



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2025 – 10:55 am BST

PDB ID : 9IHR / pdb\_00009ihr  
EMDB ID : EMD-52878  
Title : Closed state with NUQM and with flavoprotein (classification state 1) of Pichia pastoris mitochondrial complex I in cMSP26 nanodiscs  
Authors : Grba, D.N.; Hirst, J.  
Deposited on : 2025-02-21  
Resolution : 2.80 Å(reported)  
Based on initial model : .

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

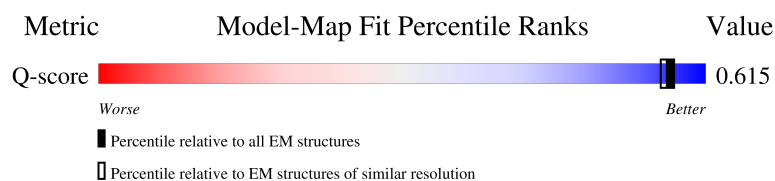
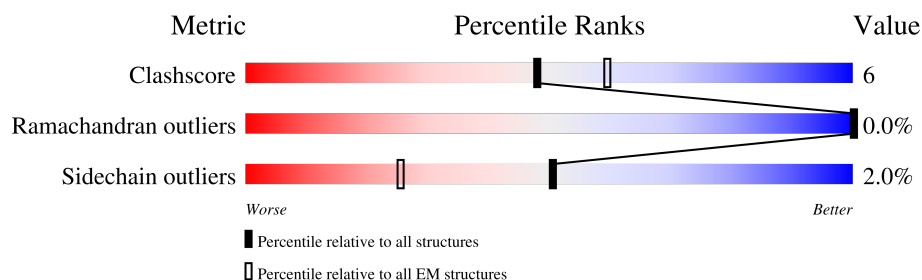
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*





The reported resolution of this entry is 2.80 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.








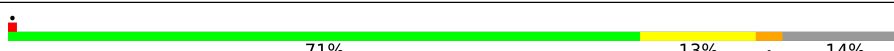
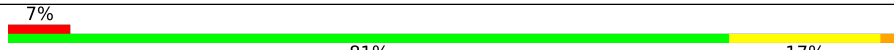

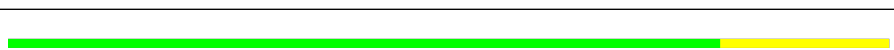

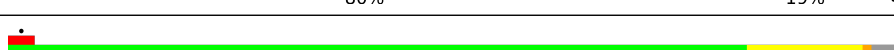
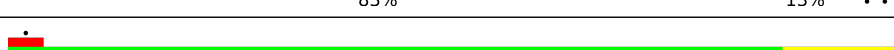

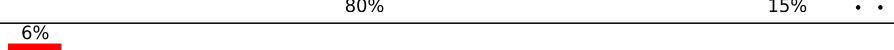
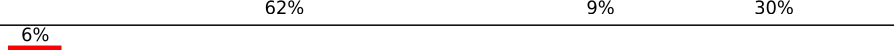
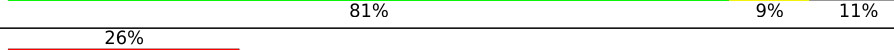





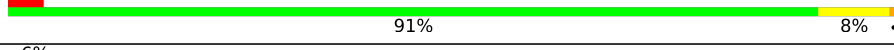
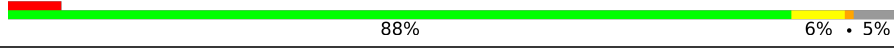


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11806 ( 2.30 - 3.30 )

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  $\geq 3$ , 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	1	190	
2	A	141	
3	B	204	
4	C	289	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	482	
6	E	241	
7	F	473	
8	G	726	
9	H	353	
10	I	222	
11	J	161	
12	K	82	
13	L	642	
14	M	491	
15	N	523	
16	O	193	
17	P	384	
18	Q	159	
19	R	139	
20	S	90	
21	T	138	
22	U	130	
23	V	134	
24	W	122	
25	X	184	
26	Y	216	
27	Z	147	
28	a	150	
29	b	79	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	c	182	
31	d	78	
32	e	106	
33	f	86	
34	g	239	
35	h	182	
36	i	74	
37	j	59	
38	k	61	
39	l	156	
40	m	81	
41	n	111	
42	o	87	
43	p	92	
44	q	140	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	SF4	F	501	-	-	X	-
46	SF4	I	302	-	-	X	-

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 70216 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 Altered inheritance of mitochondria protein 41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	169	Total	C	N	O	S	0	0
			1383	879	231	272	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	141	Total	C	N	O	S	0	0
			1133	764	166	199	4		

- Molecule 3 is a protein called BA75\_00622T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	175	Total	C	N	O	S	0	0
			1407	901	241	249	16		

- Molecule 4 is a protein called NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	240	Total	C	N	O	S	0	0
			1970	1273	331	361	5		

- Molecule 5 is a protein called NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	451	Total	C	N	O	S	0	0
			3621	2310	619	674	18		

- Molecule 6 is a protein called NUHM (24 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	183	Total	C	N	O	S	0	0
			1446	920	239	273	14		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	453	Total	C	N	O	S	0	0
			3500	2213	612	654	21		

- Molecule 8 is a protein called NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	696	Total	C	N	O	S	0	0
			5344	3345	939	1037	23		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	353	Total	C	N	O	S	0	0
			2809	1903	414	478	14		

- Molecule 10 is a protein called NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	192	Total	C	N	O	S	0	0
			1556	988	259	299	10		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	161	Total	C	N	O	S	0	0
			1313	878	180	252	3		

- Molecule 12 is a protein called NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	80	Total	C	N	O	S	0	0
			617	400	93	118	6		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	642	Total	C	N	O	S	0	0
			5115	3454	766	866	29		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	491	Total	C	N	O	S	0	0
			3868	2597	593	663	15		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	506	Total	C	N	O	S	0	0
			4045	2723	594	714	14		

- Molecule 16 is a protein called NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	193	Total	C	N	O	S	0	0
			1575	1019	257	294	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	ACE	-	acetylation	UNP E1UWB9

- Molecule 17 is a protein called NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	368	Total	C	N	O	S	0	0
			2922	1862	510	547	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	112	Total	C	N	O	S	0	0
			924	585	161	176	2		

- Molecule 19 is a protein called NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	124	Total	C	N	O	S	0	0
			978	610	179	186	3		

- Molecule 20 is a protein called NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	90	Total	C	N	O		0	0
			697	454	117	126			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	ACE	-	acetylation	UNP E1UWD3

- Molecule 21 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	95	Total	C	N	O	S	0	0
			745	467	119	158	1		

- Molecule 22 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	88	Total	C	N	O		0	0
			681	427	102	152			

- Molecule 23 is a protein called NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	126	Total	C	N	O	S	0	0
			1025	658	165	201	1		

- Molecule 24 is a protein called BA75\_04796T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	115	Total	C	N	O	S	0	0
			979	626	177	171	5		



- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	184	Total	C	N	O	S	0	0
			1450	905	253	282	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	0	ACE	-	acetylation	UNP E1UWB8

- Molecule 26 is a protein called NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	205	Total	C	N	O	S	0	0
			1578	1012	274	289	3		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	142	Total	C	N	O	S	0	0
			1176	758	212	202	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	ACE	-	acetylation	UNP E1UWD8

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	149	Total	C	N	O	S	0	0
			1215	756	228	225	6		

- Molecule 29 is a protein called NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	78	Total	C	N	O	S	0	0
			641	419	111	109	2		

- Molecule 30 is a protein called BA75\_00589T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	182	Total	C	N	O	S	0	0
			1418	902	248	266	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	0	ACE	-	acetylation	UNP E1UWC1

- Molecule 31 is a protein called Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	75	Total	C	N	O	S	0	0
			616	406	106	103	1		

- Molecule 32 is a protein called BA75\_05084T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	105	Total	C	N	O	S	0	0
			848	531	154	157	6		

- Molecule 33 is a protein called NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	78	Total	C	N	O	S	0	0
			642	428	113	101			

- Molecule 34 is a protein called NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	158	Total	C	N	O	S	0	0
			1280	815	210	252	3		

- Molecule 35 is a protein called NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	131	Total	C	N	O	S	0	0
			1078	699	183	196			

- Molecule 36 is a protein called NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	69	Total	C	N	O	S	0	0
			552	358	95	97	2		

- Molecule 37 is a protein called Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	53	Total	C	N	O	S	0	0
			460	319	76	64	1		

- Molecule 38 is a protein called NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	45	Total	C	N	O	S	0	0
			368	240	71	56	1		

- Molecule 39 is a protein called NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	132	Total	C	N	O	S	0	0
			1082	706	175	200	1		

- Molecule 40 is a protein called NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
40	m	77	Total	C	N	O	0	0
			642	418	116	108		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	105	Total	C	N	O	S	0	0
			861	550	155	155	1		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	80	Total	C	N	O	S	0	0
			682	428	126	122	6		

- Molecule 43 is a protein called NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	90	Total	C	N	O	S	0	0
			740	457	135	144	4		

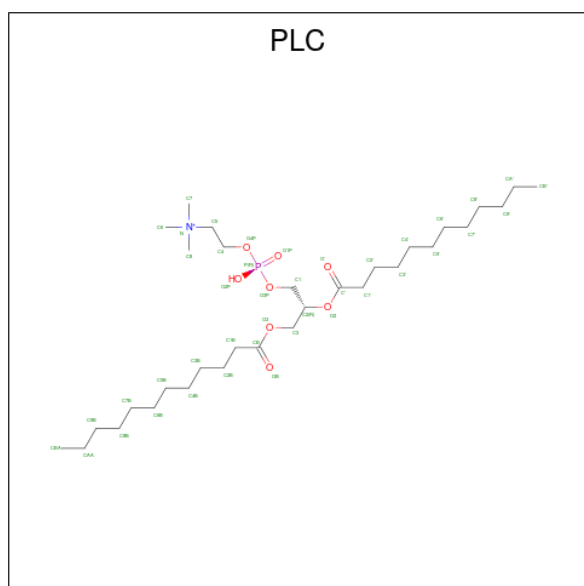
- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	140	Total	C	N	O	S	0	0
			1156	741	201	211	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	0	ACE	-	acetylation	UNP E1UWE0

- Molecule 45 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula:  $C_{32}H_{65}NO_8P$ ).



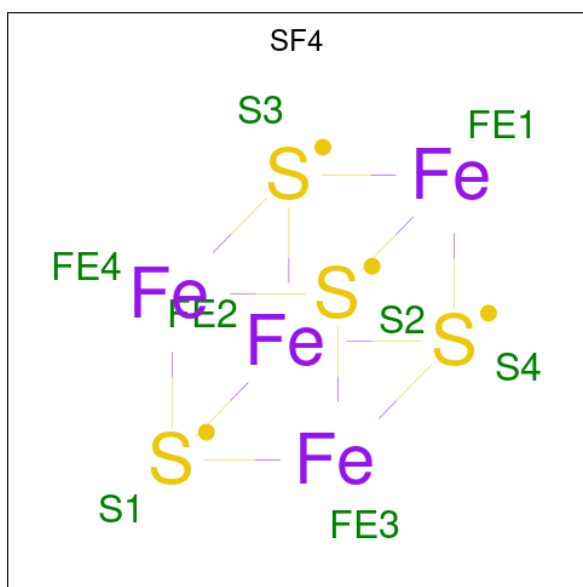
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			31	21	1	8	1	

*Continued on next page...*

*Continued from previous page...*

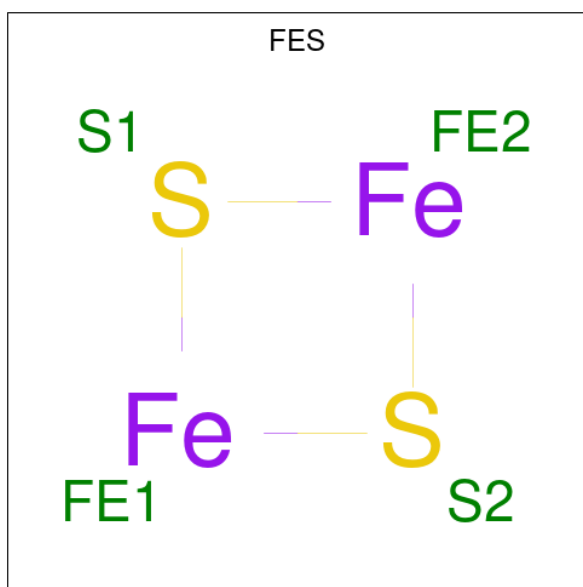
Mol	Chain	Residues	Atoms					AltConf
45	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	H	1	Total	C	N	O	P	0
			24	14	1	8	1	
45	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	L	1	Total	C	N	O	P	0
			32	22	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	M	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	P	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	Z	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	a	1	Total	C	N	O	P	0
			22	12	1	8	1	
45	b	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	d	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	h	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	q	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	q	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



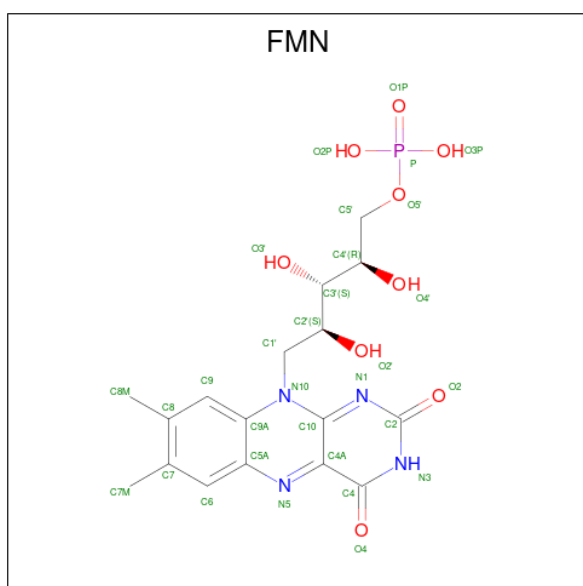
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



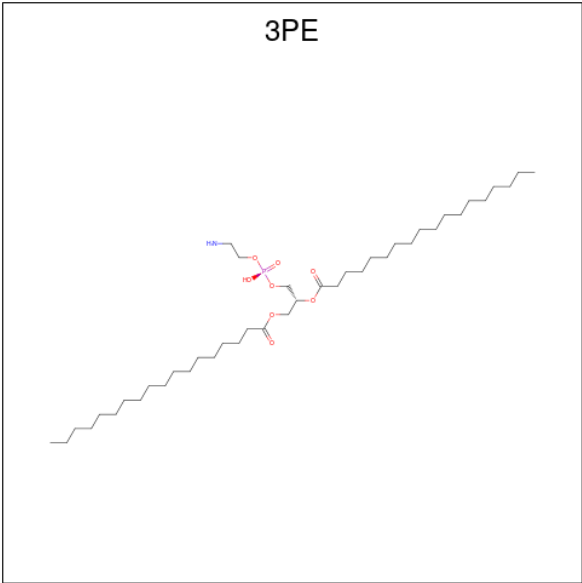
Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms		AltConf
49	G	1	Total	K	0
			1	1	

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
50	H	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	L	1	Total	C	N	O	P	0
			29	19	1	8	1	
50	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	L	1	Total	C	N	O	P	0
			46	36	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	L	1	Total	C	N	O	P	0
			33	23	1	8	1	
50	M	1	Total	C	N	O	P	0
			35	25	1	8	1	

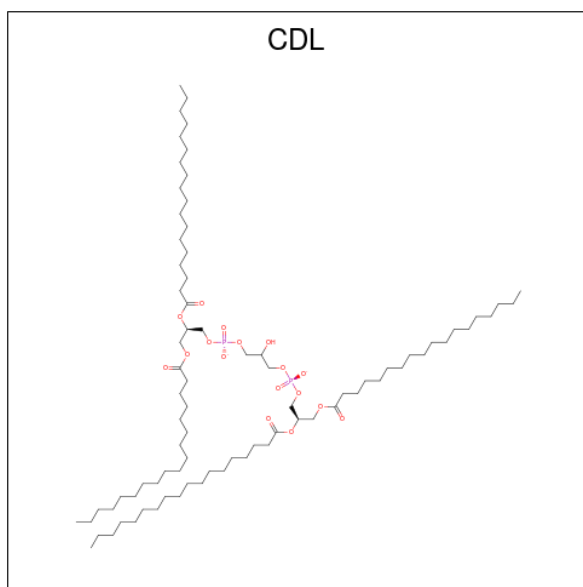
Continued on next page...



*Continued from previous page...*

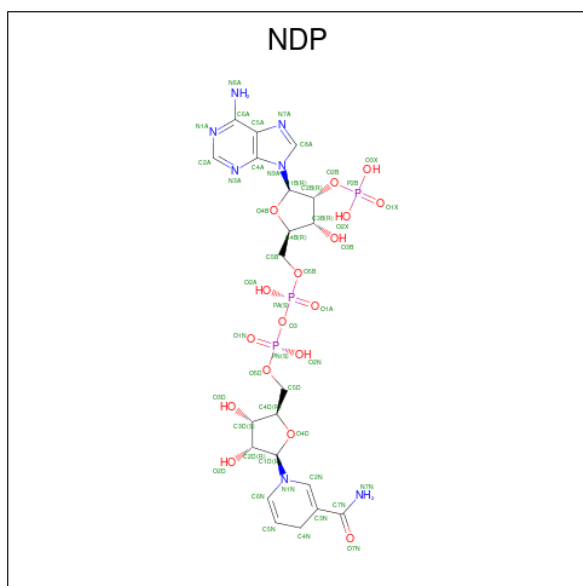
Mol	Chain	Residues	Atoms					AltConf
50	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	Y	1	Total	C	N	O	P	0
			26	16	1	8	1	
50	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	b	1	Total	C	N	O	P	0
			36	26	1	8	1	
50	b	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	b	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	f	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	g	1	Total	C	N	O	P	0
			46	36	1	8	1	
50	j	1	Total	C	N	O	P	0
			27	17	1	8	1	
50	m	1	Total	C	N	O	P	0
			25	15	1	8	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
51	O	1	Total	C	O	P	0
			75	56	17	2	
51	P	1	Total	C	O	P	0
			42	23	17	2	
51	Z	1	Total	C	O	P	0
			49	30	17	2	
51	a	1	Total	C	O	P	0
			60	41	17	2	
51	b	1	Total	C	O	P	0
			59	40	17	2	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

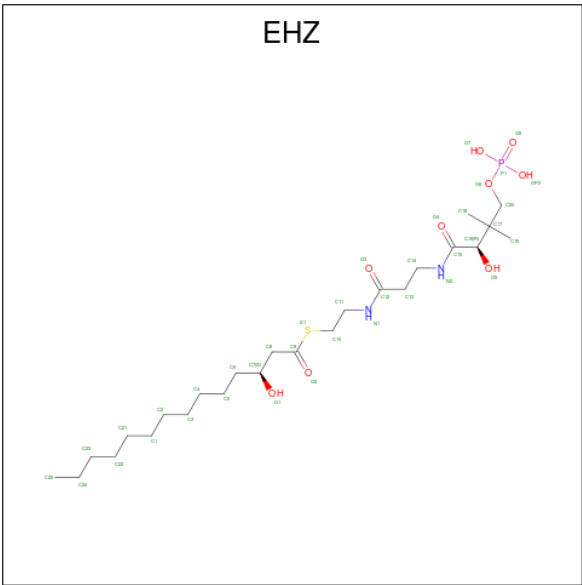


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		AltConf
53	R	1	Total	Zn	0
			1	1	

- Molecule 54 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EH2) (formula:  $C_{25}H_{49}N_2O_9PS$ ).

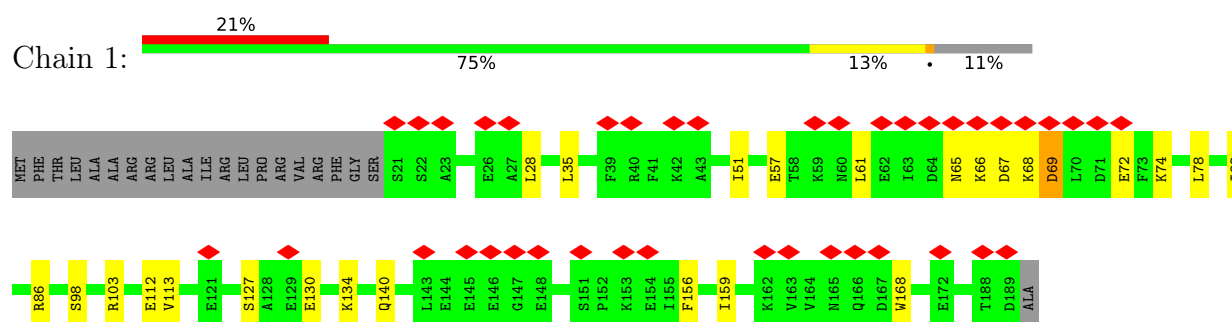


Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

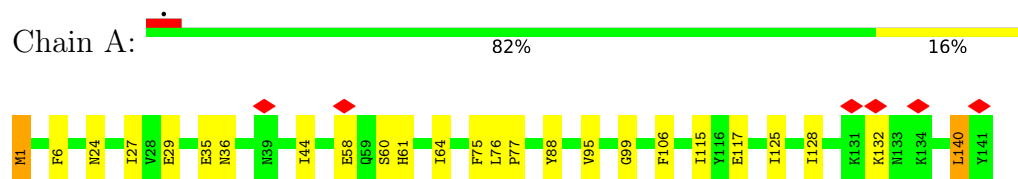
### 3 Residue-property plots

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.

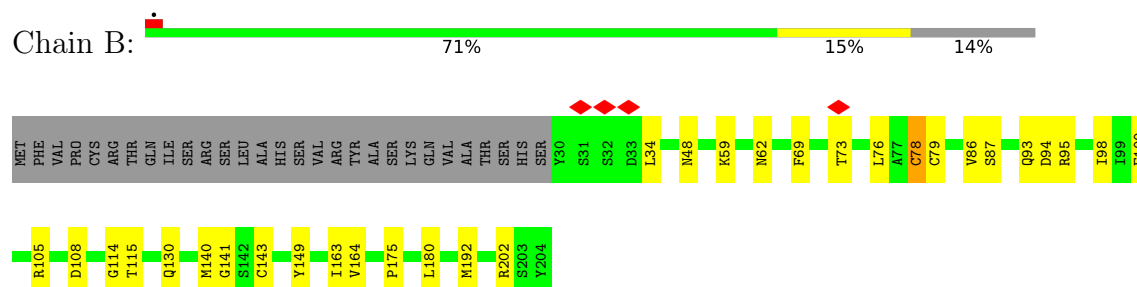
- Molecule 1: Altered inheritance of mitochondria protein 41, mitochondrial



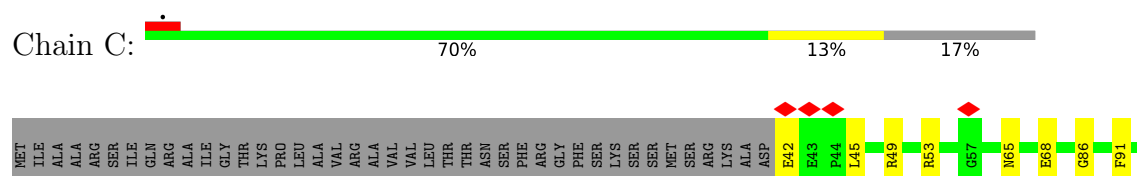
- Molecule 2: NADH-ubiquinone oxidoreductase chain 3



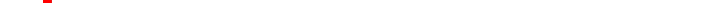
- Molecule 3: BA75\_00622T0

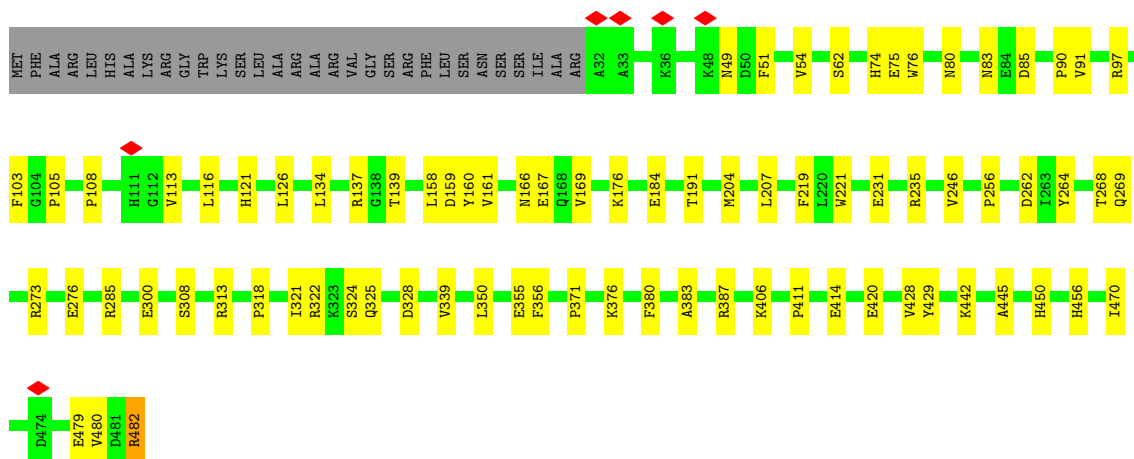


- Molecule 4: NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



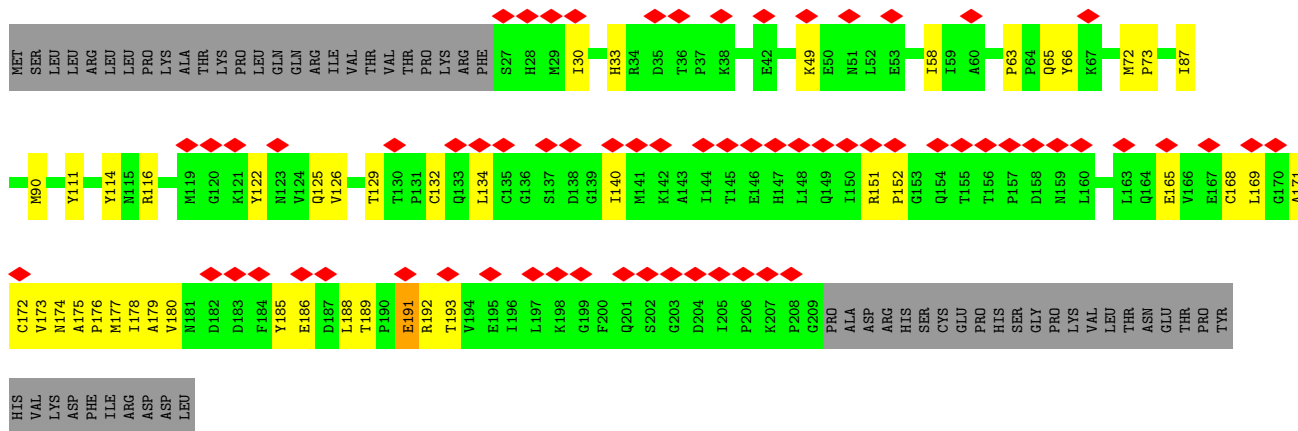
- Molecule 5: NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain D:  77% 16% 6%



- Molecule 6: NUHM (24 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

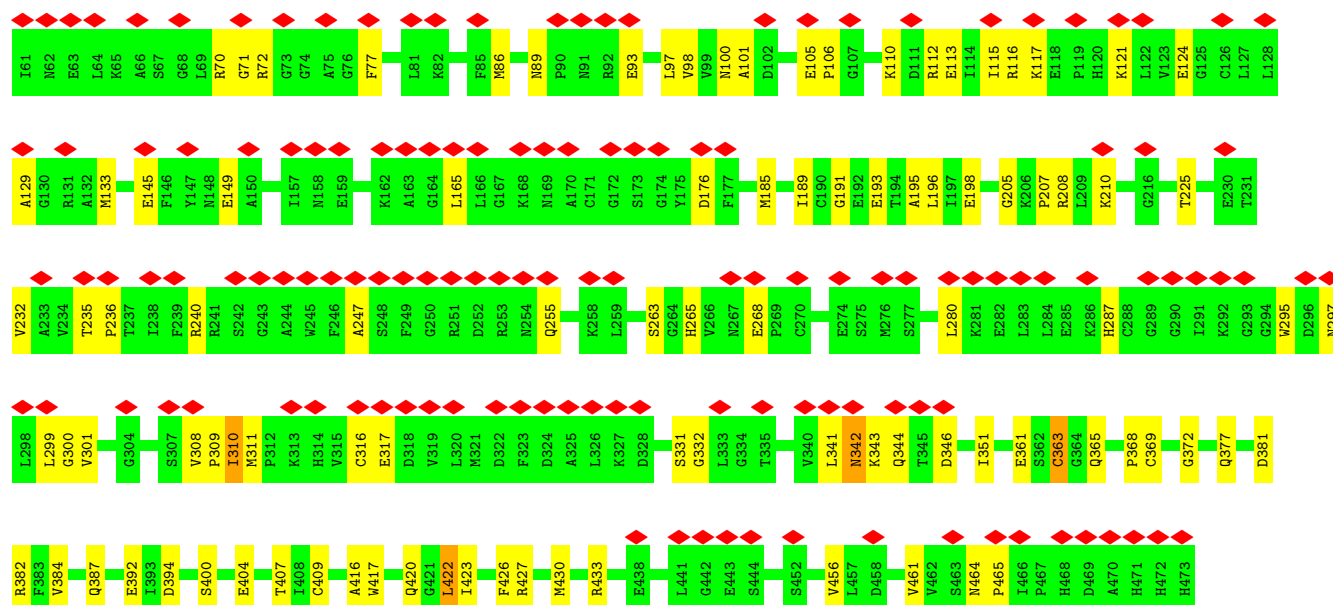
Chain E: 



- Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

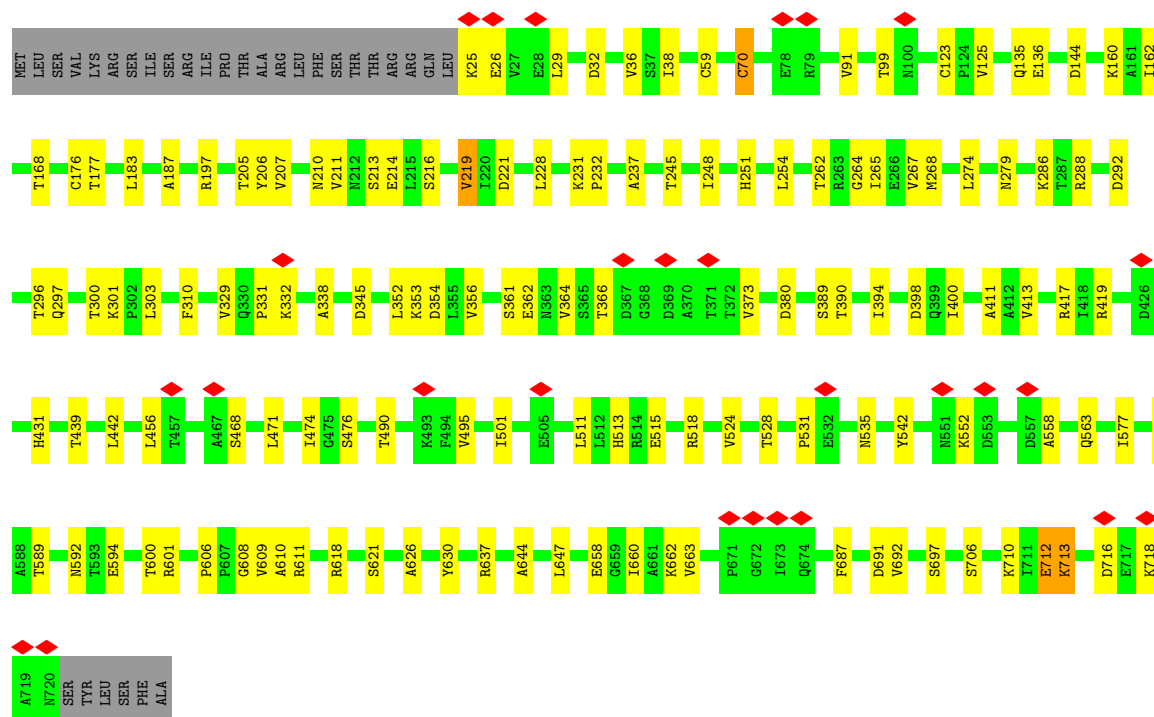
Chain F:  36% 72% 22%





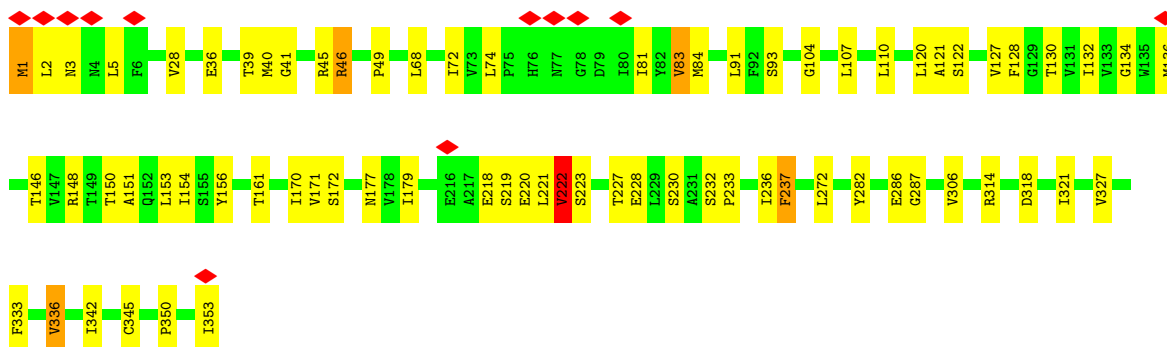
- Molecule 8: NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain G: 77% 18%



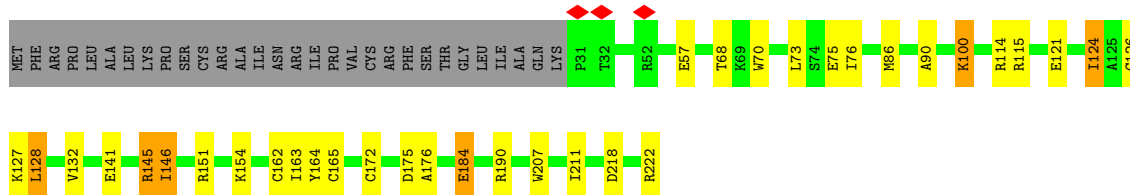
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain H: 79% 19%



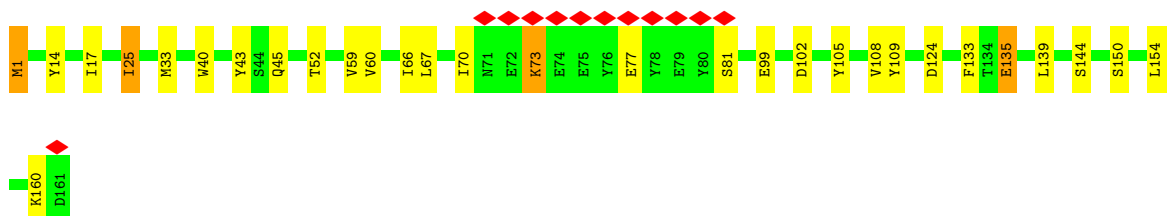
- Molecule 10: NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain I: 71% 13% 14%



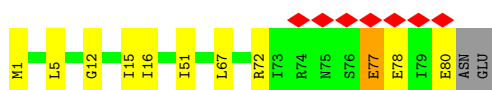
- Molecule 11: NADH-ubiquinone oxidoreductase chain 6

Chain J: 7% 81% 17%



- Molecule 12: NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

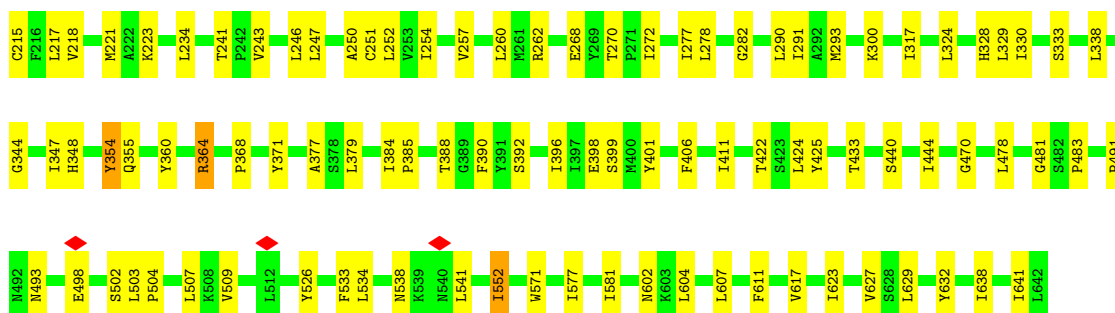
Chain K: 9% 84% 12%



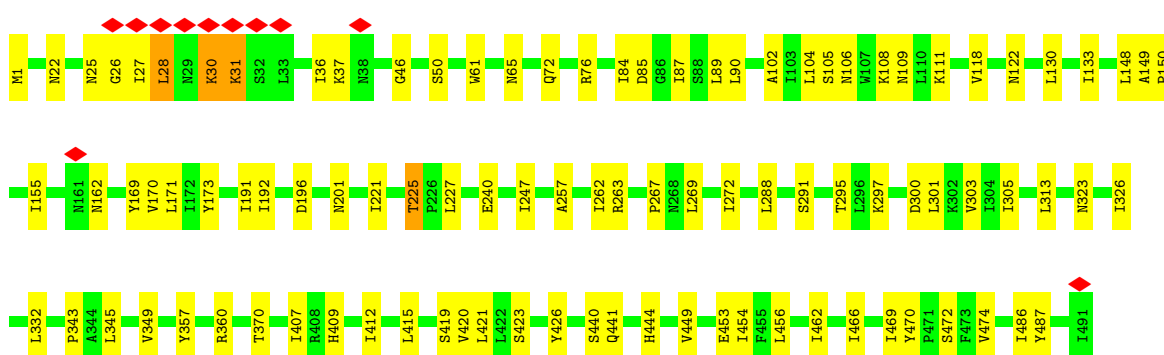
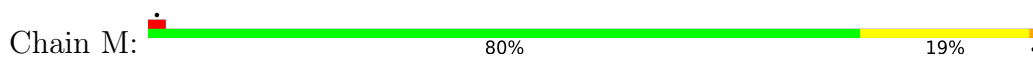
- Molecule 13: NADH-ubiquinone oxidoreductase chain 5

Chain L: 80% 19%

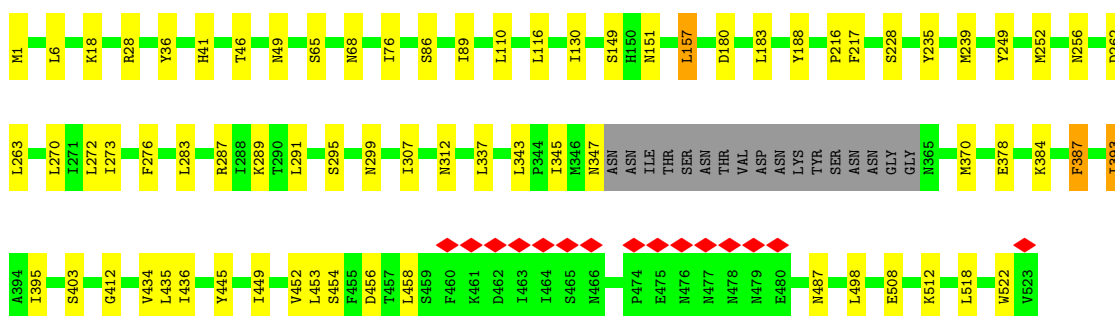
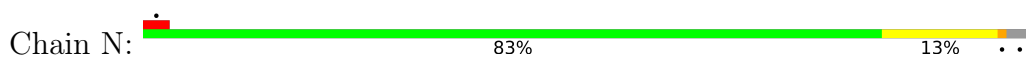




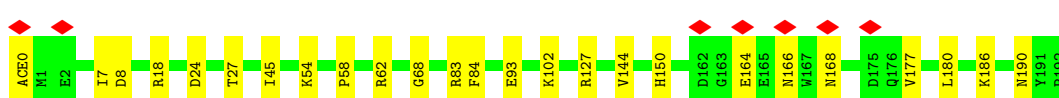
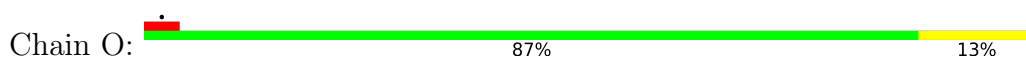
- Molecule 14: NADH-ubiquinone oxidoreductase chain 4



- Molecule 15: NADH-ubiquinone oxidoreductase chain 2




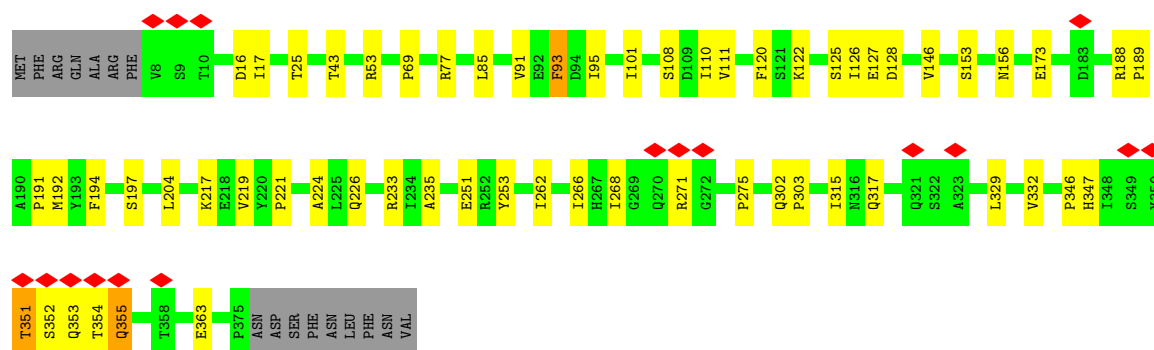
- Molecule 16: NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 17: NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

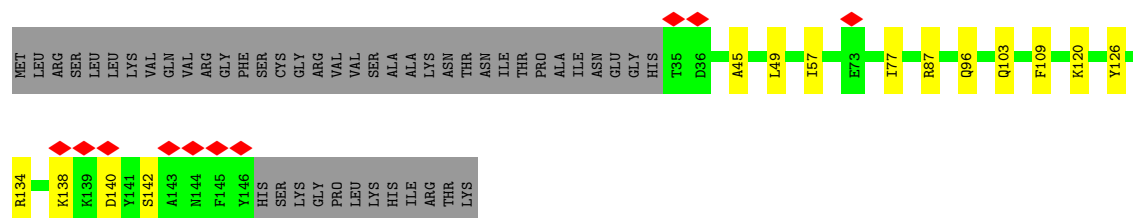


Chain P: 




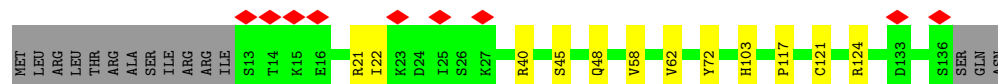
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 




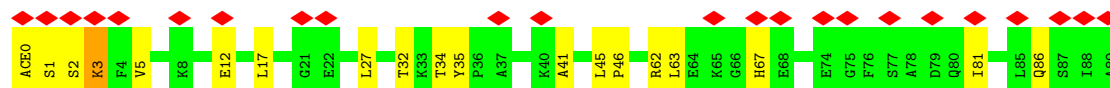
- Molecule 19: NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain R: 



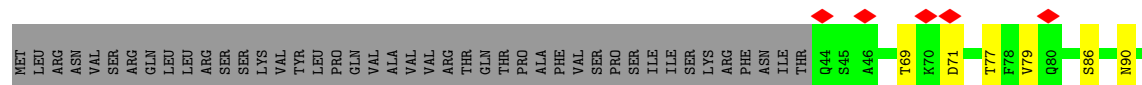
- Molecule 20: NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

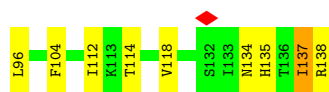
Chain S: 



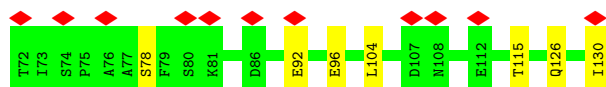
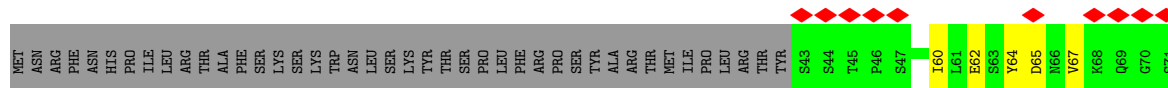
- Molecule 21: Acyl carrier protein

Chain T: 

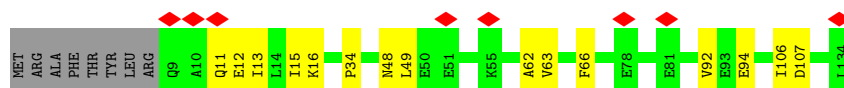
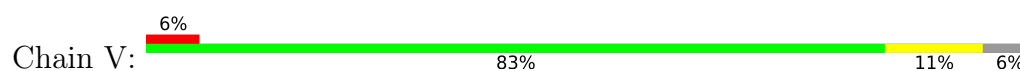




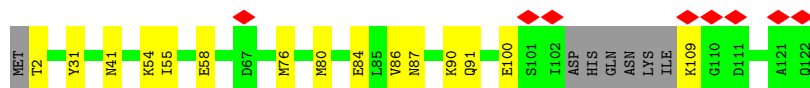
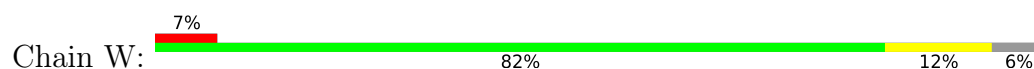
- Molecule 22: Acyl carrier protein



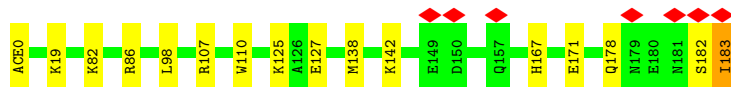
- Molecule 23: NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



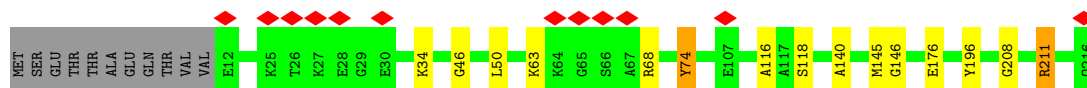
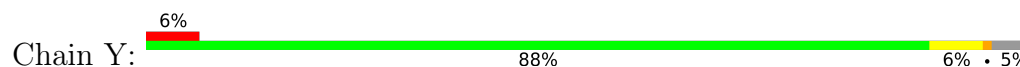
- Molecule 24: BA75\_04796T0



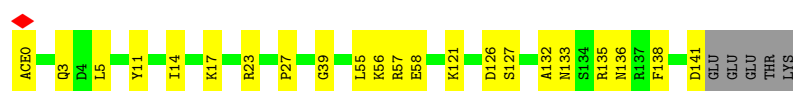
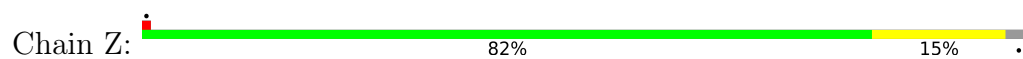
- Molecule 25: NADH-ubiquinone oxidoreductase



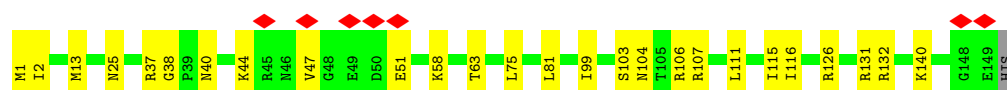
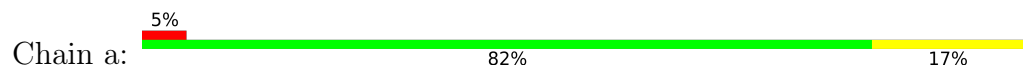
- Molecule 26: NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



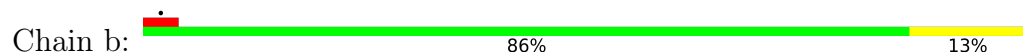
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



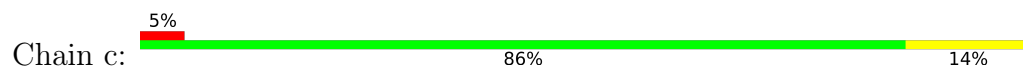
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



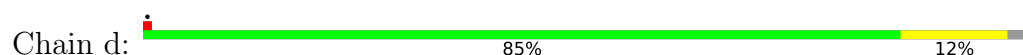
- Molecule 29: NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 30: BA75\_00589T0



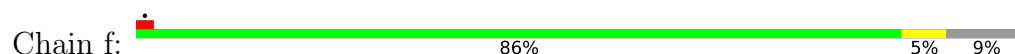
- Molecule 31: Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM

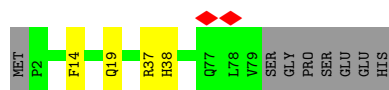


- Molecule 32: BA75\_05084T0

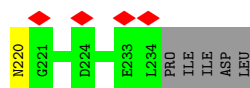
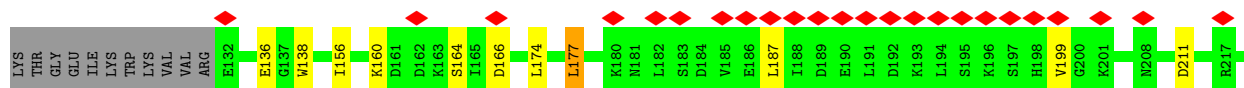
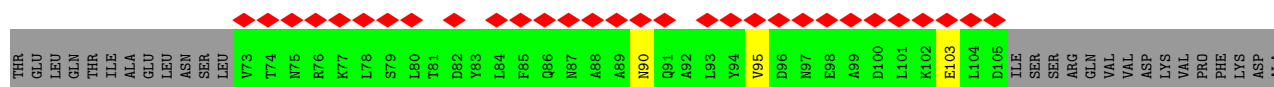


- Molecule 33: NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

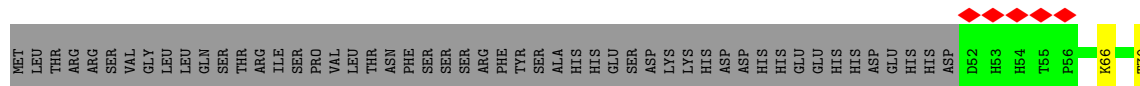




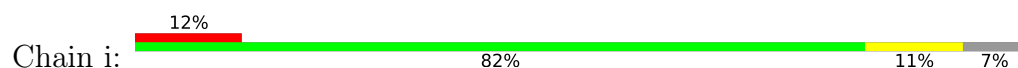
- Molecule 34: NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



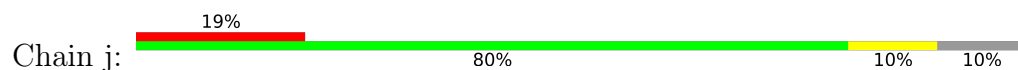
- Molecule 35: NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

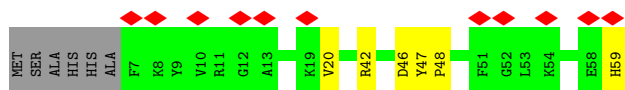


- Molecule 36: NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

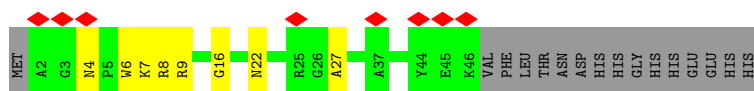


- Molecule 37: Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

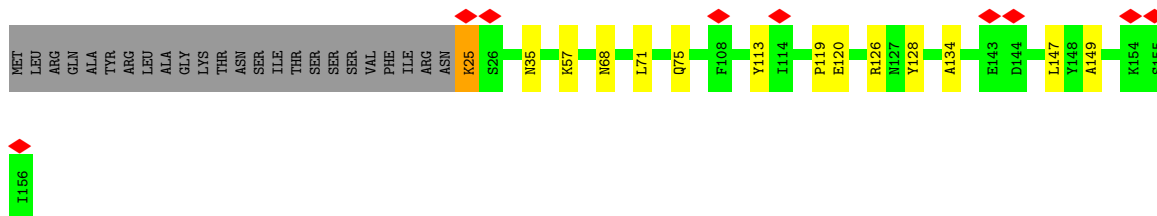
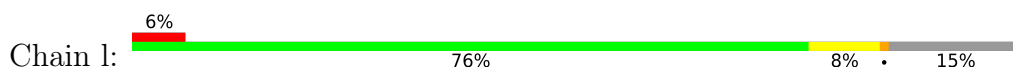




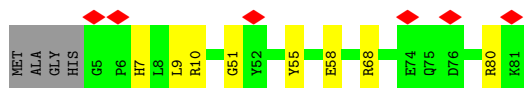
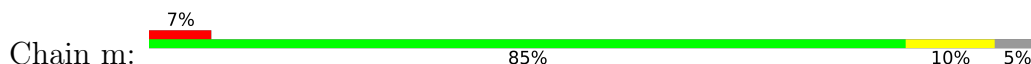
- Molecule 38: NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



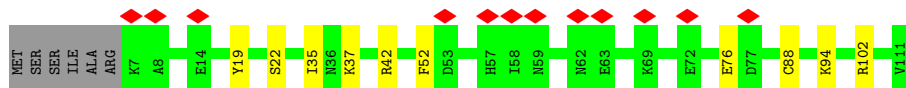
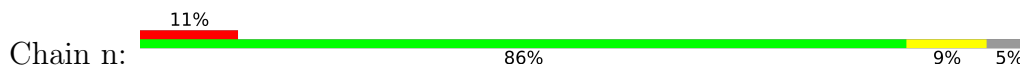
- Molecule 39: NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



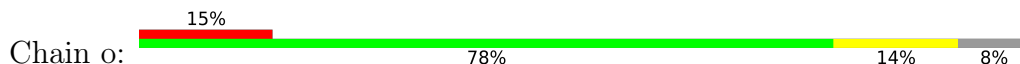
- Molecule 40: NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



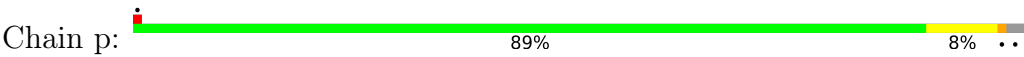
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



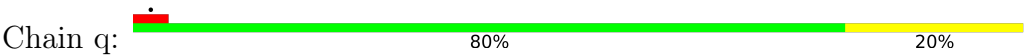
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 43: NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53716	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47.79	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.031	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0127	Depositor
Map size ( $\text{\AA}$ )	501.66, 501.66, 501.66	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.929, 0.929, 0.929	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, 3PE, FME, FES, 2MR, FMN, PLC, SF4, ACE, ZN, EHZ, NDP, K

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	1	0.08	0/1405	0.24	0/1896
2	A	0.08	0/1151	0.22	0/1564
3	B	0.09	0/1450	0.24	0/1969
4	C	0.08	0/2033	0.24	0/2770
5	D	0.09	0/3698	0.23	0/5007
6	E	0.08	0/1480	0.24	0/2008
7	F	0.09	0/3579	0.25	0/4832
8	G	0.08	0/5436	0.24	0/7370
9	H	0.08	0/2880	0.24	0/3939
10	I	0.09	0/1596	0.25	0/2164
11	J	0.08	0/1329	0.24	0/1816
12	K	0.07	0/610	0.20	0/828
13	L	0.08	0/5236	0.23	0/7128
14	M	0.09	0/3940	0.24	0/5379
15	N	0.08	0/4110	0.22	0/5609
16	O	0.18	1/1621 (0.1%)	0.24	0/2199
17	P	0.08	0/2985	0.23	0/4035
18	Q	0.07	0/945	0.21	0/1273
19	R	0.08	0/998	0.23	0/1350
20	S	0.26	1/710 (0.1%)	0.30	1/961 (0.1%)
21	T	0.06	0/752	0.19	0/1021
22	U	0.07	0/688	0.21	0/936
23	V	0.08	0/1044	0.20	0/1411
24	W	0.07	0/999	0.19	0/1340
25	X	0.18	1/1475 (0.1%)	0.22	0/1990
26	Y	0.07	0/1615	0.21	0/2175
27	Z	0.20	1/1210 (0.1%)	0.21	0/1639
28	a	0.08	0/1241	0.21	0/1670
29	b	0.08	0/666	0.21	0/911
30	c	0.19	1/1448 (0.1%)	0.25	0/1964
31	d	0.08	0/633	0.18	0/854
32	e	0.07	0/865	0.20	0/1158



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	f	0.07	0/663	0.19	0/896
34	g	0.07	0/1293	0.21	0/1735
35	h	0.08	0/1114	0.24	0/1516
36	i	0.11	0/571	0.29	0/777
37	j	0.09	0/484	0.24	0/658
38	k	0.07	0/382	0.22	0/514
39	l	0.08	0/1119	0.25	0/1520
40	m	0.09	0/661	0.21	0/893
41	n	0.07	0/884	0.20	0/1197
42	o	0.08	0/696	0.22	0/933
43	p	0.07	0/756	0.21	0/1020
44	q	0.20	1/1192 (0.1%)	0.25	0/1620
All	All	0.10	6/69643 (0.0%)	0.23	1/94445 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S	0	ACE	C-N	6.19	1.45	1.33
25	X	0	ACE	C-N	6.18	1.45	1.33
16	O	0	ACE	C-N	6.18	1.45	1.33
30	c	0	ACE	C-N	6.18	1.45	1.33
44	q	0	ACE	C-N	6.13	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S	2	SER	CB-CA-C	-5.58	110.12	116.54

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	1	1383	0	1390	12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1133	0	1167	24	0
3	B	1407	0	1372	21	0
4	C	1970	0	1905	26	0
5	D	3621	0	3531	56	0
6	E	1446	0	1435	26	0
7	F	3500	0	3459	70	0
8	G	5344	0	5333	82	0
9	H	2809	0	2880	51	0
10	I	1556	0	1499	30	0
11	J	1313	0	1320	30	0
12	K	617	0	657	11	0
13	L	5115	0	5338	80	0
14	M	3868	0	4127	64	0
15	N	4045	0	4327	48	0
16	O	1575	0	1523	15	0
17	P	2922	0	2915	42	0
18	Q	924	0	891	8	0
19	R	978	0	964	8	0
20	S	697	0	736	11	0
21	T	745	0	734	11	0
22	U	681	0	664	7	0
23	V	1025	0	1035	9	0
24	W	979	0	980	9	0
25	X	1450	0	1422	10	0
26	Y	1578	0	1567	13	0
27	Z	1176	0	1165	19	0
28	a	1215	0	1197	21	0
29	b	641	0	620	8	0
30	c	1418	0	1452	19	0
31	d	616	0	624	8	0
32	e	848	0	830	9	0
33	f	642	0	640	4	0
34	g	1280	0	1302	12	0
35	h	1078	0	1036	14	0
36	i	552	0	540	7	0
37	j	460	0	455	2	0
38	k	368	0	348	6	0
39	l	1082	0	1033	11	0
40	m	642	0	635	7	0
41	n	861	0	866	7	0
42	o	682	0	677	7	0
43	p	740	0	700	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	q	1156	0	1115	17	0
45	A	31	0	36	2	0
45	B	31	0	36	1	0
45	D	42	0	64	2	0
45	H	24	0	22	0	0
45	L	109	0	146	7	0
45	M	123	0	183	4	0
45	N	42	0	64	0	0
45	P	31	0	36	3	0
45	Y	72	0	98	1	0
45	Z	42	0	64	0	0
45	a	22	0	18	0	0
45	b	39	0	55	2	0
45	d	42	0	64	4	0
45	h	42	0	64	2	0
45	q	78	0	113	4	0
46	B	8	0	0	0	0
46	F	8	0	0	2	0
46	G	16	0	0	1	0
46	I	16	0	0	3	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	0	0
49	G	1	0	0	0	0
50	H	31	0	36	0	0
50	L	338	0	489	23	0
50	M	35	0	44	0	0
50	N	40	0	57	1	0
50	Y	77	0	108	9	0
50	b	142	0	183	5	0
50	f	51	0	82	7	0
50	g	46	0	69	2	0
50	j	27	0	28	0	0
50	m	25	0	24	0	0
51	O	75	0	97	5	0
51	P	42	0	28	0	0
51	Z	49	0	42	0	0
51	a	60	0	64	2	0
51	b	59	0	62	3	0
52	P	48	0	26	1	0
53	R	1	0	0	0	0
54	T	37	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	U	37	0	0	1	0
All	All	70216	0	70927	798	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 6.

The worst 5 of 798 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:B:163:ILE:HG22	3:B:164:VAL:HG13	1.66	0.77
6:E:63:PRO:HG2	6:E:66:TYR:HB2	1.68	0.76
19:R:103:HIS:CD2	19:R:121:CYS:SG	2.80	0.74
8:G:59:CYS:HB3	8:G:70:CYS:HB3	1.71	0.73
13:L:388:THR:HG22	13:L:470:GLY:H	1.52	0.72

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	167/190 (88%)	158 (95%)	9 (5%)	0	100	100
2	A	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
3	B	173/204 (85%)	168 (97%)	5 (3%)	0	100	100
4	C	238/289 (82%)	234 (98%)	4 (2%)	0	100	100
5	D	448/482 (93%)	438 (98%)	10 (2%)	0	100	100
6	E	181/241 (75%)	175 (97%)	6 (3%)	0	100	100
7	F	451/473 (95%)	428 (95%)	23 (5%)	0	100	100
8	G	694/726 (96%)	679 (98%)	15 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	351/353 (99%)	343 (98%)	6 (2%)	2 (1%)	22	51
10	I	190/222 (86%)	187 (98%)	3 (2%)	0	100	100
11	J	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
12	K	78/82 (95%)	76 (97%)	2 (3%)	0	100	100
13	L	640/642 (100%)	628 (98%)	11 (2%)	1 (0%)	44	73
14	M	489/491 (100%)	472 (96%)	17 (4%)	0	100	100
15	N	502/523 (96%)	491 (98%)	10 (2%)	1 (0%)	44	73
16	O	191/193 (99%)	190 (100%)	1 (0%)	0	100	100
17	P	366/384 (95%)	356 (97%)	10 (3%)	0	100	100
18	Q	110/159 (69%)	110 (100%)	0	0	100	100
19	R	122/139 (88%)	121 (99%)	1 (1%)	0	100	100
20	S	88/90 (98%)	85 (97%)	3 (3%)	0	100	100
21	T	93/138 (67%)	92 (99%)	1 (1%)	0	100	100
22	U	86/130 (66%)	82 (95%)	4 (5%)	0	100	100
23	V	124/134 (92%)	121 (98%)	3 (2%)	0	100	100
24	W	111/122 (91%)	110 (99%)	1 (1%)	0	100	100
25	X	182/184 (99%)	180 (99%)	2 (1%)	0	100	100
26	Y	203/216 (94%)	195 (96%)	8 (4%)	0	100	100
27	Z	140/147 (95%)	138 (99%)	2 (1%)	0	100	100
28	a	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
29	b	76/79 (96%)	75 (99%)	1 (1%)	0	100	100
30	c	180/182 (99%)	175 (97%)	5 (3%)	0	100	100
31	d	73/78 (94%)	72 (99%)	1 (1%)	0	100	100
32	e	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
33	f	76/86 (88%)	76 (100%)	0	0	100	100
34	g	152/239 (64%)	149 (98%)	3 (2%)	0	100	100
35	h	129/182 (71%)	126 (98%)	3 (2%)	0	100	100
36	i	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
37	j	51/59 (86%)	51 (100%)	0	0	100	100
38	k	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
39	l	130/156 (83%)	127 (98%)	3 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	m	75/81 (93%)	75 (100%)	0	0	100	100
41	n	103/111 (93%)	103 (100%)	0	0	100	100
42	o	78/87 (90%)	75 (96%)	3 (4%)	0	100	100
43	p	88/92 (96%)	86 (98%)	2 (2%)	0	100	100
44	q	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
All	All	8425/9219 (91%)	8223 (98%)	198 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	H	222	VAL
9	H	2	LEU
15	N	522	TRP
13	L	552	ILE

### 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	1	152/168 (90%)	146 (96%)	6 (4%)	27	61
2	A	128/128 (100%)	125 (98%)	3 (2%)	45	78
3	B	154/180 (86%)	151 (98%)	3 (2%)	52	82
4	C	214/254 (84%)	213 (100%)	1 (0%)	86	95
5	D	384/408 (94%)	378 (98%)	6 (2%)	58	85
6	E	163/218 (75%)	157 (96%)	6 (4%)	29	63
7	F	369/387 (95%)	357 (97%)	12 (3%)	33	67
8	G	582/610 (95%)	569 (98%)	13 (2%)	47	79
9	H	307/307 (100%)	297 (97%)	10 (3%)	33	67
10	I	166/192 (86%)	159 (96%)	7 (4%)	25	58
11	J	149/149 (100%)	145 (97%)	4 (3%)	40	74

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	70/72 (97%)	69 (99%)	1 (1%)	62	87
13	L	576/576 (100%)	565 (98%)	11 (2%)	52	82
14	M	439/439 (100%)	432 (98%)	7 (2%)	58	85
15	N	474/489 (97%)	466 (98%)	8 (2%)	56	84
16	O	169/169 (100%)	164 (97%)	5 (3%)	36	70
17	P	317/332 (96%)	314 (99%)	3 (1%)	75	92
18	Q	95/135 (70%)	94 (99%)	1 (1%)	70	90
19	R	104/118 (88%)	103 (99%)	1 (1%)	73	91
20	S	77/77 (100%)	74 (96%)	3 (4%)	27	61
21	T	87/128 (68%)	84 (97%)	3 (3%)	32	66
22	U	80/120 (67%)	76 (95%)	4 (5%)	20	51
23	V	112/119 (94%)	110 (98%)	2 (2%)	54	83
24	W	107/114 (94%)	105 (98%)	2 (2%)	52	82
25	X	165/165 (100%)	164 (99%)	1 (1%)	84	95
26	Y	163/173 (94%)	159 (98%)	4 (2%)	42	75
27	Z	123/128 (96%)	123 (100%)	0	100	100
28	a	128/129 (99%)	127 (99%)	1 (1%)	79	93
29	b	66/67 (98%)	64 (97%)	2 (3%)	36	70
30	c	159/159 (100%)	157 (99%)	2 (1%)	65	88
31	d	62/65 (95%)	61 (98%)	1 (2%)	58	85
32	e	91/92 (99%)	90 (99%)	1 (1%)	70	90
33	f	64/71 (90%)	64 (100%)	0	100	100
34	g	143/215 (66%)	140 (98%)	3 (2%)	48	80
35	h	118/167 (71%)	115 (98%)	3 (2%)	42	75
36	i	59/63 (94%)	58 (98%)	1 (2%)	56	84
37	j	46/50 (92%)	44 (96%)	2 (4%)	25	57
38	k	32/47 (68%)	32 (100%)	0	100	100
39	l	116/137 (85%)	114 (98%)	2 (2%)	56	84
40	m	64/66 (97%)	63 (98%)	1 (2%)	58	85
41	n	95/100 (95%)	94 (99%)	1 (1%)	70	90
42	o	74/79 (94%)	74 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	p	83/85 (98%)	82 (99%)	1 (1%)	67 89
44	q	125/125 (100%)	123 (98%)	2 (2%)	58 85
All	All	7451/8072 (92%)	7301 (98%)	150 (2%)	50 81

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	U	104	LEU
39	l	25	LYS
23	V	12	GLU
30	c	1	SER
8	G	713	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	521	ASN
18	Q	129	GLN
16	O	168	ASN
17	P	353	GLN
24	W	41	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	FME	H	1	9	8,9,10	1.51	1 (12%)	7,9,11	1.73	3 (42%)
15	FME	N	1	15	8,9,10	1.51	1 (12%)	7,9,11	1.54	1 (14%)
11	FME	J	1	11	8,9,10	1.51	1 (12%)	7,9,11	1.71	3 (42%)
14	FME	M	1	14	8,9,10	1.51	1 (12%)	7,9,11	1.67	2 (28%)
2	FME	A	1	2	8,9,10	1.51	1 (12%)	7,9,11	1.71	2 (28%)
13	FME	L	1	13	8,9,10	1.50	1 (12%)	7,9,11	1.73	3 (42%)
12	FME	K	1	12	8,9,10	1.50	1 (12%)	7,9,11	1.68	2 (28%)
5	2MR	D	137	5	10,12,13	2.43	2 (20%)	5,13,15	1.65	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FME	H	1	9	-	2/7/9/11	-
15	FME	N	1	15	-	0/7/9/11	-
11	FME	J	1	11	-	4/7/9/11	-
14	FME	M	1	14	-	4/7/9/11	-
2	FME	A	1	2	-	4/7/9/11	-
13	FME	L	1	13	-	3/7/9/11	-
12	FME	K	1	12	-	4/7/9/11	-
5	2MR	D	137	5	-	1/10/13/15	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	137	2MR	CZ-NH2	5.39	1.45	1.33
5	D	137	2MR	CZ-NE	5.08	1.45	1.34
2	A	1	FME	CN-N	3.67	1.45	1.33
9	H	1	FME	CN-N	3.67	1.45	1.33
15	N	1	FME	CN-N	3.66	1.45	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	FME	CE-SD-CG	2.83	110.13	100.40
11	J	1	FME	CE-SD-CG	2.67	109.57	100.40
5	D	137	2MR	CD-NE-CZ	-2.66	118.43	123.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	1	FME	CE-SD-CG	2.64	109.47	100.40
9	H	1	FME	CE-SD-CG	2.62	109.39	100.40

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	FME	O1-CN-N-CA
2	A	1	FME	C-CA-CB-CG
5	D	137	2MR	O-C-CA-CB
11	J	1	FME	O-C-CA-CB
12	K	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	H	1	FME	1	0
11	J	1	FME	1	0
2	A	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 61 ligands modelled in this entry, 2 are monoatomic - leaving 59 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	$\# Z  > 2$
45	PLC	H	401	-	23,23,41	0.67	0	29,31,49	0.68	1 (3%)
45	PLC	N	601	-	41,41,41	0.51	0	47,49,49	0.53	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	SF4	G	802	8	0,12,12	-	-	-		
50	3PE	L	711	-	32,32,50	1.06	4 (12%)	35,37,55	1.15	2 (5%)
45	PLC	M	1002	-	38,38,41	0.52	0	44,46,49	0.50	0
50	3PE	g	301	-	45,45,50	0.90	4 (8%)	48,50,55	1.08	2 (4%)
50	3PE	b	105	-	30,30,50	1.09	4 (13%)	33,35,55	1.16	2 (6%)
50	3PE	j	101	-	26,26,50	1.16	4 (15%)	29,31,55	1.20	2 (6%)
50	3PE	m	101	-	24,24,50	1.20	4 (16%)	27,29,55	1.26	2 (7%)
50	3PE	Y	303	-	25,25,50	1.19	4 (16%)	28,30,55	1.34	3 (10%)
46	SF4	F	501	7	0,12,12	-	-	-		
51	CDL	a	201	-	59,59,99	1.11	8 (13%)	65,71,111	1.15	4 (6%)
51	CDL	O	201	-	74,74,99	1.00	8 (10%)	80,86,111	1.13	4 (5%)
52	NDP	P	501	-	45,52,52	4.30	23 (51%)	53,80,80	2.11	5 (9%)
54	EHZ	T	201	21	29,36,37	1.70	5 (17%)	35,44,47	1.50	4 (11%)
45	PLC	A	201	-	30,30,41	0.58	0	36,38,49	0.55	0
45	PLC	M	1003	-	41,41,41	0.50	0	47,49,49	0.52	0
50	3PE	L	708	-	34,34,50	1.03	4 (11%)	37,39,55	1.16	2 (5%)
45	PLC	q	401	-	35,35,41	0.55	0	41,43,49	0.57	0
45	PLC	M	1001	-	41,41,41	0.51	0	47,49,49	0.51	0
45	PLC	d	101	-	41,41,41	0.50	0	47,49,49	0.52	0
50	3PE	M	1004	-	34,34,50	1.03	4 (11%)	37,39,55	1.15	2 (5%)
45	PLC	a	202	-	21,21,41	0.68	0	27,29,49	0.66	0
45	PLC	B	302	-	30,30,41	0.58	0	36,38,49	0.58	0
54	EHZ	U	201	22	29,36,37	1.70	5 (17%)	35,44,47	1.54	5 (14%)
50	3PE	L	701	-	28,28,50	1.13	4 (14%)	31,33,55	1.12	2 (6%)
51	CDL	b	102	-	58,58,99	1.12	8 (13%)	64,70,111	1.20	4 (6%)
46	SF4	I	301	10	0,12,12	-	-	-		
46	SF4	B	301	3	0,12,12	-	-	-		
45	PLC	b	101	-	38,38,41	0.52	0	44,46,49	0.55	0
50	3PE	L	706	-	50,50,50	0.86	4 (8%)	53,55,55	1.11	2 (3%)
50	3PE	b	106	-	34,34,50	1.03	4 (11%)	37,39,55	1.12	2 (5%)
48	FMN	F	502	-	33,33,33	2.81	10 (30%)	48,50,50	1.86	15 (31%)
50	3PE	b	103	-	39,39,50	0.96	4 (10%)	42,44,55	1.13	2 (4%)
51	CDL	P	503	-	41,41,99	1.28	7 (17%)	47,53,111	1.32	3 (6%)
50	3PE	L	710	-	50,50,50	0.86	4 (8%)	53,55,55	1.11	2 (3%)
50	3PE	L	707	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)
45	PLC	h	201	-	41,41,41	0.51	0	47,49,49	0.53	0
45	PLC	Y	301	-	35,35,41	0.55	0	41,43,49	0.55	0
45	PLC	L	704	-	31,31,41	0.57	0	37,39,49	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	PLC	q	402	-	41,41,41	0.50	0	47,49,49	0.49	0
45	PLC	L	702	-	34,34,41	0.56	0	40,42,49	0.54	0
46	SF4	G	801	8	0,12,12	-	-	-	-	-
50	3PE	L	709	-	45,45,50	0.90	4 (8%)	48,50,55	1.09	2 (4%)
50	3PE	N	602	-	39,39,50	0.97	4 (10%)	42,44,55	1.12	2 (4%)
50	3PE	Y	302	-	50,50,50	0.86	4 (8%)	53,55,55	1.12	2 (3%)
47	FES	E	301	6	0,4,4	-	-	-	-	-
45	PLC	D	501	-	41,41,41	0.50	0	47,49,49	0.56	0
45	PLC	L	705	-	41,41,41	0.50	0	47,49,49	0.63	1 (2%)
45	PLC	Y	304	-	35,35,41	0.54	0	41,43,49	0.57	0
50	3PE	f	101	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
46	SF4	I	302	10	0,12,12	-	-	-	-	-
50	3PE	H	402	-	30,30,50	1.09	4 (13%)	33,35,55	1.15	2 (6%)
51	CDL	Z	202	-	48,48,99	1.22	8 (16%)	54,60,111	1.27	4 (7%)
45	PLC	Z	201	-	41,41,41	0.51	0	47,49,49	0.50	0
45	PLC	P	502	-	30,30,41	0.58	0	36,38,49	0.58	0
50	3PE	L	703	-	41,41,50	0.94	4 (9%)	44,46,55	1.13	2 (4%)
50	3PE	b	104	-	35,35,50	1.02	4 (11%)	38,40,55	1.13	2 (5%)
47	FES	G	803	8	0,4,4	-	-	-	-	-

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
45	PLC	H	401	-	-	19/26/26/45	-
45	PLC	N	601	-	-	13/45/45/45	-
46	SF4	G	802	8	-	-	0/6/5/5
50	3PE	L	711	-	-	15/36/36/54	-
45	PLC	M	1002	-	-	14/42/42/45	-
50	3PE	g	301	-	-	21/49/49/54	-
50	3PE	b	105	-	-	17/34/34/54	-
50	3PE	j	101	-	-	17/30/30/54	-
50	3PE	m	101	-	-	12/27/27/54	-
50	3PE	Y	303	-	-	11/28/28/54	-
46	SF4	F	501	7	-	-	0/6/5/5
51	CDL	a	201	-	-	32/70/70/110	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	O	201	-	-	34/85/85/110	-
52	NDP	P	501	-	-	10/30/77/77	0/5/5/5
54	EHZ	T	201	21	-	22/42/44/45	-
45	PLC	A	201	-	-	14/34/34/45	-
45	PLC	M	1003	-	-	18/45/45/45	-
50	3PE	L	708	-	-	16/38/38/54	-
47	FES	G	803	8	-	-	0/1/1/1
45	PLC	q	401	-	-	12/39/39/45	-
45	PLC	M	1001	-	-	16/45/45/45	-
45	PLC	d	101	-	-	15/45/45/45	-
50	3PE	M	1004	-	-	21/38/38/54	-
45	PLC	a	202	-	-	6/23/23/45	-
45	PLC	B	302	-	-	14/34/34/45	-
54	EHZ	U	201	22	-	15/42/44/45	-
50	3PE	L	701	-	-	10/32/32/54	-
51	CDL	b	102	-	-	19/69/69/110	-
46	SF4	I	301	10	-	-	0/6/5/5
46	SF4	B	301	3	-	-	0/6/5/5
45	PLC	b	101	-	-	8/42/42/45	-
50	3PE	L	706	-	-	22/54/54/54	-
50	3PE	b	106	-	-	15/38/38/54	-
48	FMN	F	502	-	-	8/18/18/18	0/3/3/3
50	3PE	b	103	-	-	21/43/43/54	-
51	CDL	P	503	-	-	17/50/50/110	-
50	3PE	L	710	-	-	27/54/54/54	-
45	PLC	h	201	-	-	10/45/45/45	-
45	PLC	Y	301	-	-	9/39/39/45	-
45	PLC	L	704	-	-	15/35/35/45	-
45	PLC	q	402	-	-	13/45/45/45	-
45	PLC	L	702	-	-	14/38/38/45	-
50	3PE	L	709	-	-	28/49/49/54	-
46	SF4	G	801	8	-	-	0/6/5/5
50	3PE	N	602	-	-	17/43/43/54	-
50	3PE	Y	302	-	-	17/54/54/54	-
47	FES	E	301	6	-	-	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PLC	D	501	-	-	11/45/45/45	-
45	PLC	L	705	-	-	19/45/45/45	-
45	PLC	Y	304	-	-	13/39/39/45	-
50	3PE	f	101	-	-	21/54/54/54	-
50	3PE	H	402	-	-	17/34/34/54	-
51	CDL	Z	202	-	-	32/58/58/110	-
46	SF4	I	302	10	-	-	0/6/5/5
45	PLC	Z	201	-	-	17/45/45/45	-
45	PLC	P	502	-	-	8/34/34/45	-
50	3PE	L	703	-	-	25/45/45/54	-
50	3PE	b	104	-	-	17/39/39/54	-
50	3PE	L	707	-	-	16/54/54/54	-

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	O4B-C1B	15.01	1.62	1.41
52	P	501	NDP	C6N-C5N	12.26	1.55	1.33
52	P	501	NDP	C7N-N7N	8.37	1.55	1.33
52	P	501	NDP	O4D-C1D	8.16	1.61	1.42
48	F	502	FMN	C4A-N5	7.38	1.45	1.30

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	P	501	NDP	C5A-C6A-N6A	8.59	133.41	120.35
52	P	501	NDP	C1B-N9A-C4A	-7.63	113.24	126.64
52	P	501	NDP	N6A-C6A-N1A	-6.05	106.02	118.57
52	P	501	NDP	N3A-C2A-N1A	-5.52	120.04	128.68
51	P	503	CDL	OB6-CB5-C51	5.14	120.55	111.09

There are no chirality outliers.

5 of 850 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	PLC	C1'-C'-O2-C2
45	A	201	PLC	O'-C'-O2-C2
45	A	201	PLC	C1-O3P-P-O1P
45	A	201	PLC	C1-O3P-P-O2P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
45	B	302	PLC	O4P-C4-C5-N

There are no ring outliers.

39 monomers are involved in 95 short contacts:

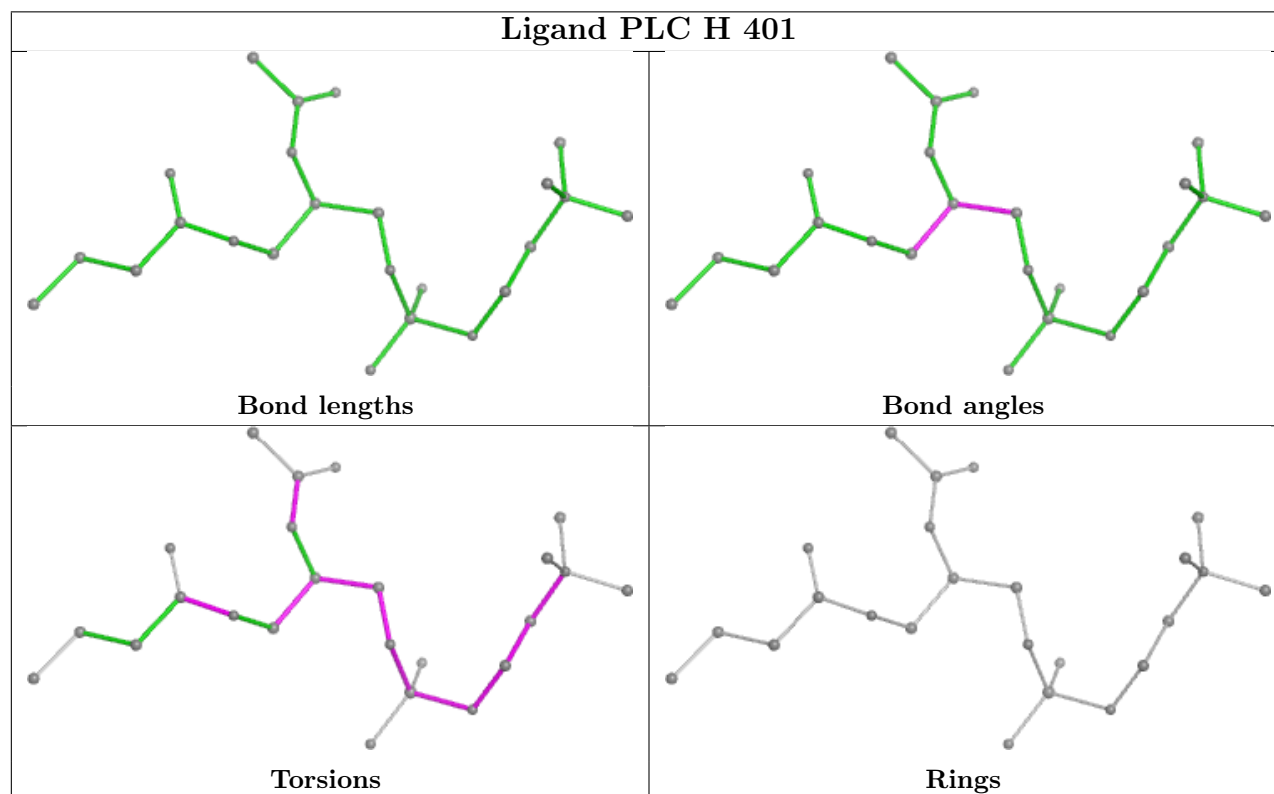
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	G	802	SF4	1	0
50	L	711	3PE	2	0
45	M	1002	PLC	3	0
50	g	301	3PE	2	0
50	b	105	3PE	1	0
50	Y	303	3PE	1	0
46	F	501	SF4	2	0
51	a	201	CDL	2	0
51	O	201	CDL	5	0
52	P	501	NDP	1	0
45	A	201	PLC	2	0
45	M	1003	PLC	1	0
50	L	708	3PE	3	0
45	q	401	PLC	3	0
45	d	101	PLC	4	0
45	B	302	PLC	1	0
54	U	201	EHZ	1	0
51	b	102	CDL	3	0
46	I	301	SF4	1	0
45	b	101	PLC	2	0
50	L	706	3PE	7	0
50	b	106	3PE	2	0
50	L	710	3PE	4	0
50	L	707	3PE	5	0
45	h	201	PLC	2	0
45	Y	301	PLC	1	0
45	L	704	PLC	1	0
45	q	402	PLC	1	0
45	L	702	PLC	3	0
50	L	709	3PE	2	0
50	N	602	3PE	1	0
50	Y	302	3PE	8	0
45	D	501	PLC	2	0
45	L	705	PLC	3	0
50	f	101	3PE	7	0
46	I	302	SF4	2	0

*Continued on next page...*

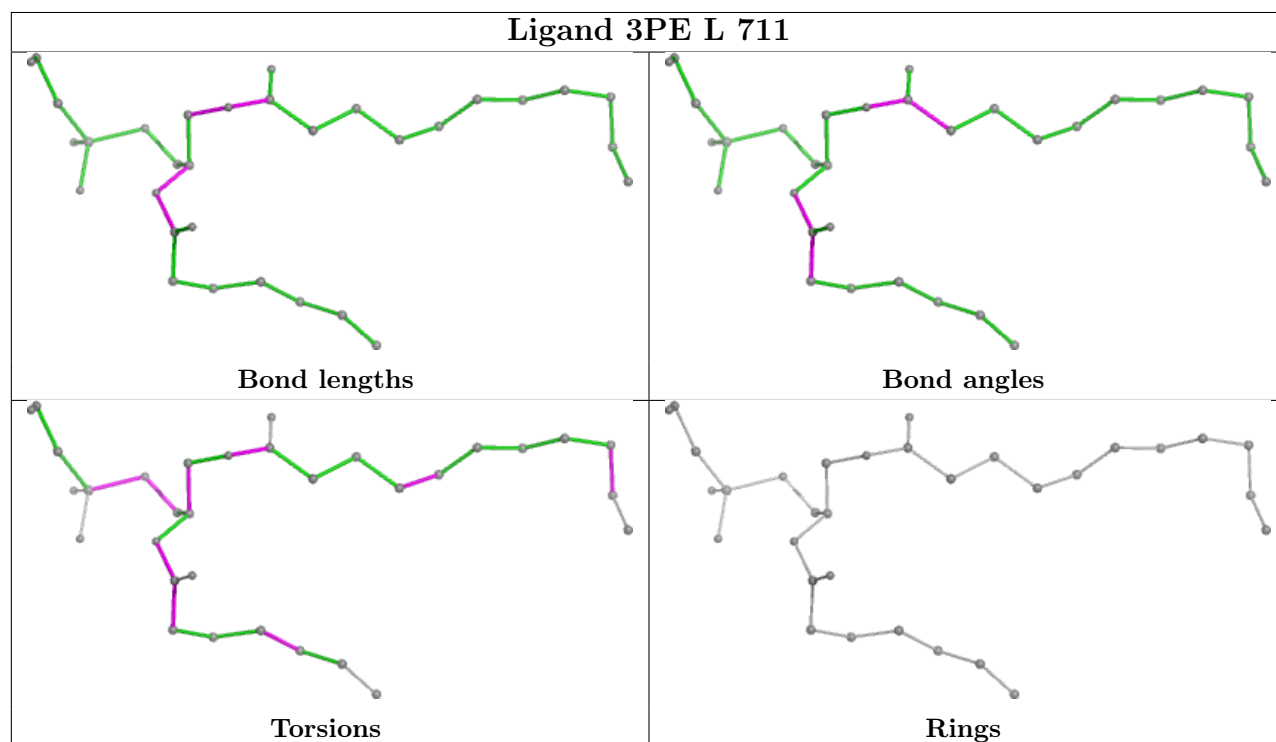
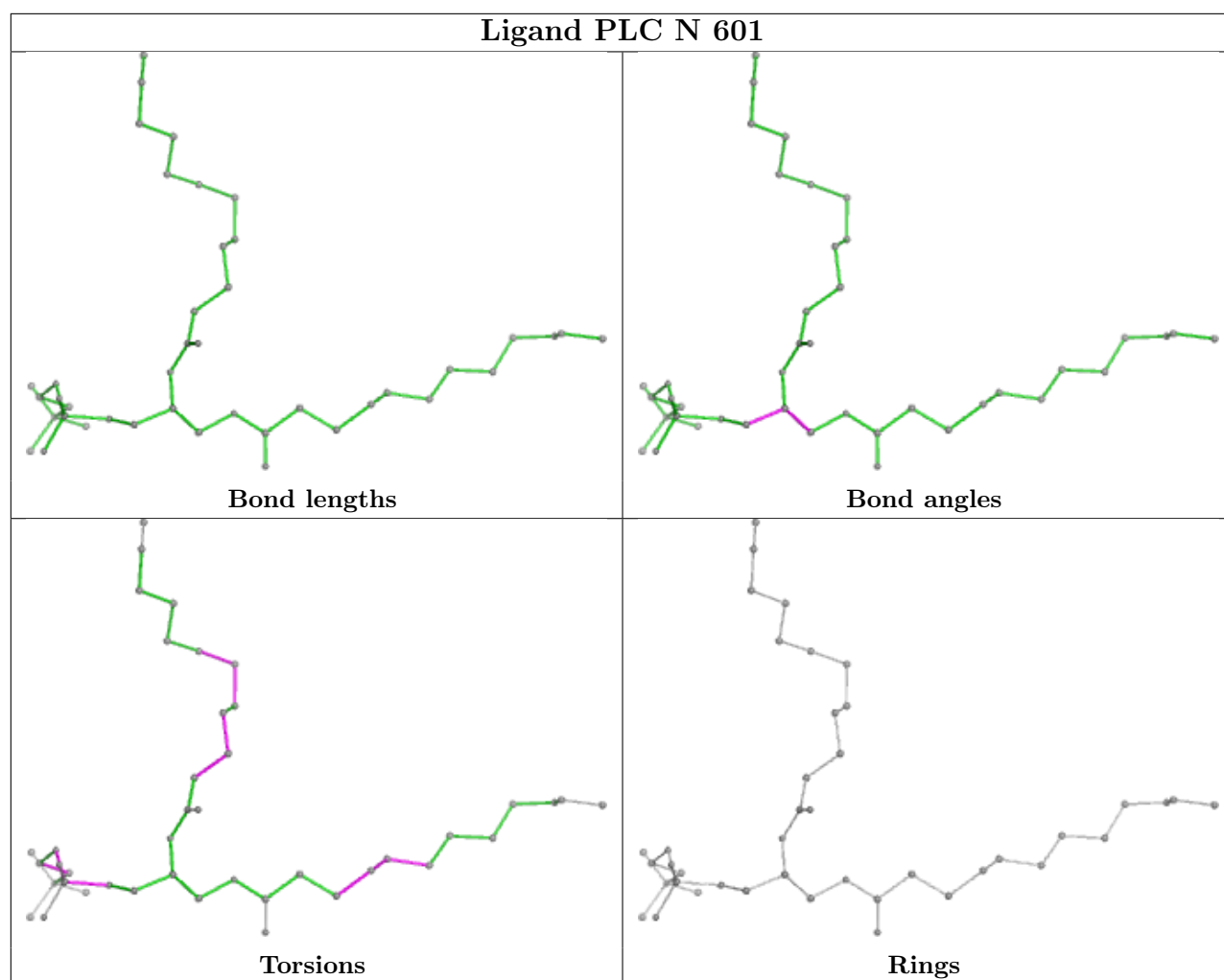
*Continued from previous page...*

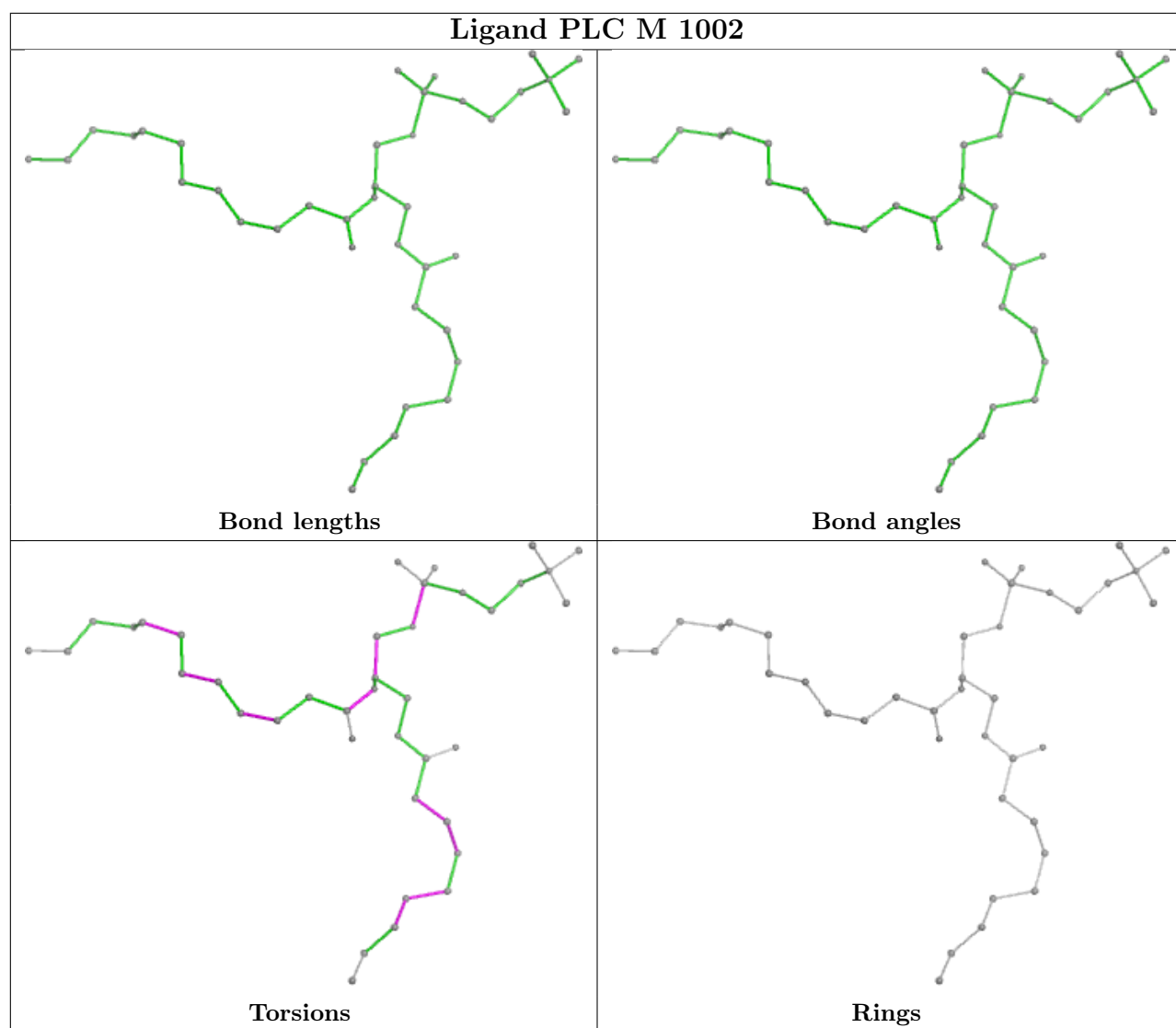
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	P	502	PLC	3	0
50	L	703	3PE	2	0
50	b	104	3PE	2	0

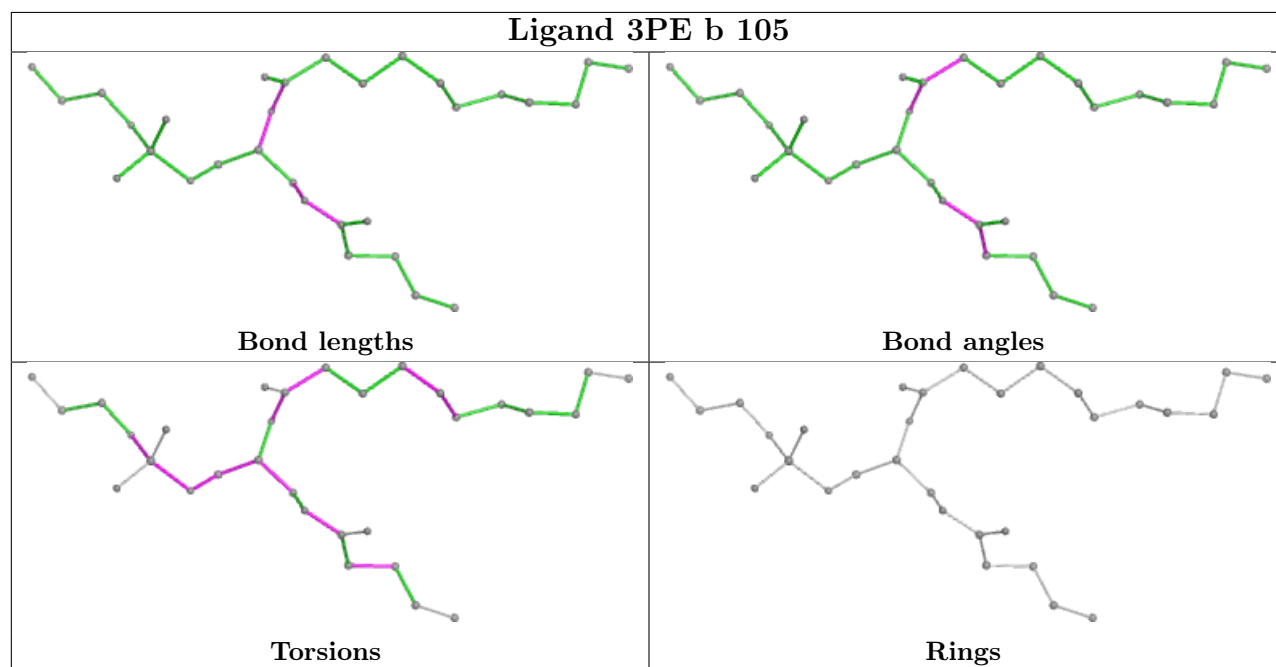
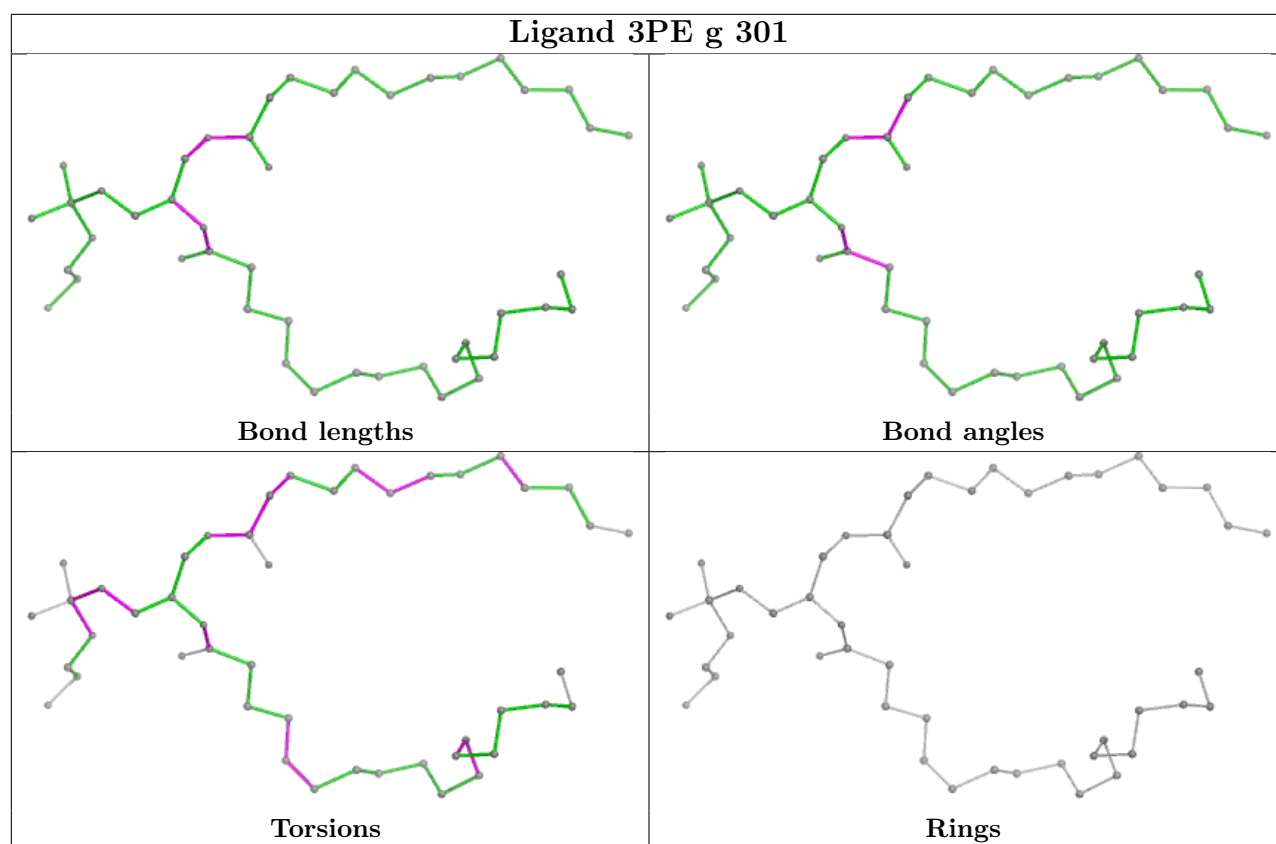
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

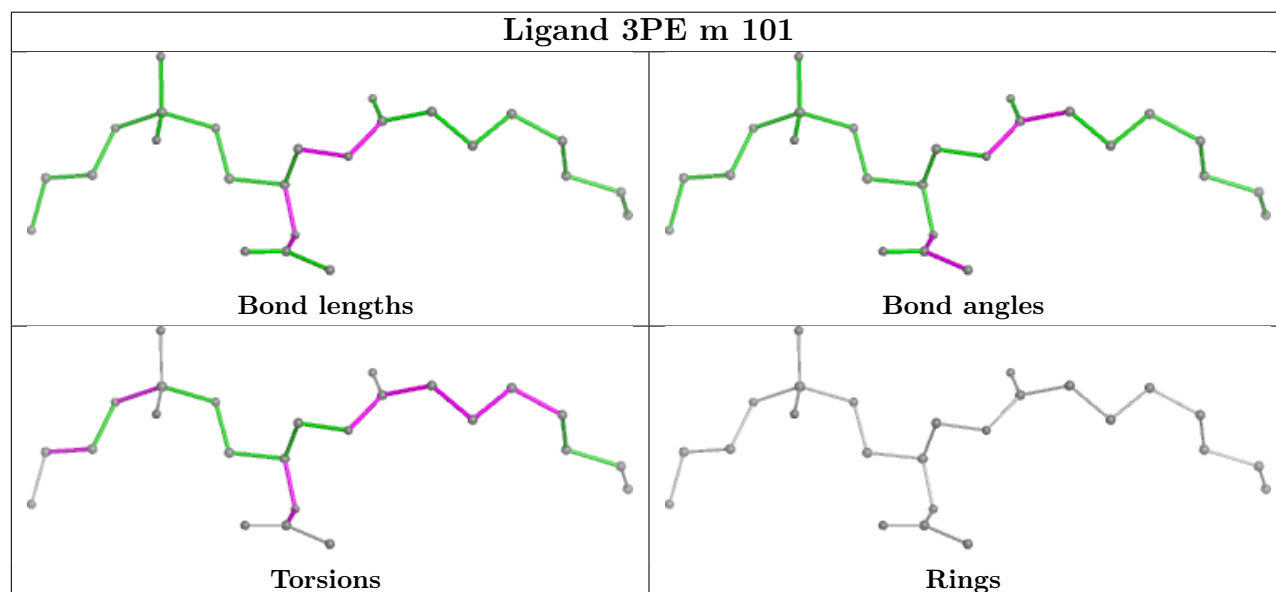
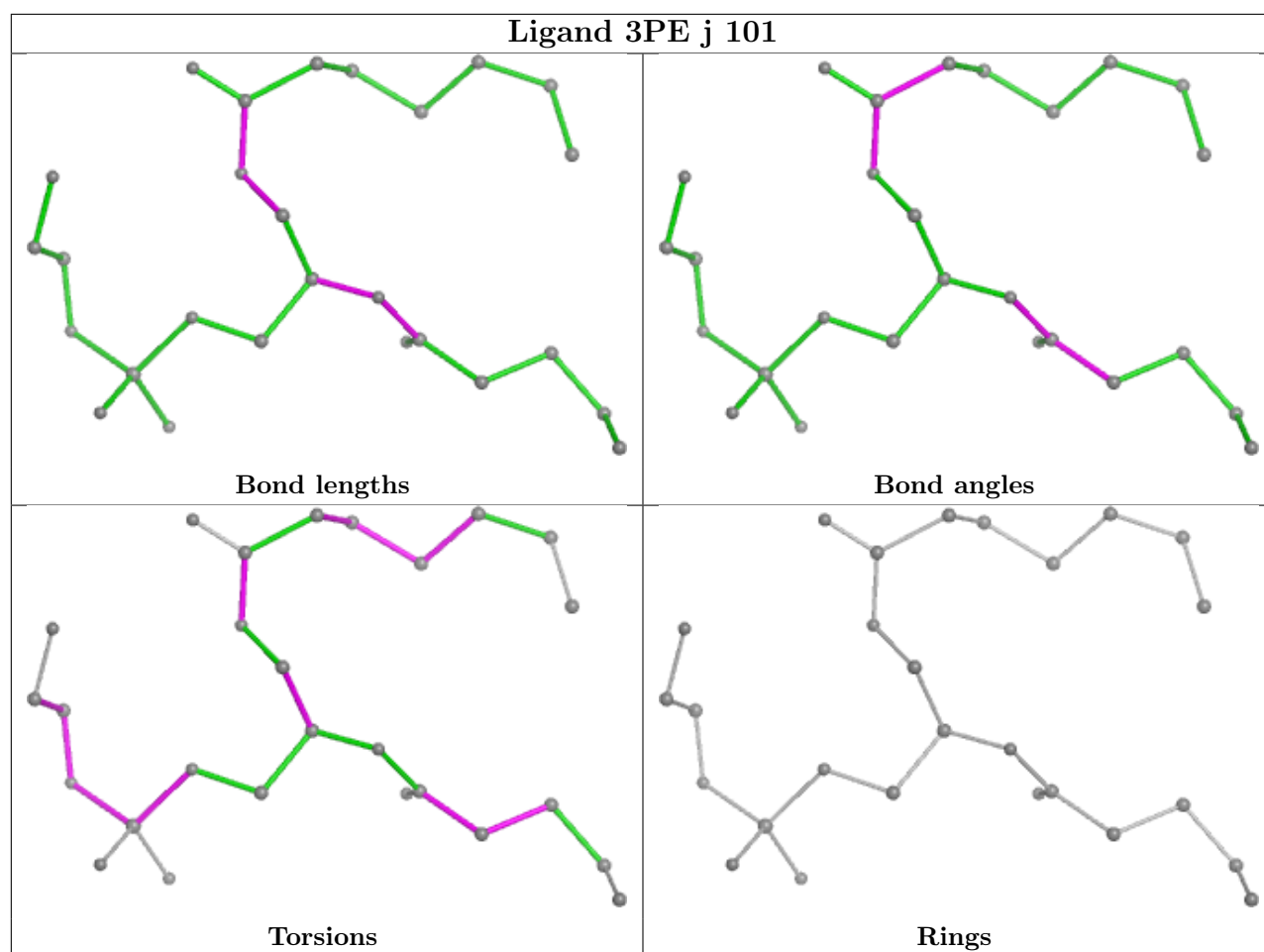


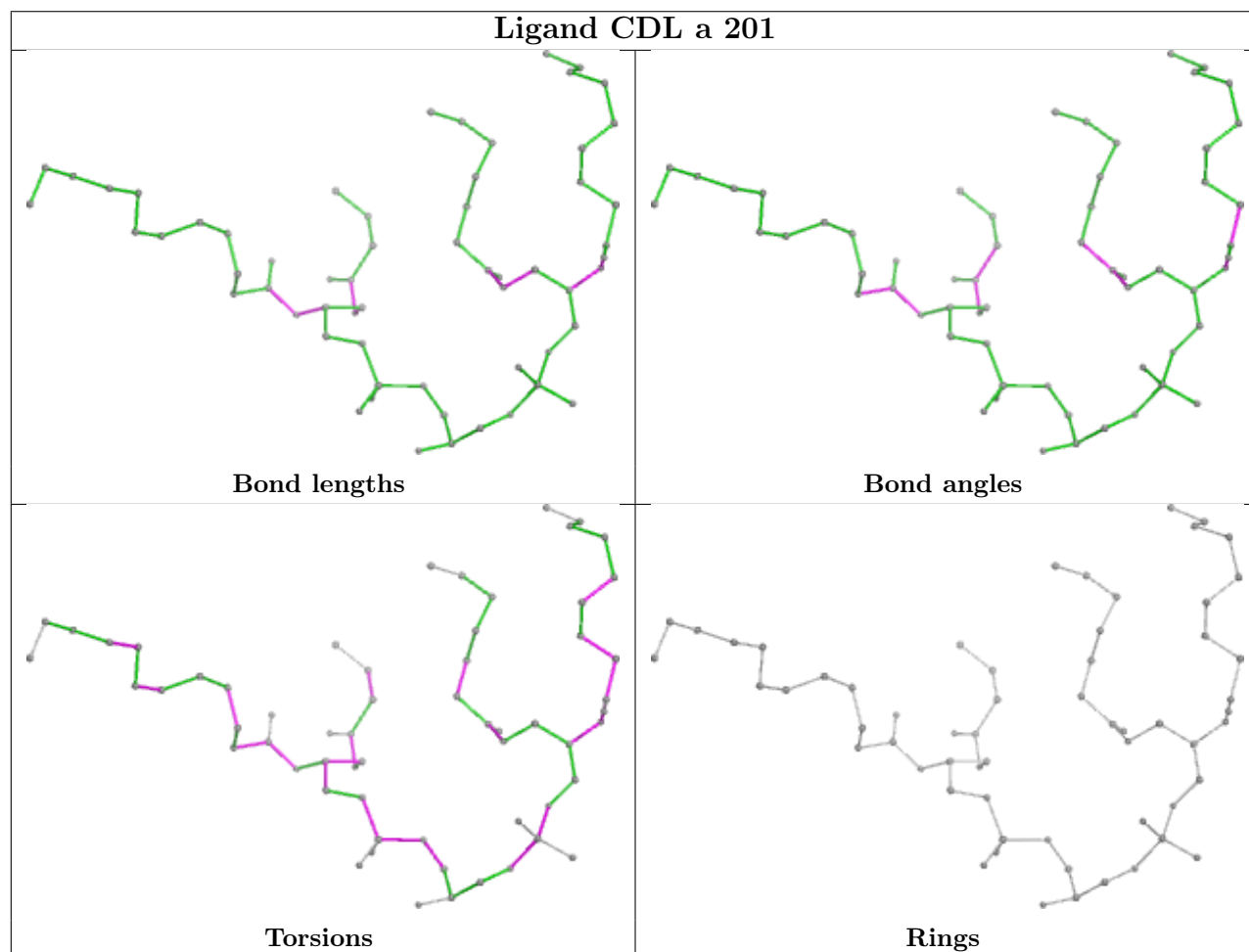
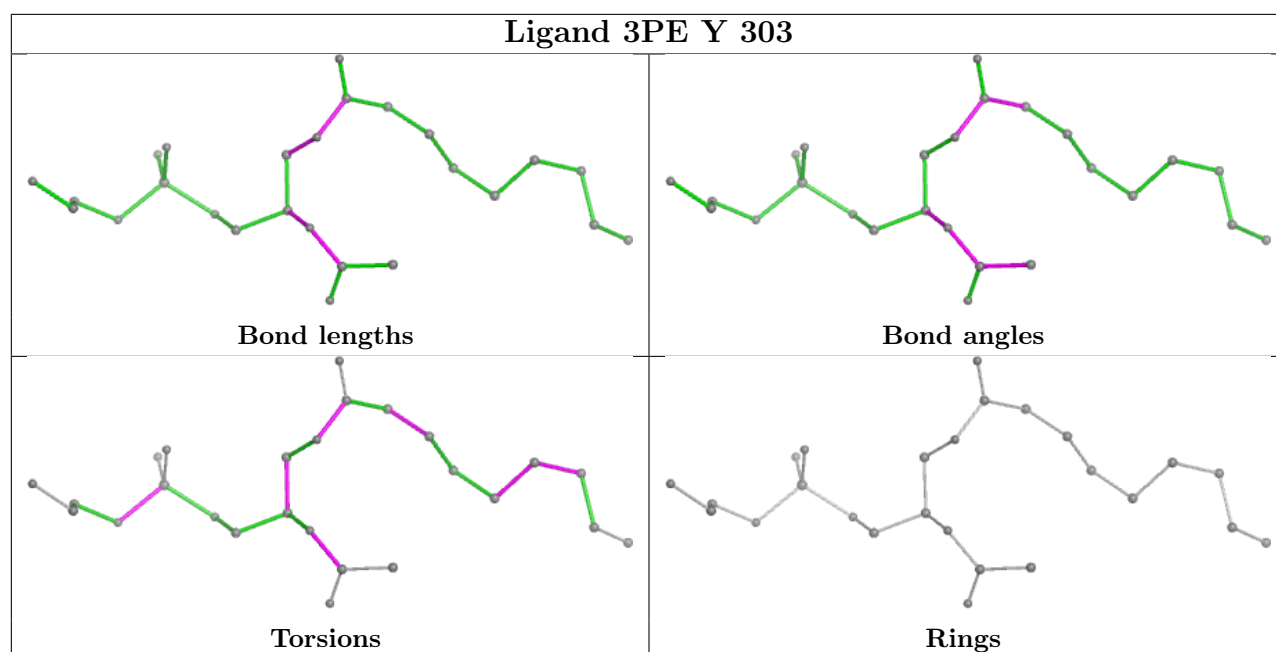


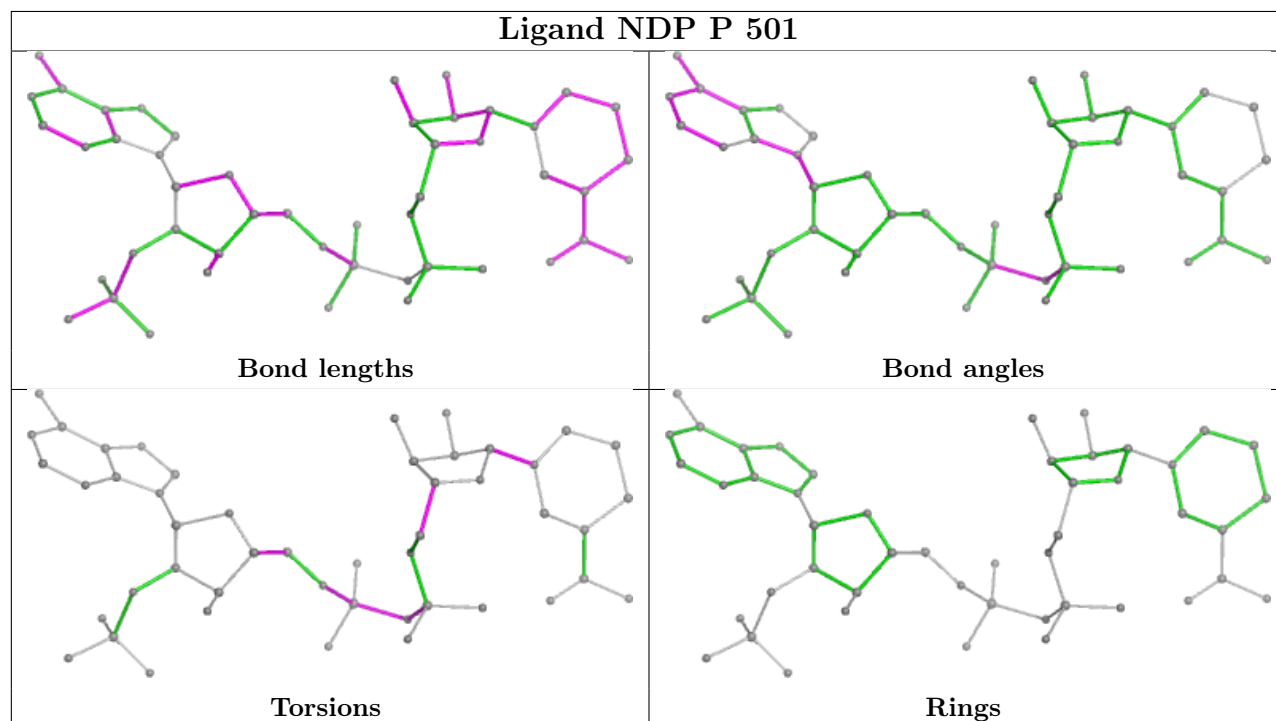
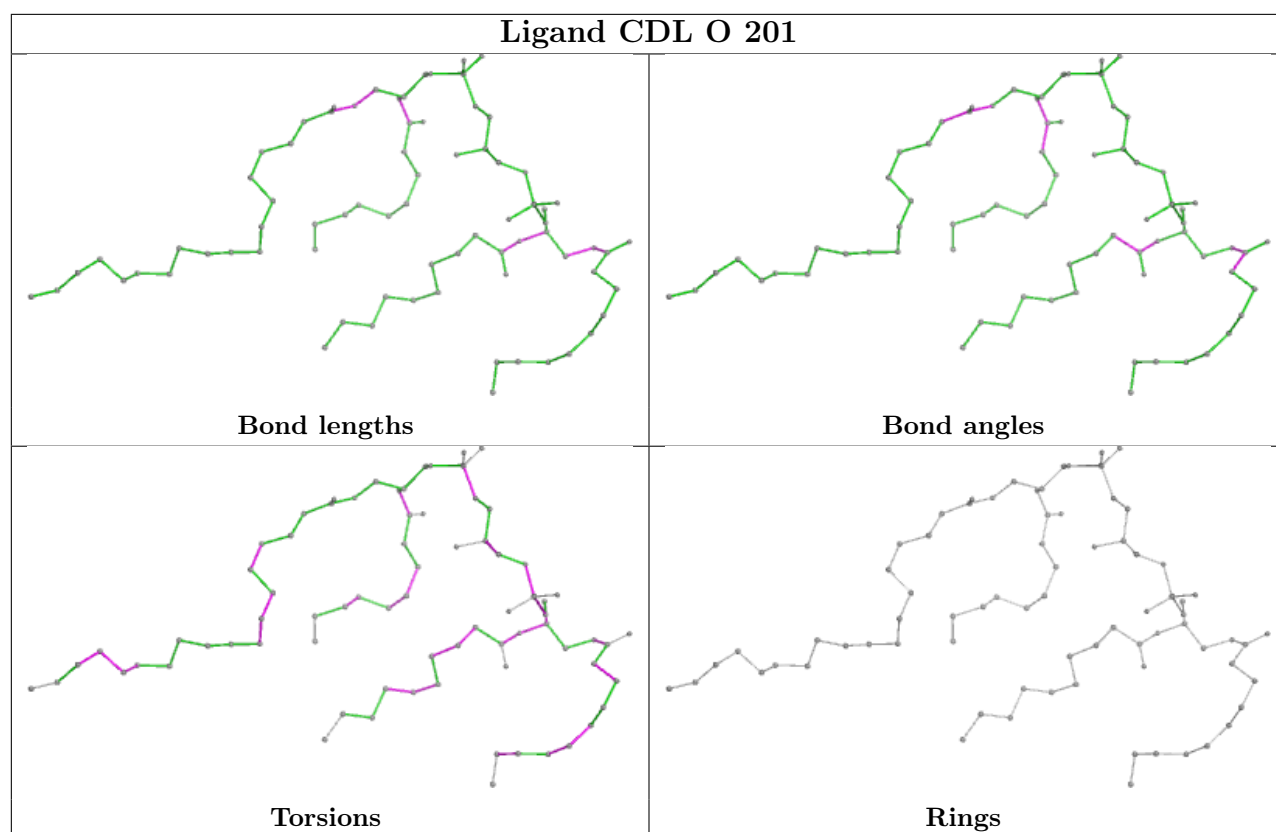


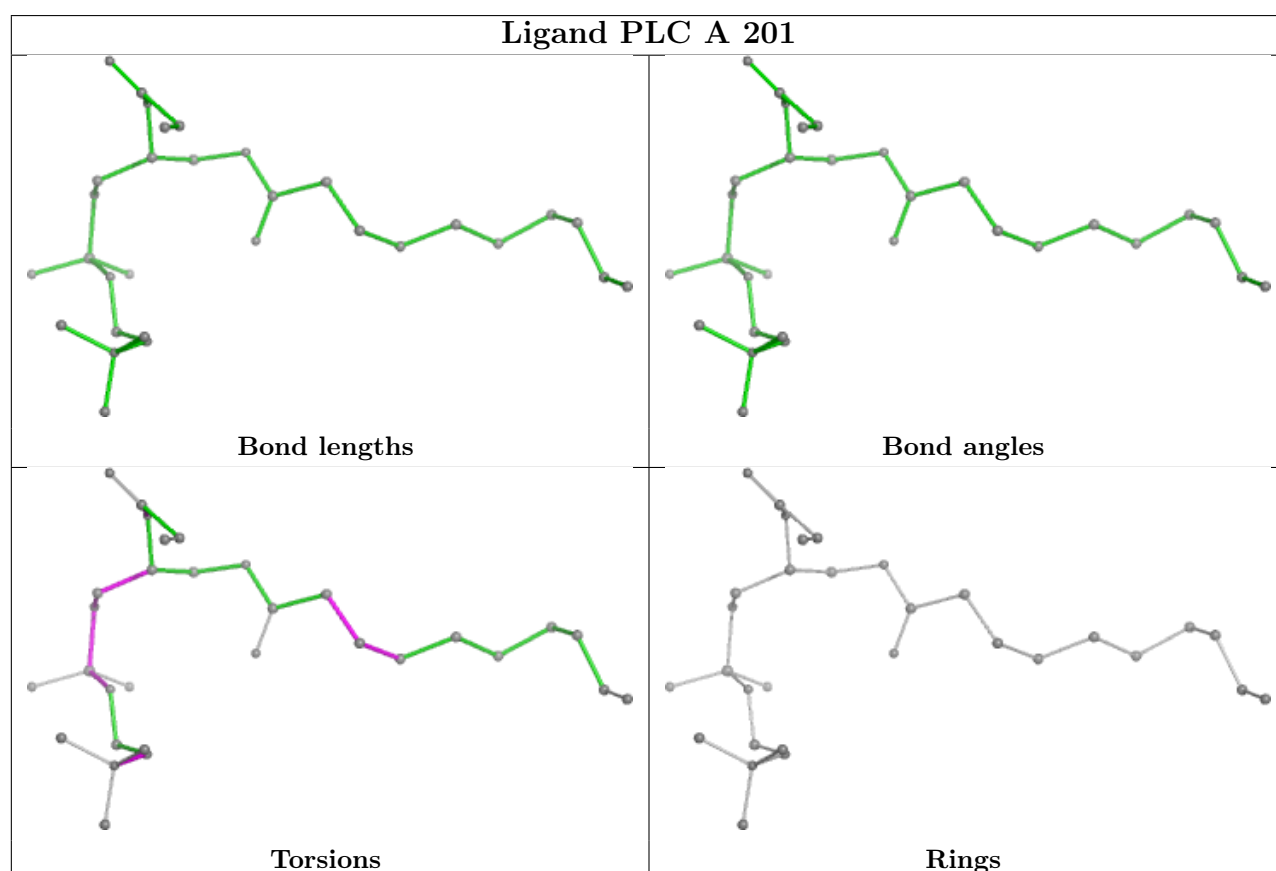
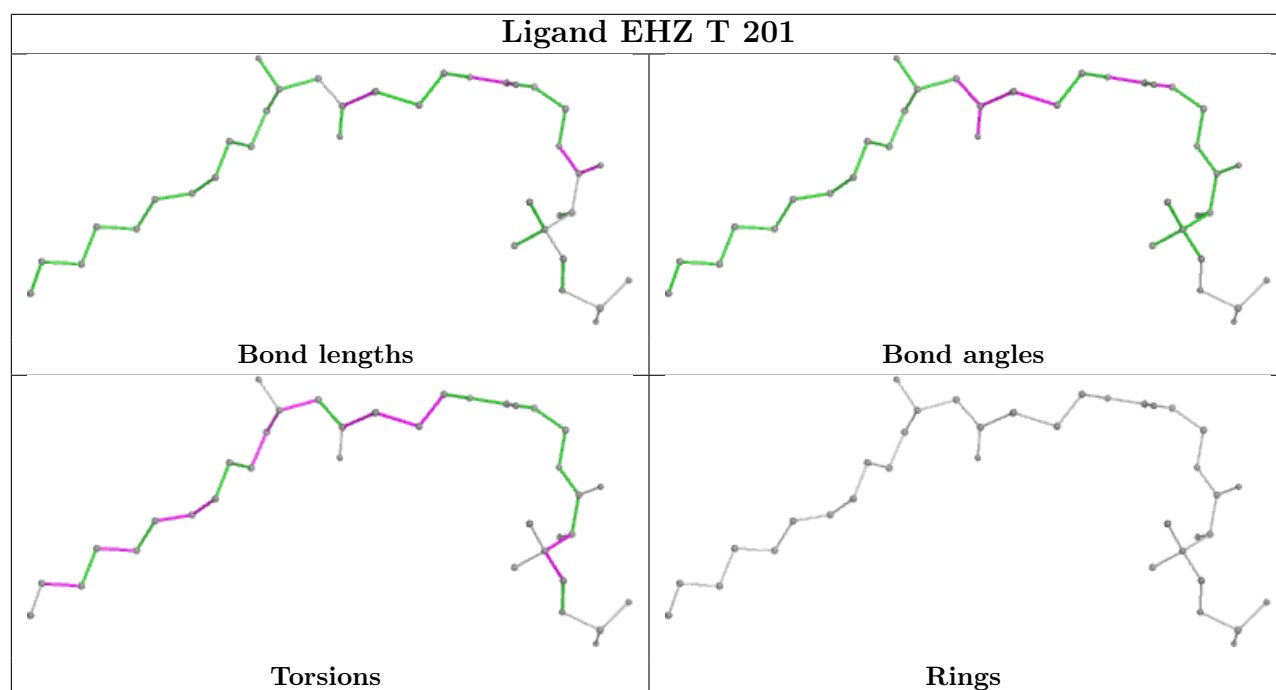


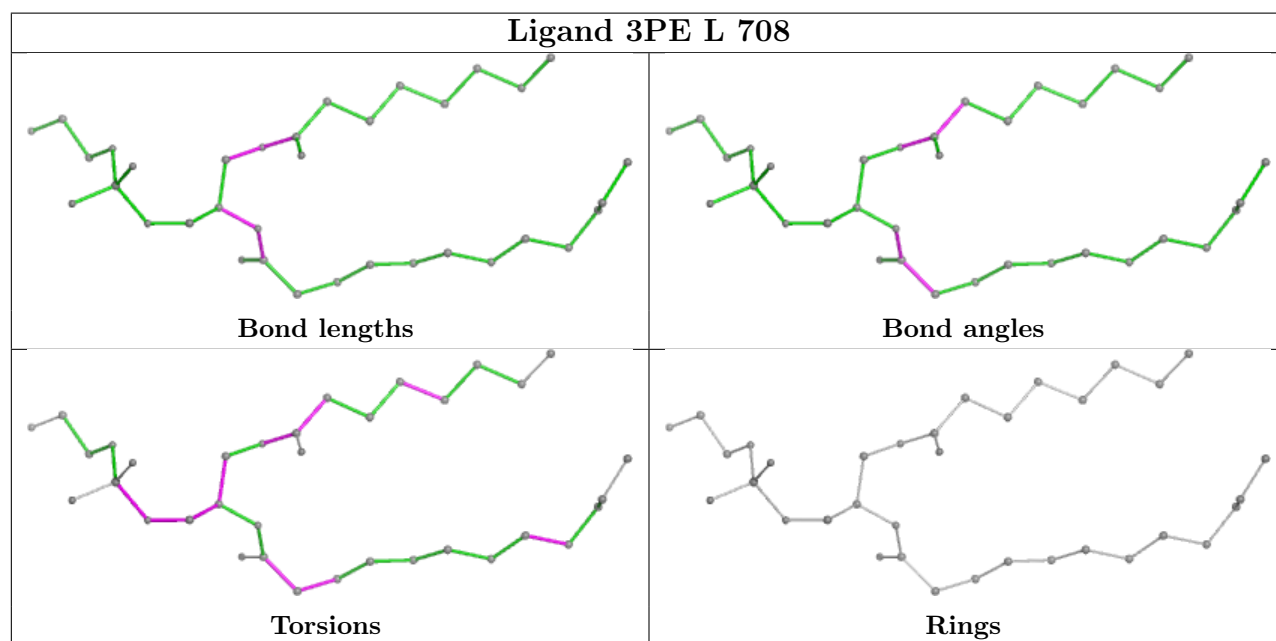
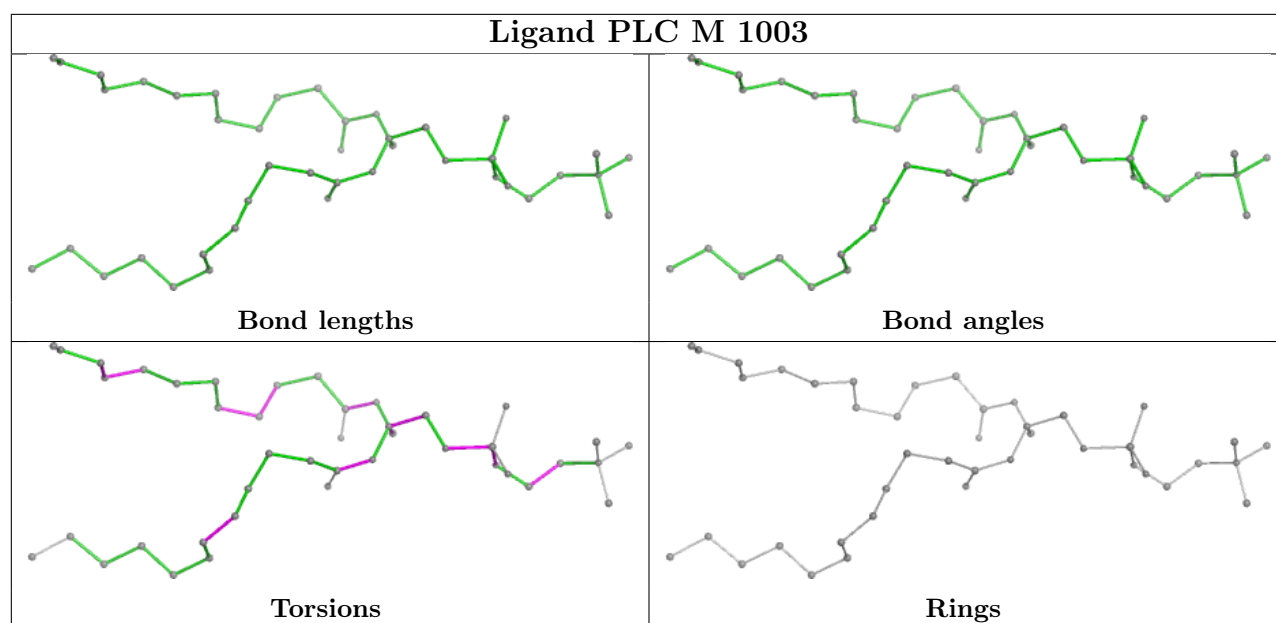




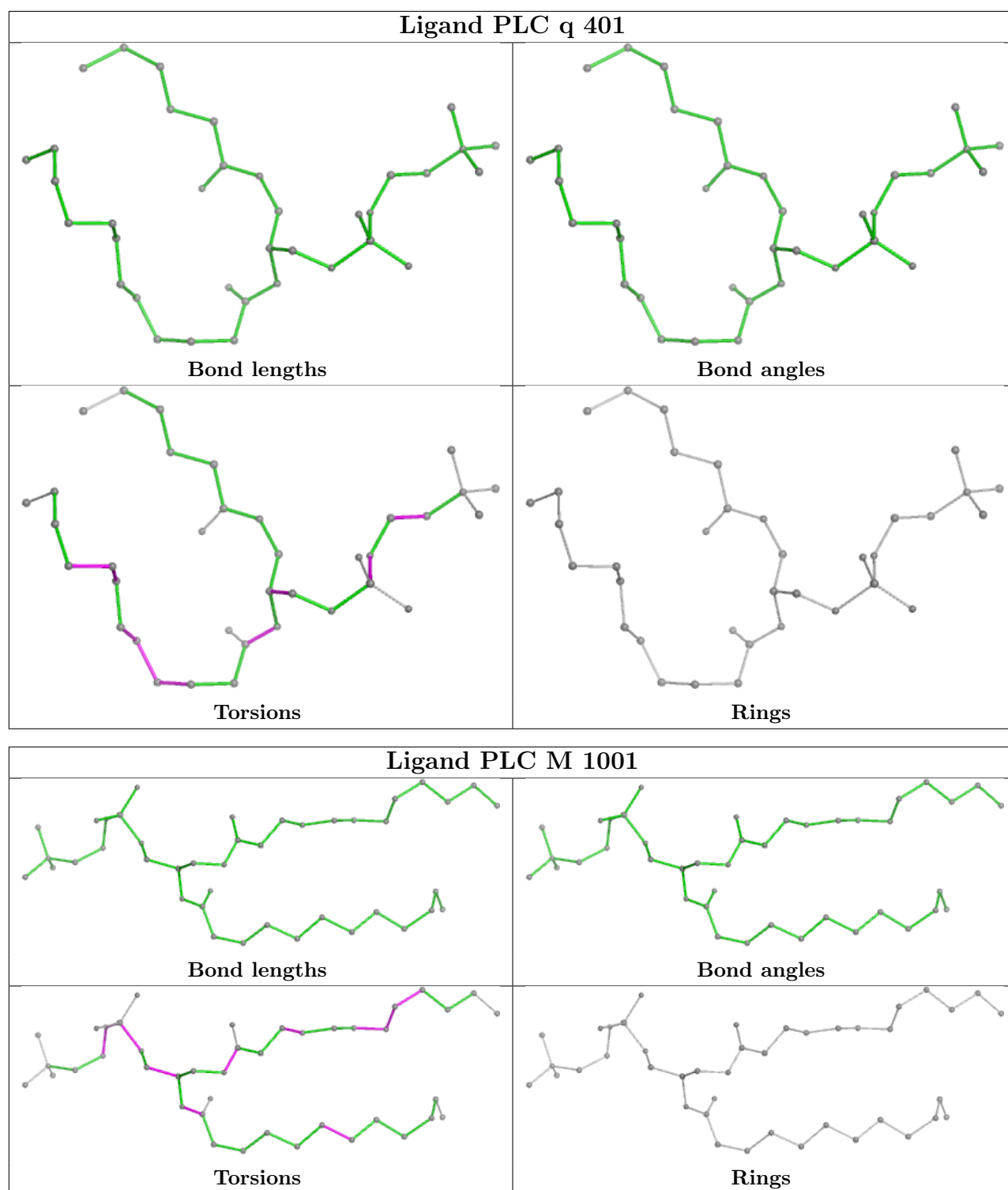


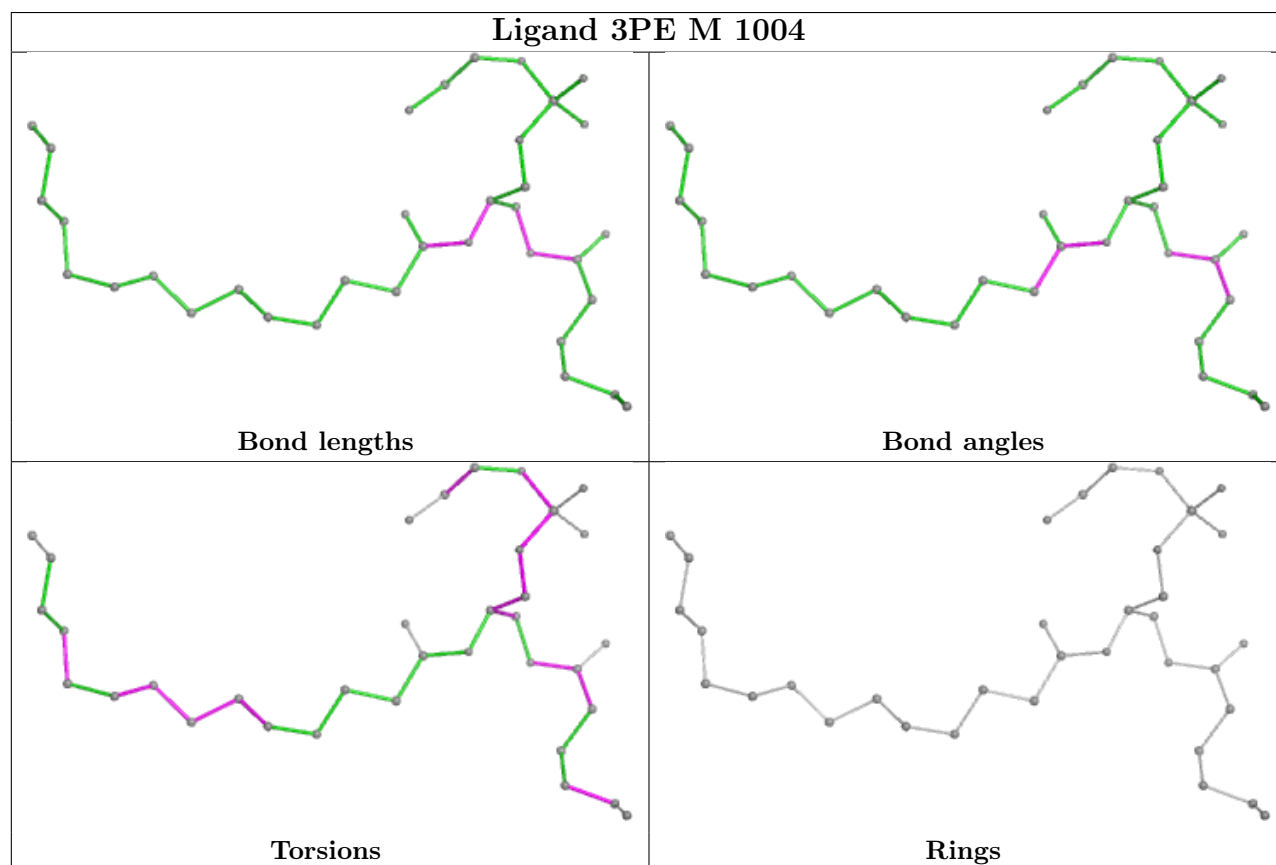
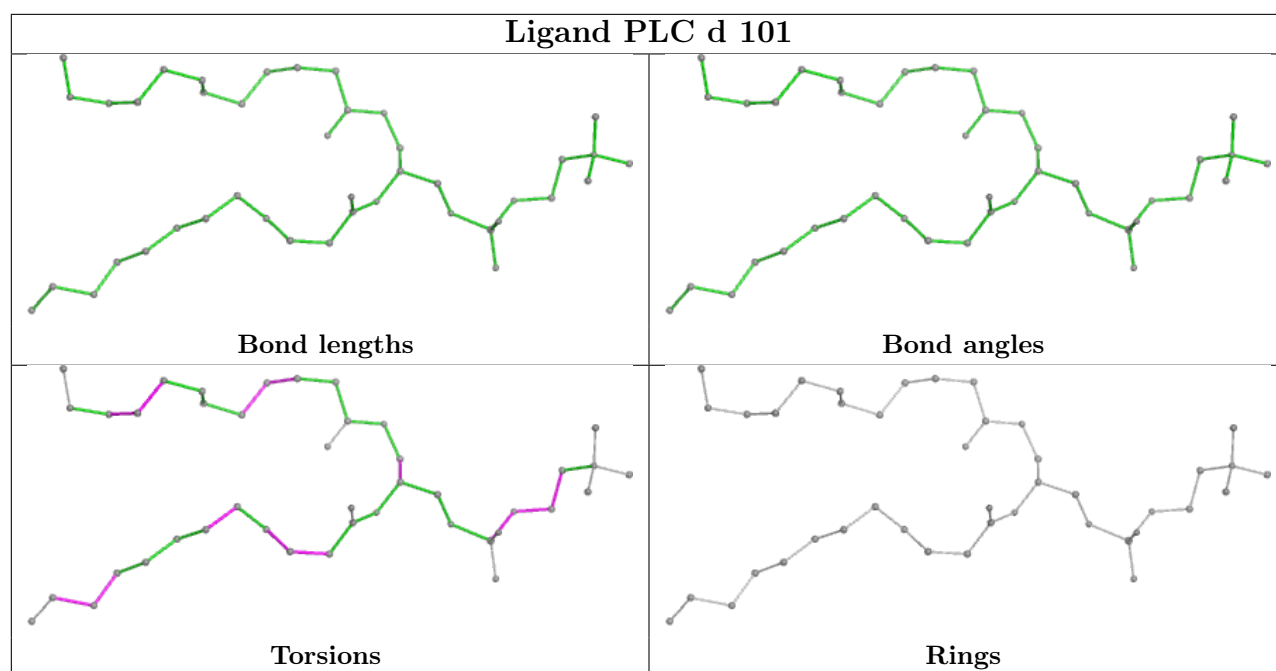


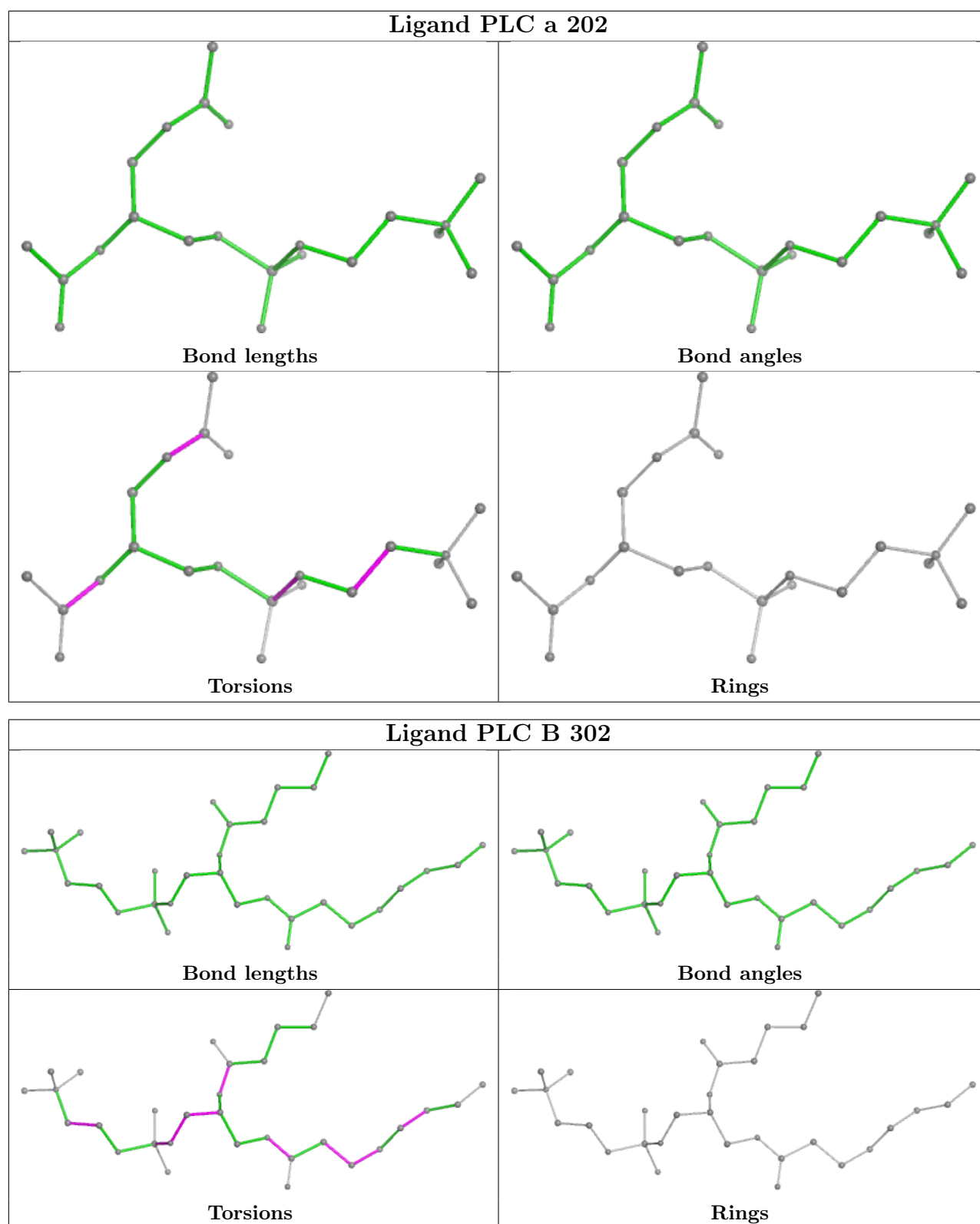


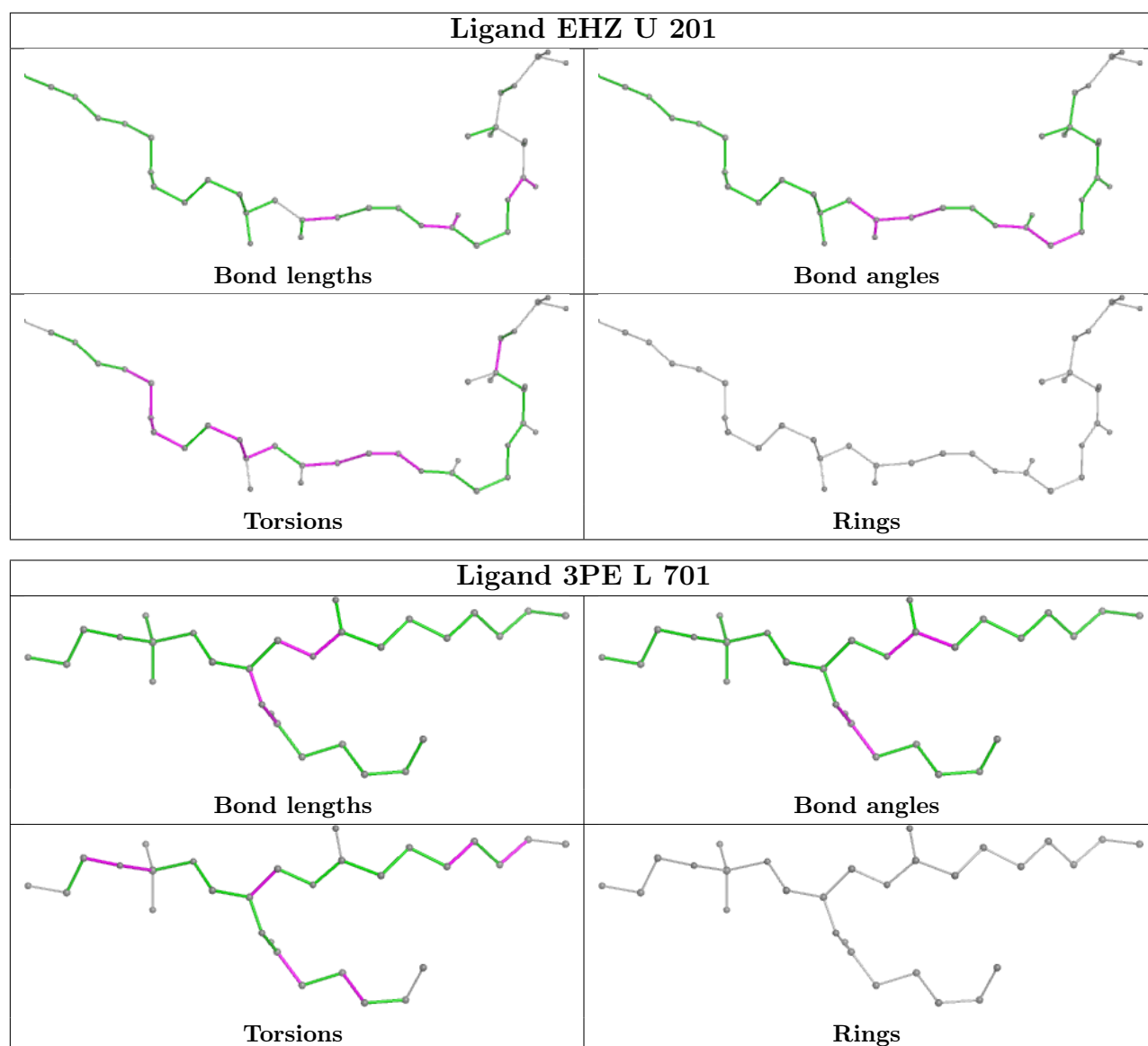


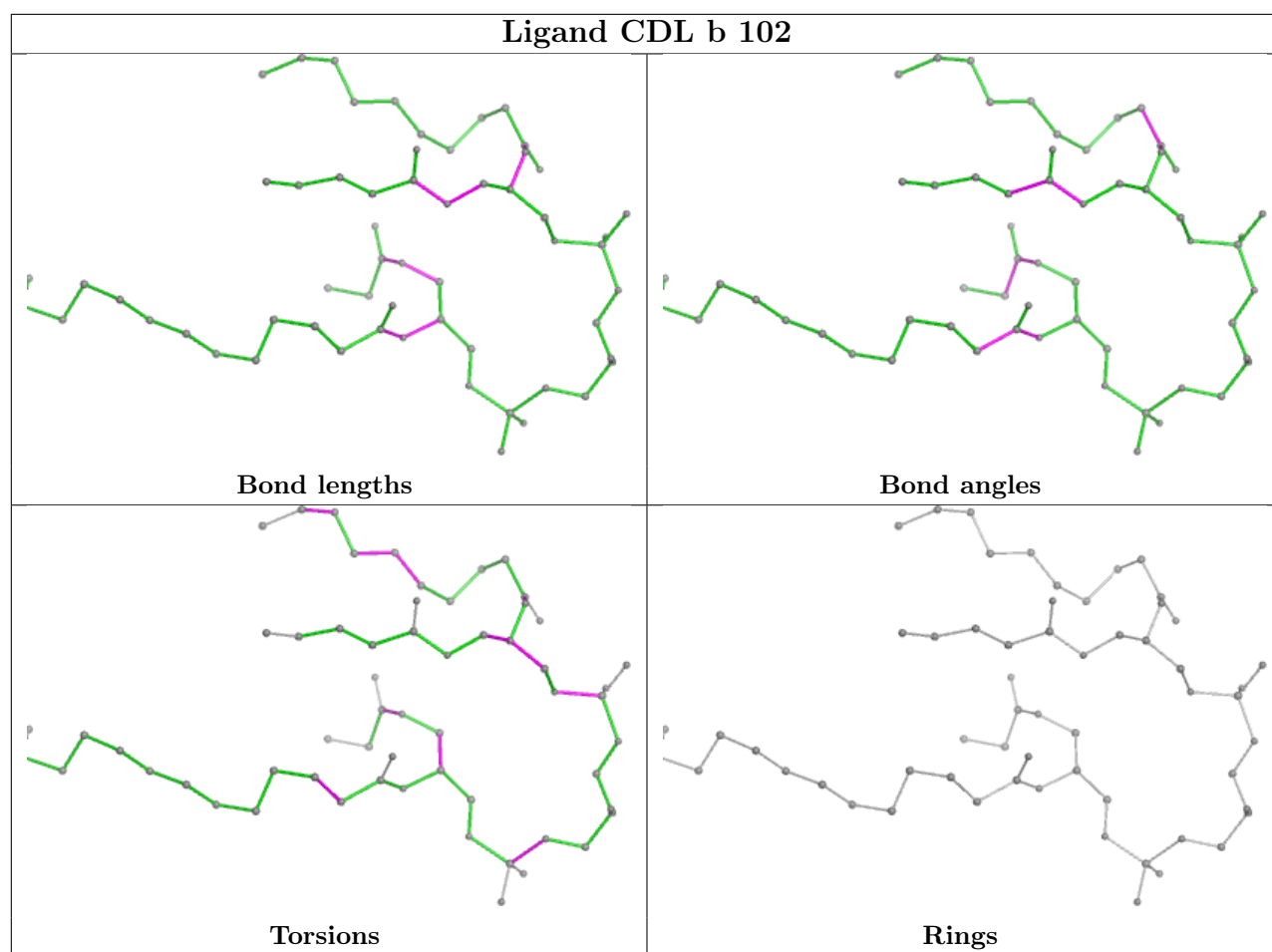


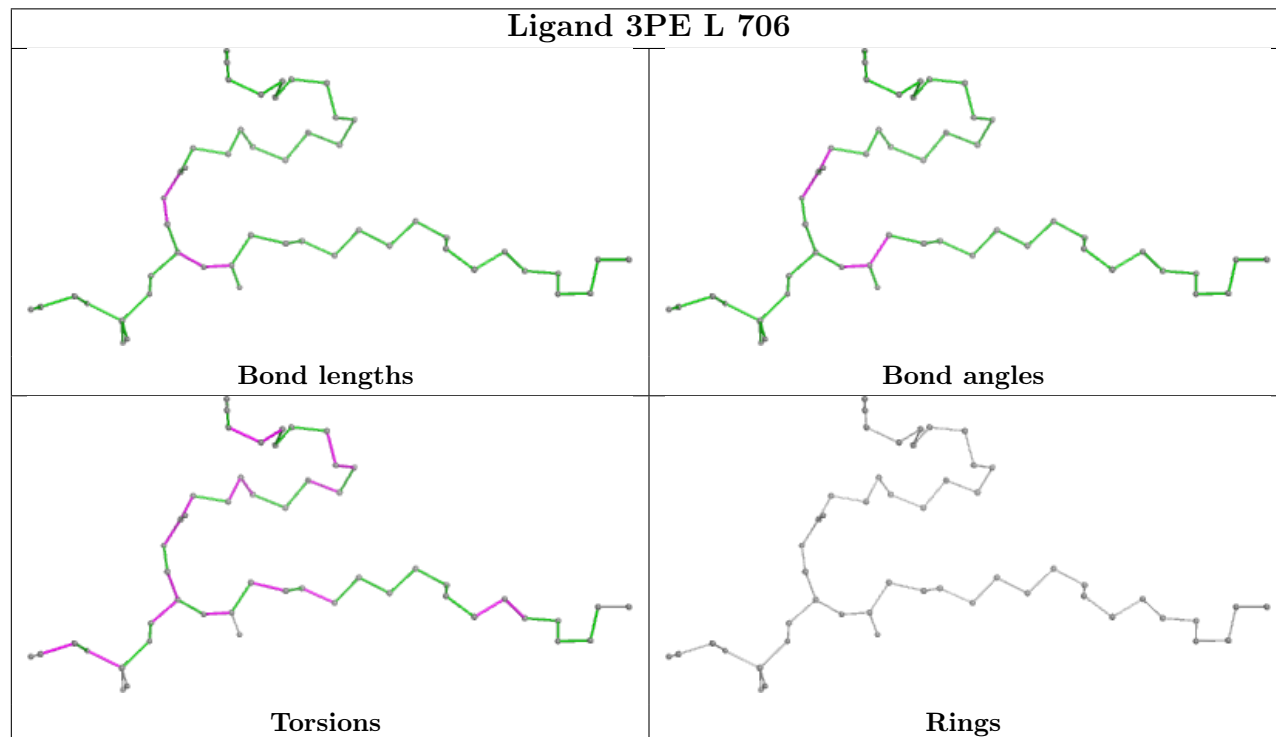
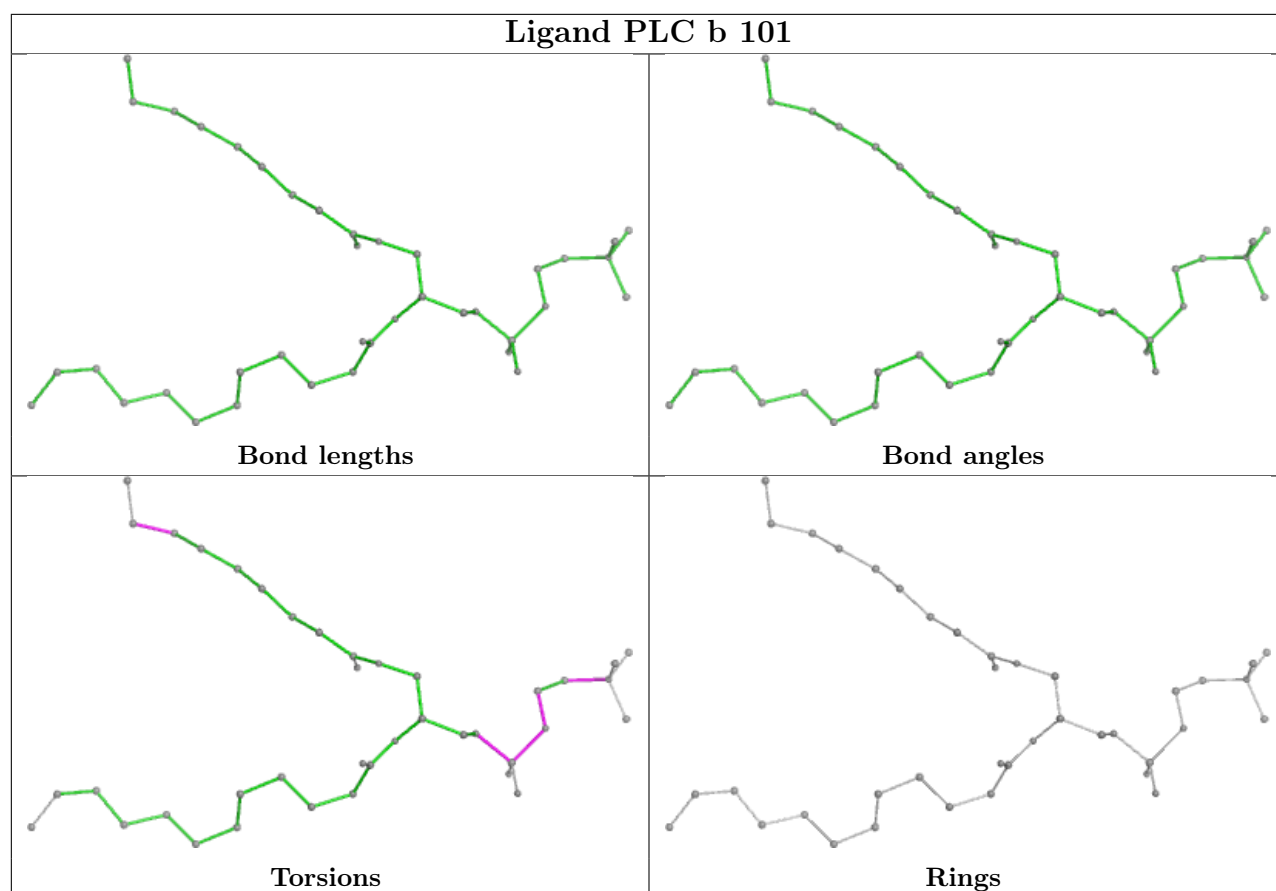


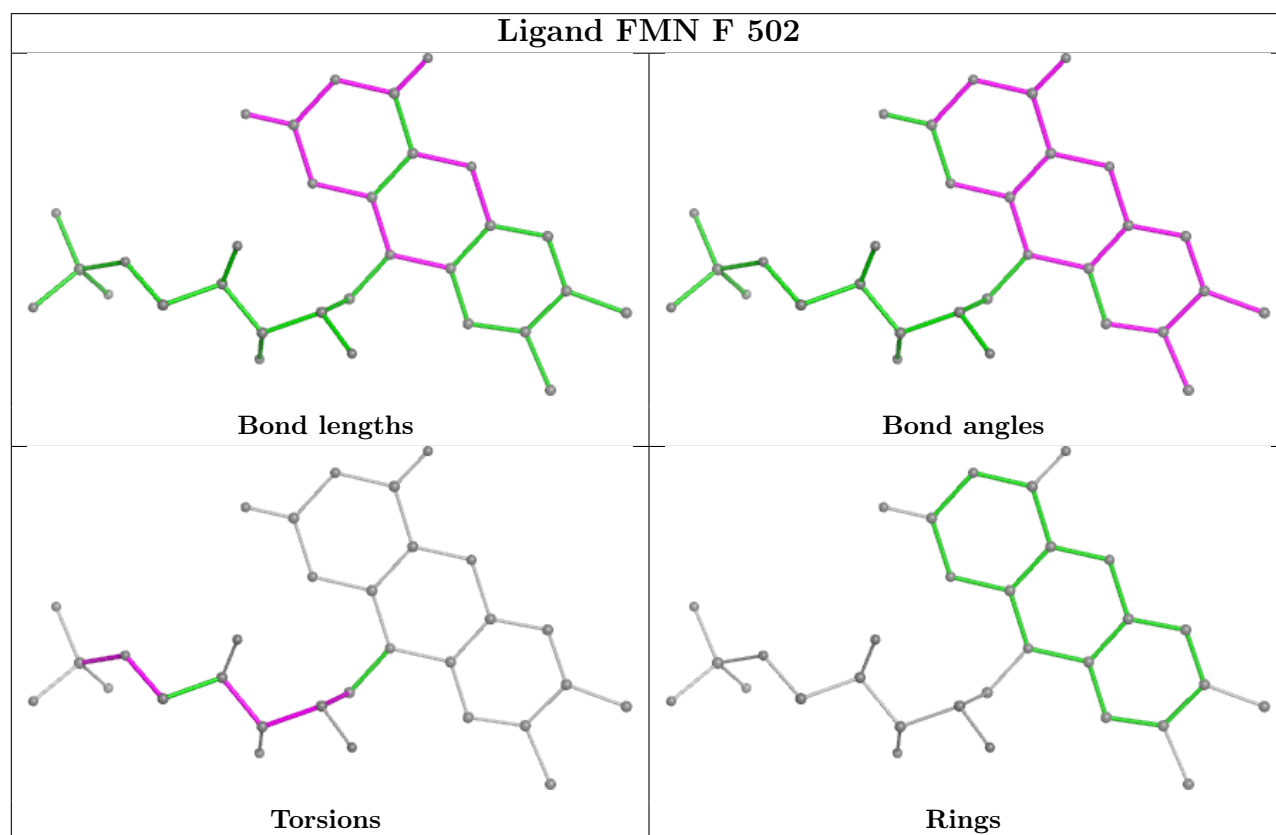
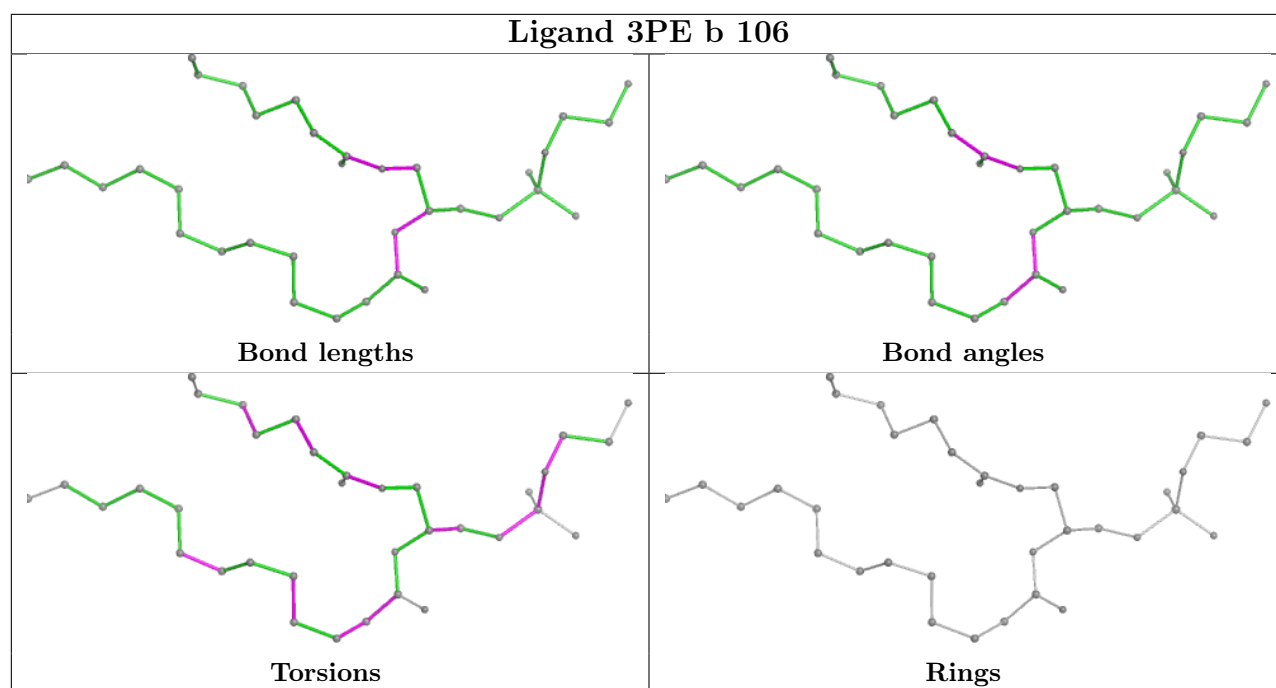


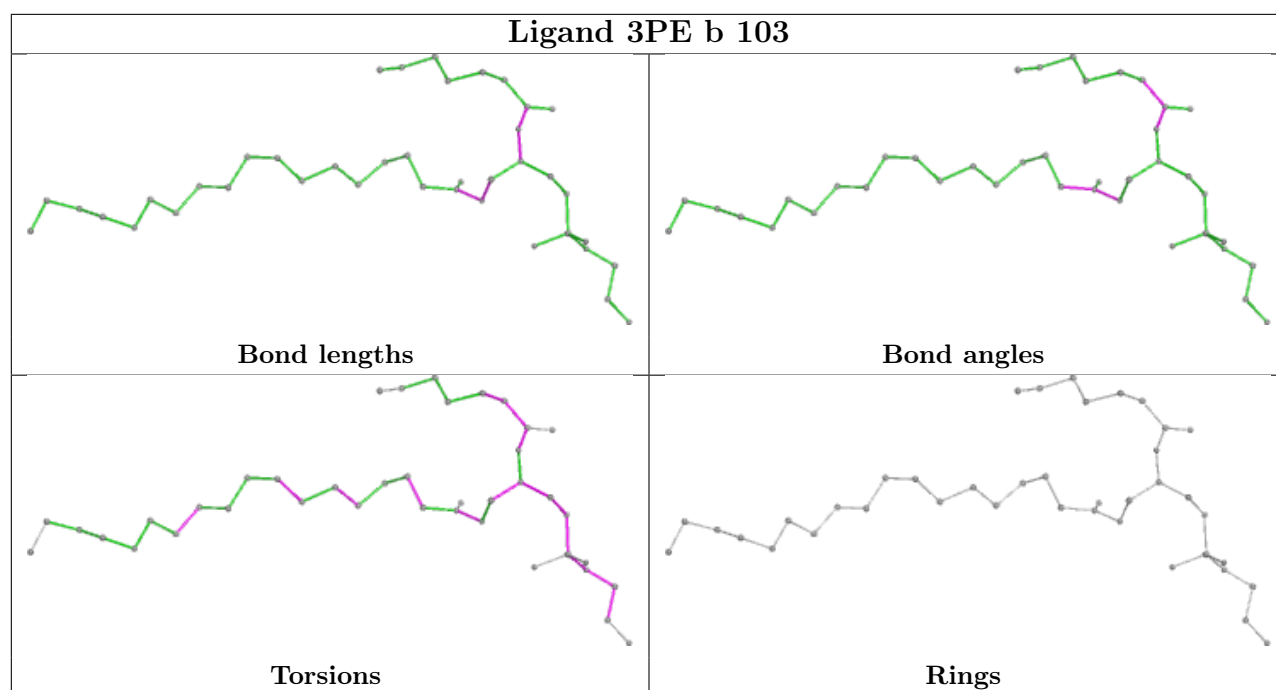




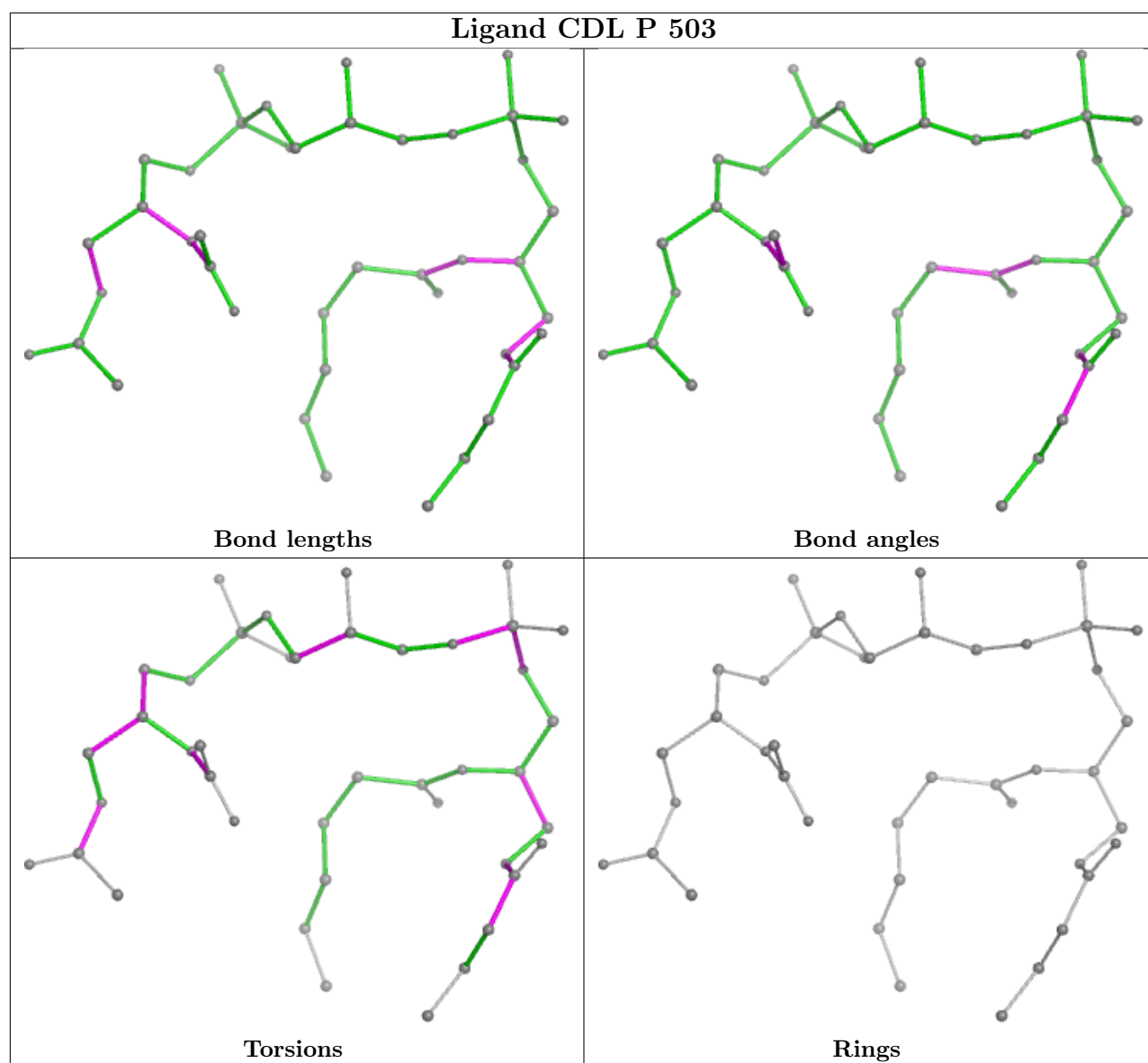


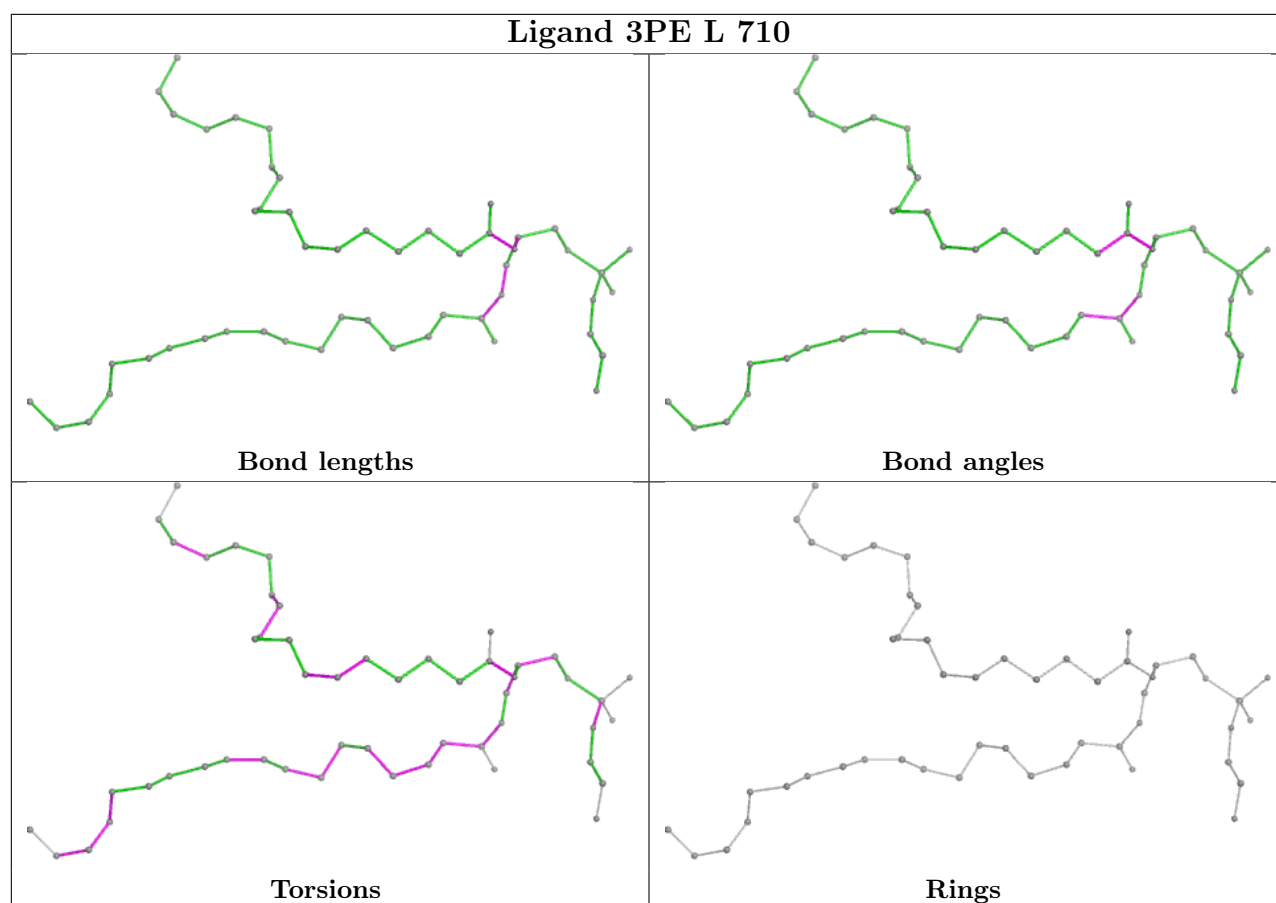


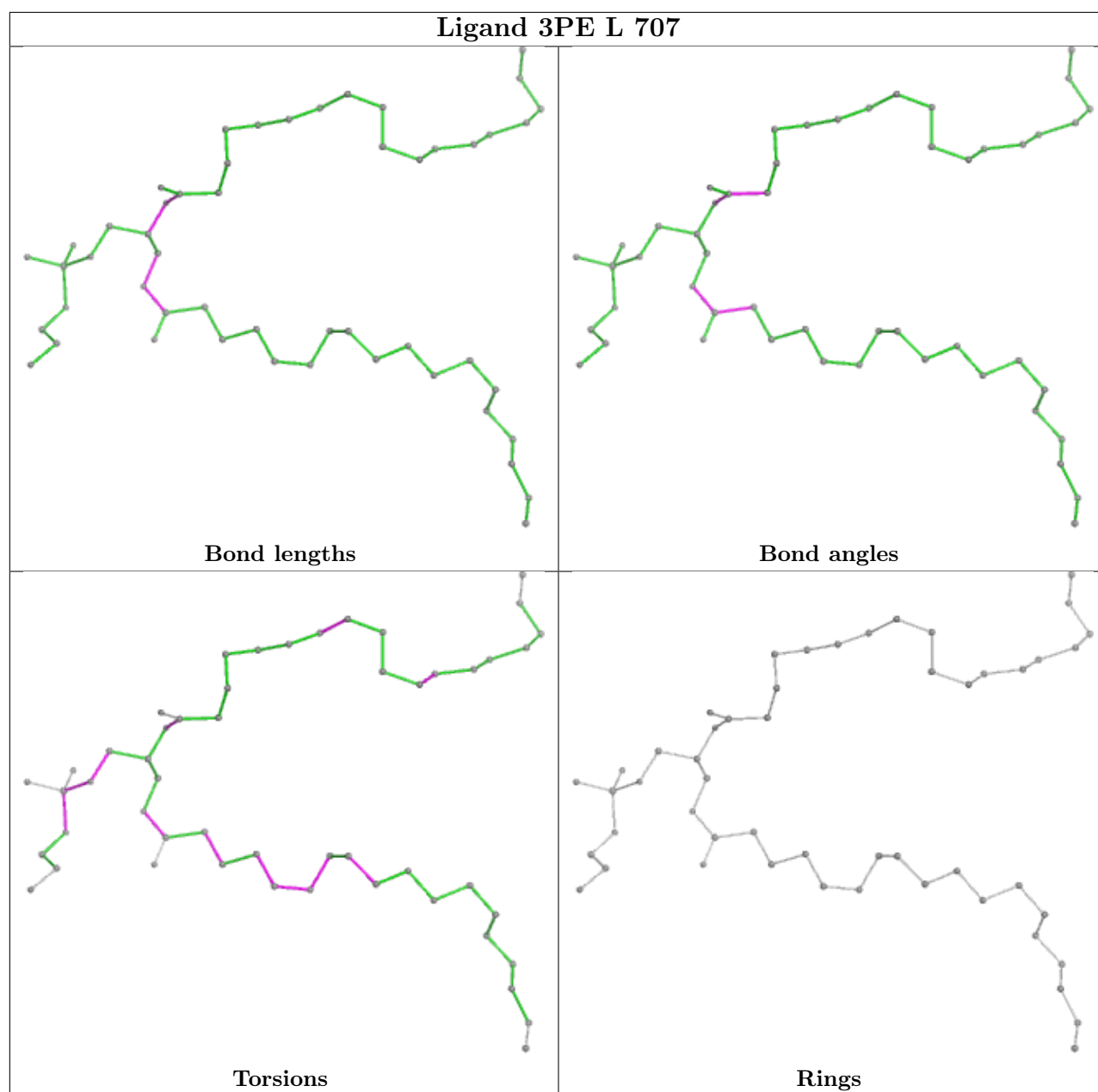


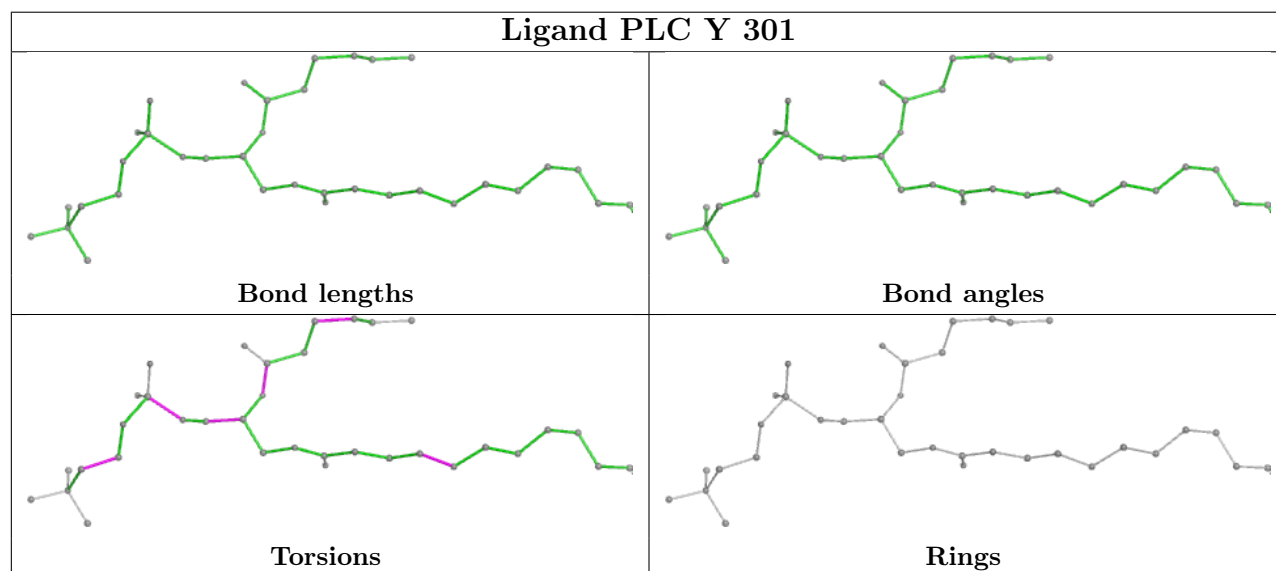
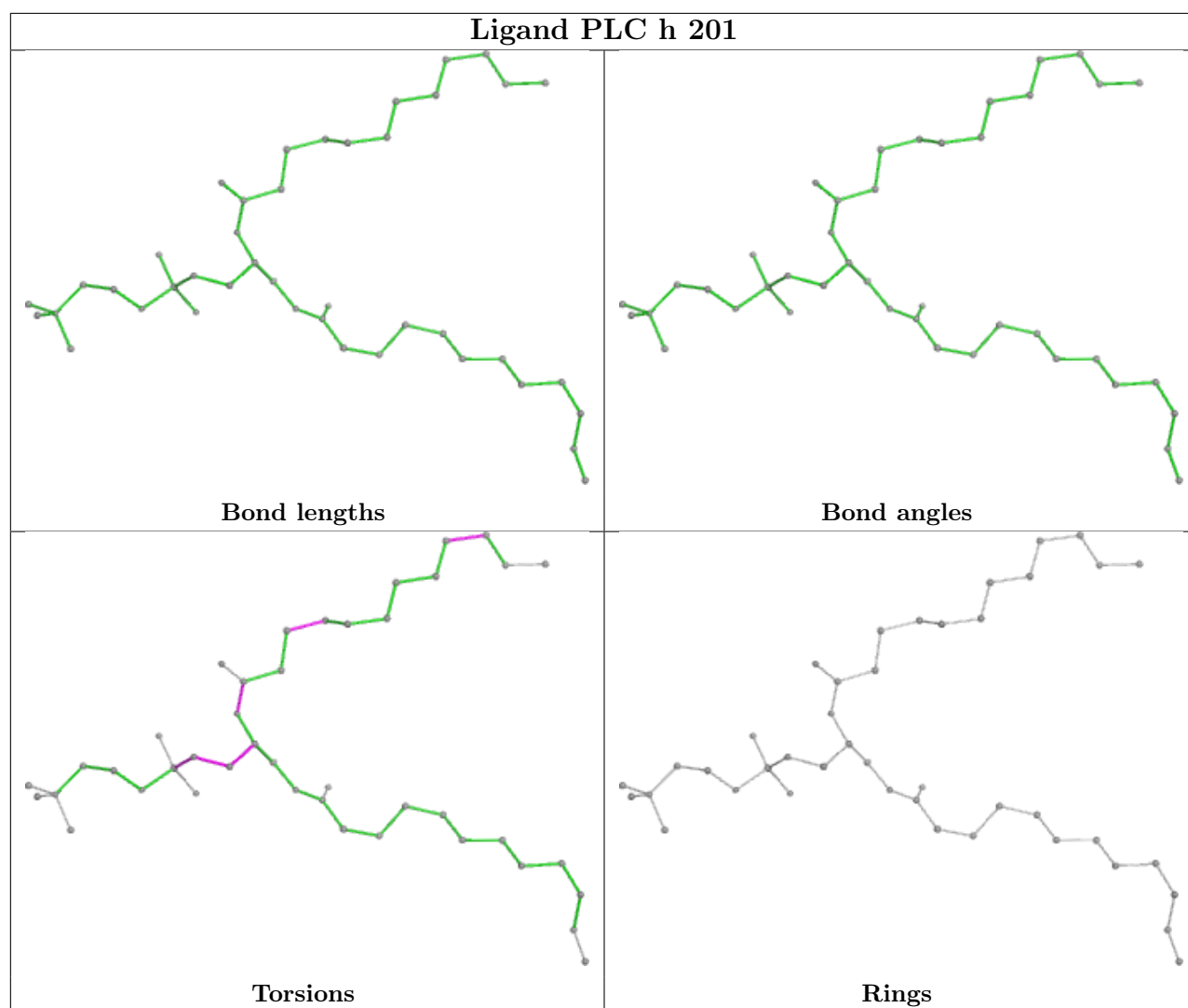


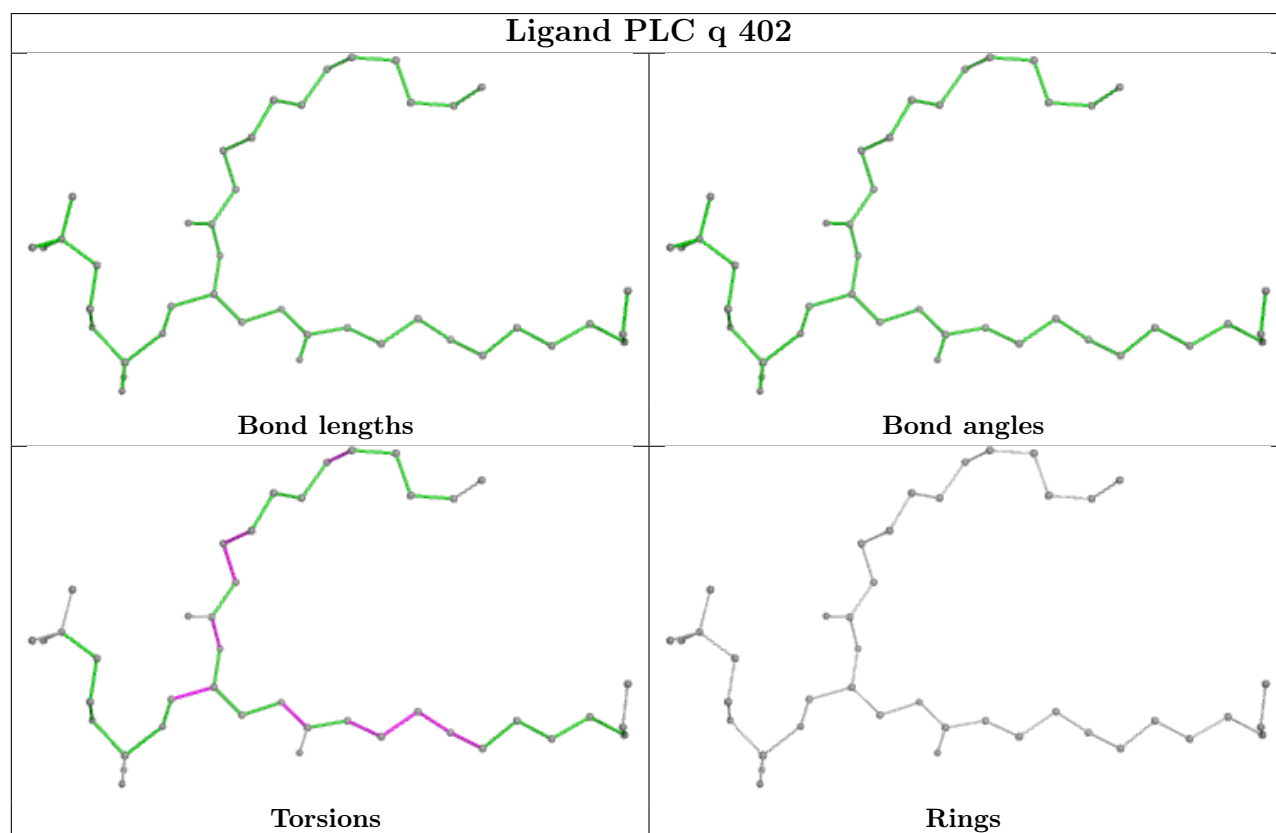
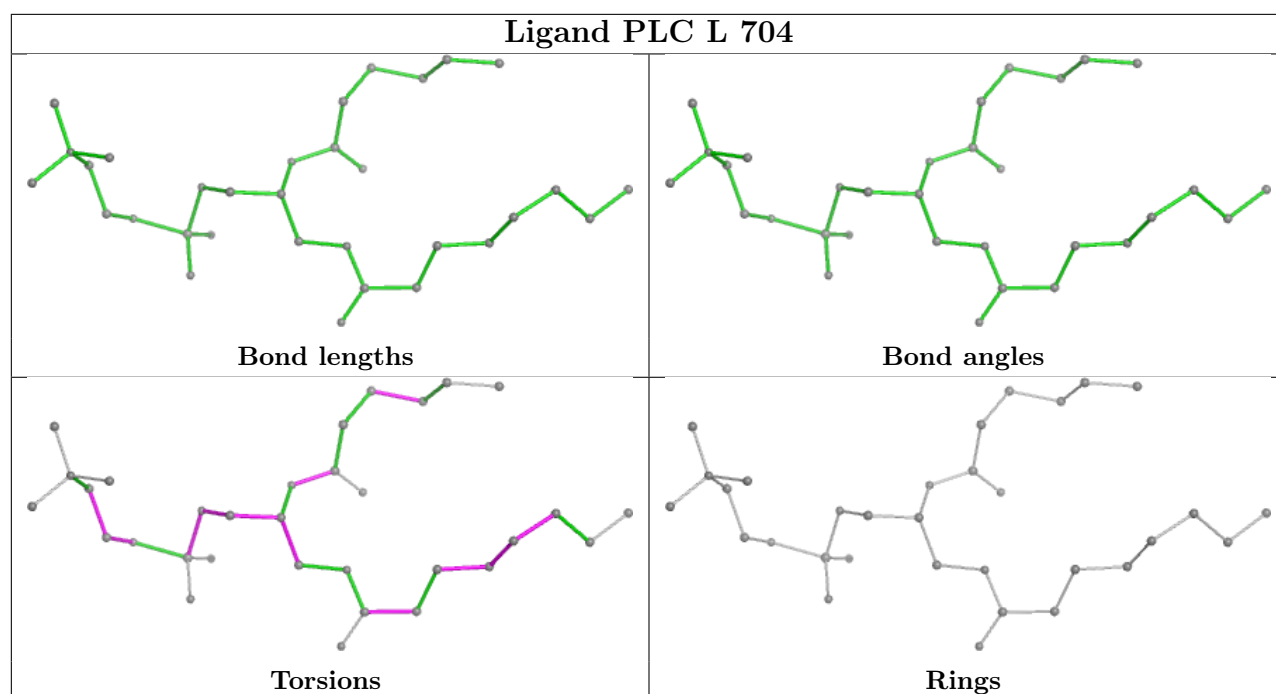


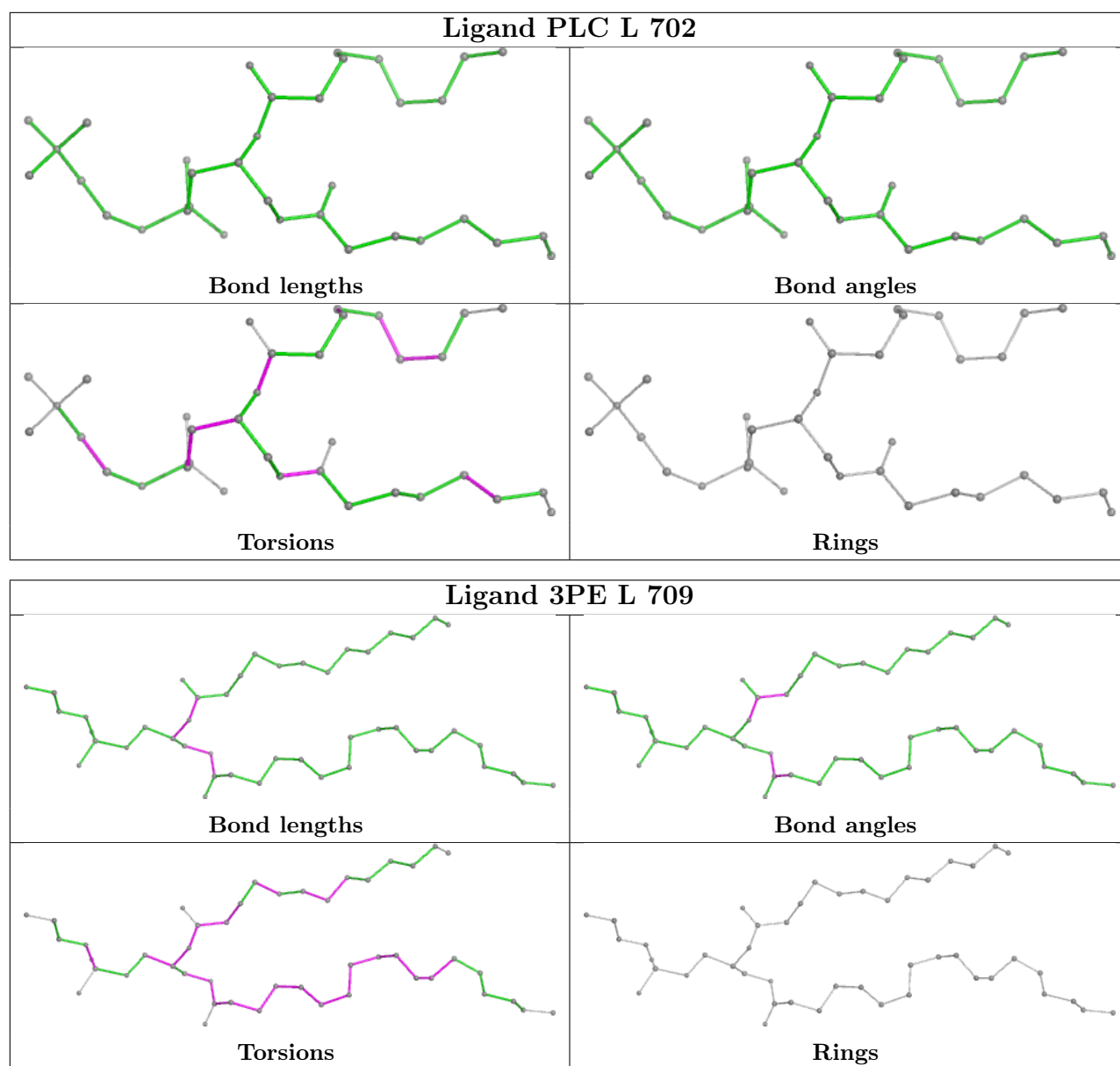


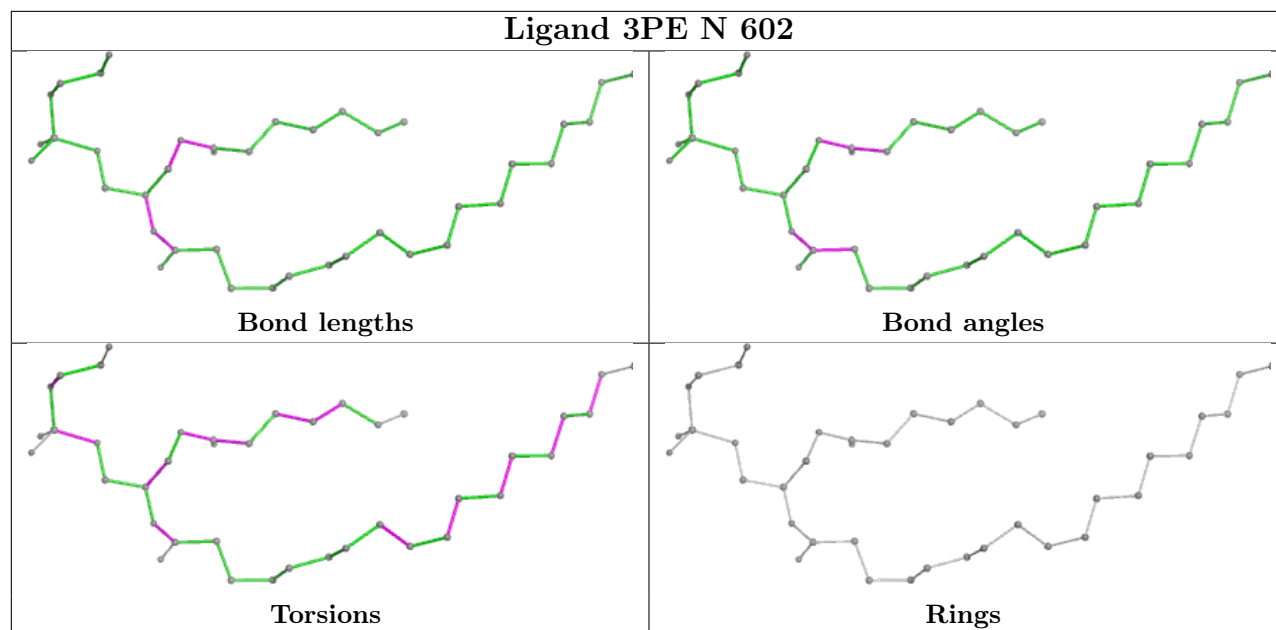


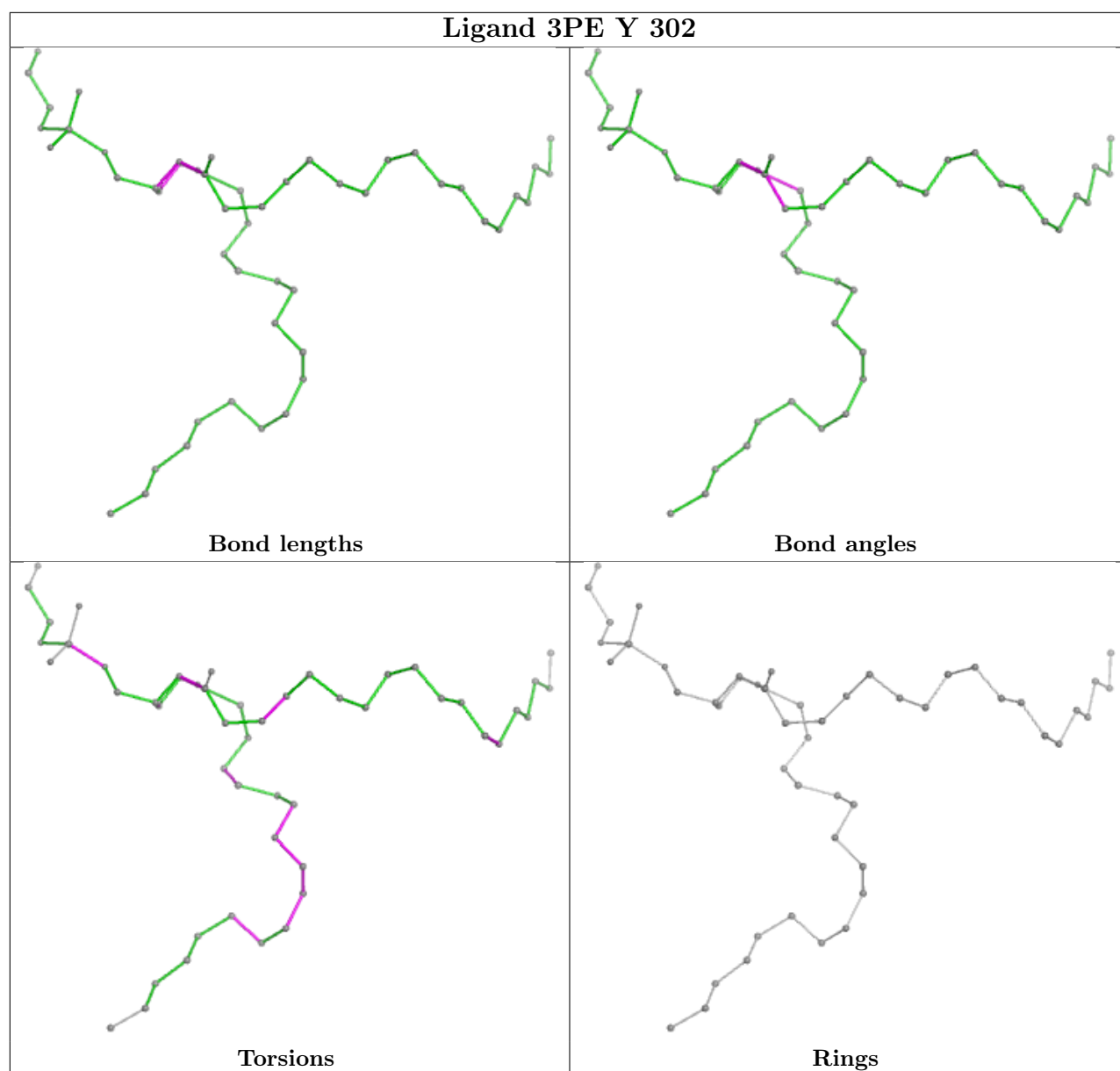




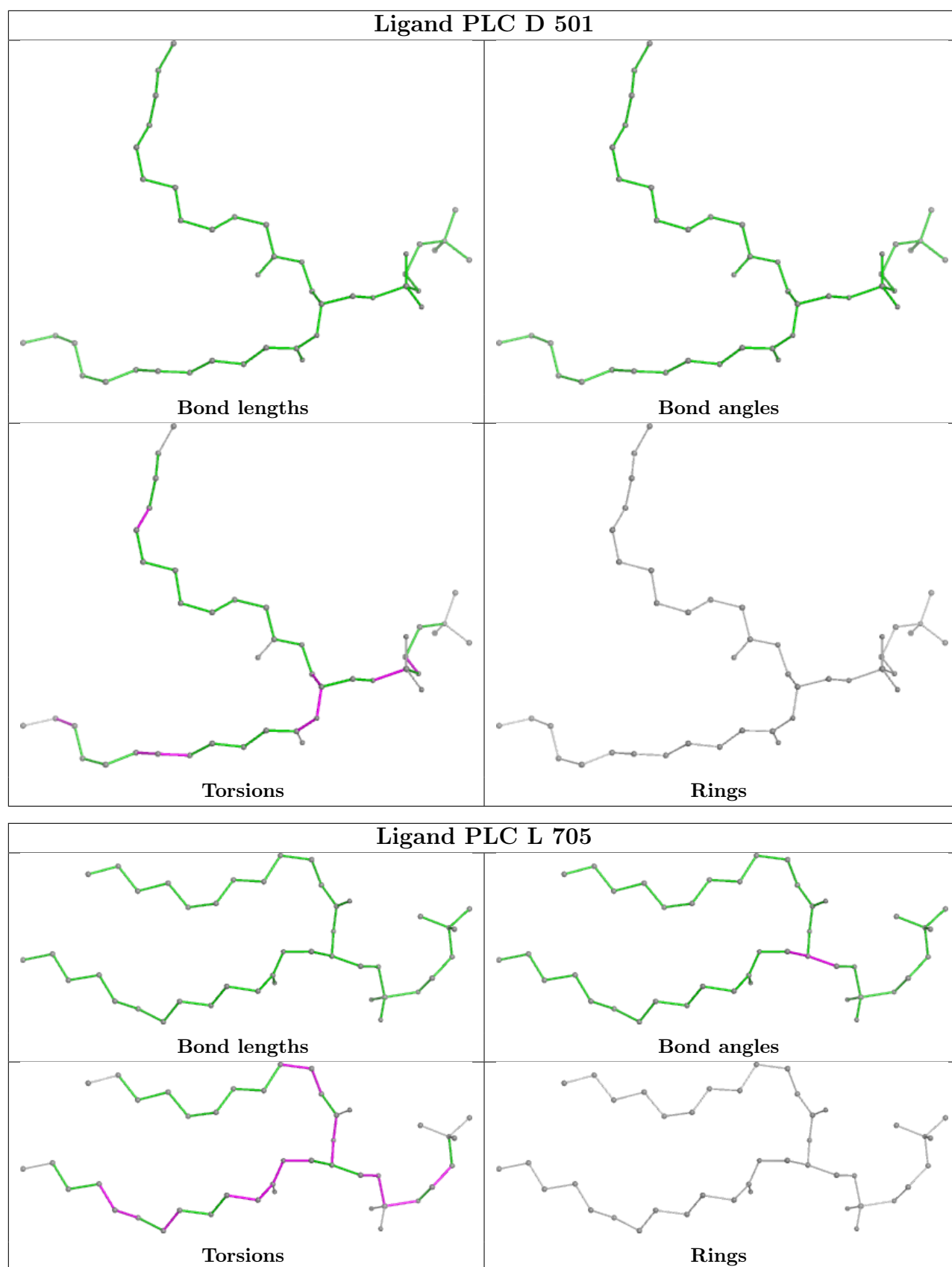


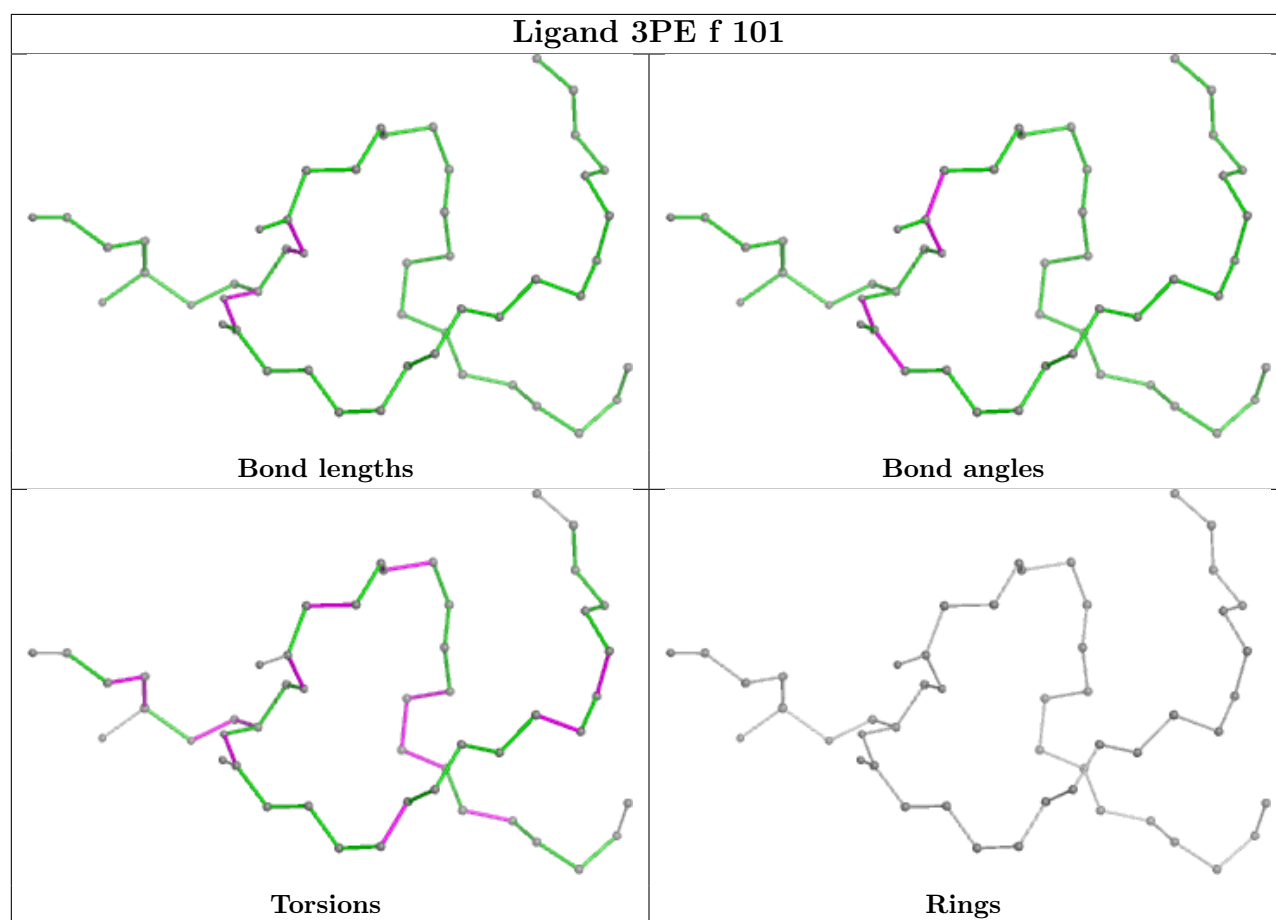
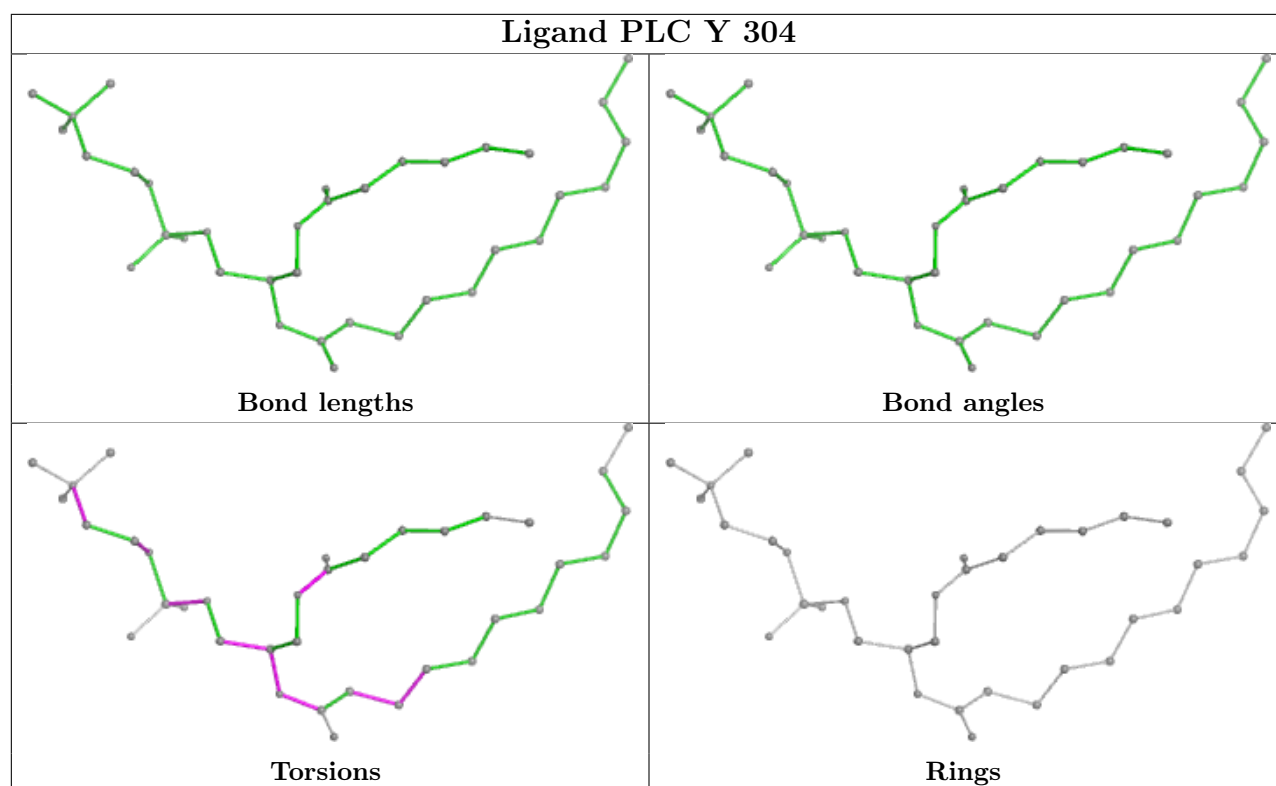


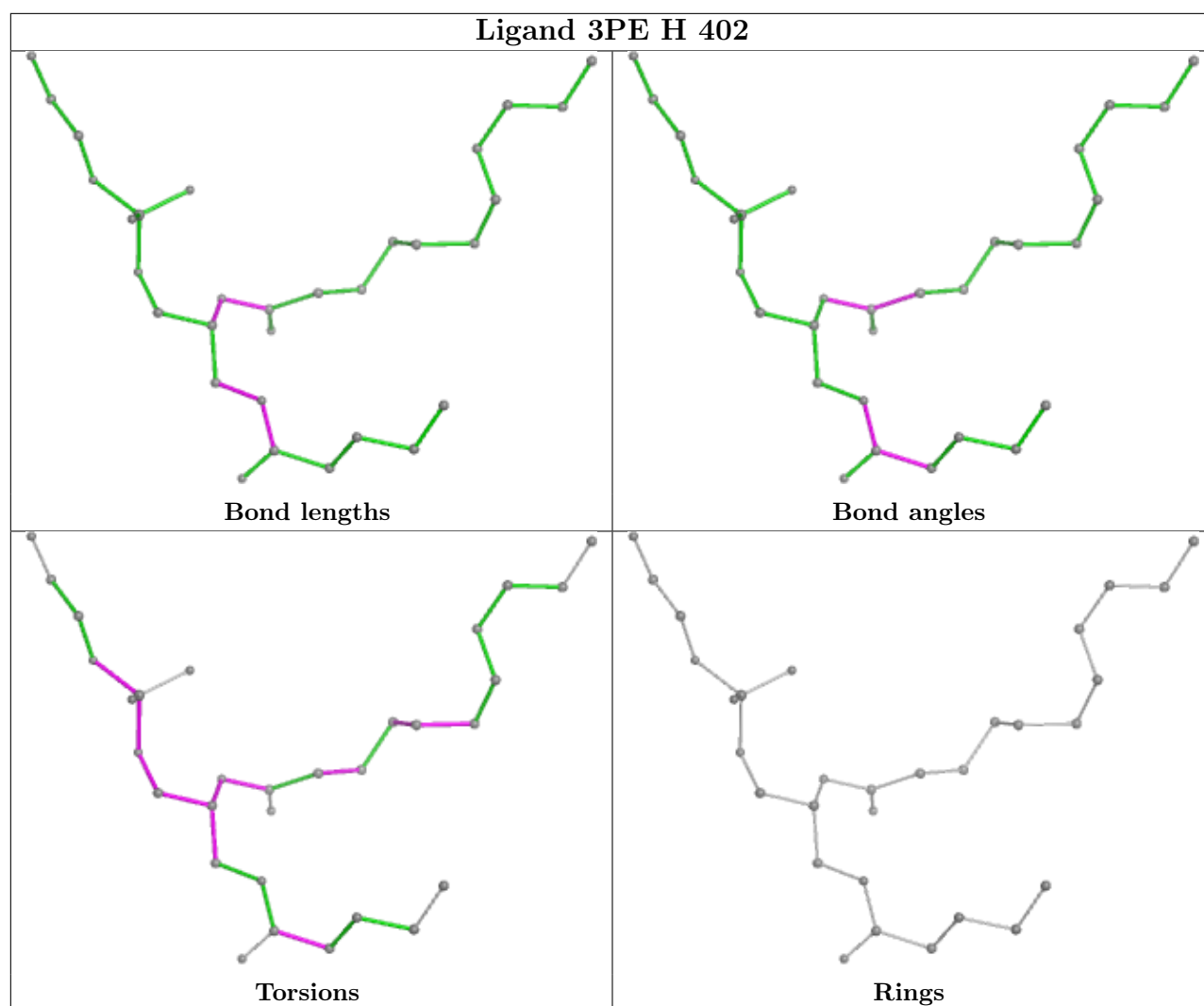


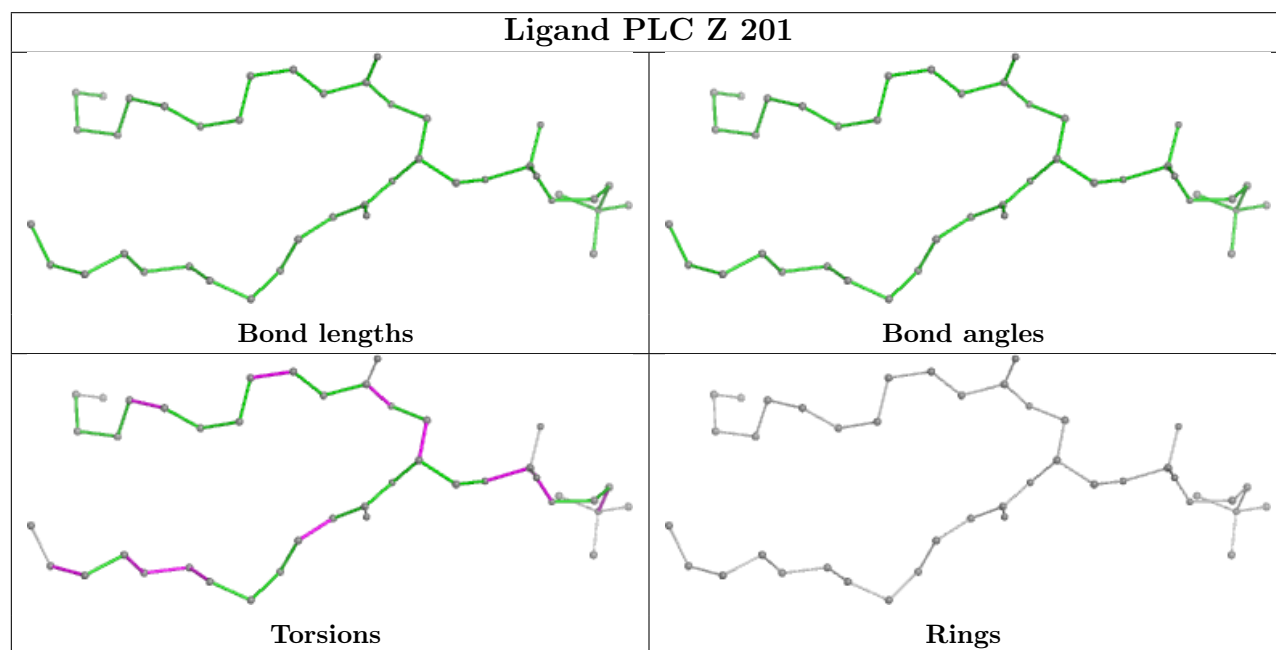
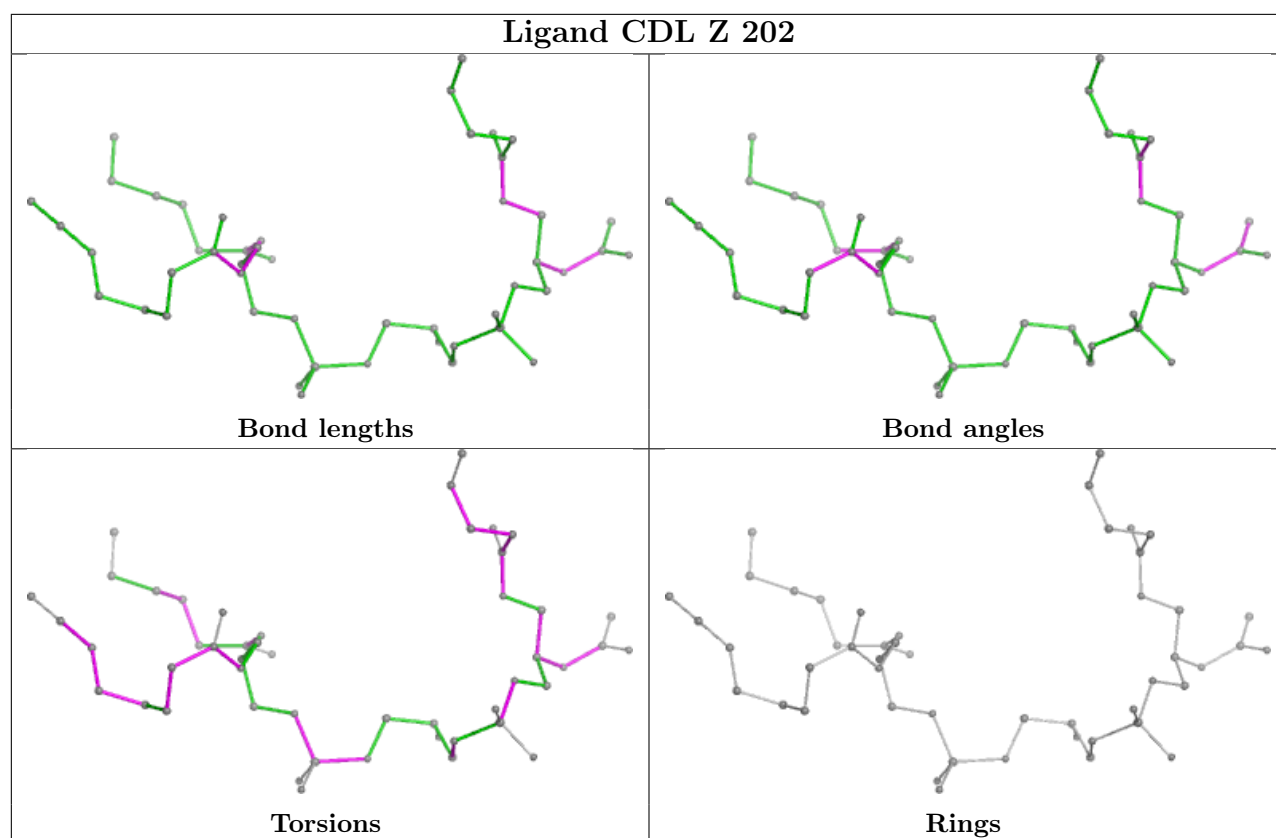


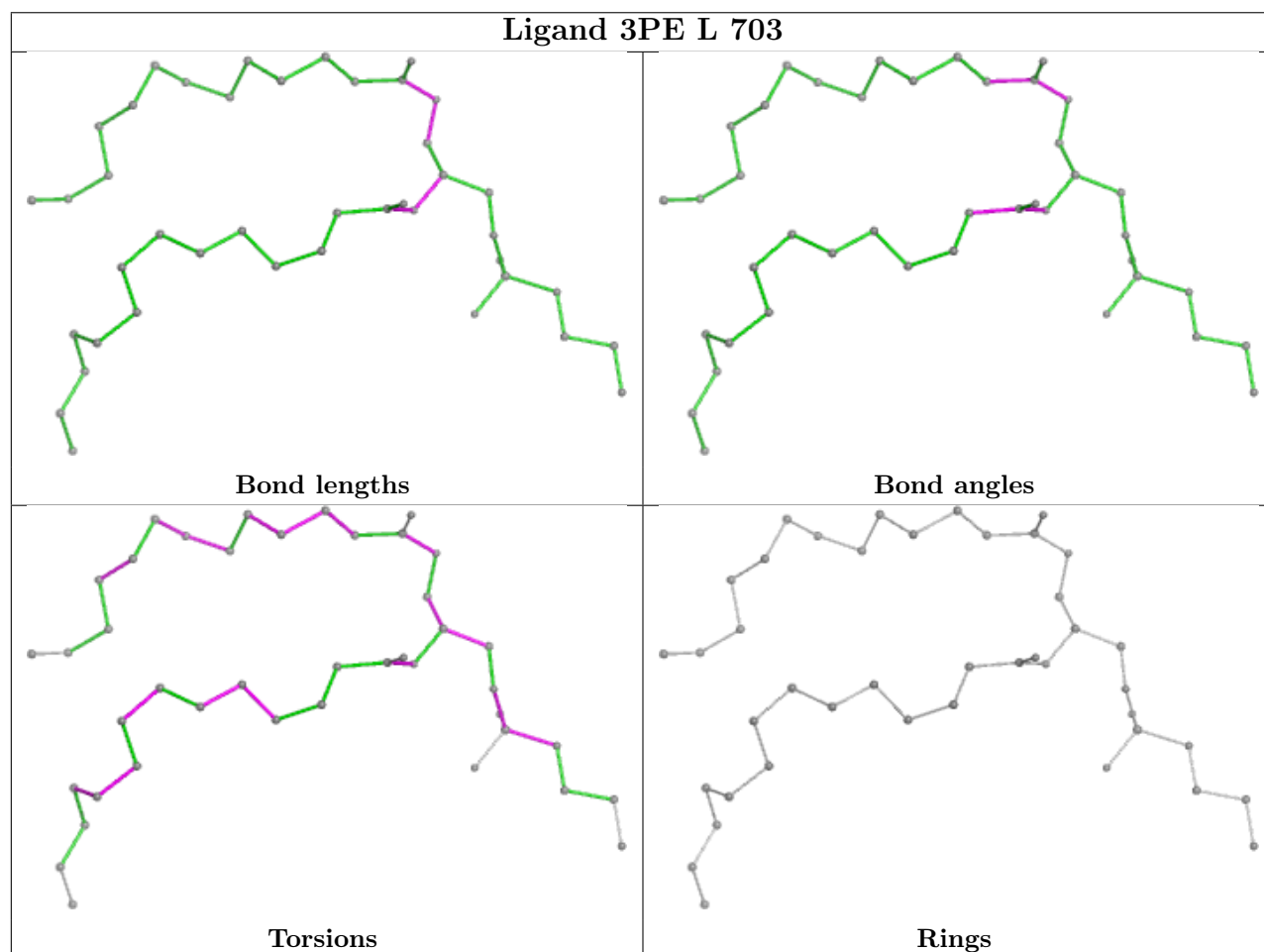
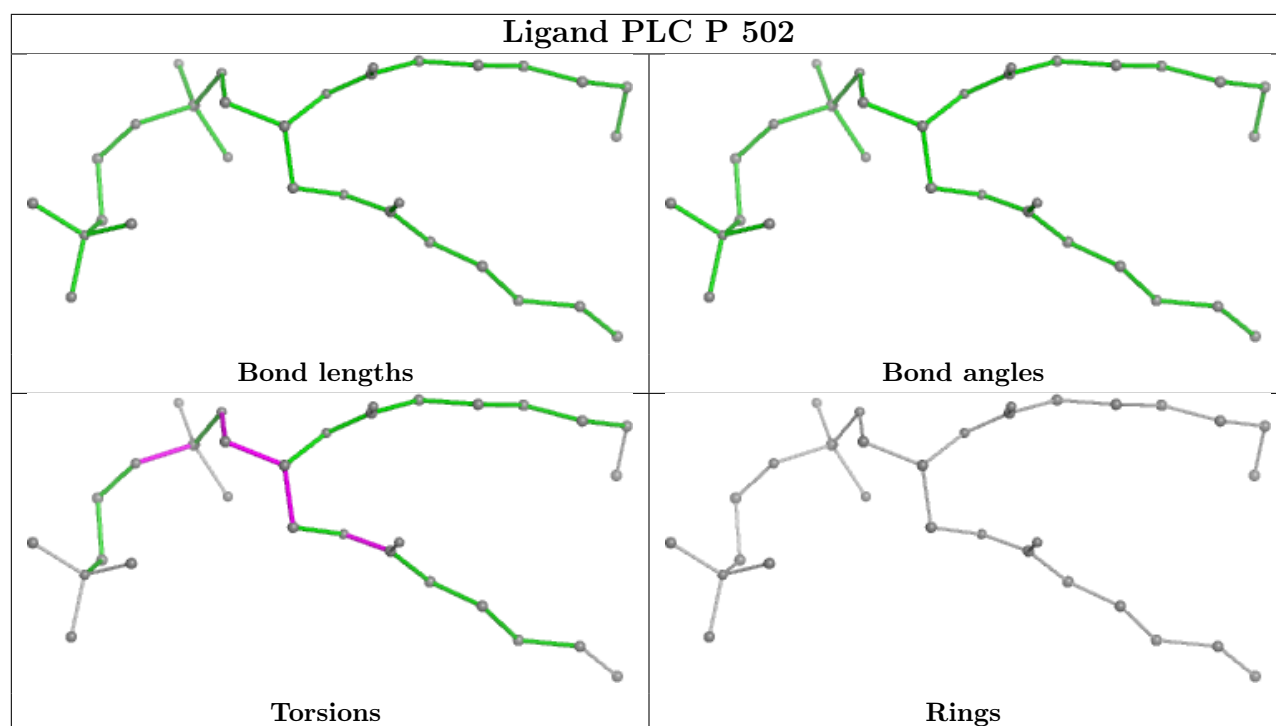


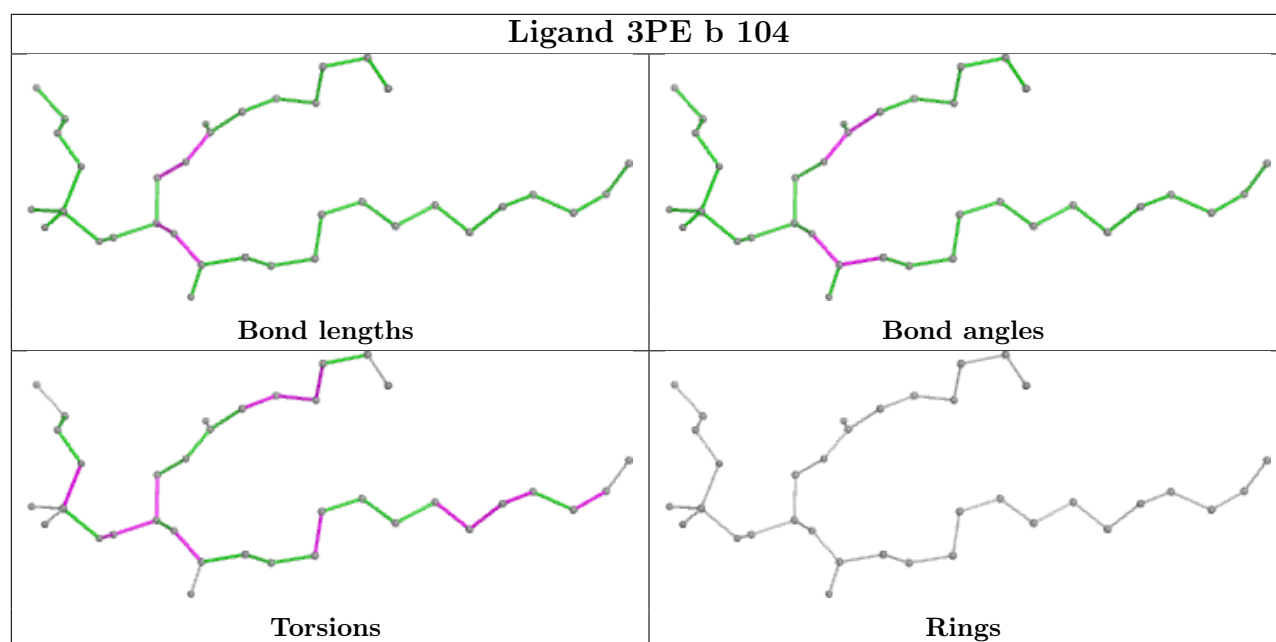












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

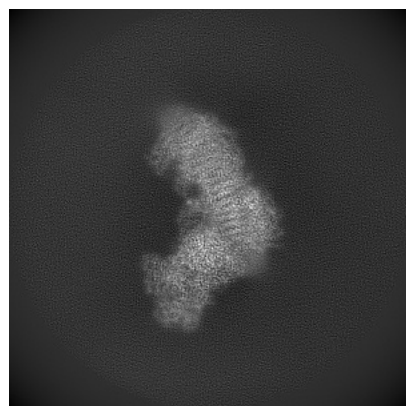
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52878. These allow visual inspection of the internal detail of the map and identification of artifacts.

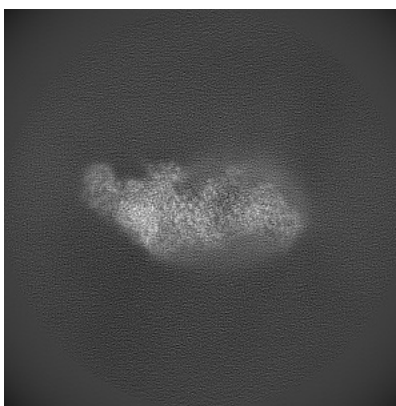
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

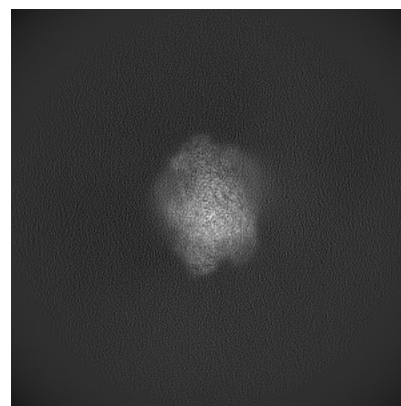
#### 6.1.1 Primary map



X

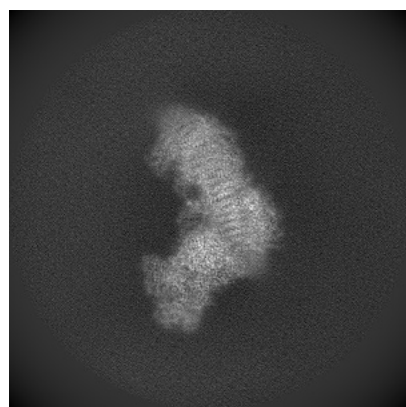


Y

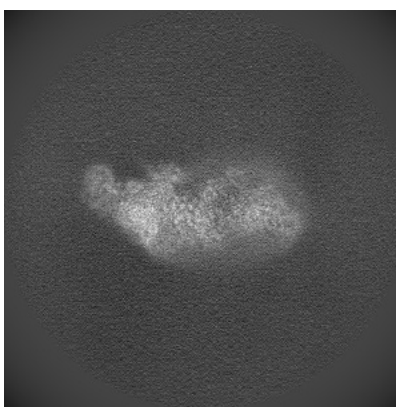


Z

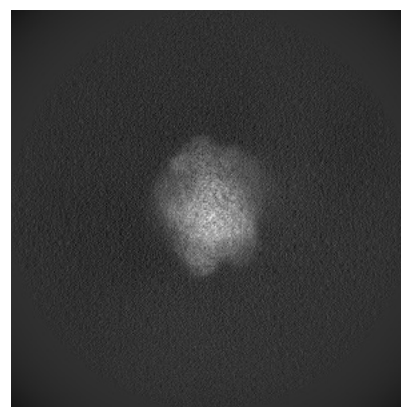
#### 6.1.2 Raw map



X



Y

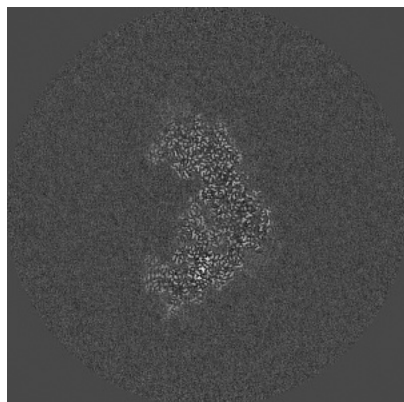


Z

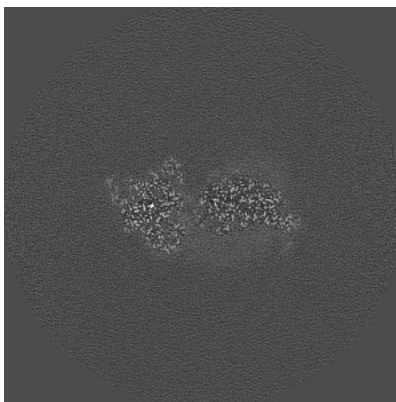
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

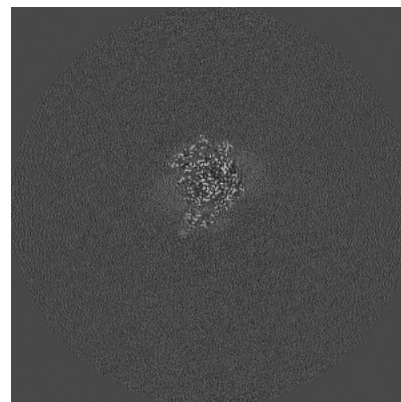
### 6.2.1 Primary map



X Index: 270

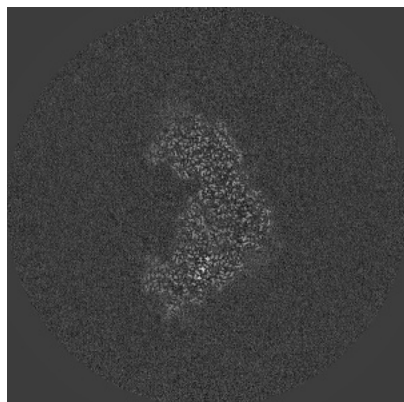


Y Index: 270

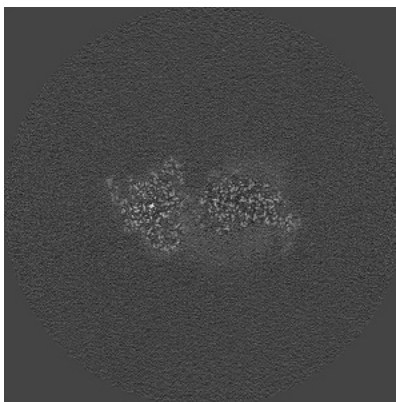


Z Index: 270

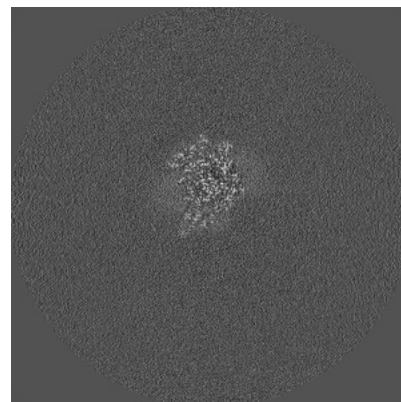
### 6.2.2 Raw map



X Index: 270



Y Index: 270



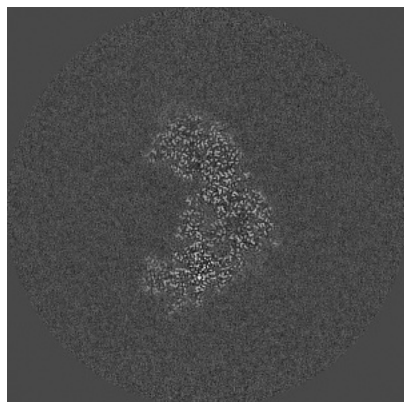
Z Index: 270

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

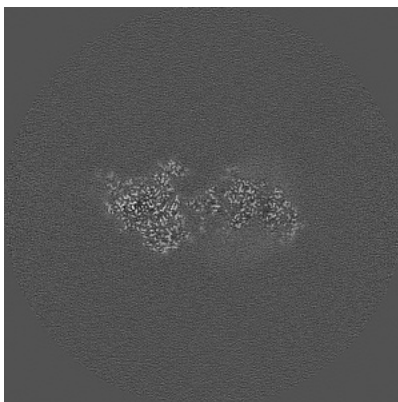


## 6.3 Largest variance slices [i](#)

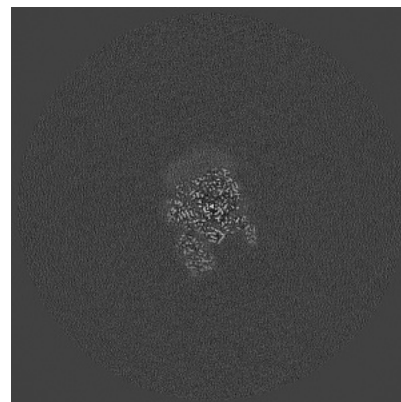
### 6.3.1 Primary map



X Index: 268

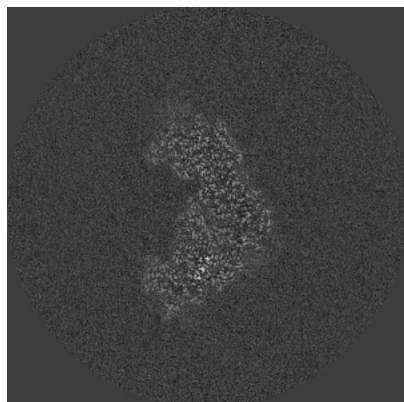


Y Index: 261

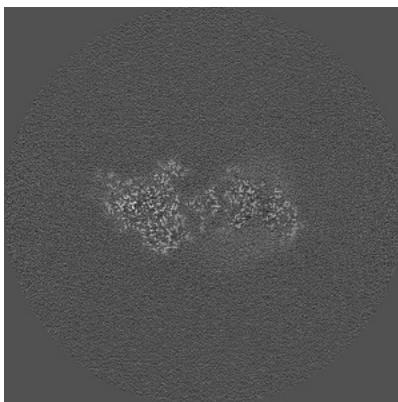


Z Index: 198

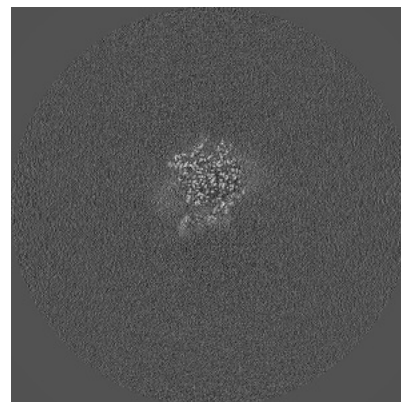
### 6.3.2 Raw map



X Index: 270



Y Index: 261

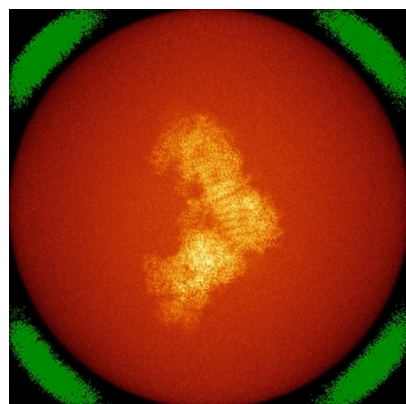


Z Index: 272

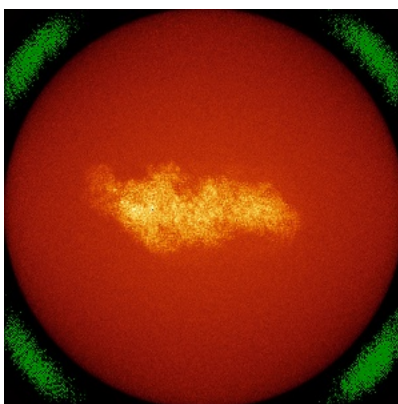
The images above show the largest variance slices of the map in three orthogonal directions.

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

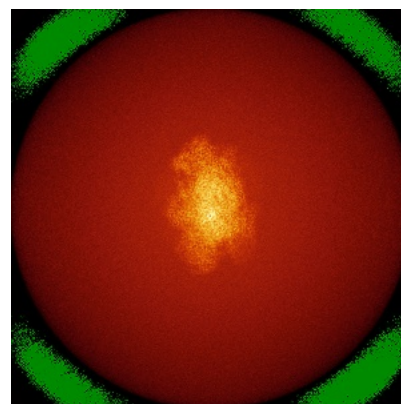
### 6.4.1 Primary map



X

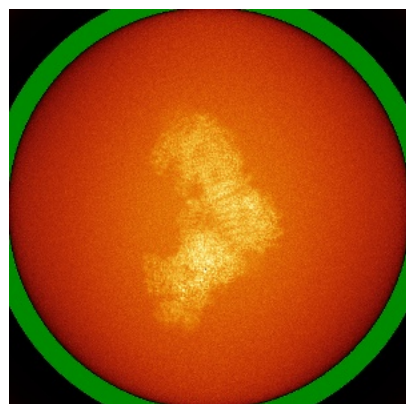


Y

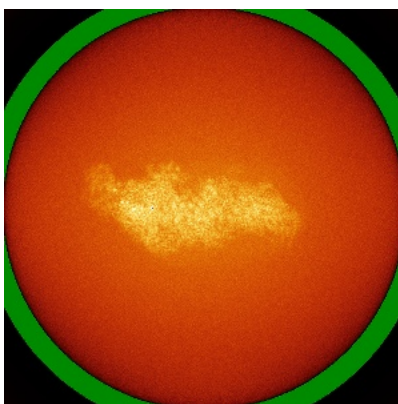


Z

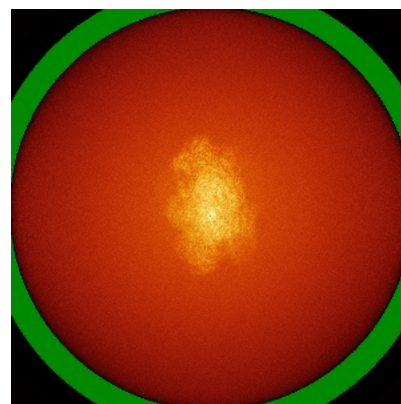
### 6.4.2 Raw map



X



Y

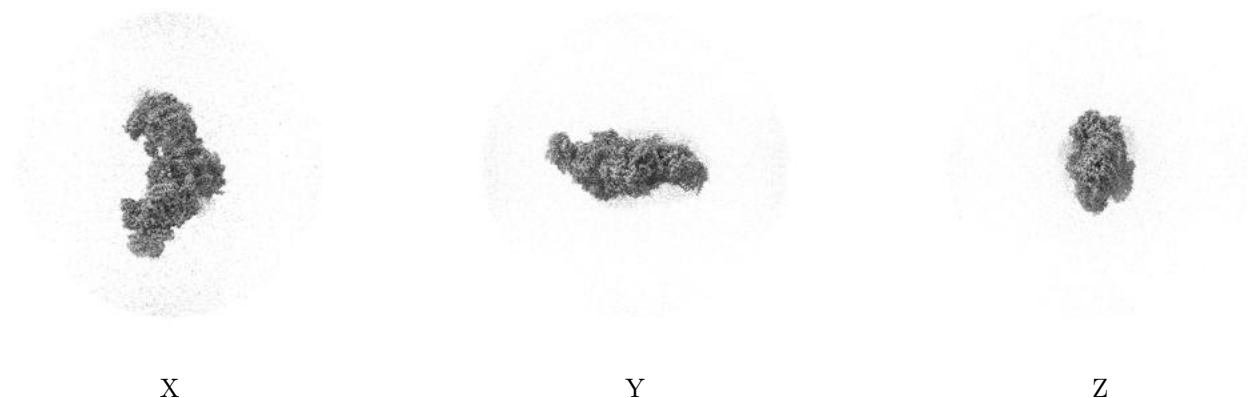


Z

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.

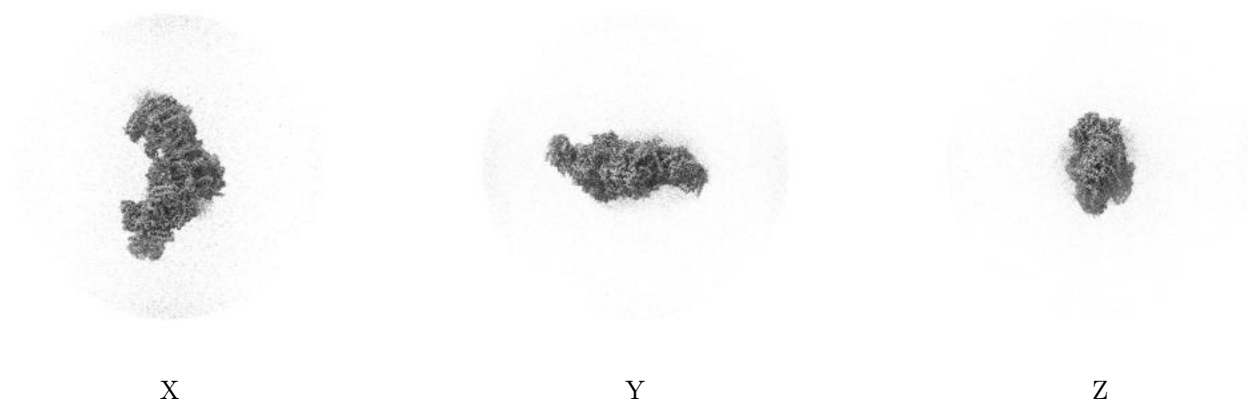
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0127. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

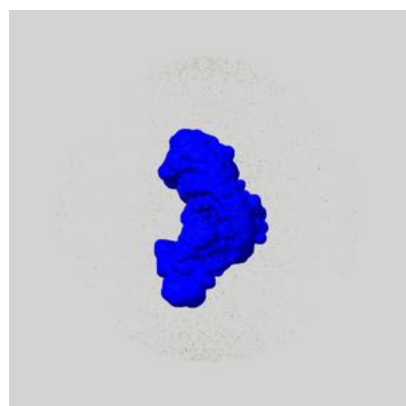
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

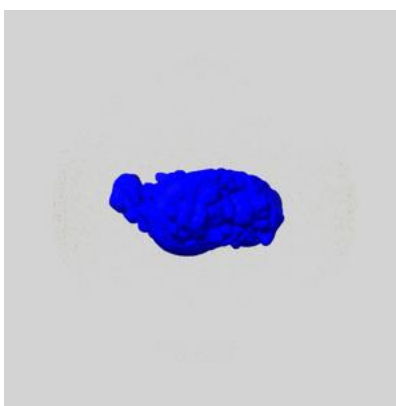
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

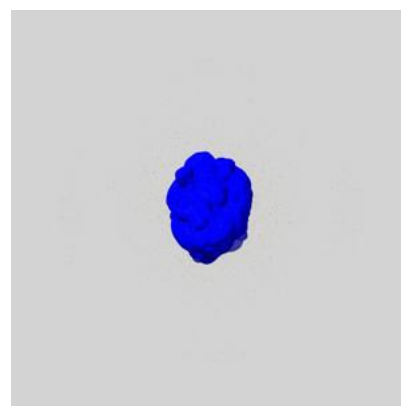
### 6.6.1 emd\_52878\_msk\_1.map [i](#)



X



Y

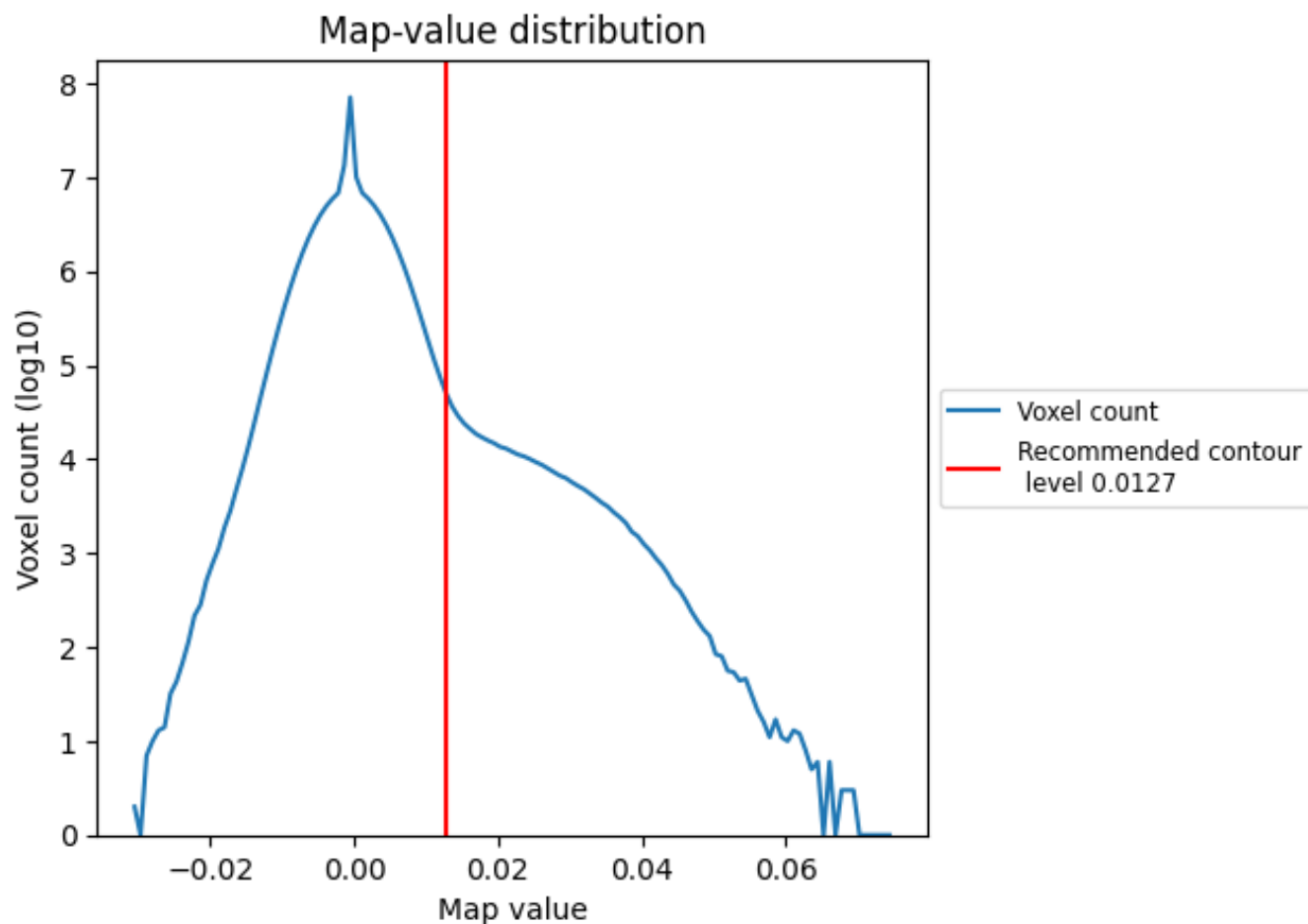


Z

## 7 Map analysis [i](#)

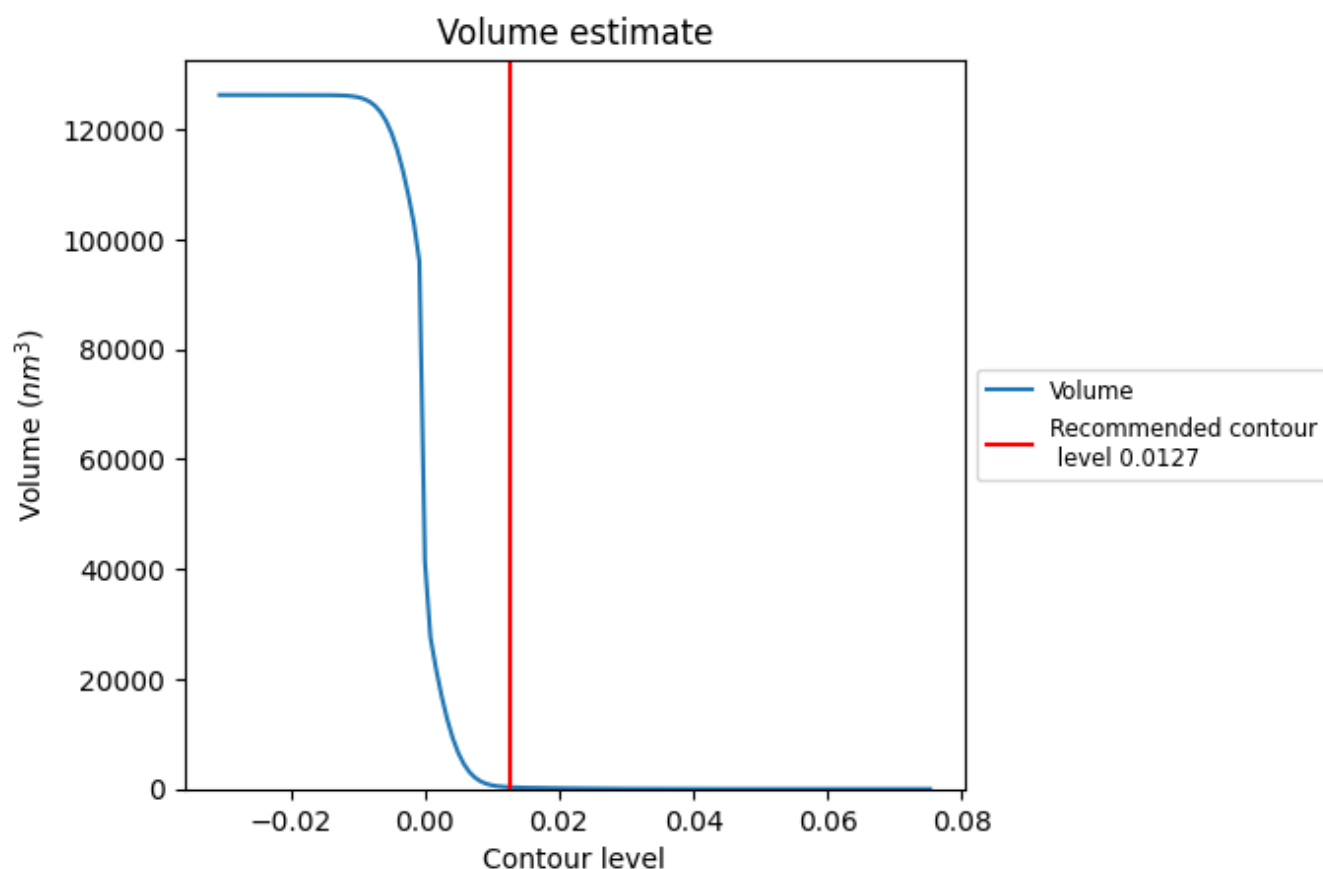
This section contains the results of statistical analysis of the map.

### 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.

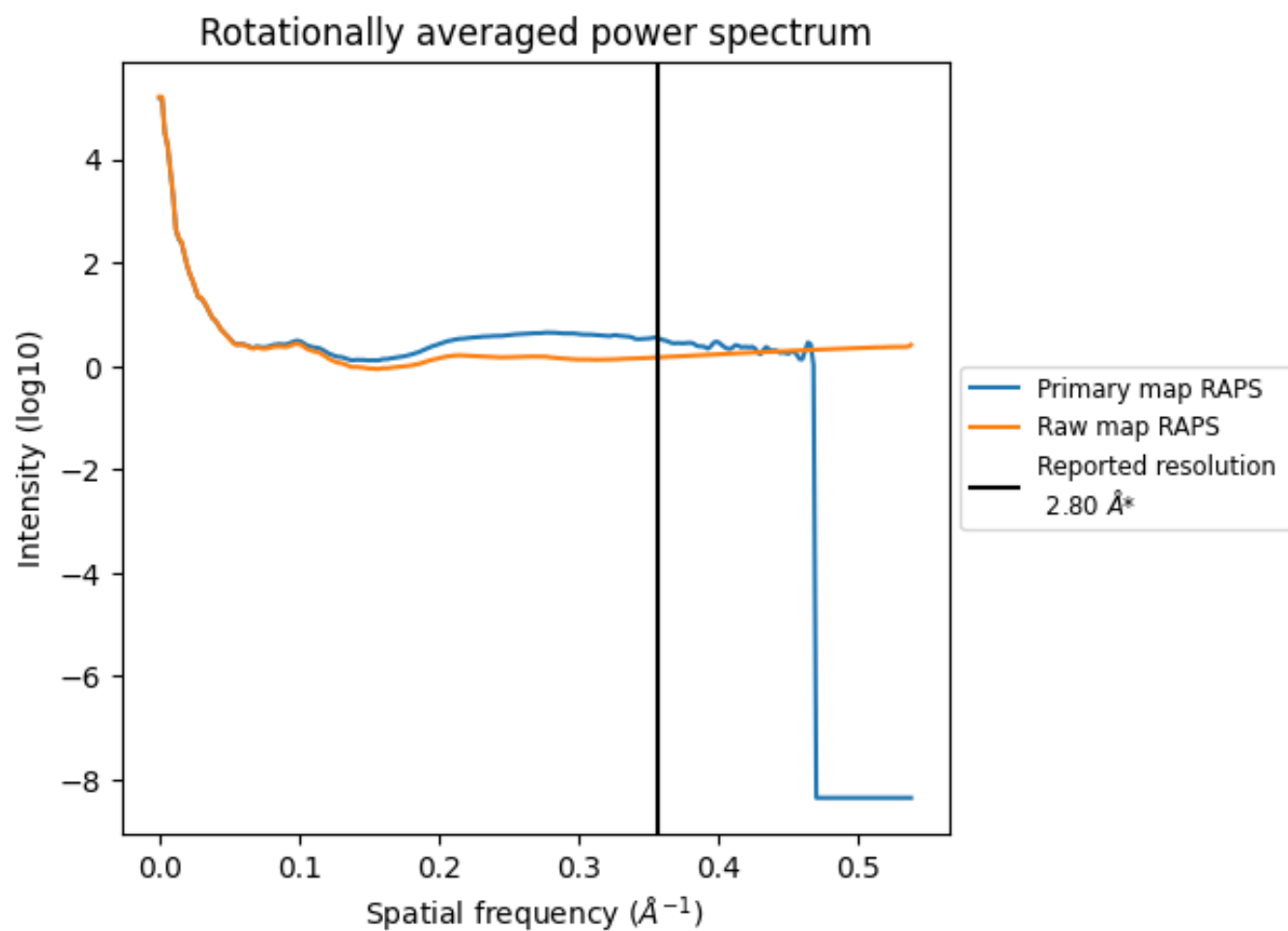
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm<sup>3</sup>; this corresponds to an approximate mass of 289 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 ⓘ



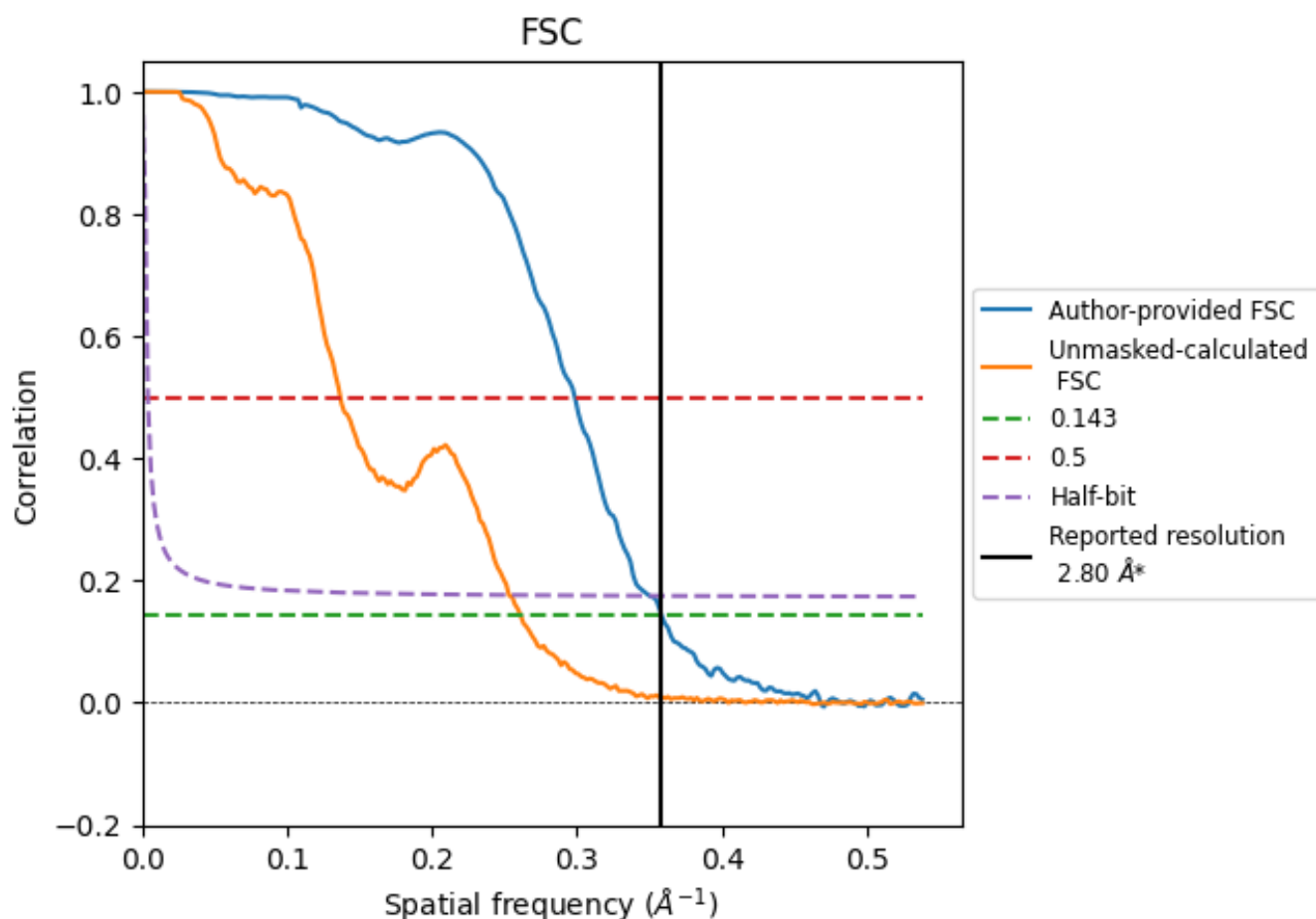
\*Reported resolution corresponds to spatial frequency of  $0.357 \text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.357 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

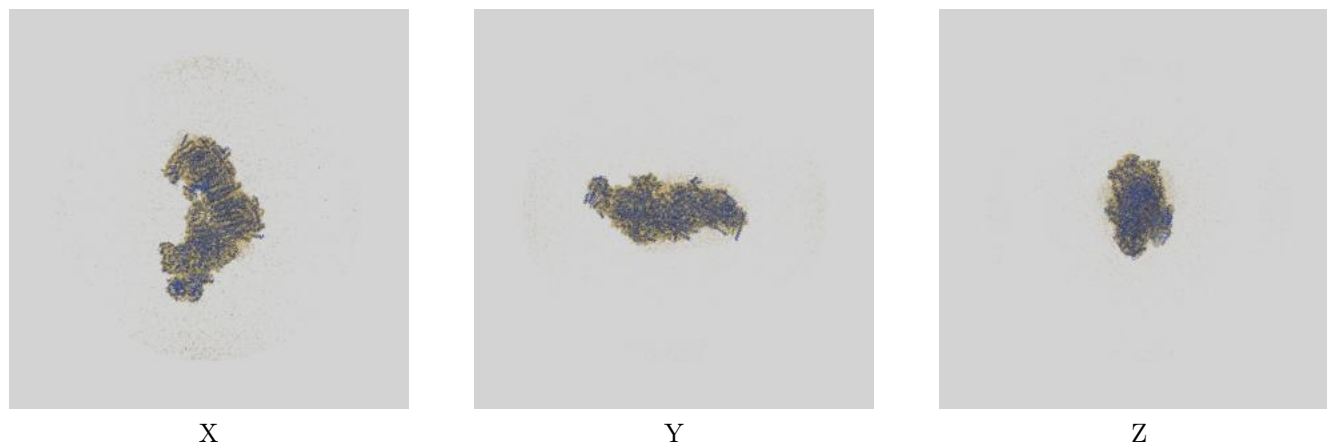
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.79	3.35	2.86
Unmasked-calculated*	3.83	7.31	3.95

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.8 by more than 10 %

## 9 Map-model fit [i](#)

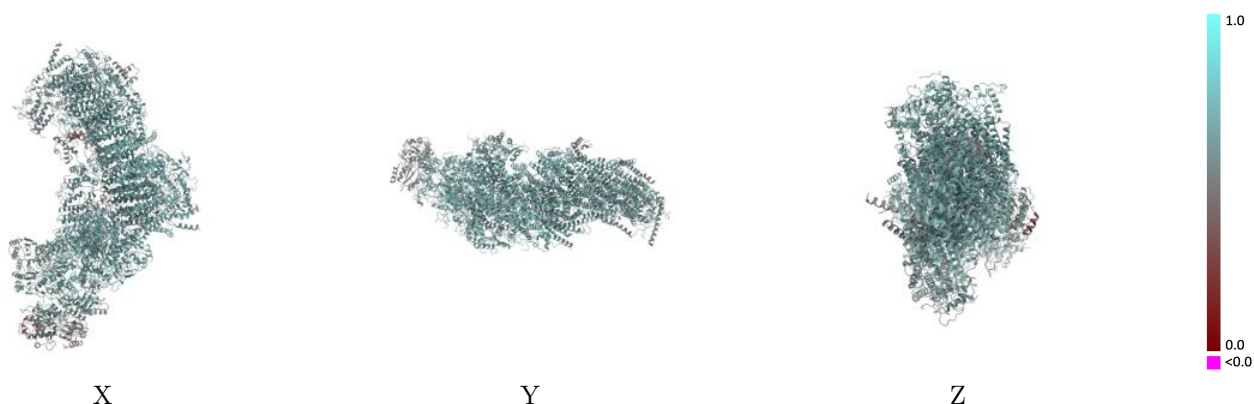
This section contains information regarding the fit between EMDB map EMD-52878 and PDB model 9IHR. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

### 9.1 Map-model overlay [i](#)



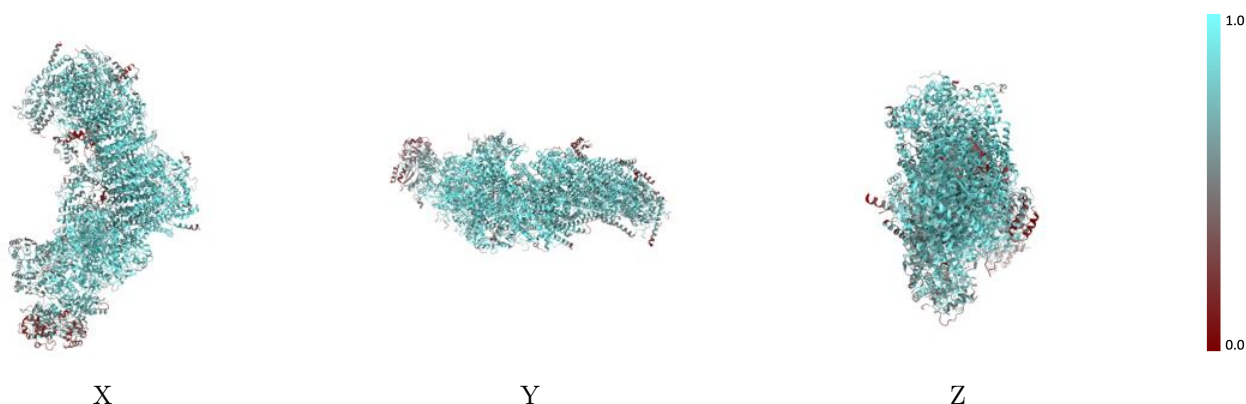
The images above show the 3D surface view of the map at the recommended contour level 0.0127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



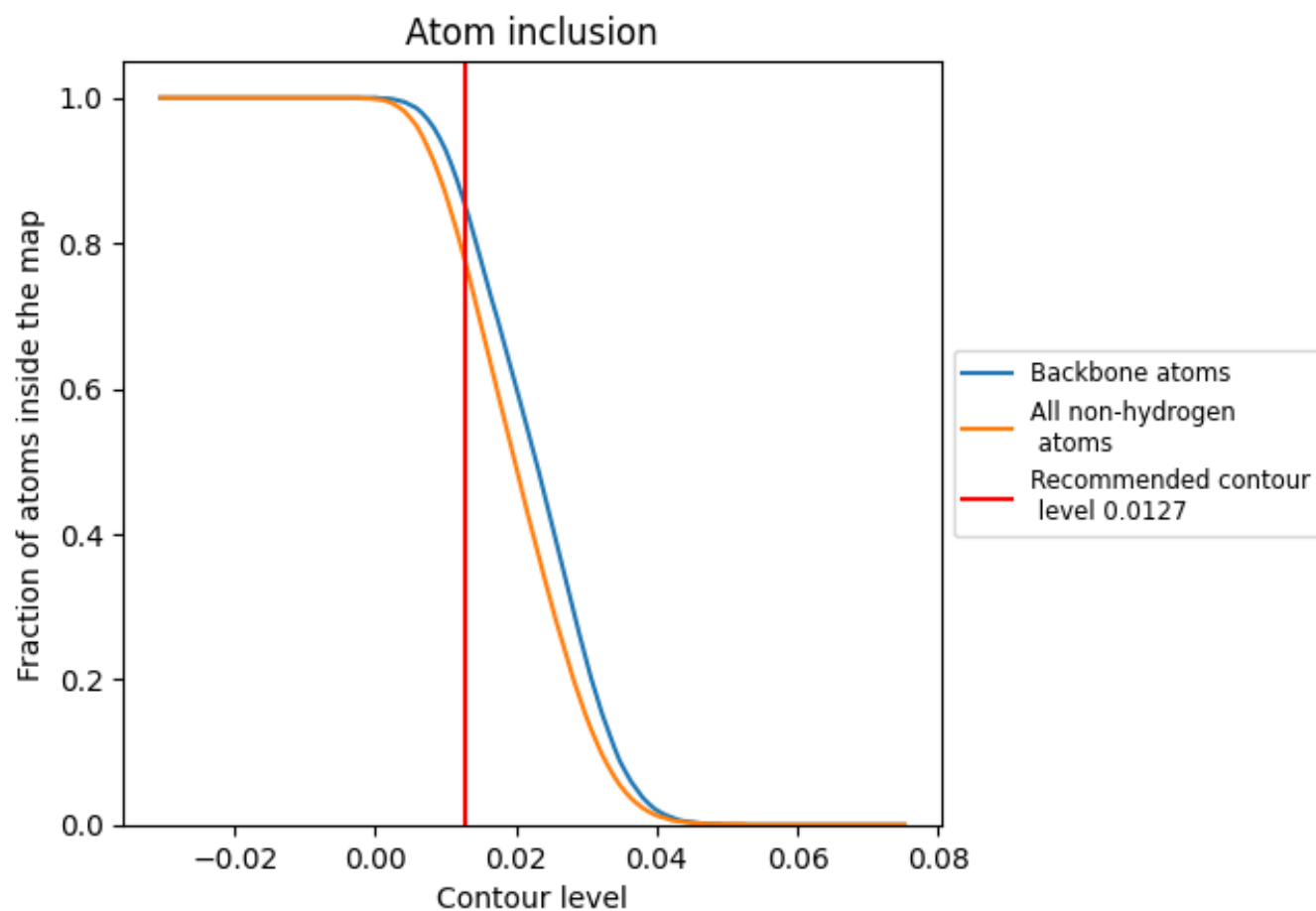
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0127).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.0127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.6150
1	 0.5800	 0.5340
A	 0.7960	 0.6320
B	 0.9000	 0.6630
C	 0.8640	 0.6430
D	 0.8890	 0.6600
E	 0.5280	 0.5090
F	 0.5090	 0.5040
G	 0.7890	 0.6120
H	 0.8450	 0.6440
I	 0.9040	 0.6630
J	 0.7650	 0.6120
K	 0.8130	 0.6240
L	 0.8150	 0.6270
M	 0.8800	 0.6540
N	 0.8820	 0.6610
O	 0.8230	 0.6370
P	 0.8000	 0.6190
Q	 0.7730	 0.6260
R	 0.7920	 0.6160
S	 0.5570	 0.5330
T	 0.7250	 0.5980
U	 0.5500	 0.5300
V	 0.7620	 0.6140
W	 0.8210	 0.6360
X	 0.8390	 0.6410
Y	 0.7600	 0.6250
Z	 0.8400	 0.6360
a	 0.8360	 0.6360
b	 0.7370	 0.6320
c	 0.7770	 0.6060
d	 0.8370	 0.6400
e	 0.8450	 0.6370
f	 0.7640	 0.6150
g	 0.4590	 0.5130



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
h	 0.7250	 0.6030
i	 0.6720	 0.5630
j	 0.6130	 0.5550
k	 0.6100	 0.5360
l	 0.7270	 0.5970
m	 0.7580	 0.6230
n	 0.6710	 0.5570
o	 0.6510	 0.5670
p	 0.8490	 0.6290
q	 0.8270	 0.6340