



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2026 – 01:38 pm BST

PDB ID : 9IHO / pdb_00009iho
EMDB ID : EMD-52875
Title : Open state without NUQM and without flavoprotein (classification state 4) of Pichia pastoris mitochondrial complex I in cMSP26 nanodiscs
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2025-02-21
Resolution : 3.80 Å(reported)
Based on initial model : 9ihr

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:

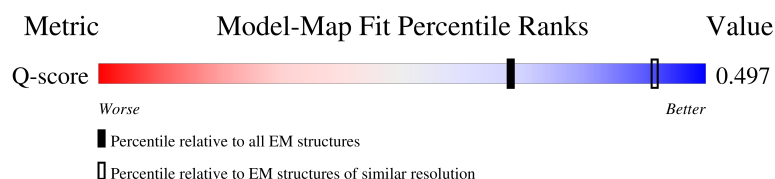
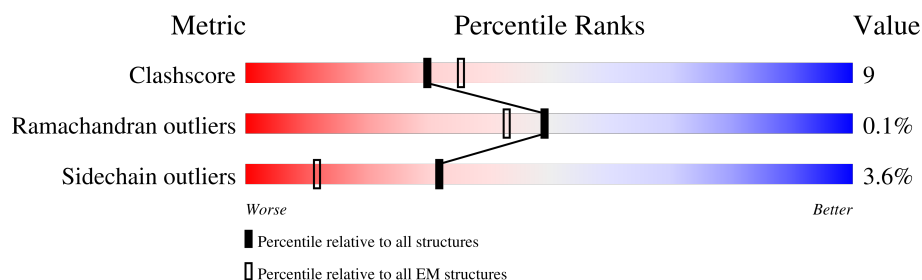
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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 ≥ 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	141	35% 65% 29% • •
2	B	204	9% 62% 22% • 14%
3	C	289	26% 55% 24% • 19%
4	D	482	15% 70% 19% • 9%

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Mol	Chain	Length	Quality of chain
5	G	726	
6	H	353	
7	I	222	
8	J	161	
9	K	82	
10	L	642	
11	M	491	
12	N	523	
13	O	193	
14	P	384	
15	Q	159	
16	R	139	
17	S	90	
18	T	138	
19	U	130	
20	V	134	
21	W	122	
22	X	184	
23	Y	216	
24	Z	147	
25	a	150	
26	b	79	
27	c	182	
28	d	78	
29	e	106	

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Mol	Chain	Length	Quality of chain
30	f	86	
31	g	239	
32	h	182	
33	i	74	
34	j	59	
35	k	61	
36	l	156	
37	m	81	
38	n	111	
39	o	87	
40	p	92	
41	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
42	SF4	G	801	-	-	X	-
42	SF4	G	802	-	-	X	-
42	SF4	I	302	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 61836 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	137	Total	C	N	O	S	0	0
			1099	745	159	191	4		

- Molecule 2 is a protein called BA75_00622T0.

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

- Molecule 3 is a protein called NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	233	Total	C	N	O	S	0	0
			1922	1242	324	351	5		

- Molecule 4 is a protein called NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	440	Total	C	N	O	S	0	0
			3536	2259	602	657	18		

- Molecule 5 is a protein called NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	556	Total	C	N	O	S	0	0
			4295	2693	751	836	15		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 7 is a protein called NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	155	Total	C	N	O	S	0	0
			1250	836	174	237	3		

- Molecule 9 is a protein called NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 13 is a protein called NUXM subunit of mitochondrial NADH:ubiquinone oxidore-

ductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	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 14 is a protein called NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	359	Total	C	N	O	S	0	0
			2851	1821	496	531	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	88	Total	C	N	O	S	0	0
			727	462	122	141	2		

- Molecule 16 is a protein called NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 17 is a protein called NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
17	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 18 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	93	Total	C	N	O	S	0	0
			730	459	116	154	1		

- Molecule 19 is a protein called Acyl carrier protein.

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

- Molecule 20 is a protein called NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 21 is a protein called BA75_04796T0.

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

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	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 23 is a protein called NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

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

- Molecule 26 is a protein called NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 27 is a protein called BA75_00589T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	146	Total	C	N	O	S	0	0
			1143	727	203	211	2		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 28 is a protein called Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM.

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

- Molecule 29 is a protein called BA75_05084T0.

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

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

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

- Molecule 31 is a protein called NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 32 is a protein called NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

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

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

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

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

- Molecule 35 is a protein called NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

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

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

- Molecule 37 is a protein called NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

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

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

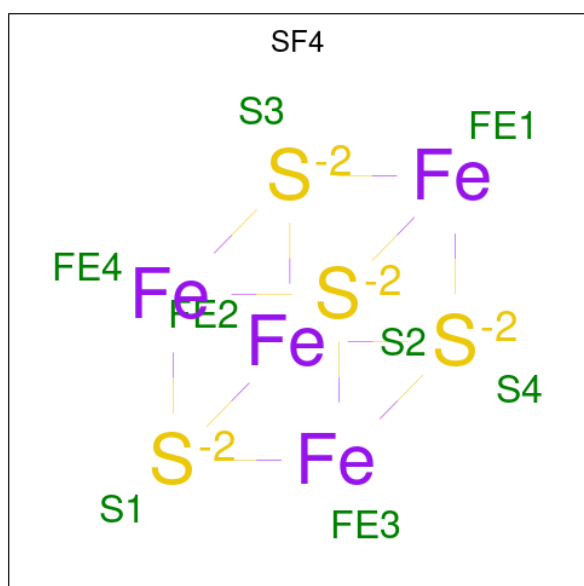
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit.

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

There is a discrepancy between the modelled and reference sequences:

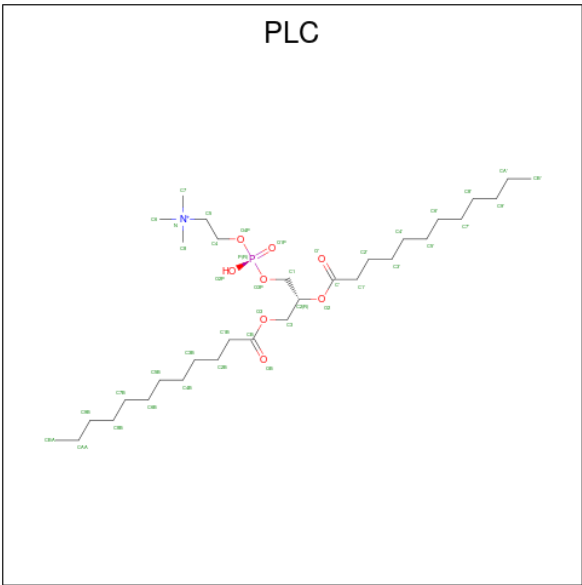
Chain	Residue	Modelled	Actual	Comment	Reference
q	0	ACE	-	acetylation	UNP E1UWE0

- Molecule 42 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 43 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $\text{C}_{32}\text{H}_{65}\text{NO}_8\text{P}$).



Mol	Chain	Residues	Atoms					AltConf
43	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
43	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	H	1	Total	C	N	O	P	0
			24	14	1	8	1	
43	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
43	L	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	P	1	Total	C	N	O	P	0
			31	21	1	8	1	
43	P	1	Total	C	N	O	P	0
			31	21	1	8	1	
43	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
43	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
43	Z	1	Total	C	N	O	P	0
			42	32	1	8	1	

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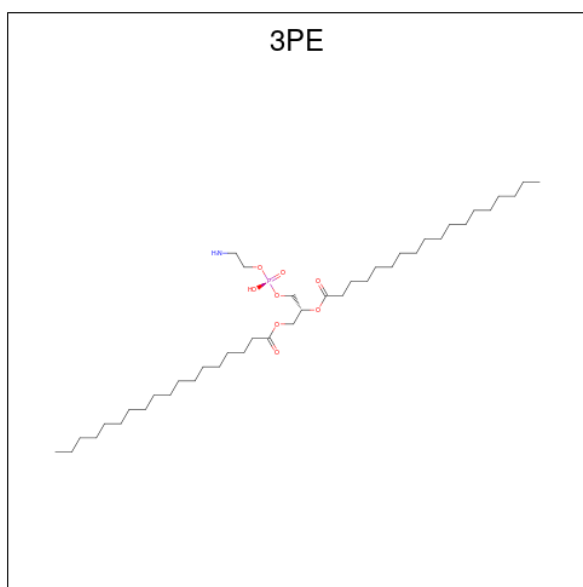
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Mol	Chain	Residues	Atoms					AltConf
43	a	1	Total	C	N	O	P	0
			22	12	1	8	1	
43	b	1	Total	C	N	O	P	0
			39	29	1	8	1	
43	d	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	d	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	g	1	Total	C	N	O	P	0
			39	29	1	8	1	
43	q	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	q	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 44 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



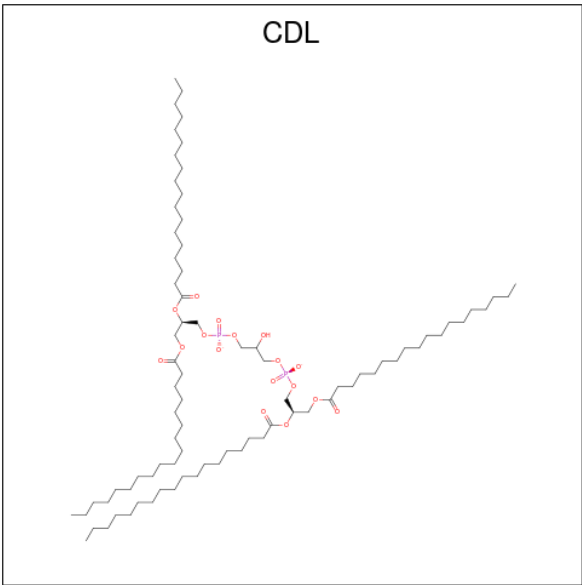
Mol	Chain	Residues	Atoms					AltConf
45	J	1	Total	C	N	O	P	0
			51	41	1	8	1	

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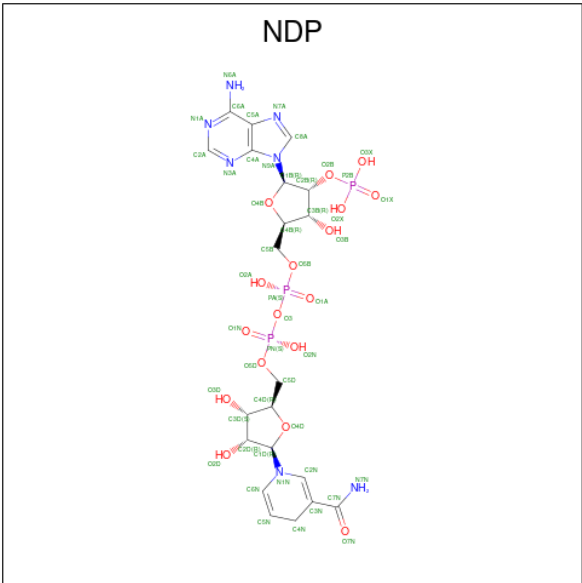
Mol	Chain	Residues	Atoms					AltConf
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	L	1	Total	C	N	O	P	0
			29	19	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	Y	1	Total	C	N	O	P	0
			25	15	1	8	1	
45	Z	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	b	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	h	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	j	1	Total	C	N	O	P	0
			27	17	1	8	1	
45	m	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 46 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
46	O	1	Total	C	O	P	0
			75	56	17	2	
46	Z	1	Total	C	O	P	0
			49	30	17	2	
46	b	1	Total	C	O	P	0
			59	40	17	2	
46	q	1	Total	C	O	P	0
			60	41	17	2	

- Molecule 47 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

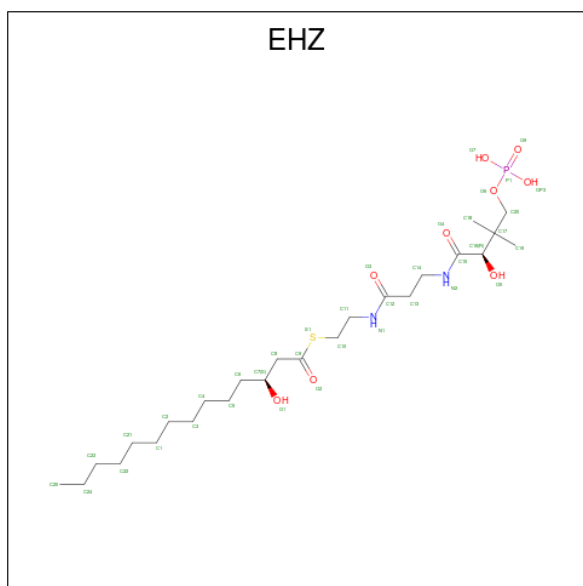


Mol	Chain	Residues	Atoms					AltConf
47	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 49 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

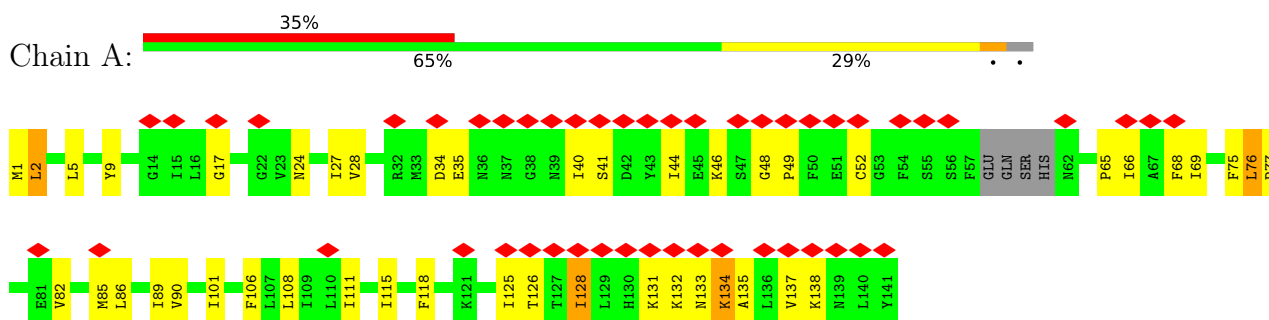


Mol	Chain	Residues	Atoms						AltConf
49	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
49	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

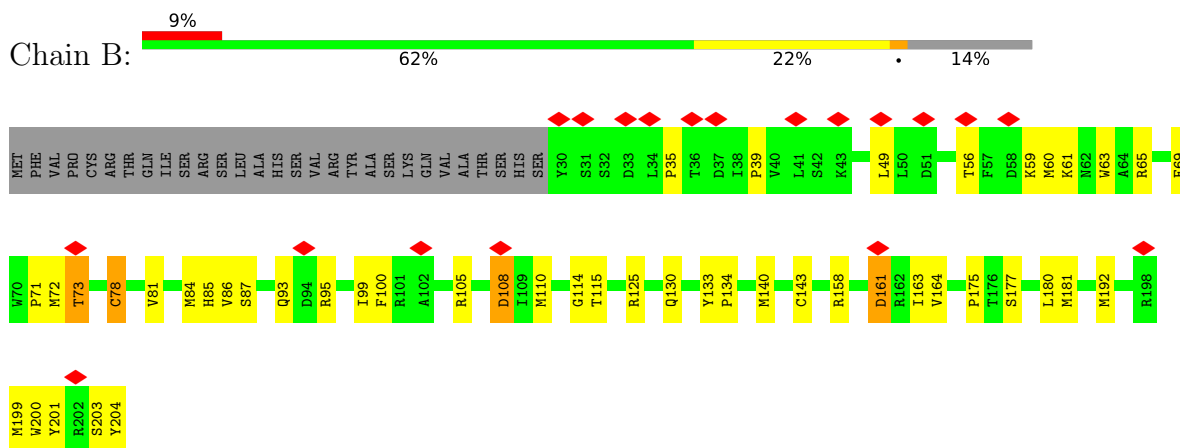
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

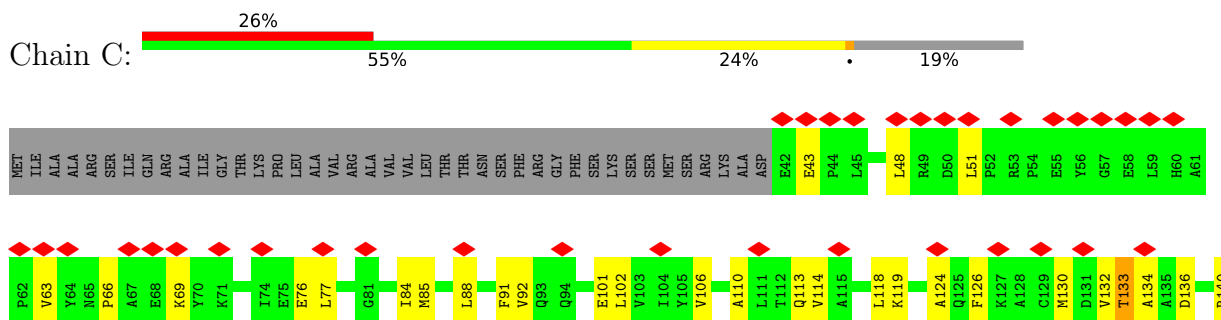
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

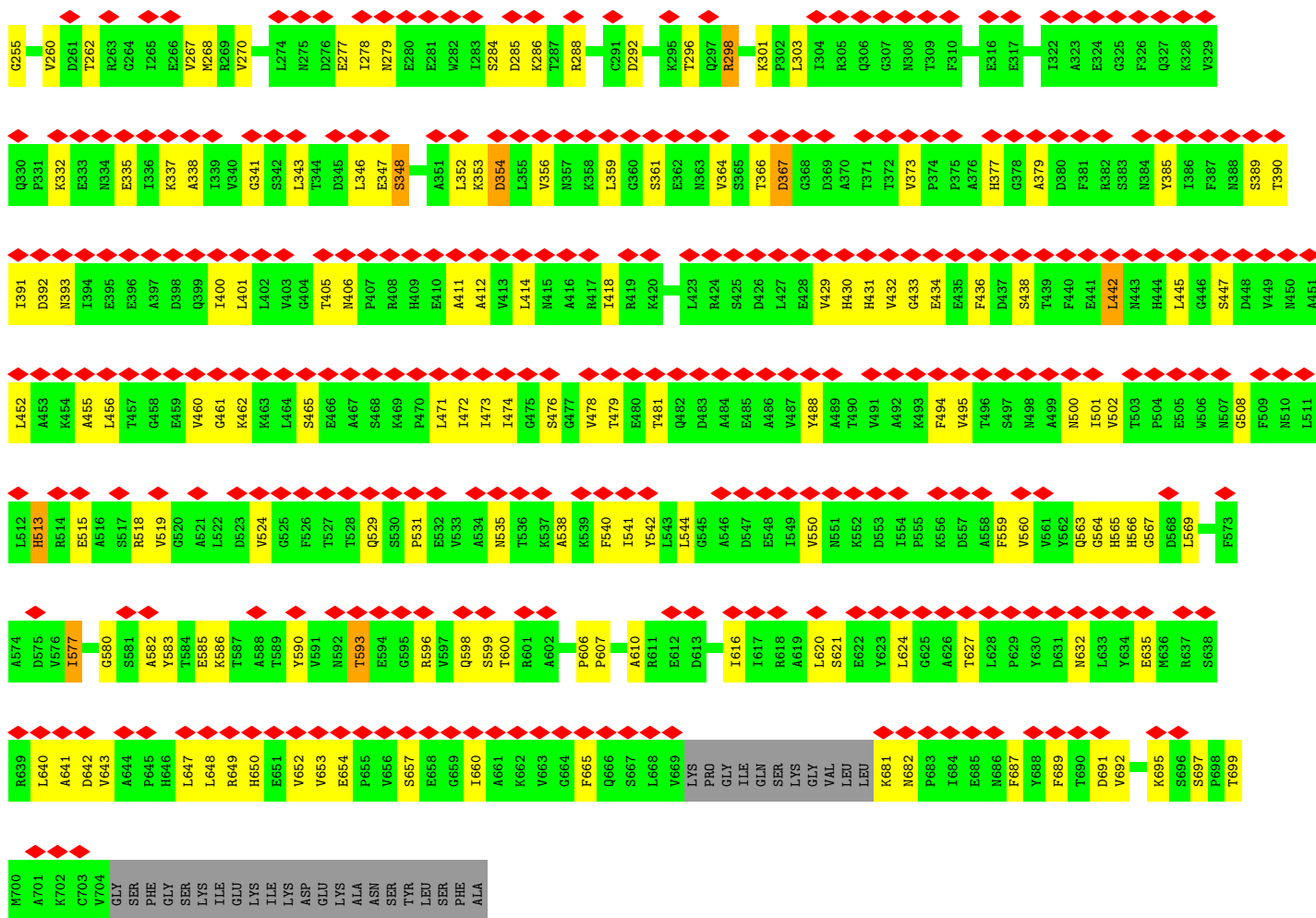


- Molecule 2: BA75_00622T0

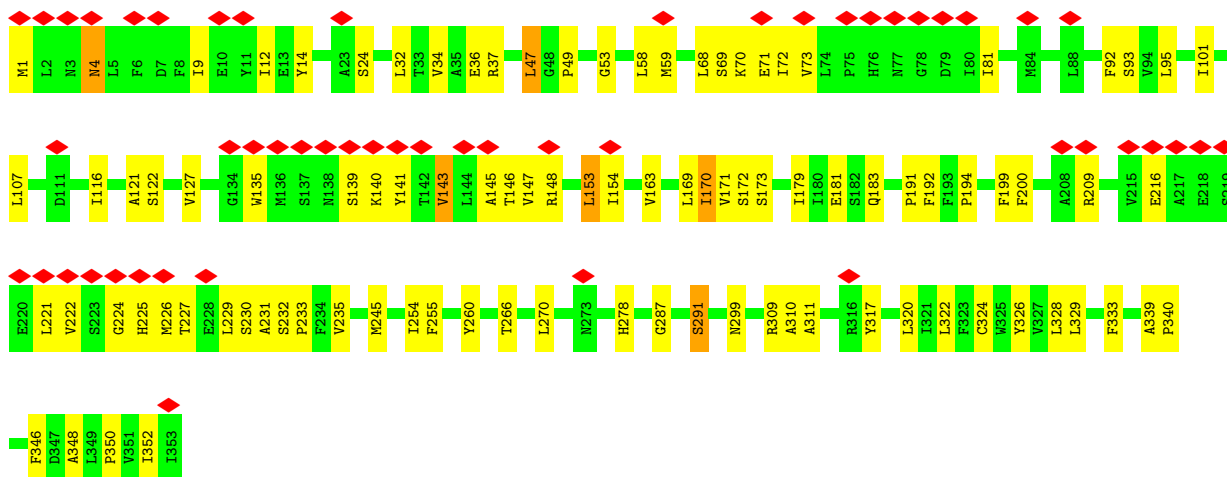


- Molecule 3: NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

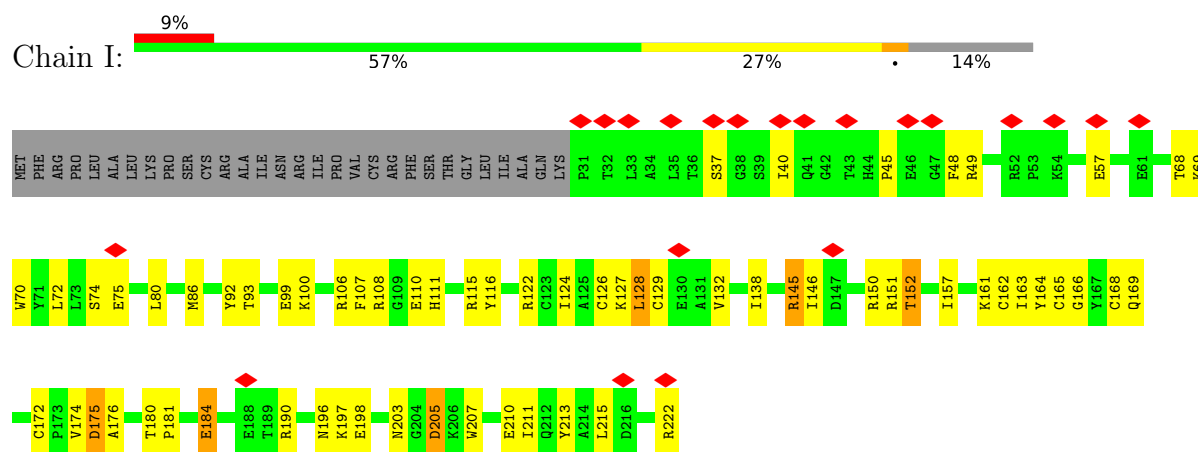




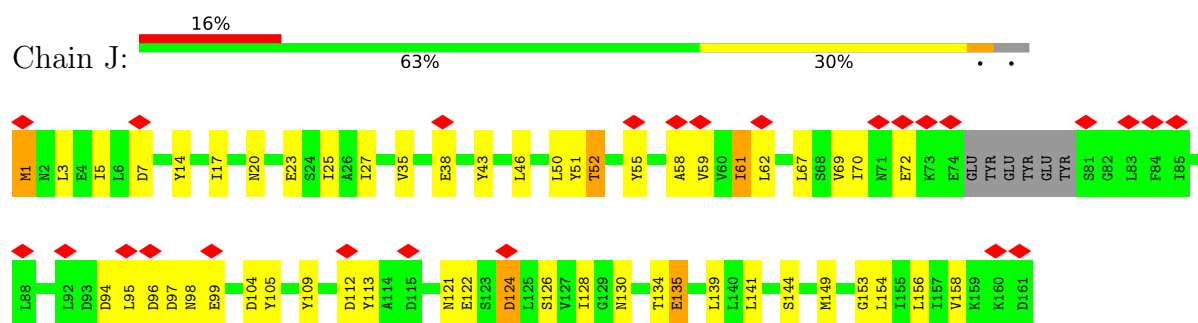
• Molecule 6: NADH-ubiquinone oxidoreductase chain 1



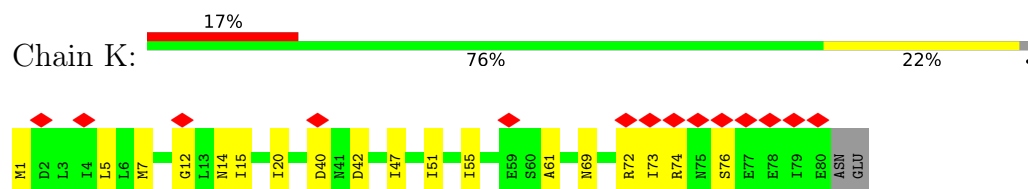
• Molecule 7: NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



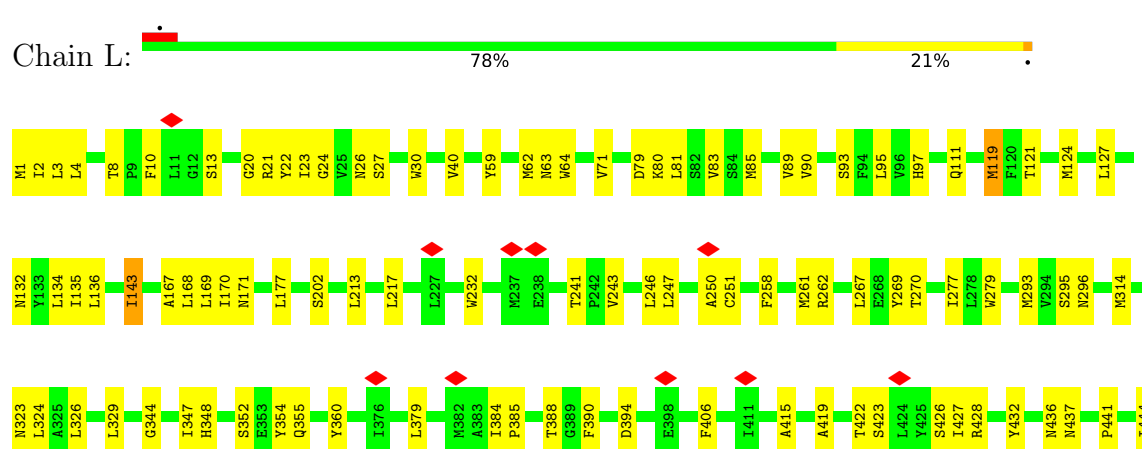
• Molecule 8: NADH-ubiquinone oxidoreductase chain 6

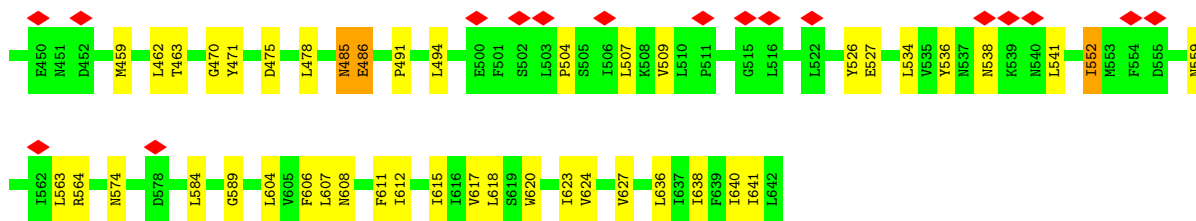


• Molecule 9: NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

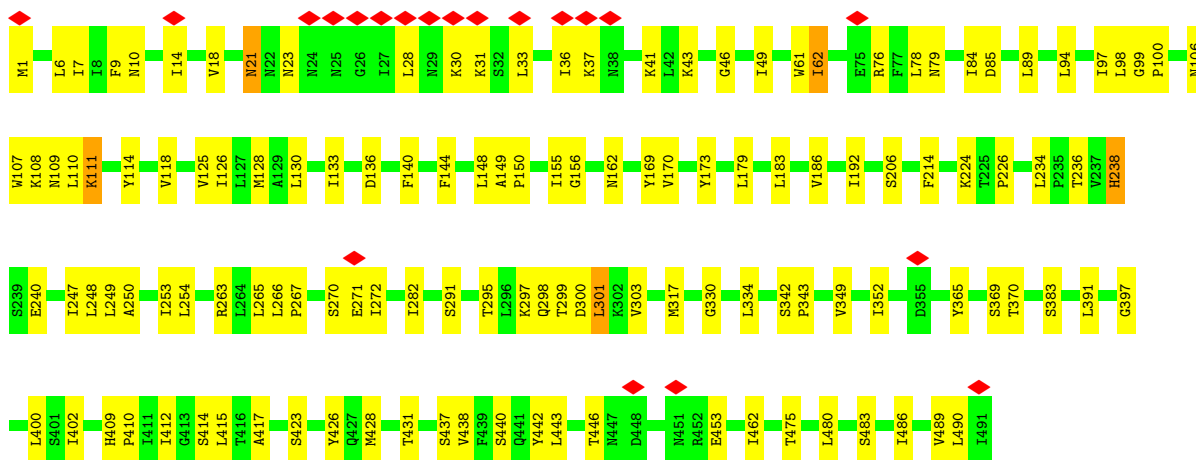
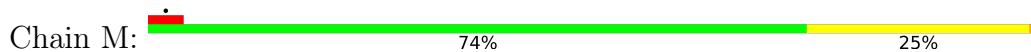


• Molecule 10: NADH-ubiquinone oxidoreductase chain 5

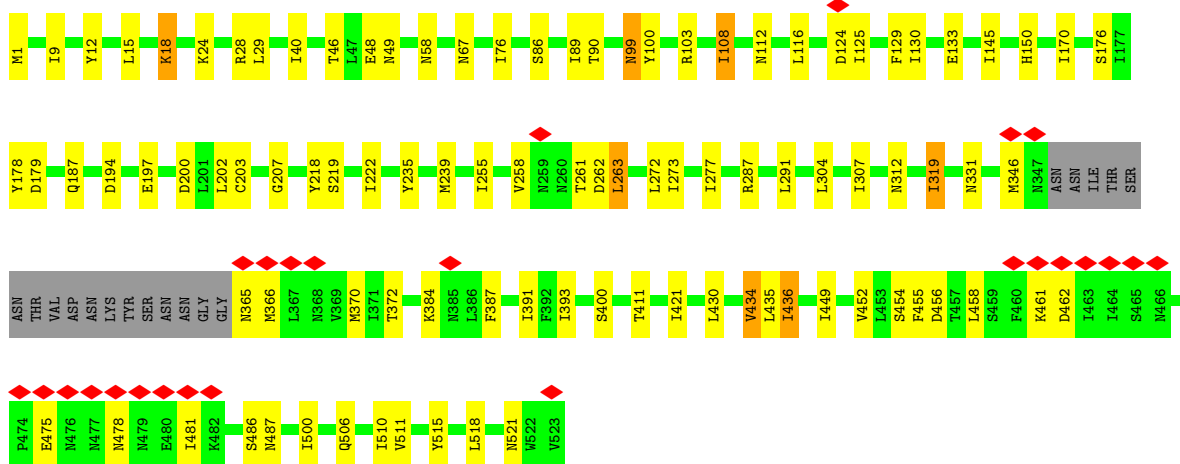
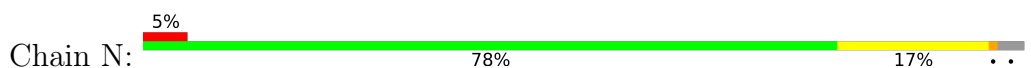




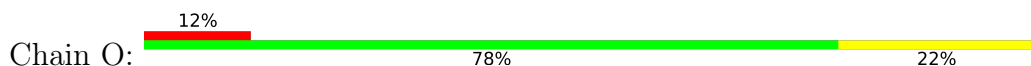
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4

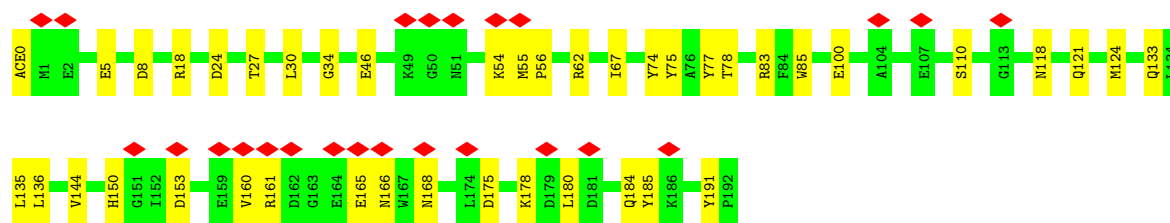


• Molecule 12: NADH-ubiquinone oxidoreductase chain 2

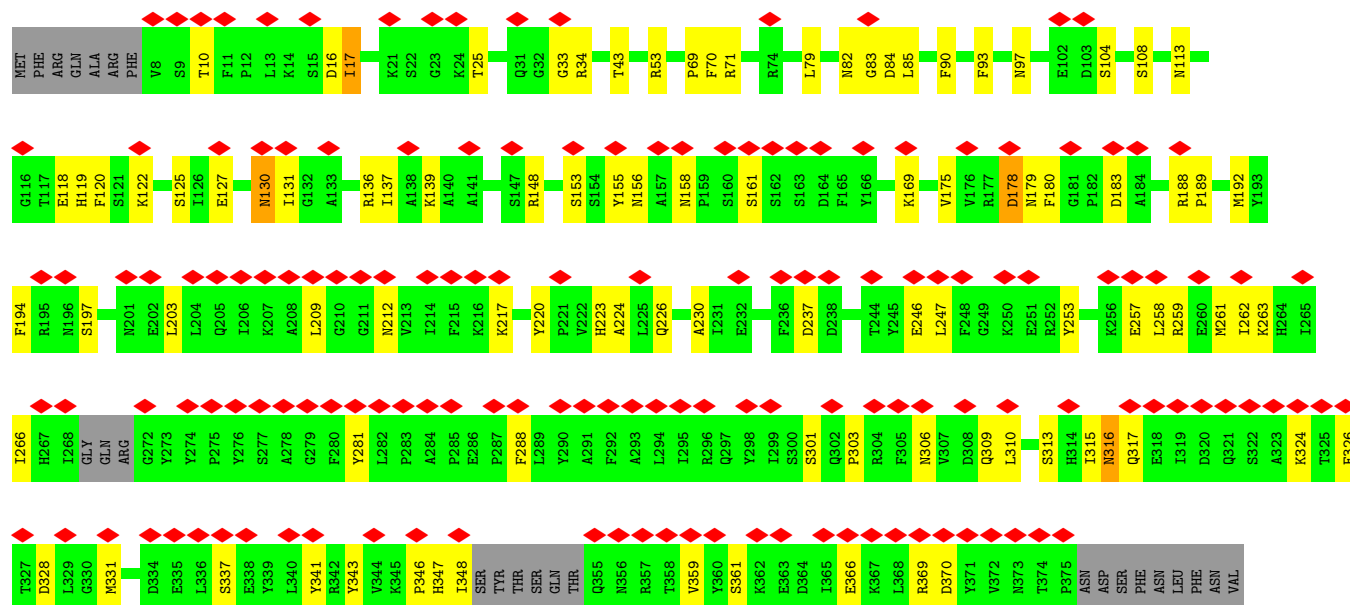
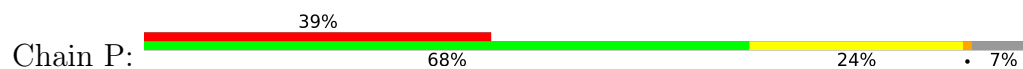


• Molecule 13: NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

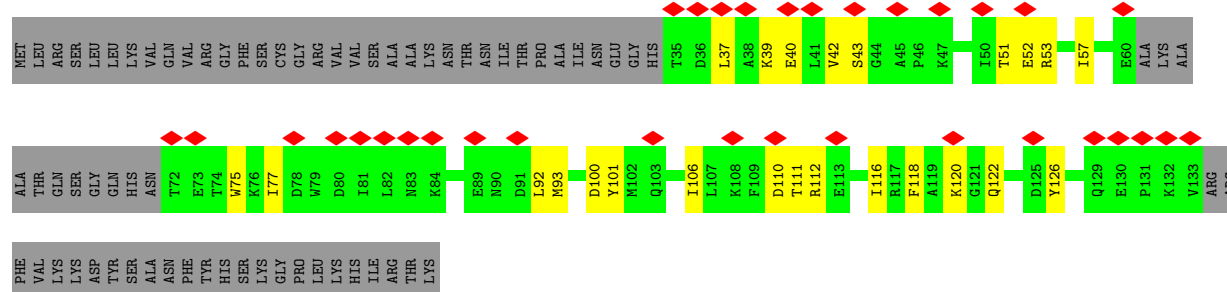




- Molecule 14: NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

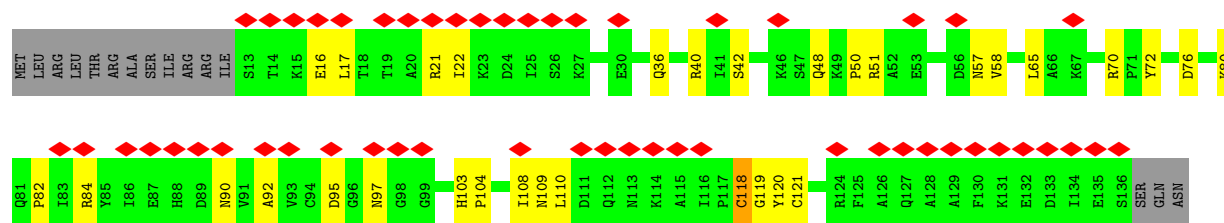


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

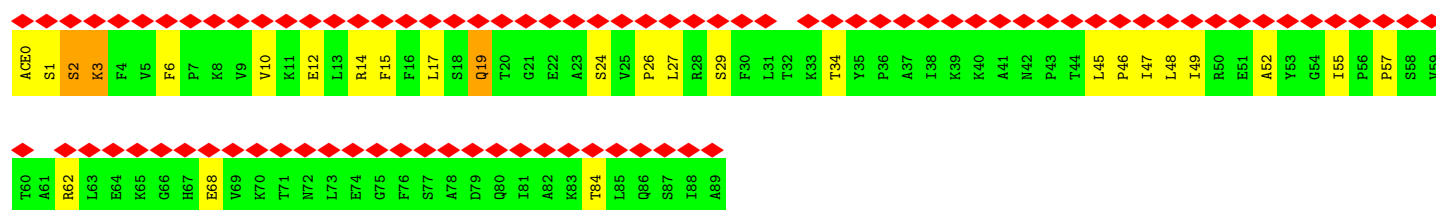


- Molecule 16: NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

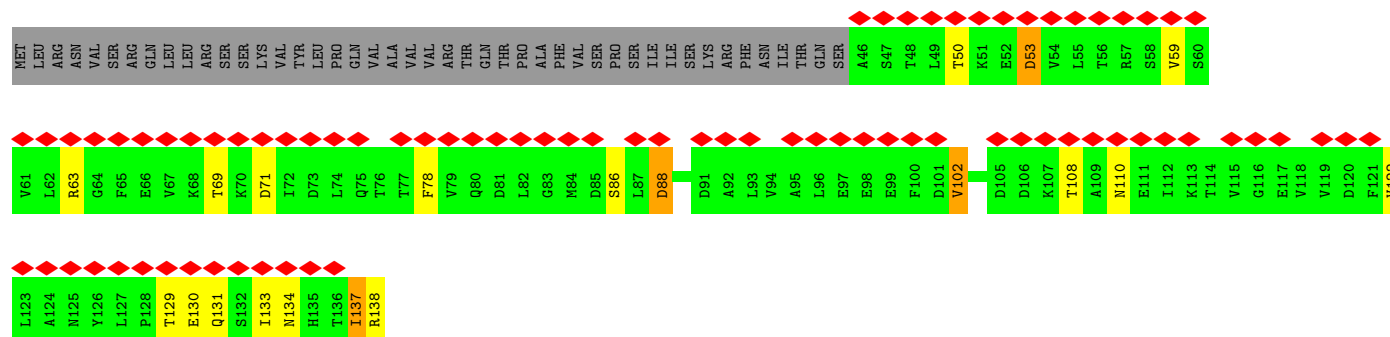




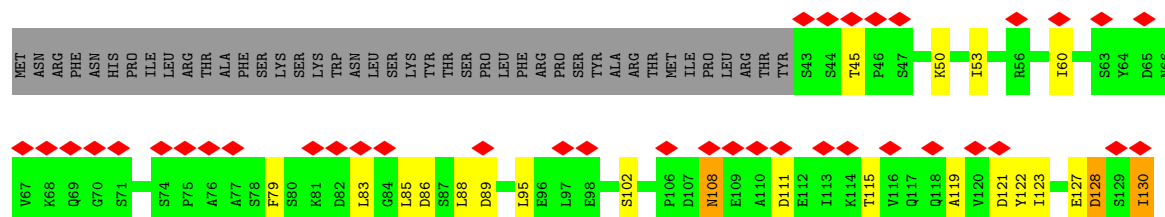
- Molecule 17: NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 18: Acyl carrier protein

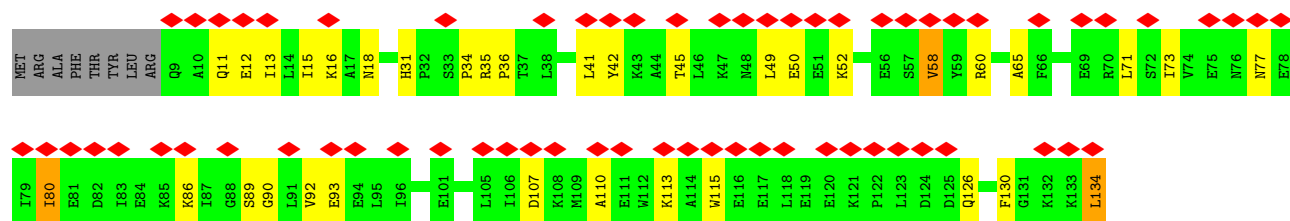


- Molecule 19: Acyl carrier protein

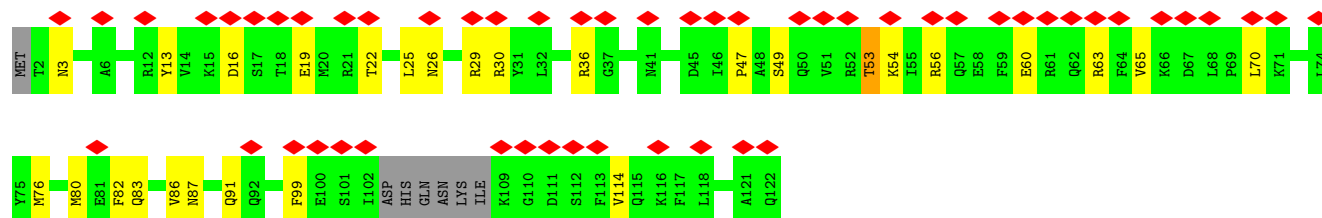
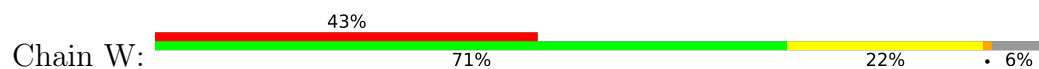


- Molecule 20: NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

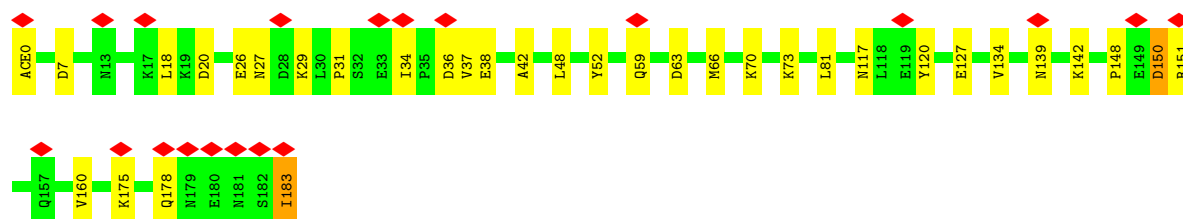
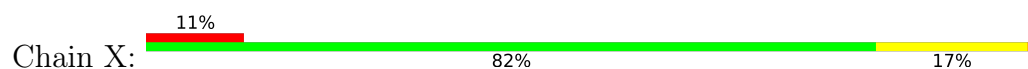




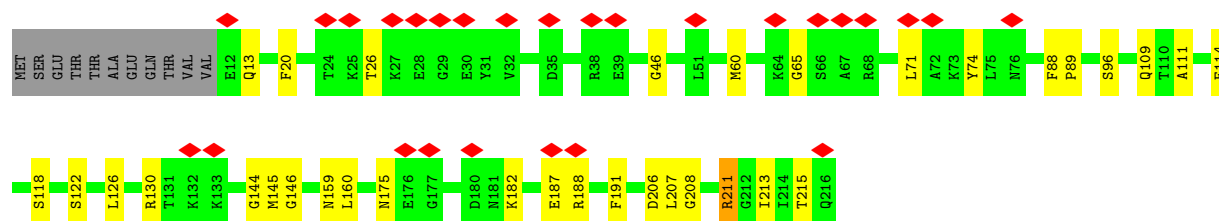
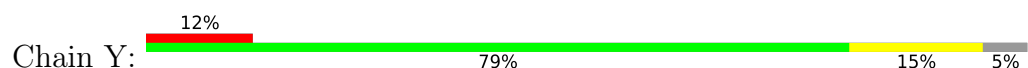
• Molecule 21: BA75_04796T0



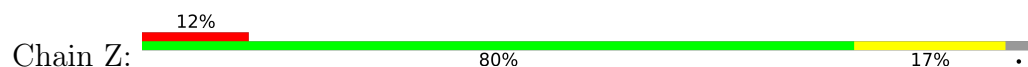
• Molecule 22: NADH-ubiquinone oxidoreductase

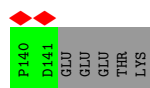


• Molecule 23: NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

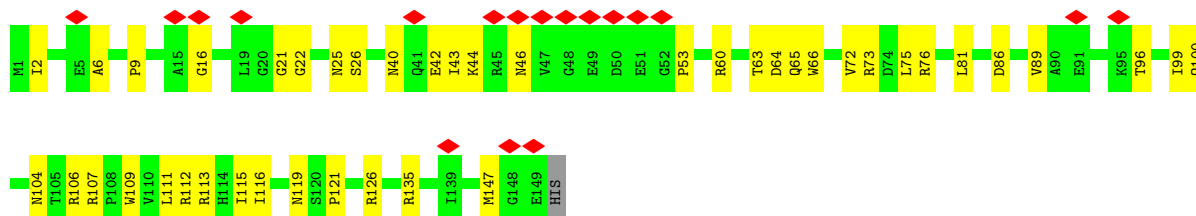


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

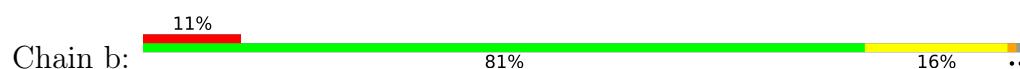




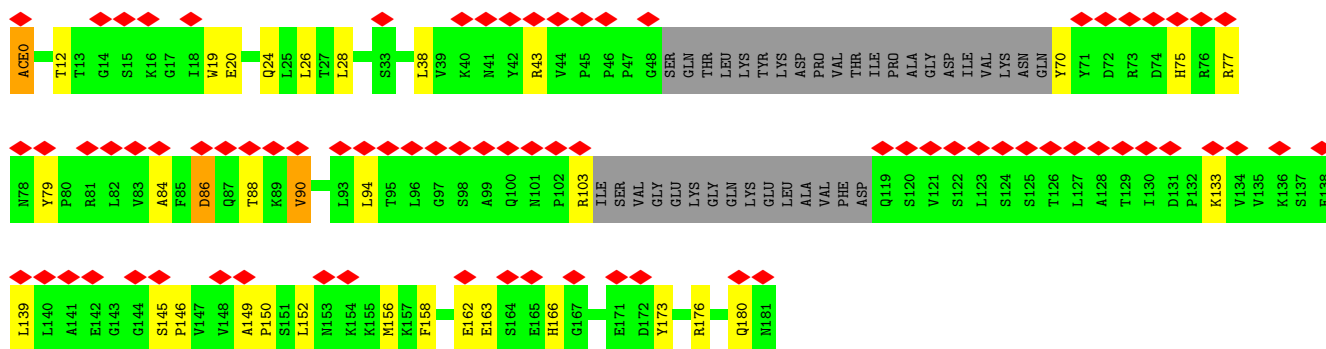
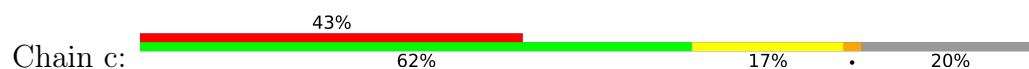
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



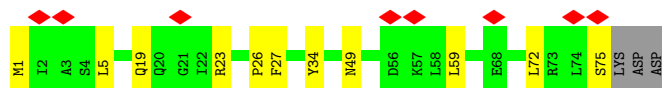
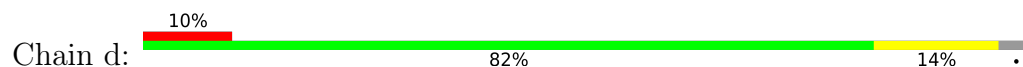
- Molecule 26: NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



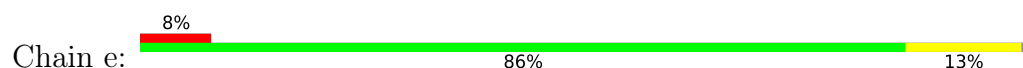
- Molecule 27: BA75_00589T0

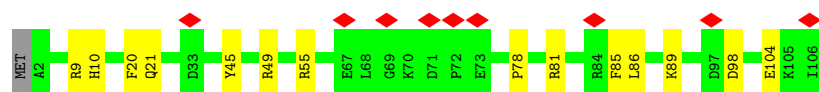


- Molecule 28: Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM

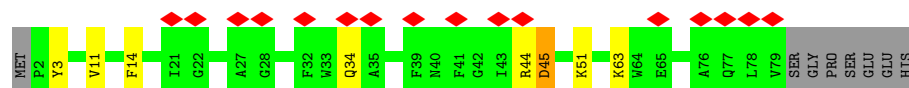
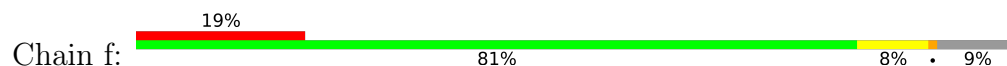


- Molecule 29: BA75_05084T0

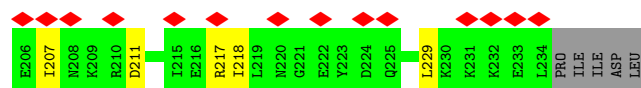
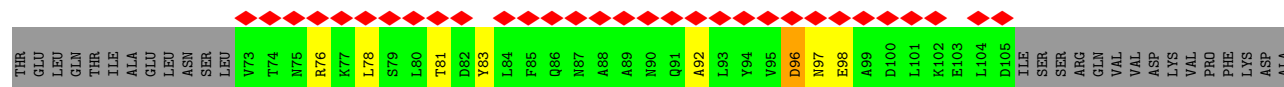
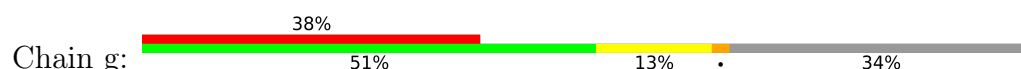




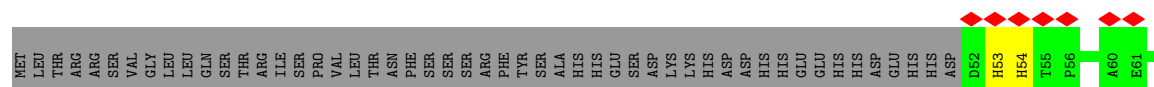
- Molecule 30: NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 31: NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 32: NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

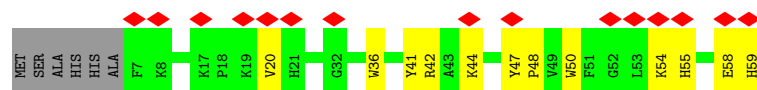


- Molecule 33: NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

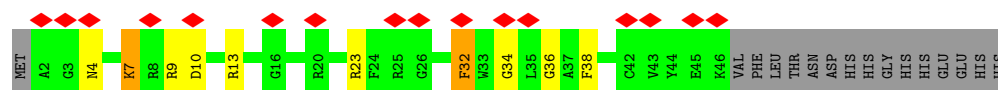




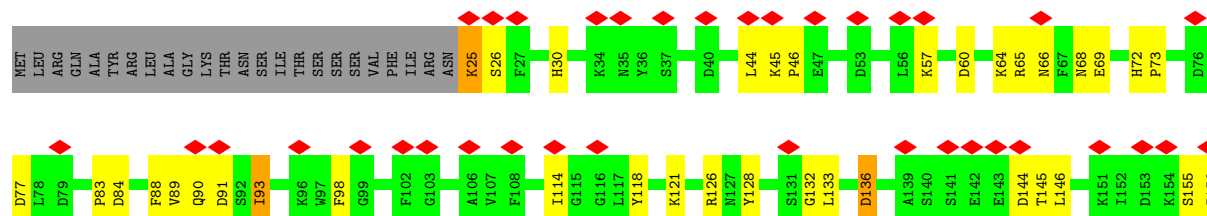
- Molecule 34: Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



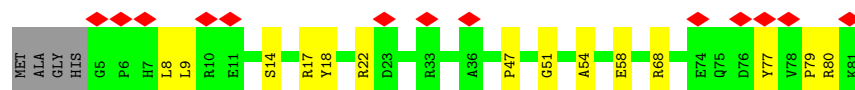
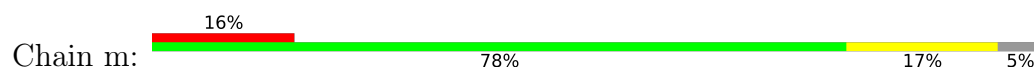
- Molecule 35: NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



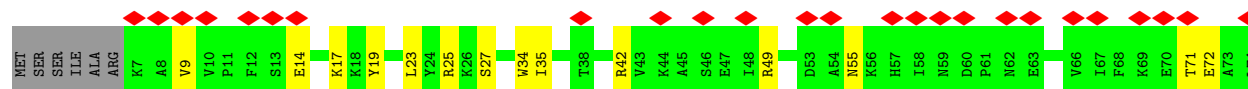
- Molecule 36: NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

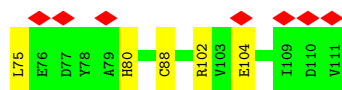


- Molecule 37: NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

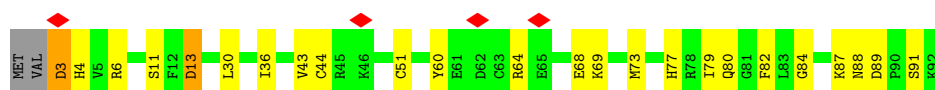




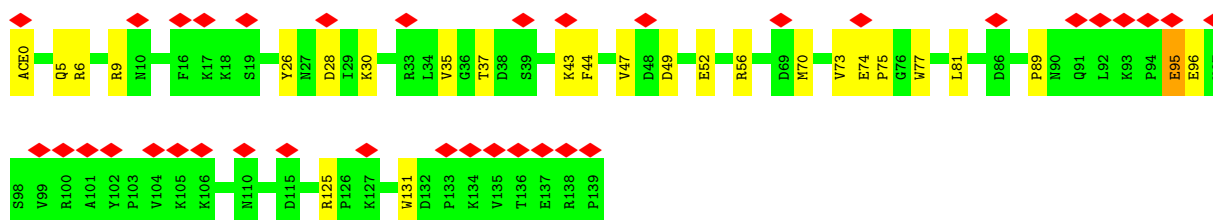
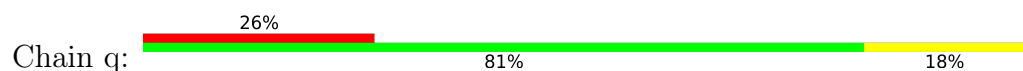
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 40: NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 41: 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	18608	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	0.072	Depositor
Minimum map value	-0.025	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	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: FME, CDL, K, SF4, PLC, ZN, 2MR, ACE, NDP, EHZ, 3PE

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	0.19	0/1115	0.30	0/1514
2	B	0.20	0/1450	0.28	0/1969
3	C	0.17	0/1981	0.26	0/2694
4	D	0.19	0/3612	0.28	0/4892
5	G	0.14	0/4371	0.28	0/5932
6	H	0.21	0/2880	0.28	0/3939
7	I	0.24	0/1596	0.33	0/2164
8	J	0.22	0/1262	0.28	0/1723
9	K	0.22	0/610	0.25	0/828
10	L	0.21	0/5236	0.28	0/7128
11	M	0.23	0/3940	0.29	0/5379
12	N	0.23	0/4110	0.27	0/5609
13	O	0.24	1/1621 (0.1%)	0.30	0/2199
14	P	0.15	0/2911	0.27	0/3932
15	Q	0.16	0/742	0.26	0/1000
16	R	0.15	0/998	0.26	0/1350
17	S	0.26	1/710 (0.1%)	0.27	0/961
18	T	0.11	0/737	0.24	0/1001
19	U	0.14	0/688	0.26	0/936
20	V	0.14	0/1044	0.27	0/1411
21	W	0.14	0/999	0.26	0/1340
22	X	0.24	1/1475 (0.1%)	0.28	0/1990
23	Y	0.18	0/1615	0.27	0/2175
24	Z	0.26	1/1210 (0.1%)	0.25	0/1639
25	a	0.19	0/1241	0.26	0/1670
26	b	0.16	0/666	0.25	0/911
27	c	0.23	1/1167 (0.1%)	0.27	0/1581
28	d	0.19	0/633	0.22	0/854
29	e	0.20	0/865	0.25	0/1158
30	f	0.17	0/663	0.22	0/896
31	g	0.15	0/1293	0.26	0/1735
32	h	0.18	0/1114	0.27	0/1516

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.16	0/571	0.25	0/777
34	j	0.15	0/484	0.26	0/658
35	k	0.14	0/382	0.24	0/514
36	l	0.17	0/1119	0.29	0/1520
37	m	0.18	0/661	0.27	0/893
38	n	0.14	0/884	0.23	0/1197
39	o	0.14	0/696	0.27	0/933
40	p	0.20	0/756	0.25	0/1020
41	q	0.25	1/1192 (0.1%)	0.29	0/1620
All	All	0.20	6/61300 (0.0%)	0.27	0/83158

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	S	0	ACE	C-N	6.20	1.45	1.33
27	c	0	ACE	C-N	6.14	1.45	1.33
22	X	0	ACE	C-N	6.11	1.45	1.33
41	q	0	ACE	C-N	6.06	1.45	1.33
24	Z	0	ACE	C-N	6.03	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1099	0	1140	38	0
2	B	1407	0	1372	42	0
3	C	1922	0	1861	61	0
4	D	3536	0	3437	79	0
5	G	4295	0	4257	133	0
6	H	2809	0	2880	66	0
7	I	1556	0	1499	60	0
8	J	1250	0	1274	44	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	617	0	657	16	0
10	L	5115	0	5338	98	0
11	M	3868	0	4127	88	0
12	N	4045	0	4327	68	0
13	O	1575	0	1523	27	0
14	P	2851	0	2847	69	0
15	Q	727	0	701	13	0
16	R	978	0	964	19	0
17	S	697	0	736	20	0
18	T	730	0	721	16	0
19	U	681	0	664	15	0
20	V	1025	0	1035	30	0
21	W	979	0	980	19	0
22	X	1450	0	1422	23	0
23	Y	1578	0	1567	25	0
24	Z	1176	0	1165	19	0
25	a	1215	0	1197	41	0
26	b	641	0	620	13	0
27	c	1143	0	1165	29	0
28	d	616	0	624	8	0
29	e	848	0	830	11	0
30	f	642	0	640	9	0
31	g	1280	0	1302	27	0
32	h	1078	0	1036	12	0
33	i	552	0	540	12	0
34	j	460	0	455	8	0
35	k	368	0	348	8	0
36	l	1082	0	1033	26	0
37	m	642	0	635	12	0
38	n	861	0	866	13	0
39	o	682	0	677	15	0
40	p	740	0	700	20	0
41	q	1156	0	1115	17	0
42	B	8	0	0	1	0
42	G	16	0	0	6	0
42	I	16	0	0	3	0
43	B	31	0	36	3	0
43	D	42	0	64	3	0
43	H	24	0	22	0	0
43	L	151	0	210	13	0
43	M	84	0	128	4	0
43	P	62	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	Y	72	0	98	4	0
43	Z	42	0	64	3	0
43	a	22	0	18	0	0
43	b	39	0	55	0	0
43	d	84	0	128	3	0
43	g	39	0	55	5	0
43	q	78	0	113	5	0
44	G	1	0	0	0	0
45	J	51	0	82	4	0
45	L	259	0	380	19	0
45	M	86	0	126	6	0
45	N	40	0	57	1	0
45	Y	25	0	24	1	0
45	Z	36	0	46	1	0
45	b	71	0	93	3	0
45	h	46	0	69	5	0
45	j	27	0	28	4	0
45	m	46	0	69	4	0
46	O	75	0	97	3	0
46	Z	49	0	42	1	0
46	b	59	0	62	3	0
46	q	60	0	64	5	0
47	P	48	0	25	2	0
48	R	1	0	0	0	0
49	T	37	0	0	0	0
49	U	37	0	0	2	0
All	All	61836	0	62604	1133	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 9.

The worst 5 of 1133 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)
5:G:175:HIS:HA	42:G:801:SF4:S4	1.96	1.04
7:I:111:HIS:CD2	7:I:168:CYS:SG	2.49	1.03
7:I:111:HIS:CE1	42:I:302:SF4:S2	2.55	0.97
14:P:156:ASN:HD21	14:P:317:GLN:HA	1.39	0.86
16:R:103:HIS:CD2	16:R:121:CYS:SG	2.68	0.86

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	133/141 (94%)	126 (95%)	6 (4%)	1 (1%)	16	48
2	B	173/204 (85%)	166 (96%)	7 (4%)	0	100	100
3	C	231/289 (80%)	221 (96%)	10 (4%)	0	100	100
4	D	435/482 (90%)	406 (93%)	29 (7%)	0	100	100
5	G	548/726 (76%)	515 (94%)	33 (6%)	0	100	100
6	H	351/353 (99%)	323 (92%)	27 (8%)	1 (0%)	36	67
7	I	190/222 (86%)	181 (95%)	9 (5%)	0	100	100
8	J	151/161 (94%)	144 (95%)	7 (5%)	0	100	100
9	K	78/82 (95%)	75 (96%)	3 (4%)	0	100	100
10	L	640/642 (100%)	622 (97%)	17 (3%)	1 (0%)	43	73
11	M	489/491 (100%)	470 (96%)	19 (4%)	0	100	100
12	N	502/523 (96%)	492 (98%)	10 (2%)	0	100	100
13	O	191/193 (99%)	185 (97%)	6 (3%)	0	100	100
14	P	353/384 (92%)	342 (97%)	11 (3%)	0	100	100
15	Q	84/159 (53%)	84 (100%)	0	0	100	100
16	R	122/139 (88%)	115 (94%)	7 (6%)	0	100	100
17	S	88/90 (98%)	83 (94%)	4 (4%)	1 (1%)	11	41
18	T	91/138 (66%)	85 (93%)	6 (7%)	0	100	100
19	U	86/130 (66%)	80 (93%)	6 (7%)	0	100	100
20	V	124/134 (92%)	119 (96%)	5 (4%)	0	100	100
21	W	111/122 (91%)	109 (98%)	2 (2%)	0	100	100
22	X	182/184 (99%)	176 (97%)	6 (3%)	0	100	100
23	Y	203/216 (94%)	190 (94%)	13 (6%)	0	100	100
24	Z	140/147 (95%)	135 (96%)	5 (4%)	0	100	100
25	a	147/150 (98%)	144 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	b	76/79 (96%)	71 (93%)	5 (7%)	0	100	100
27	c	140/182 (77%)	127 (91%)	13 (9%)	0	100	100
28	d	73/78 (94%)	72 (99%)	1 (1%)	0	100	100
29	e	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
30	f	76/86 (88%)	74 (97%)	2 (3%)	0	100	100
31	g	152/239 (64%)	144 (95%)	8 (5%)	0	100	100
32	h	129/182 (71%)	123 (95%)	6 (5%)	0	100	100
33	i	67/74 (90%)	65 (97%)	2 (3%)	0	100	100
34	j	51/59 (86%)	51 (100%)	0	0	100	100
35	k	43/61 (70%)	41 (95%)	2 (5%)	0	100	100
36	l	130/156 (83%)	121 (93%)	8 (6%)	1 (1%)	16	48
37	m	75/81 (93%)	71 (95%)	4 (5%)	0	100	100
38	n	103/111 (93%)	101 (98%)	2 (2%)	0	100	100
39	o	78/87 (90%)	75 (96%)	3 (4%)	0	100	100
40	p	88/92 (96%)	83 (94%)	5 (6%)	0	100	100
41	q	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
All	All	7365/8315 (89%)	7037 (96%)	323 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	l	145	THR
6	H	222	VAL
17	S	2	SER
1	A	2	LEU
10	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	A	124/128 (97%)	115 (93%)	9 (7%)	13	39
2	B	154/180 (86%)	149 (97%)	5 (3%)	34	56
3	C	208/254 (82%)	202 (97%)	6 (3%)	37	58
4	D	375/408 (92%)	359 (96%)	16 (4%)	26	50
5	G	469/610 (77%)	450 (96%)	19 (4%)	27	51
6	H	307/307 (100%)	294 (96%)	13 (4%)	26	50
7	I	166/192 (86%)	158 (95%)	8 (5%)	23	47
8	J	143/149 (96%)	132 (92%)	11 (8%)	12	37
9	K	70/72 (97%)	70 (100%)	0	100	100
10	L	576/576 (100%)	564 (98%)	12 (2%)	47	64
11	M	439/439 (100%)	425 (97%)	14 (3%)	34	56
12	N	474/489 (97%)	455 (96%)	19 (4%)	28	52
13	O	169/169 (100%)	165 (98%)	4 (2%)	43	62
14	P	309/332 (93%)	302 (98%)	7 (2%)	44	63
15	Q	76/135 (56%)	74 (97%)	2 (3%)	40	60
16	R	104/118 (88%)	101 (97%)	3 (3%)	37	58
17	S	77/77 (100%)	72 (94%)	5 (6%)	15	42
18	T	85/128 (66%)	78 (92%)	7 (8%)	10	35
19	U	80/120 (67%)	73 (91%)	7 (9%)	9	33
20	V	112/119 (94%)	107 (96%)	5 (4%)	24	48
21	W	107/114 (94%)	102 (95%)	5 (5%)	23	48
22	X	165/165 (100%)	158 (96%)	7 (4%)	26	50
23	Y	163/173 (94%)	158 (97%)	5 (3%)	35	57
24	Z	123/128 (96%)	121 (98%)	2 (2%)	55	68
25	a	128/129 (99%)	127 (99%)	1 (1%)	73	76
26	b	66/67 (98%)	65 (98%)	1 (2%)	57	69
27	c	128/159 (80%)	123 (96%)	5 (4%)	28	52
28	d	62/65 (95%)	62 (100%)	0	100	100
29	e	91/92 (99%)	90 (99%)	1 (1%)	65	73
30	f	64/71 (90%)	63 (98%)	1 (2%)	55	68
31	g	143/215 (66%)	135 (94%)	8 (6%)	19	45
32	h	118/167 (71%)	113 (96%)	5 (4%)	26	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	i	59/63 (94%)	57 (97%)	2 (3%)	32	55
34	j	46/50 (92%)	44 (96%)	2 (4%)	26	50
35	k	32/47 (68%)	30 (94%)	2 (6%)	16	42
36	l	116/137 (85%)	107 (92%)	9 (8%)	11	36
37	m	64/66 (97%)	63 (98%)	1 (2%)	55	68
38	n	95/100 (95%)	93 (98%)	2 (2%)	47	64
39	o	74/79 (94%)	73 (99%)	1 (1%)	59	70
40	p	83/85 (98%)	81 (98%)	2 (2%)	43	62
41	q	125/125 (100%)	123 (98%)	2 (2%)	55	68
All	All	6569/7299 (90%)	6333 (96%)	236 (4%)	32	54

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	N	48	GLU
36	l	45	LYS
15	Q	40	GLU
36	l	25	LYS
30	f	45	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
24	Z	19	ASN
41	q	42	ASN
24	Z	136	ASN
32	h	92	HIS
12	N	123	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$
1	FME	A	1	1	8,9,10	1.50	1 (12%)	7,9,11	1.61	3 (42%)
8	FME	J	1	8	8,9,10	1.51	1 (12%)	7,9,11	1.62	1 (14%)
11	FME	M	1	11	8,9,10	1.50	1 (12%)	7,9,11	1.65	1 (14%)
9	FME	K	1	9	8,9,10	1.54	1 (12%)	7,9,11	1.32	1 (14%)
12	FME	N	1	12	8,9,10	1.48	1 (12%)	7,9,11	1.72	3 (42%)
10	FME	L	1	10	8,9,10	1.50	1 (12%)	7,9,11	1.78	3 (42%)
4	2MR	D	137	4	10,12,13	2.38	2 (20%)	5,13,15	2.21	2 (40%)
6	FME	H	1	6	8,9,10	1.51	1 (12%)	7,9,11	1.75	3 (42%)

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
1	FME	A	1	1	-	2/7/9/11	-
8	FME	J	1	8	-	5/7/9/11	-
11	FME	M	1	11	-	4/7/9/11	-
9	FME	K	1	9	-	5/7/9/11	-
12	FME	N	1	12	-	0/7/9/11	-
10	FME	L	1	10	-	5/7/9/11	-
4	2MR	D	137	4	-	3/10/13/15	-
6	FME	H	1	6	-	4/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	137	2MR	CZ-NE	5.14	1.45	1.34
4	D	137	2MR	CZ-NH2	5.05	1.44	1.33
9	K	1	FME	CN-N	3.79	1.46	1.33
6	H	1	FME	CN-N	3.66	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	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(°)
4	D	137	2MR	NE-CZ-NH2	3.66	122.83	119.48
6	H	1	FME	CE-SD-CG	2.85	110.19	100.40
10	L	1	FME	CE-SD-CG	2.66	109.54	100.40
4	D	137	2MR	CQ2-NH2-CZ	-2.64	118.03	123.86
11	M	1	FME	CE-SD-CG	2.53	109.10	100.40

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O-C-CA-CB
6	H	1	FME	N-CA-CB-CG
6	H	1	FME	C-CA-CB-CG
8	J	1	FME	O1-CN-N-CA
8	J	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are monoatomic - leaving 50 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	$\# Z > 2$
43	PLC	L	701	10	41,41,41	0.50	0	47,49,49	0.72	2 (4%)
45	3PE	L	704	-	34,34,50	1.02	4 (11%)	37,39,55	1.14	2 (5%)
43	PLC	L	709	-	31,31,41	0.56	0	37,39,49	0.58	0
45	3PE	N	601	-	39,39,50	0.97	4 (10%)	42,44,55	1.17	2 (4%)
43	PLC	Y	302	-	35,35,41	0.53	0	41,43,49	0.62	0
43	PLC	d	102	-	41,41,41	0.52	0	47,49,49	0.51	0
45	3PE	h	201	-	45,45,50	0.91	3 (6%)	48,50,55	1.09	2 (4%)
43	PLC	L	708	-	34,34,41	0.56	0	40,42,49	0.61	0
45	3PE	j	101	-	26,26,50	1.16	4 (15%)	29,31,55	1.17	2 (6%)
47	NDP	P	501	-	49,52,52	3.98	24 (48%)	66,80,80	2.13	15 (22%)
45	3PE	M	502	-	34,34,50	1.03	4 (11%)	37,39,55	1.16	2 (5%)
43	PLC	M	503	-	41,41,41	0.53	0	47,49,49	0.56	0
45	3PE	L	703	-	50,50,50	0.86	3 (6%)	53,55,55	1.09	2 (3%)
45	3PE	L	707	-	28,28,50	1.13	3 (10%)	31,33,55	1.16	2 (6%)
45	3PE	m	101	-	45,45,50	0.90	4 (8%)	48,50,55	1.11	2 (4%)
49	EHZ	T	201	18	29,36,37	1.68	5 (17%)	35,44,47	1.46	3 (8%)
46	CDL	q	203	-	59,59,99	1.12	8 (13%)	65,71,111	1.19	4 (6%)
43	PLC	g	301	-	38,38,41	0.55	0	44,46,49	0.49	0
46	CDL	Z	203	-	48,48,99	1.22	8 (16%)	54,60,111	1.23	4 (7%)
43	PLC	a	201	-	21,21,41	0.68	0	27,29,49	0.65	0
45	3PE	Z	201	-	35,35,50	1.01	4 (11%)	38,40,55	1.14	2 (5%)
45	3PE	J	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.11	2 (3%)
46	CDL	O	201	-	74,74,99	0.99	7 (9%)	80,86,111	1.16	4 (5%)
46	CDL	b	102	-	58,58,99	1.12	7 (12%)	64,70,111	1.24	4 (6%)
43	PLC	M	504	-	41,41,41	0.50	0	47,49,49	0.57	0
43	PLC	B	302	-	30,30,41	0.58	0	36,38,49	0.54	0
43	PLC	b	101	-	38,38,41	0.55	0	44,46,49	0.58	0
42	SF4	G	802	5	0,12,12	-	-	-	-	-
43	PLC	d	101	-	41,41,41	0.53	0	47,49,49	0.50	0
43	PLC	q	202	-	35,35,41	0.56	0	41,43,49	0.57	0
43	PLC	Y	303	-	35,35,41	0.55	0	41,43,49	0.55	0
43	PLC	H	401	-	23,23,41	0.66	0	29,31,49	0.68	0
42	SF4	I	302	7	0,12,12	-	-	-	-	-
42	SF4	G	801	5	0,12,12	-	-	-	-	-
45	3PE	L	706	-	41,41,50	0.95	3 (7%)	44,46,55	1.15	2 (4%)
43	PLC	L	710	-	41,41,41	0.53	0	47,49,49	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	M	501	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
43	PLC	Z	202	-	41,41,41	0.52	0	47,49,49	0.59	1 (2%)
43	PLC	P	502	14	30,30,41	0.60	0	36,38,49	0.54	0
42	SF4	B	301	2	0,12,12	-	-	-	-	-
43	PLC	q	201	41	41,41,41	0.50	0	47,49,49	0.56	0
45	3PE	L	702	-	50,50,50	0.86	3 (6%)	53,55,55	1.14	2 (3%)
45	3PE	b	103	-	30,30,50	1.09	4 (13%)	33,35,55	1.17	2 (6%)
45	3PE	L	705	-	50,50,50	0.85	4 (8%)	53,55,55	1.11	2 (3%)
43	PLC	D	501	-	41,41,41	0.51	0	47,49,49	0.57	0
45	3PE	b	104	-	39,39,50	0.96	4 (10%)	42,44,55	1.15	2 (4%)
42	SF4	I	301	7	0,12,12	-	-	-	-	-
45	3PE	Y	301	-	24,24,50	1.20	4 (16%)	27,29,55	1.36	2 (7%)
43	PLC	P	503	-	30,30,41	0.58	0	36,38,49	0.62	0
49	EHZ	U	201	19	29,36,37	1.68	5 (17%)	35,44,47	1.52	7 (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
43	PLC	L	701	10	-	16/45/45/45	-
45	3PE	L	704	-	-	15/38/38/54	-
43	PLC	L	709	-	-	12/35/35/45	-
45	3PE	N	601	-	-	20/43/43/54	-
43	PLC	Y	302	-	-	14/39/39/45	-
43	PLC	d	102	-	-	19/45/45/45	-
45	3PE	h	201	-	-	17/49/49/54	-
43	PLC	L	708	-	-	12/38/38/45	-
45	3PE	j	101	-	-	15/30/30/54	-
47	NDP	P	501	-	-	14/34/77/77	0/5/5/5
45	3PE	M	502	-	-	18/38/38/54	-
43	PLC	M	503	-	-	15/45/45/45	-
45	3PE	L	703	-	-	27/54/54/54	-
45	3PE	L	707	-	-	6/32/32/54	-
45	3PE	m	101	-	-	22/49/49/54	-
49	EHZ	T	201	18	-	21/42/44/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	CDL	q	203	-	-	28/70/70/110	-
43	PLC	g	301	-	-	13/42/42/45	-
46	CDL	Z	203	-	-	29/58/58/110	-
43	PLC	a	201	-	-	8/23/23/45	-
45	3PE	Z	201	-	-	13/39/39/54	-
45	3PE	J	201	-	-	25/54/54/54	-
46	CDL	O	201	-	-	35/85/85/110	-
46	CDL	b	102	-	-	24/69/69/110	-
43	PLC	M	504	-	-	19/45/45/45	-
43	PLC	B	302	-	-	10/34/34/45	-
43	PLC	b	101	-	-	7/42/42/45	-
43	PLC	q	202	-	-	15/39/39/45	-
43	PLC	d	101	-	-	13/45/45/45	-
42	SF4	G	802	5	-	-	0/6/5/5
43	PLC	Y	303	-	-	14/39/39/45	-
43	PLC	H	401	-	-	6/26/26/45	-
42	SF4	I	302	7	-	-	0/6/5/5
42	SF4	G	801	5	-	-	0/6/5/5
45	3PE	L	706	-	-	22/45/45/54	-
43	PLC	L	710	-	-	15/45/45/45	-
45	3PE	M	501	-	-	25/54/54/54	-
43	PLC	Z	202	-	-	23/45/45/45	-
43	PLC	P	502	14	-	15/34/34/45	-
43	PLC	q	201	41	-	26/45/45/45	-
42	SF4	B	301	2	-	-	0/6/5/5
45	3PE	L	702	-	-	18/54/54/54	-
45	3PE	b	103	-	-	19/34/34/54	-
45	3PE	L	705	-	-	23/54/54/54	-
43	PLC	D	501	-	-	11/45/45/45	-
45	3PE	b	104	-	-	24/43/43/54	-
45	3PE	Y	301	-	-	15/27/27/54	-
42	SF4	I	301	7	-	-	0/6/5/5
43	PLC	P	503	-	-	12/34/34/45	-
49	EHZ	U	201	19	-	14/42/44/45	-

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	P	501	NDP	C6N-C5N	12.05	1.54	1.33
47	P	501	NDP	C2B-C1B	-8.58	1.31	1.53
47	P	501	NDP	O4B-C1B	8.36	1.61	1.42
47	P	501	NDP	C7N-N7N	8.29	1.55	1.33
47	P	501	NDP	O4D-C1D	8.00	1.61	1.42

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	P	501	NDP	C4A-N9A-C1B	-5.81	112.74	126.59
47	P	501	NDP	N6A-C6A-N1A	-5.75	105.75	118.35
47	P	501	NDP	N3A-C2A-N1A	-5.50	120.00	128.60
47	P	501	NDP	C1B-N9A-C8A	5.24	138.97	127.14
47	P	501	NDP	C5A-C4A-N3A	-5.03	120.19	126.75

There are no chirality outliers.

5 of 784 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	B	302	PLC	C4-O4P-P-O1P
43	D	501	PLC	C1'-C'-O2-C2
43	D	501	PLC	O'-C'-O2-C2
43	H	401	PLC	C4-O4P-P-O1P
43	L	701	PLC	C2-C1-O3P-P

There are no ring outliers.

44 monomers are involved in 113 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	L	701	PLC	6	0
45	L	704	3PE	2	0
43	L	709	PLC	3	0
45	N	601	3PE	1	0
43	Y	302	PLC	2	0
43	d	102	PLC	1	0
45	h	201	3PE	5	0
43	L	708	PLC	4	0
45	j	101	3PE	4	0
47	P	501	NDP	2	0
45	M	502	3PE	1	0
43	M	503	PLC	2	0
45	L	703	3PE	3	0

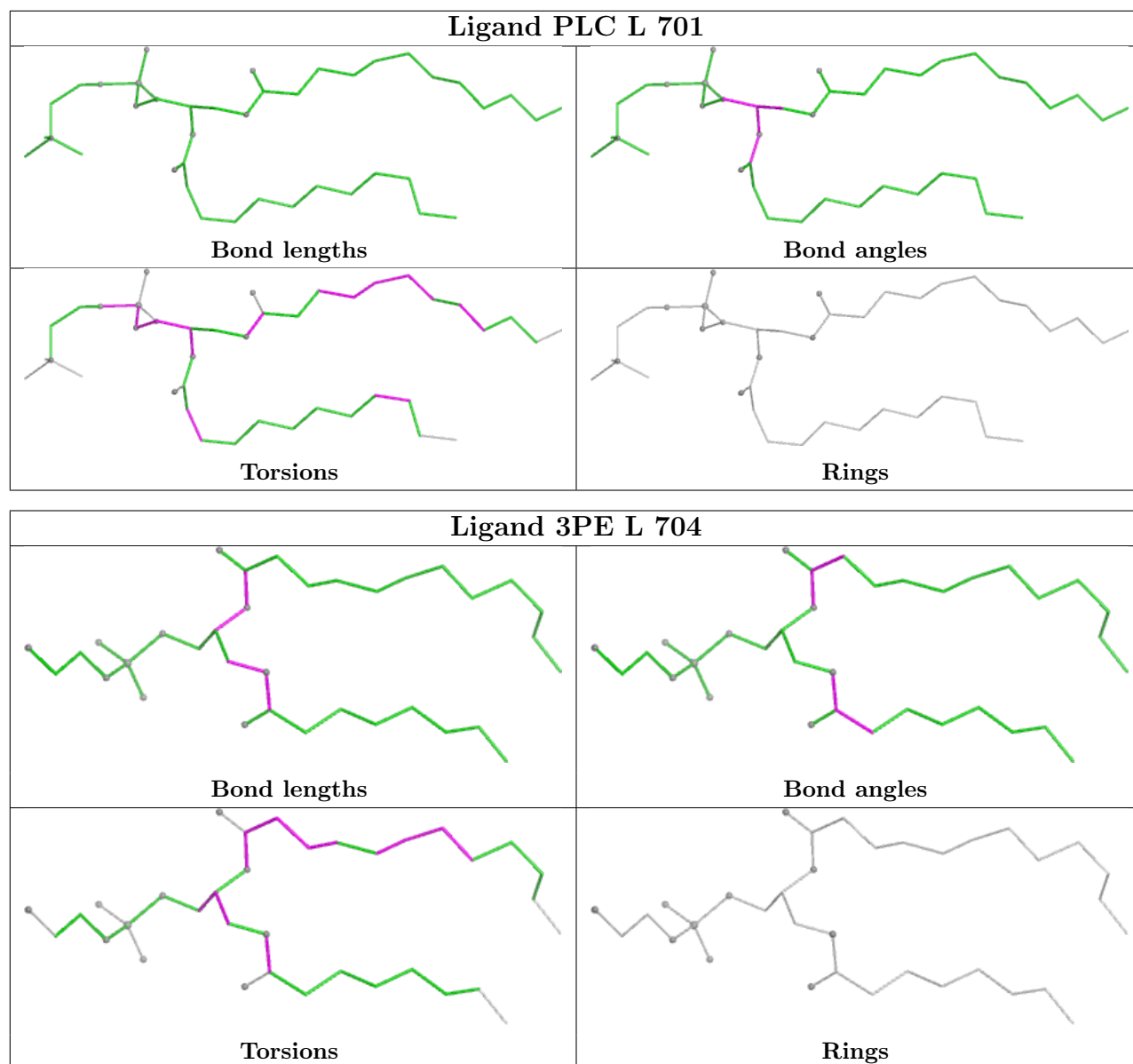
Continued on next page...

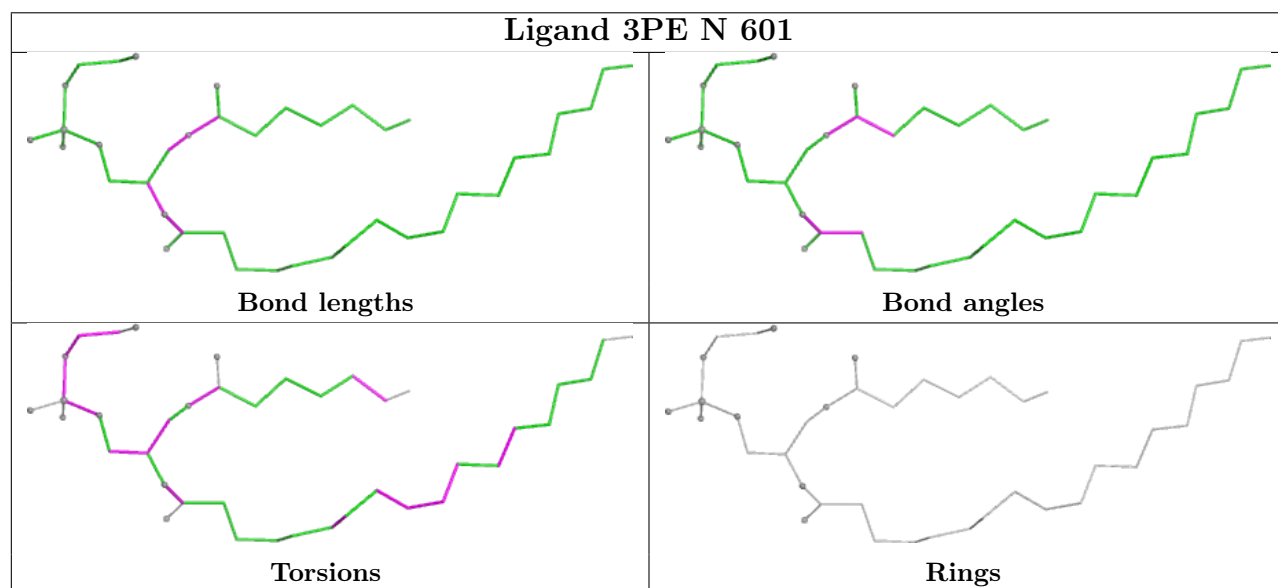
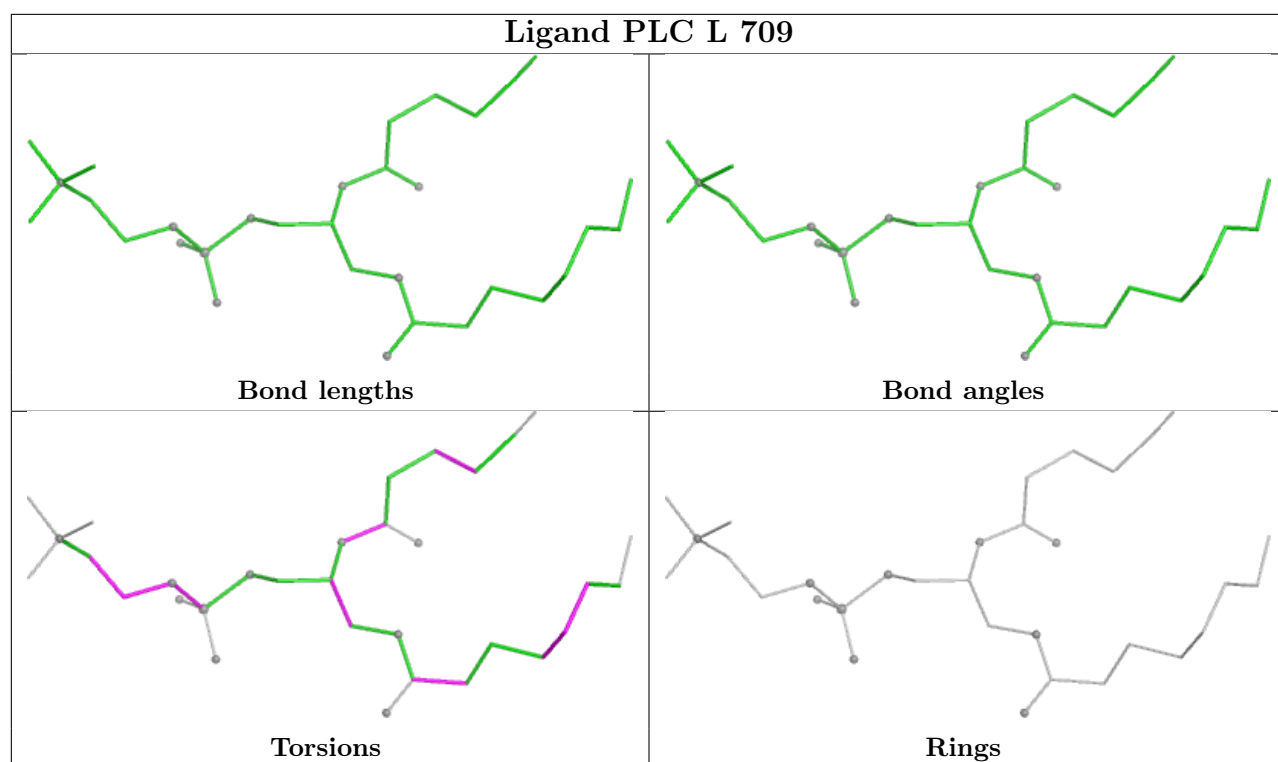
Continued from previous page...

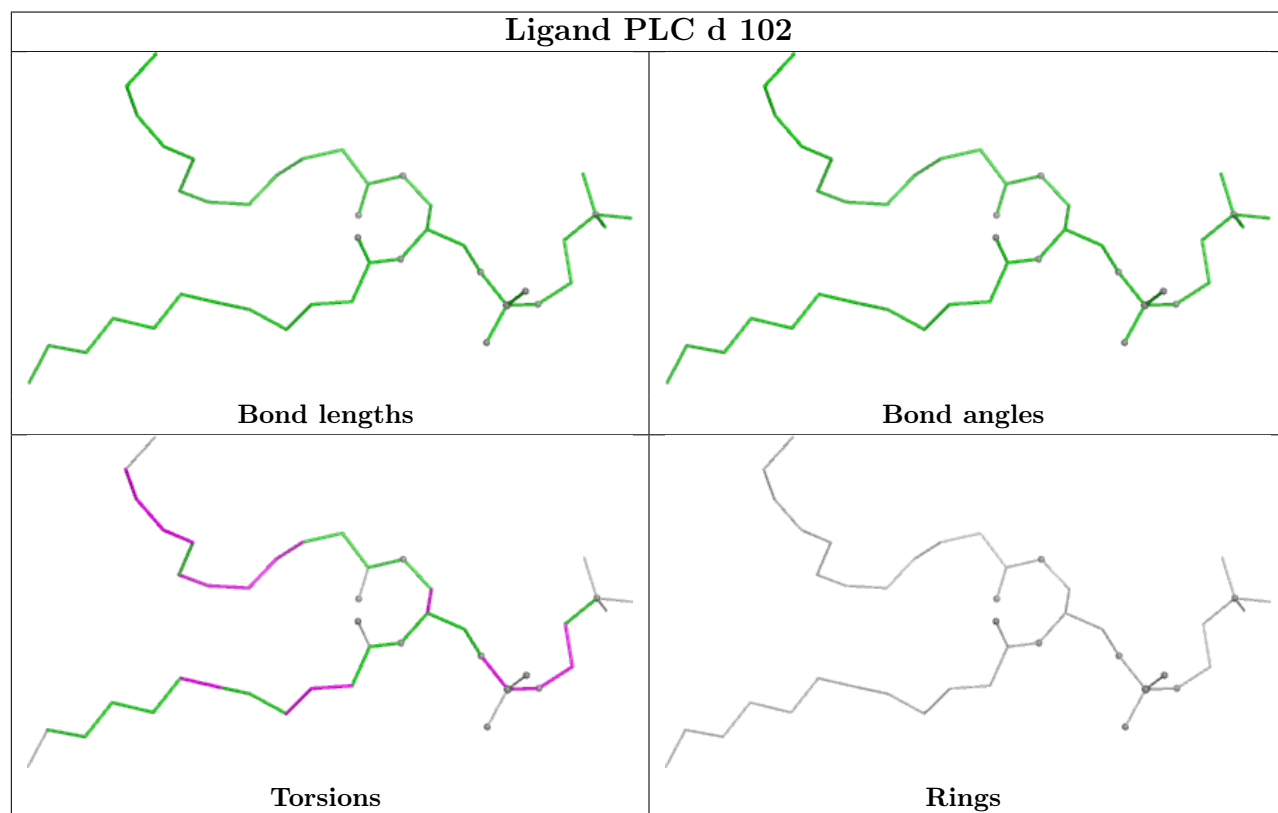
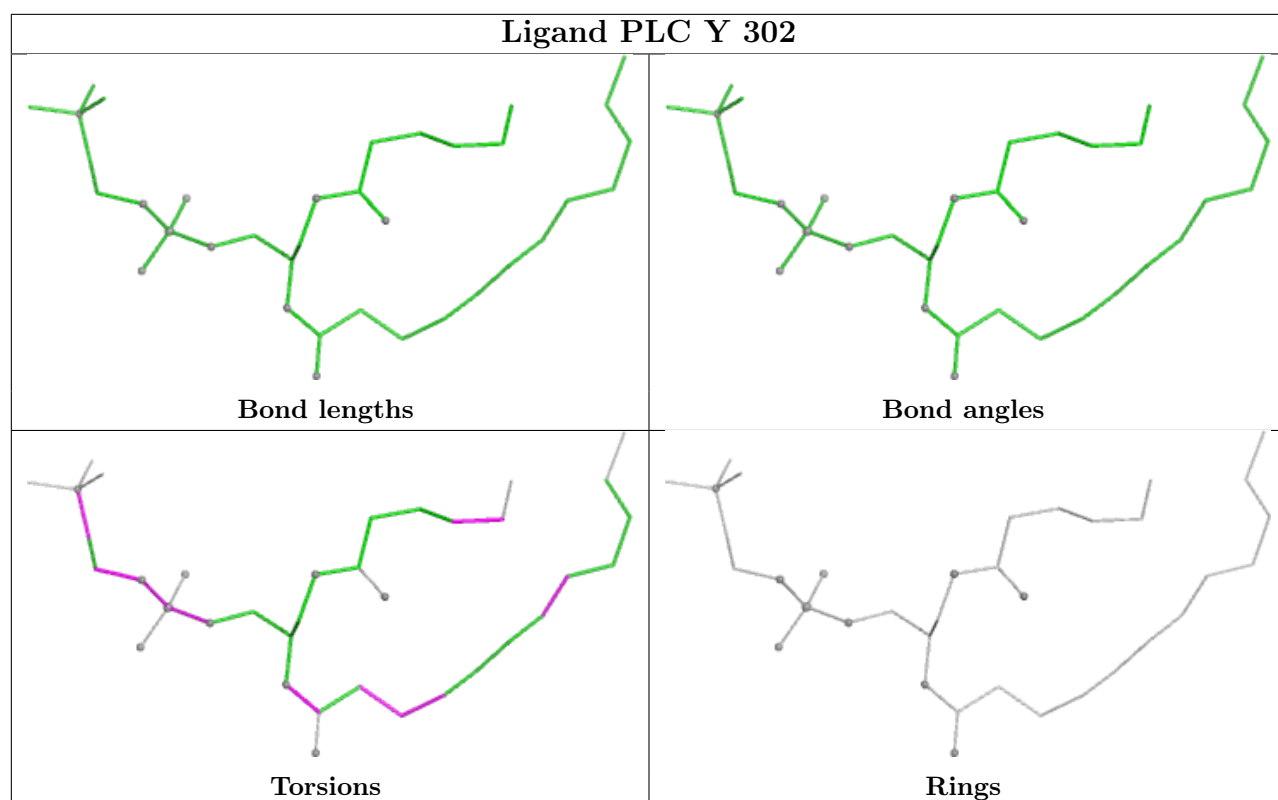
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	m	101	3PE	4	0
46	q	203	CDL	5	0
43	g	301	PLC	5	0
46	Z	203	CDL	1	0
45	Z	201	3PE	1	0
45	J	201	3PE	4	0
46	O	201	CDL	3	0
46	b	102	CDL	3	0
43	M	504	PLC	2	0
43	B	302	PLC	3	0
42	G	802	SF4	2	0
43	d	101	PLC	2	0
43	q	202	PLC	2	0
43	Y	303	PLC	2	0
42	I	302	SF4	2	0
42	G	801	SF4	4	0
45	L	706	3PE	5	0
45	M	501	3PE	5	0
43	Z	202	PLC	3	0
43	P	502	PLC	2	0
42	B	301	SF4	1	0
43	q	201	PLC	4	0
45	L	702	3PE	6	0
45	b	103	3PE	2	0
45	L	705	3PE	4	0
43	D	501	PLC	3	0
45	b	104	3PE	1	0
42	I	301	SF4	1	0
45	Y	301	3PE	1	0
43	P	503	PLC	1	0
49	U	201	EHZ	2	0

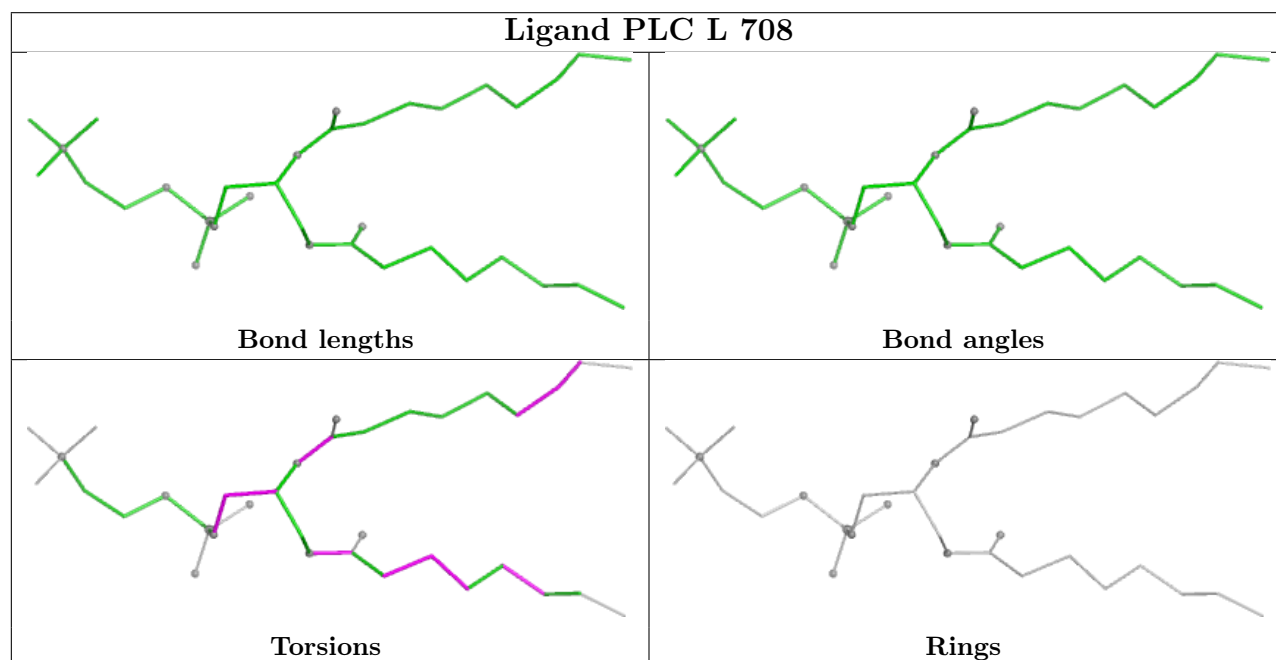
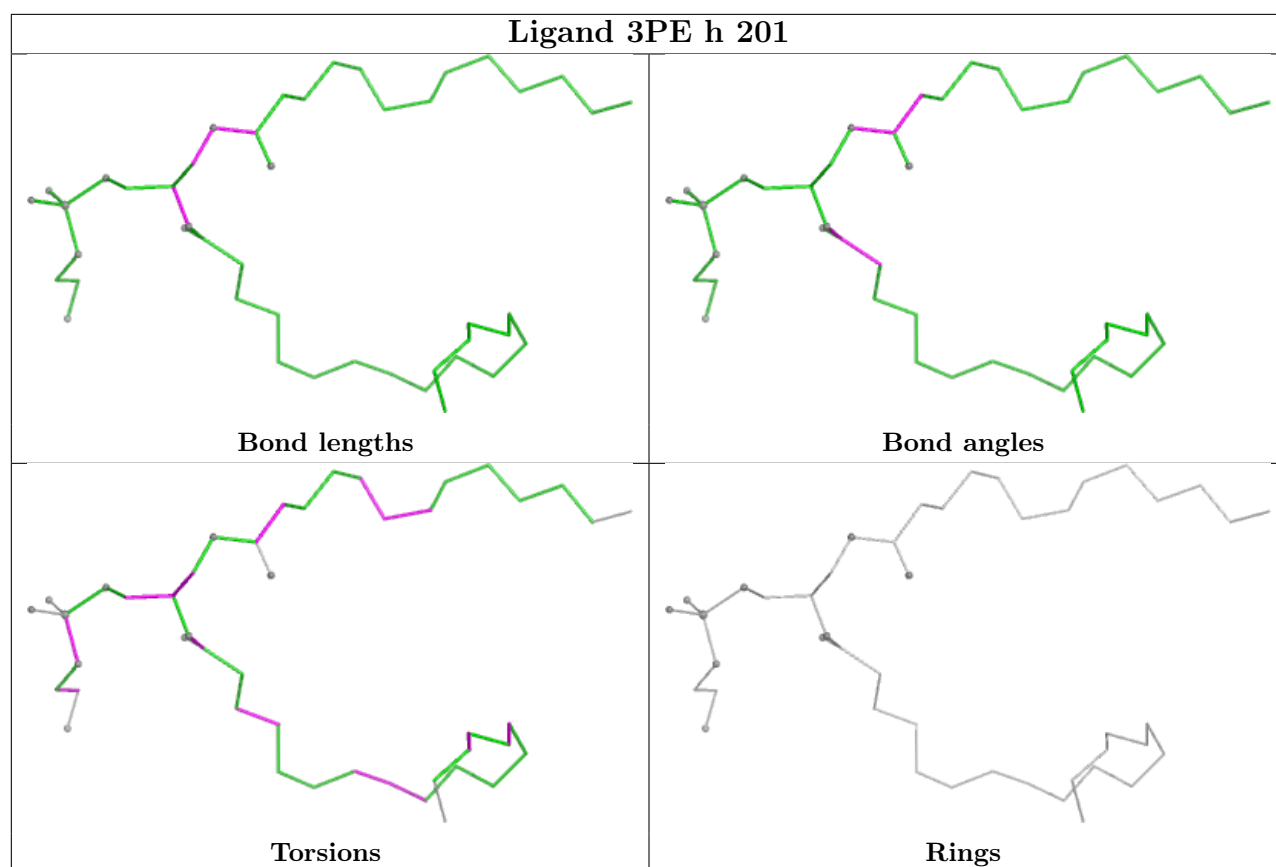
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

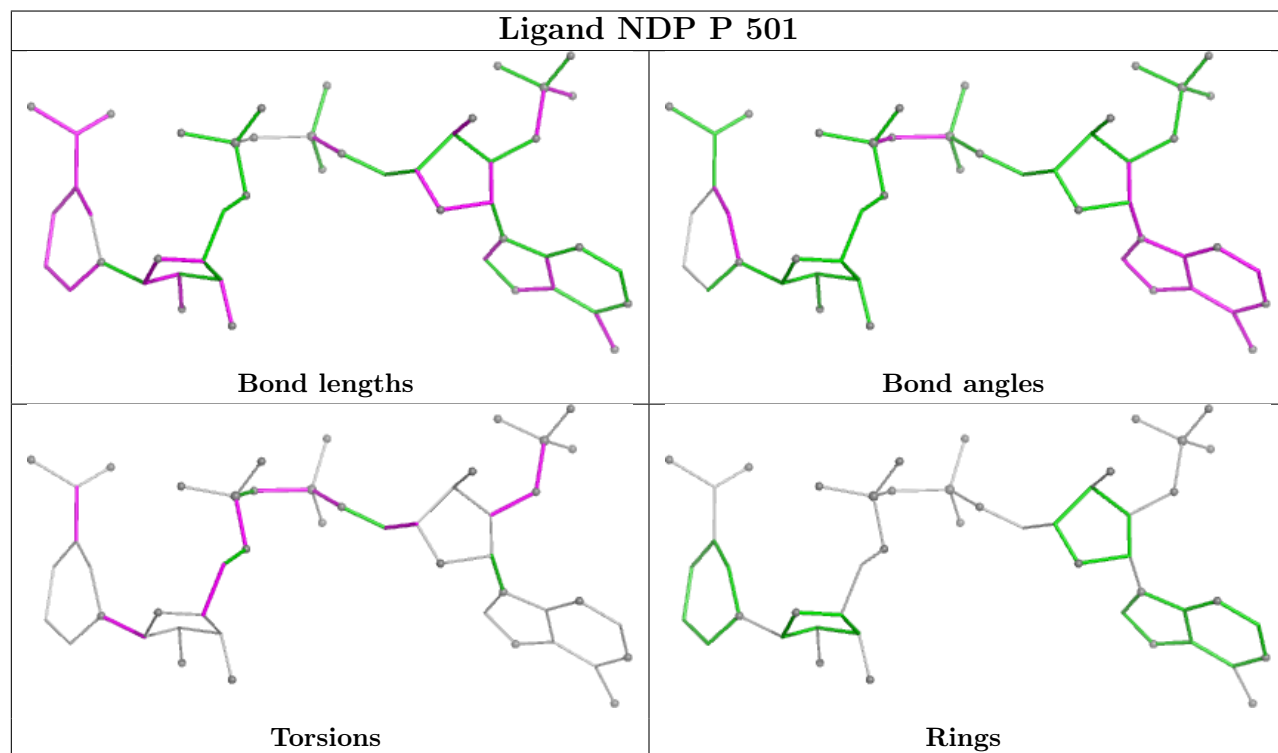
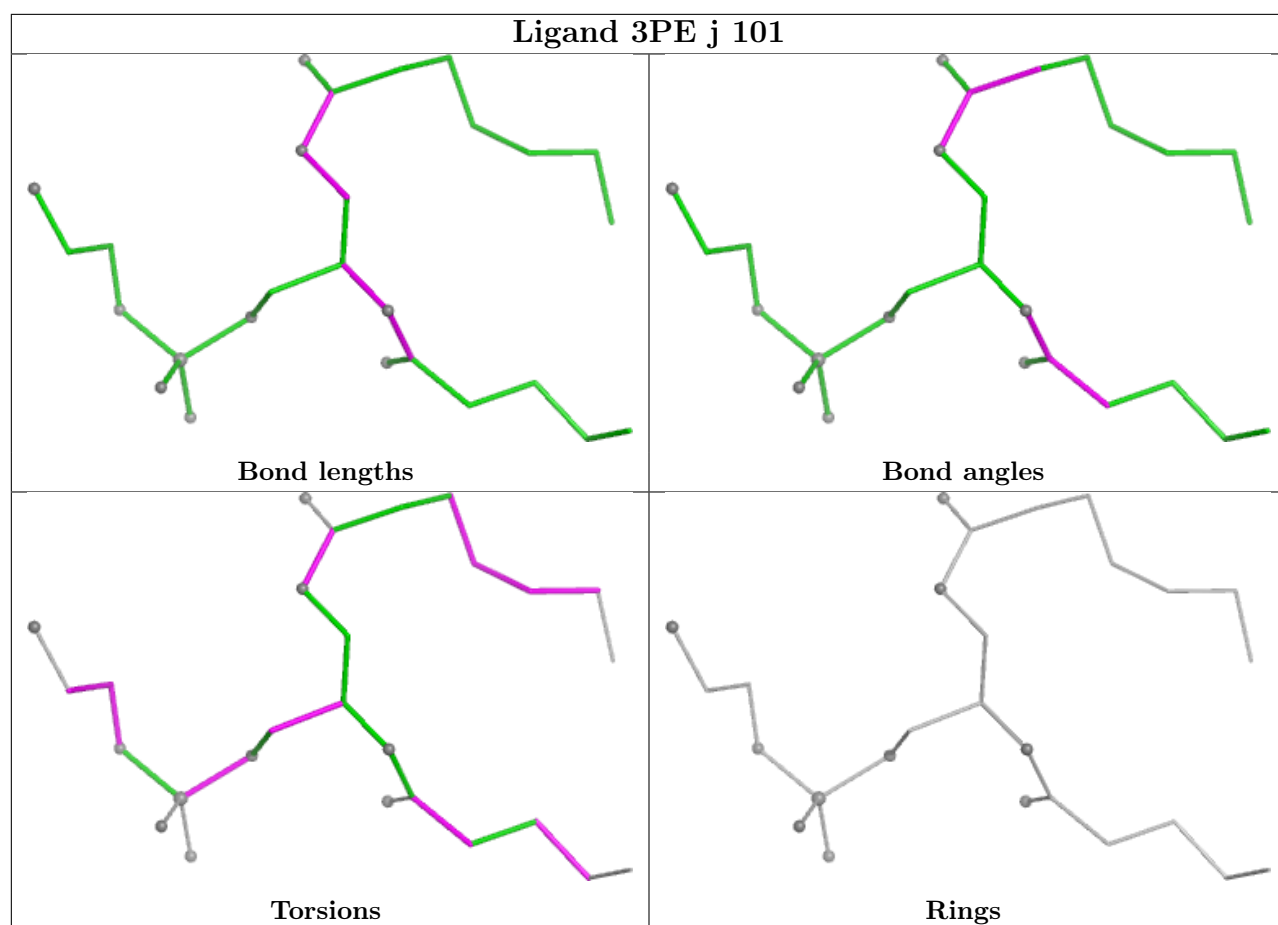
equivalents in the CSD to analyse the geometry.

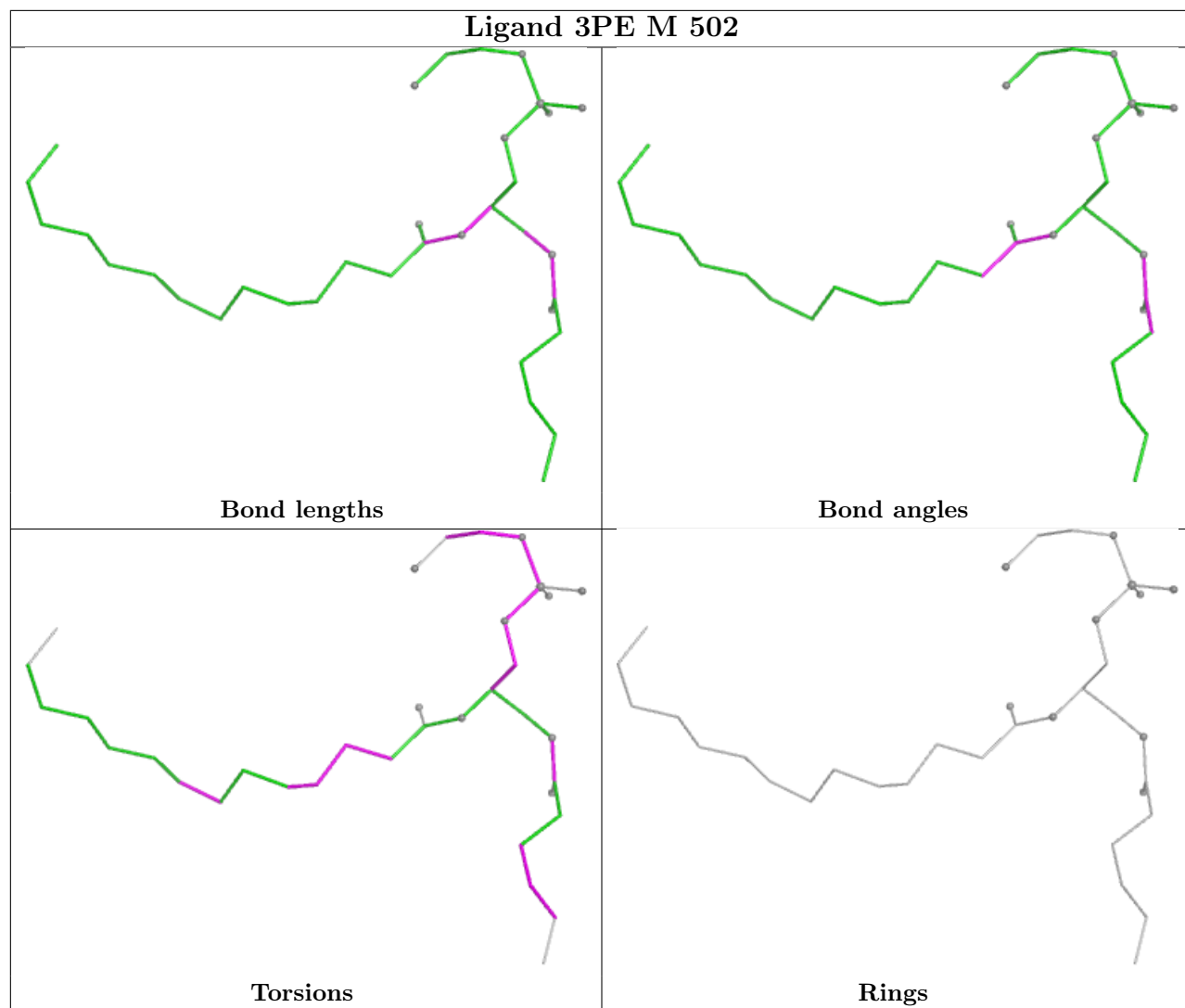


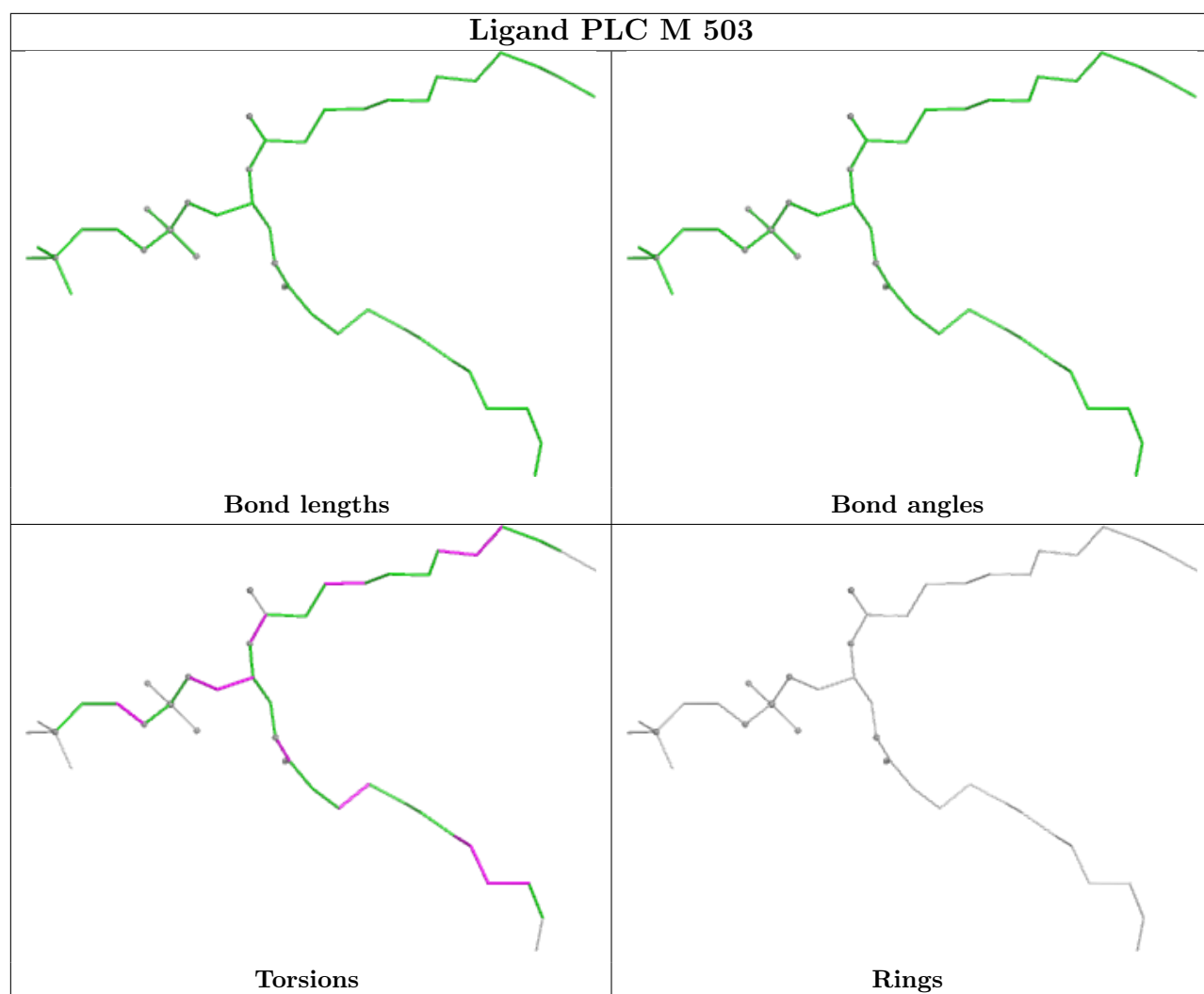


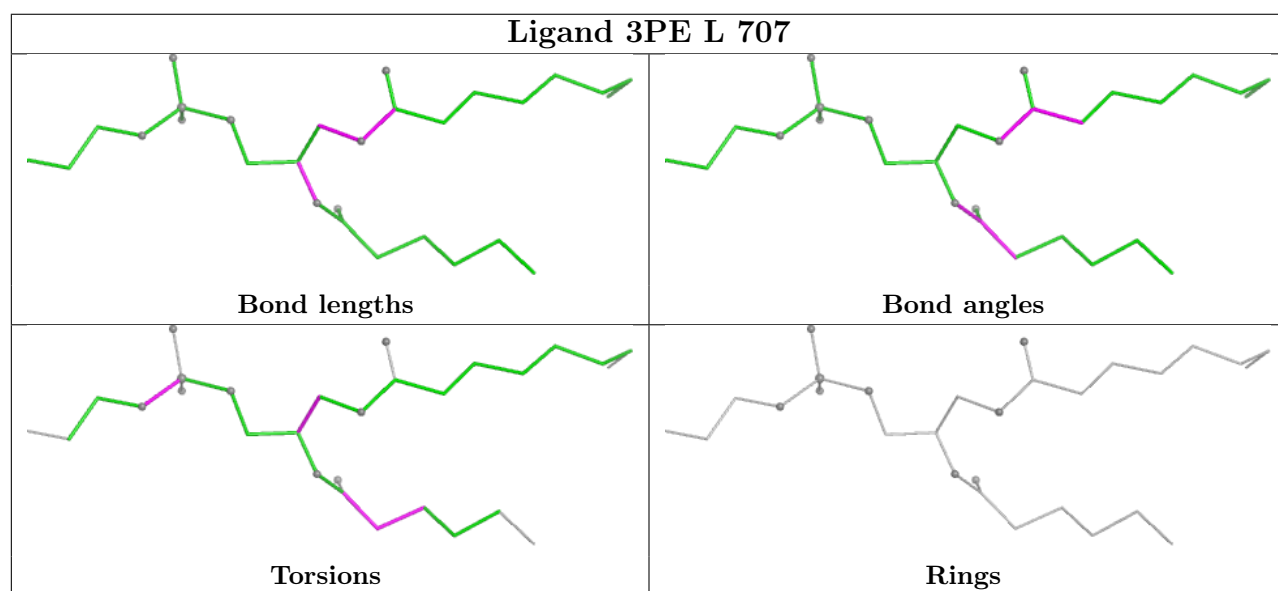
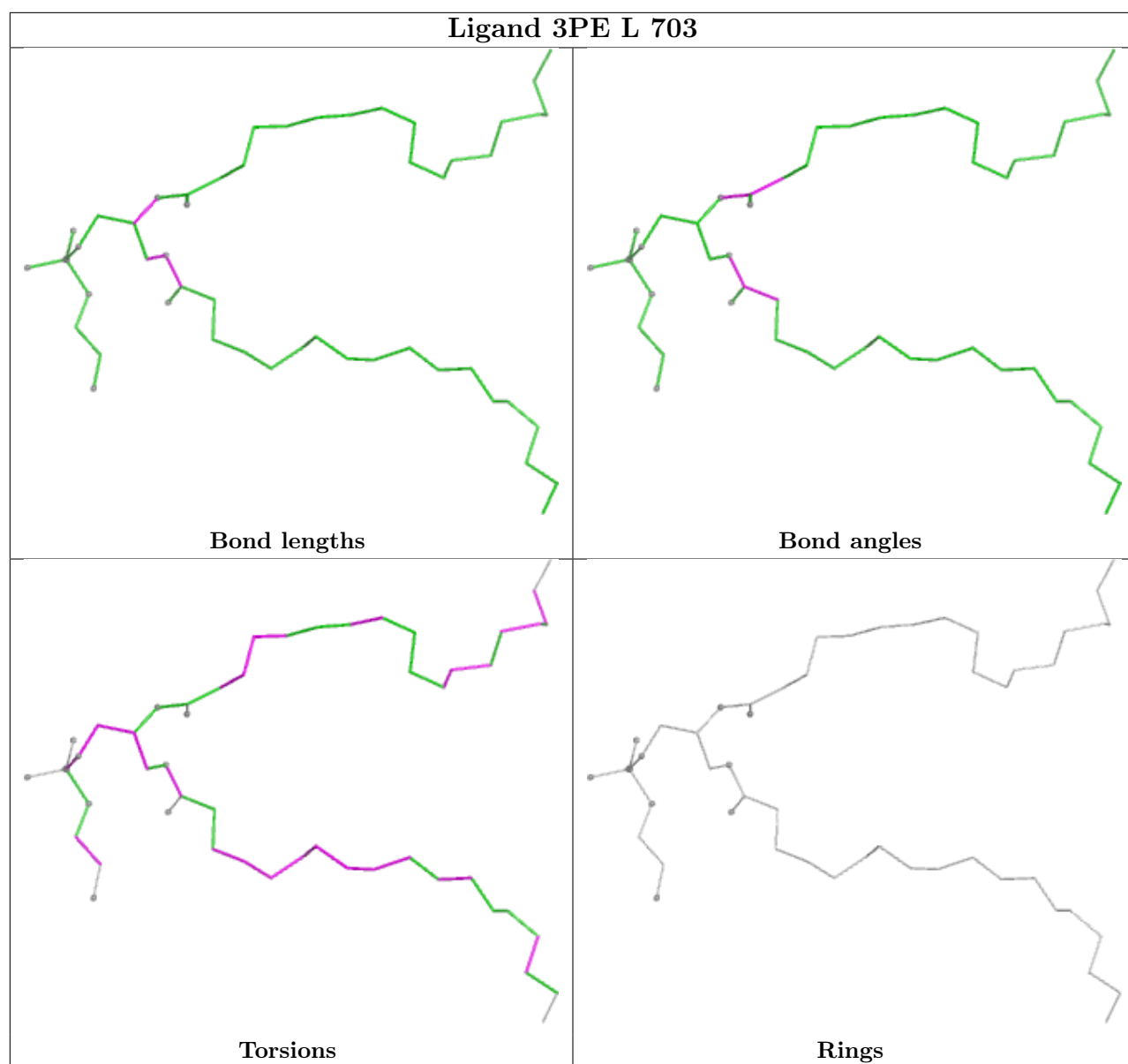


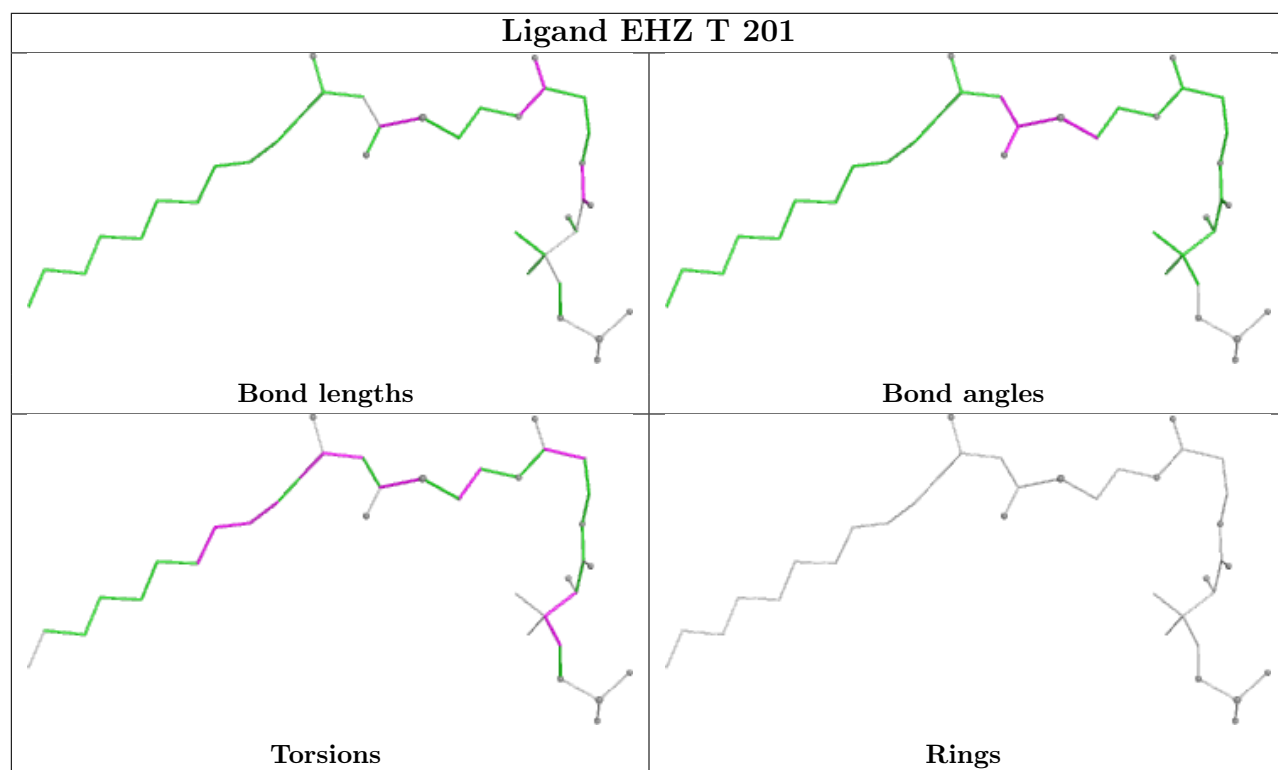
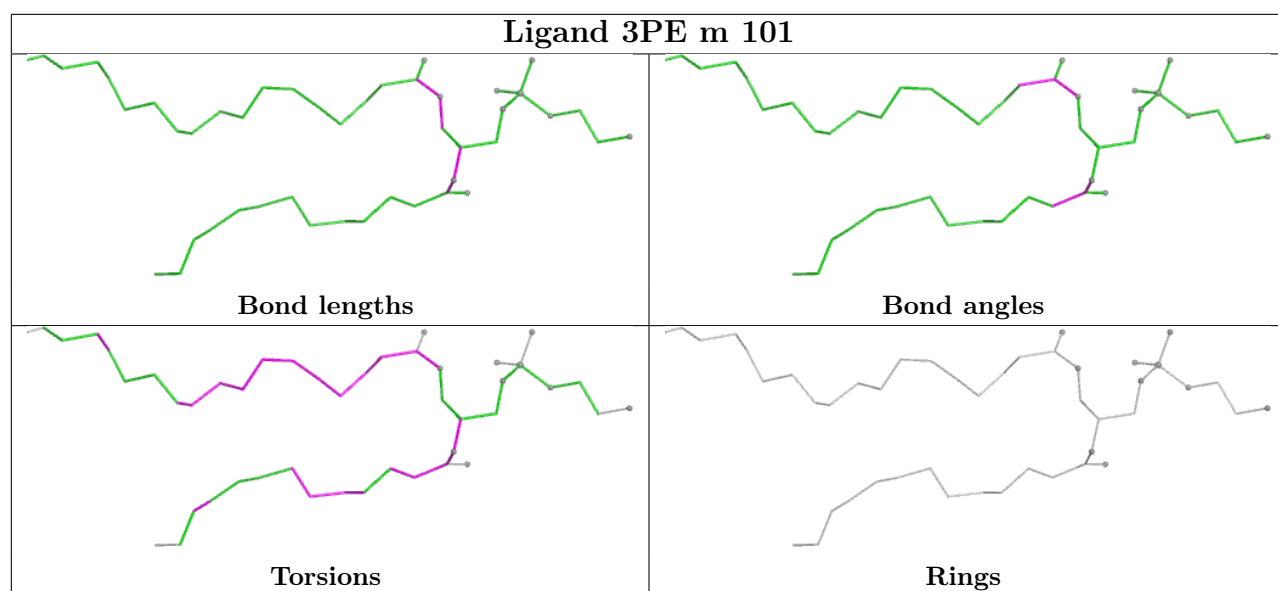


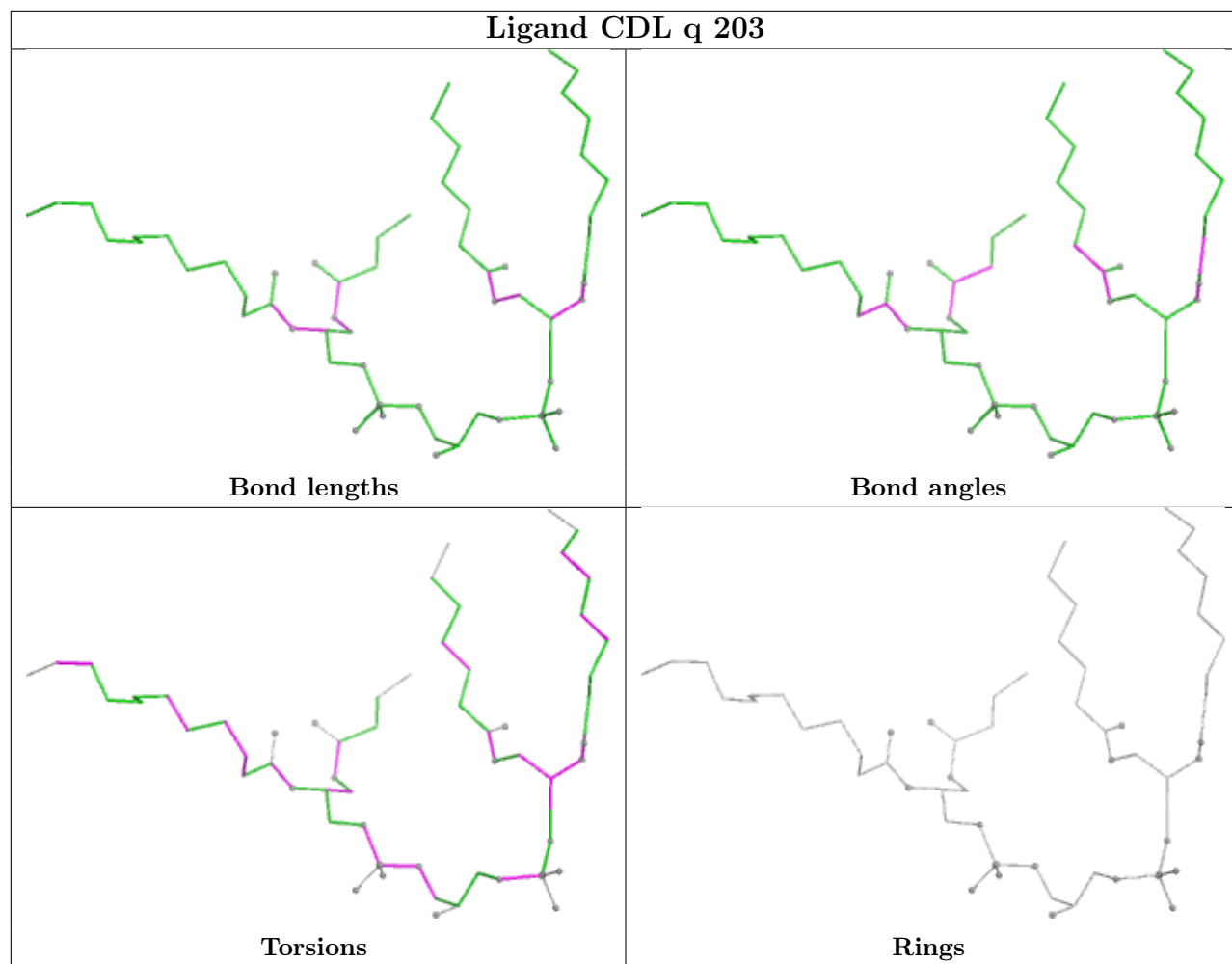


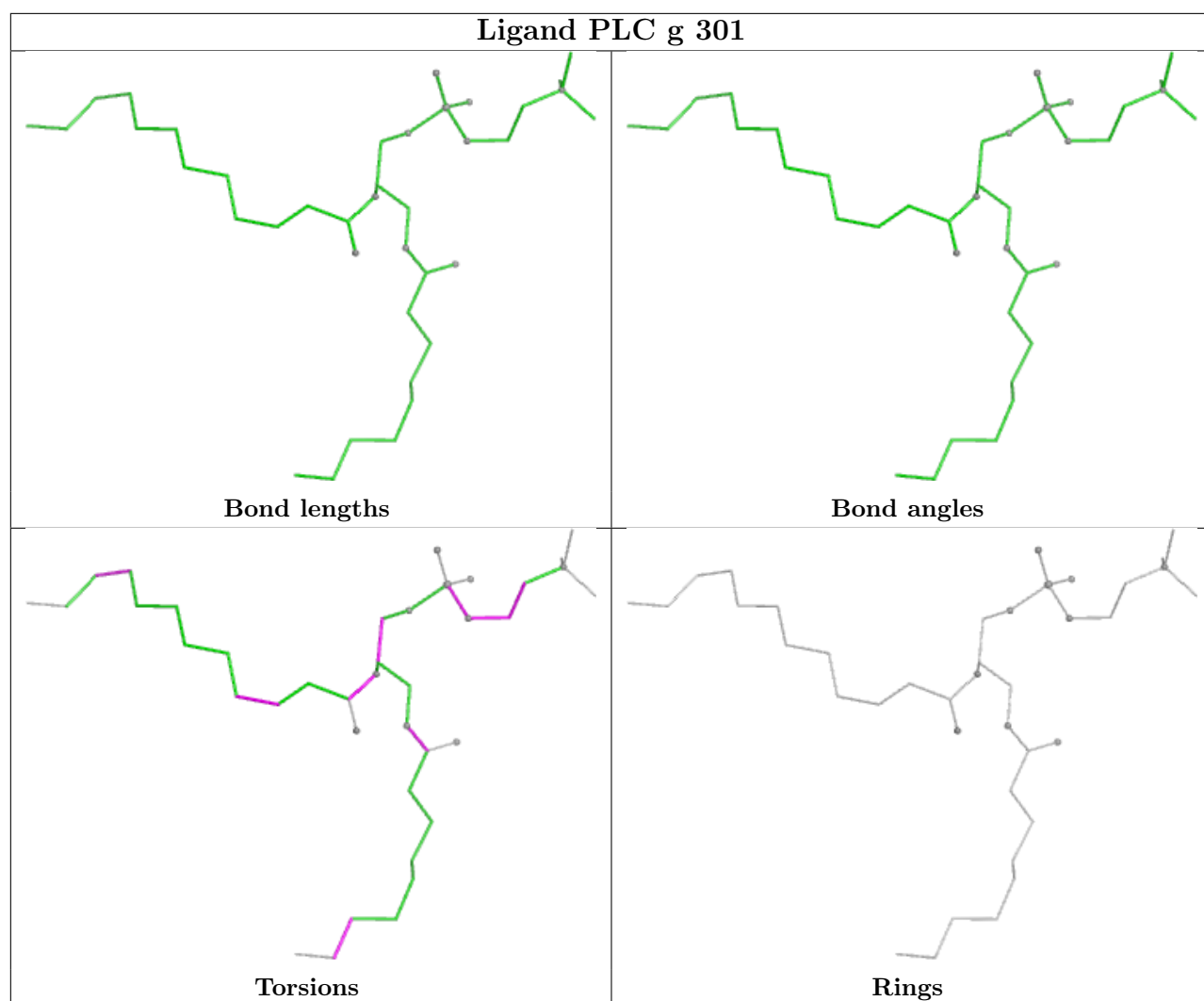


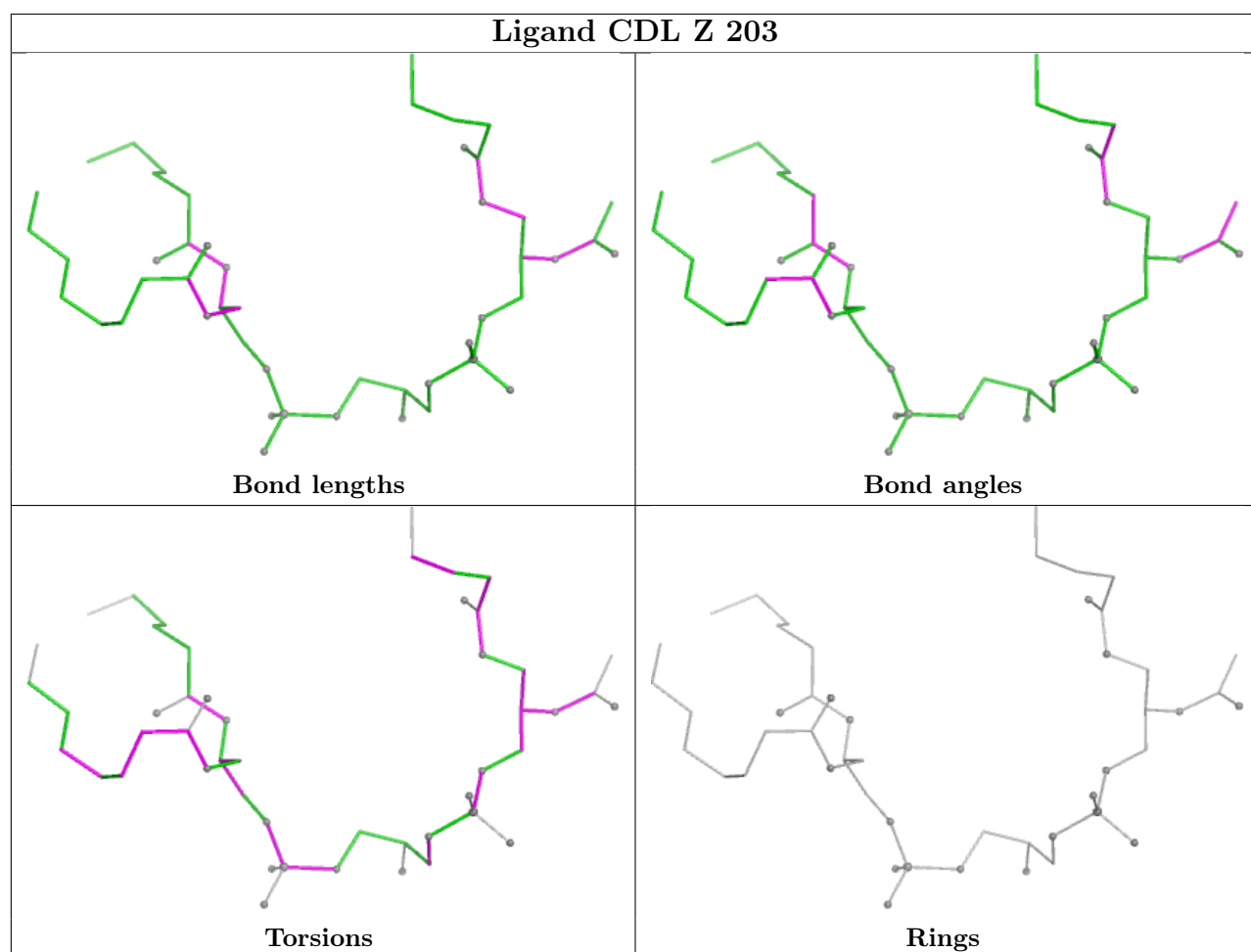


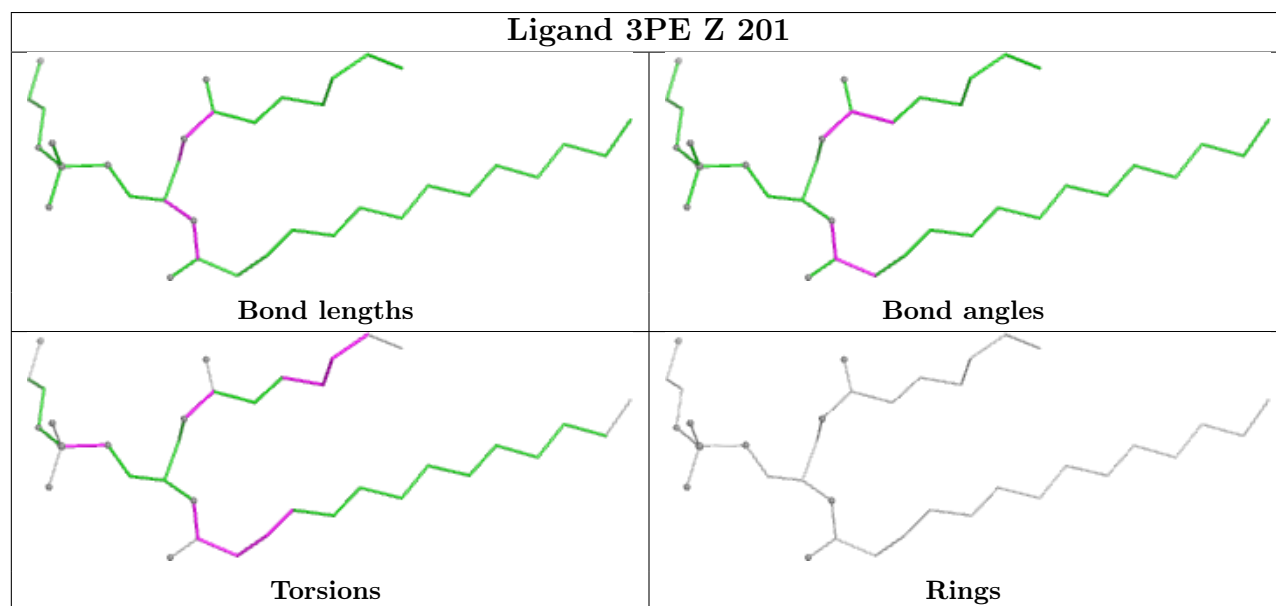
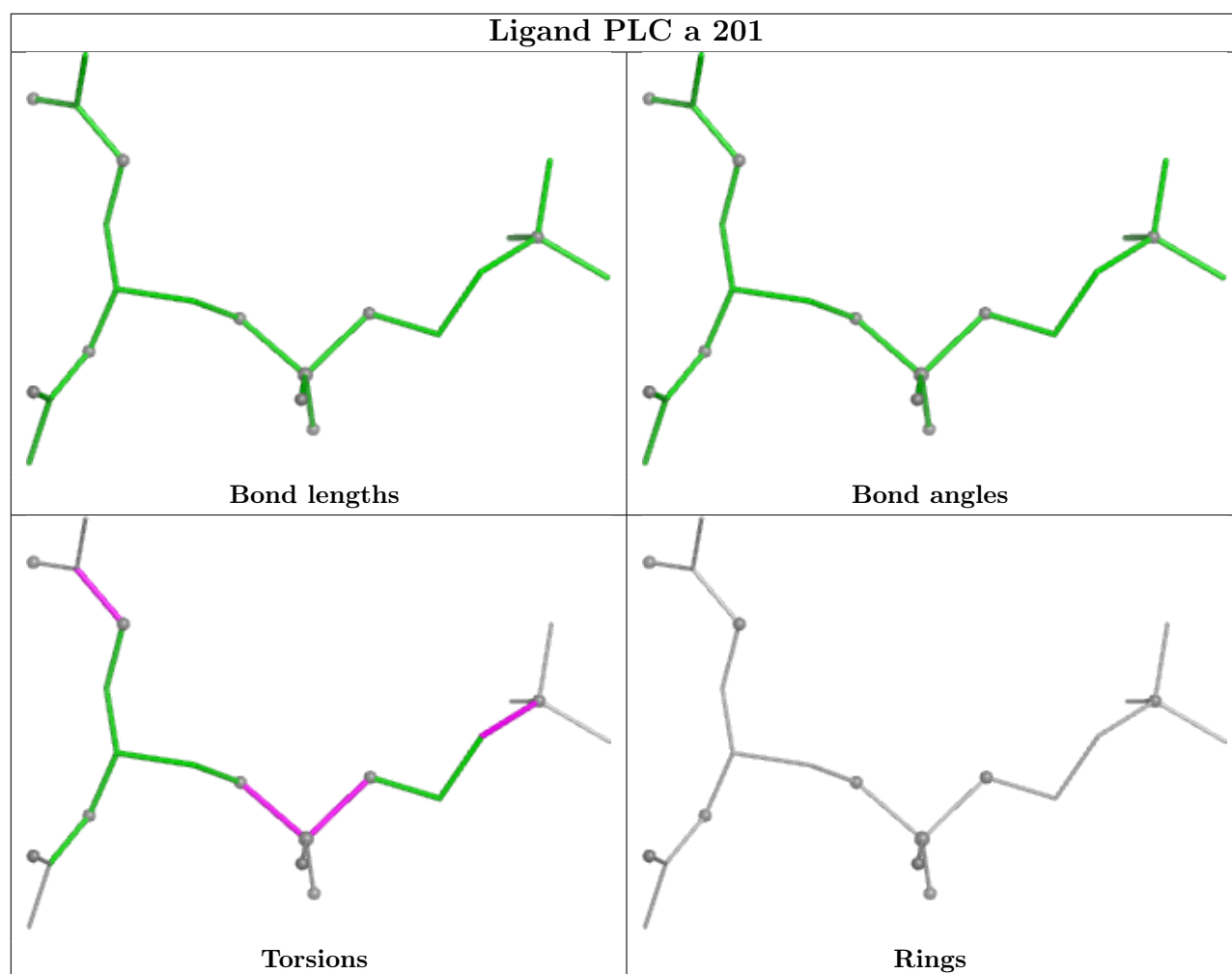


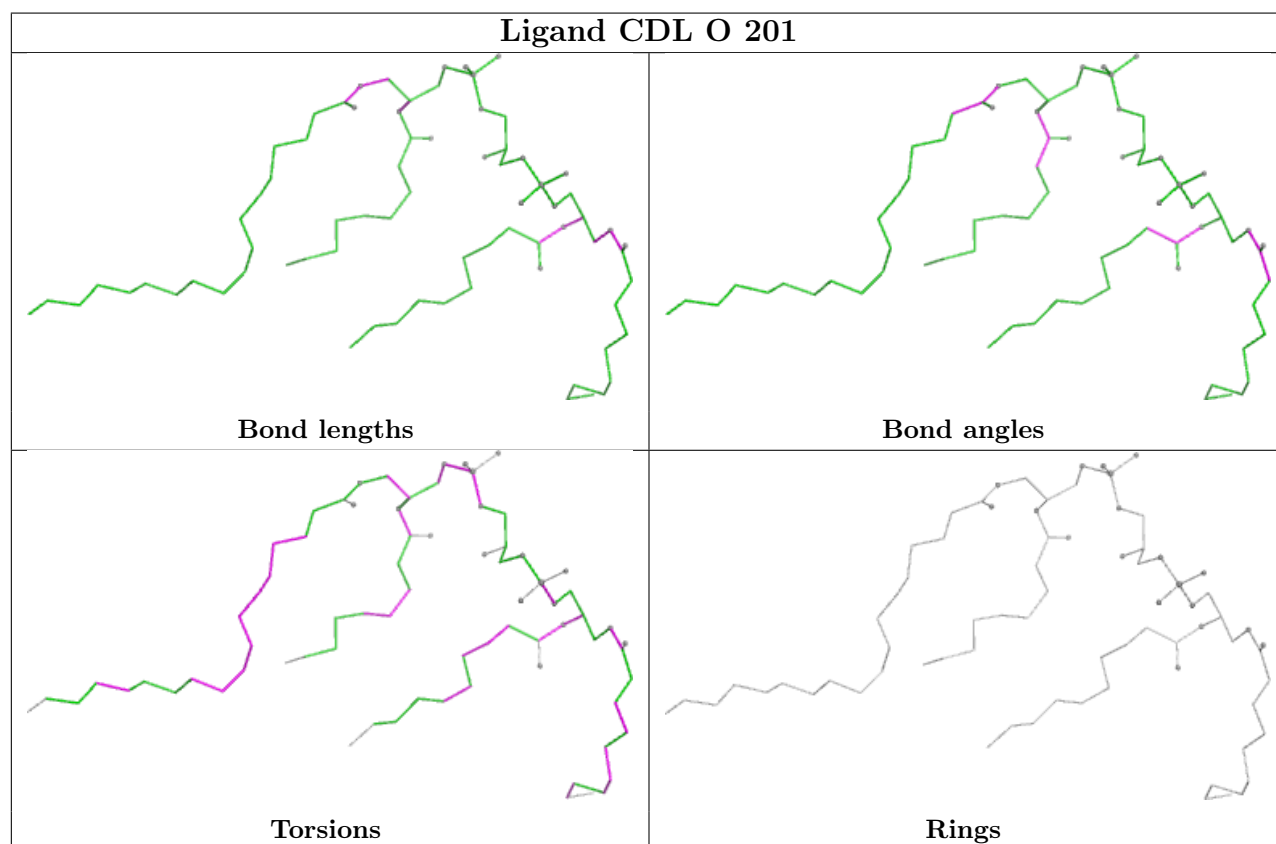
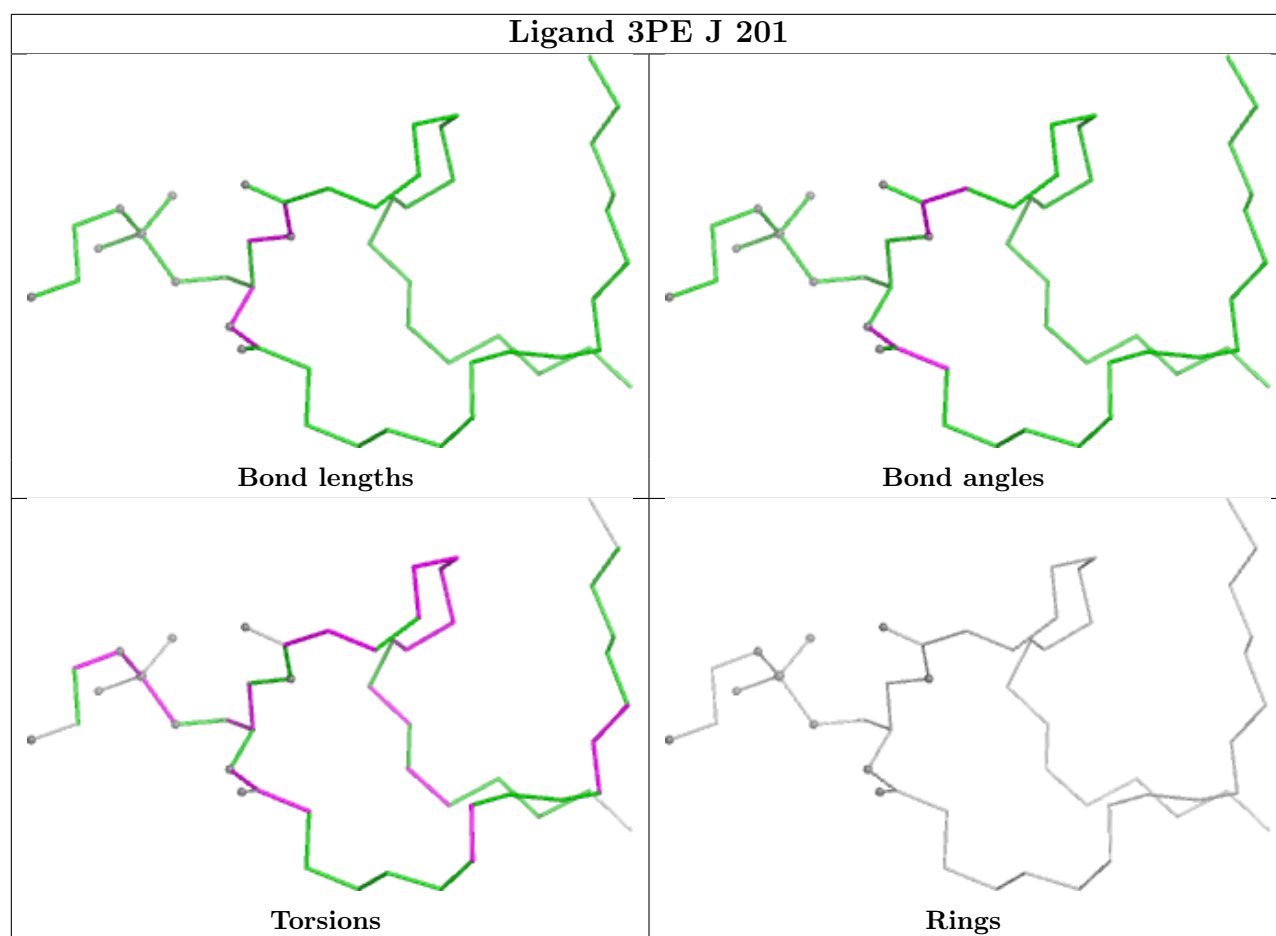


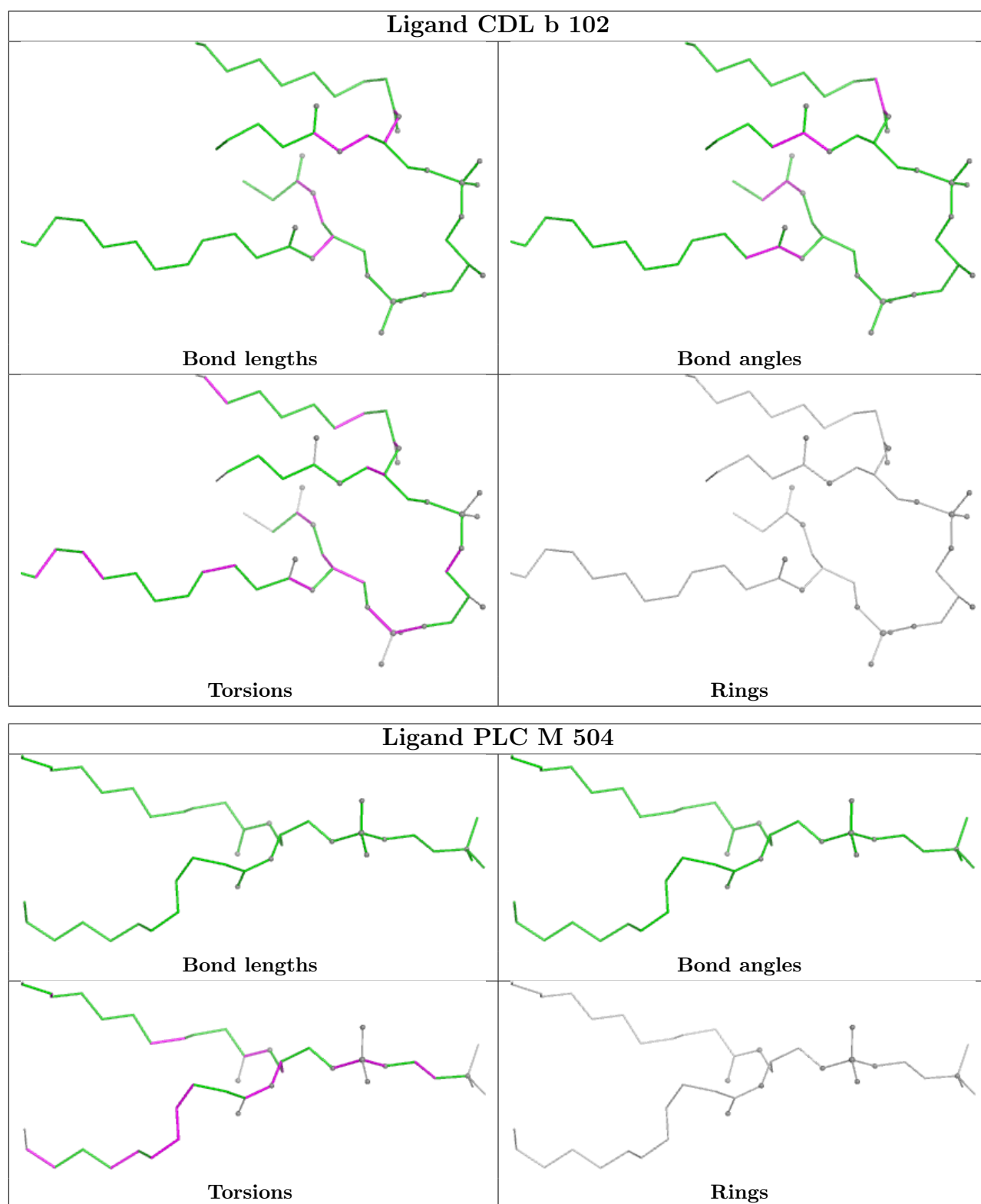


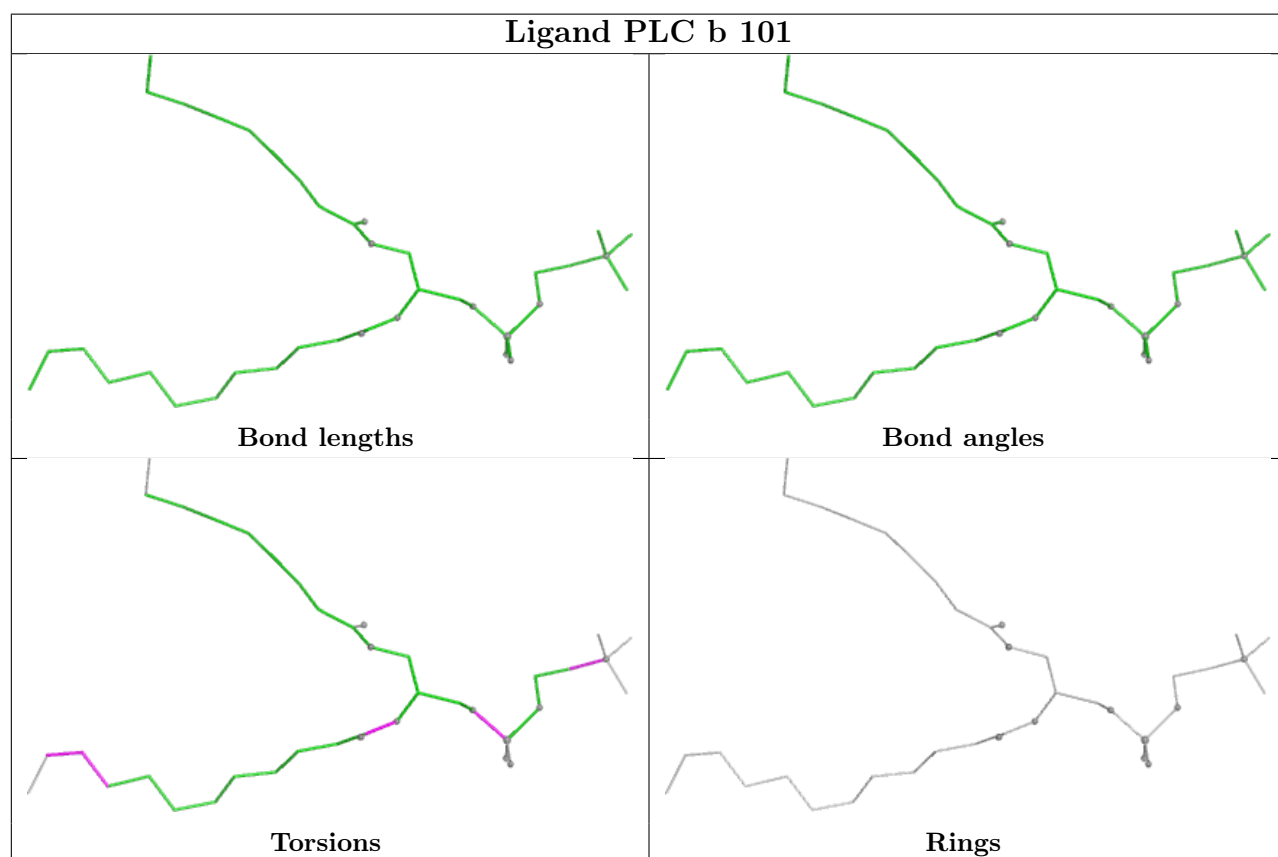
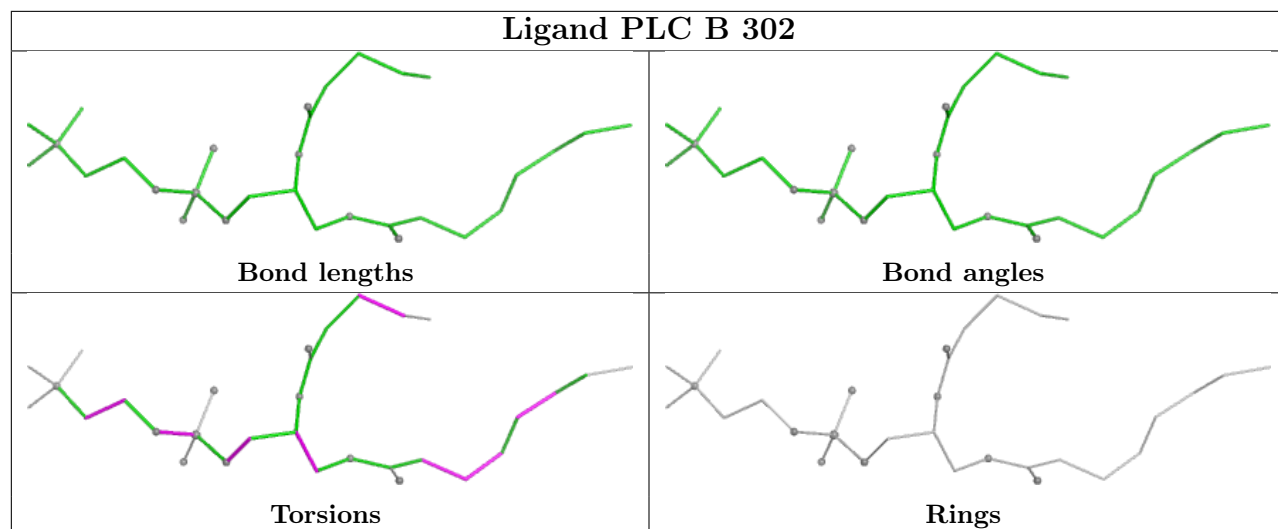


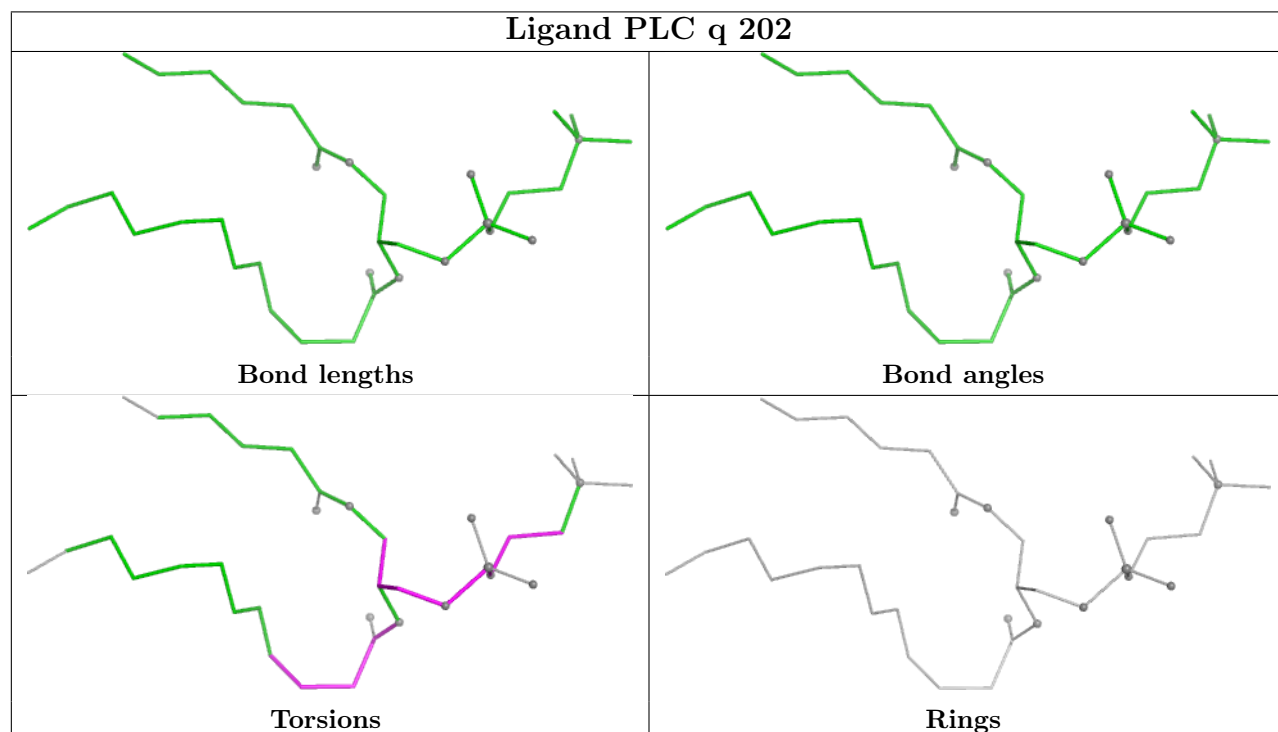
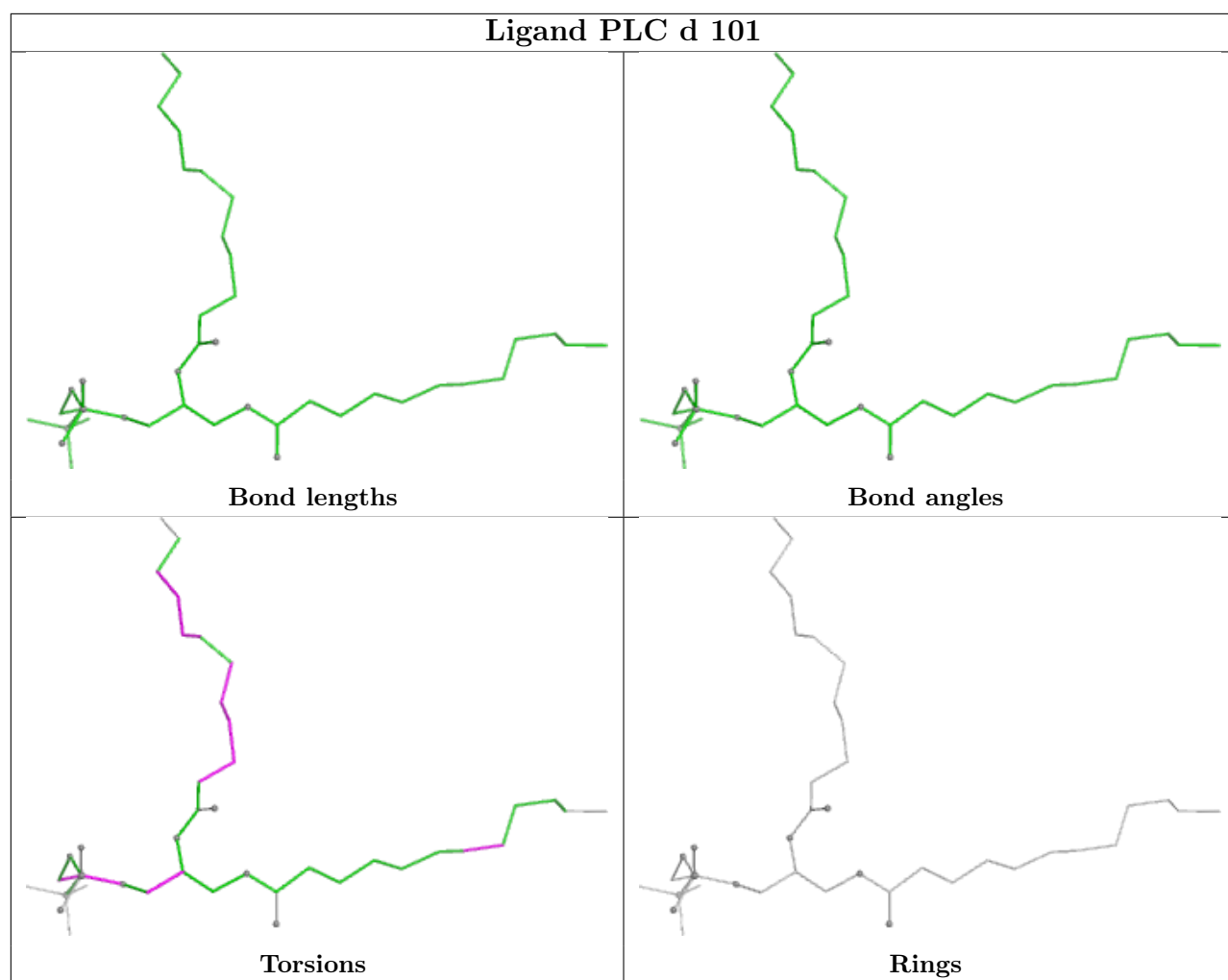




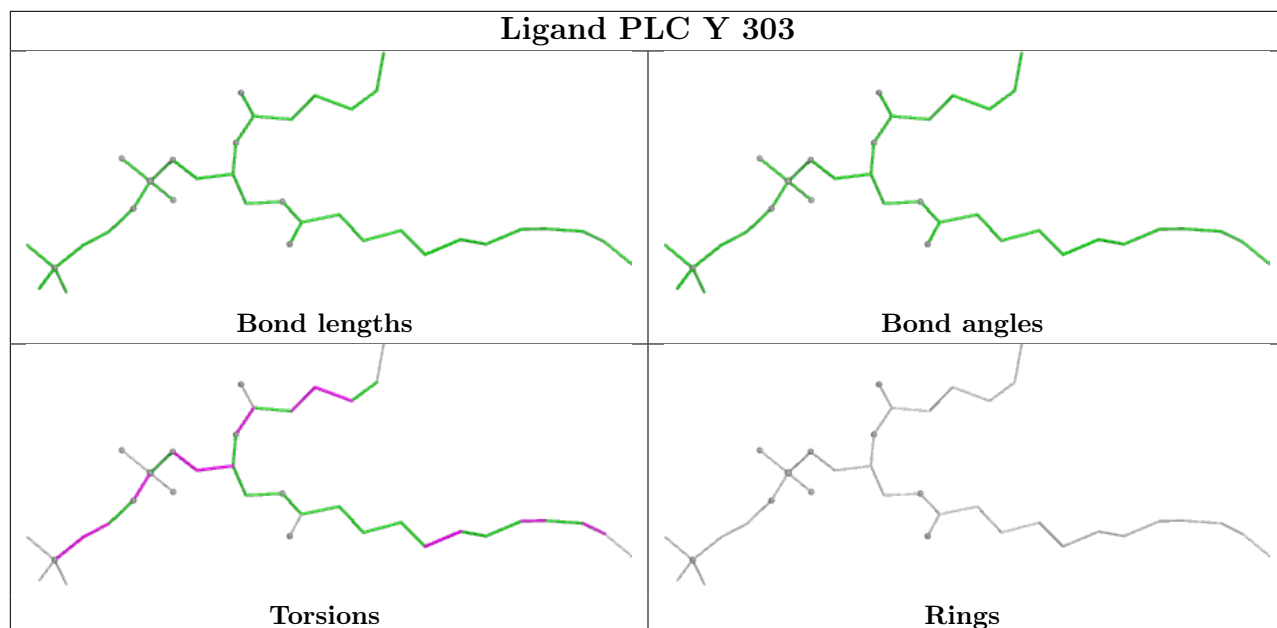




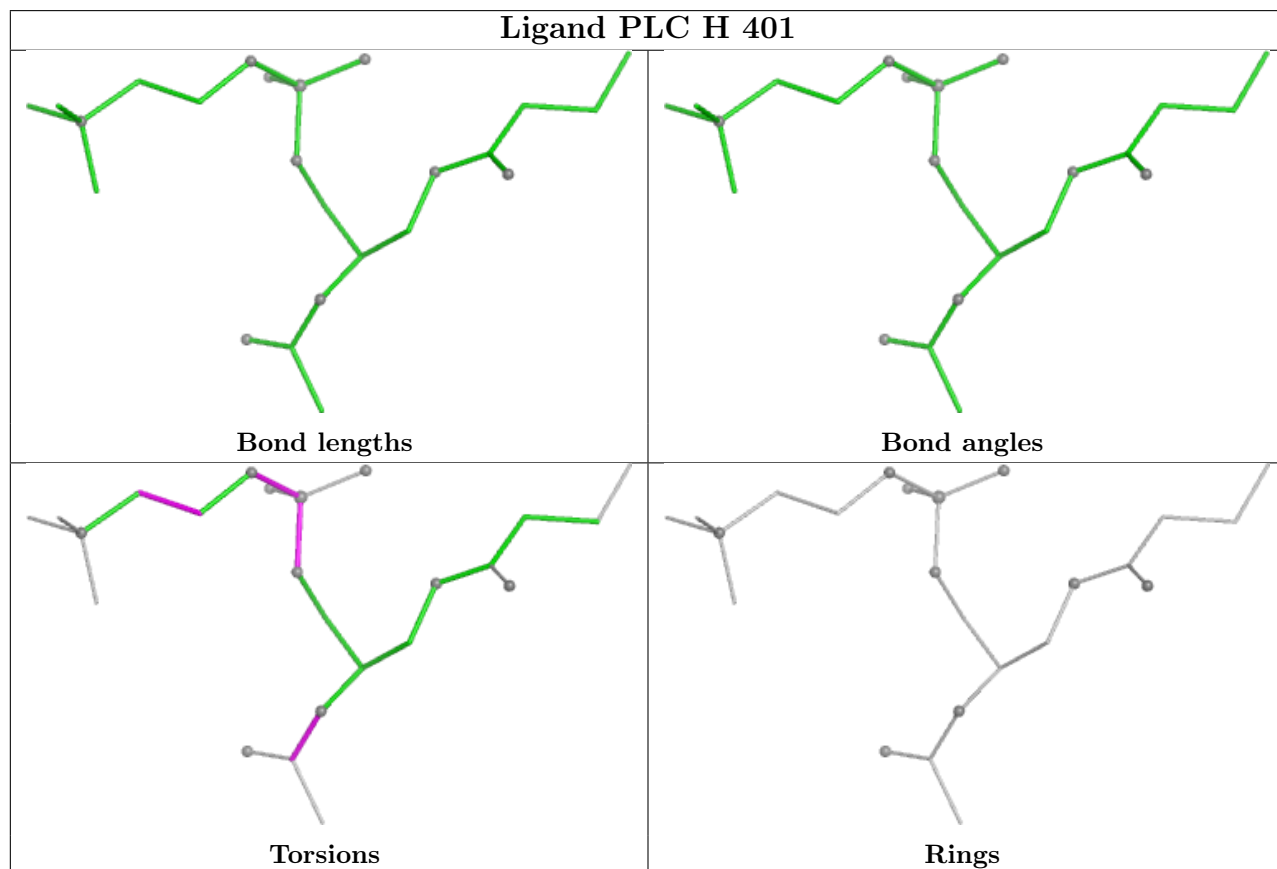


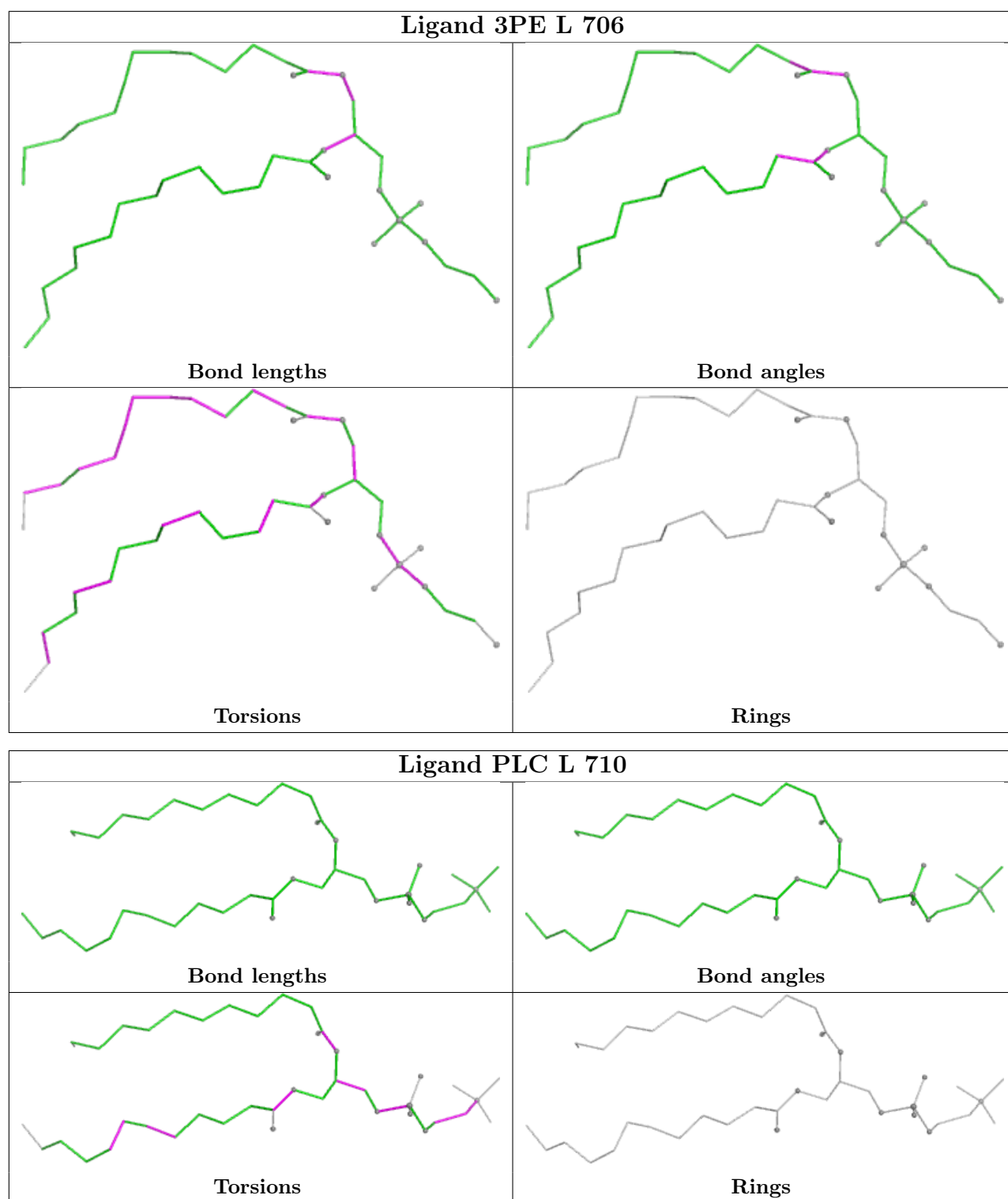


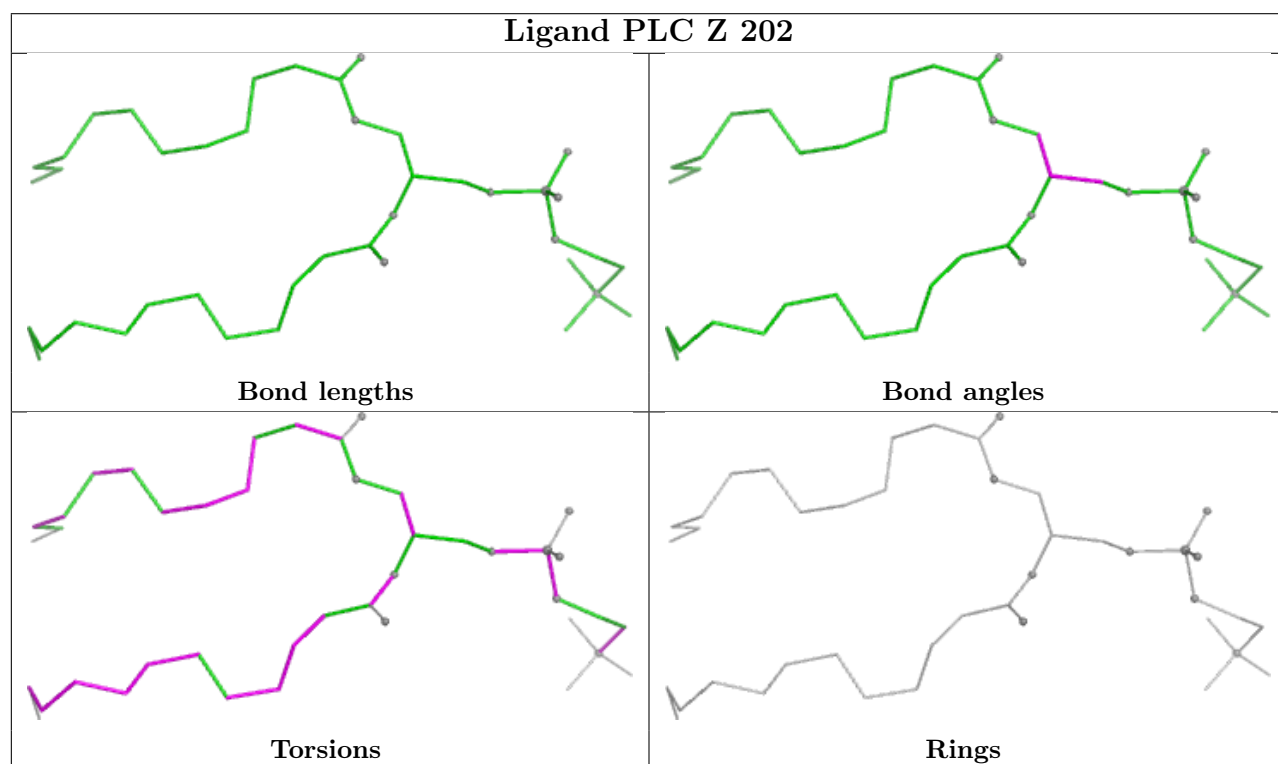
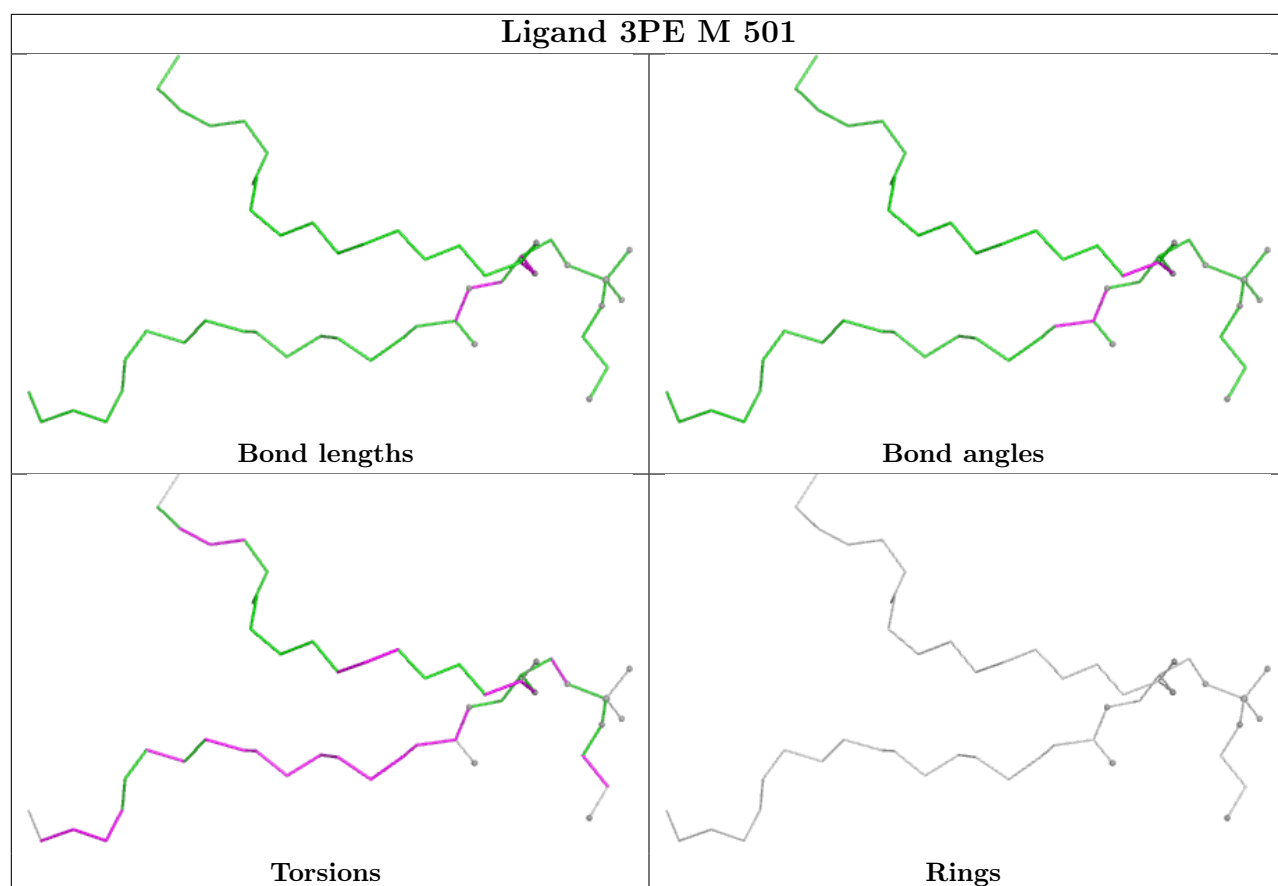
Ligand PLC Y 303

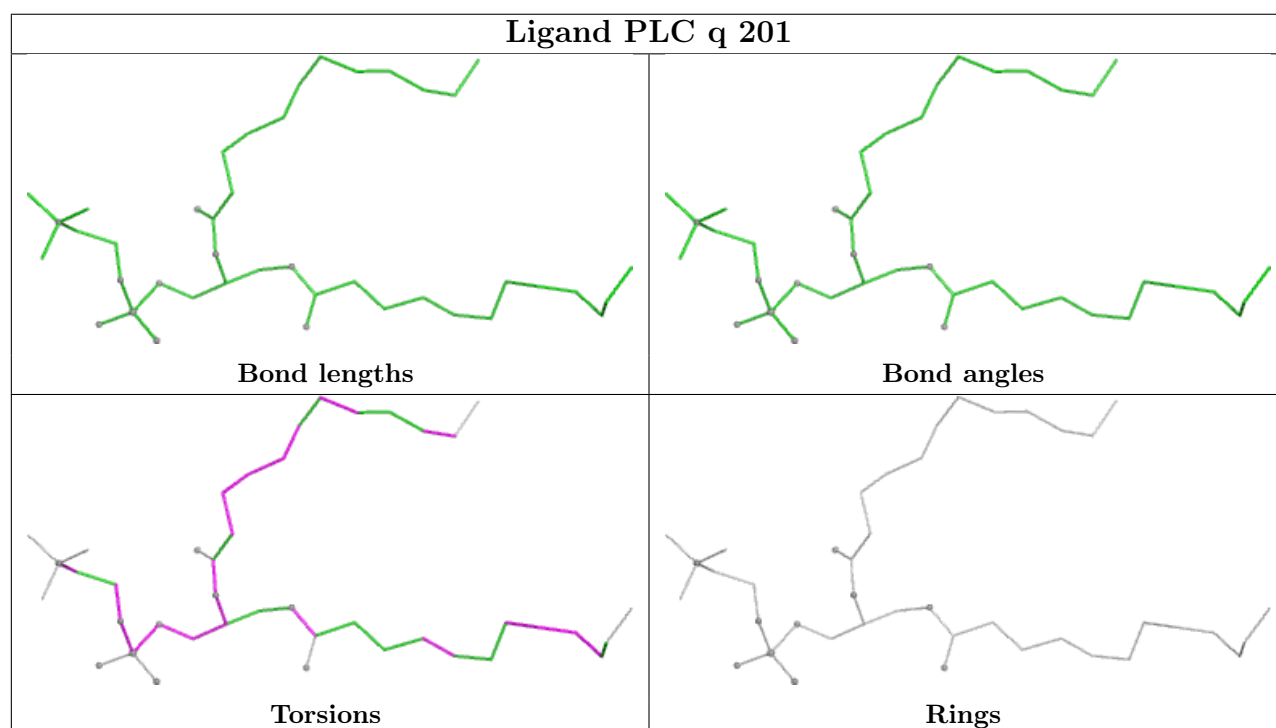
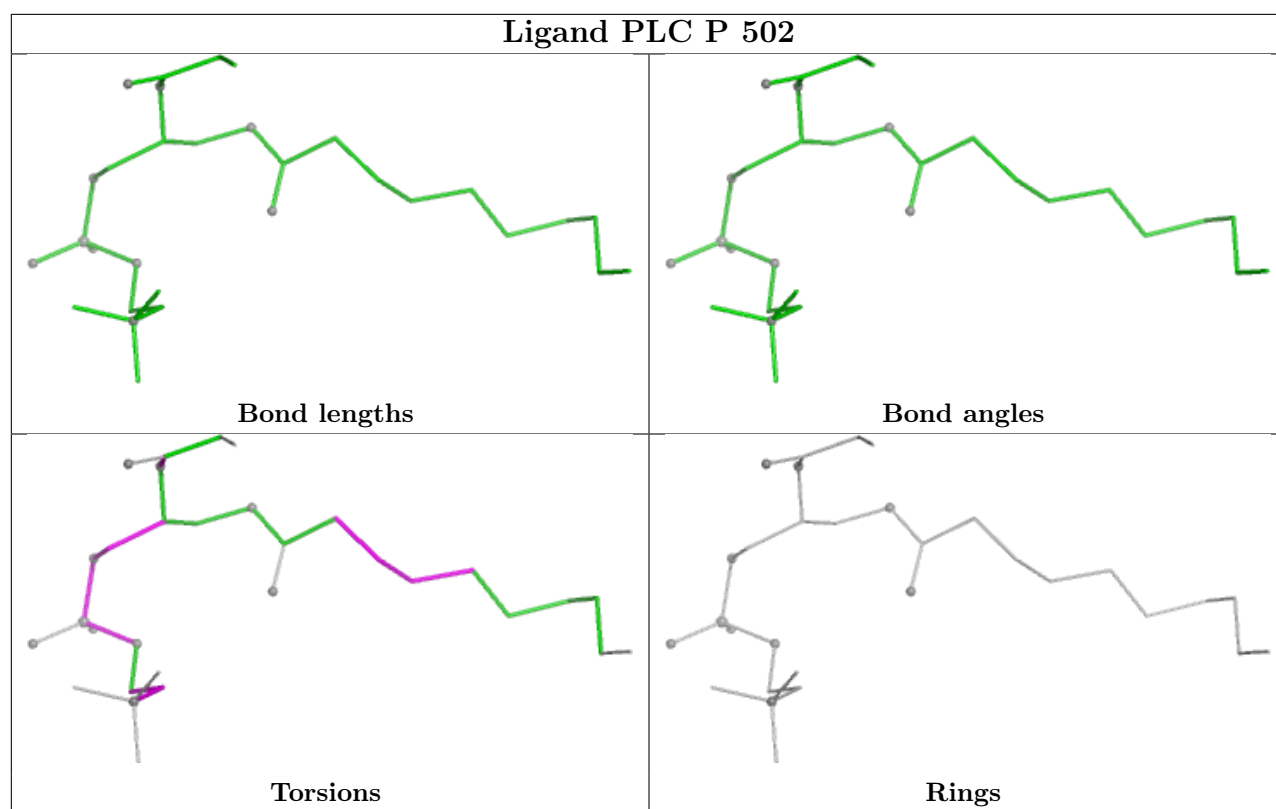


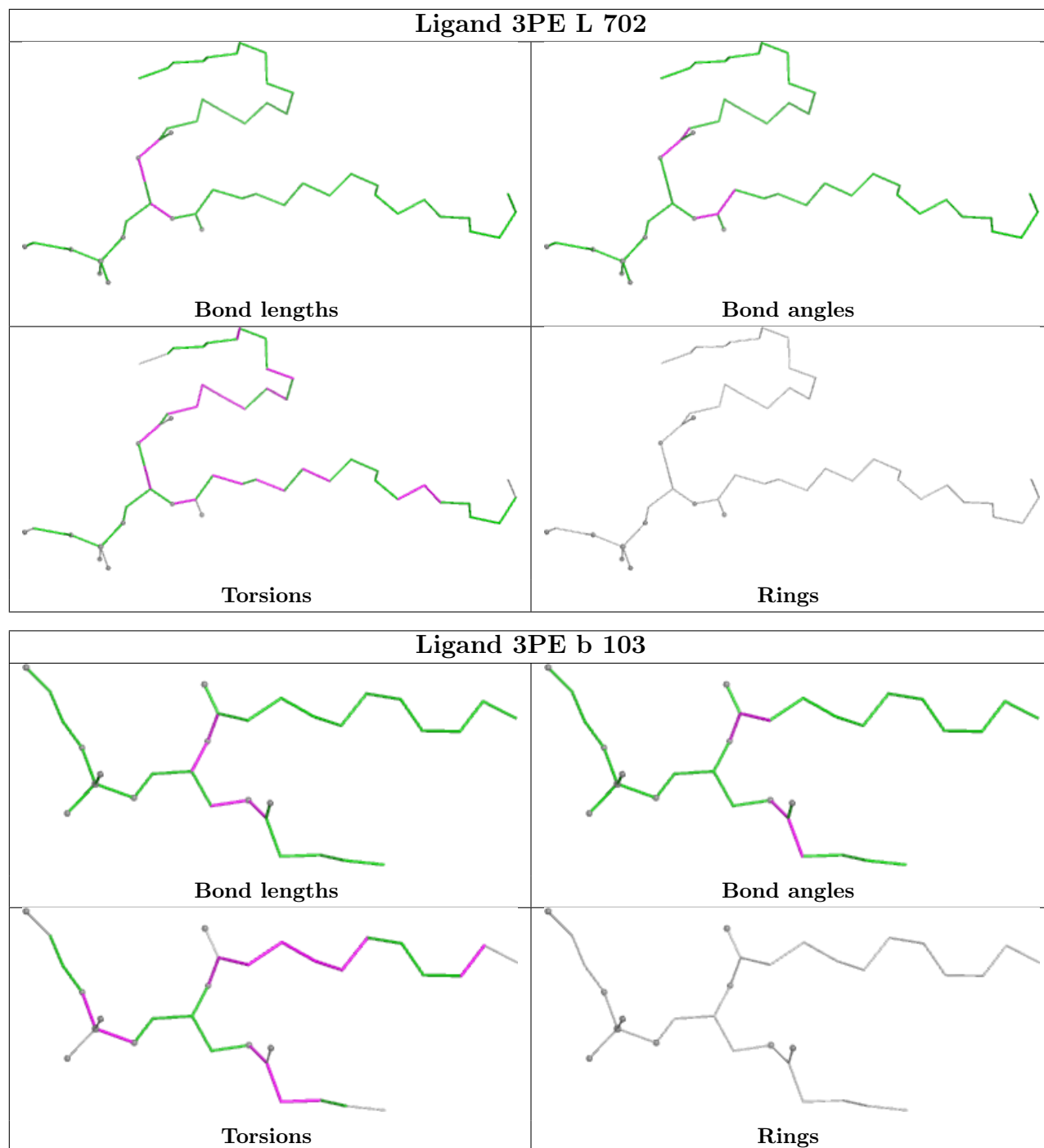
Ligand PLC H 401

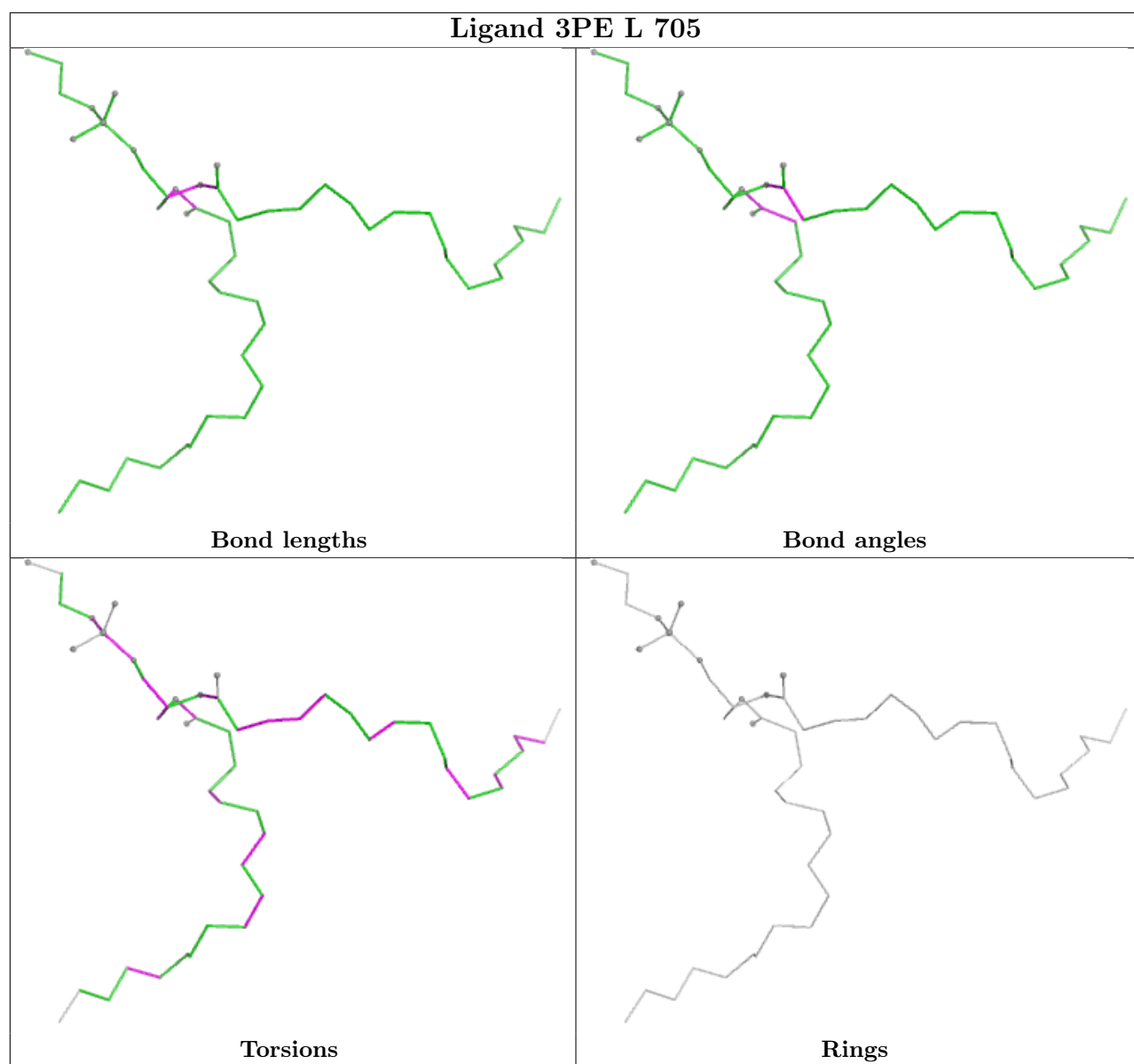


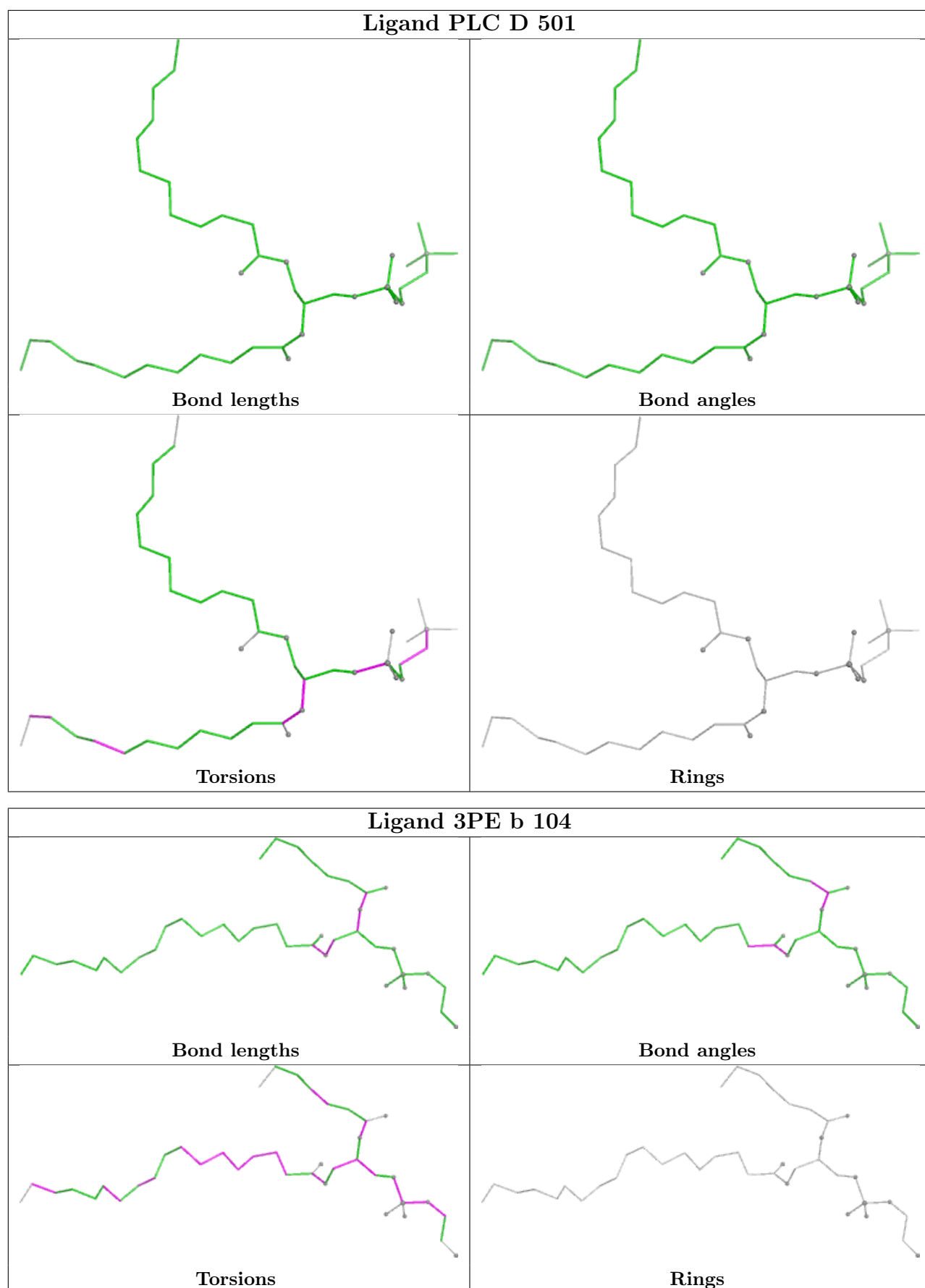


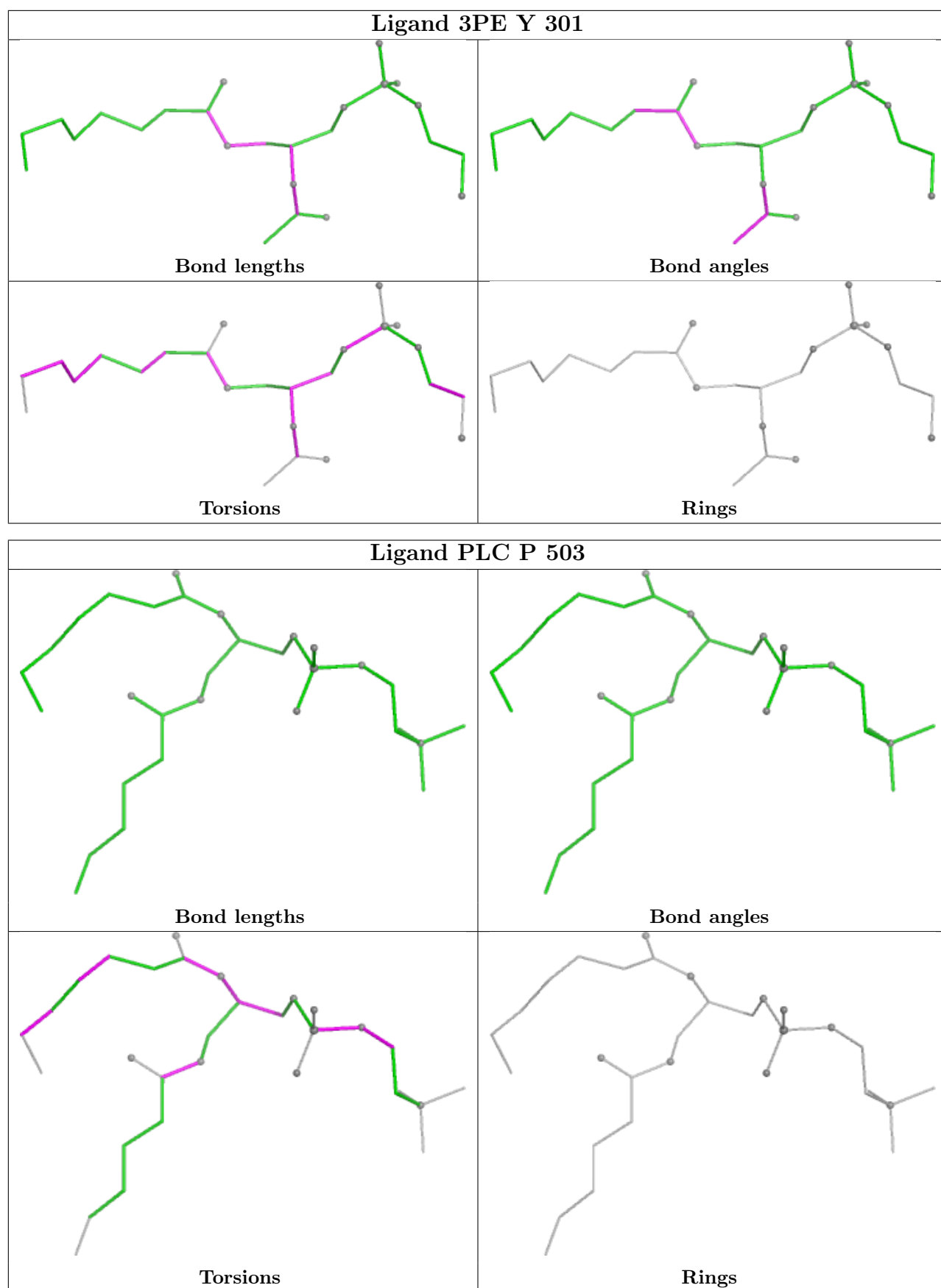


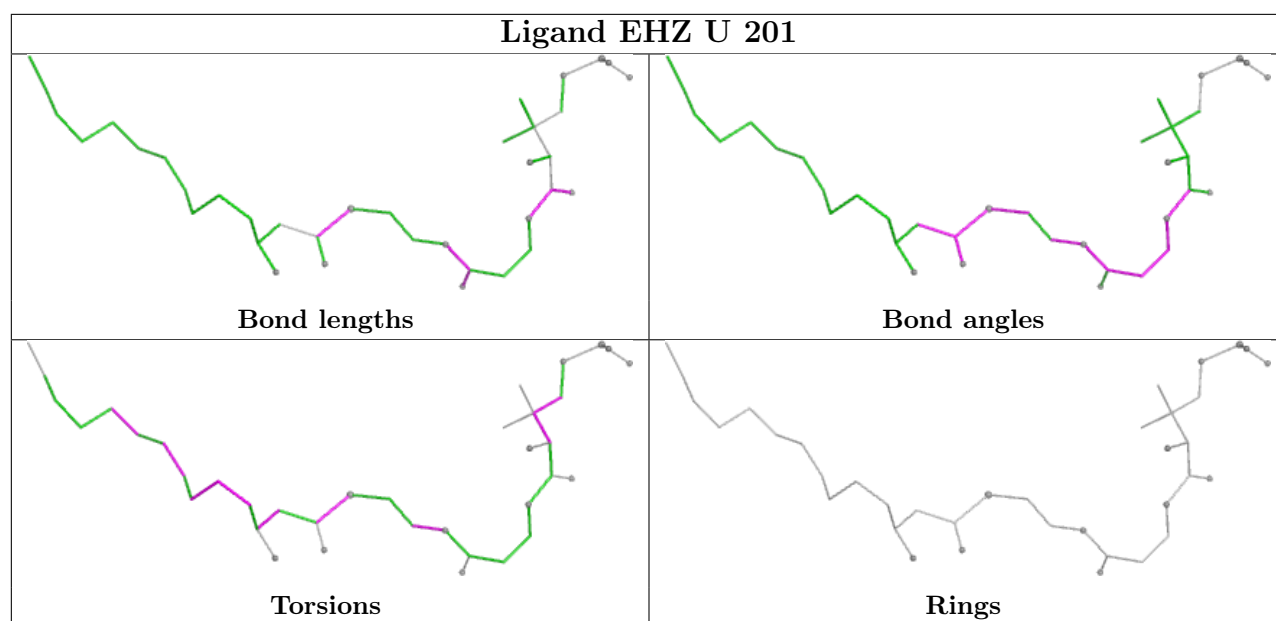












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

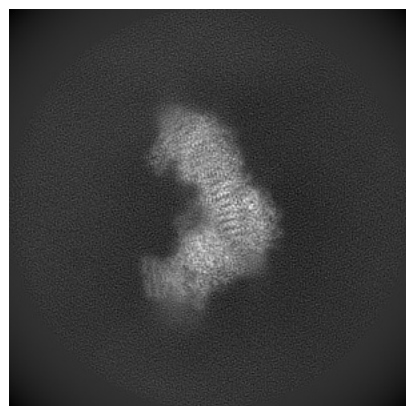
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52875. These allow visual inspection of the internal detail of the map and identification of artifacts.

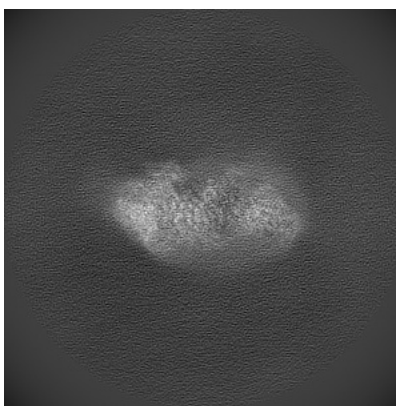
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

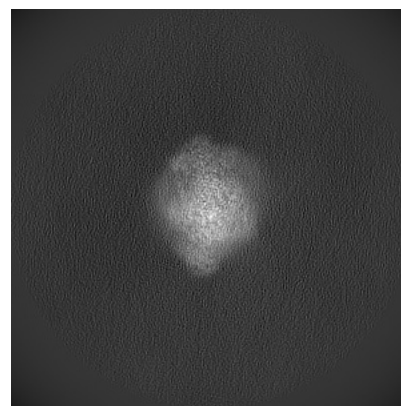
6.1.1 Primary map



X

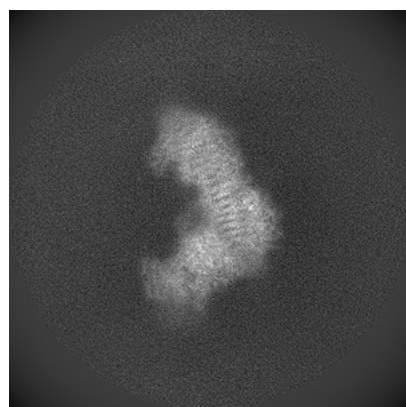


Y

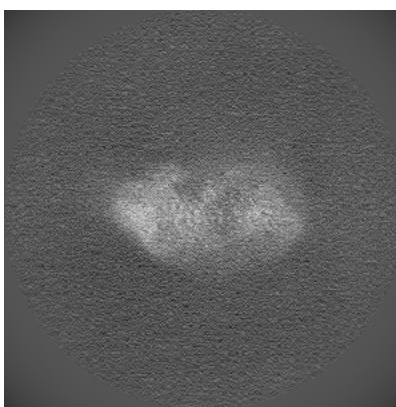


Z

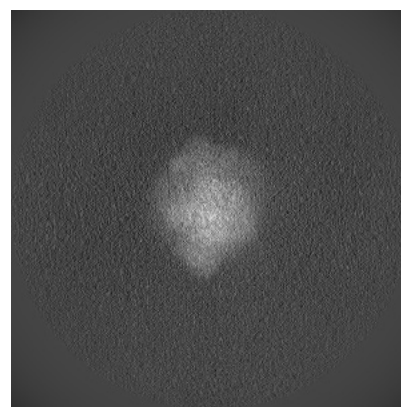
6.1.2 Raw map



X



Y

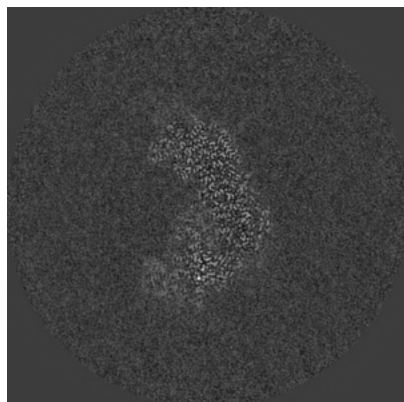


Z

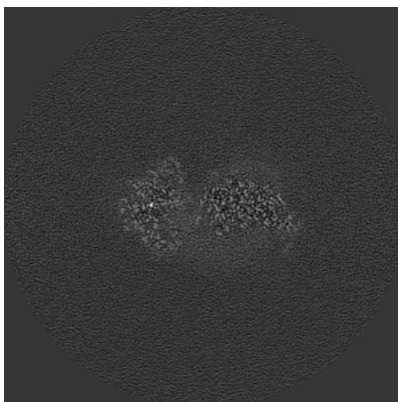
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

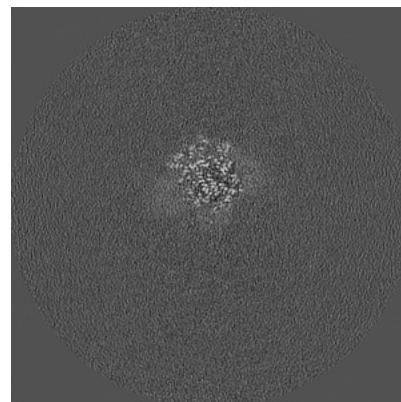
6.2.1 Primary map



X Index: 270

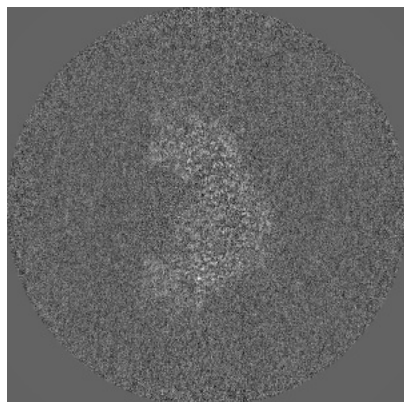


Y Index: 270

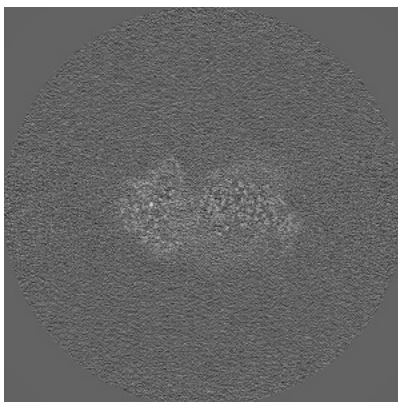


Z Index: 270

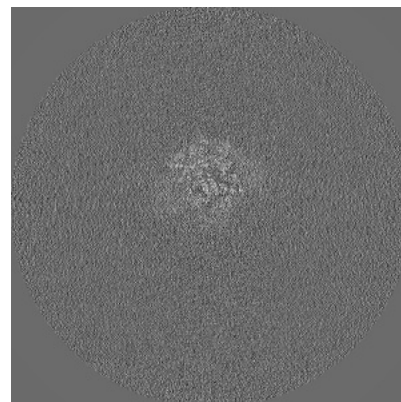
6.2.2 Raw map



X Index: 270



Y Index: 270

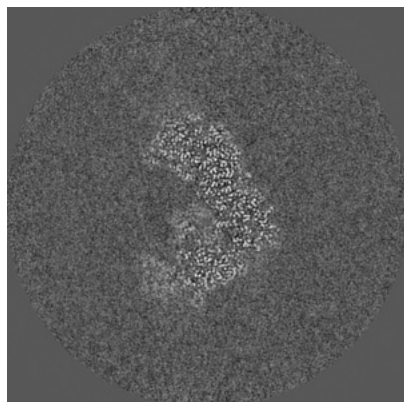


Z Index: 270

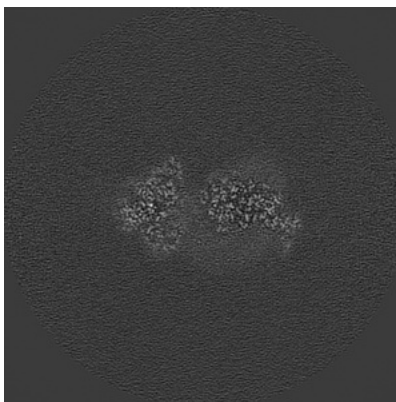
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

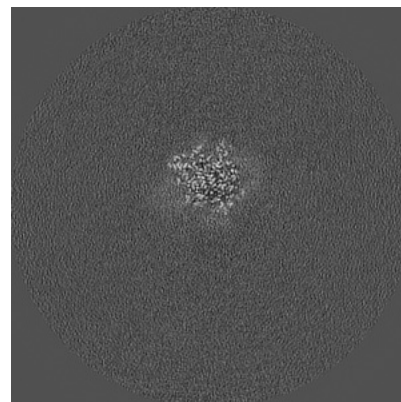
6.3.1 Primary map



X Index: 265

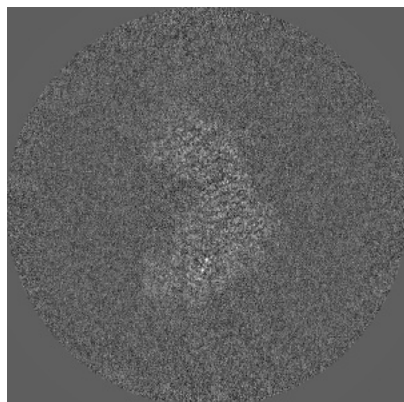


Y Index: 268

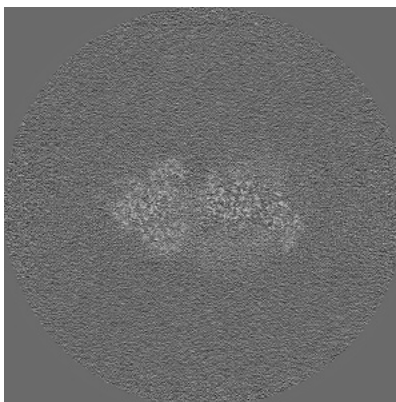


Z Index: 272

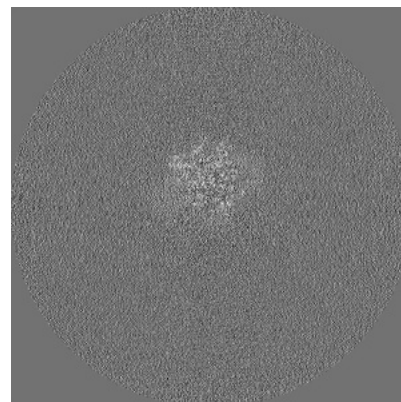
6.3.2 Raw map



X Index: 272



Y Index: 266

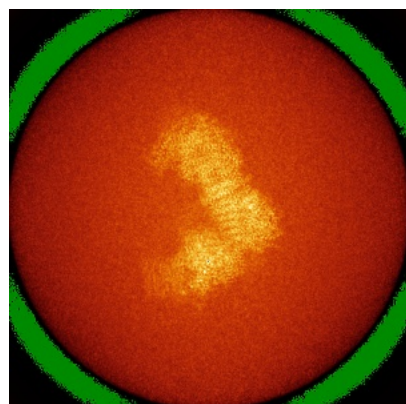


Z Index: 272

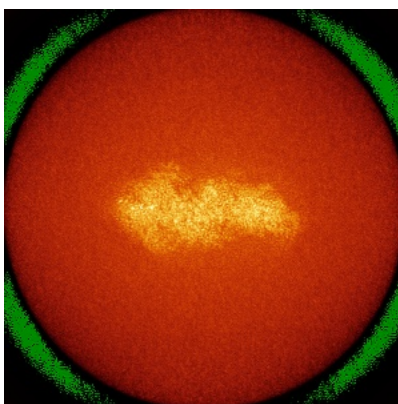
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

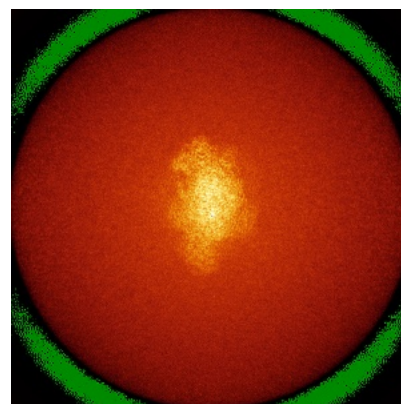
6.4.1 Primary map



X

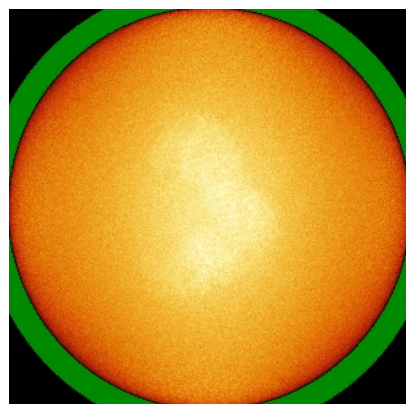


Y

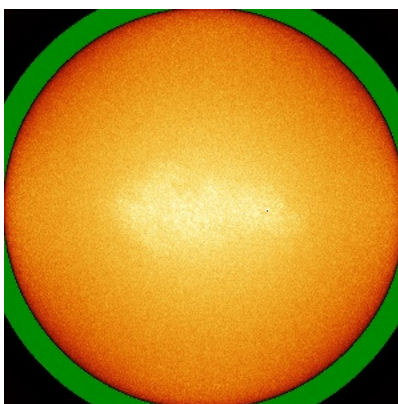


Z

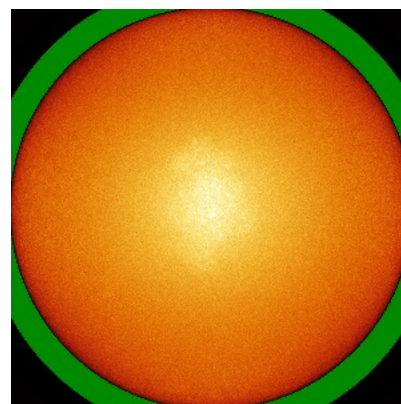
6.4.2 Raw map



X



Y

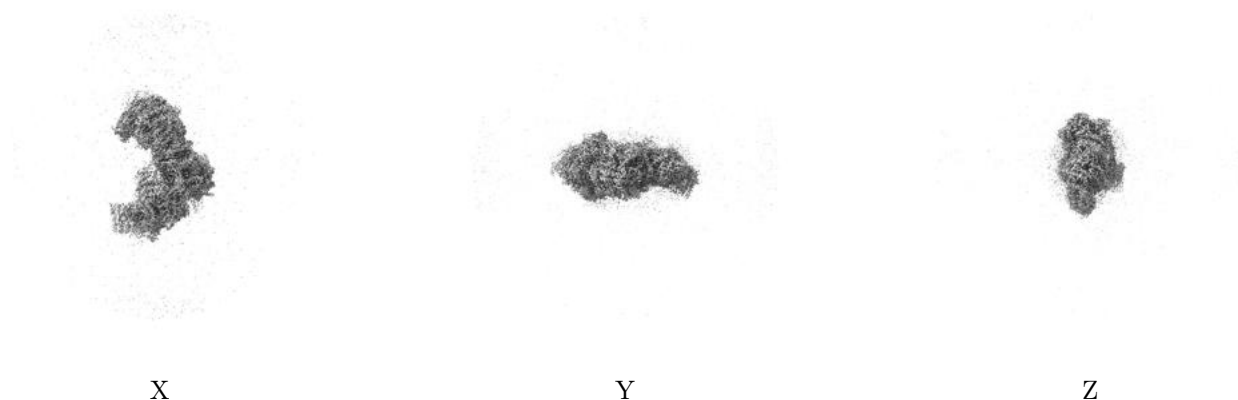


Z

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.

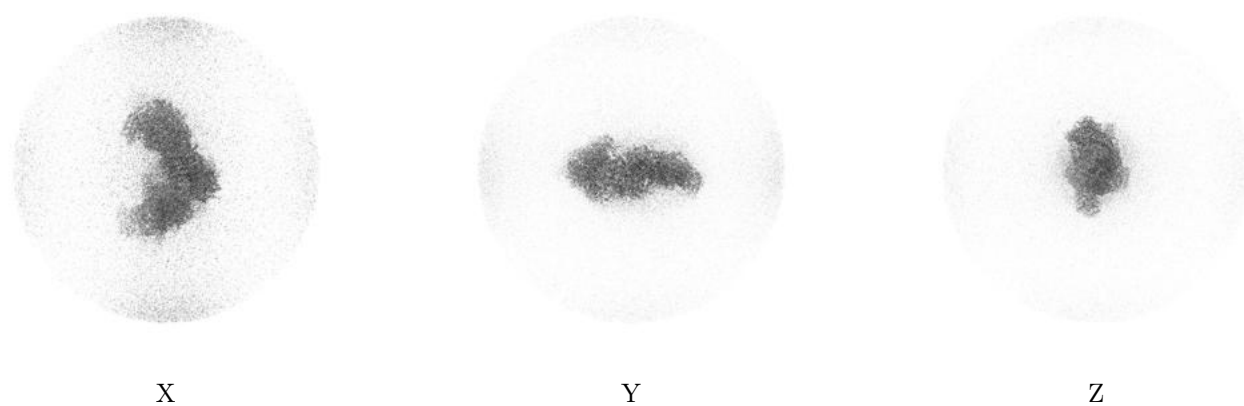
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

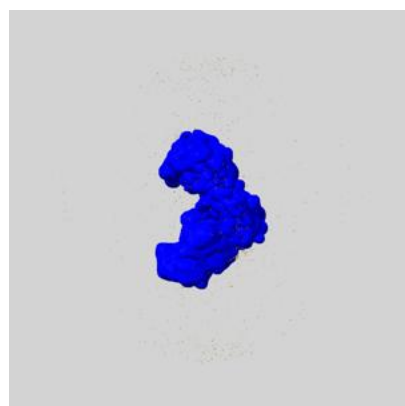
6.6 Mask visualisation [i](#)

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

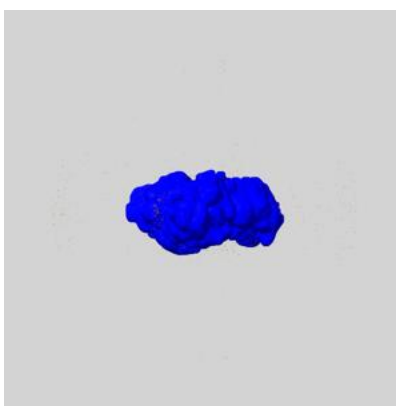
A mask typically either:

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

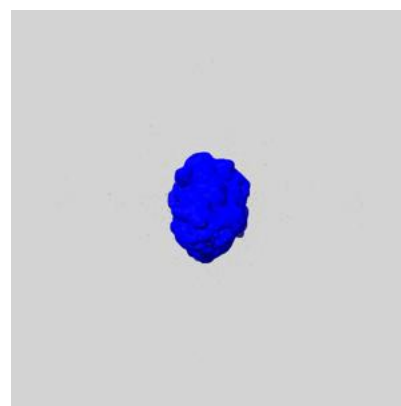
6.6.1 emd_52875_msk_1.map [i](#)



X



Y

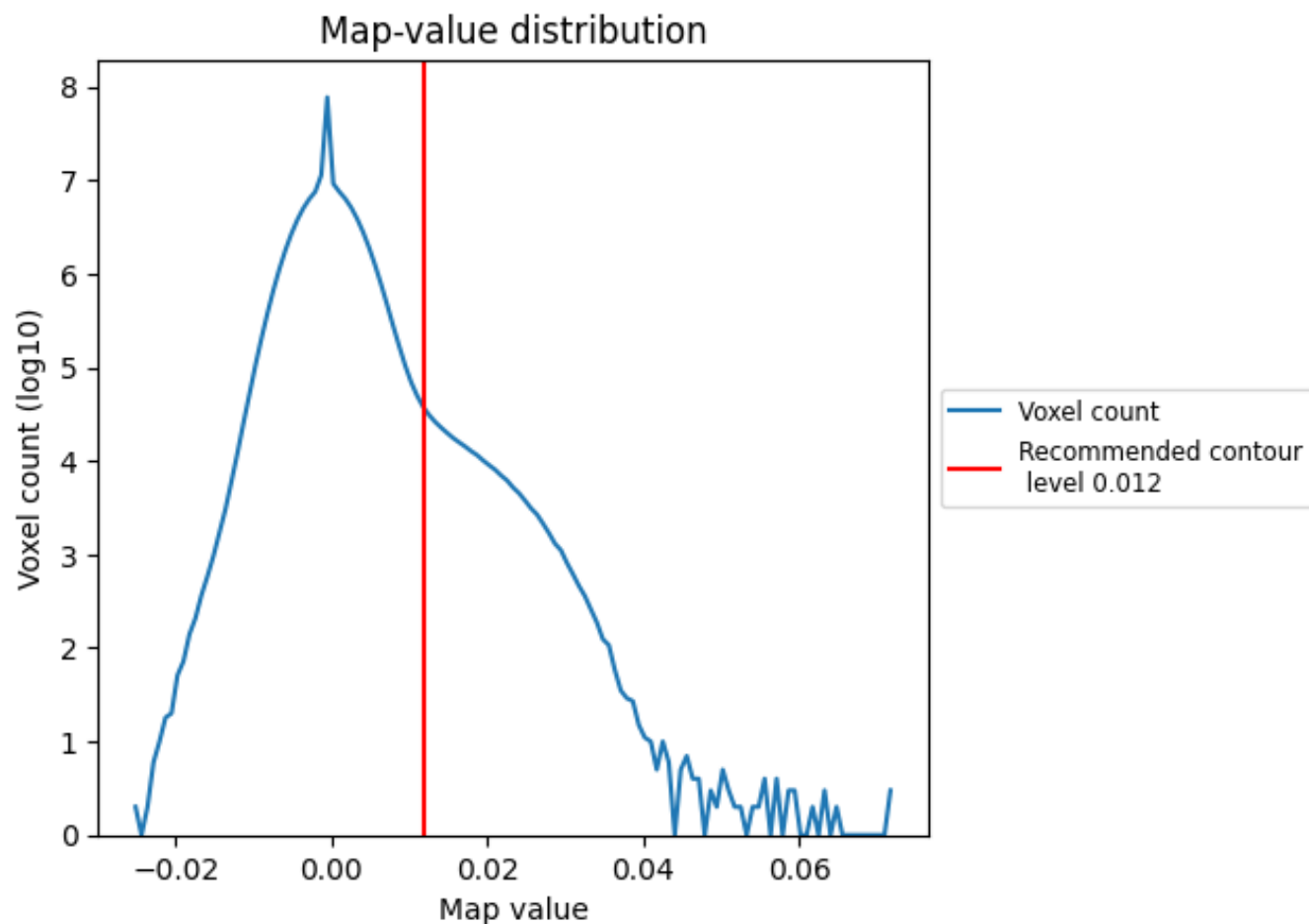


Z

7 Map analysis [i](#)

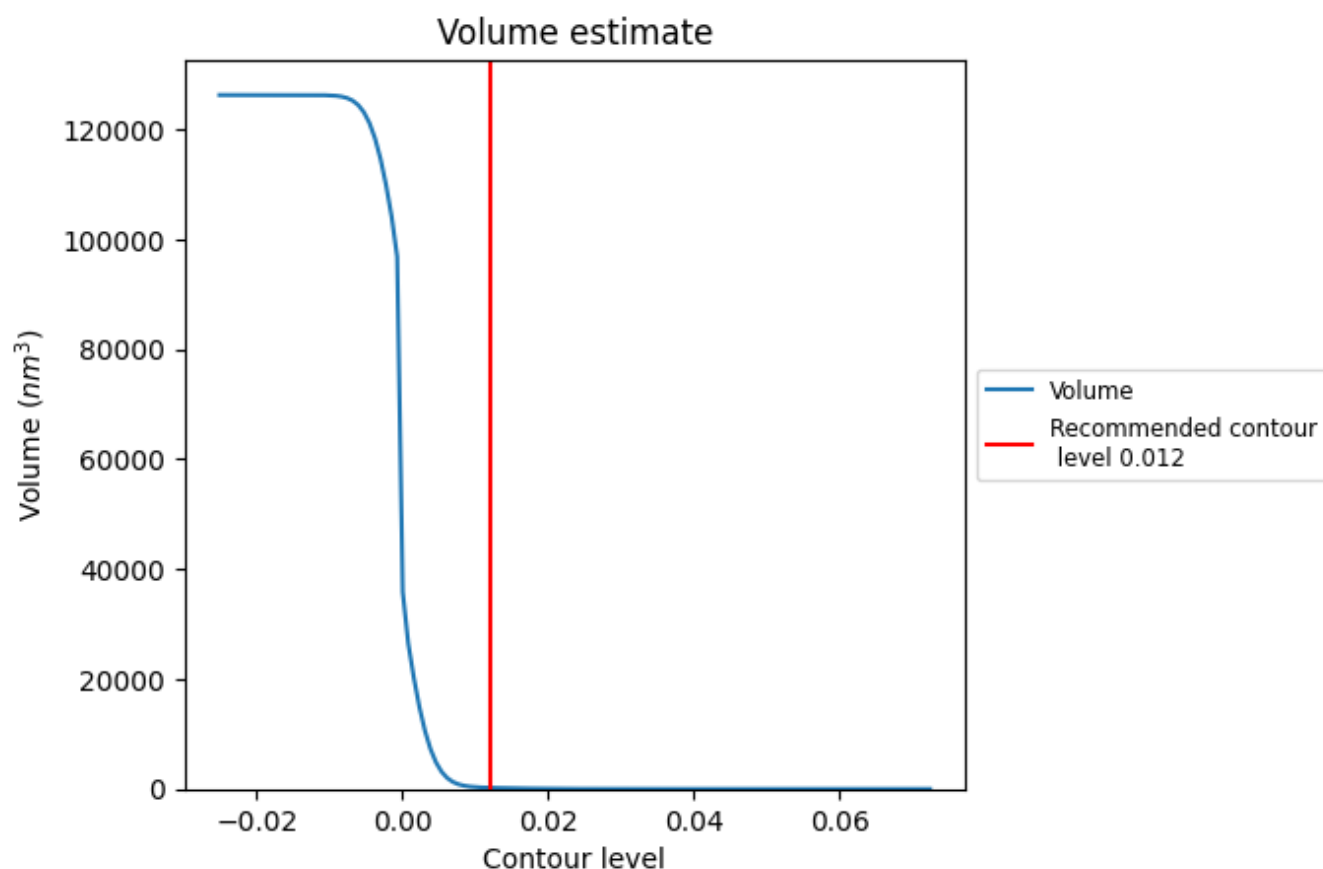
This section contains the results of statistical analysis of the map.

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.

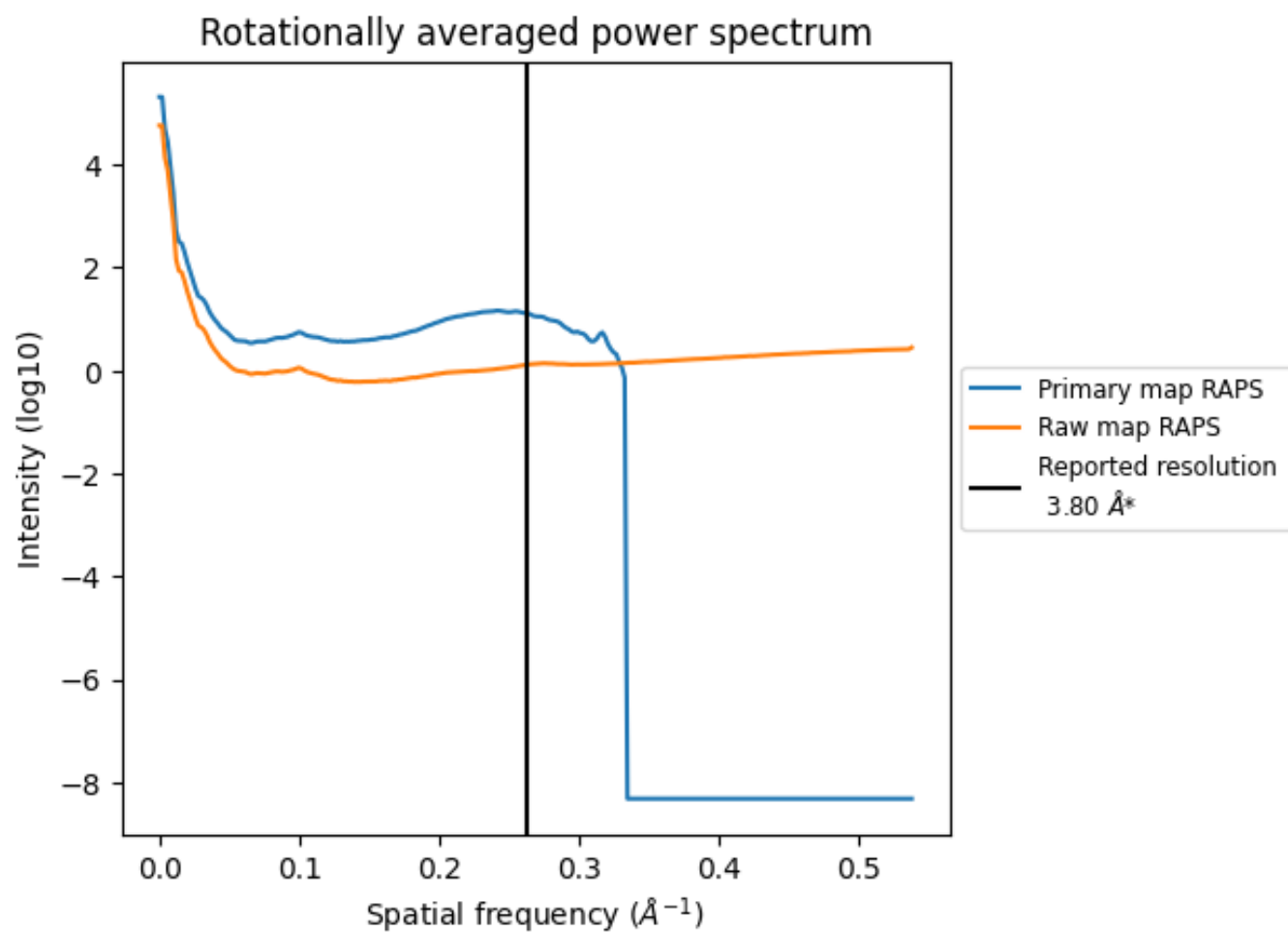
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 nm³; this corresponds to an approximate mass of 193 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 ⓘ

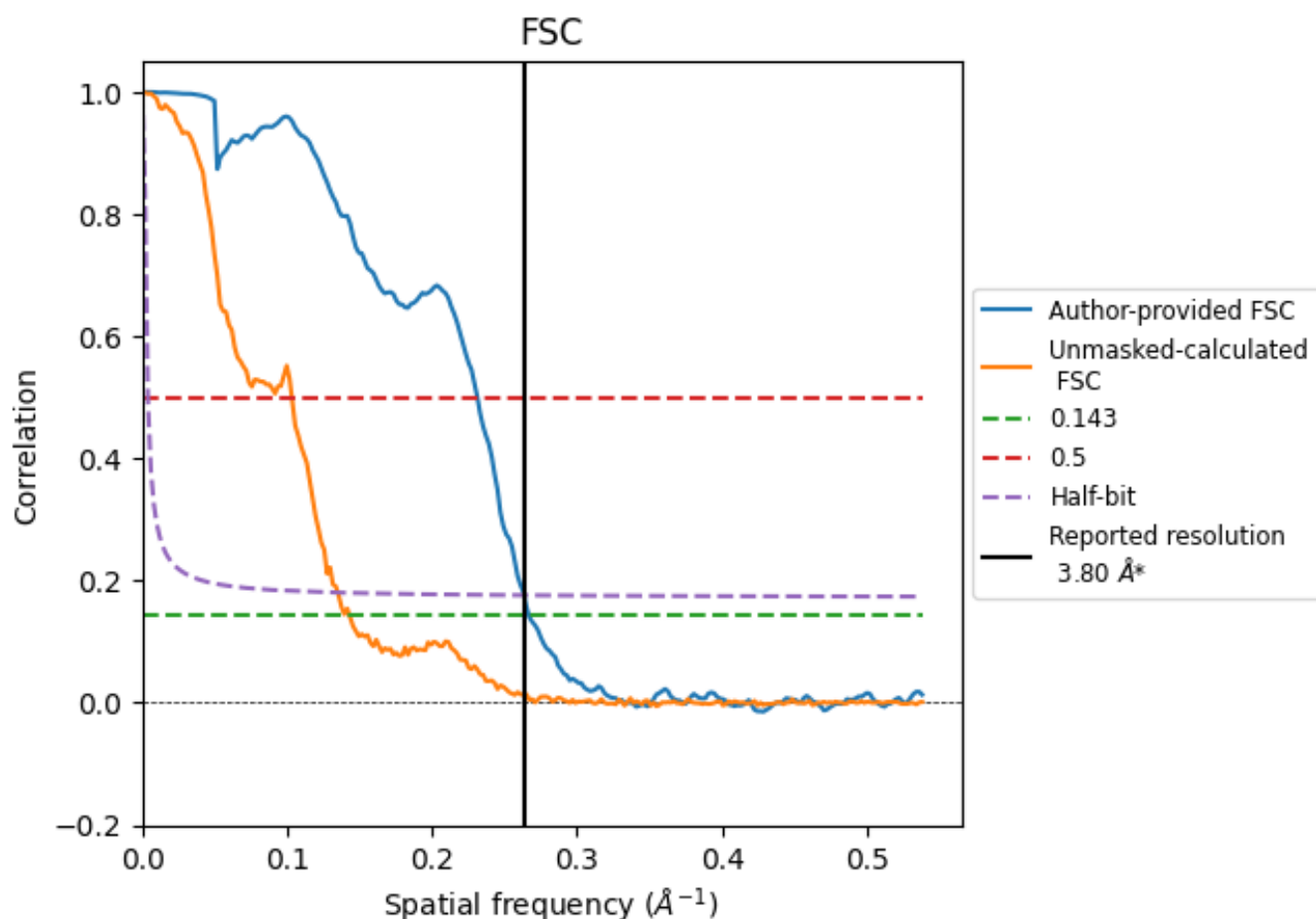


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

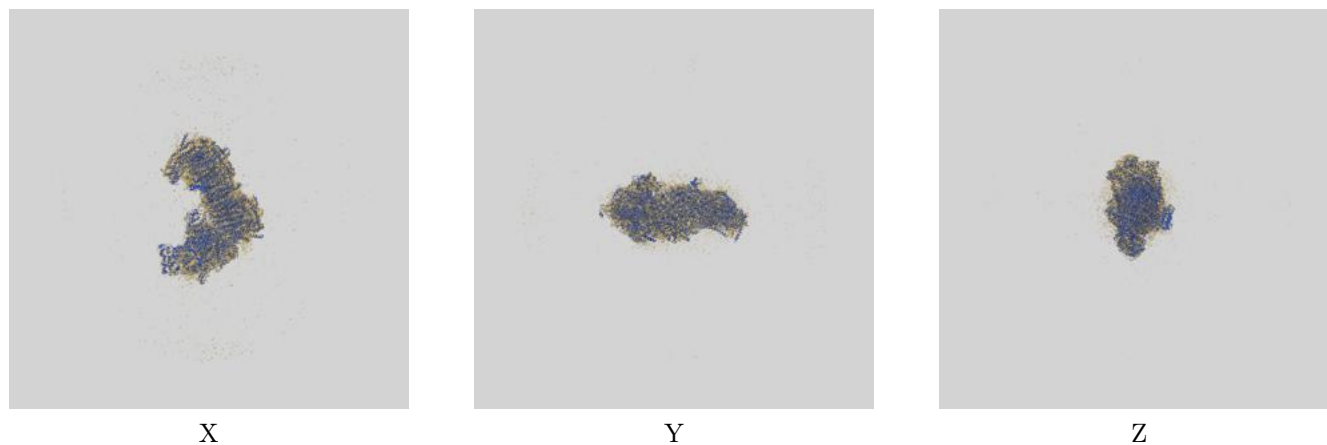
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.75	4.32	3.79
Unmasked-calculated*	6.99	9.69	7.41

*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 6.99 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

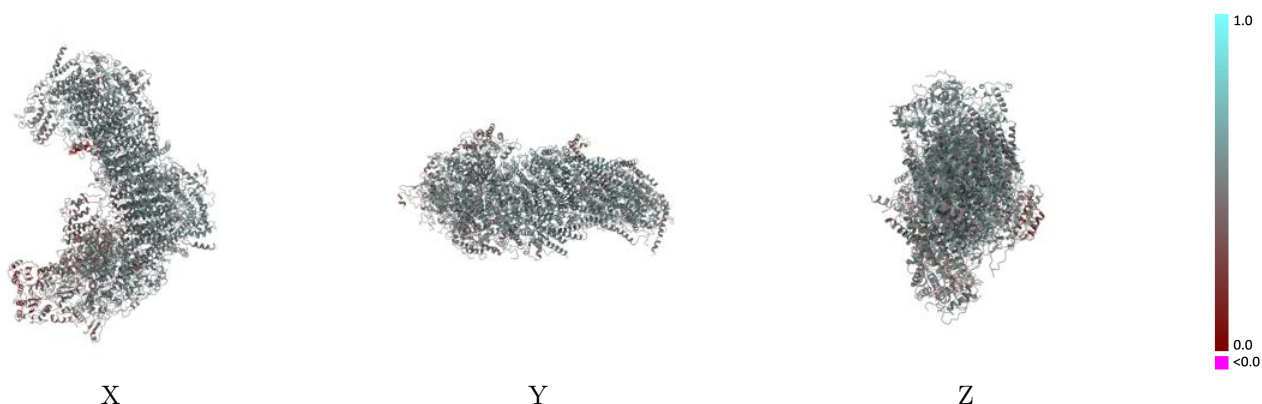
This section contains information regarding the fit between EMDB map EMD-52875 and PDB model 9IHO. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



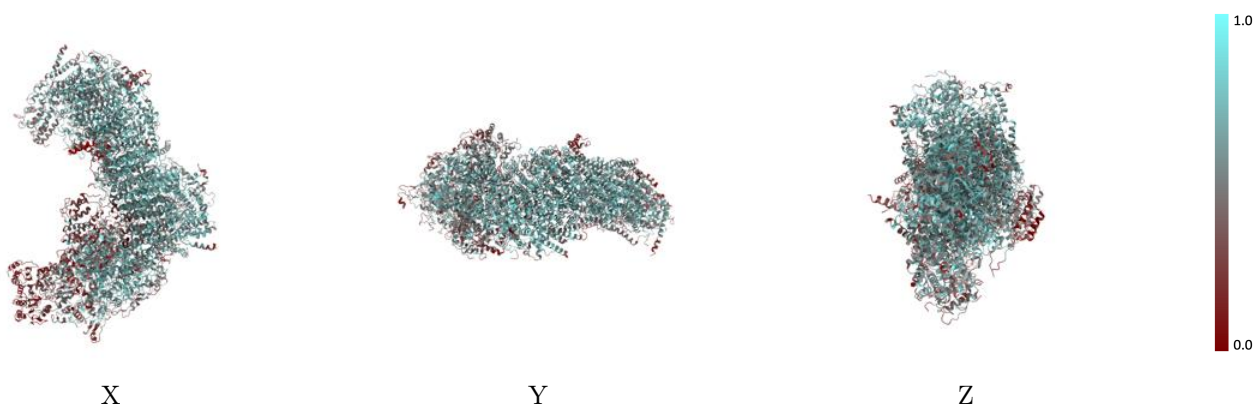
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



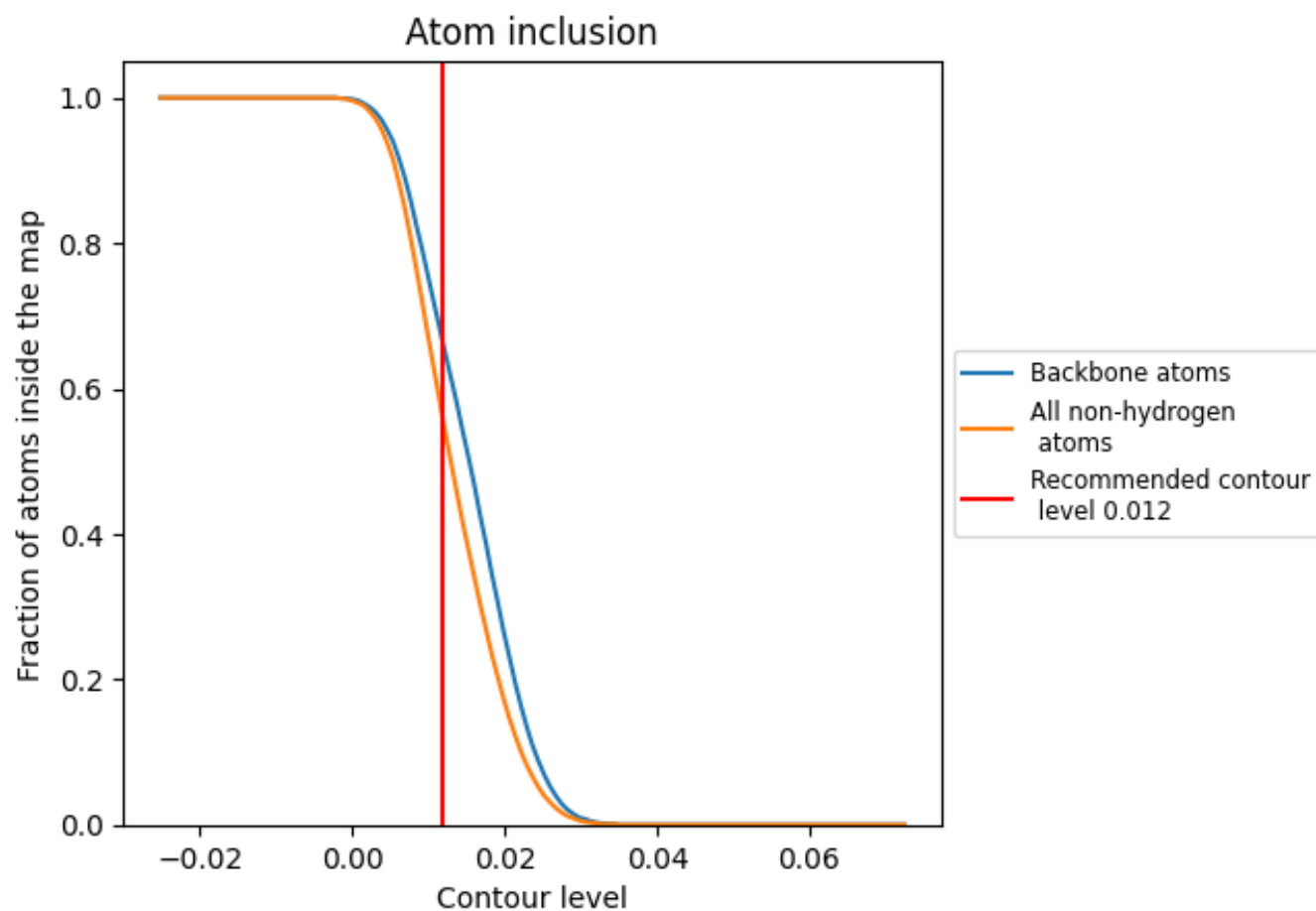
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 55% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.4970
A	 0.5050	 0.4810
B	 0.6360	 0.5220
C	 0.5140	 0.4760
D	 0.6090	 0.5090
G	 0.3130	 0.3940
H	 0.6080	 0.5200
I	 0.6780	 0.5200
J	 0.5810	 0.5190
K	 0.6090	 0.5170
L	 0.6450	 0.5340
M	 0.6850	 0.5440
N	 0.6820	 0.5390
O	 0.6340	 0.5300
P	 0.4470	 0.4570
Q	 0.4990	 0.4730
R	 0.4520	 0.4550
S	 0.0730	 0.2890
T	 0.2010	 0.4000
U	 0.4210	 0.4660
V	 0.3970	 0.4430
W	 0.4290	 0.4440
X	 0.6430	 0.5280
Y	 0.5930	 0.5210
Z	 0.6120	 0.5280
a	 0.6460	 0.5350
b	 0.5810	 0.5420
c	 0.3660	 0.4530
d	 0.6640	 0.5300
e	 0.6730	 0.5310
f	 0.5800	 0.5090
g	 0.3390	 0.4460
h	 0.5840	 0.5150
i	 0.5470	 0.5010
j	 0.4880	 0.4820



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Chain	Atom inclusion	Q-score
k	 0.4960	 0.4790
l	 0.5510	 0.4960
m	 0.5690	 0.5140
n	 0.5270	 0.4890
o	 0.5380	 0.4900
p	 0.6900	 0.5330
q	 0.5500	 0.5060