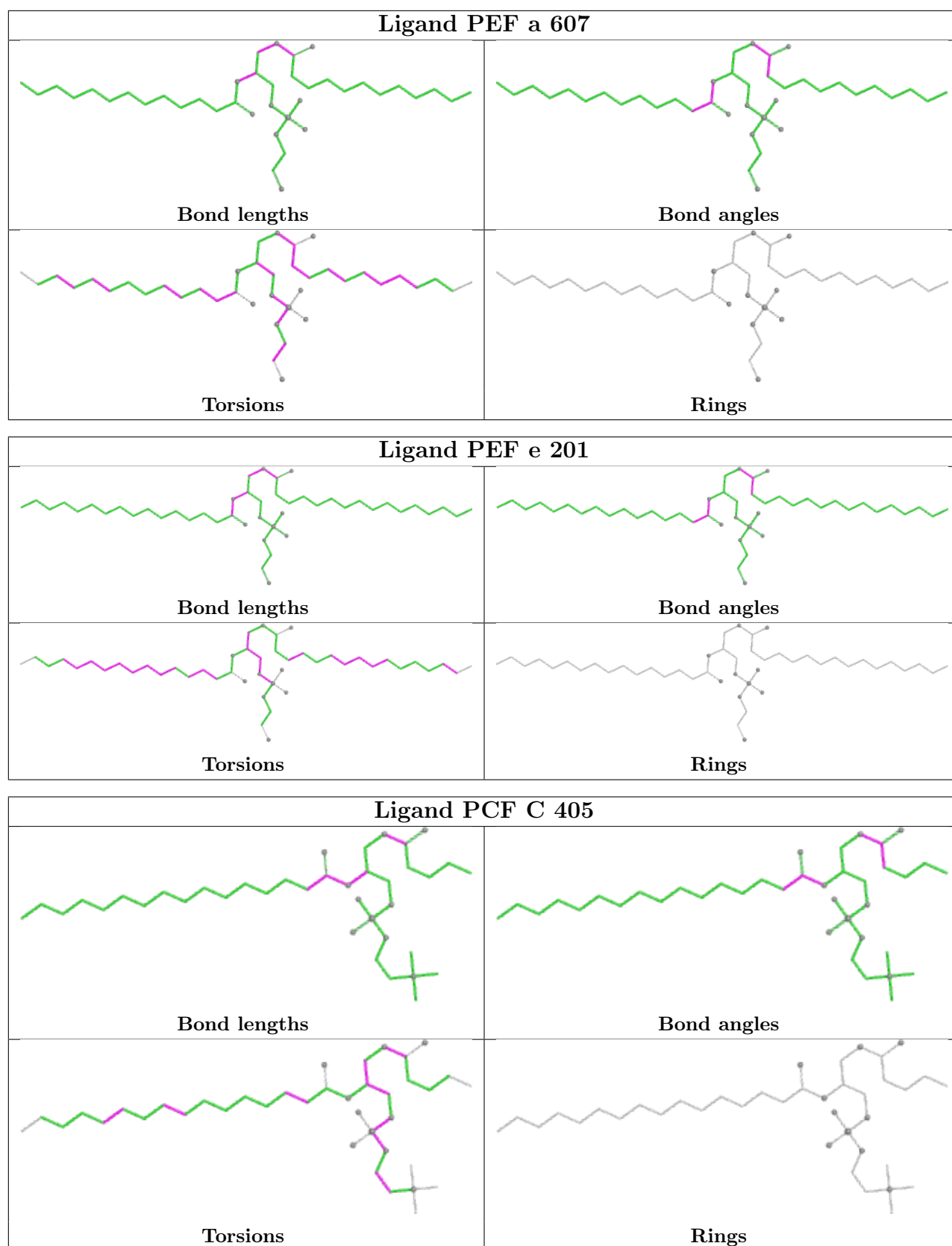


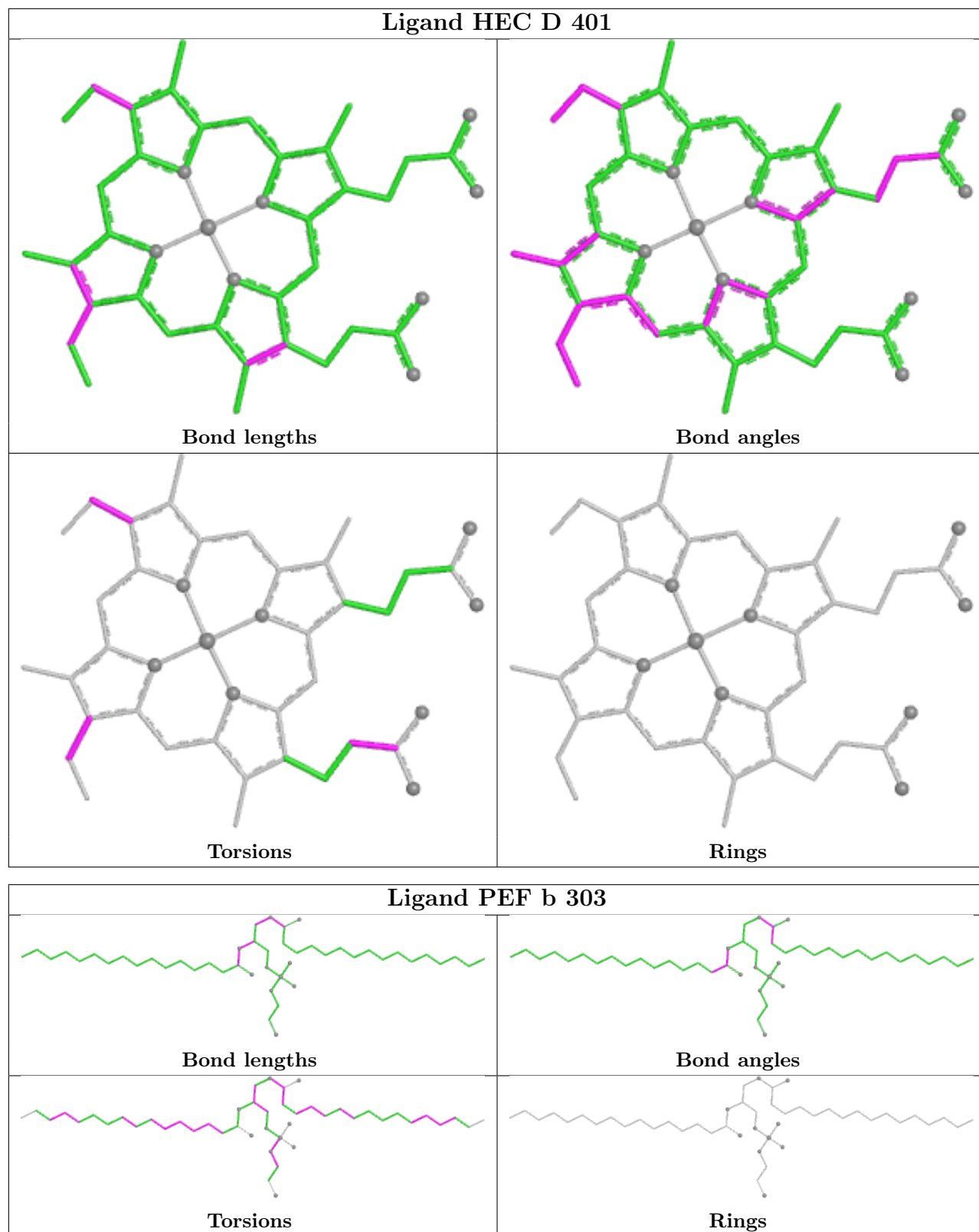


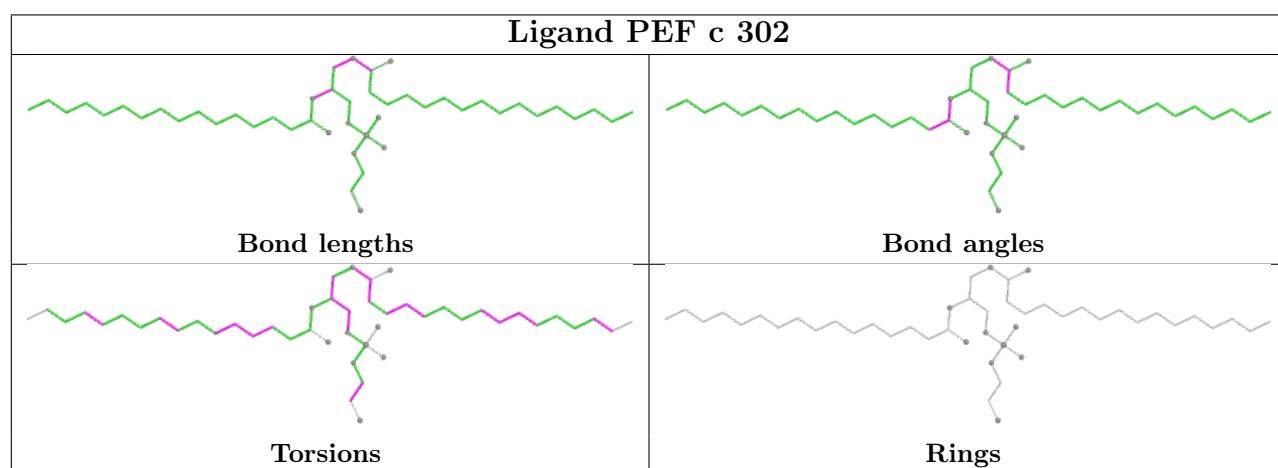
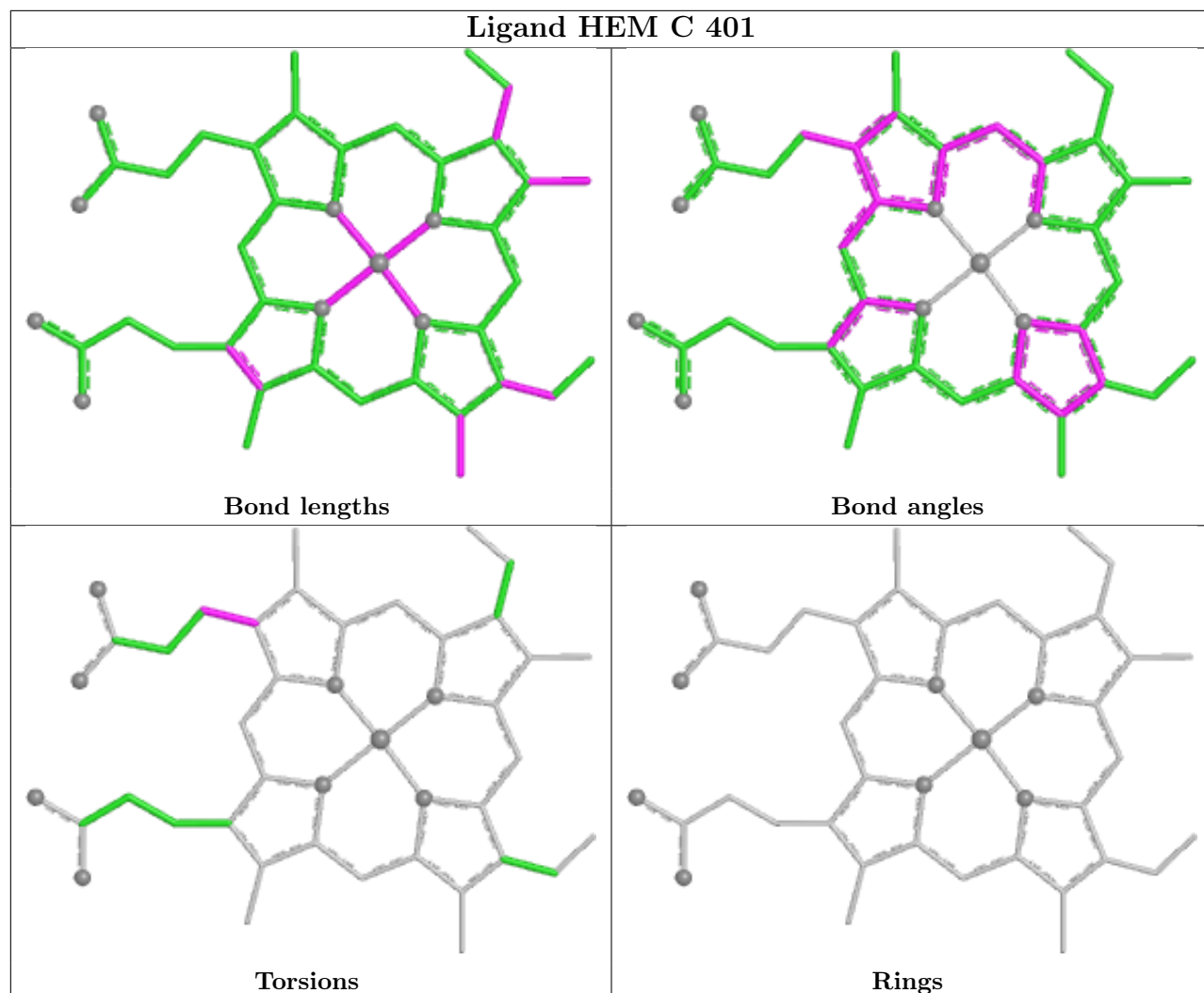


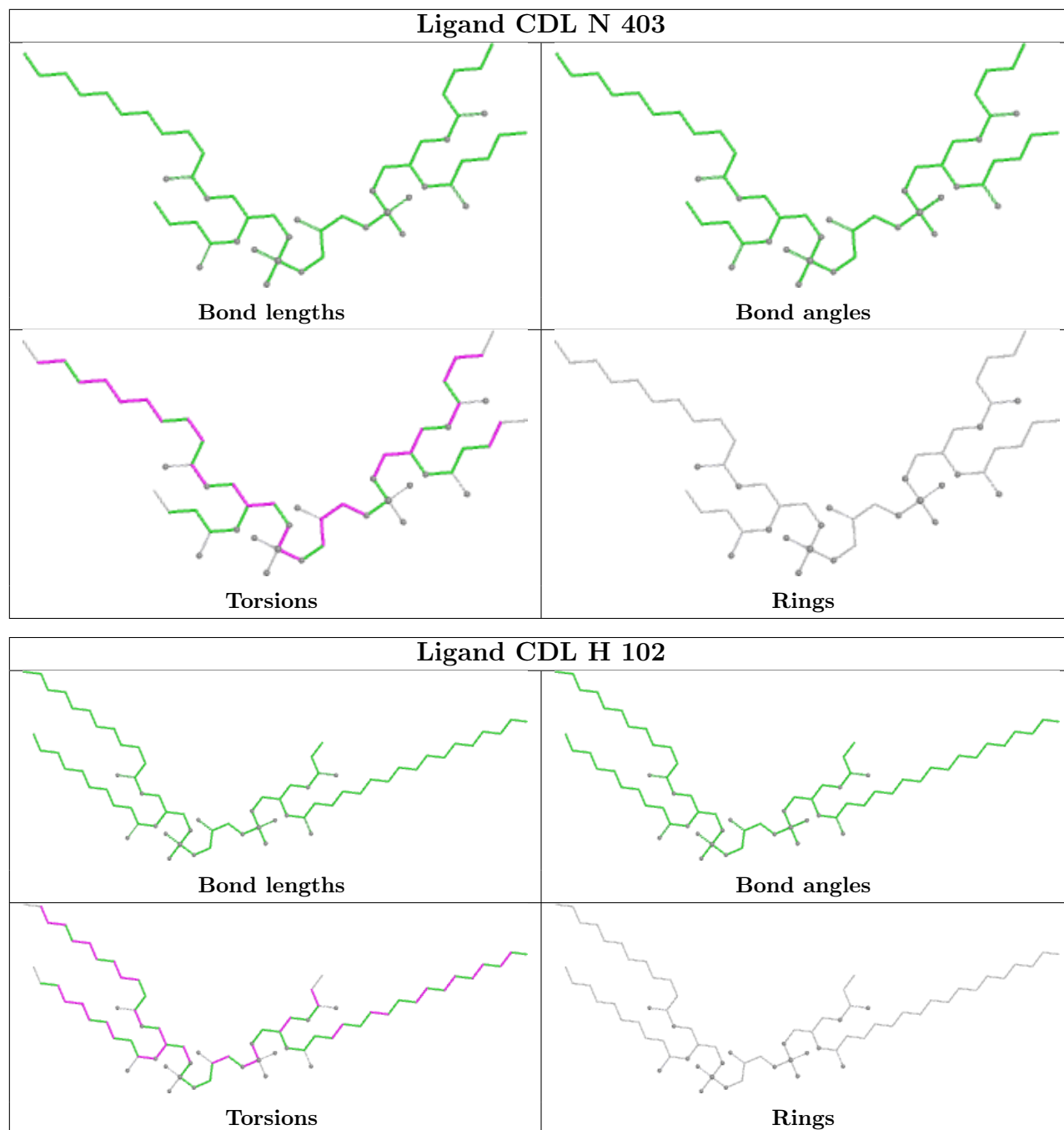


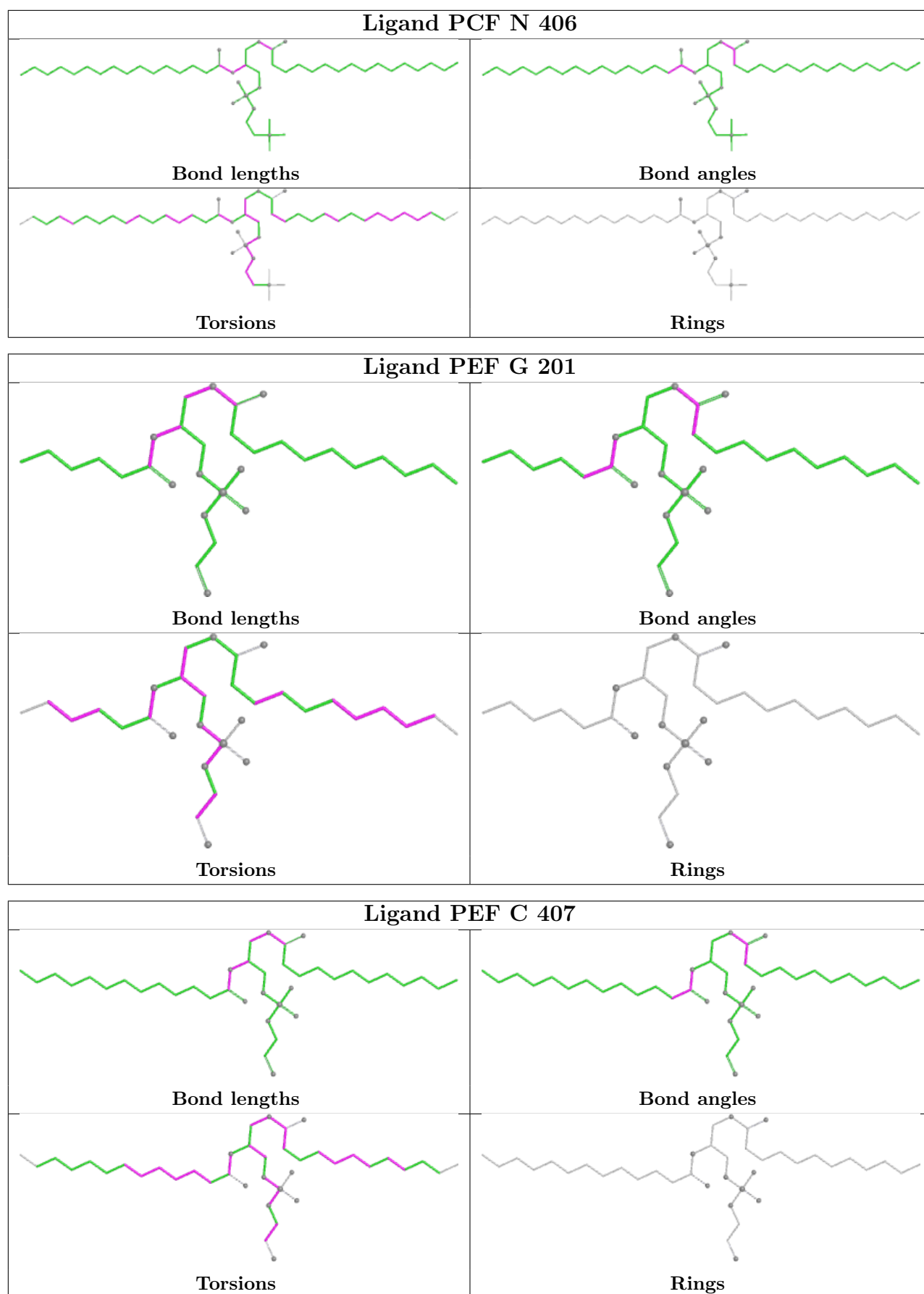


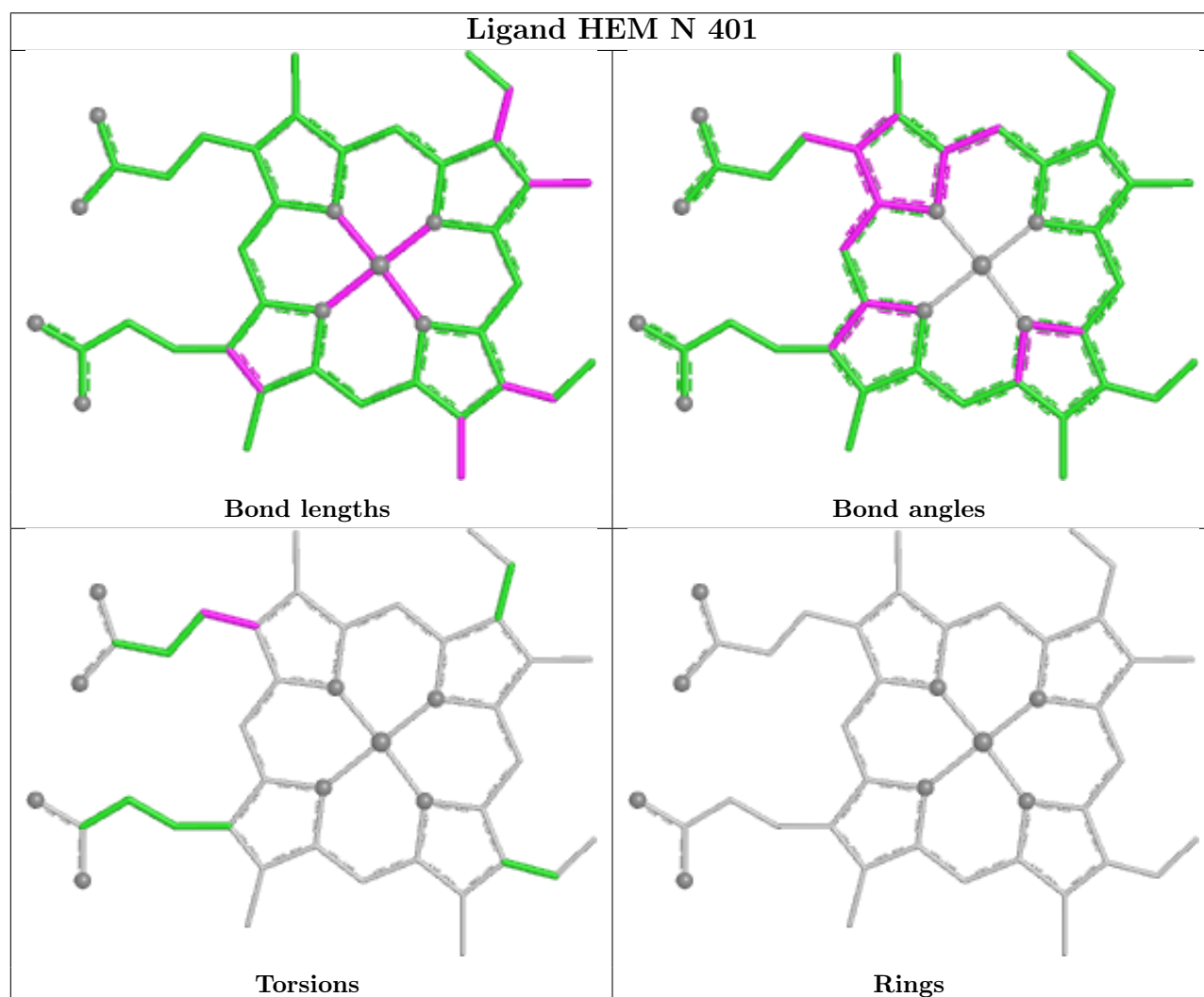
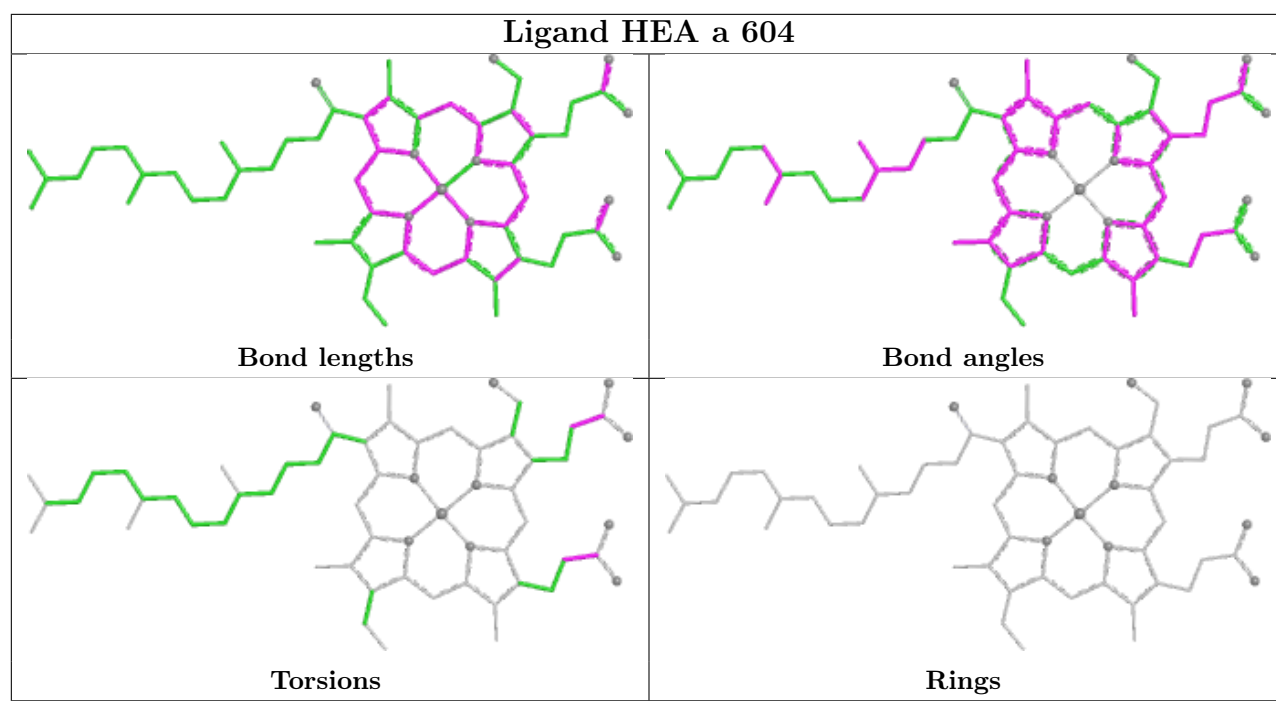


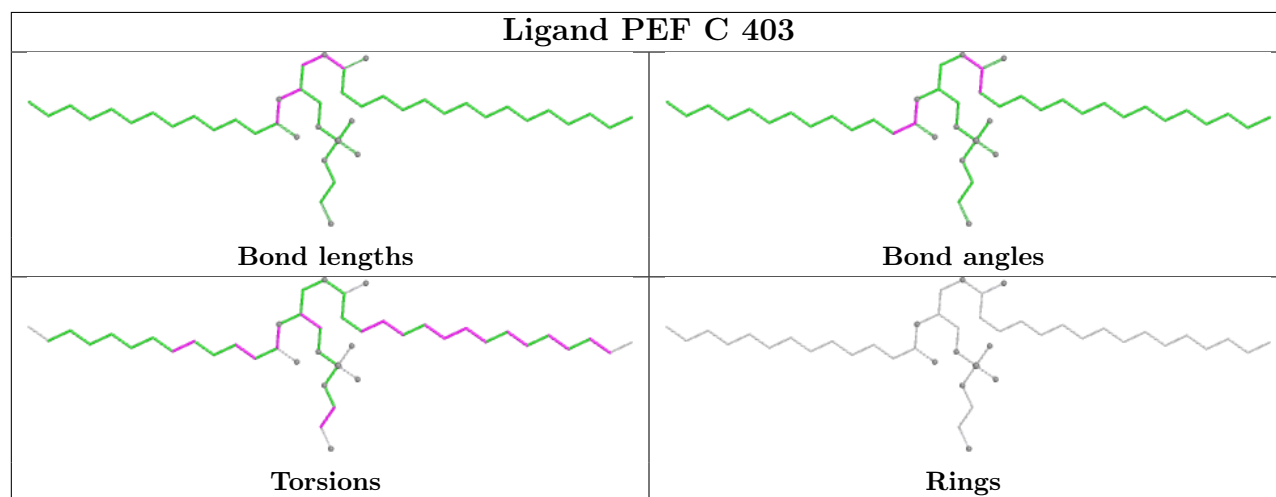
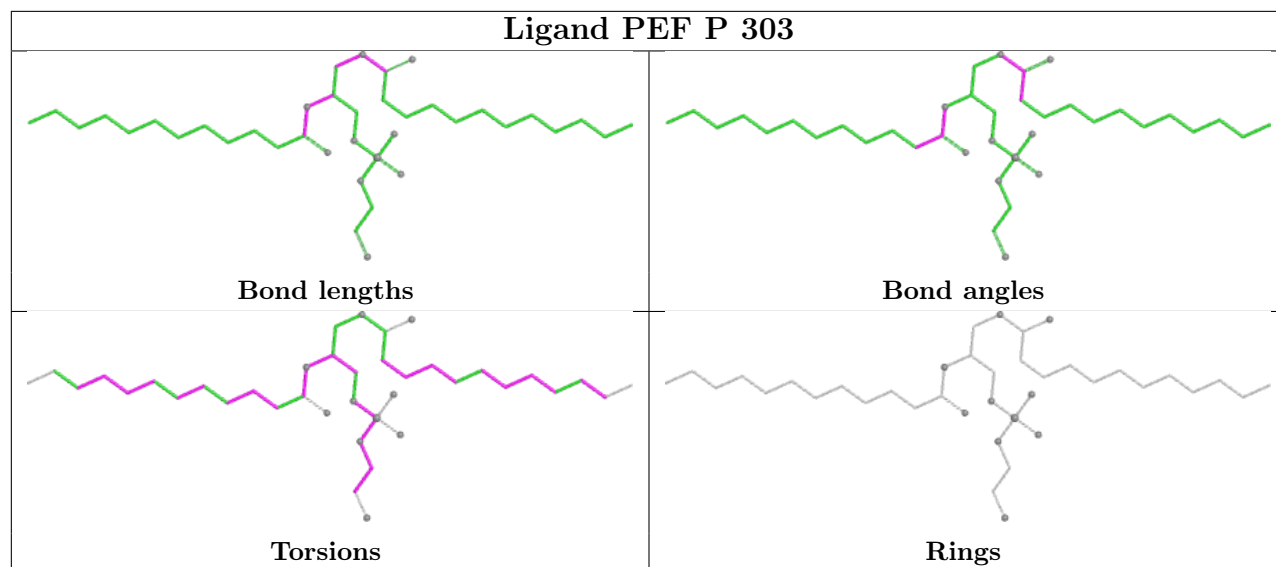


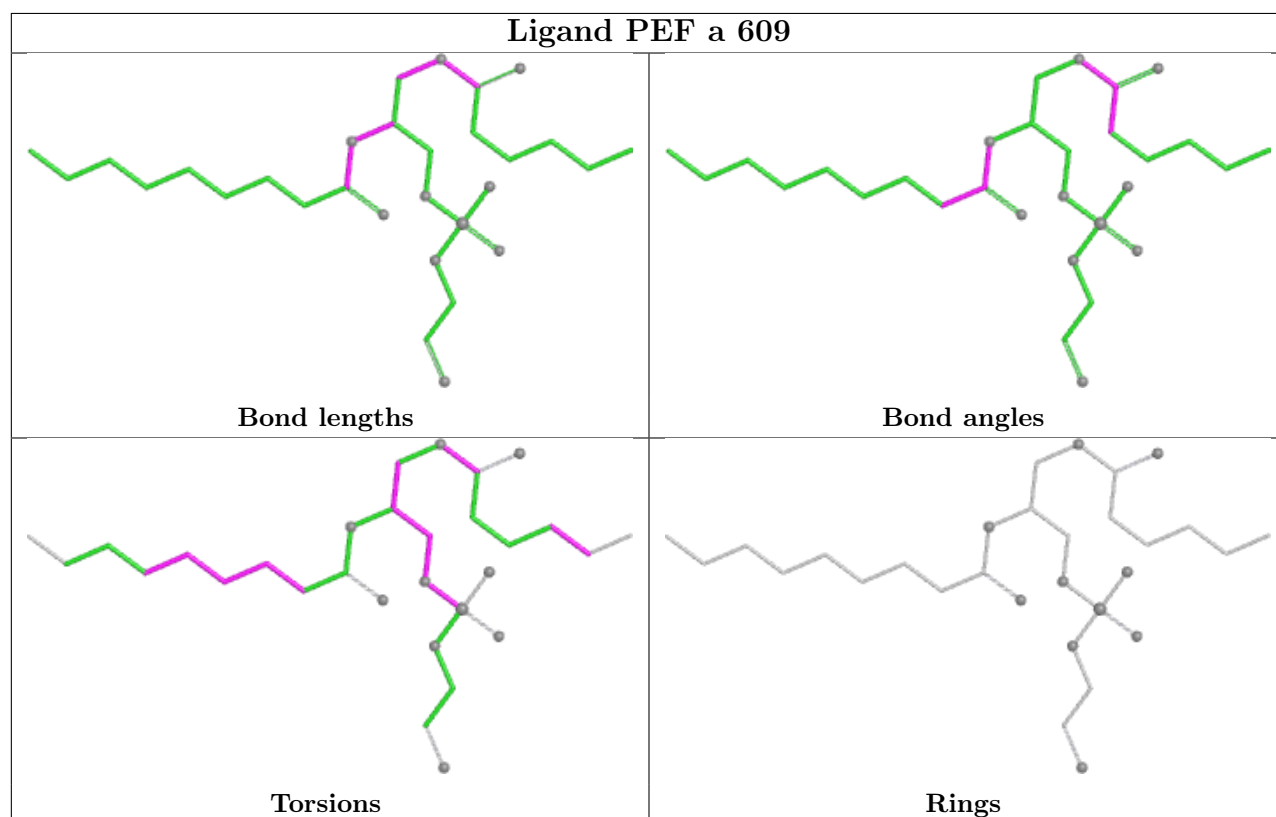
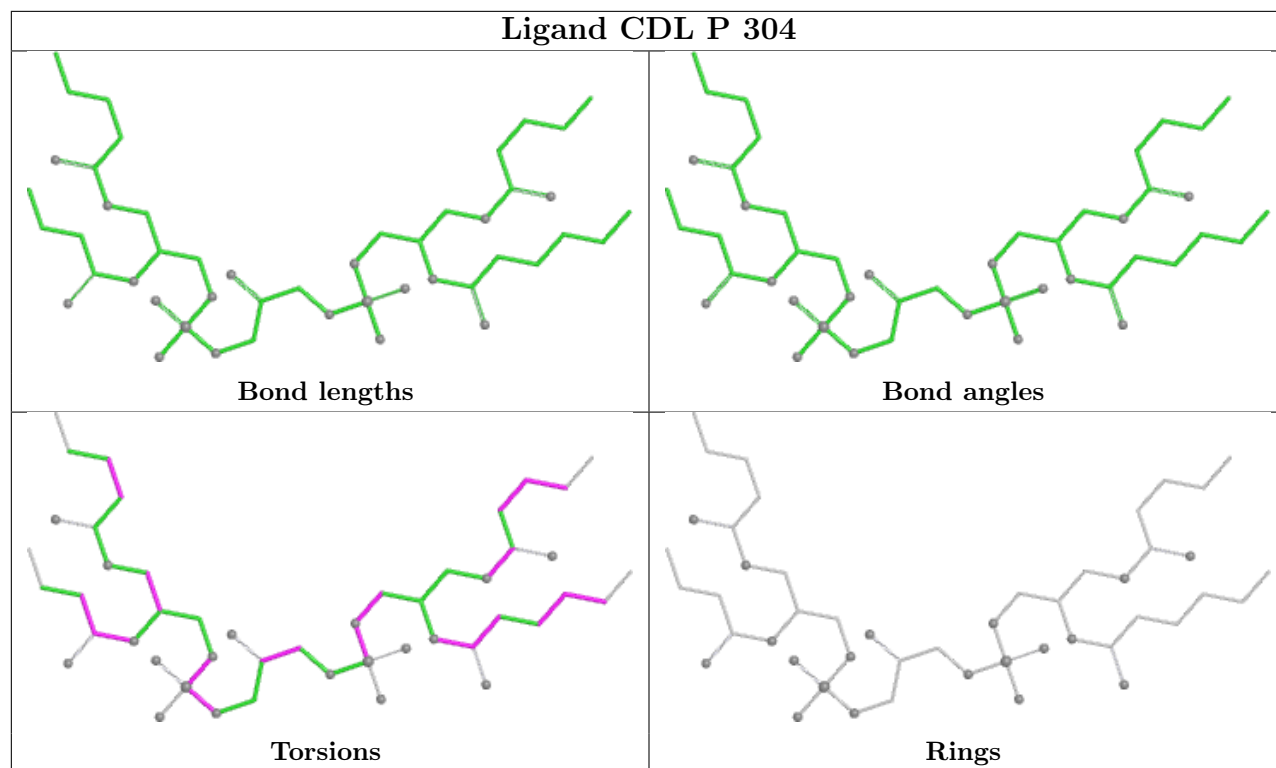


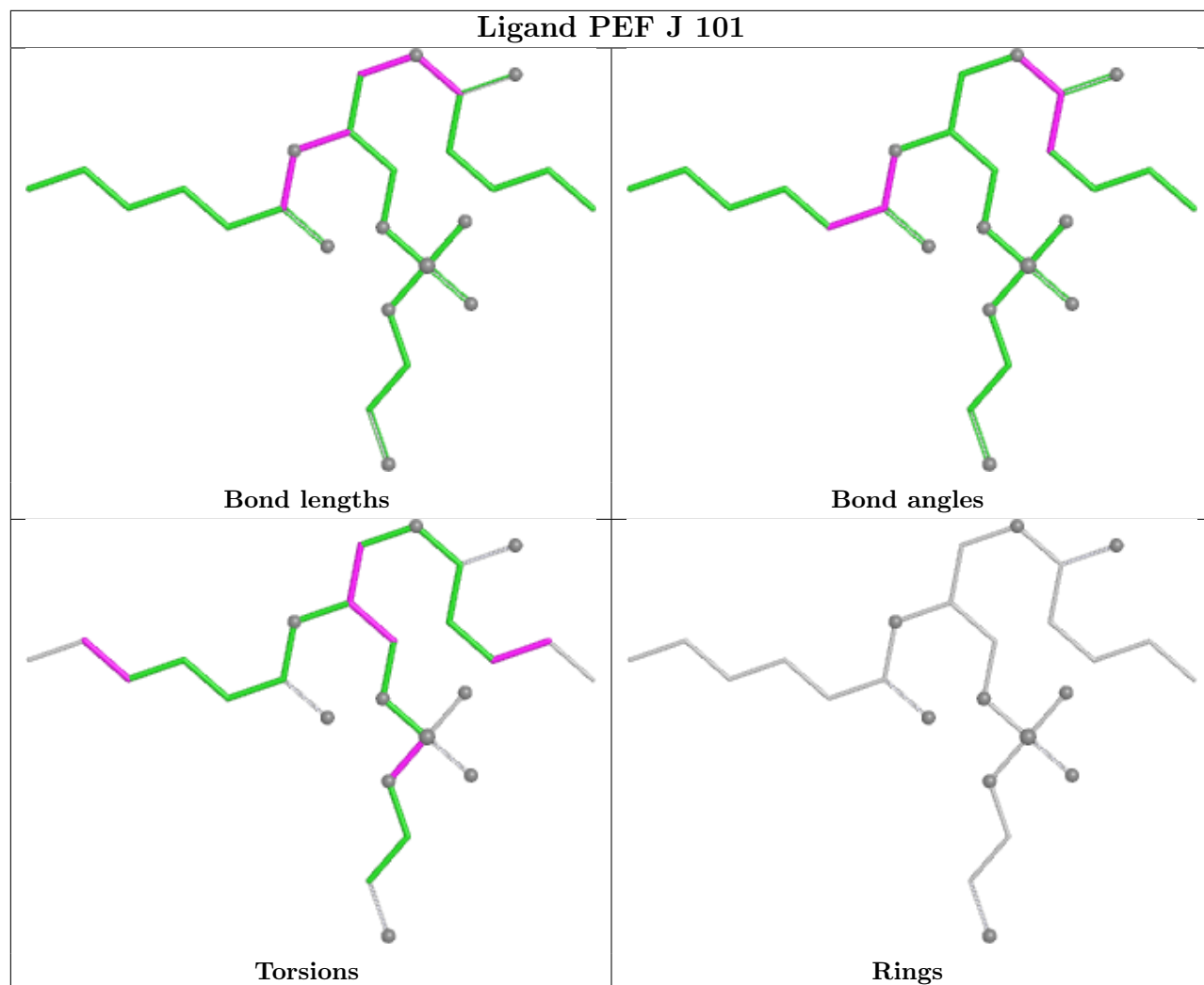


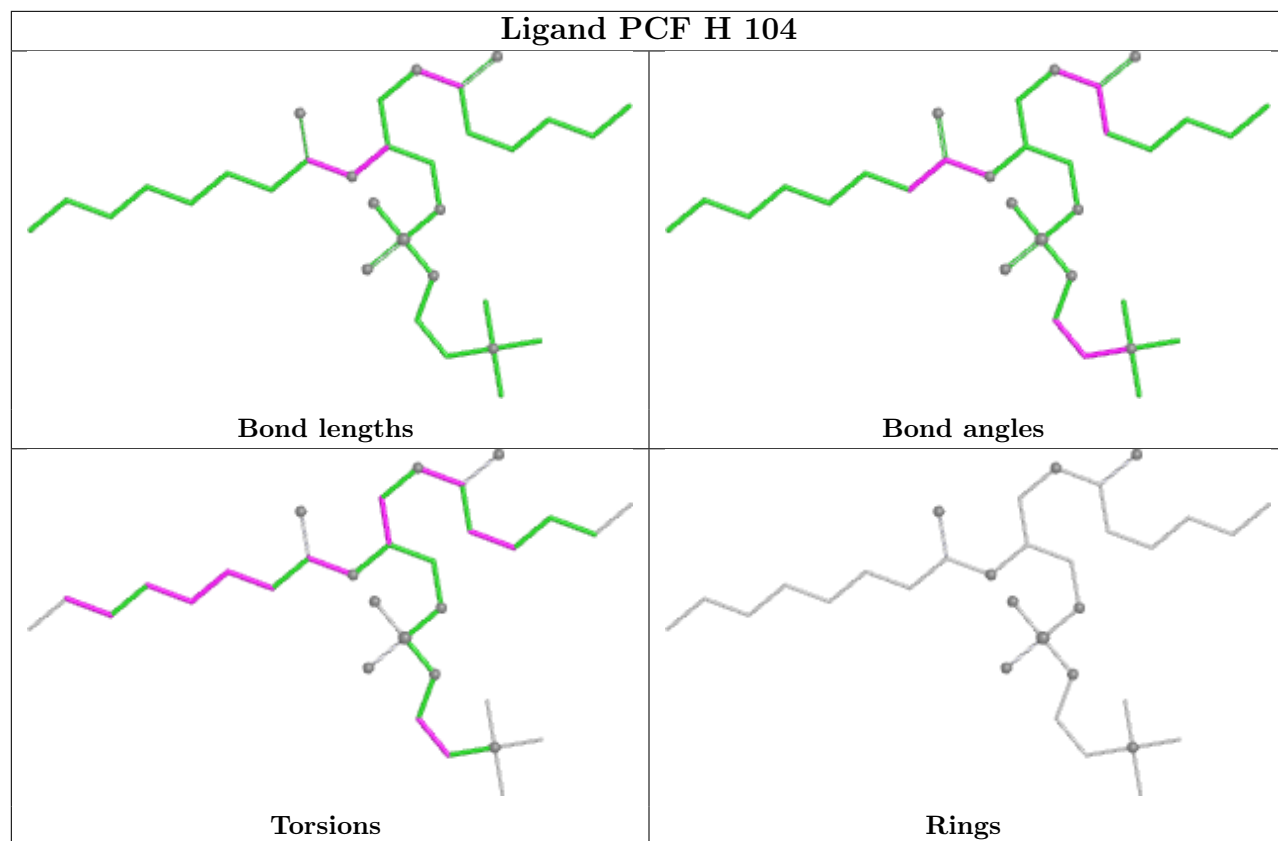


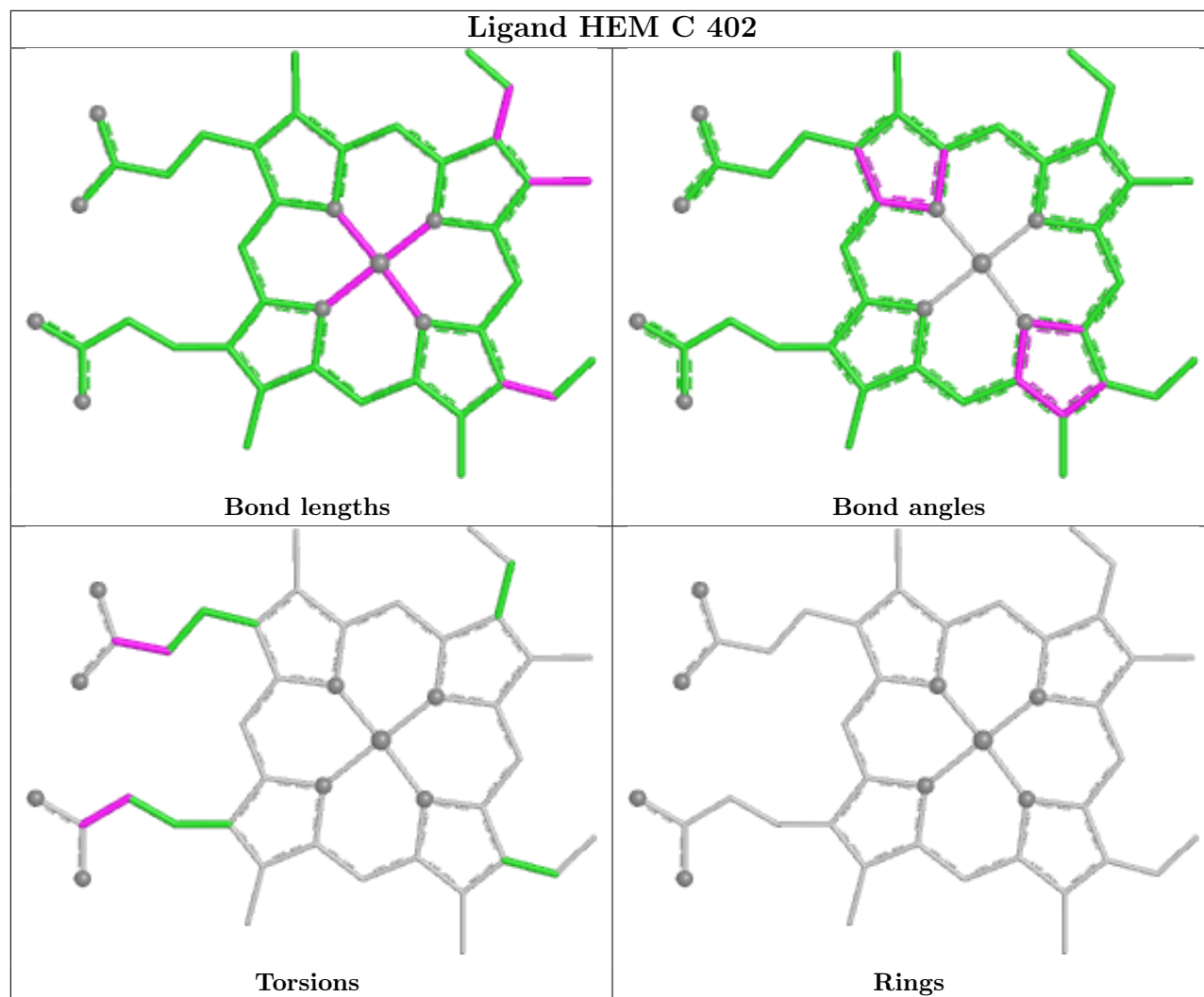












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

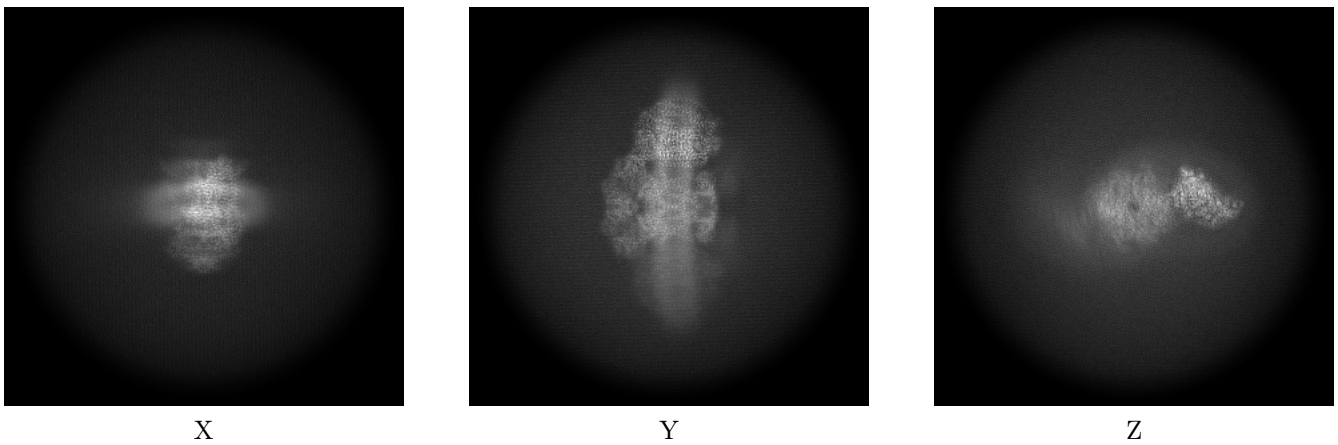
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19963. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

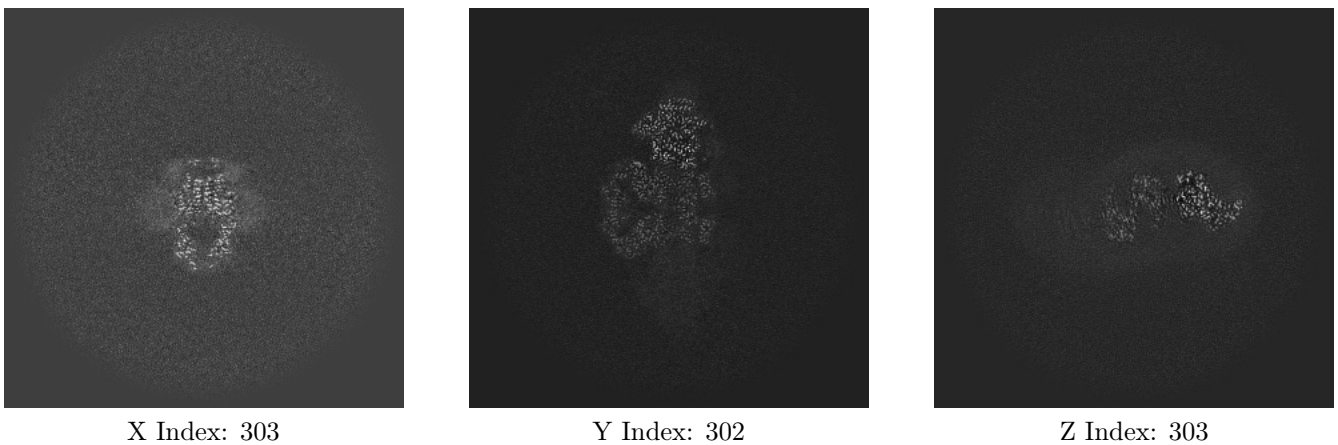
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

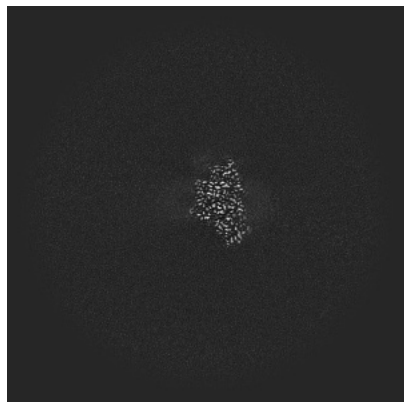
6.2.1 Primary map



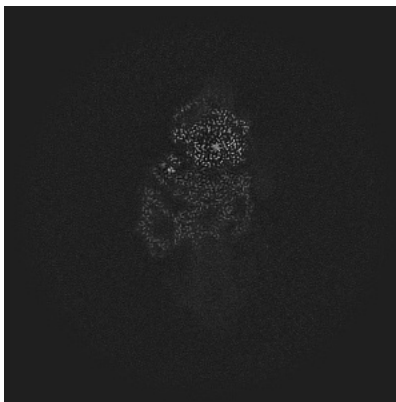
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

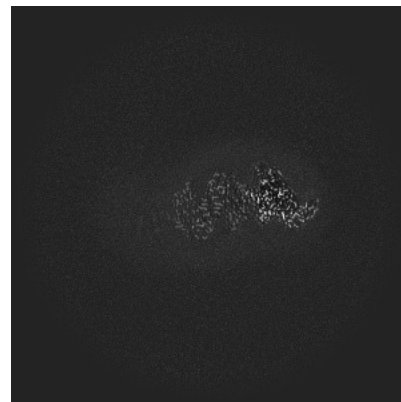
6.3.1 Primary map



X Index: 387



Y Index: 313

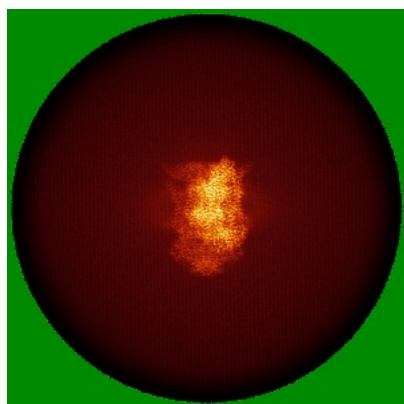


Z Index: 294

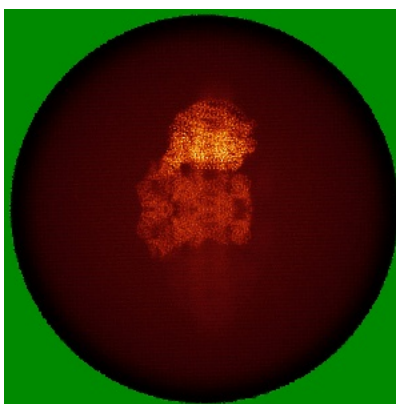
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

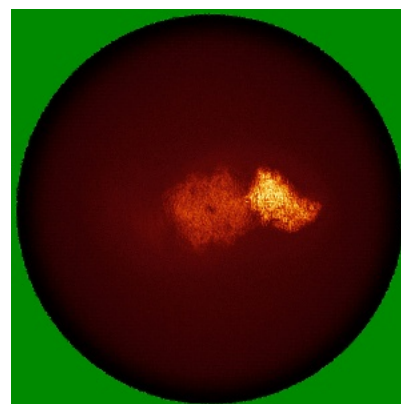
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

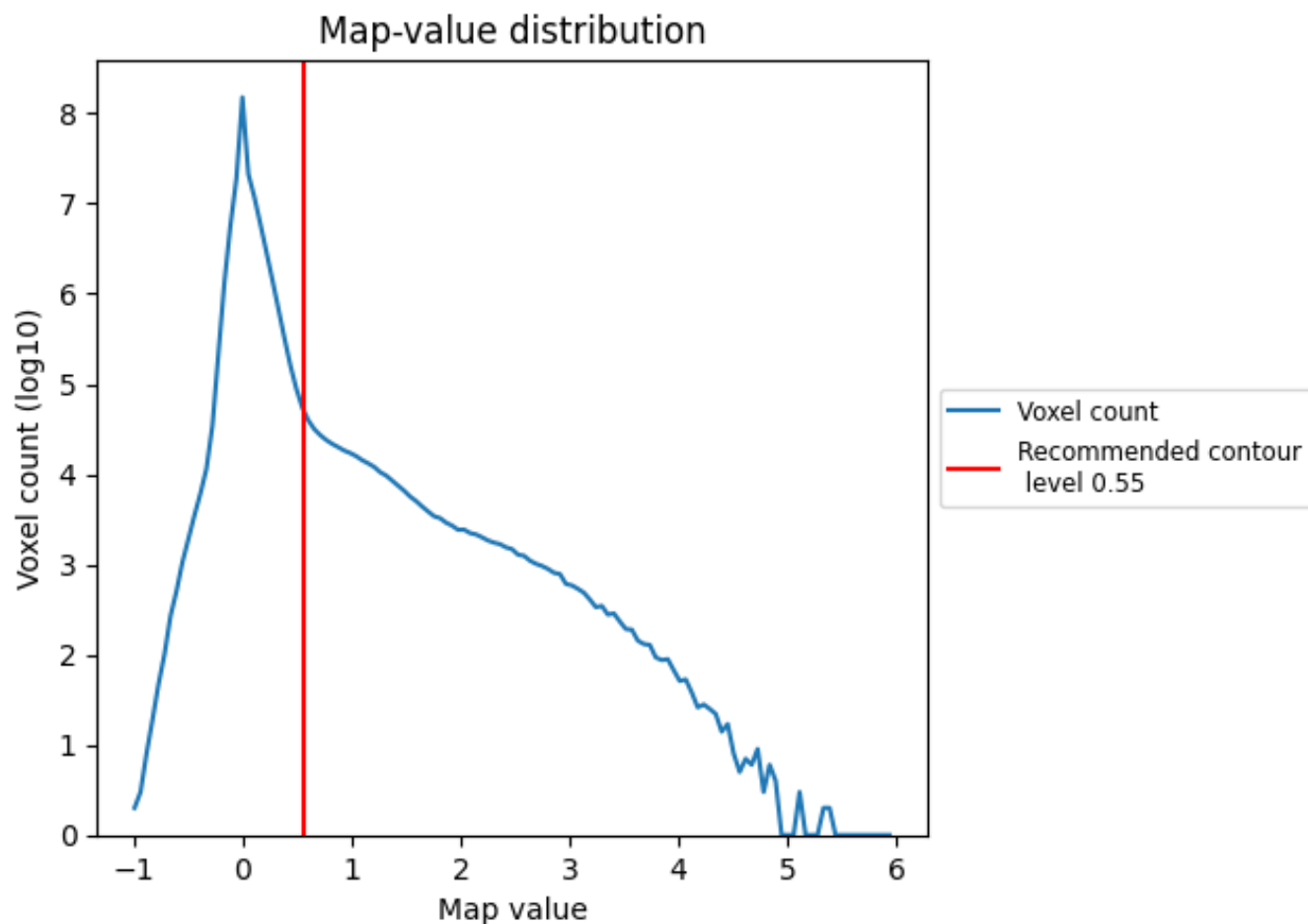
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

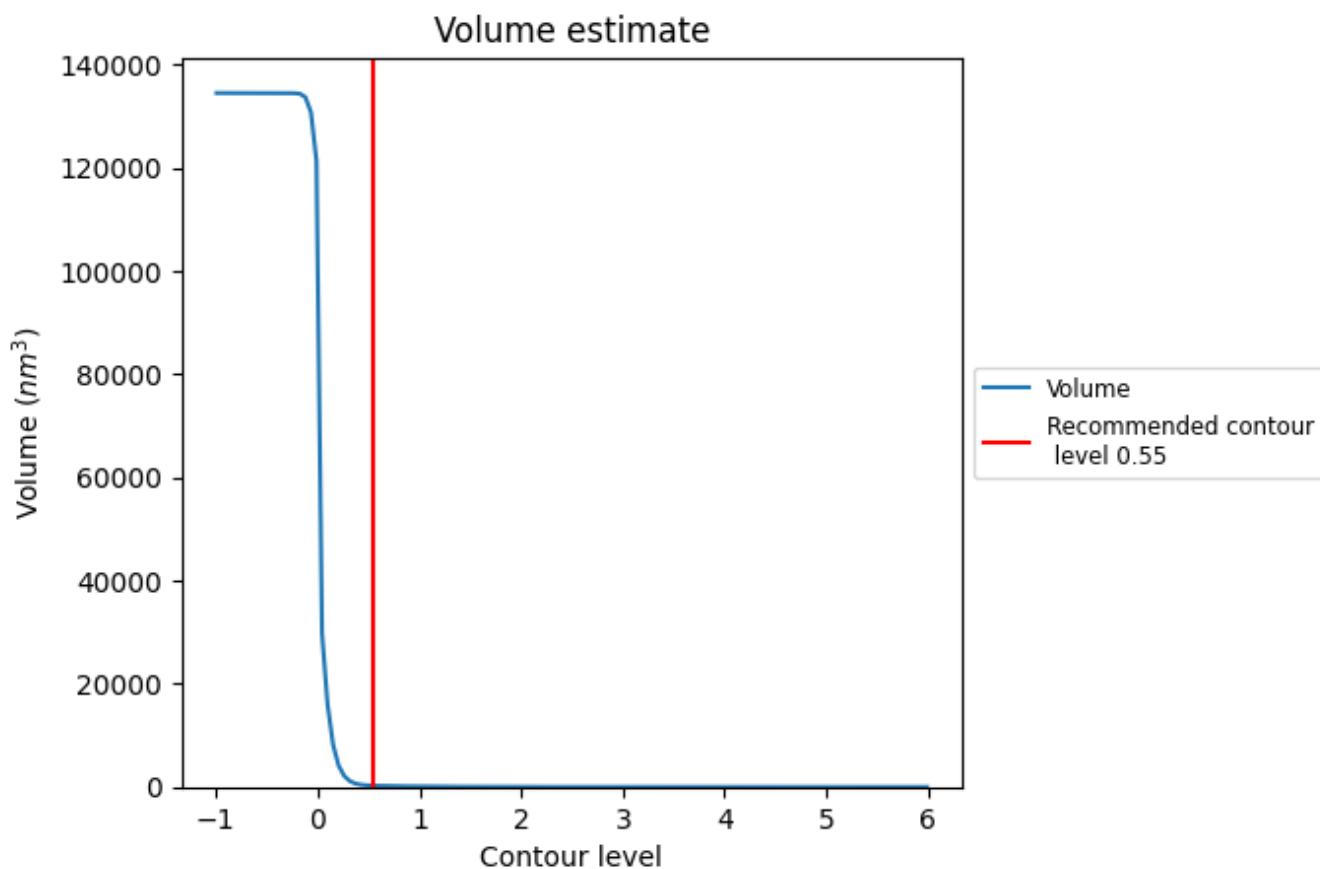
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 nm^3 ; this corresponds to an approximate mass of 227 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

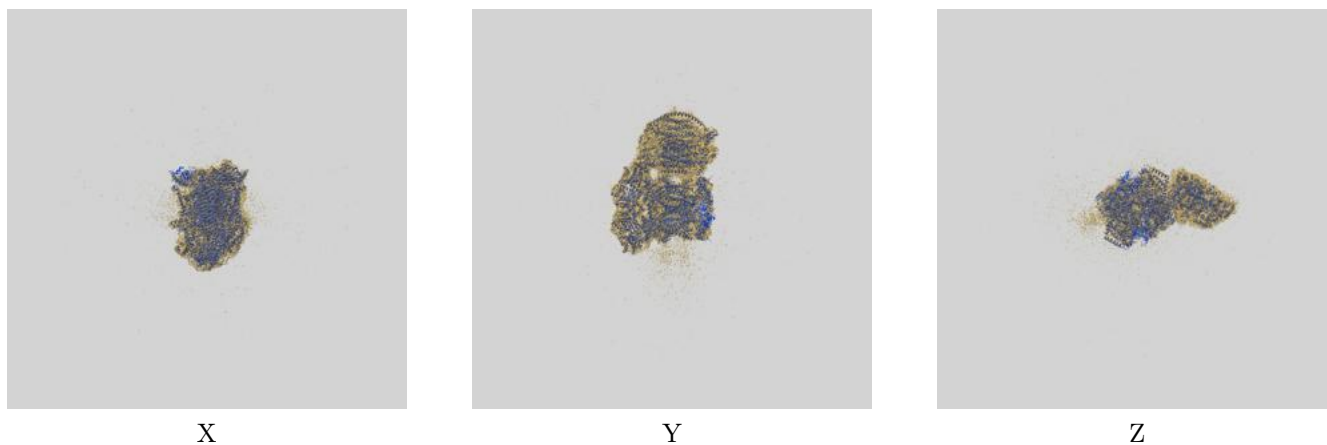
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

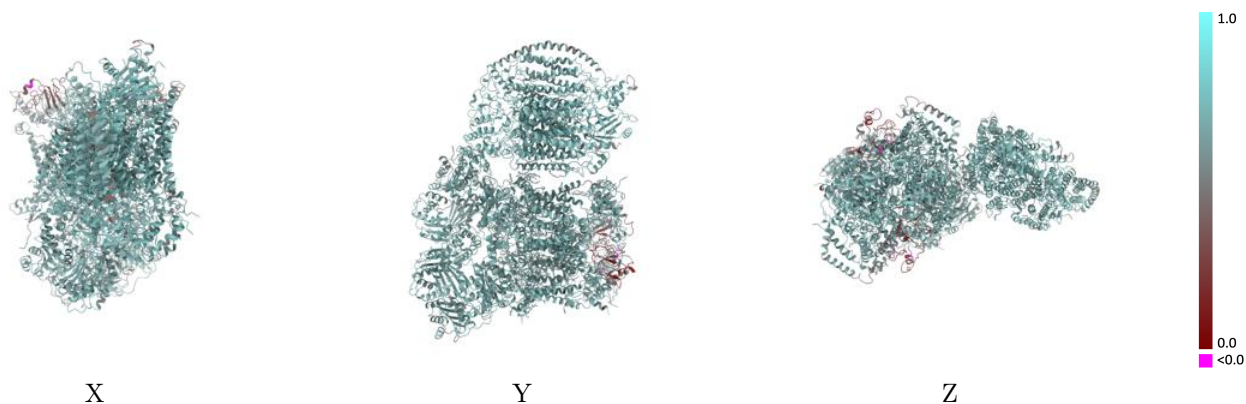
This section contains information regarding the fit between EMDB map EMD-19963 and PDB model 9ETZ. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

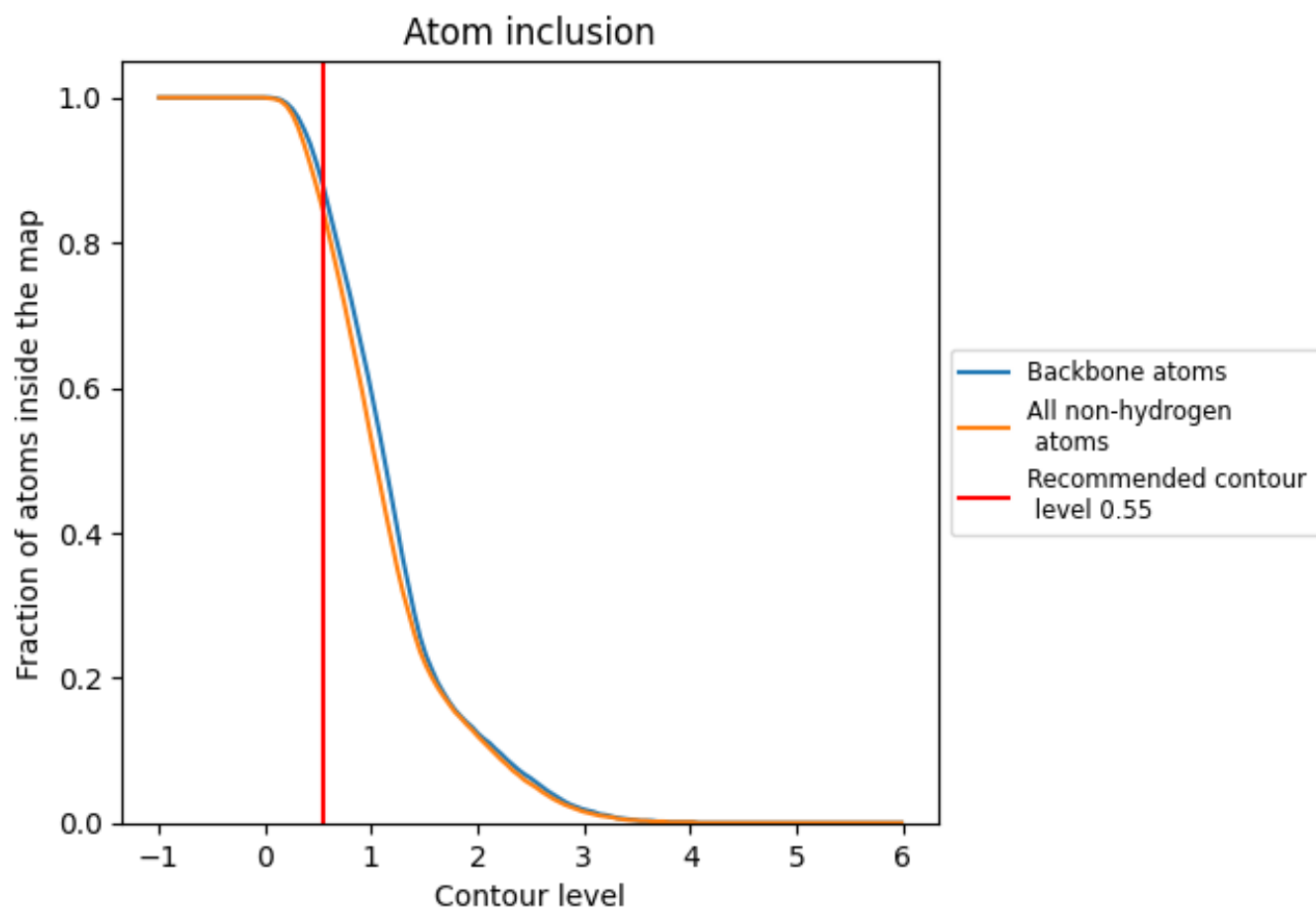


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.6390
A	 0.8520	 0.6480
B	 0.8340	 0.6430
C	 0.8950	 0.6620
D	 0.8780	 0.6470
E	 0.3550	 0.4380
F	 0.5750	 0.5590
G	 0.8510	 0.6460
H	 0.8130	 0.6340
I	 0.8380	 0.6410
J	 0.7160	 0.6240
L	 0.8330	 0.6470
M	 0.8340	 0.6430
N	 0.8920	 0.6650
O	 0.8790	 0.6590
P	 0.3340	 0.4320
Q	 0.5480	 0.5710
R	 0.8440	 0.6510
S	 0.7820	 0.6320
T	 0.8020	 0.6320
U	 0.6920	 0.6200
a	 0.9890	 0.6920
b	 0.9690	 0.6790
c	 0.9720	 0.6730
d	 0.9410	 0.6670
e	 0.9370	 0.6540
f	 0.9570	 0.6650
g	 0.9430	 0.6510
h	 0.9560	 0.6710
i	 0.9250	 0.6330
j	 0.8830	 0.6330
k	 0.8420	 0.6090
l	 0.9700	 0.6620

