



wwPDB EM Validation Summary Report ⓘ

Jun 29, 2025 – 05:06 am BST

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

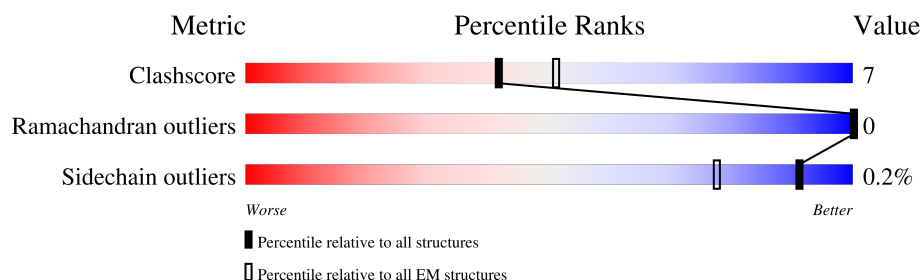
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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)
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 $\leq 5\%$. 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	
1	L	431	
2	B	352	
2	M	352	
3	C	385	
3	N	385	
4	D	247	
4	O	247	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
20	k	113	
21	l	45	
22	e	133	

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
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
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
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
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
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

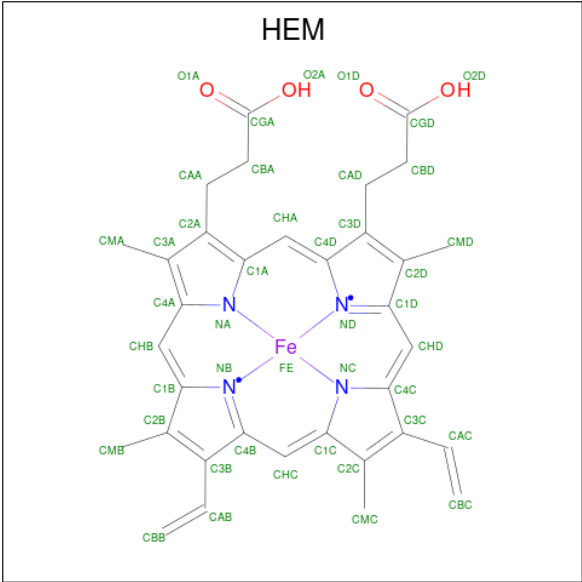
Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		

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



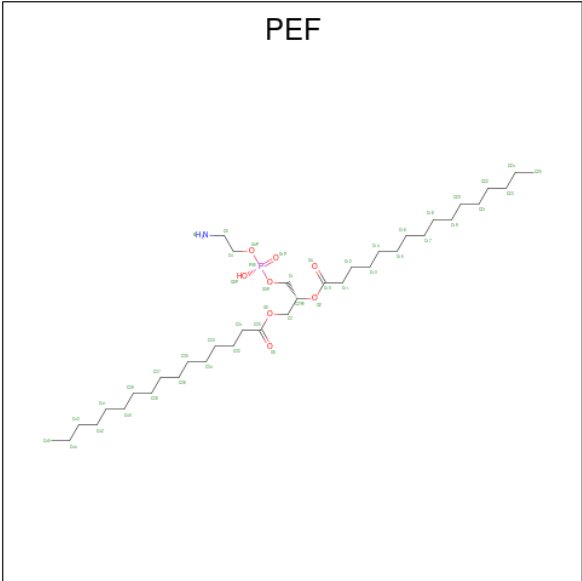
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			77	58	17	2	
23	A	1	Total	C	O	P	0
			54	35	17	2	
23	E	1	Total	C	O	P	0
			53	34	17	2	
23	H	1	Total	C	O	P	0
			66	47	17	2	
23	H	1	Total	C	O	P	0
			71	52	17	2	
23	L	1	Total	C	O	P	0
			55	36	17	2	
23	L	1	Total	C	O	P	0
			67	48	17	2	
23	N	1	Total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

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



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

- Molecule 25 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



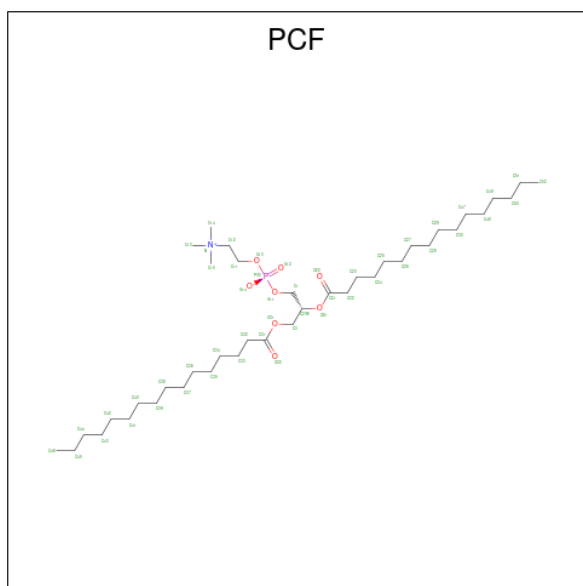
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 44	C 34	N 1	O 8	P 1	0
25	C	1	Total 47	C 37	N 1	O 8	P 1	0
25	C	1	Total 40	C 30	N 1	O 8	P 1	0
25	E	1	Total 42	C 32	N 1	O 8	P 1	0
25	G	1	Total 32	C 22	N 1	O 8	P 1	0
25	H	1	Total 34	C 24	N 1	O 8	P 1	0
25	J	1	Total 26	C 16	N 1	O 8	P 1	0
25	J	1	Total 29	C 19	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

Continued on next page...

Continued from previous page...

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

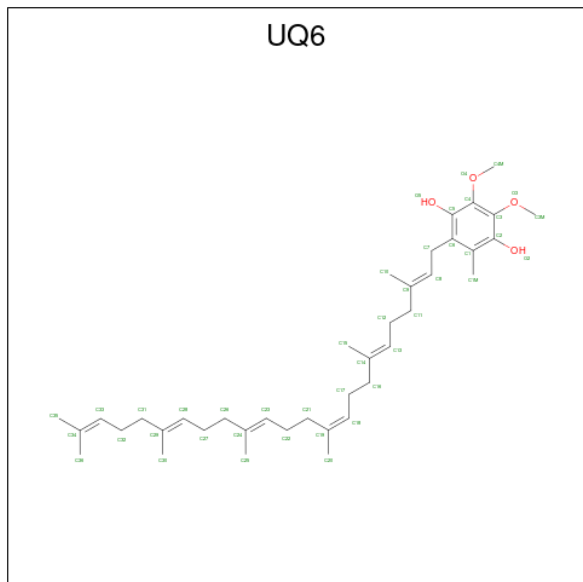
- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).



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

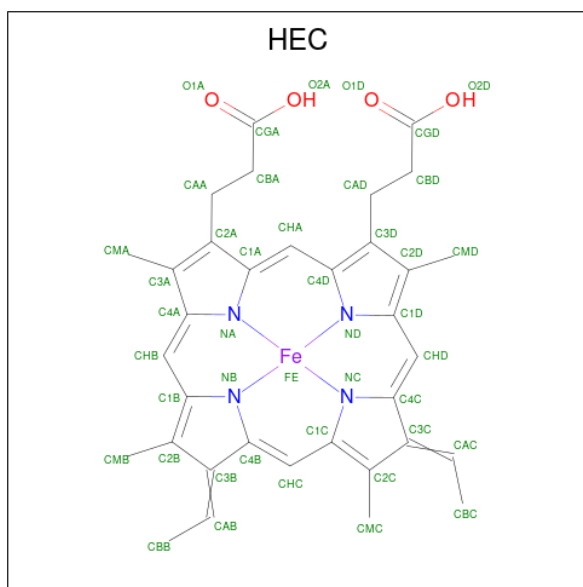
- Molecule 27 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA

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



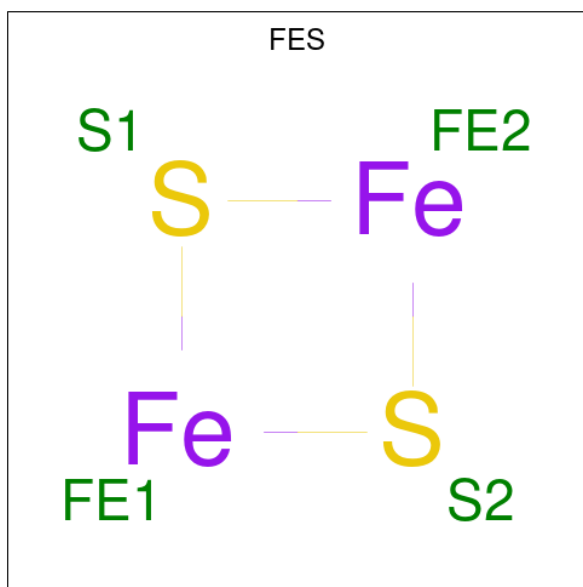
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	C	O	0
			43	39	4	
27	N	1	Total	C	O	0
			43	39	4	

- 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 43	C 34	Fe 1	N 4	O 4	0
28	O	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

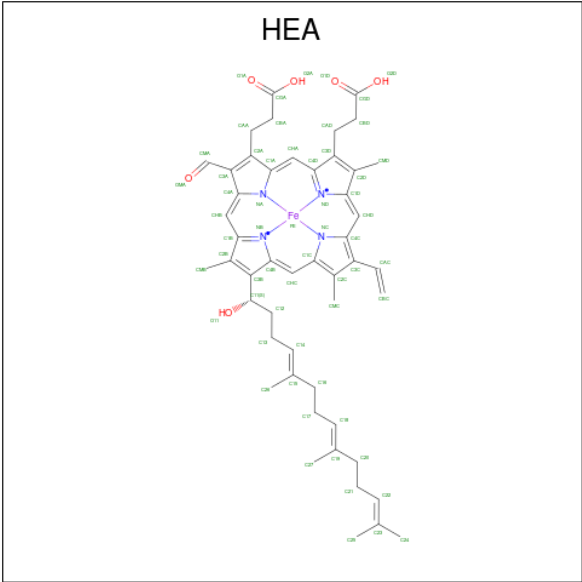


Mol	Chain	Residues	Atoms			AltConf
29	E	1	Total	Fe	S	0
			4	2	2	
29	P	1	Total	Fe	S	0
			4	2	2	

- 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: $\text{C}_{49}\text{H}_{56}\text{FeN}_4\text{O}_6$).



Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total 60	C 49	Fe 1	N 4	O 6	0
31	a	1	Total 60	C 49	Fe 1	N 4	O 6	0

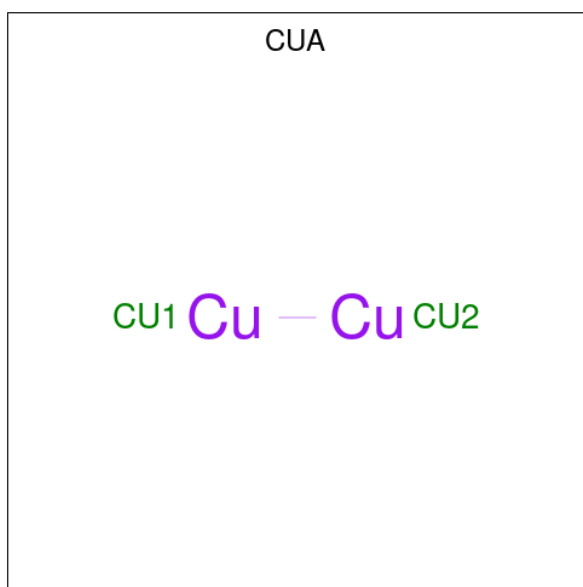
- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total	Ca	0
			1	1	

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	a	1	Total	Mg	0
			1	1	

- Molecule 34 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

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

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

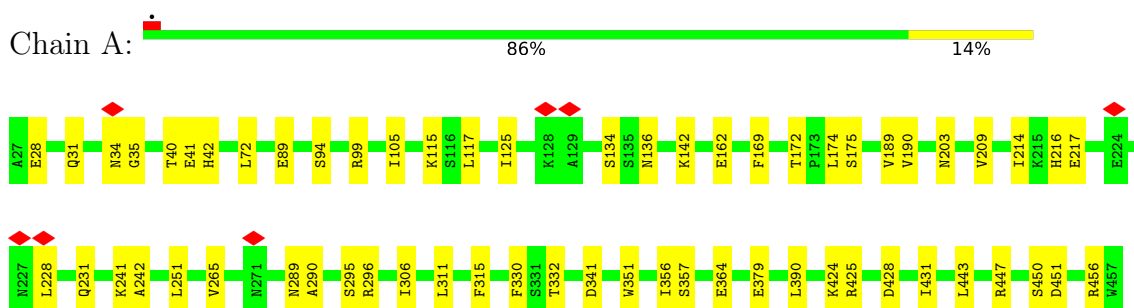
- Molecule 36 is water.

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

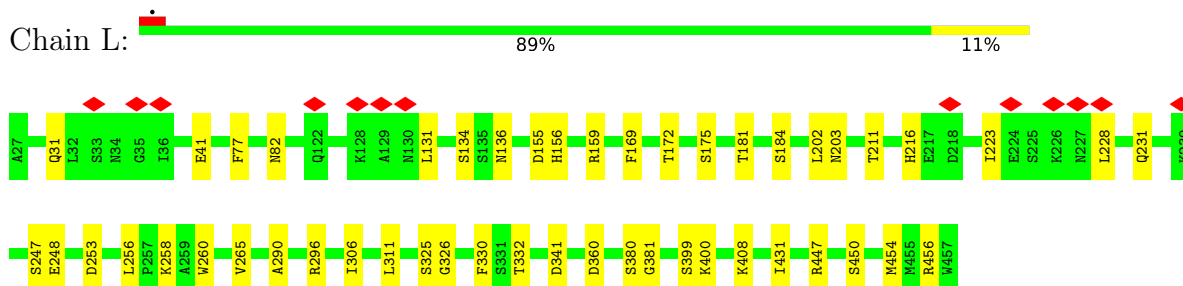
3 Residue-property plots

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.

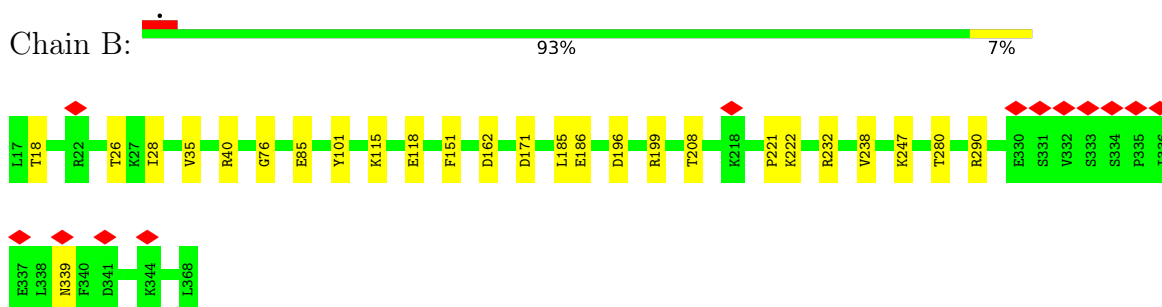
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



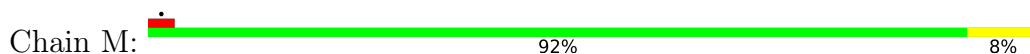
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

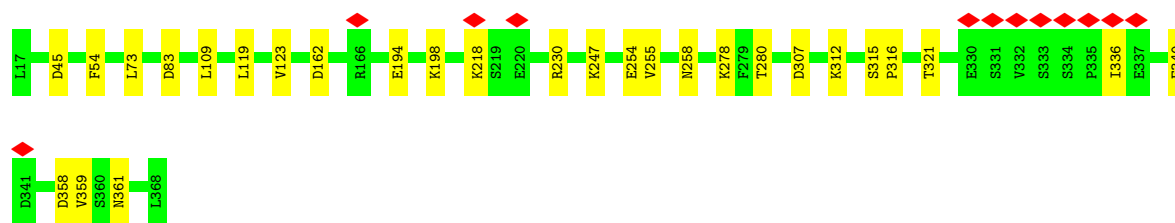


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

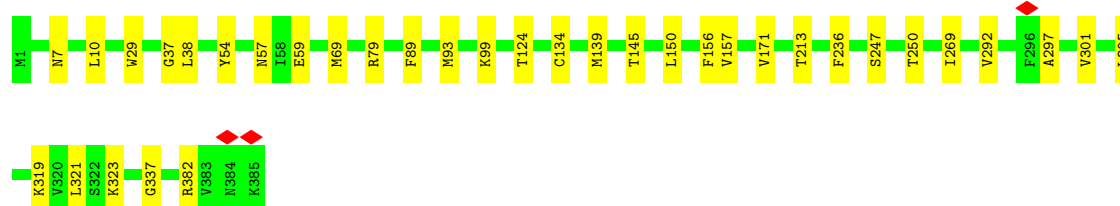


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

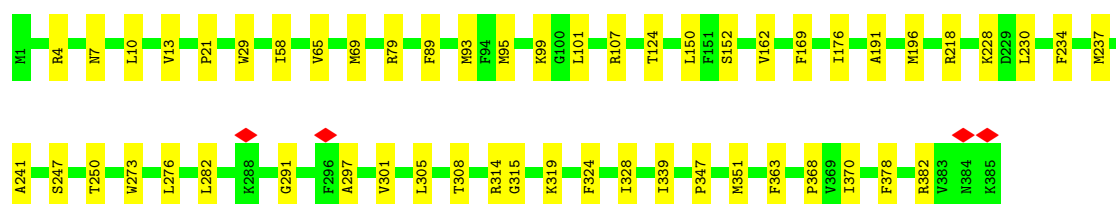
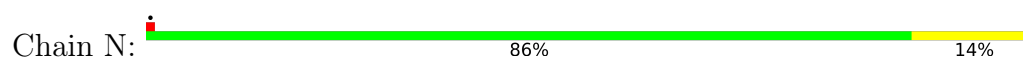




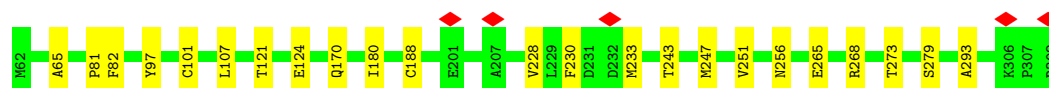
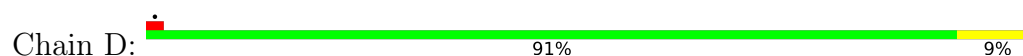
- Molecule 3: Cytochrome b



- Molecule 3: Cytochrome b



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

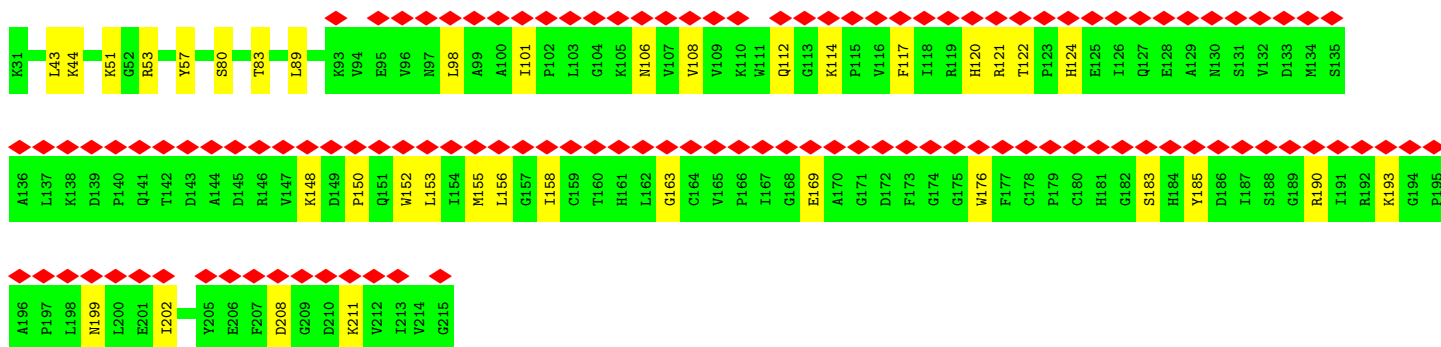


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

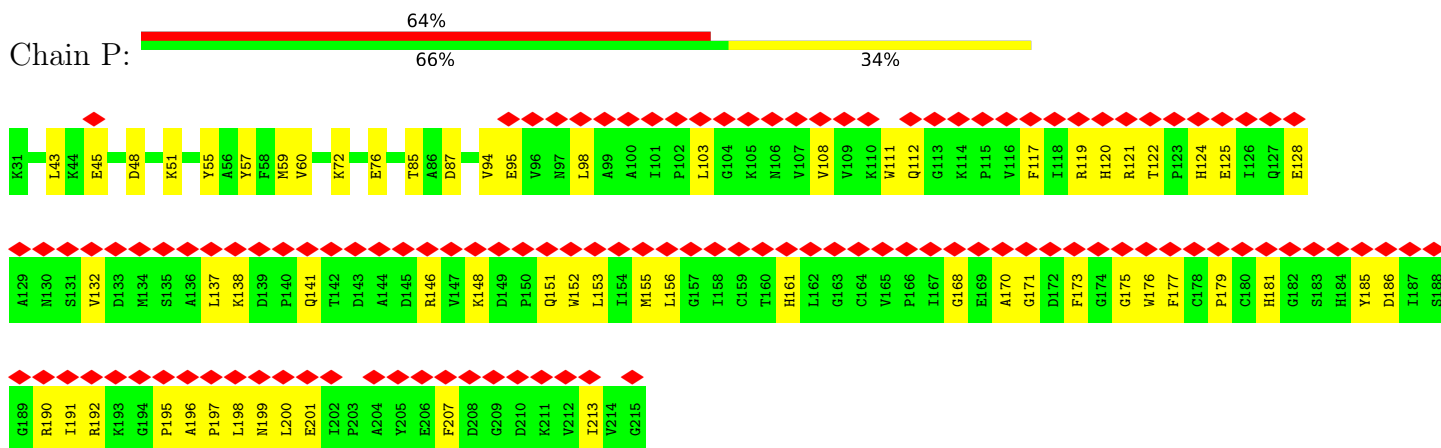


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

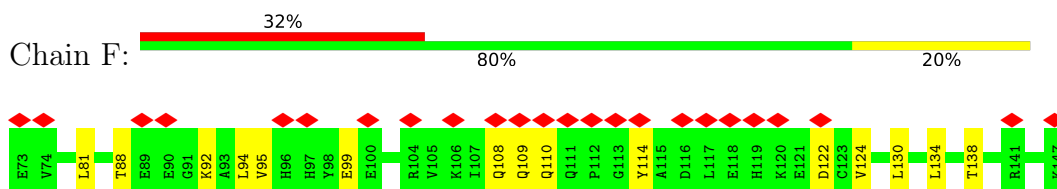




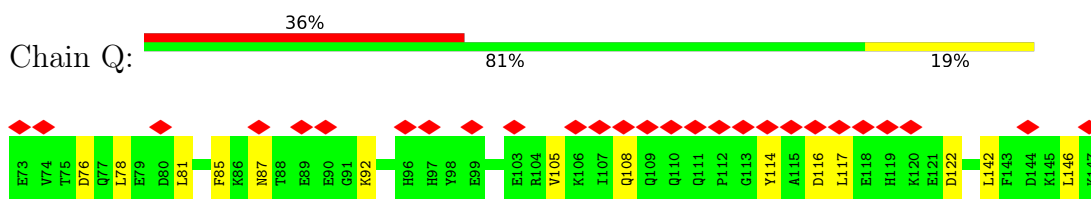
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



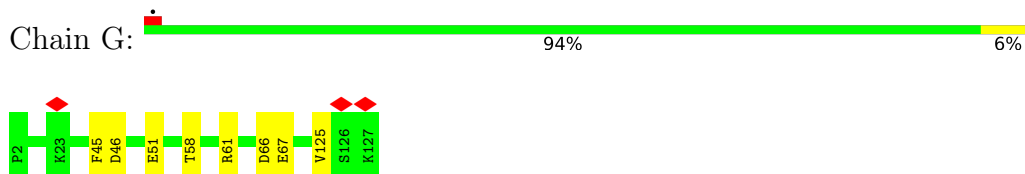
- Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



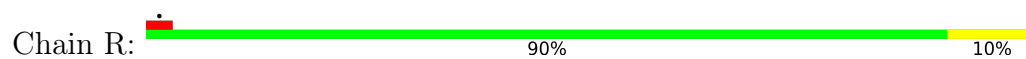
- Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



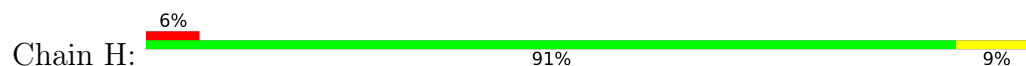
- Molecule 7: Cytochrome b-c1 complex subunit 7, mitochondrial



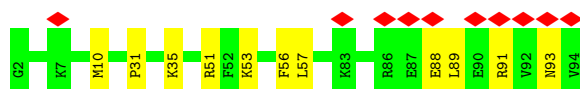
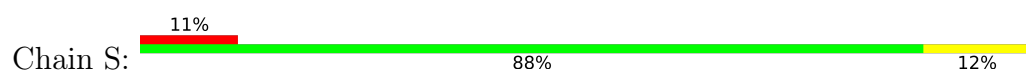
- Molecule 7: Cytochrome b-c1 complex subunit 7, mitochondrial



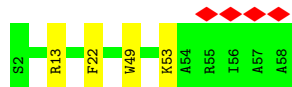
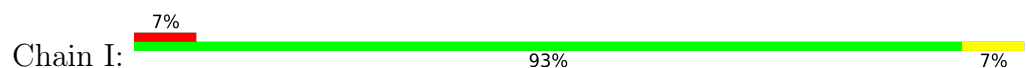
- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial



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



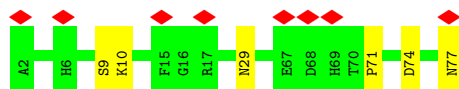
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



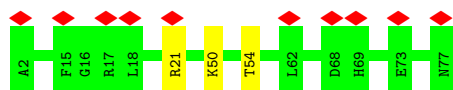
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



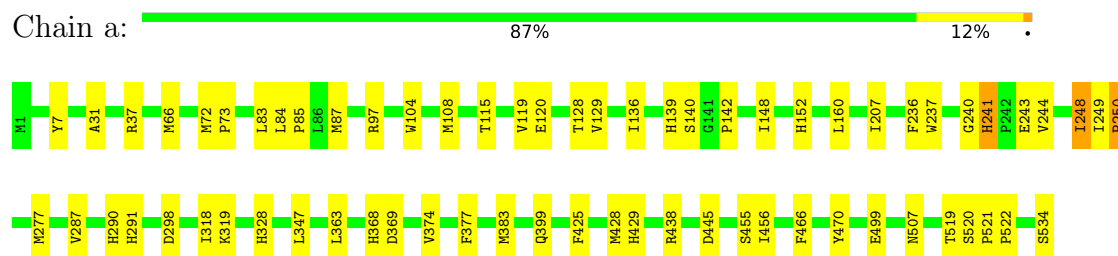
- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



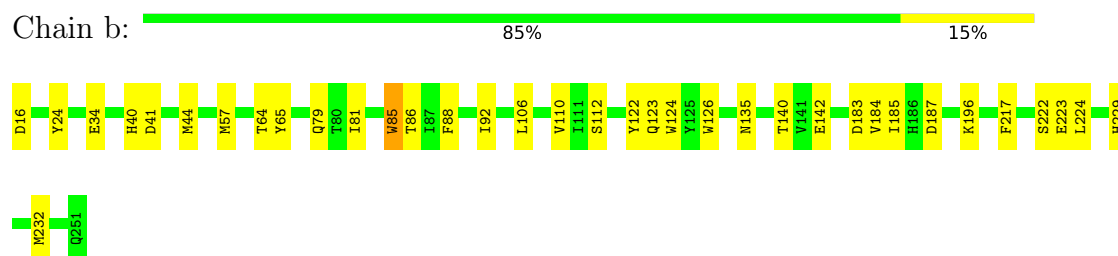
- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



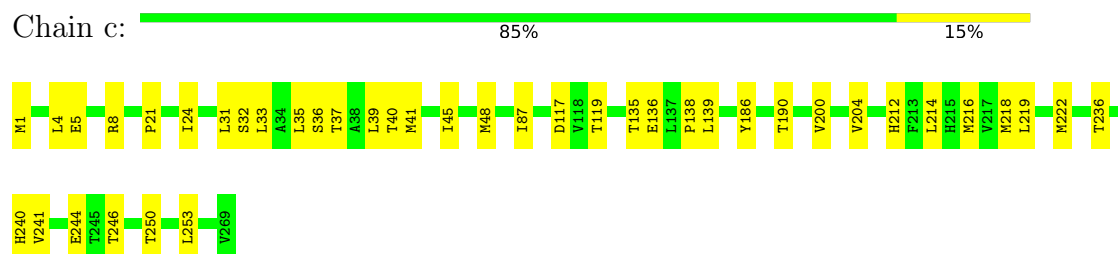
- Molecule 11: Cytochrome c oxidase subunit 1



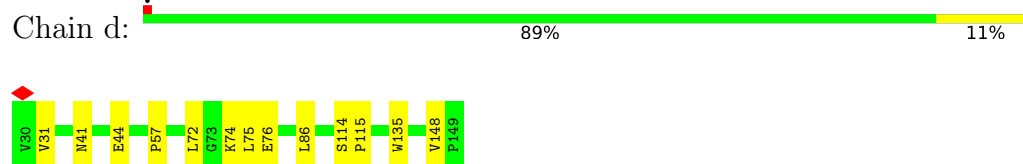
- Molecule 12: Cytochrome c oxidase subunit 2



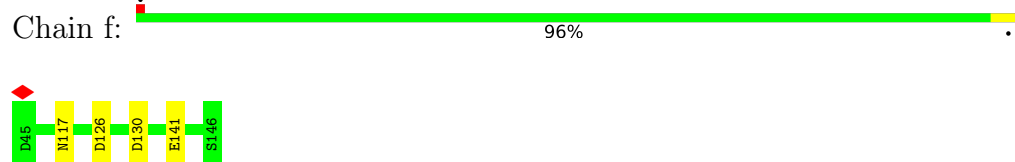
- Molecule 13: Cytochrome c oxidase subunit 3



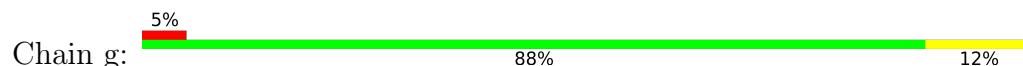
- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial



- Molecule 15: Cytochrome c oxidase subunit 6, mitochondrial

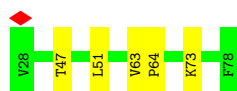


- Molecule 16: Cytochrome c oxidase subunit 7, mitochondrial





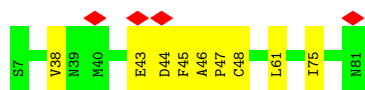
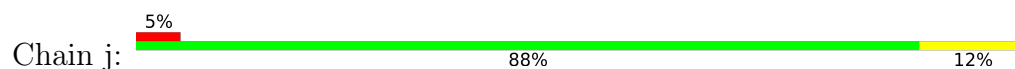
- Molecule 17: Cytochrome c oxidase subunit 8, mitochondrial



- Molecule 18: Cytochrome c oxidase subunit 9, mitochondrial



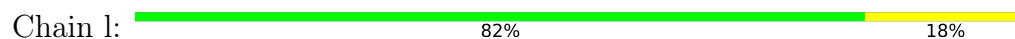
- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial



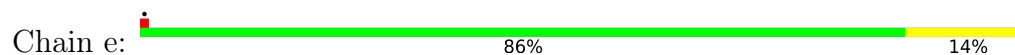
- Molecule 20: Cytochrome c oxidase subunit 13, mitochondrial



- 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 (Å)	512.9184, 511.22562, 512.9184	wwPDB
Map dimensions	606, 604, 606	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HEA, CA, CUA, PEF, ZN, MG, FES, PCF, UQ6, HEC, CDL, HEM

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	81	91
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%)	81	91
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

Continued on next page...

Continued from previous page...

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%)	81	91
12	b	209/209 (100%)	207 (99%)	2 (1%)	73	86
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%)	60	77
20	k	99/99 (100%)	98 (99%)	1 (1%)	73	86
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%)	91	97

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	P	46	ASN
11	a	404	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
25	PEF	P	301	-	42,42,46	0.93	4 (9%)	45,47,51	1.14	2 (4%)
23	CDL	H	102	-	70,70,99	0.39	0	76,82,111	0.23	0
25	PEF	h	101	-	46,46,46	0.89	3 (6%)	49,51,51	1.27	3 (6%)
23	CDL	A	502	-	53,53,99	0.44	0	59,65,111	0.25	0
25	PEF	l	101	-	46,46,46	0.89	3 (6%)	49,51,51	1.13	2 (4%)
25	PEF	N	408	-	31,31,46	1.08	4 (12%)	34,36,51	1.14	2 (5%)
25	PEF	S	102	-	35,35,46	1.02	4 (11%)	38,40,51	1.11	2 (5%)
25	PEF	E	302	-	41,41,46	0.94	4 (9%)	44,46,51	1.13	2 (4%)
25	PEF	a	607	-	39,39,46	0.96	3 (7%)	42,44,51	1.11	2 (4%)
34	CUA	b	301	12	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	HEM	N	402	3	41,50,50	1.45	3 (7%)	45,82,82	1.33	6 (13%)
25	PEF	J	101	-	25,25,46	1.19	4 (16%)	28,30,51	1.17	2 (7%)
25	PEF	a	601	-	39,39,46	0.95	4 (10%)	42,44,51	1.20	3 (7%)
25	PEF	e	201	-	46,46,46	0.89	4 (8%)	49,51,51	1.09	2 (4%)
28	HEC	D	401	4	32,50,50	2.16	3 (9%)	24,82,82	1.76	7 (29%)
26	PCF	H	104	-	31,31,49	1.32	3 (9%)	37,39,57	1.14	2 (5%)
25	PEF	H	103	-	33,33,46	1.06	3 (9%)	36,38,51	1.05	2 (5%)
23	CDL	L	501	-	54,54,99	0.43	0	60,66,111	0.26	0
28	HEC	O	401	4	32,50,50	2.24	3 (9%)	24,82,82	1.48	4 (16%)
23	CDL	S	101	-	74,74,99	0.37	0	80,86,111	0.21	0
23	CDL	N	403	-	52,52,99	0.45	0	58,64,111	0.28	0
25	PEF	C	407	-	39,39,46	0.96	4 (10%)	42,44,51	1.12	2 (4%)
25	PEF	b	303	-	46,46,46	0.88	4 (8%)	49,51,51	1.11	2 (4%)
26	PCF	I	101	-	29,29,49	1.38	4 (13%)	35,37,57	1.07	2 (5%)
24	HEM	N	401	3	41,50,50	1.48	3 (7%)	45,82,82	1.65	9 (20%)
24	HEM	C	402	3	41,50,50	1.44	3 (7%)	45,82,82	1.35	7 (15%)
23	CDL	P	304	-	47,47,99	0.44	0	53,59,111	0.30	0
25	PEF	P	303	-	38,38,46	0.96	4 (10%)	41,43,51	1.03	2 (4%)
25	PEF	J	102	-	28,28,46	1.13	4 (14%)	31,33,51	1.20	2 (6%)
25	PEF	N	405	-	42,42,46	0.92	3 (7%)	45,47,51	1.10	2 (4%)
25	PEF	b	302	-	39,39,46	0.97	4 (10%)	42,44,51	1.19	2 (4%)
31	HEA	a	603	11	57,67,67	1.32	8 (14%)	61,103,103	1.67	15 (24%)
25	PEF	C	403	-	43,43,46	0.91	4 (9%)	46,48,51	1.15	2 (4%)
25	PEF	C	404	-	46,46,46	0.89	4 (8%)	49,51,51	1.13	2 (4%)
27	UQ6	C	406	-	43,43,43	0.34	0	51,55,55	1.17	3 (5%)
31	HEA	a	604	11	57,67,67	2.01	16 (28%)	61,103,103	2.54	24 (39%)
25	PEF	U	101	-	36,36,46	1.00	3 (8%)	39,41,51	1.15	3 (7%)
23	CDL	E	303	-	52,52,99	0.44	0	58,64,111	0.29	0
26	PCF	T	101	-	46,46,49	1.12	3 (6%)	52,54,57	1.05	3 (5%)
24	HEM	C	401	3	41,50,50	1.50	5 (12%)	45,82,82	1.73	10 (22%)
25	PEF	a	608	-	46,46,46	0.93	3 (6%)	49,51,51	1.12	2 (4%)
26	PCF	e	202	-	49,49,49	1.10	3 (6%)	55,57,57	1.03	4 (7%)
23	CDL	H	101	-	65,65,99	0.42	0	71,77,111	0.26	0
23	CDL	A	501	-	76,76,99	0.38	0	82,88,111	0.27	0
26	PCF	N	406	-	49,49,49	1.08	3 (6%)	55,57,57	1.05	2 (3%)
23	CDL	L	502	-	66,66,99	0.39	0	72,78,111	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEF	G	201	-	31,31,46	1.07	4 (12%)	34,36,51	1.19	2 (5%)
26	PCF	C	405	-	38,38,49	1.21	3 (7%)	44,46,57	1.13	2 (4%)
25	PEF	c	301	-	46,46,46	0.91	3 (6%)	49,51,51	1.23	4 (8%)
25	PEF	a	609	-	29,29,46	1.12	4 (13%)	32,34,51	1.21	2 (6%)
29	FES	P	302	5	0,4,4	-	-	-	-	-
29	FES	E	301	5	0,4,4	-	-	-	-	-
25	PEF	N	404	-	39,39,46	0.96	4 (10%)	42,44,51	1.21	2 (4%)
27	UQ6	N	407	-	43,43,43	0.33	0	51,55,55	0.61	1 (1%)
25	PEF	c	302	-	46,46,46	0.89	3 (6%)	49,51,51	1.15	2 (4%)
23	CDL	c	303	-	85,85,99	0.40	0	91,97,111	0.24	0

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
25	PEF	P	301	-	-	21/46/46/50	-
23	CDL	H	102	-	-	33/81/81/110	-
25	PEF	h	101	-	-	25/50/50/50	-
23	CDL	A	502	-	-	28/64/64/110	-
25	PEF	l	101	-	-	19/50/50/50	-
25	PEF	N	408	-	-	14/35/35/50	-
25	PEF	S	102	-	-	16/39/39/50	-
25	PEF	E	302	-	-	15/45/45/50	-
25	PEF	a	607	-	-	21/43/43/50	-
24	HEM	N	402	3	-	2/12/54/54	-
25	PEF	J	101	-	-	8/29/29/50	-
25	PEF	a	601	-	-	18/43/43/50	-
25	PEF	e	201	-	-	23/50/50/50	-
28	HEC	D	401	4	-	2/10/54/54	-
26	PCF	H	104	-	-	13/35/35/53	-
25	PEF	H	103	-	-	15/37/37/50	-
23	CDL	L	501	-	-	42/64/64/110	-
28	HEC	O	401	4	-	0/10/54/54	-
23	CDL	S	101	-	-	48/85/85/110	-
23	CDL	N	403	-	-	33/63/63/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEF	C	407	-	-	23/43/43/50	-
25	PEF	b	303	-	-	26/50/50/50	-
26	PCF	I	101	-	-	10/33/33/53	-
24	HEM	N	401	3	-	2/12/54/54	-
24	HEM	C	402	3	-	4/12/54/54	-
23	CDL	P	304	-	-	26/58/58/110	-
25	PEF	P	303	-	-	23/42/42/50	-
25	PEF	J	102	-	-	12/32/32/50	-
25	PEF	N	405	-	-	15/46/46/50	-
25	PEF	b	302	-	-	20/43/43/50	-
31	HEA	a	603	11	-	17/32/76/76	-
25	PEF	C	403	-	-	15/47/47/50	-
25	PEF	C	404	-	-	23/50/50/50	-
27	UQ6	C	406	-	-	5/39/39/39	0/1/1/1
31	HEA	a	604	11	-	5/32/76/76	-
25	PEF	U	101	-	-	15/40/40/50	-
23	CDL	E	303	-	-	26/63/63/110	-
26	PCF	T	101	-	-	23/50/50/53	-
24	HEM	C	401	3	-	2/12/54/54	-
25	PEF	a	608	-	-	24/50/50/50	-
26	PCF	e	202	-	-	20/53/53/53	-
23	CDL	H	101	-	-	40/76/76/110	-
23	CDL	A	501	-	-	44/87/87/110	-
26	PCF	N	406	-	-	23/53/53/53	-
23	CDL	L	502	-	-	41/77/77/110	-
25	PEF	G	201	-	-	19/35/35/50	-
26	PCF	C	405	-	-	15/42/42/53	-
25	PEF	c	301	-	-	18/50/50/50	-
25	PEF	a	609	-	-	15/33/33/50	-
29	FES	P	302	5	-	-	0/1/1/1
29	FES	E	301	5	-	-	0/1/1/1
25	PEF	N	404	-	-	18/43/43/50	-
27	UQ6	N	407	-	-	11/39/39/39	0/1/1/1
25	PEF	c	302	-	-	21/50/50/50	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CDL	c	303	-	-	62/96/96/110	-

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	O	401	HEC	C2B-C3B	-6.92	1.33	1.40
28	D	401	HEC	C3C-C2C	-6.54	1.33	1.40
28	O	401	HEC	C3C-C2C	-6.48	1.34	1.40
28	D	401	HEC	C2B-C3B	-5.94	1.34	1.40
28	D	401	HEC	C3D-C2D	5.40	1.53	1.37

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	604	HEA	C2B-C1B-NB	5.82	116.85	109.88
31	a	604	HEA	C1D-C2D-C3D	-5.51	101.17	106.96
31	a	604	HEA	C3B-C4B-NB	5.26	116.08	109.84
31	a	604	HEA	C2D-C1D-ND	5.08	115.86	109.84
25	h	101	PEF	O2-C10-C11	5.00	122.29	111.50

There are no chirality outliers.

5 of 1059 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
23	A	501	CDL	C11-CA5-OA6-CA4

There are no ring outliers.

49 monomers are involved in 104 short contacts:

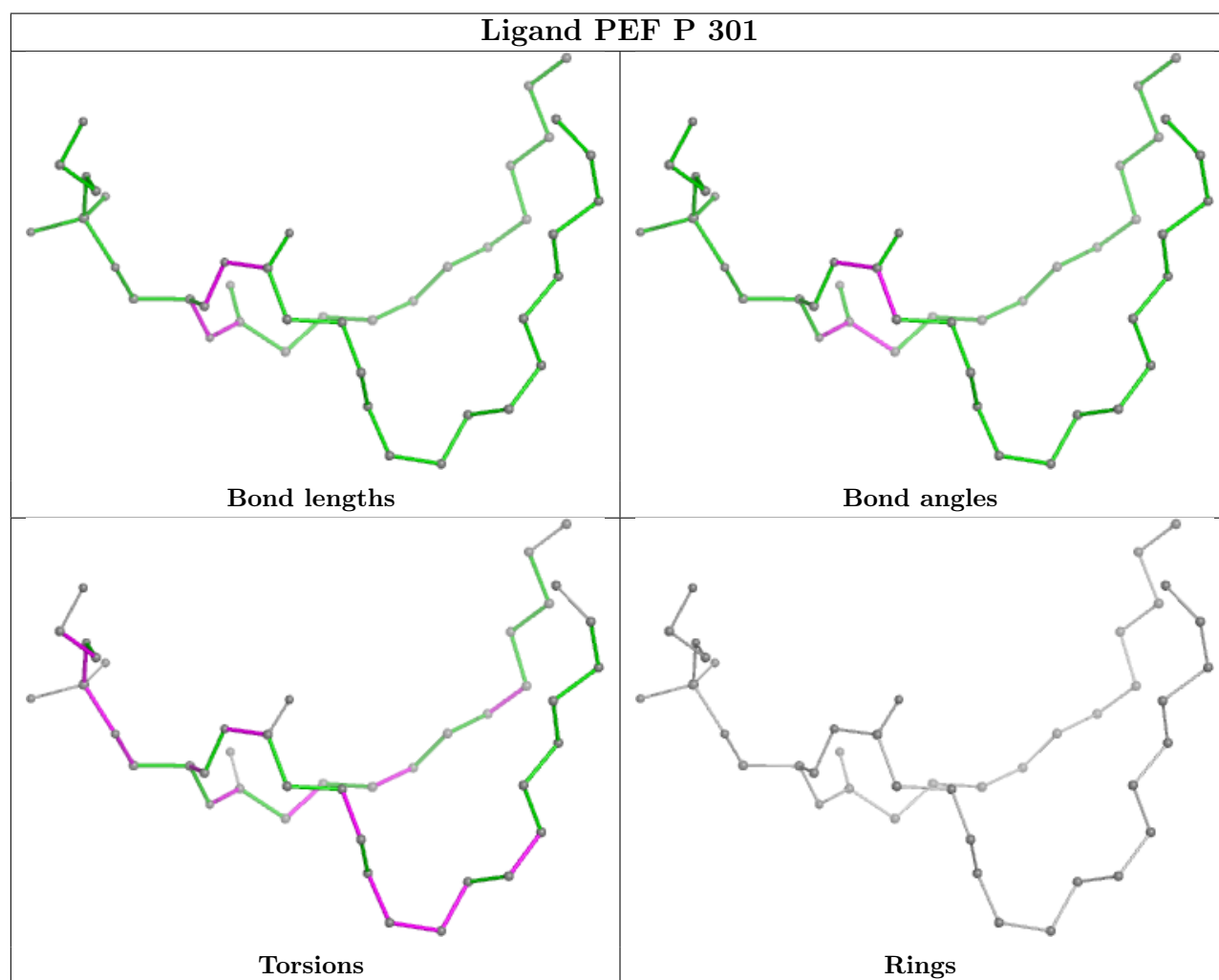
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	301	PEF	3	0
23	H	102	CDL	1	0
25	h	101	PEF	1	0
23	A	502	CDL	2	0
25	l	101	PEF	4	0
25	N	408	PEF	2	0
25	S	102	PEF	3	0

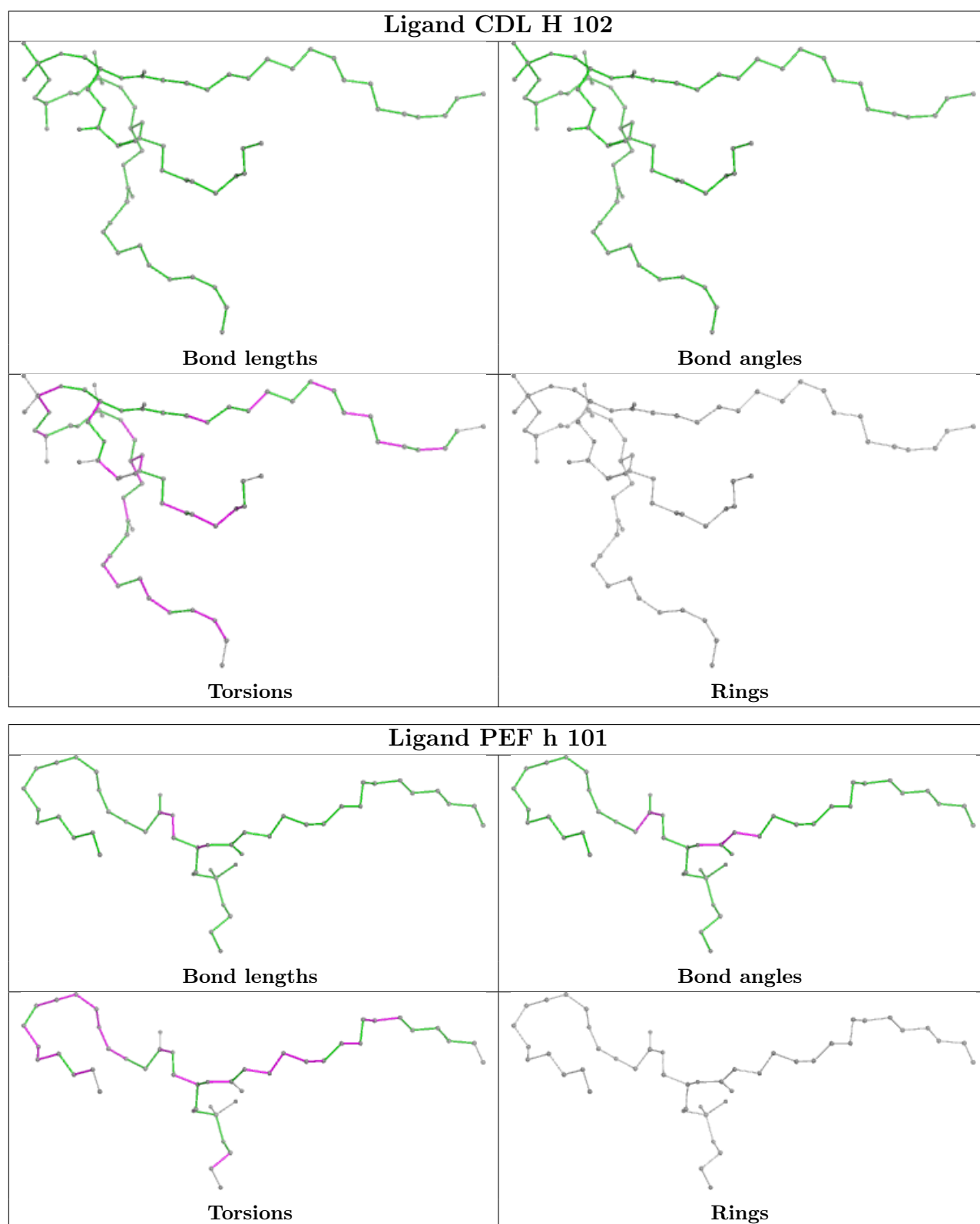
Continued on next page...

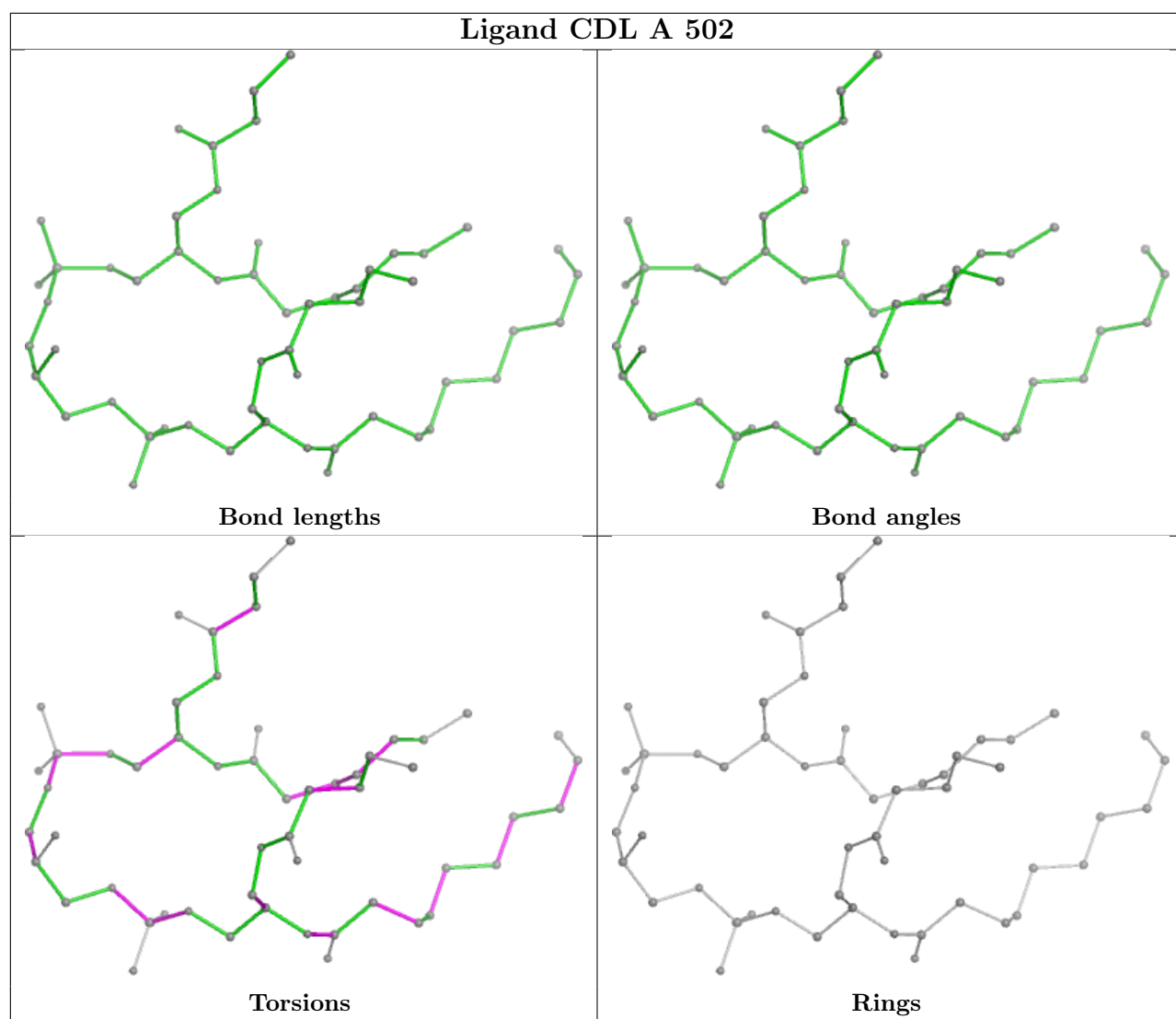
Continued from previous page...

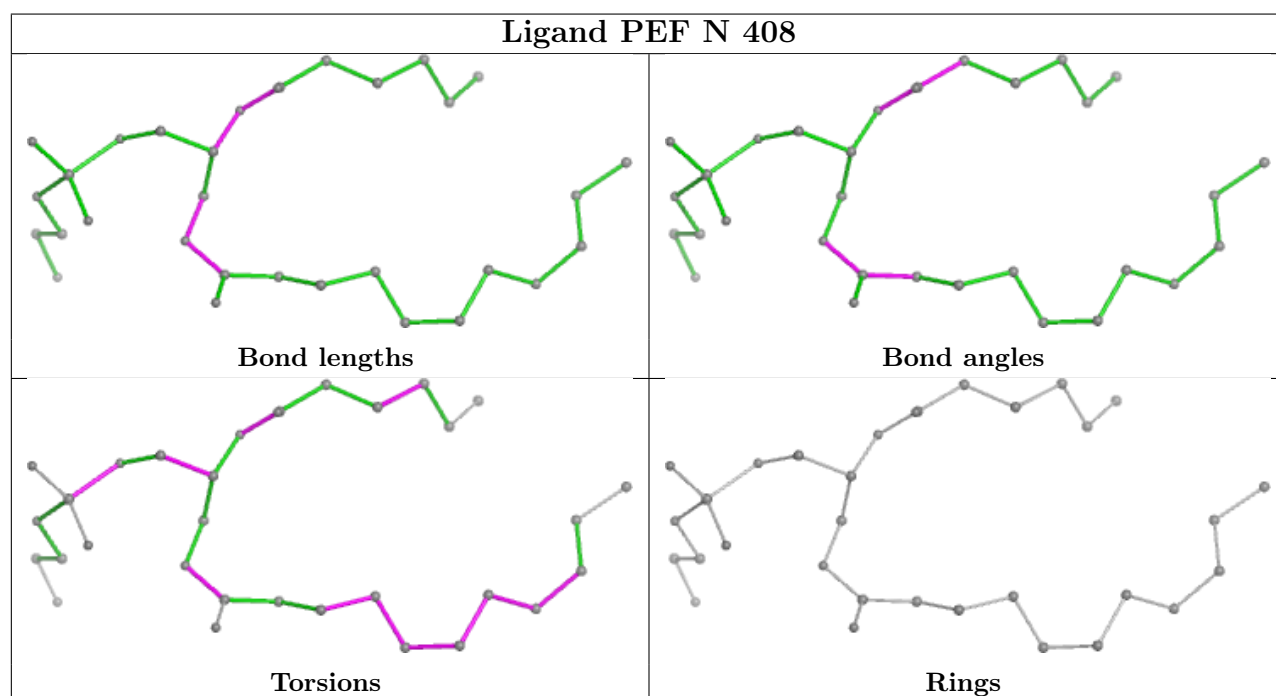
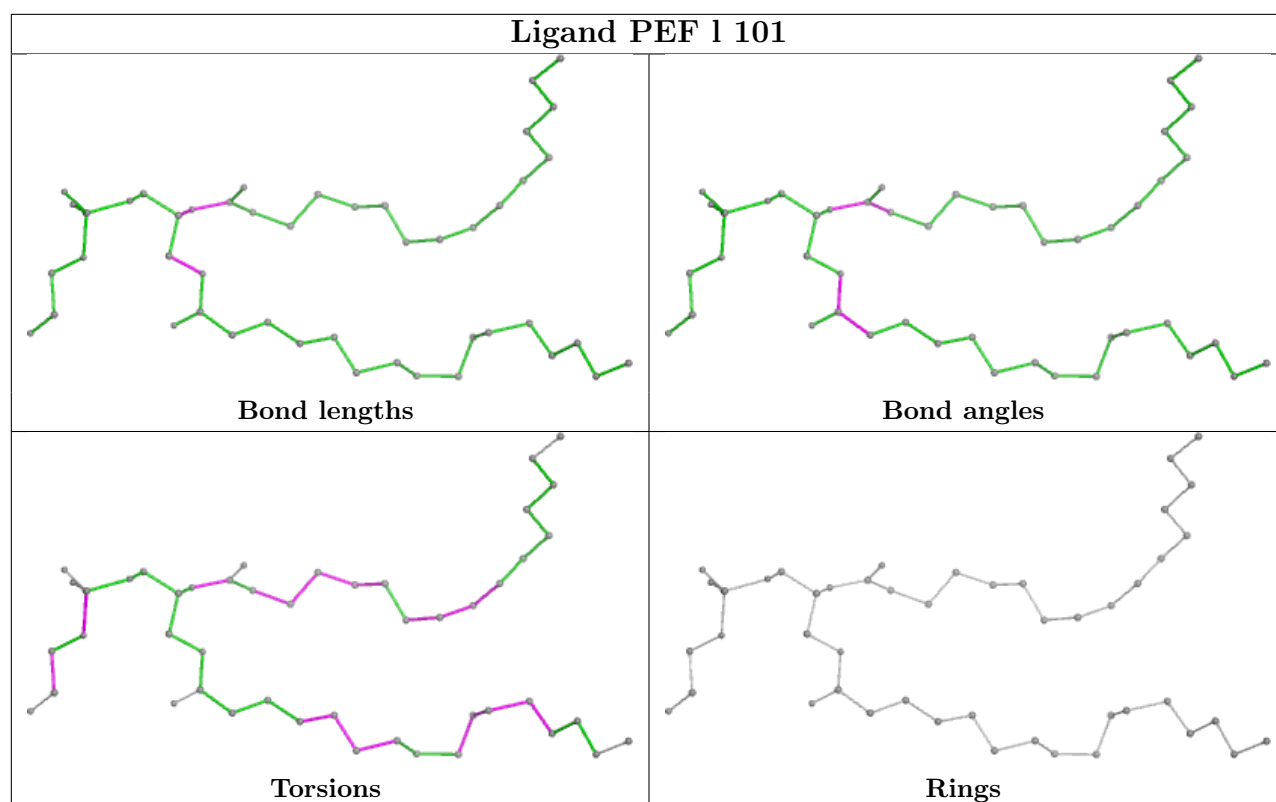
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	E	302	PEF	2	0
25	a	607	PEF	3	0
24	N	402	HEM	1	0
25	a	601	PEF	2	0
25	e	201	PEF	2	0
28	D	401	HEC	4	0
26	H	104	PCF	1	0
23	L	501	CDL	3	0
28	O	401	HEC	5	0
23	S	101	CDL	2	0
23	N	403	CDL	4	0
25	C	407	PEF	2	0
25	b	303	PEF	1	0
26	I	101	PCF	2	0
24	N	401	HEM	3	0
24	C	402	HEM	2	0
23	P	304	CDL	1	0
25	P	303	PEF	2	0
25	J	102	PEF	1	0
25	b	302	PEF	2	0
31	a	603	HEA	3	0
25	C	403	PEF	4	0
25	C	404	PEF	1	0
27	C	406	UQ6	2	0
25	U	101	PEF	2	0
23	E	303	CDL	2	0
26	T	101	PCF	4	0
24	C	401	HEM	2	0
25	a	608	PEF	2	0
26	e	202	PCF	1	0
23	H	101	CDL	3	0
23	A	501	CDL	2	0
26	N	406	PCF	3	0
23	L	502	CDL	4	0
25	G	201	PEF	1	0
26	C	405	PCF	1	0
25	c	301	PEF	1	0
25	a	609	PEF	1	0
25	N	404	PEF	2	0
27	N	407	UQ6	1	0
25	c	302	PEF	6	0
23	c	303	CDL	3	0

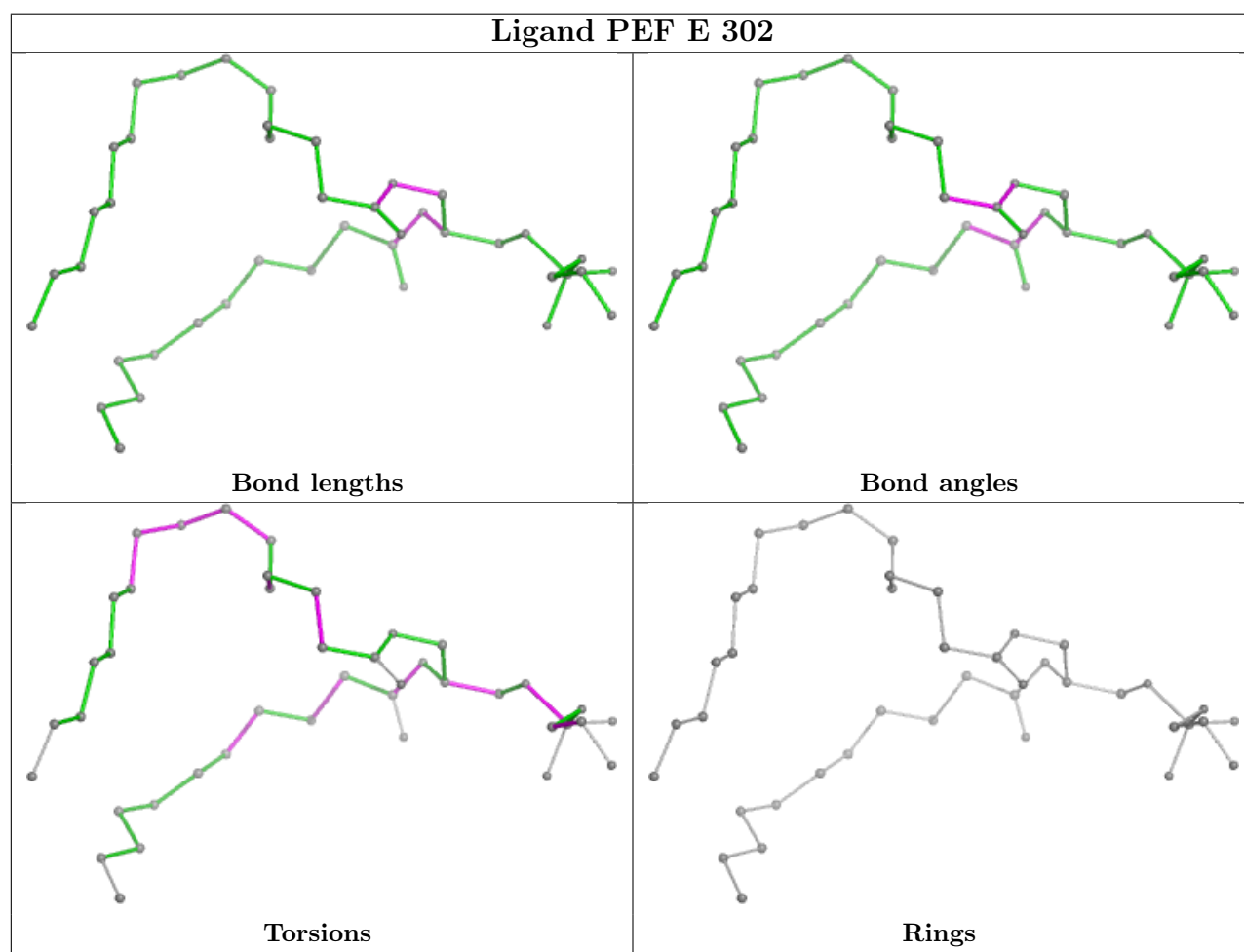
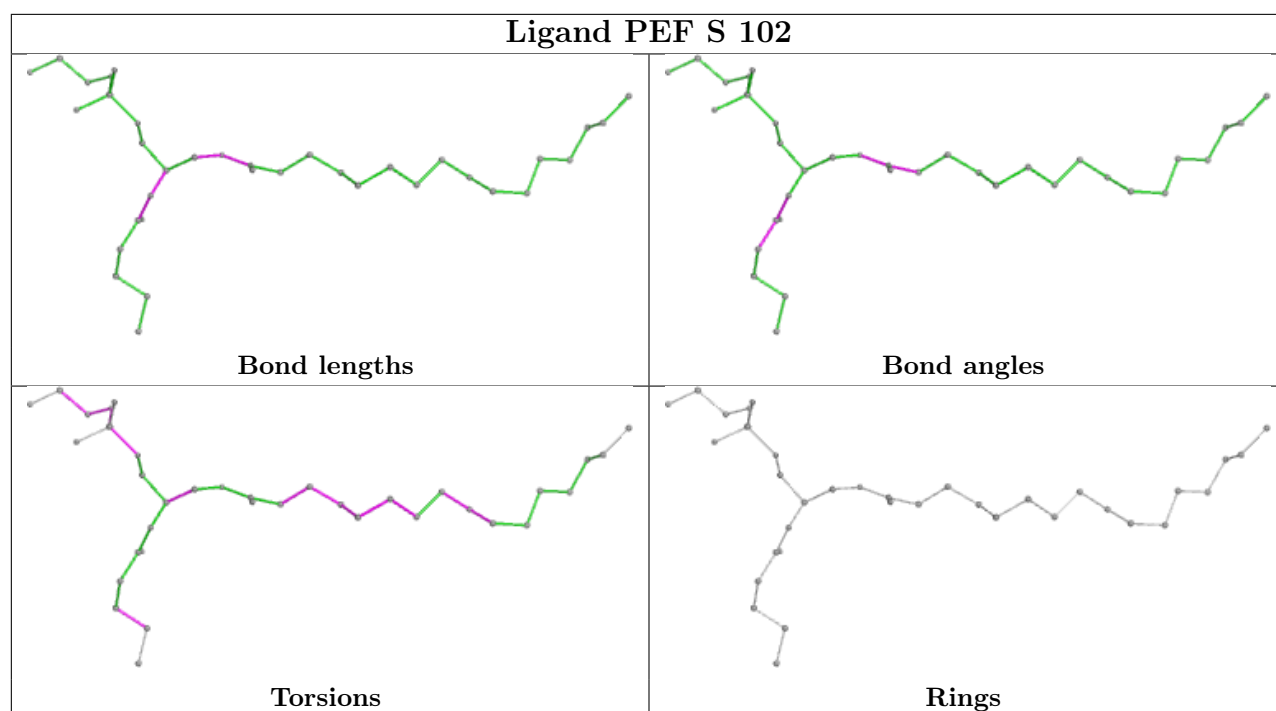
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

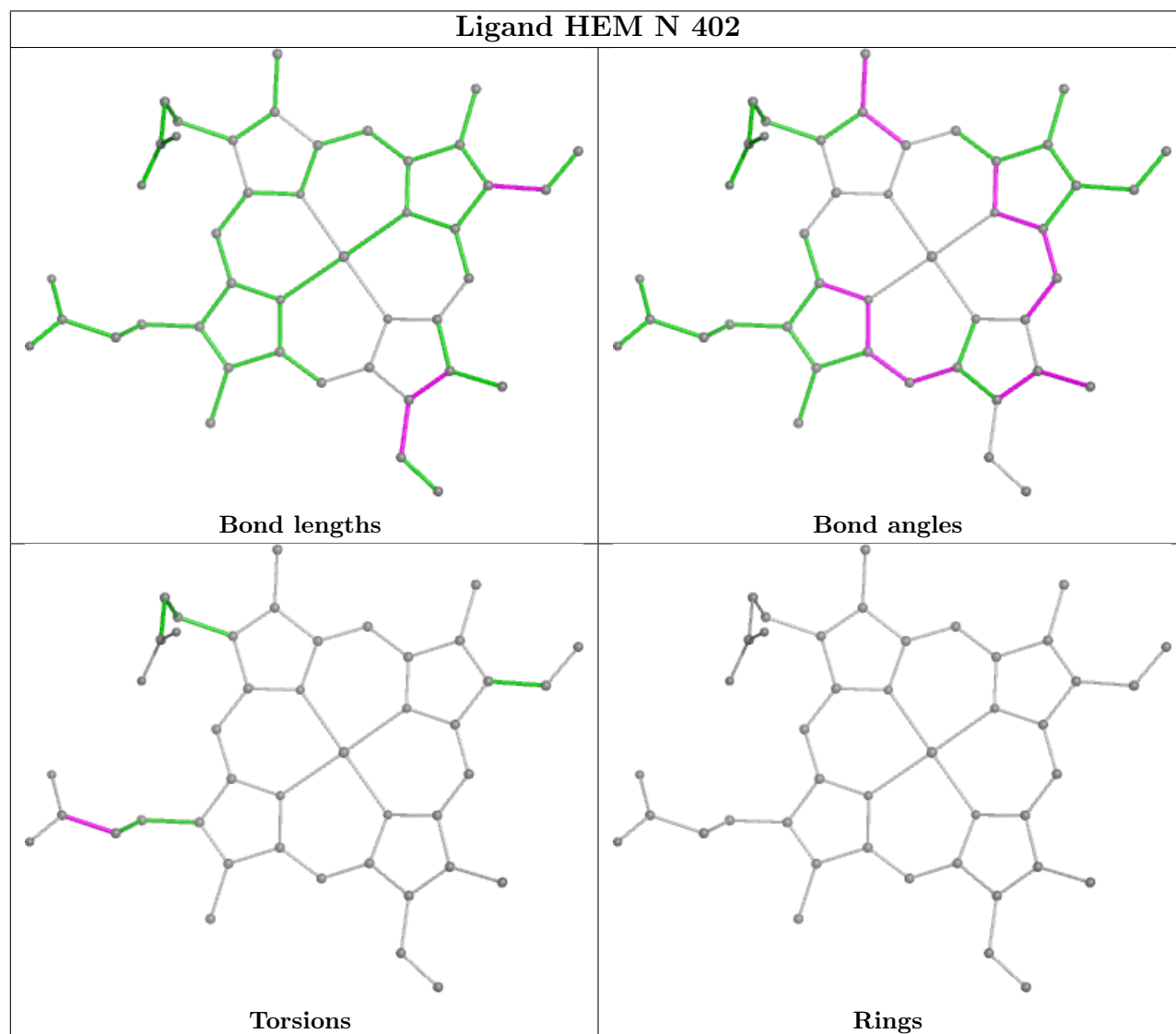
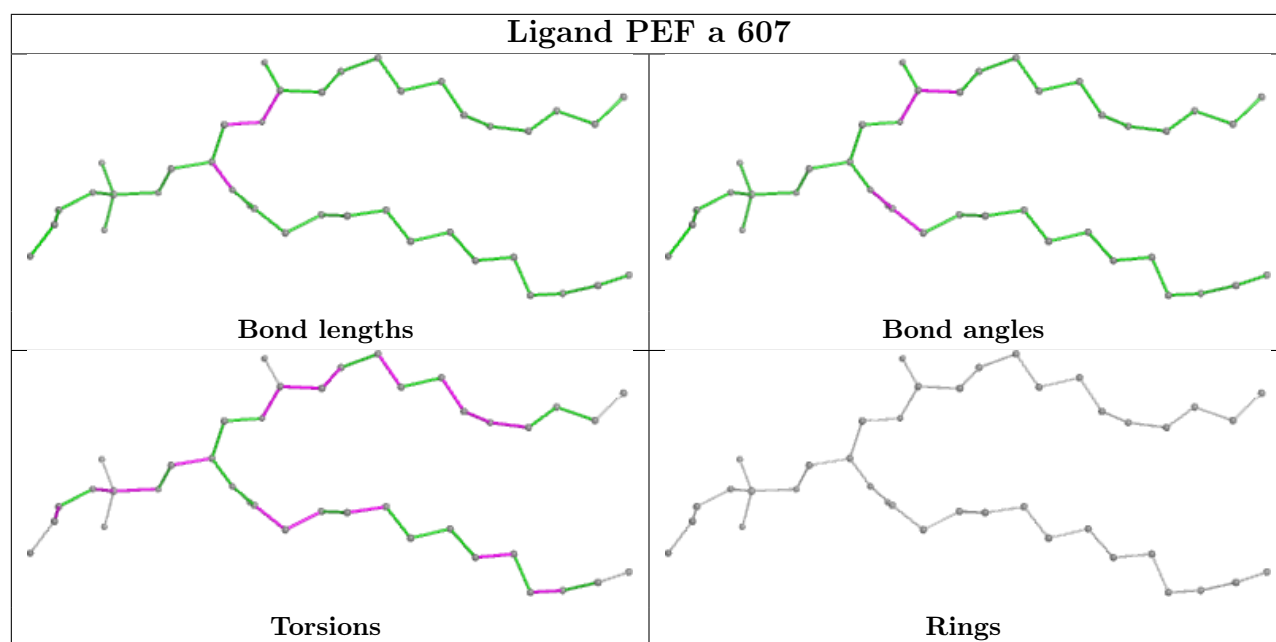


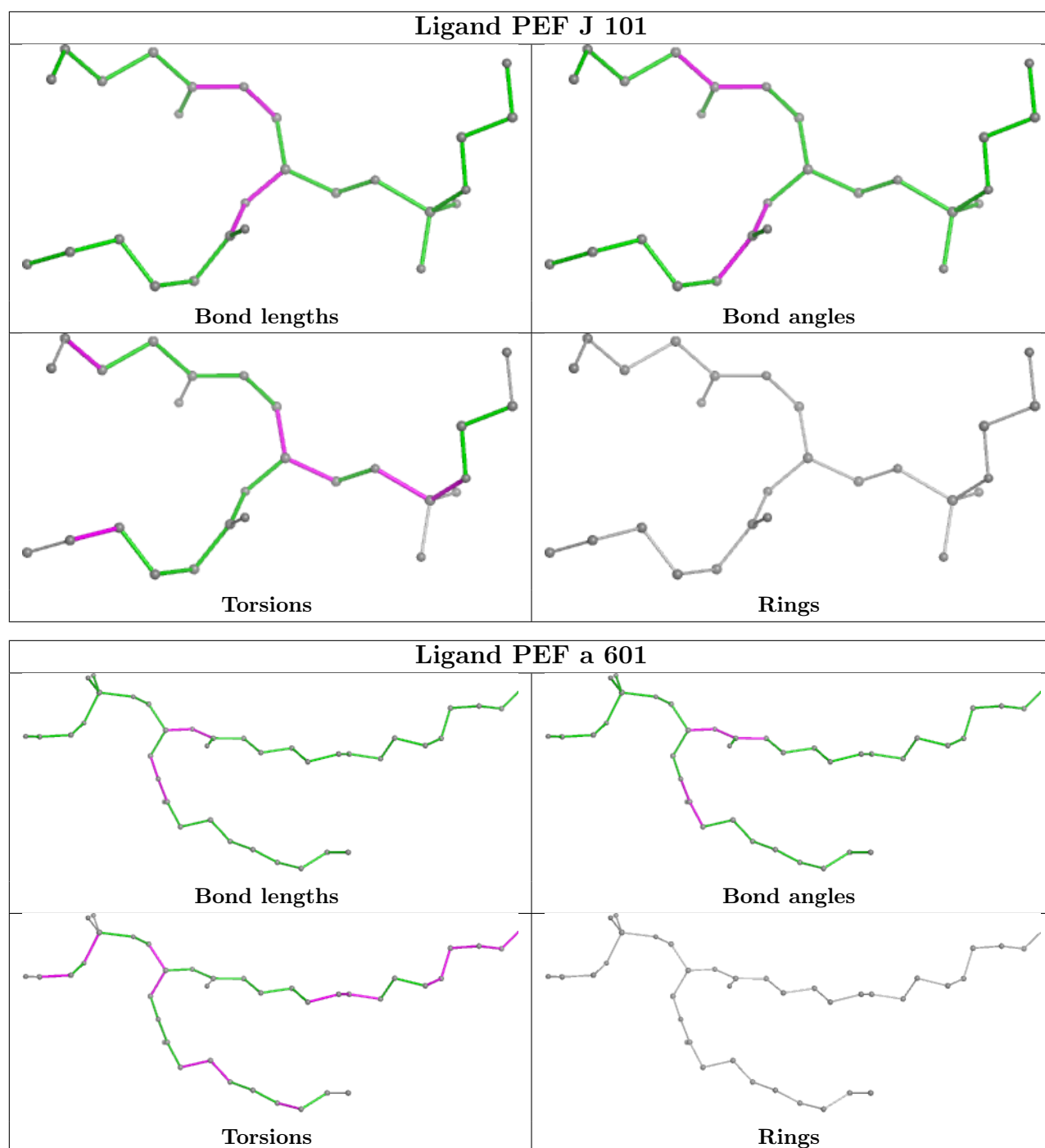


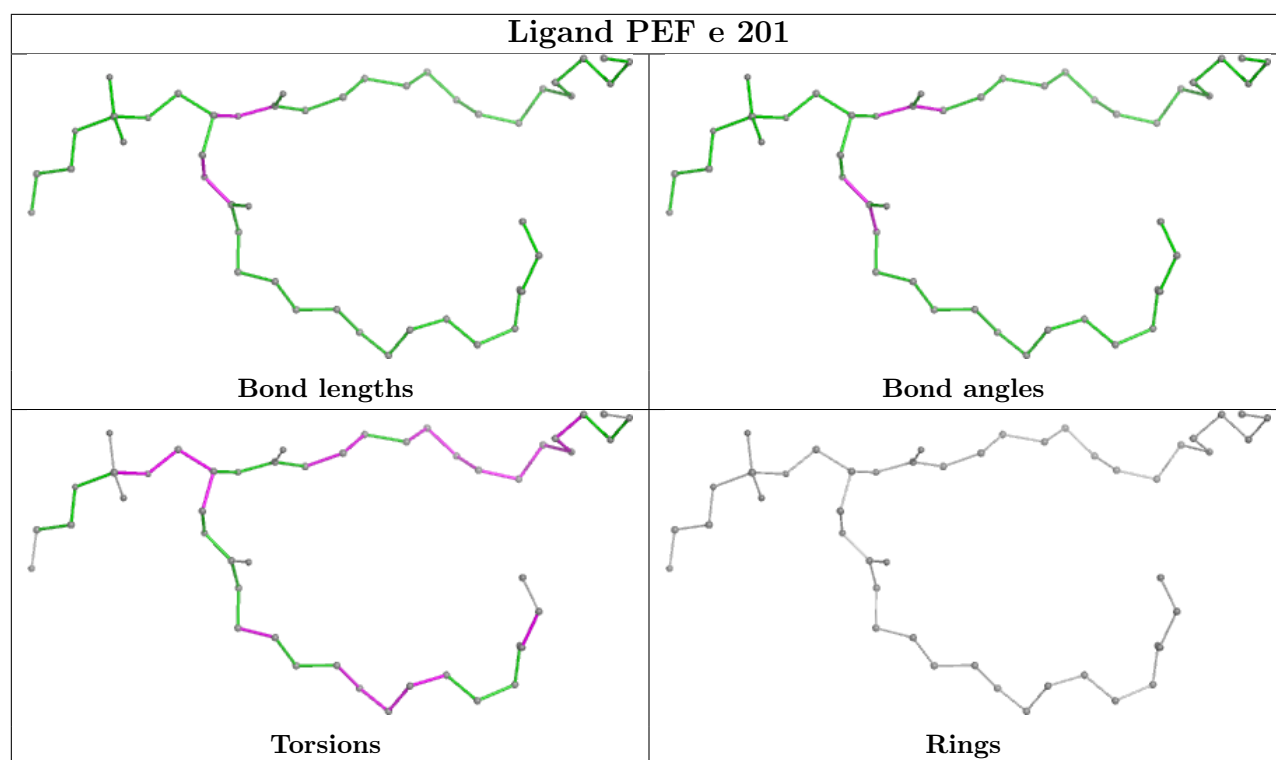


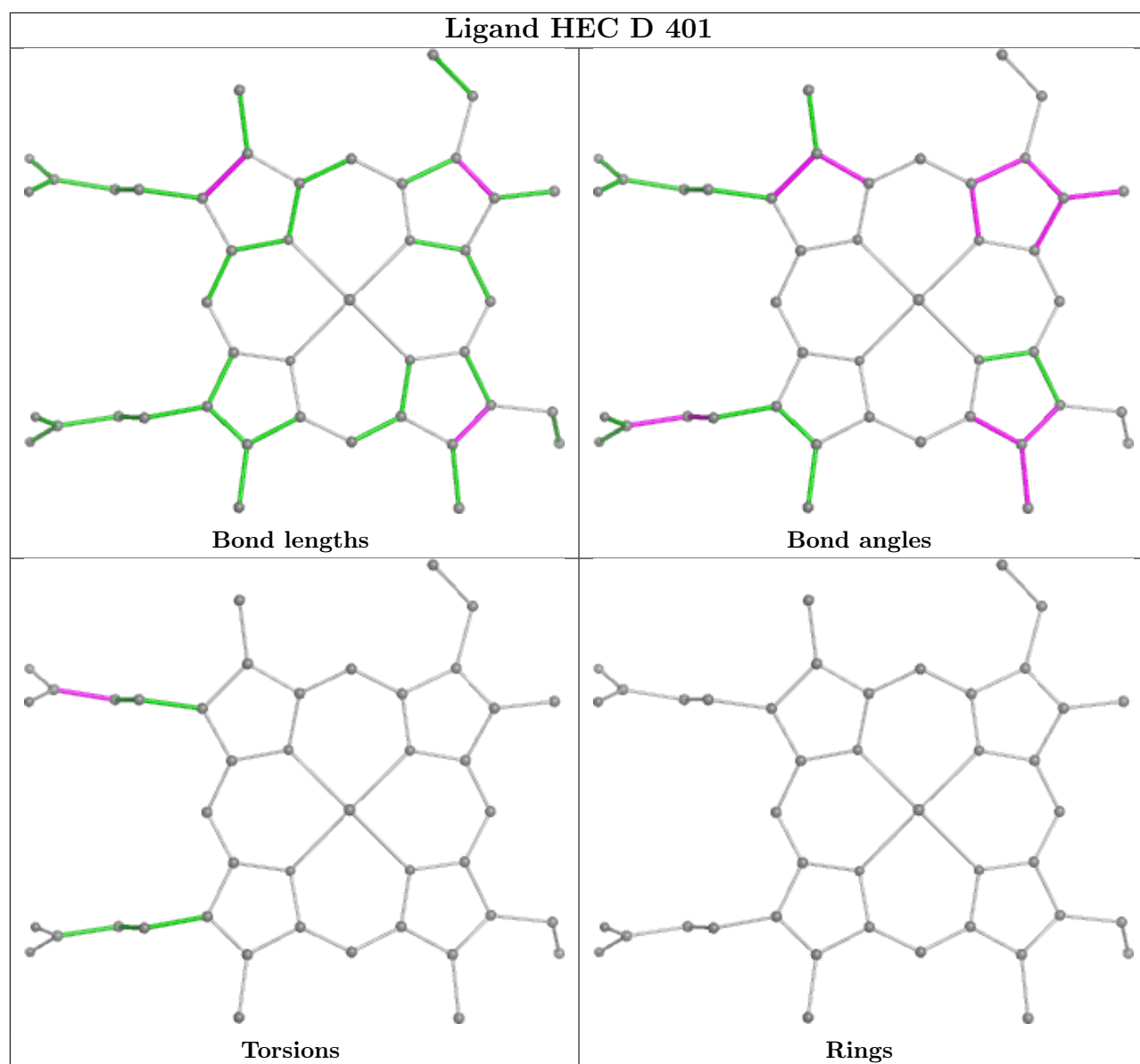


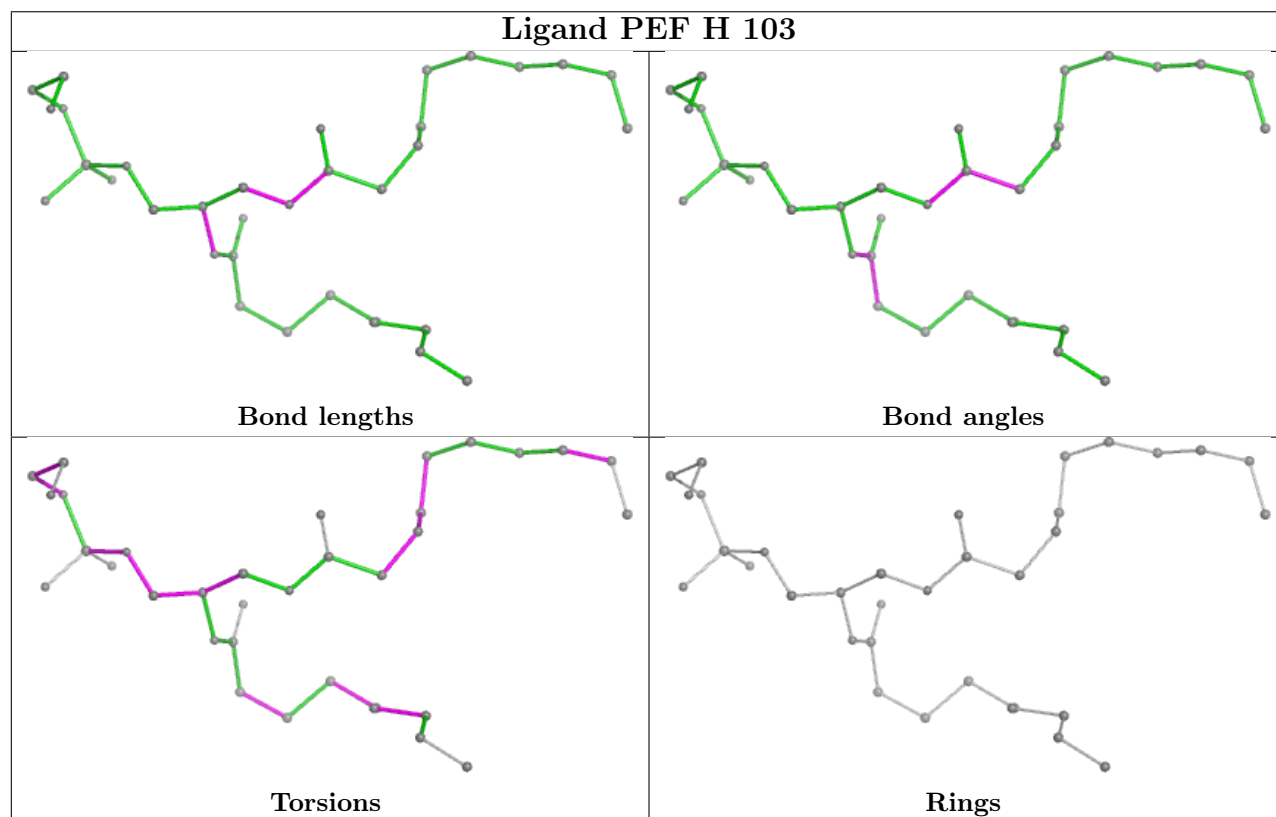
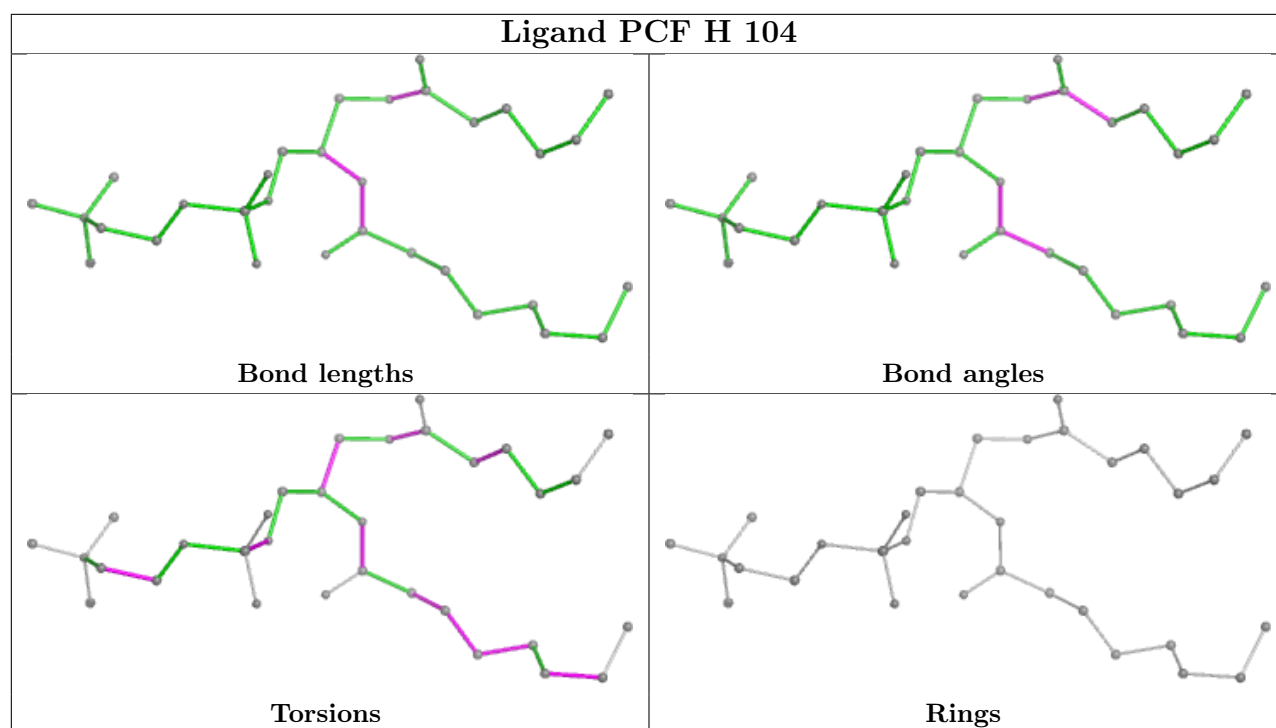


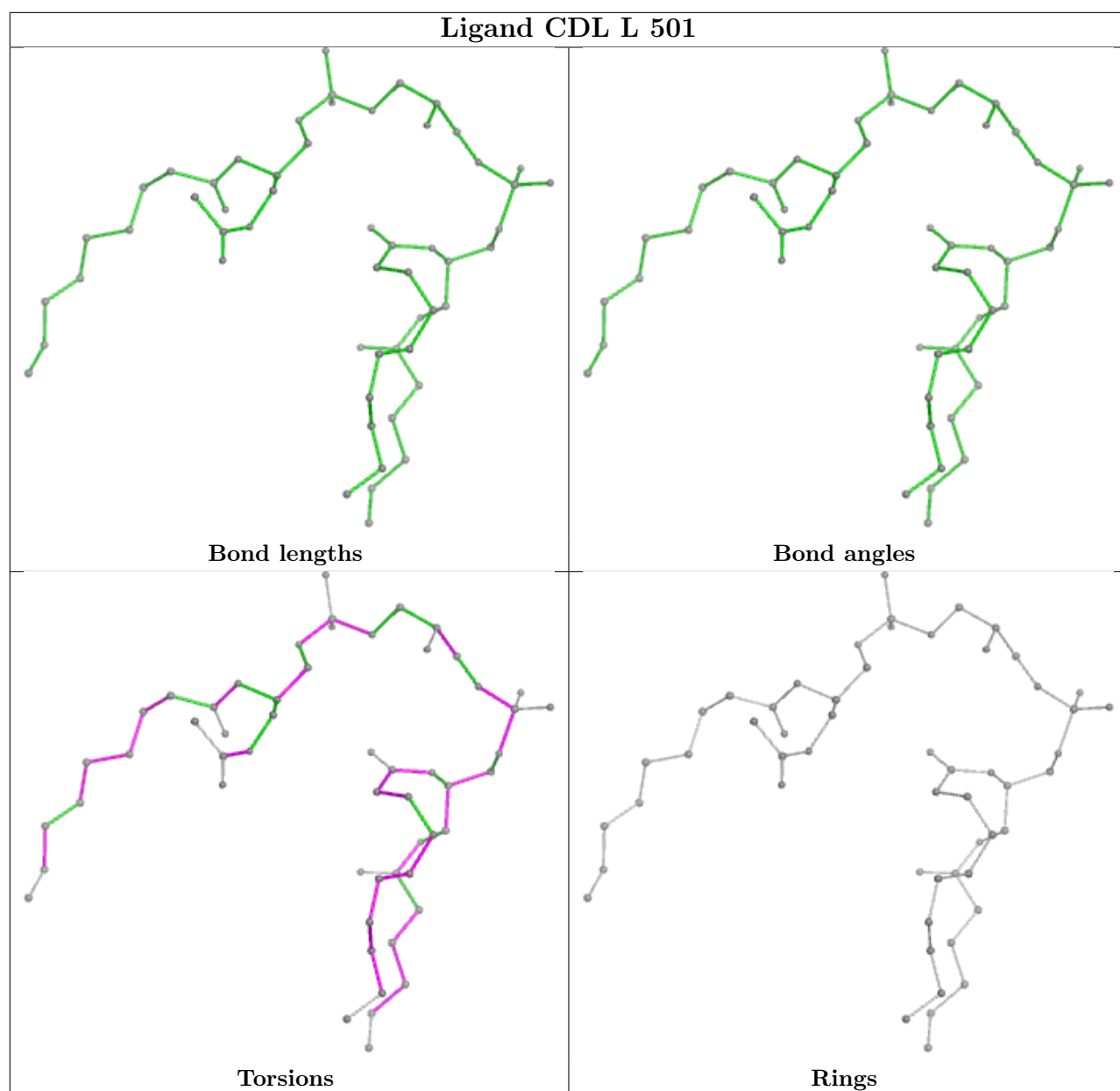


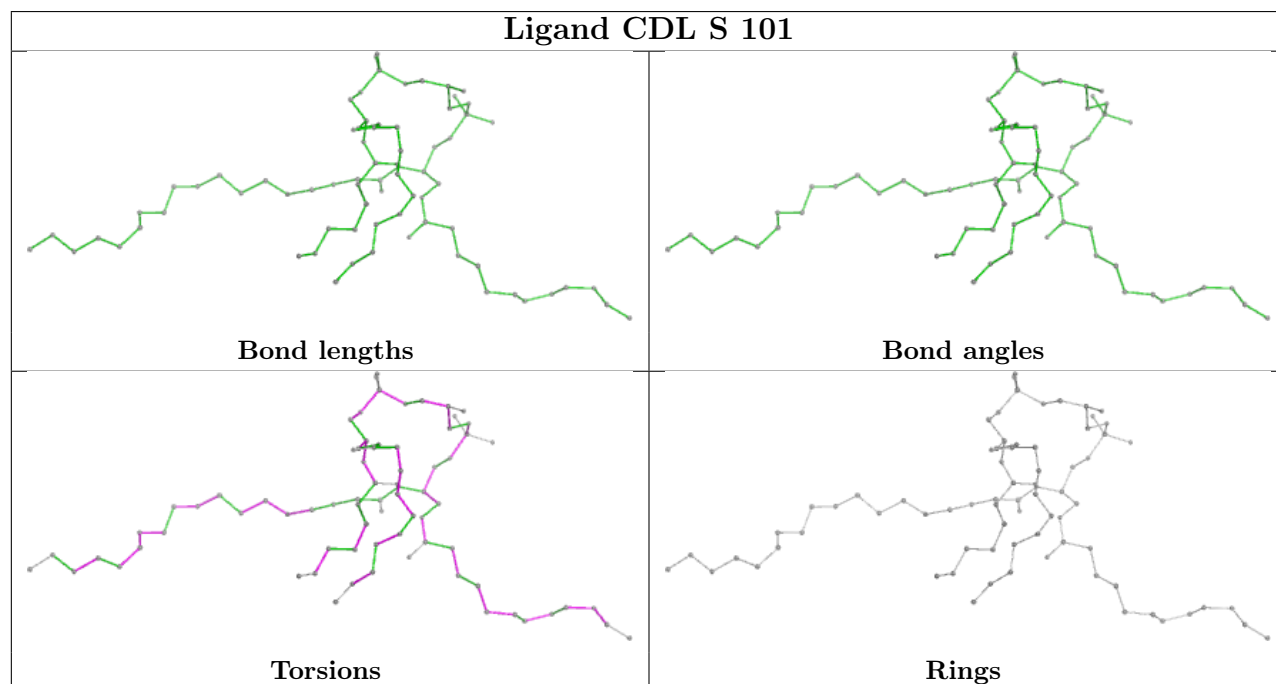
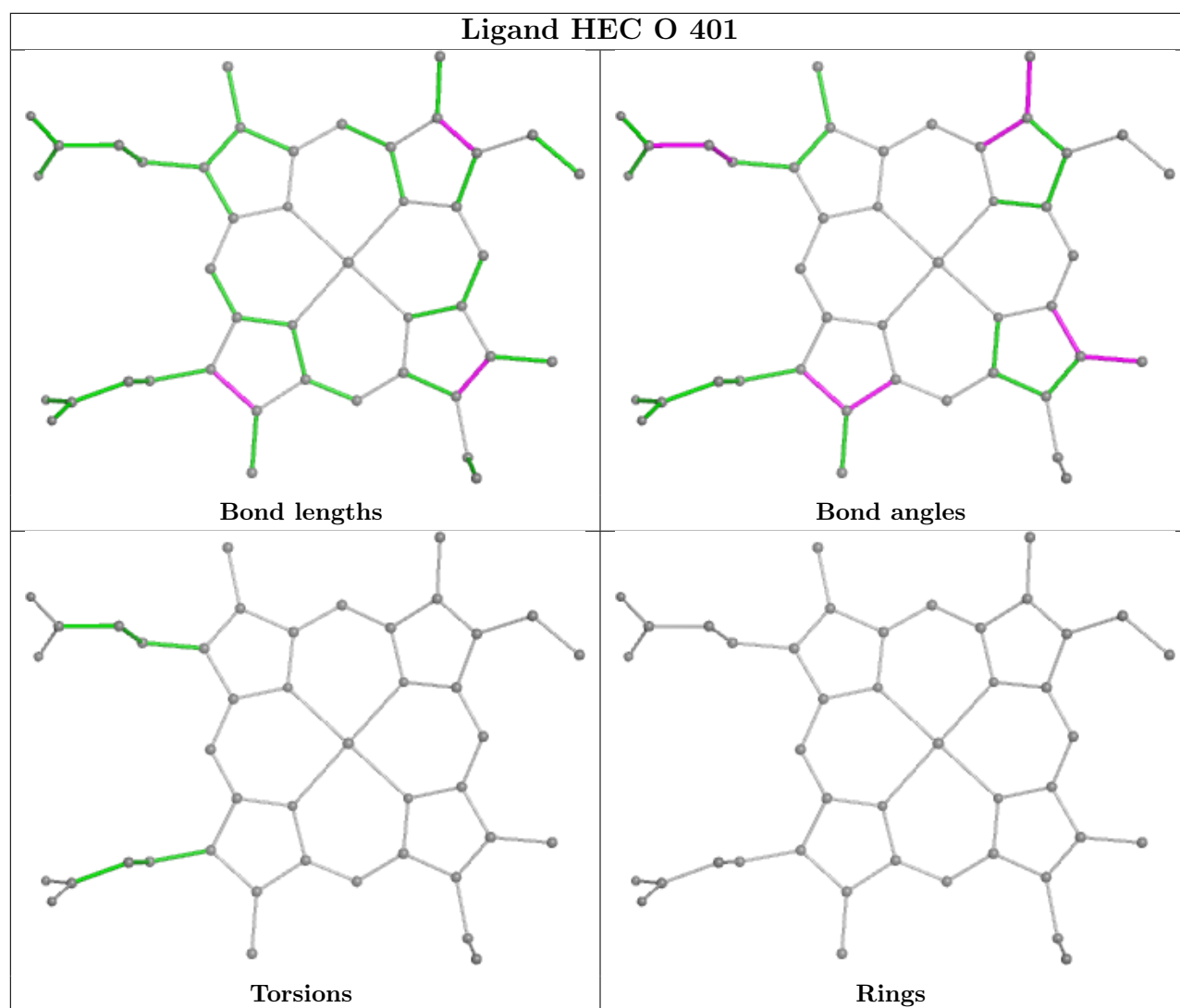


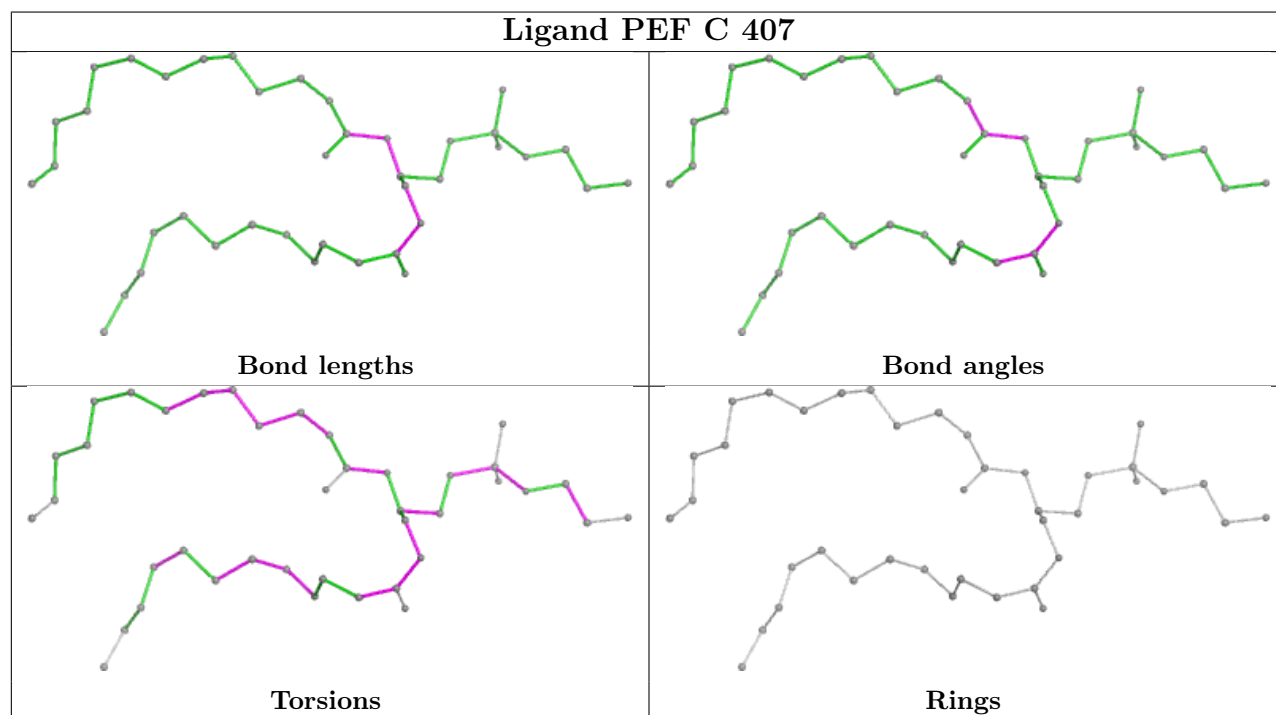
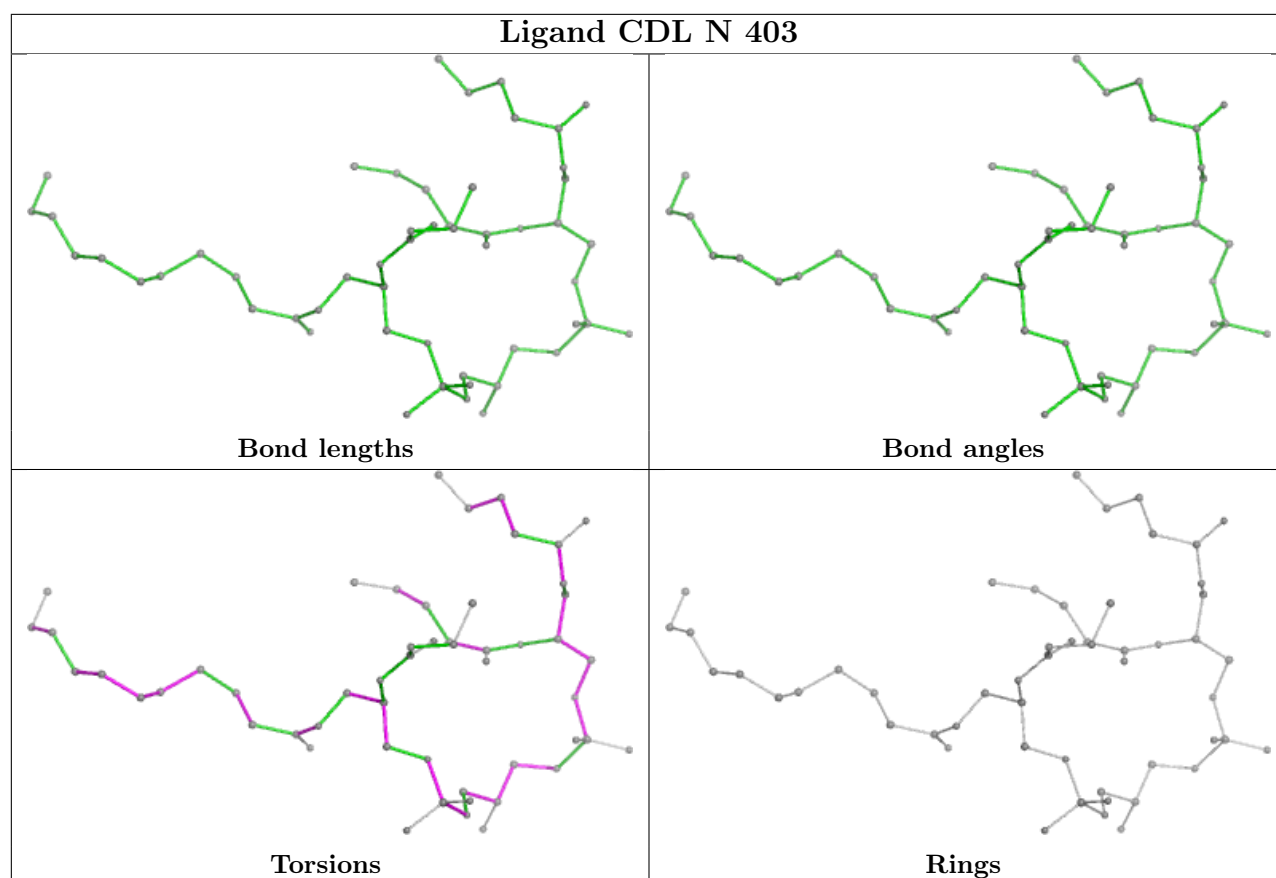


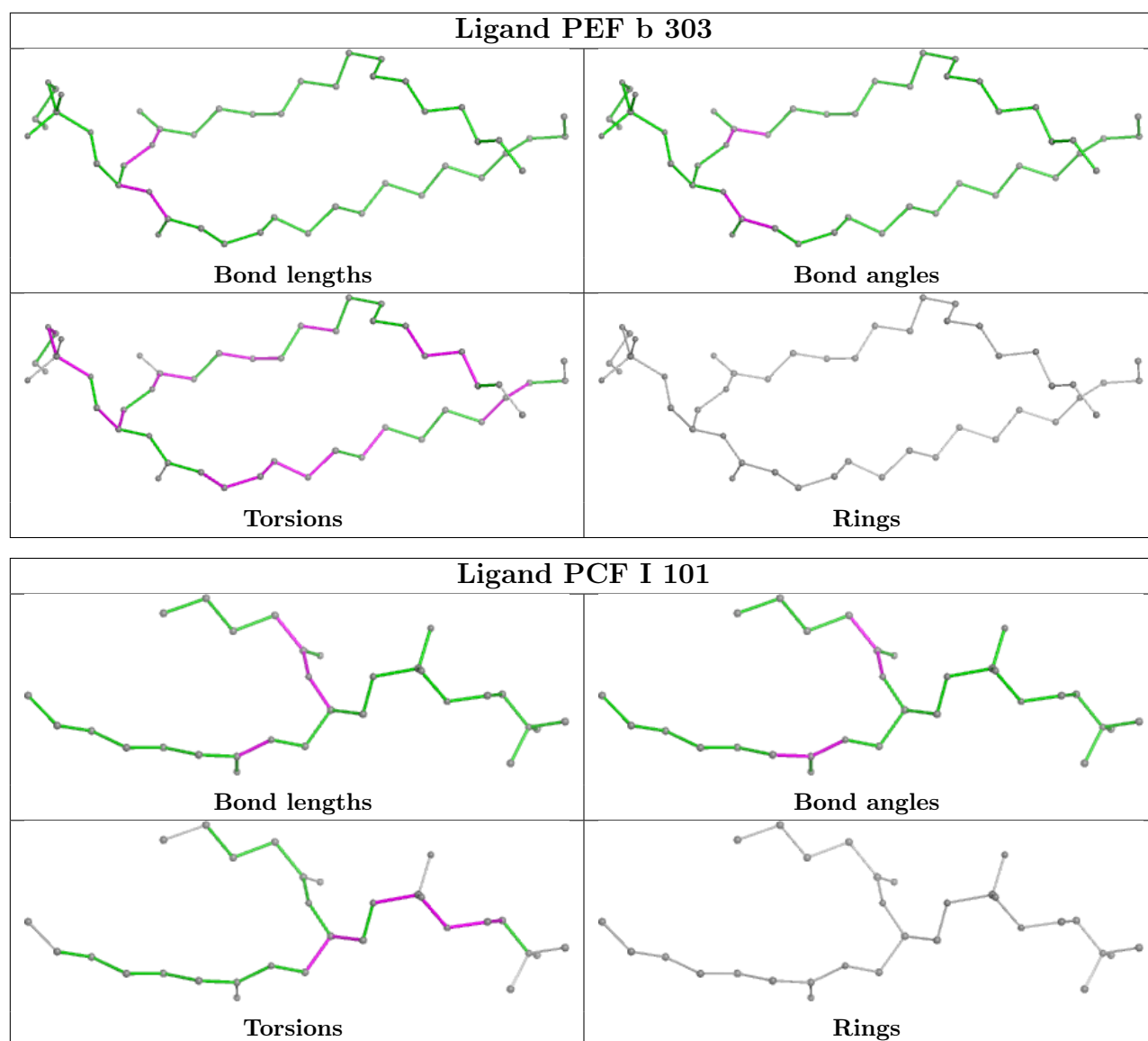


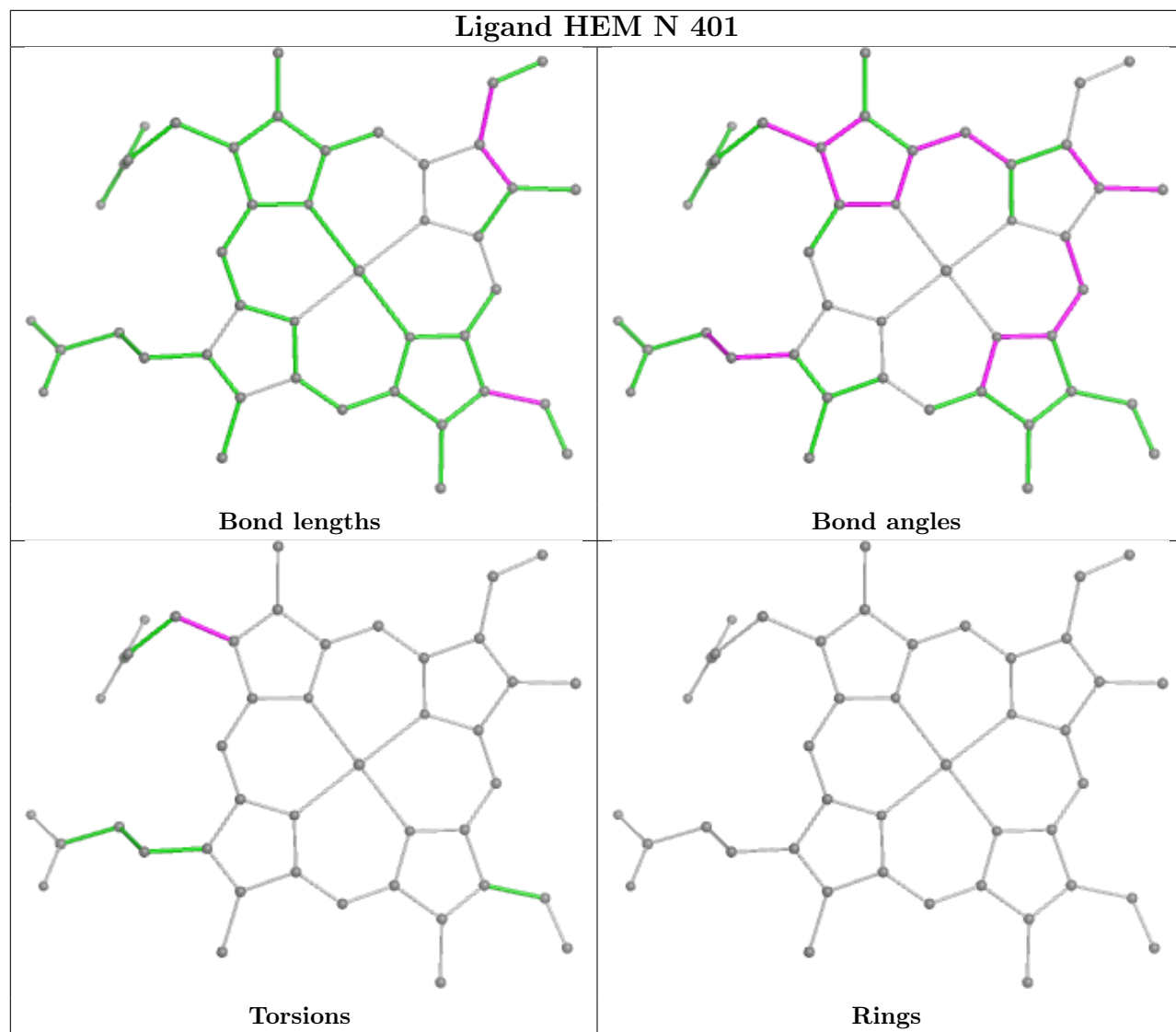


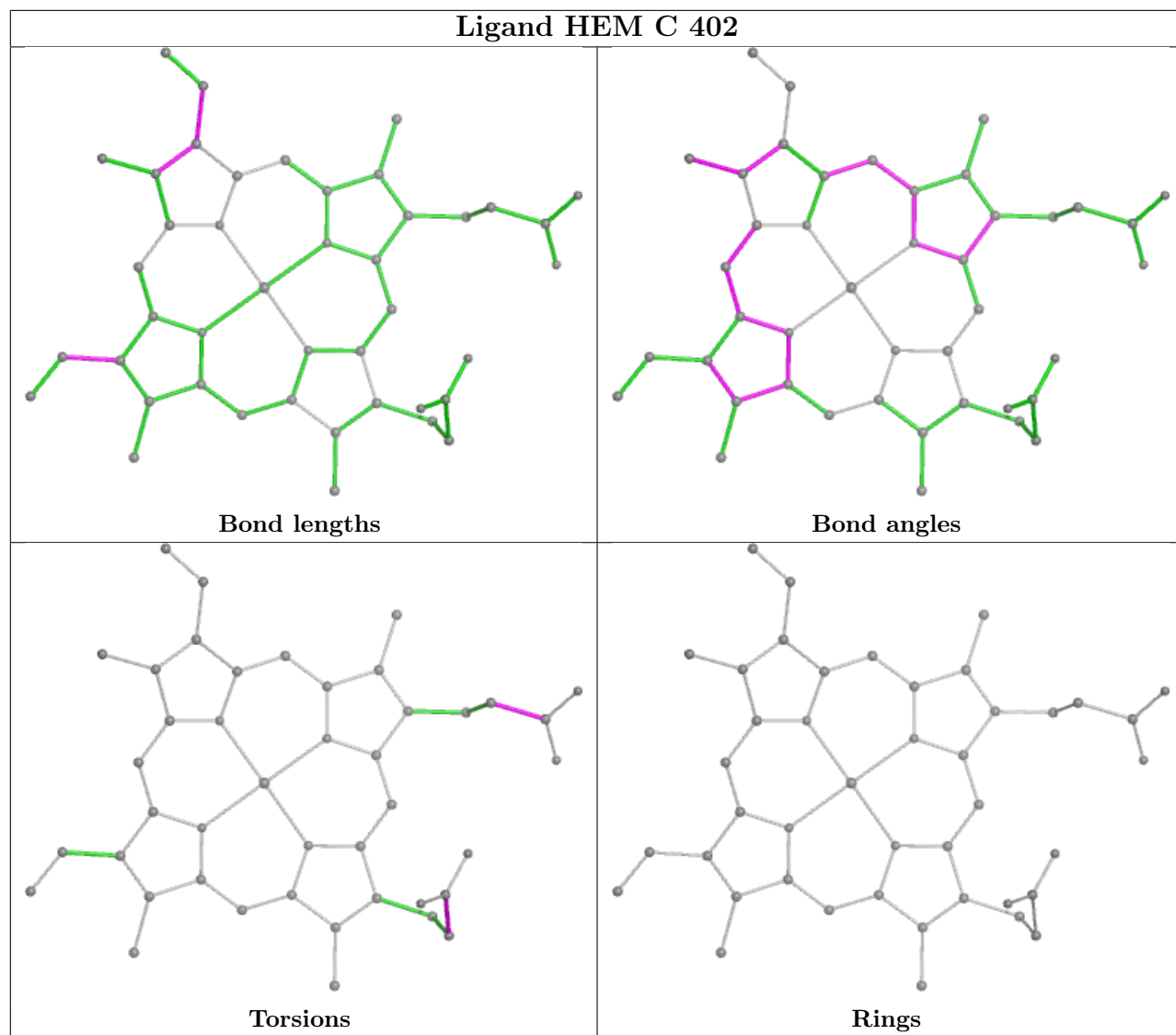




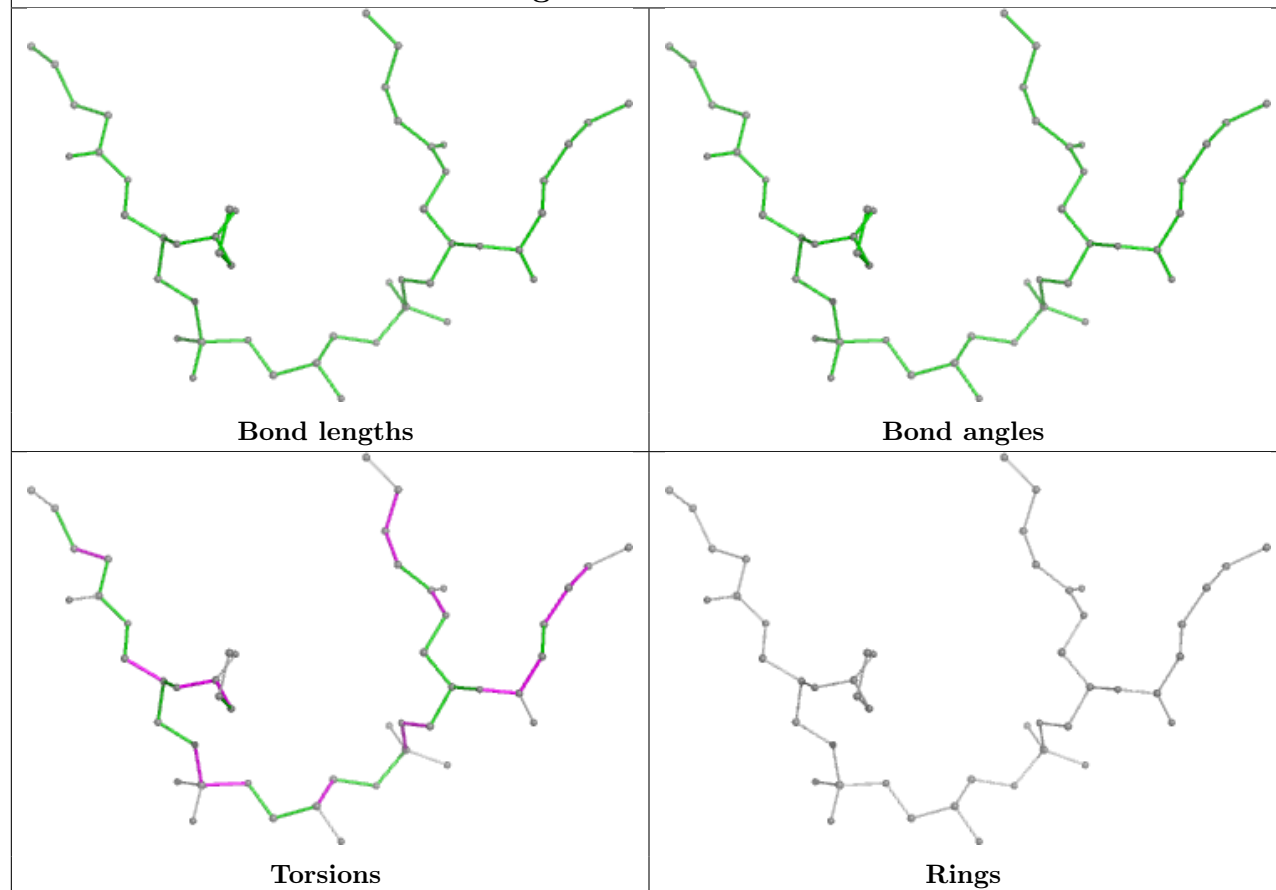




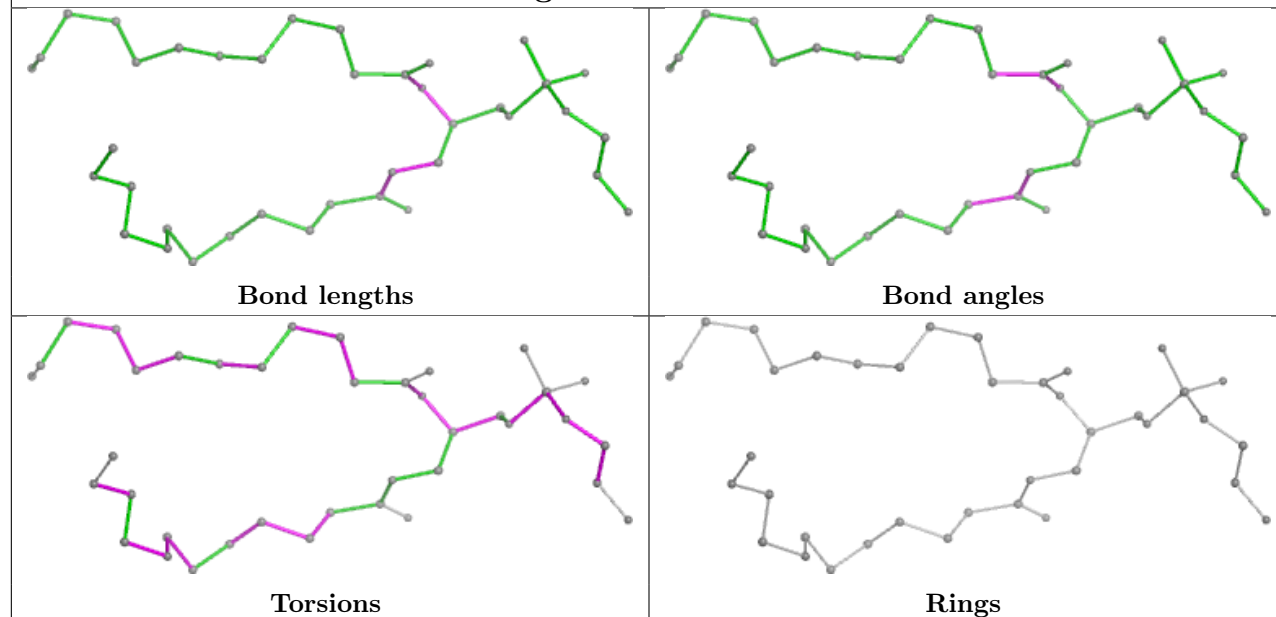


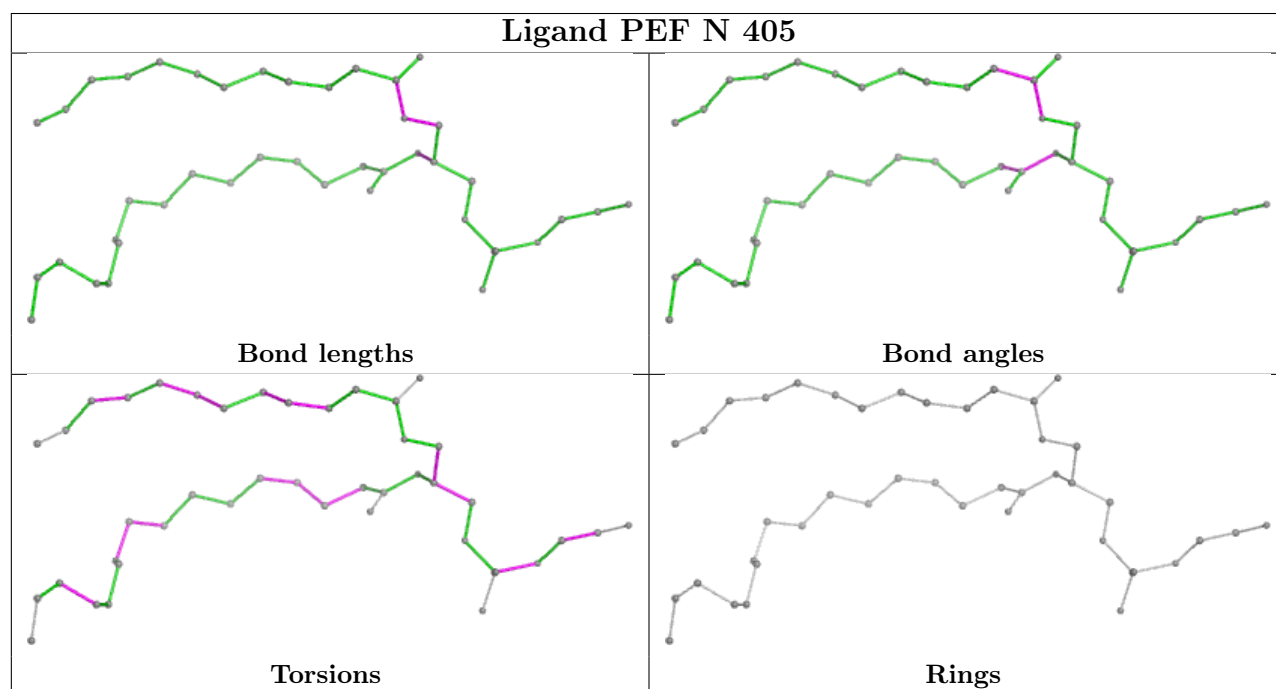
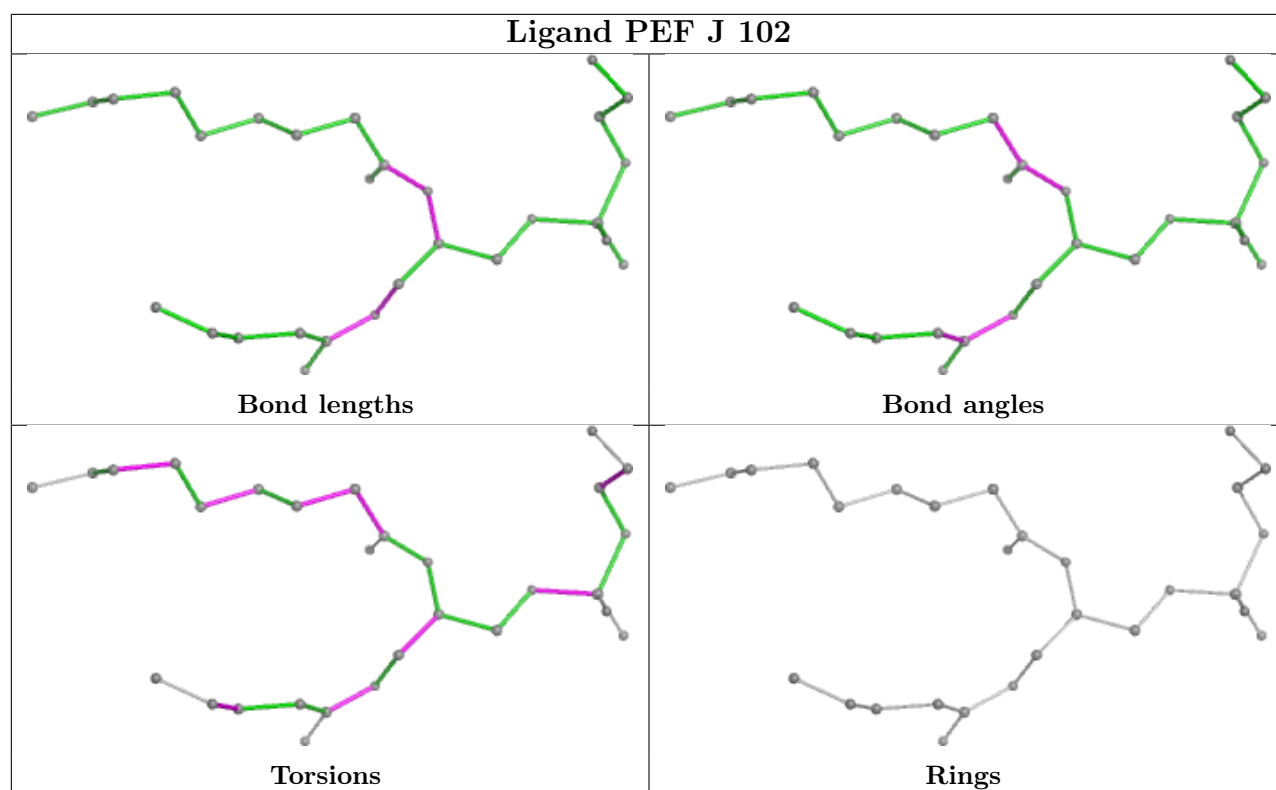


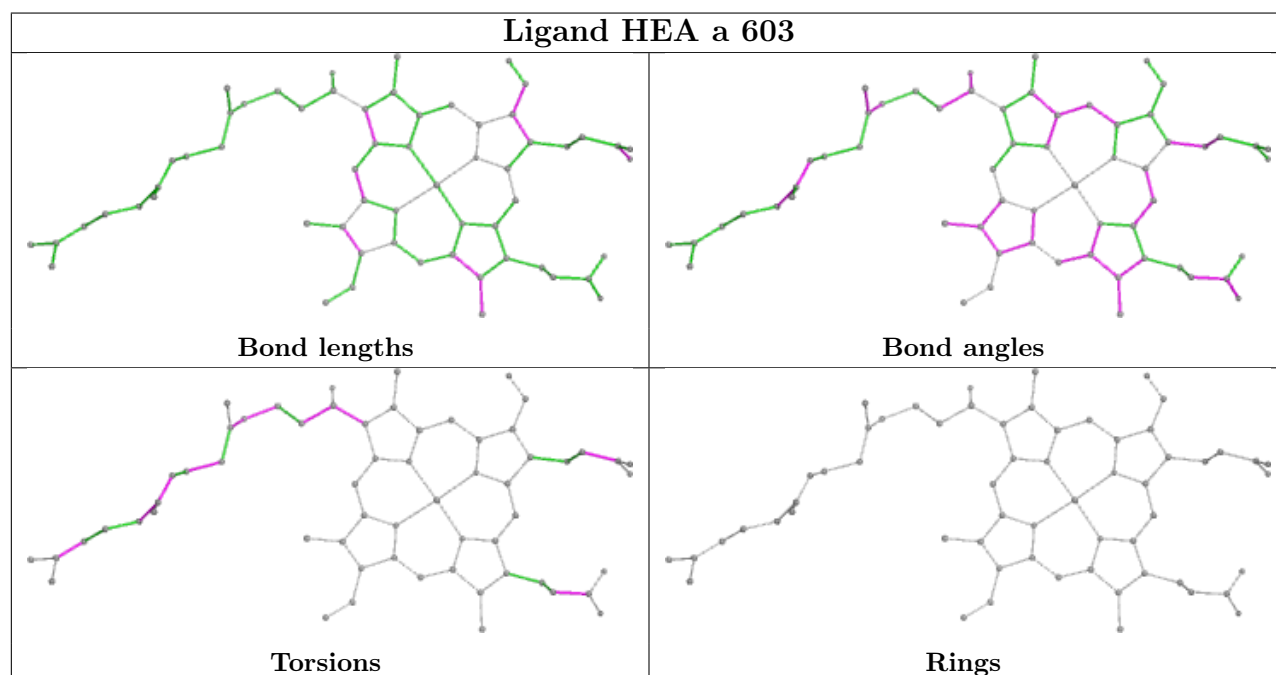
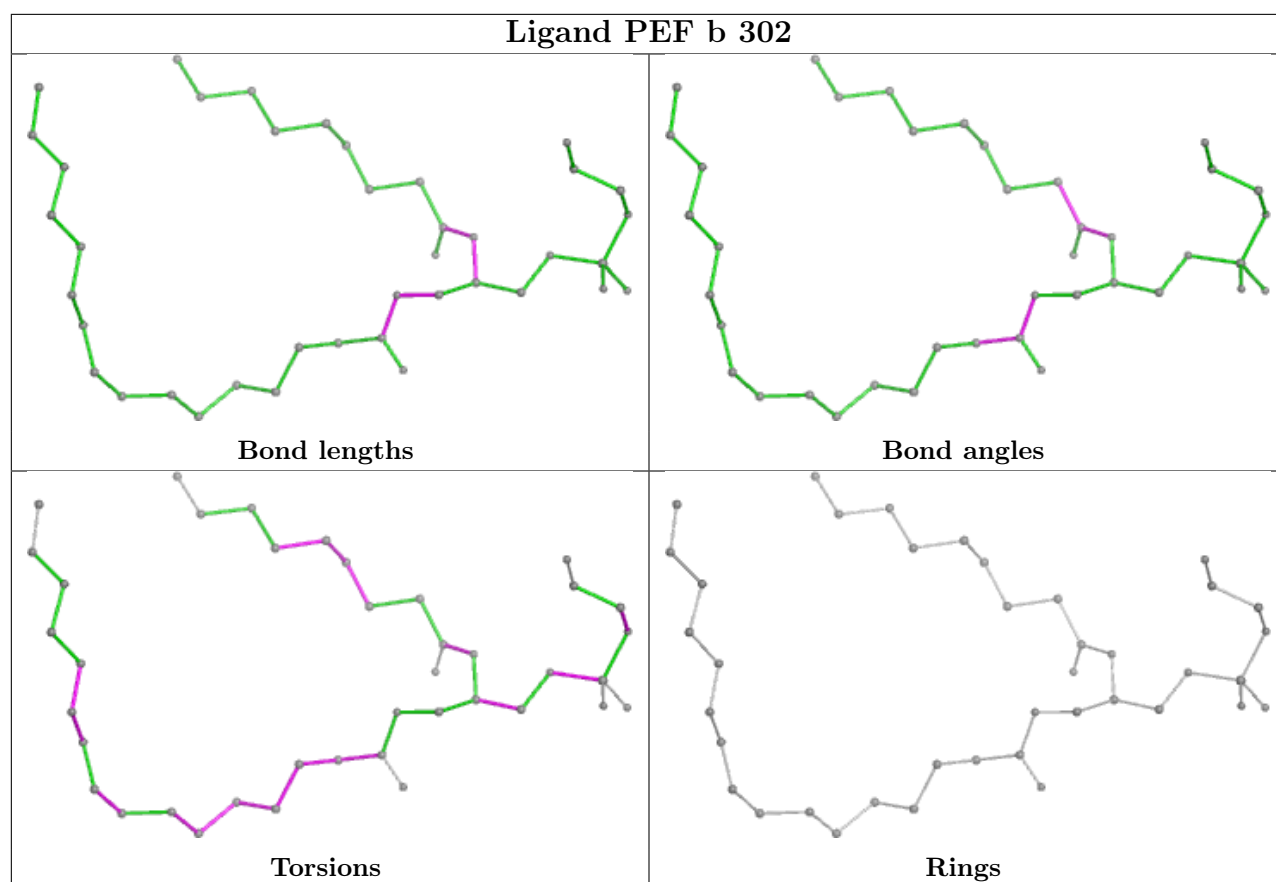
Ligand CDL P 304

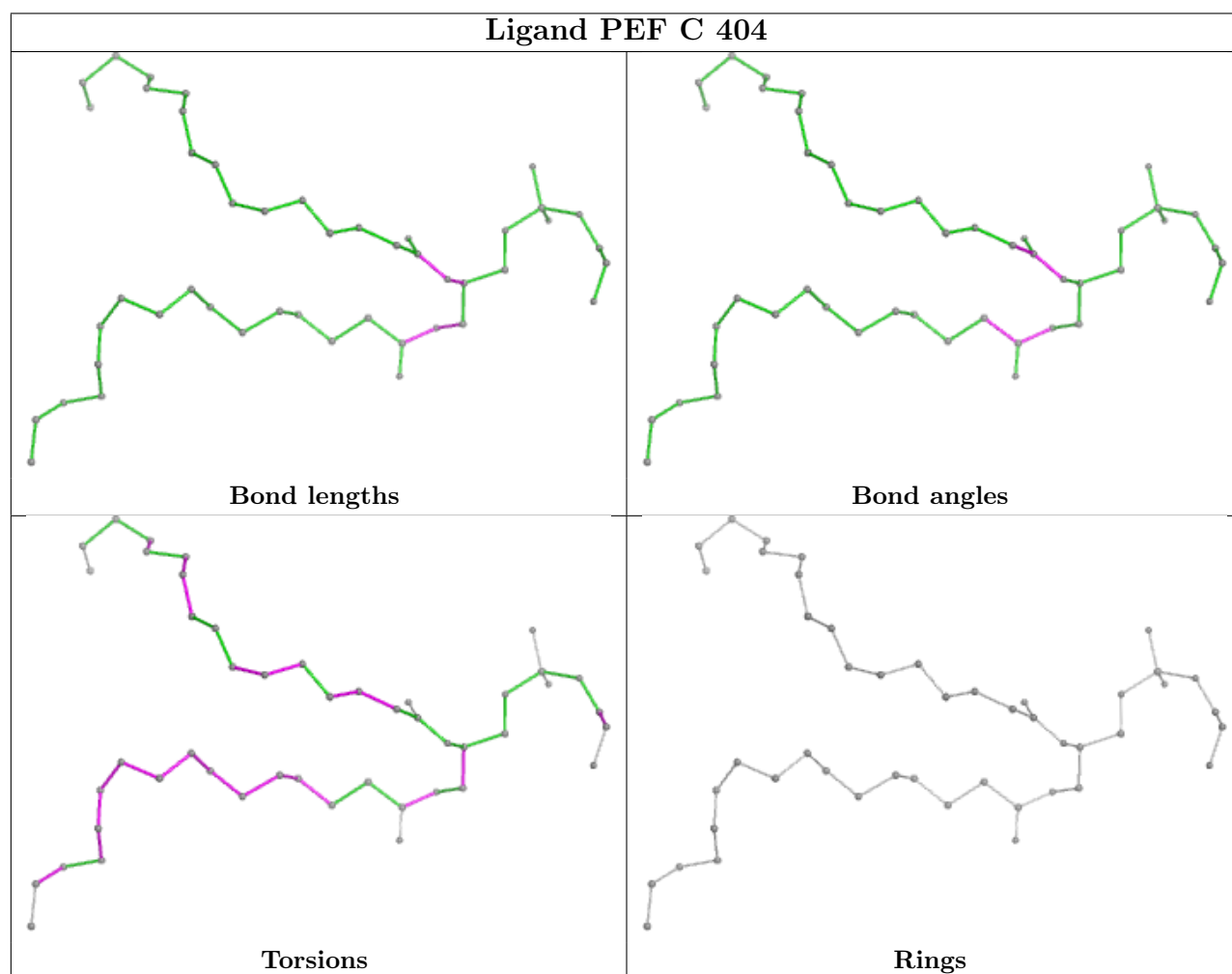
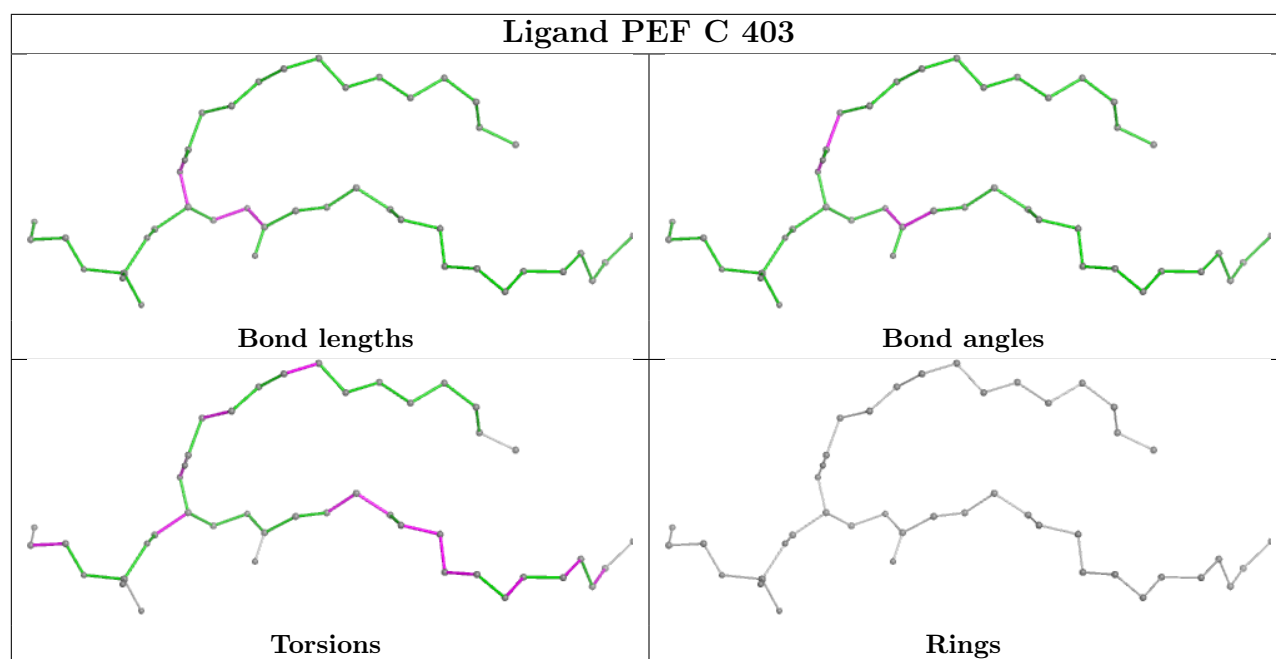


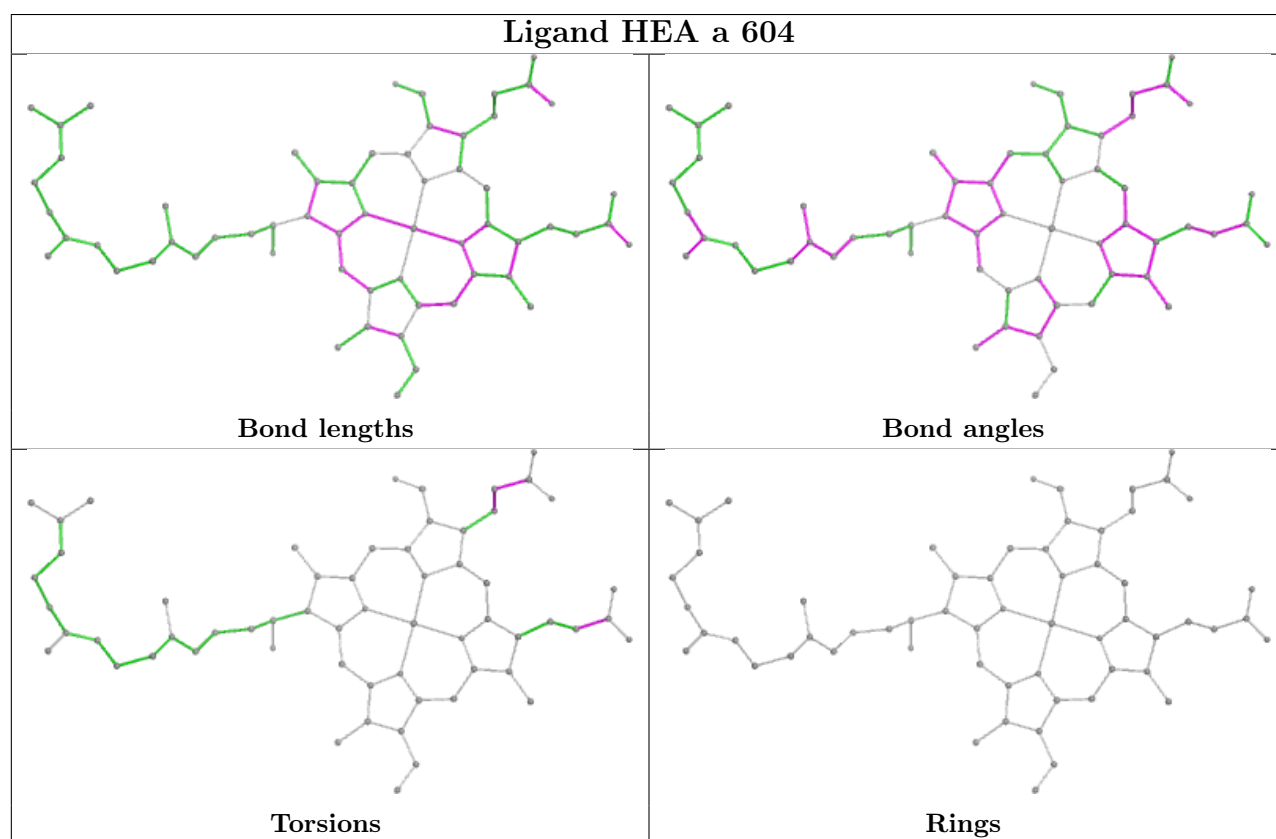
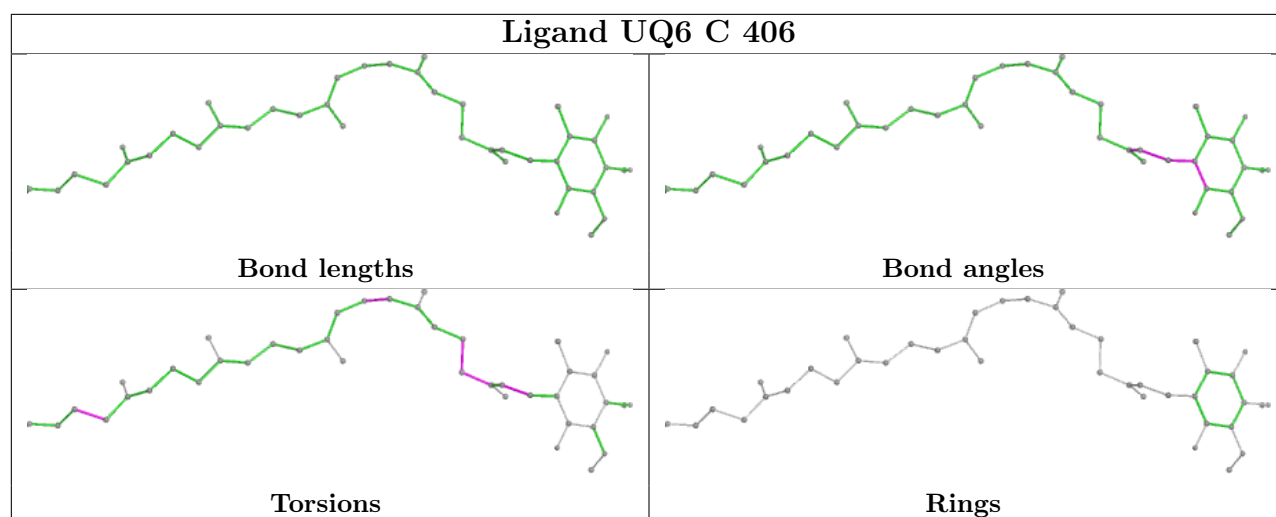
Ligand PEF P 303

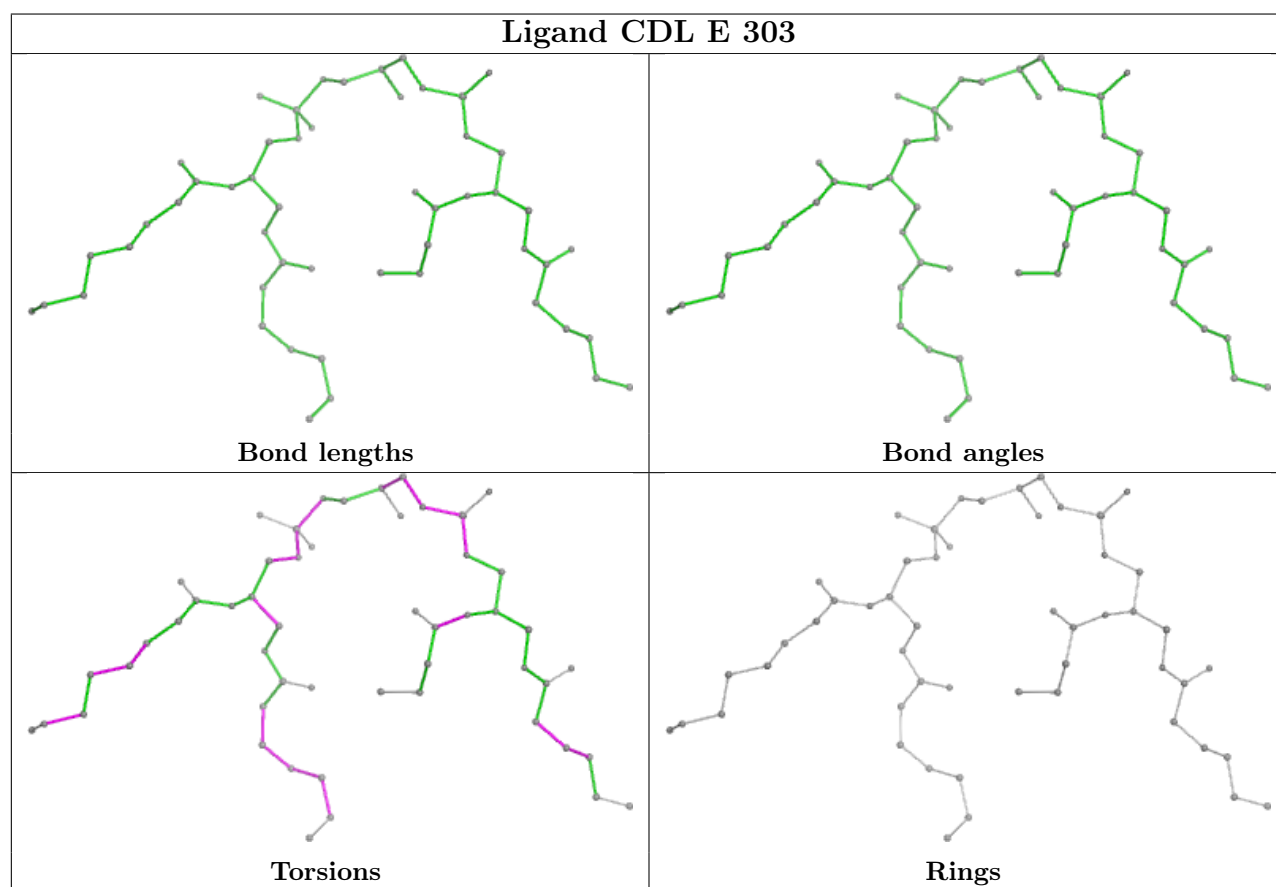
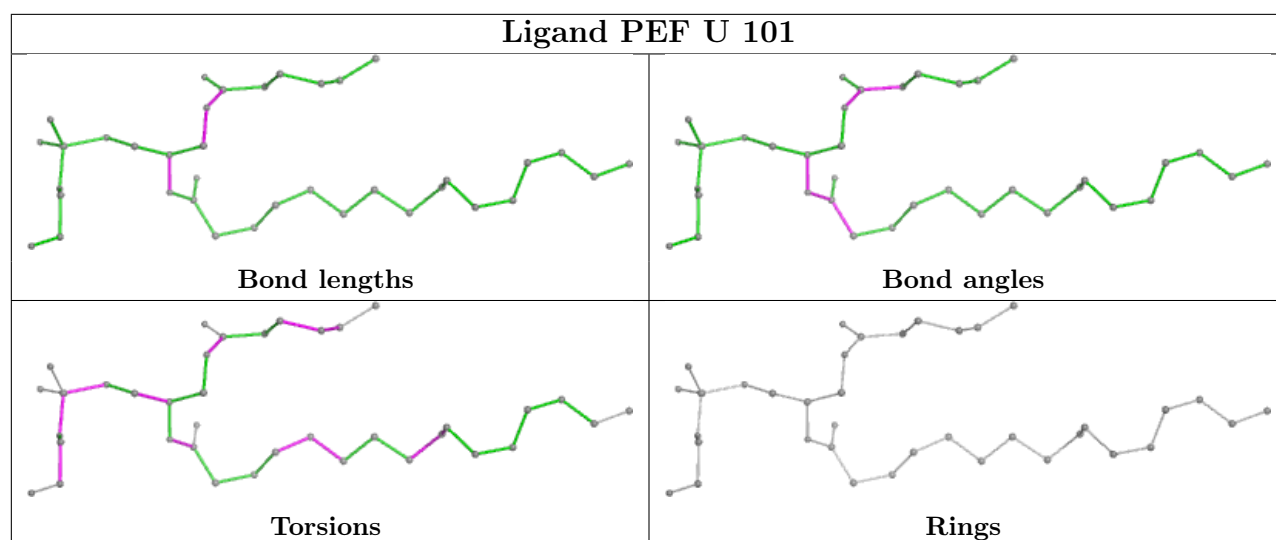


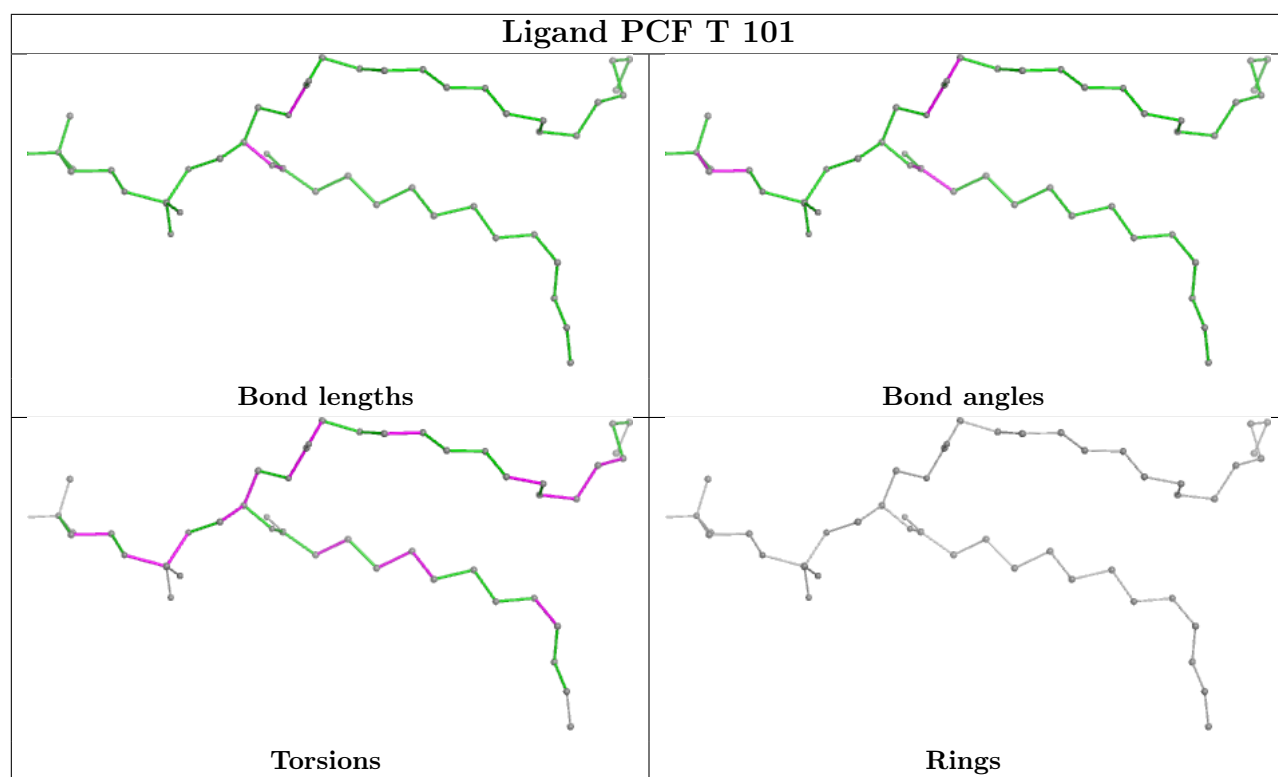


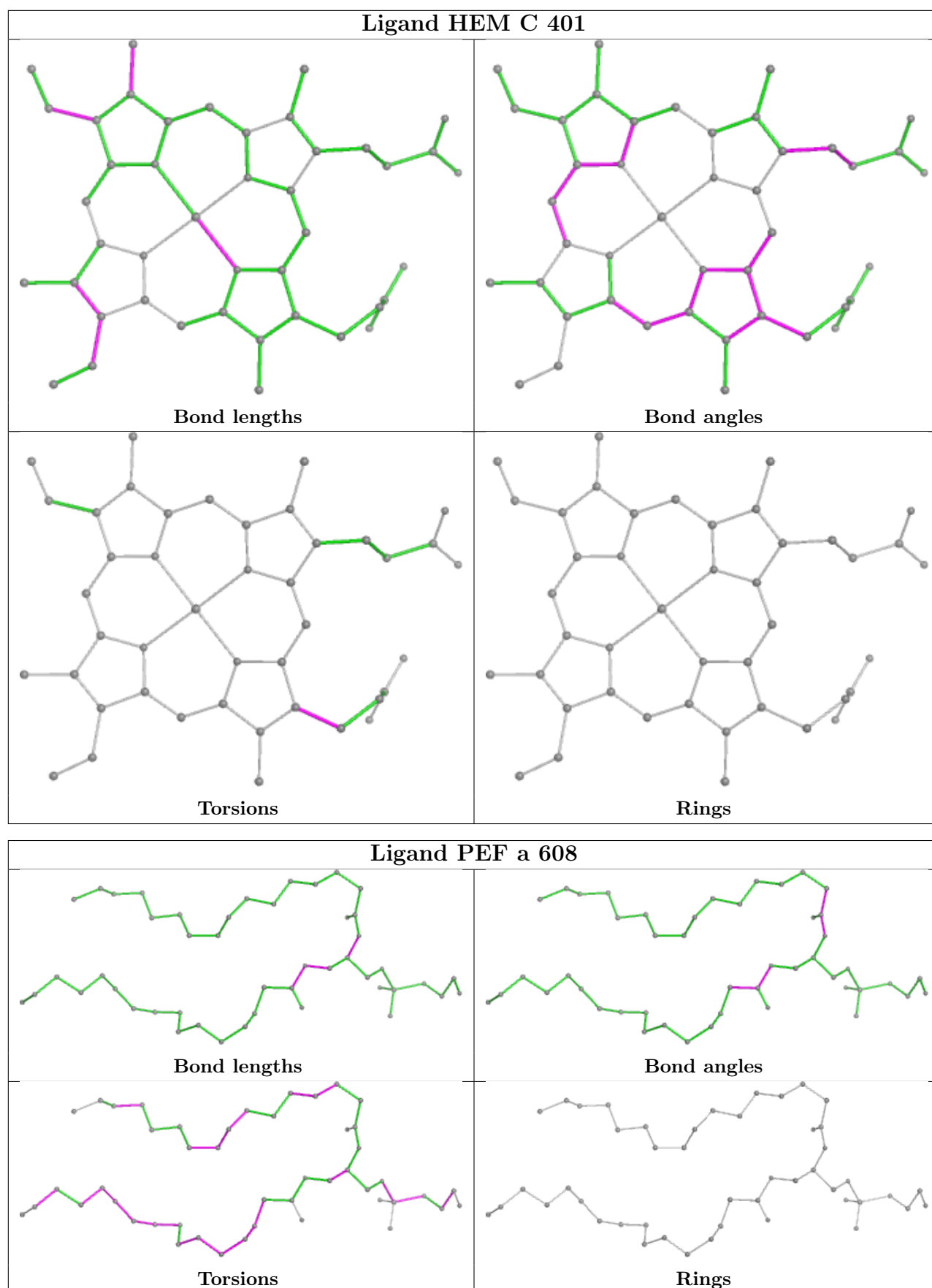


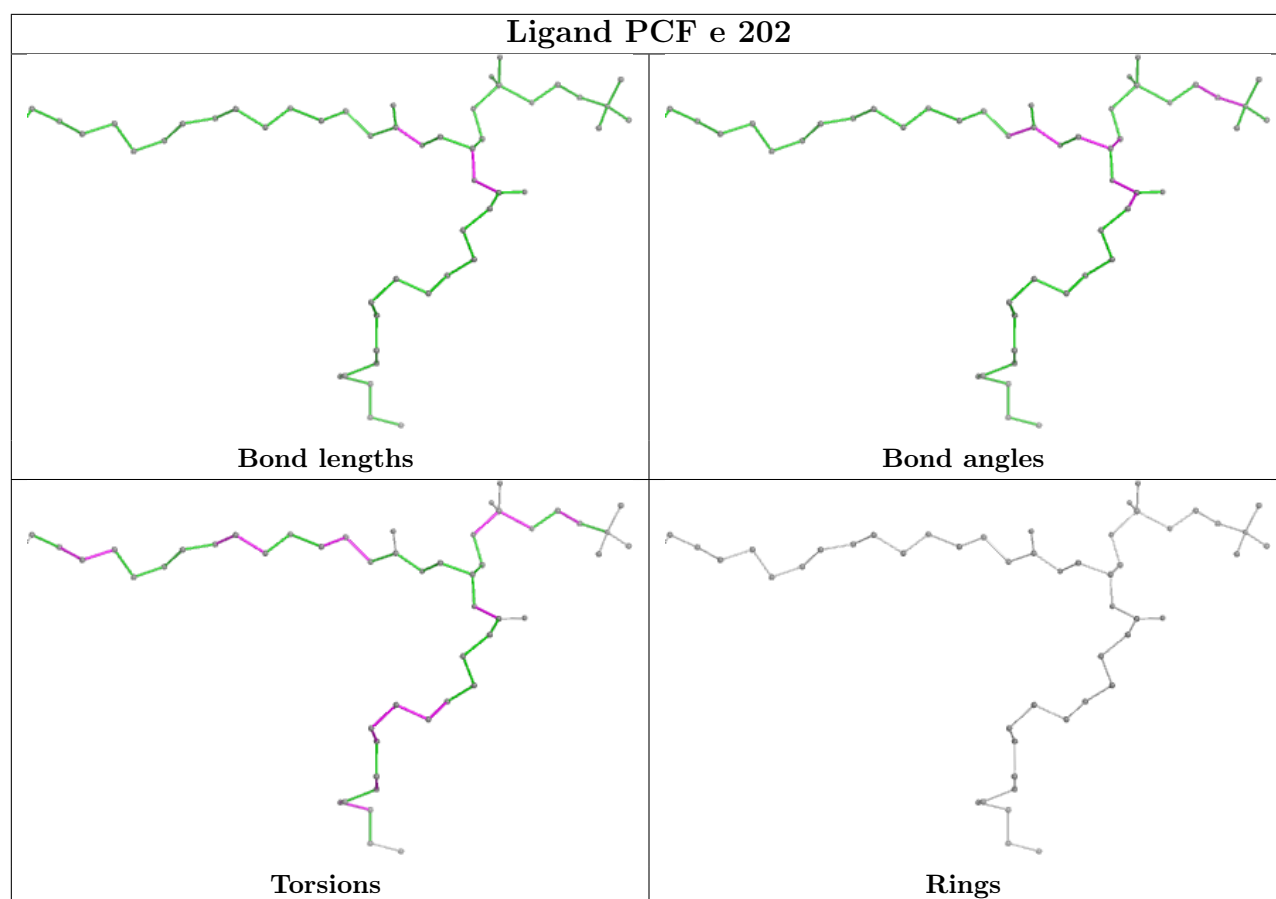


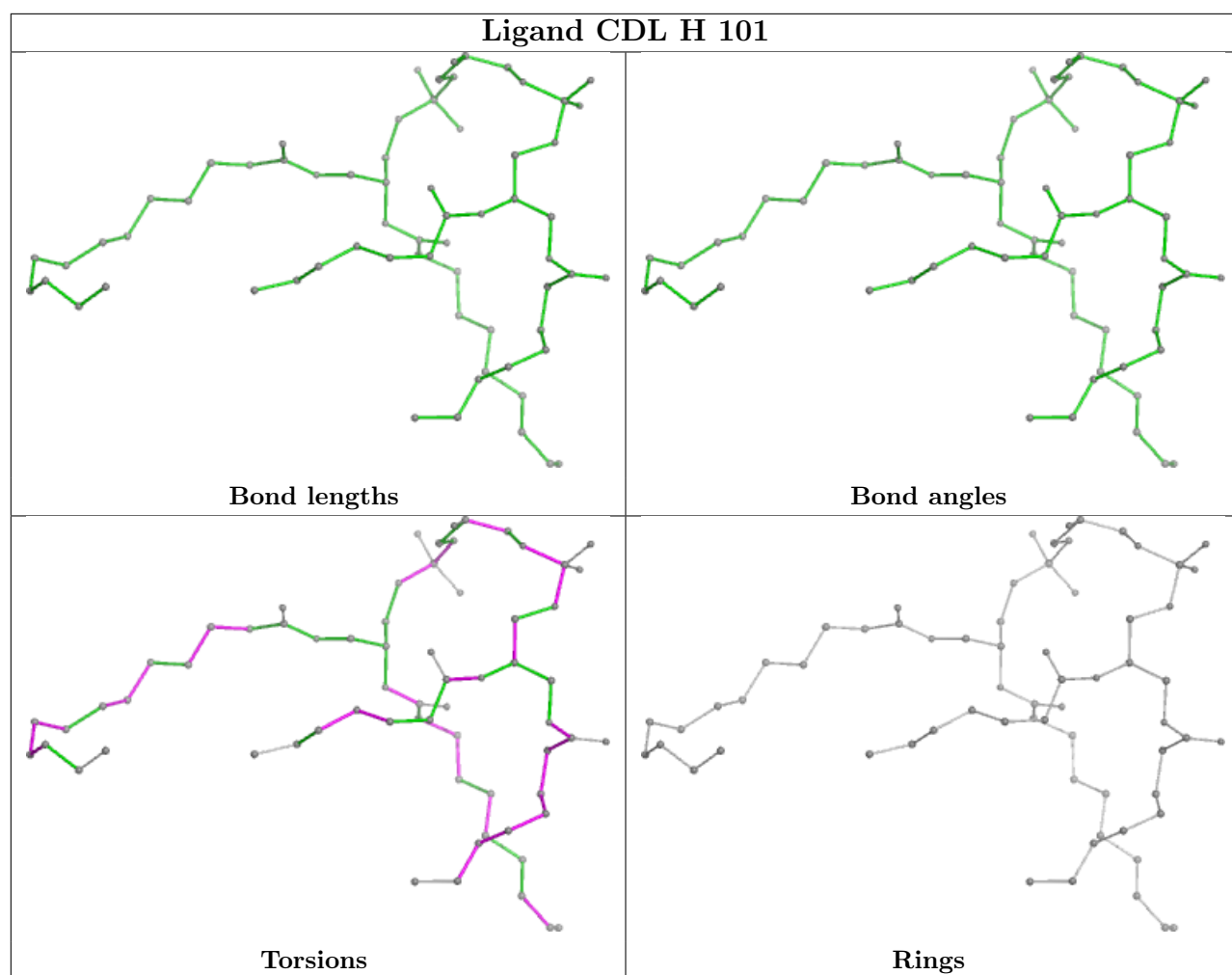


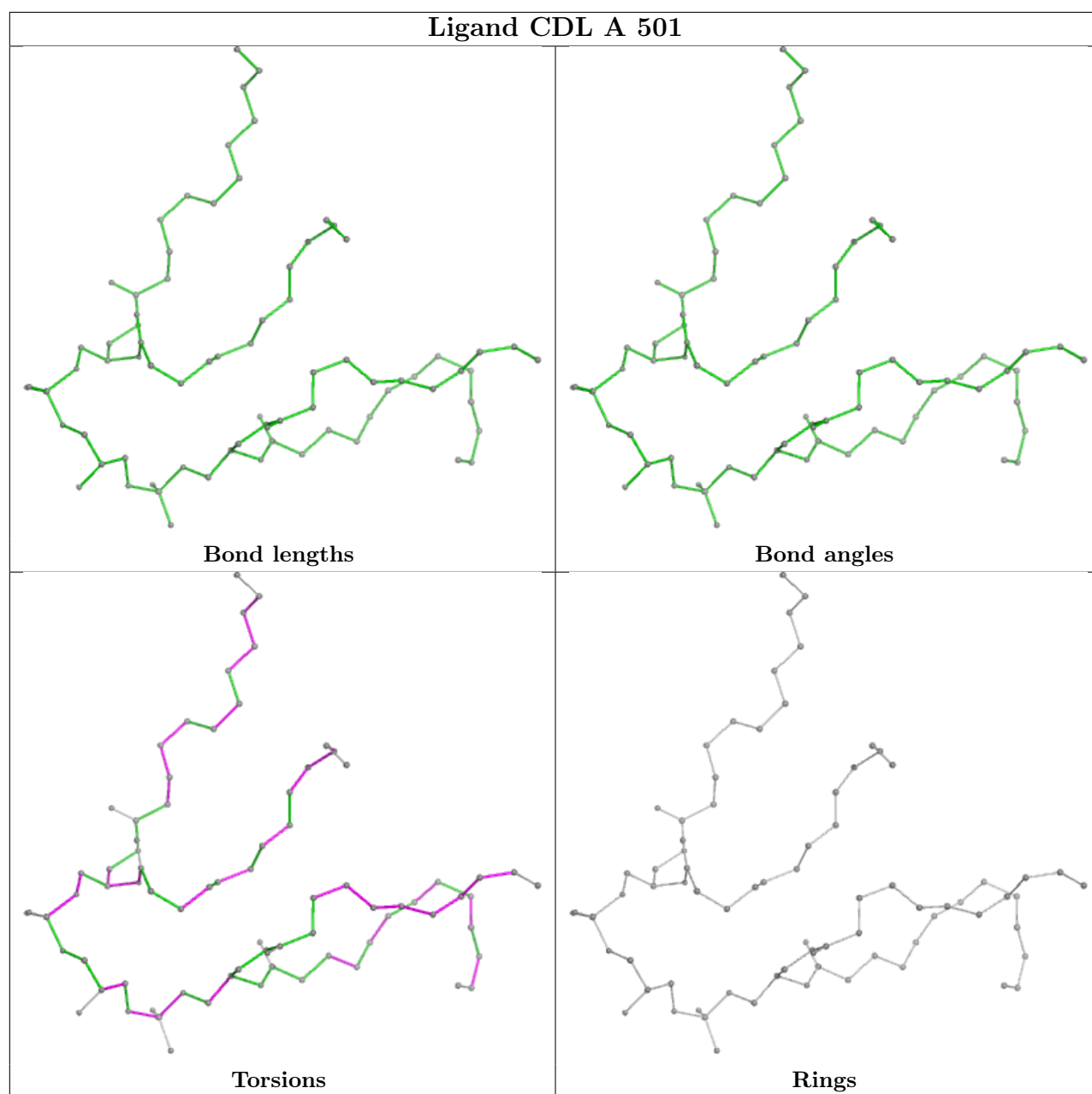


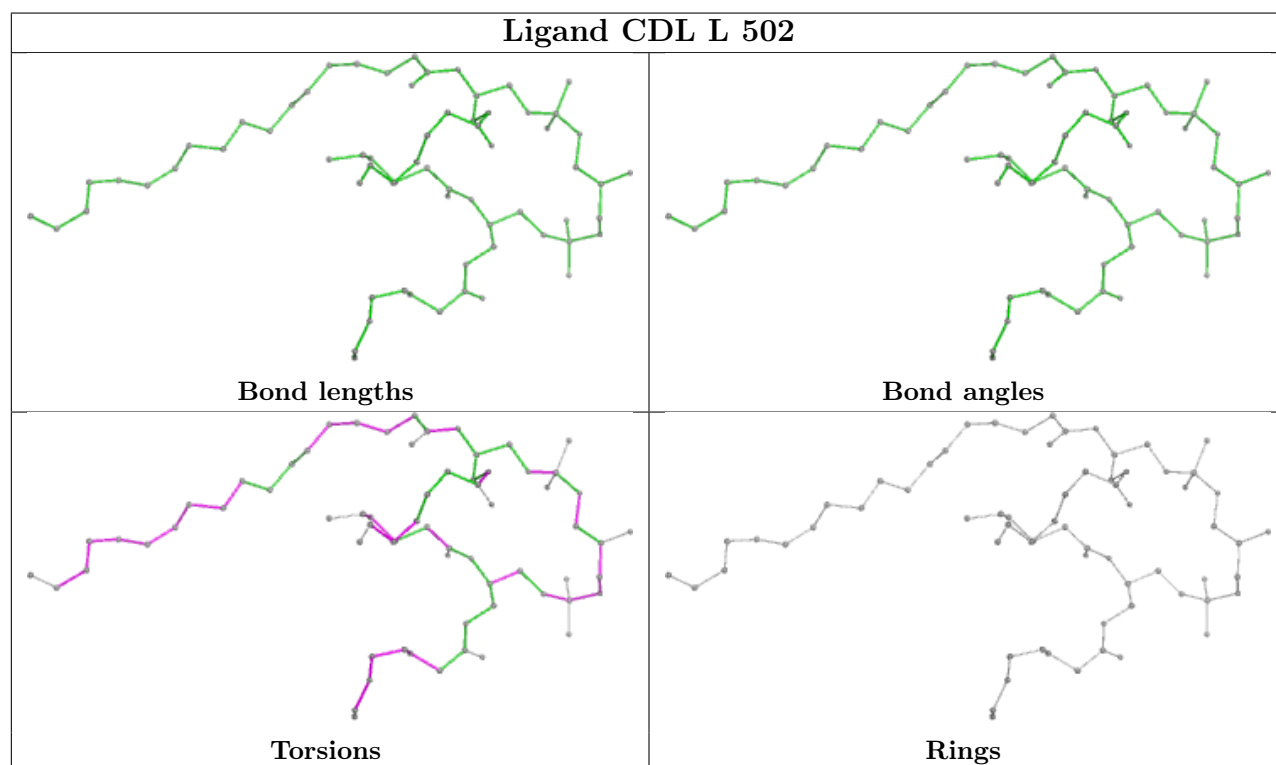
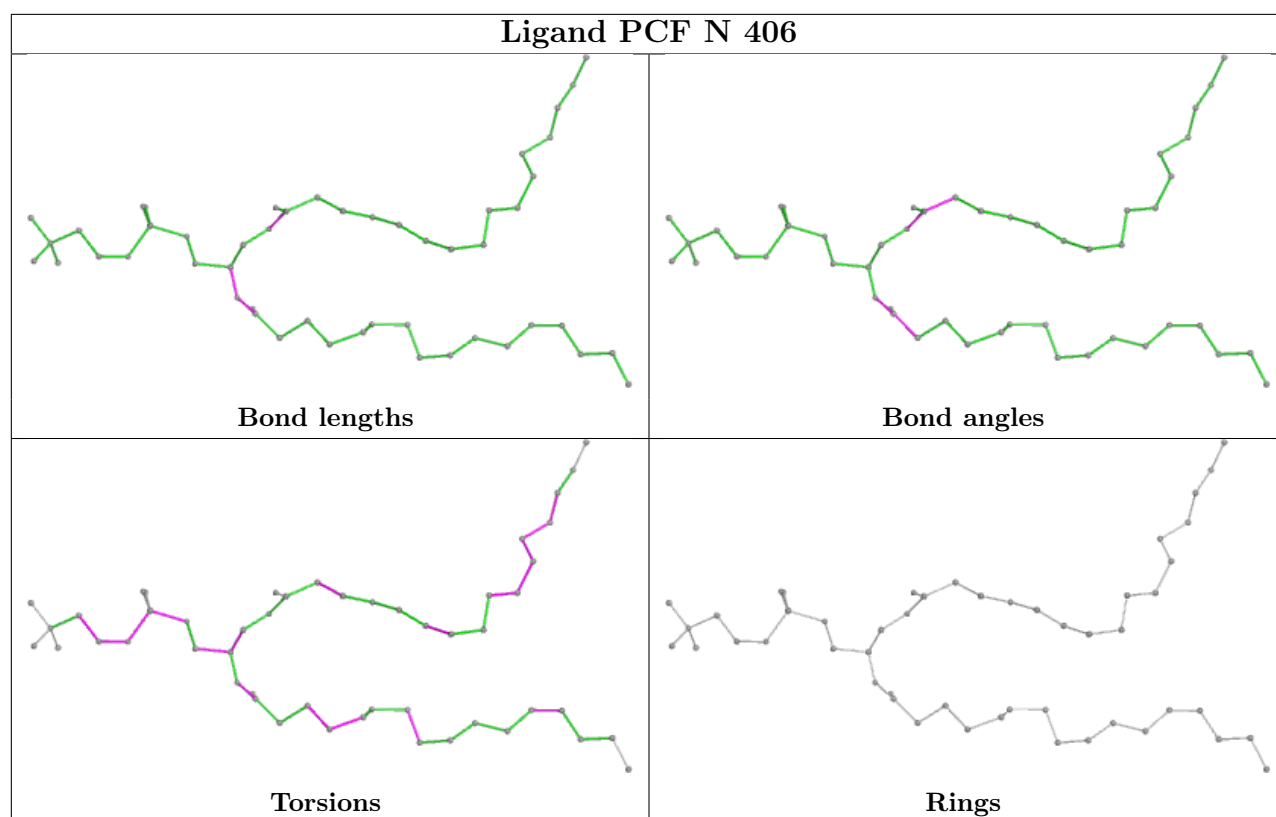


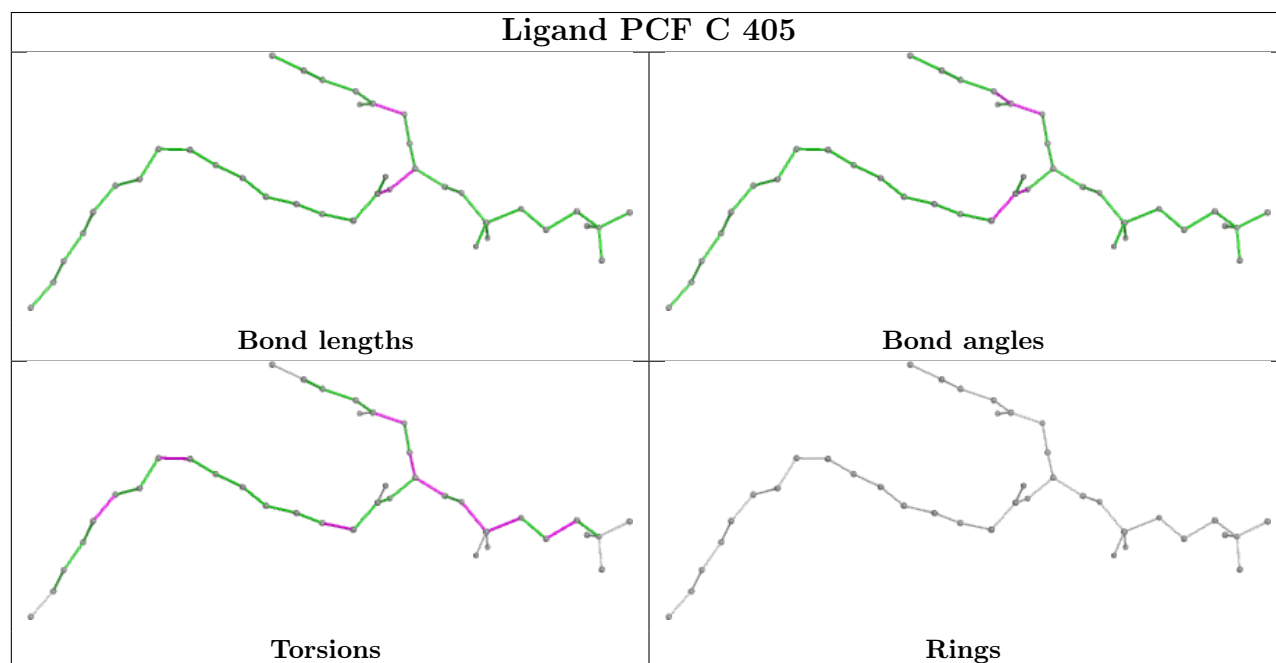
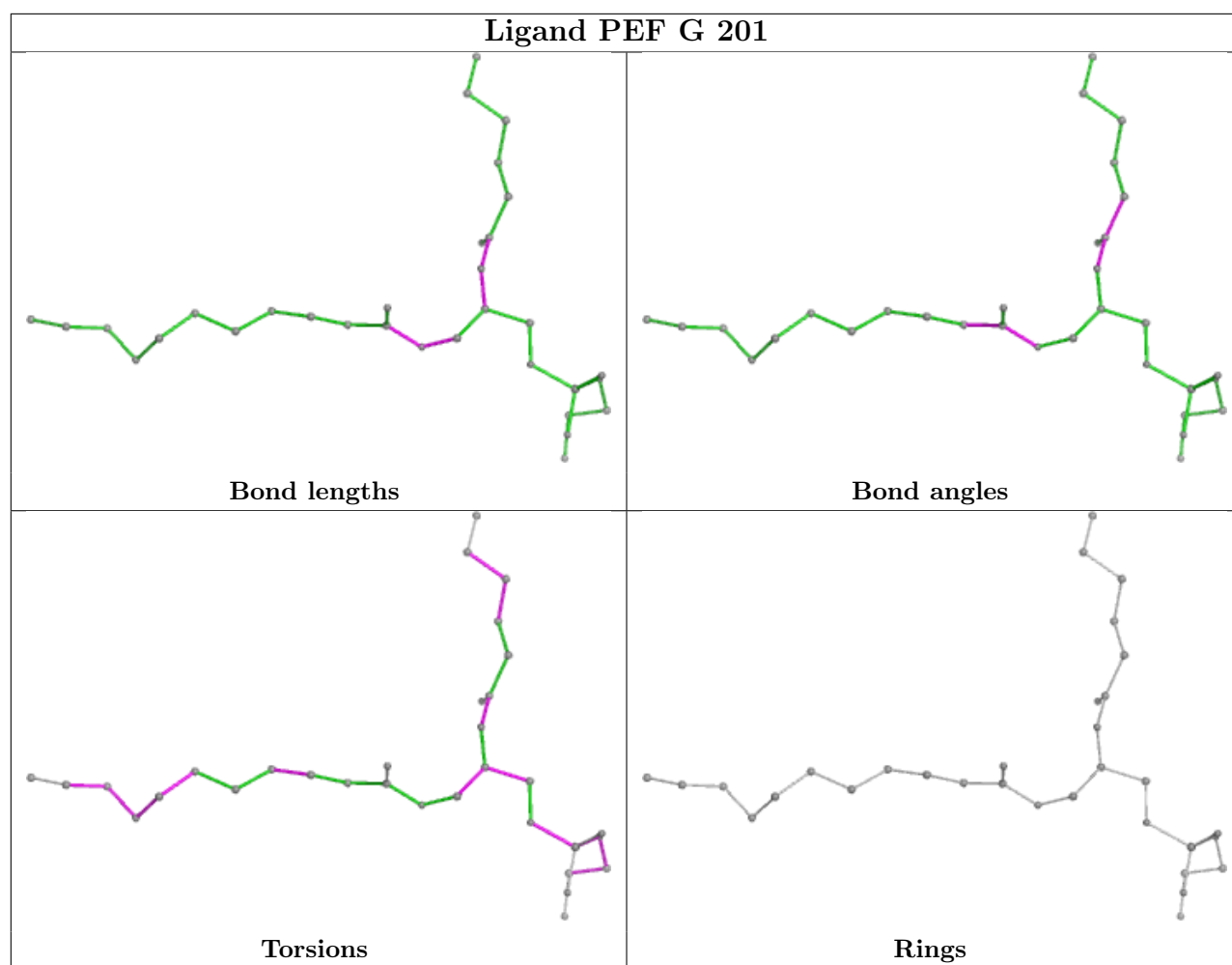


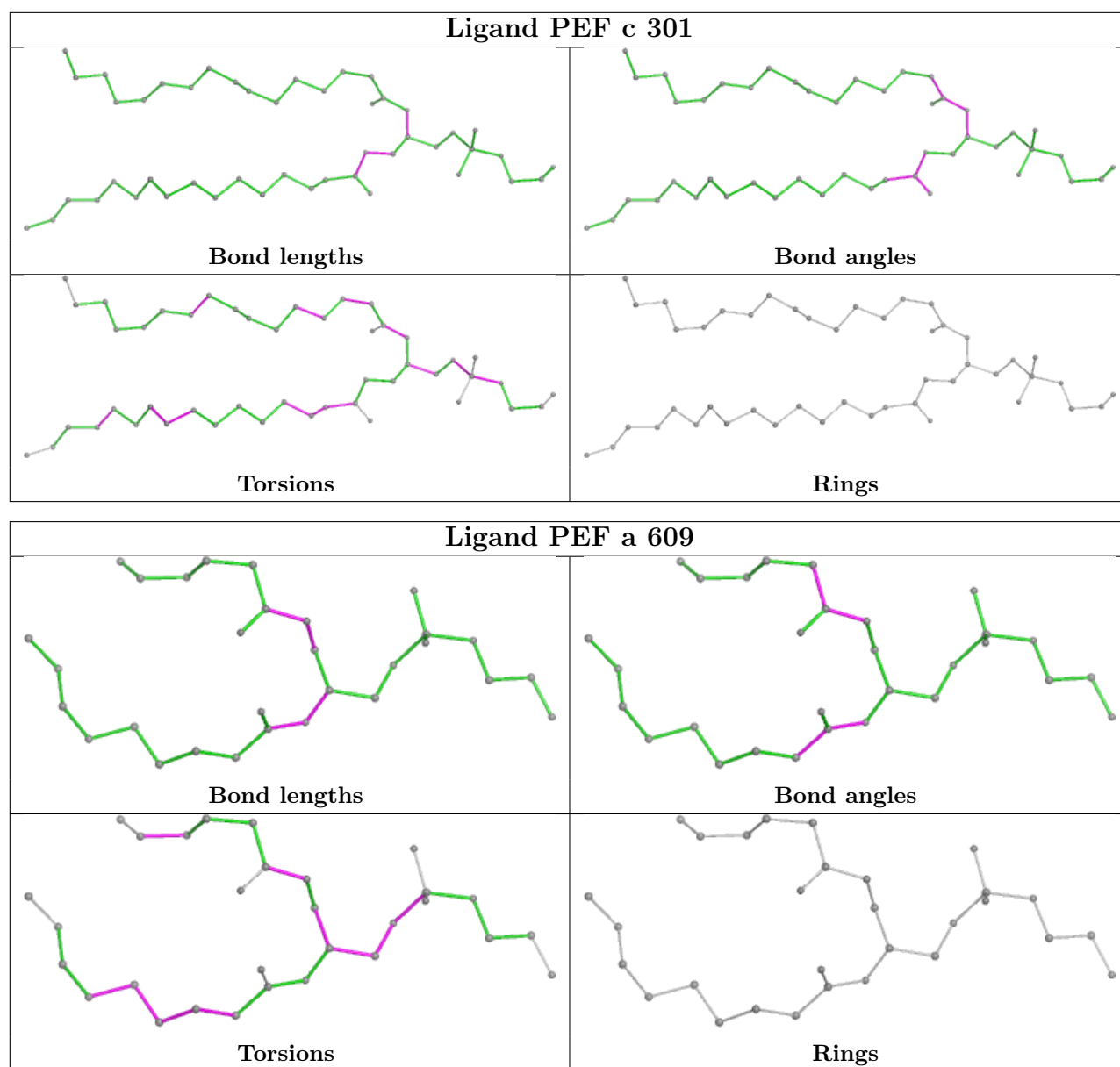


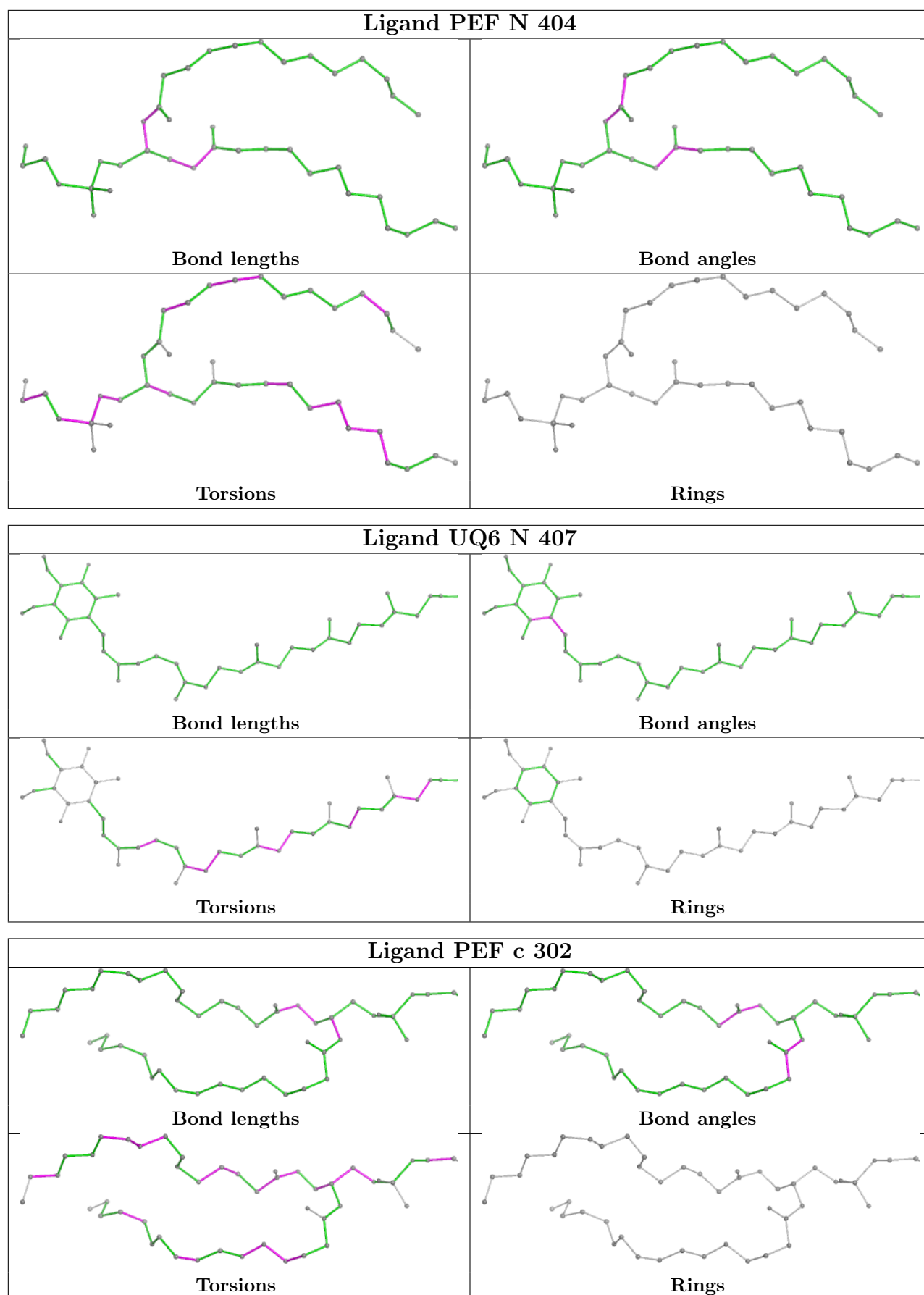


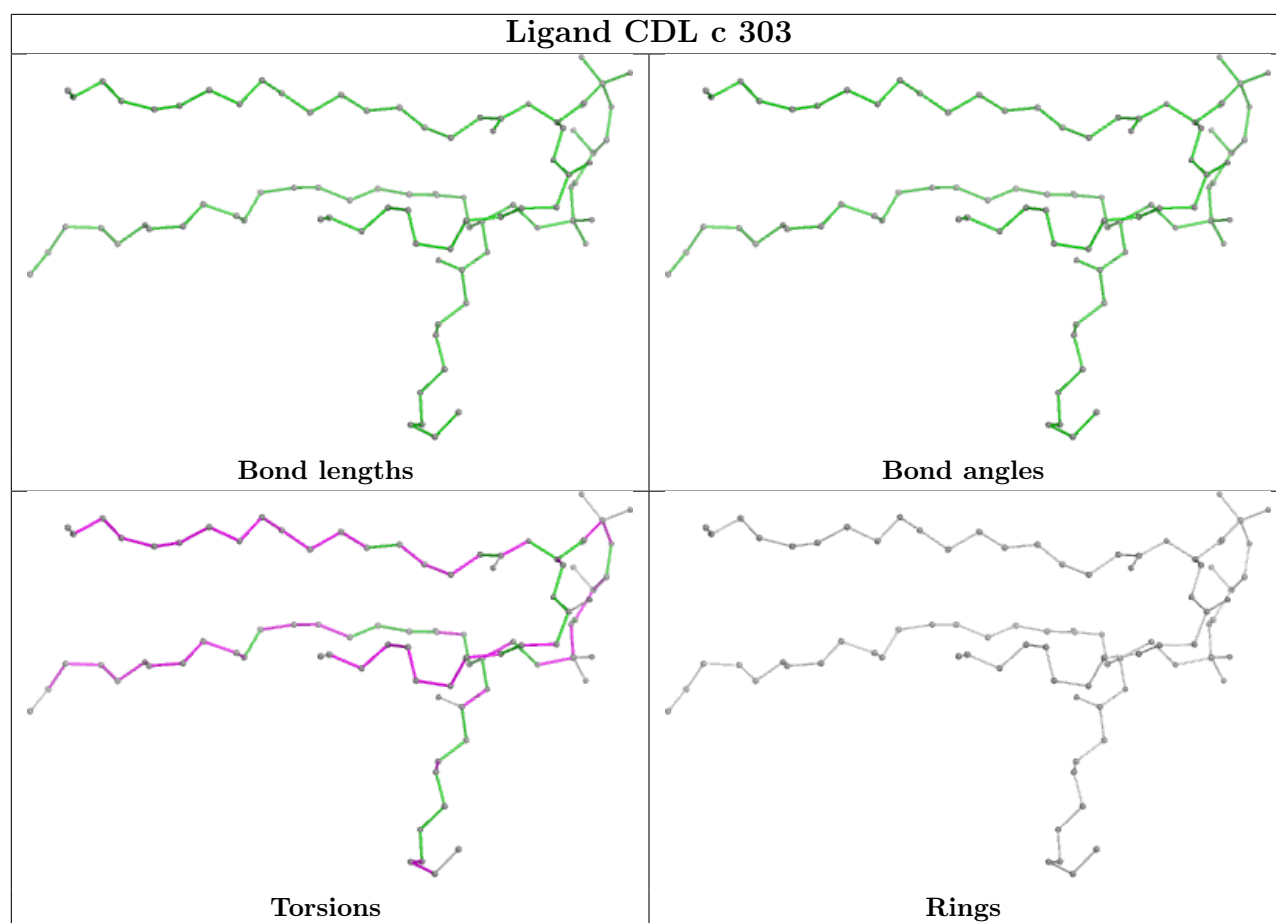












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

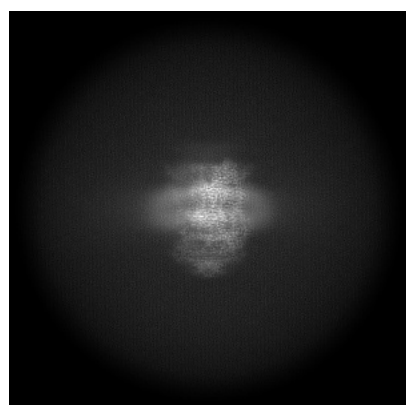
6 Map visualisation [i](#)

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.

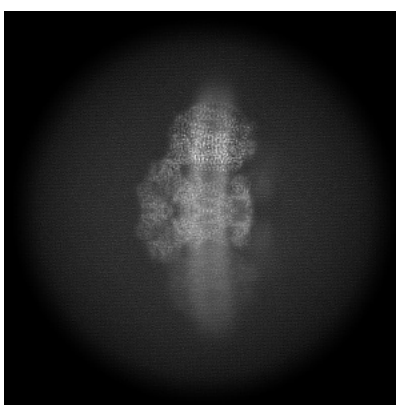
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

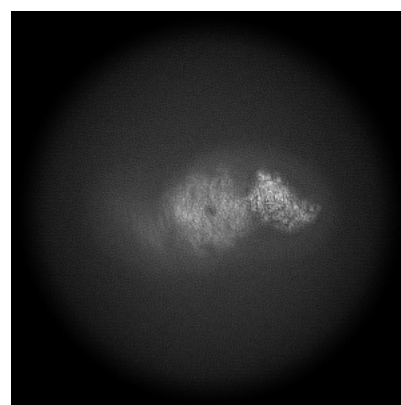
6.1.1 Primary map



X



Y

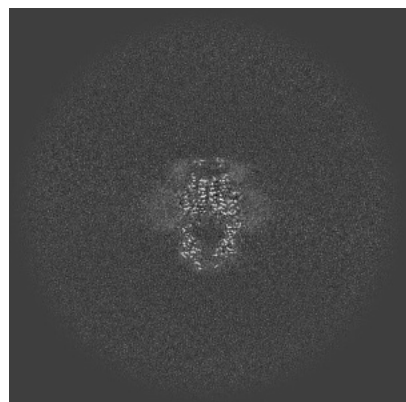


Z

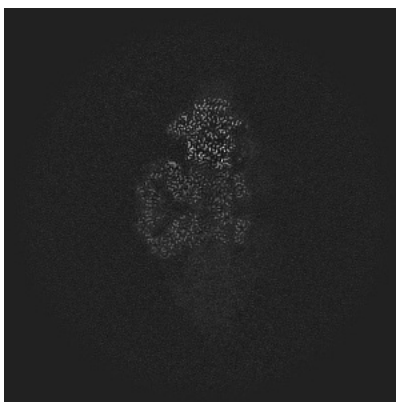
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

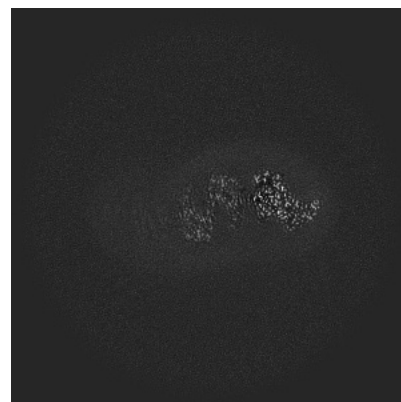
6.2.1 Primary map



X Index: 303



Y Index: 302

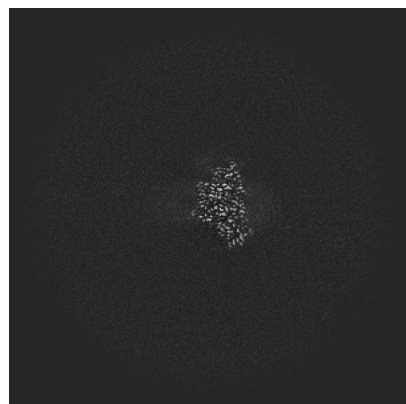


Z Index: 303

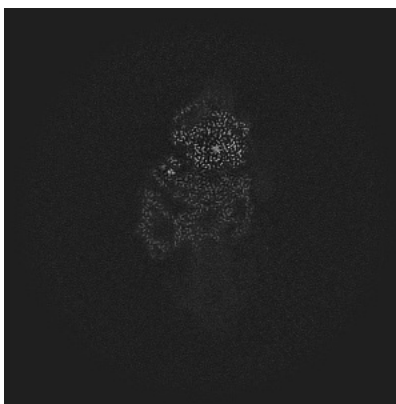
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

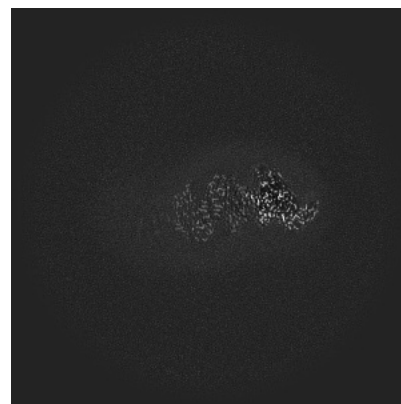
6.3.1 Primary map



X Index: 387



Y Index: 313

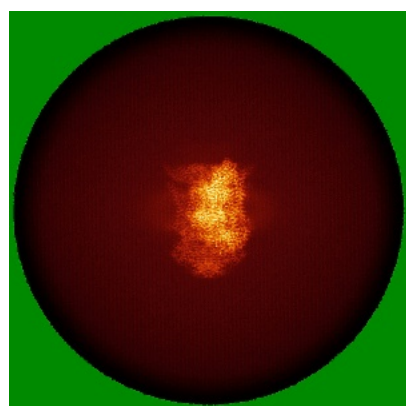


Z Index: 294

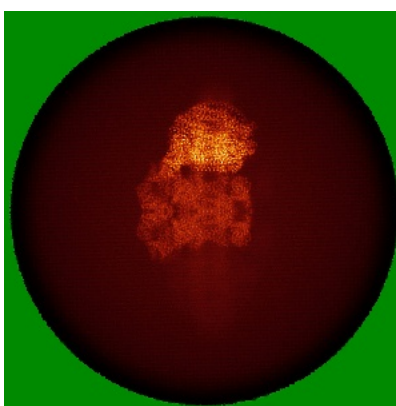
The images above show the largest variance slices of the map in three orthogonal directions.

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

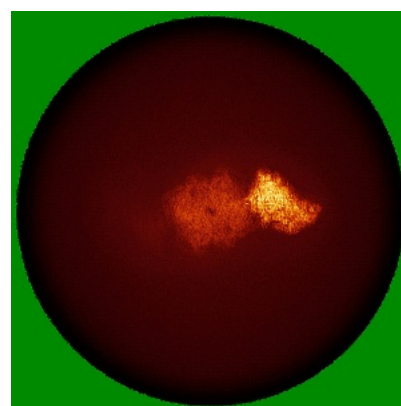
6.4.1 Primary map



X



Y

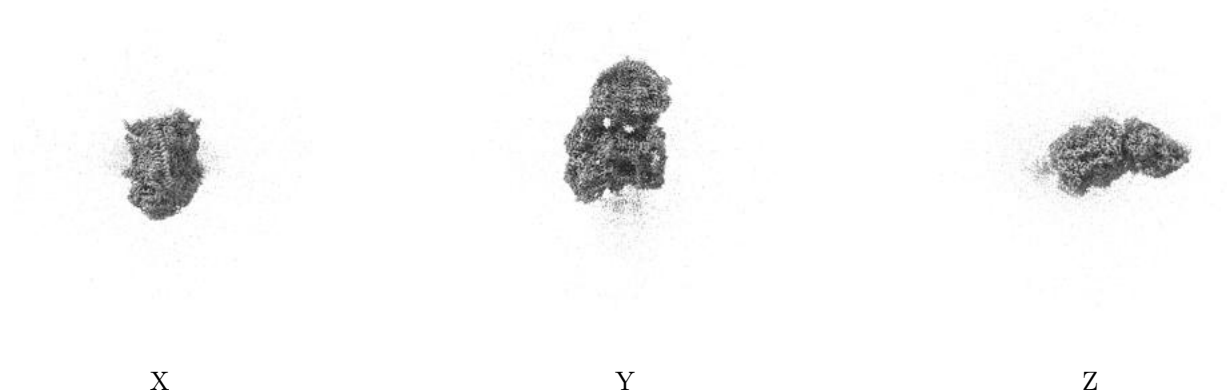


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

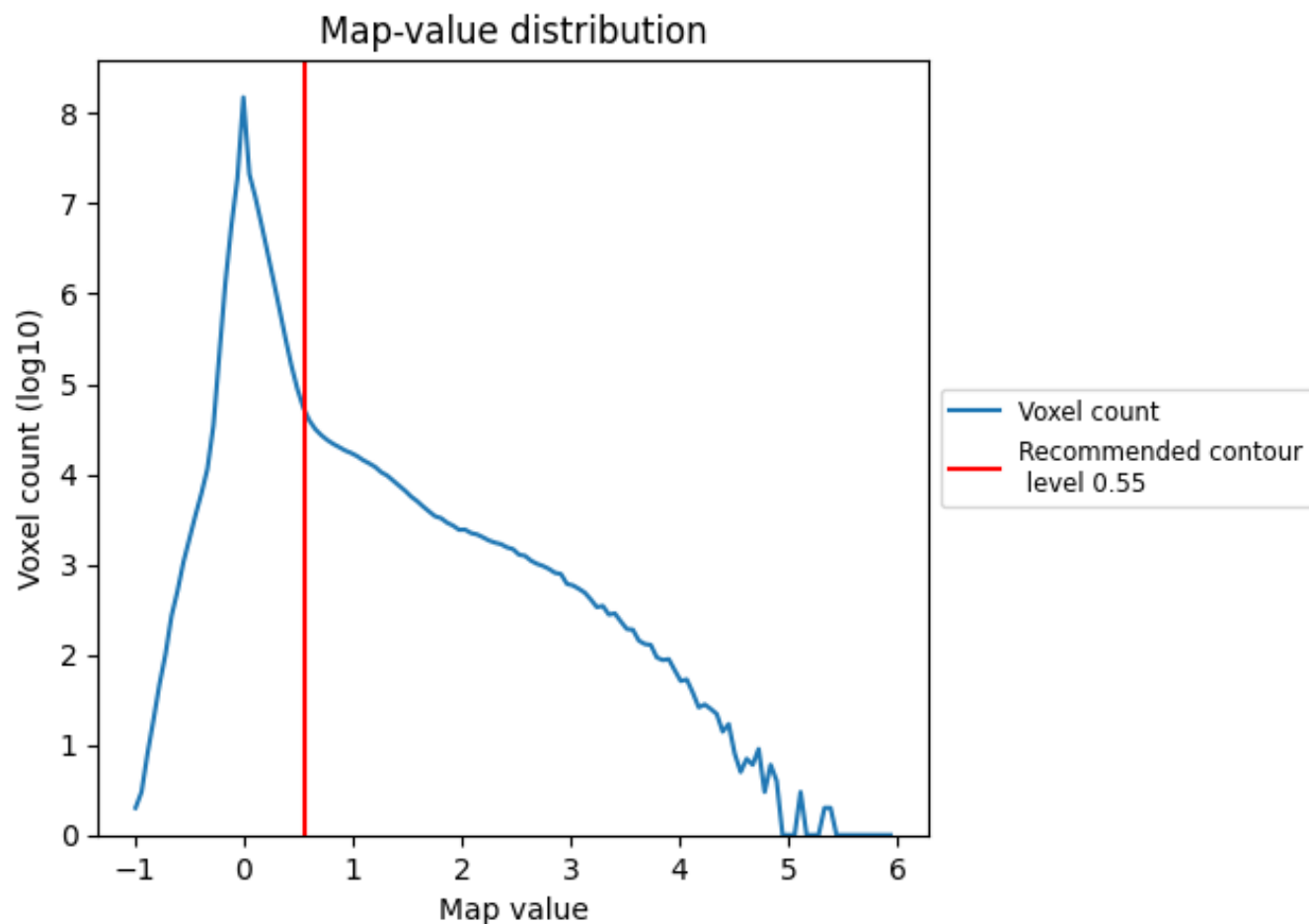
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

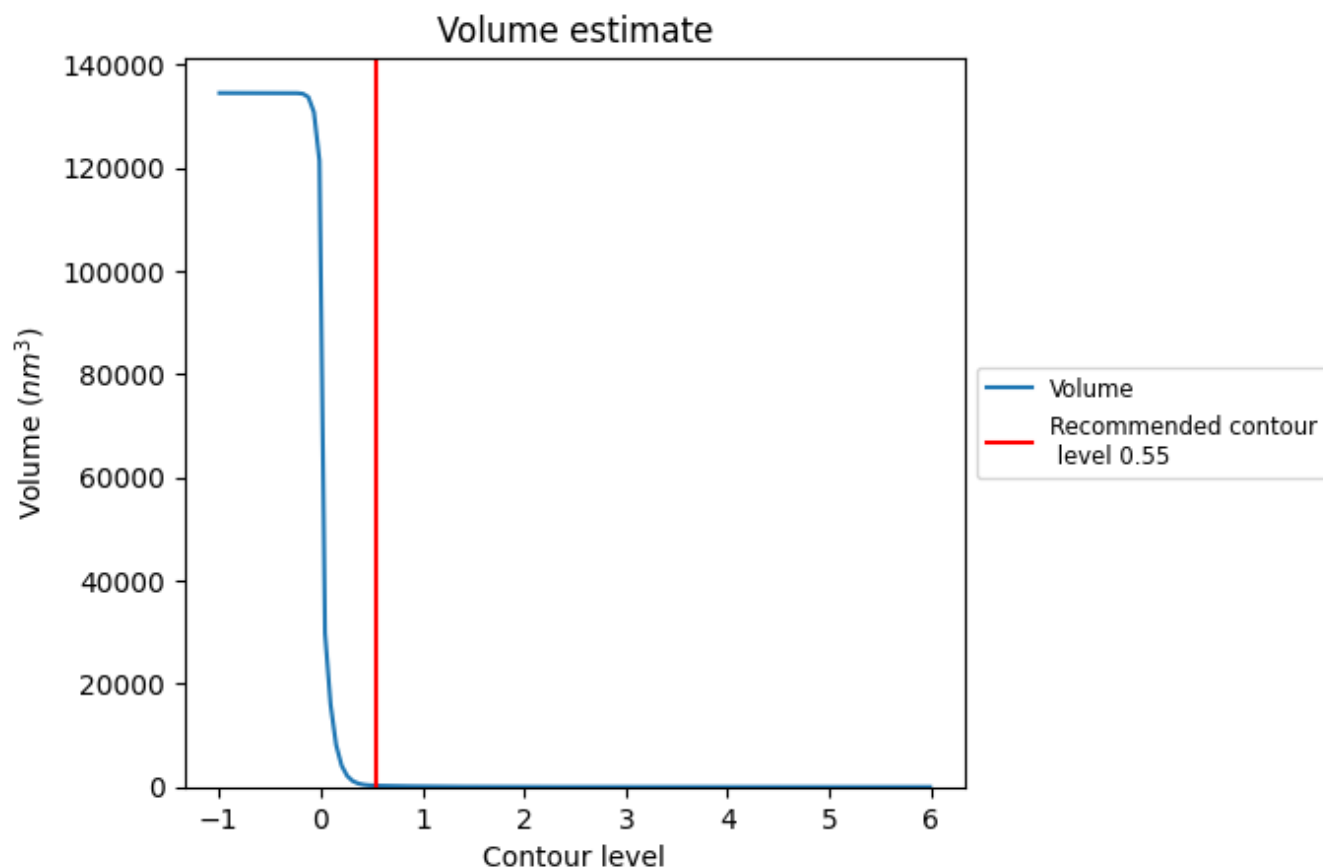
This section contains the results of statistical analysis of the map.

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 nm³; 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.

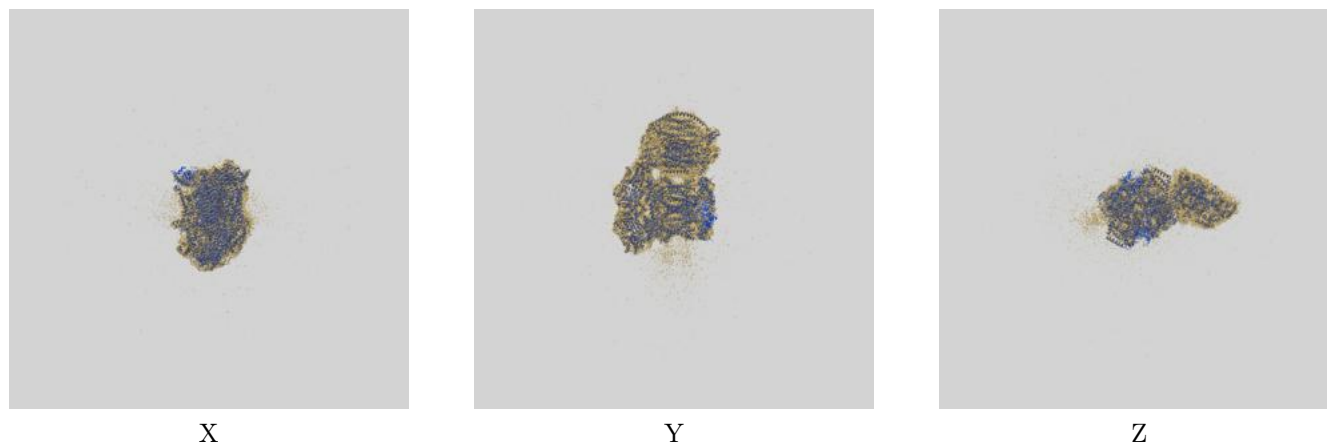
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

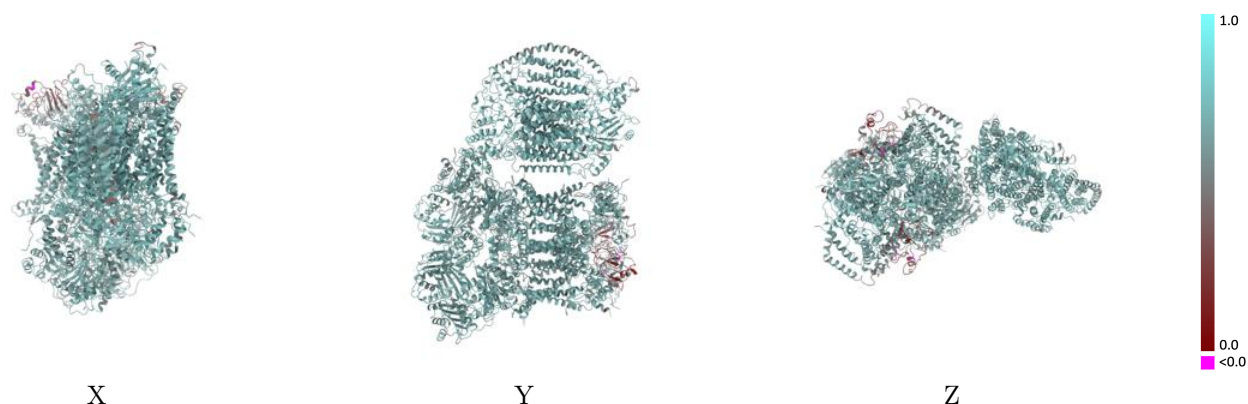
This section contains information regarding the fit between EMDB map EMD-19963 and PDB model 9ETZ. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



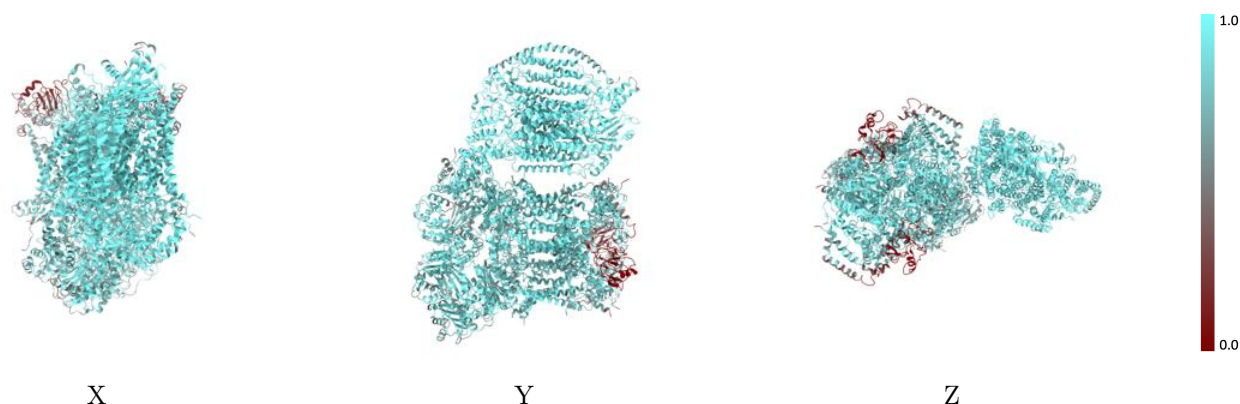
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



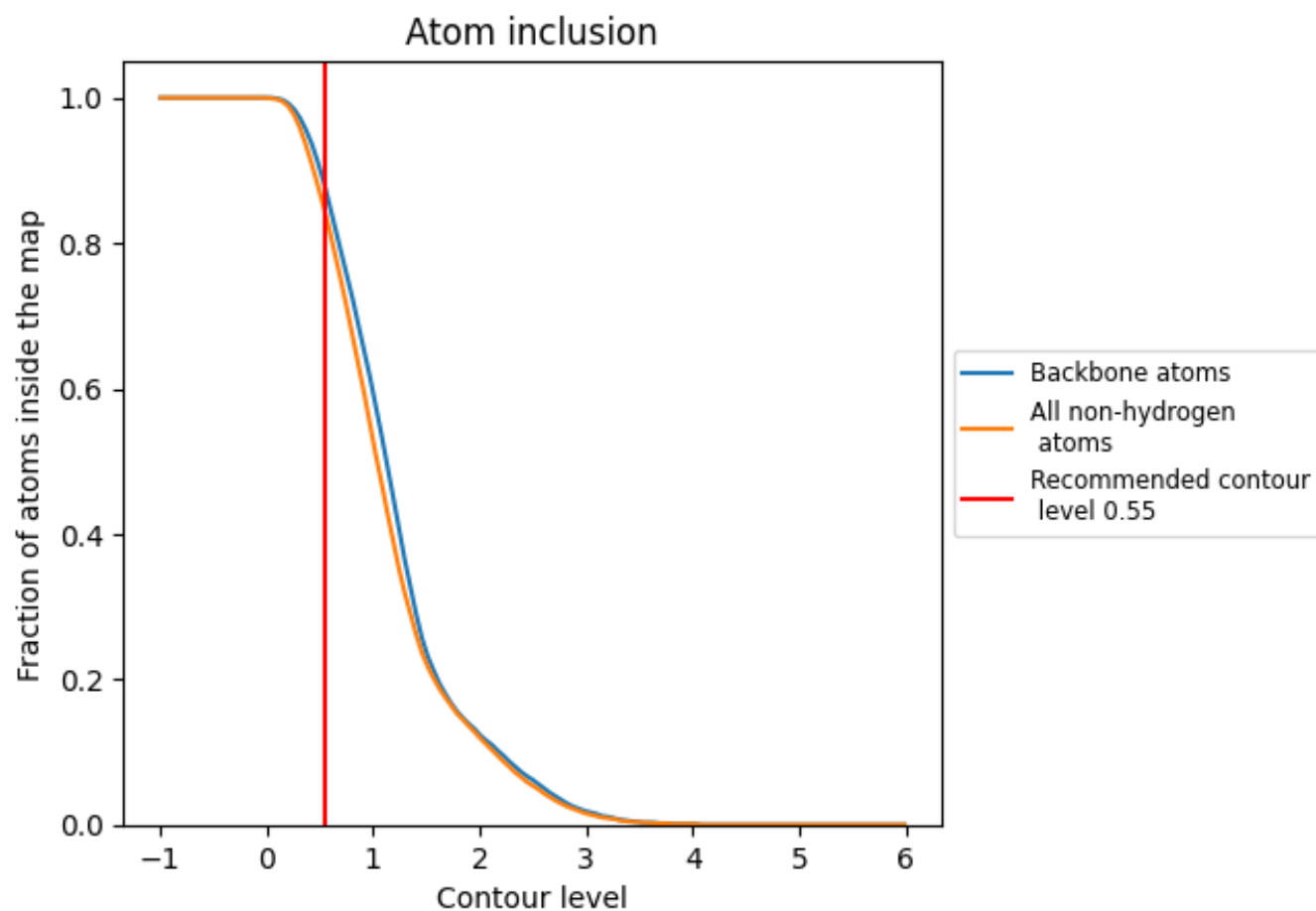
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).



































































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

