



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2025 – 10:56 am BST

PDB ID : 9IHQ / pdb_00009ihq
EMDB ID : EMD-52877
Title : Closed state with NUQM and without flavoprotein (classification state 2) of Pichia pastoris mitochondrial complex I in cMSP26 nanodiscs
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2025-02-21
Resolution : 2.90 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.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

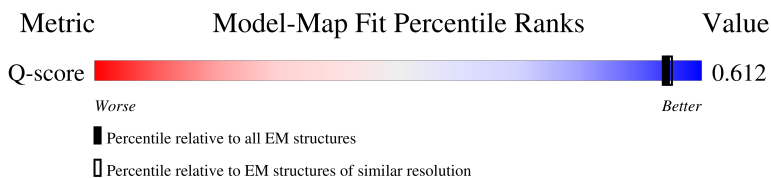
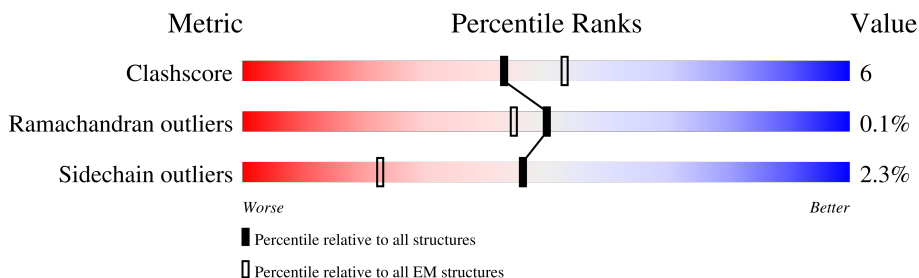
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.




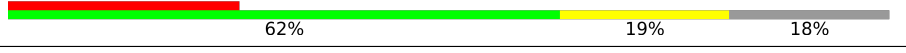

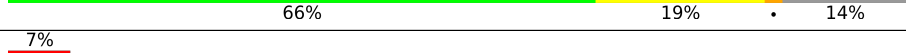
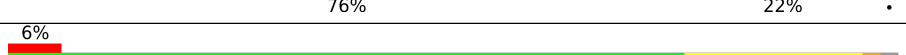

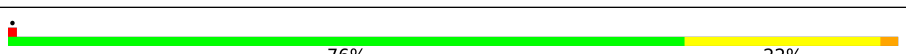



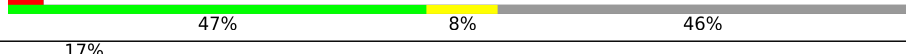

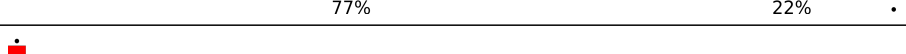
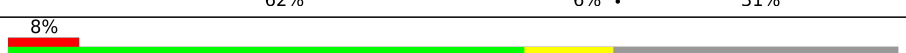


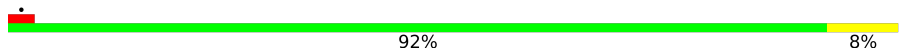








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	1	190	
2	A	141	
3	B	204	
4	C	289	

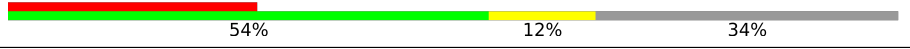



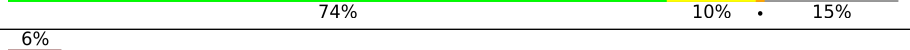
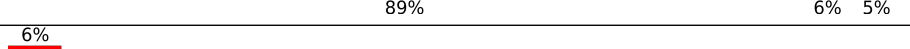
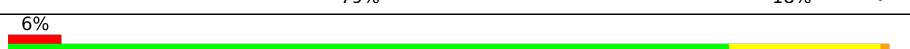
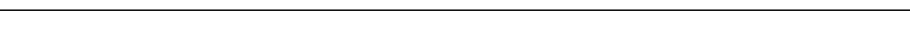
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Mol	Chain	Length	Quality of chain
5	D	482	
6	G	726	
7	H	353	
8	I	222	
9	J	161	
10	K	82	
11	L	642	
12	M	491	
13	N	523	
14	O	193	
15	P	384	
16	Q	159	
17	R	139	
18	S	90	
19	T	138	
20	U	130	
21	V	134	
22	W	122	
23	X	184	
24	Y	216	
25	Z	147	
26	a	150	
27	b	79	
28	c	182	
29	d	78	

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Mol	Chain	Length	Quality of chain
30	e	106	
31	f	86	
32	g	239	
33	h	182	
34	i	74	
35	j	59	
36	k	61	
37	l	156	
38	m	81	
39	n	111	
40	o	87	
41	p	92	
42	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
44	SF4	I	301	-	-	X	-
44	SF4	I	302	-	-	X	-

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 64071 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 NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	592	Total	C	N	O	S	0	0
			4563	2862	798	882	21		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 8 is a protein called NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 10 is a protein called NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 14 is a protein called NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	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 15 is a protein called NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	86	Total	C	N	O	S	0	0
			711	451	119	139	2		

- Molecule 17 is a protein called NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 18 is a protein called NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	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 19 is a protein called Acyl carrier protein.

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

- Molecule 20 is a protein called Acyl carrier protein.

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

- Molecule 21 is a protein called NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 22 is a protein called BA75_04796T0.

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

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	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 24 is a protein called NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	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 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

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

- Molecule 27 is a protein called NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 28 is a protein called BA75_00589T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	161	Total	C	N	O	S	0	0
			1256	799	221	234	2		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 29 is a protein called Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM.

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

- Molecule 30 is a protein called BA75_05084T0.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 36 is a protein called NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

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

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

- Molecule 38 is a protein called NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 41 is a protein called NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

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

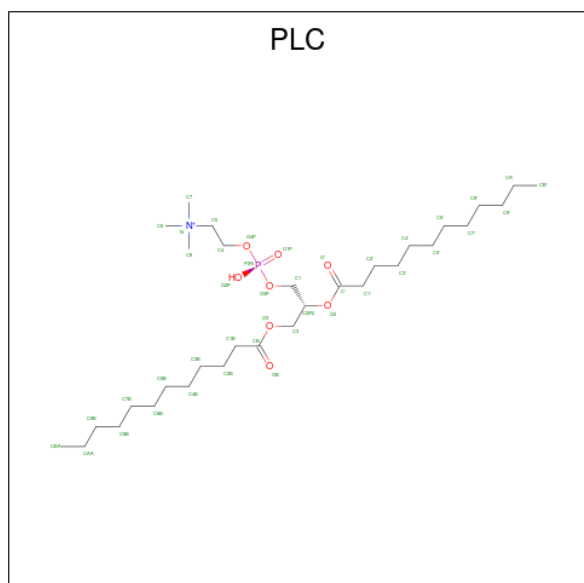
- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	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 43 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



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

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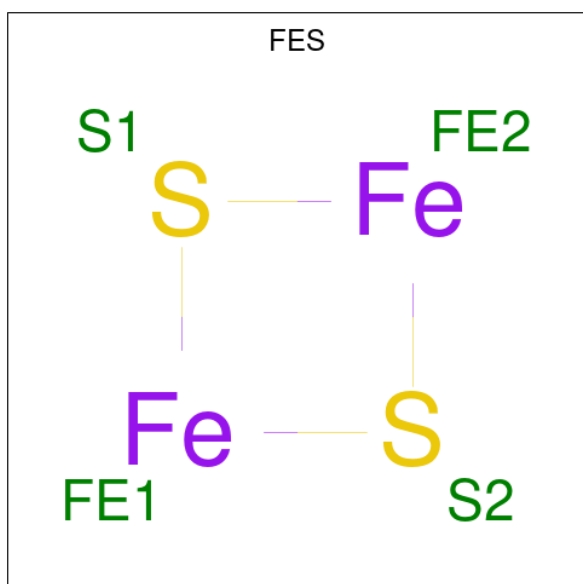
Mol	Chain	Residues	Atoms					AltConf
43	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
43	L	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	P	1	Total	C	N	O	P	0
			31	21	1	8	1	
43	Y	1	Total	C	N	O	P	0
			36	26	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	
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	h	1	Total	C	N	O	P	0
			42	32	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 IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

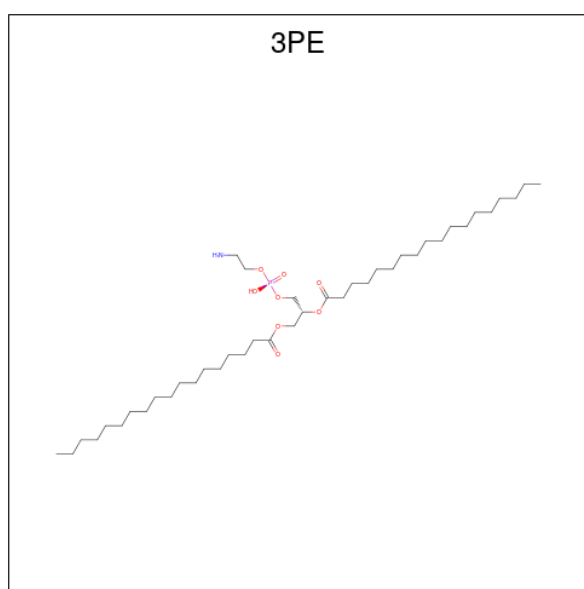


Mol	Chain	Residues	Atoms			AltConf
45	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



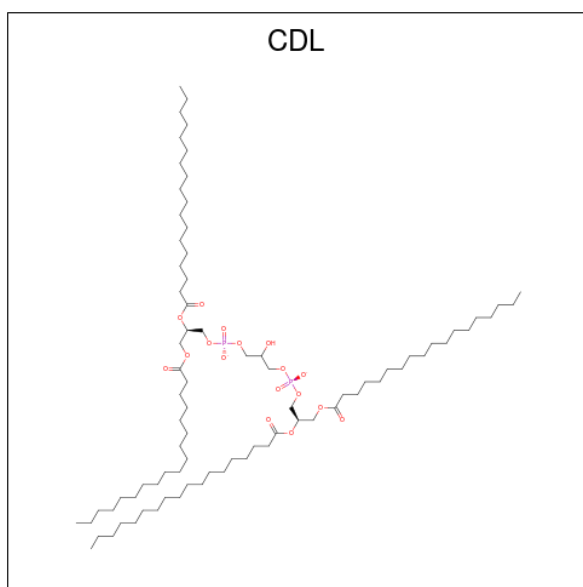
Mol	Chain	Residues	Atoms					AltConf
47	H	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	L	1	Total	C	N	O	P	0
			29	19	1	8	1	
47	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	L	1	Total	C	N	O	P	0
			33	23	1	8	1	
47	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	L	1	Total	C	N	O	P	0
			46	36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

Continued on next page...

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

- Molecule 48 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 49 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
49	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 51 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

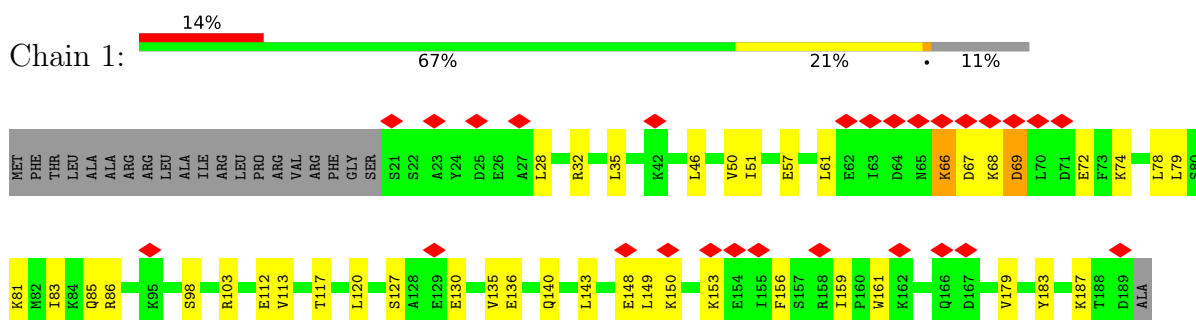


Mol	Chain	Residues	Atoms						AltConf
51	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
51	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

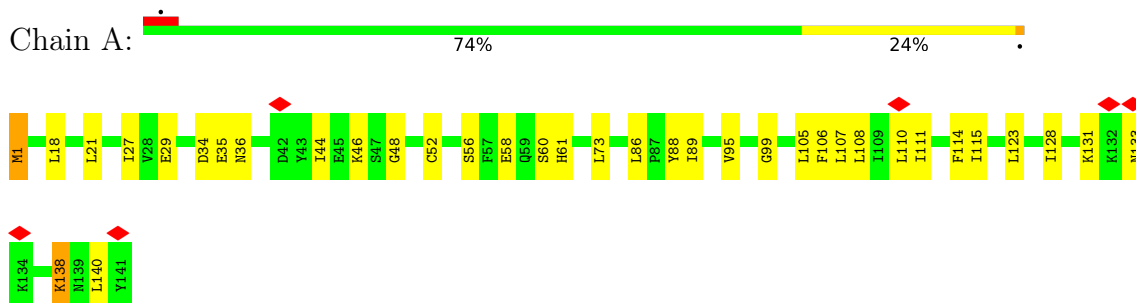
3 Residue-property plots [i](#)

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.

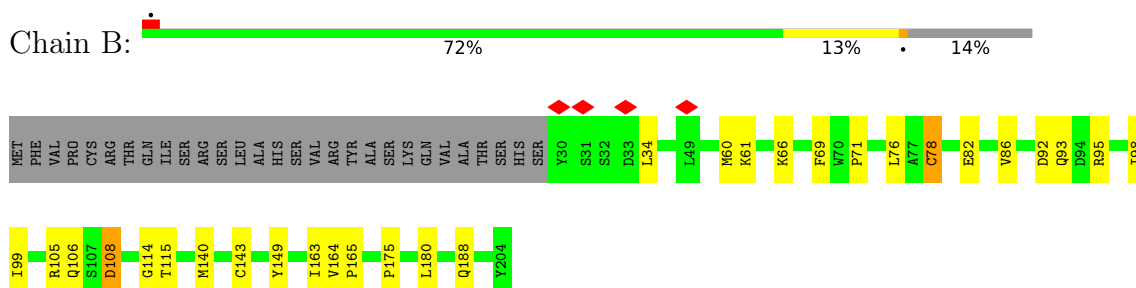
- Molecule 1: Altered inheritance of mitochondria protein 41, mitochondrial



- Molecule 2: NADH-ubiquinone oxidoreductase chain 3

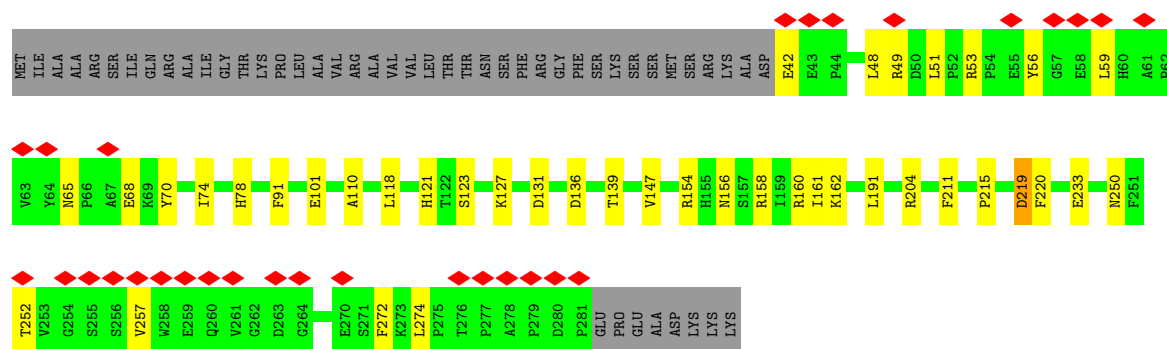


- Molecule 3: BA75_00622T0



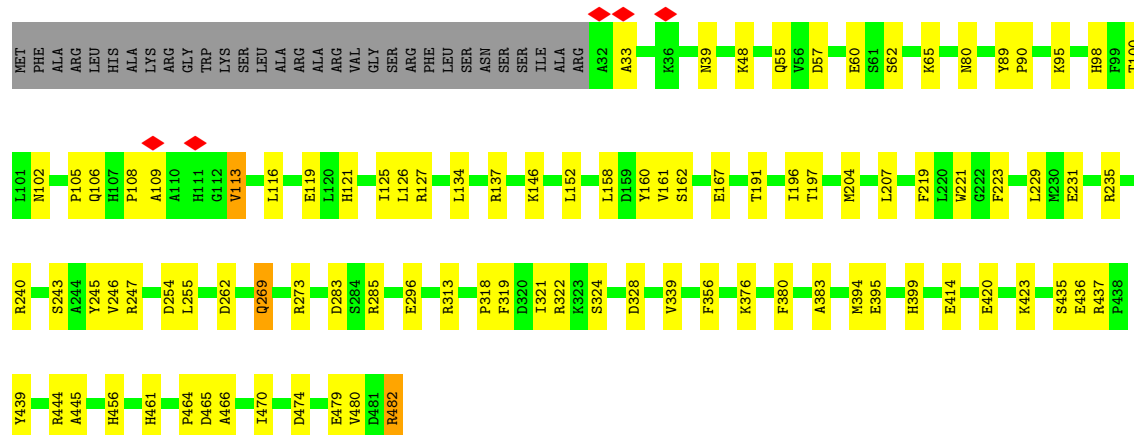
- Molecule 4: NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)





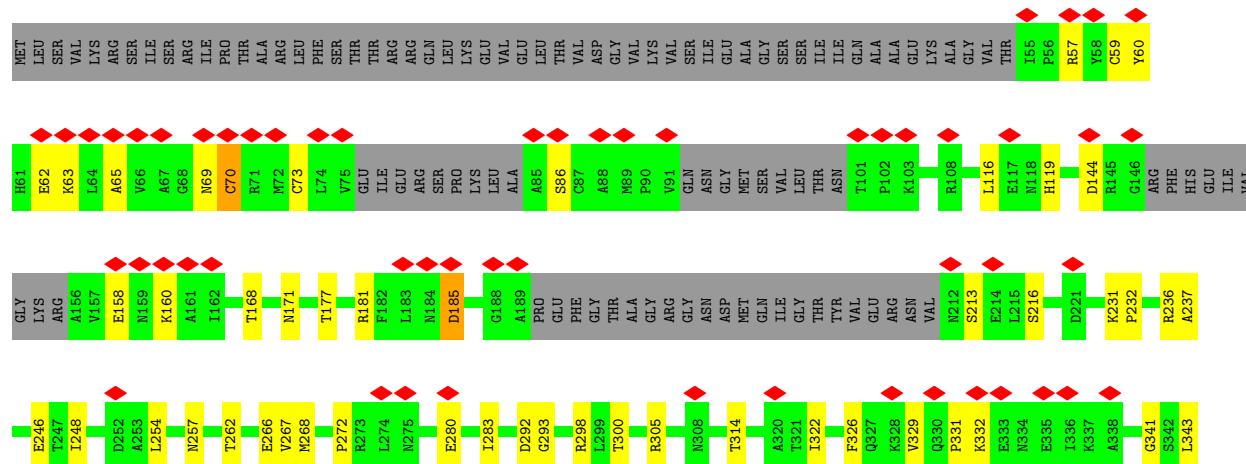
- Molecule 5: NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

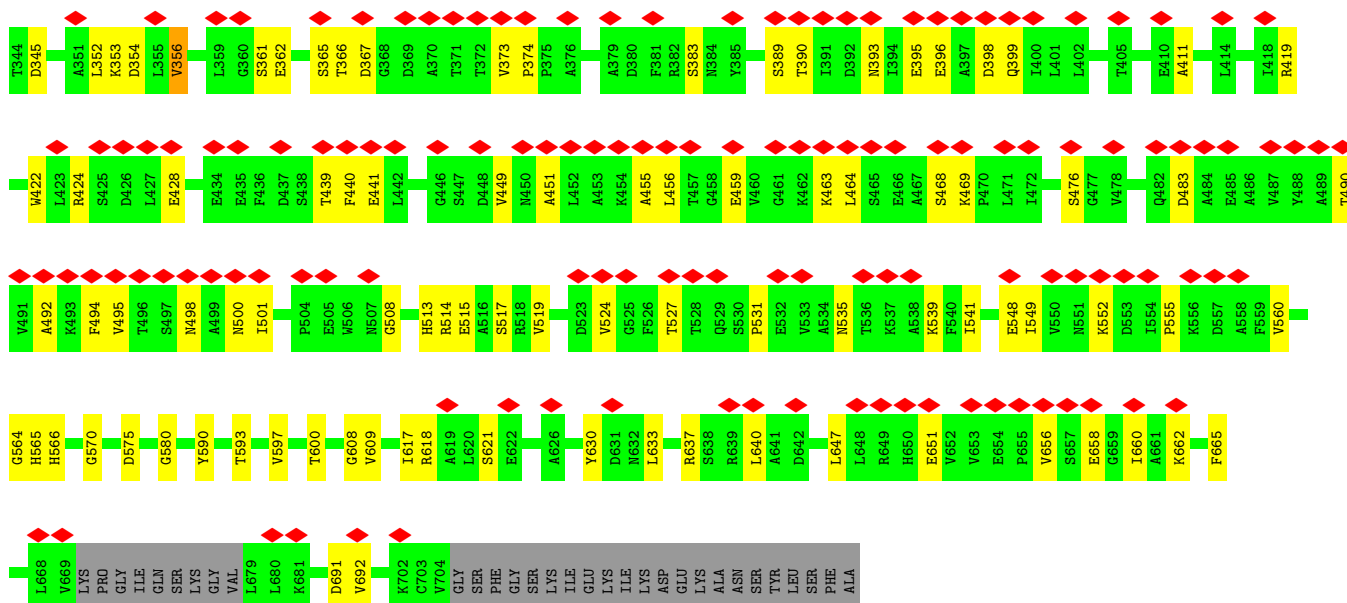
Chain D: 74% 19% 6%



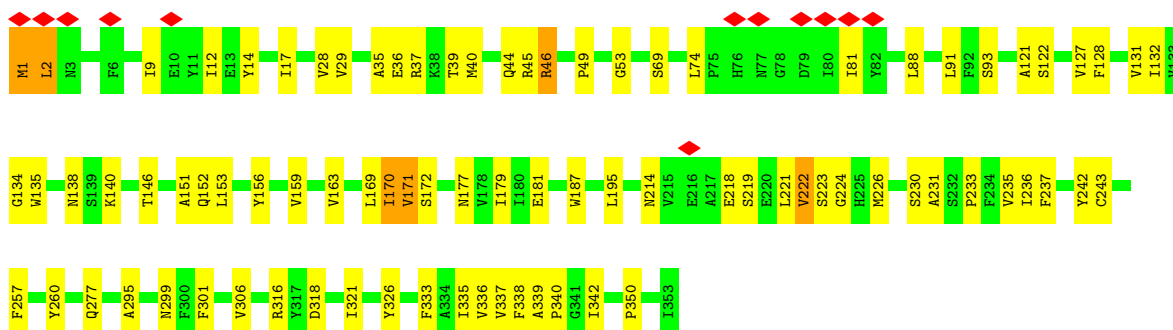
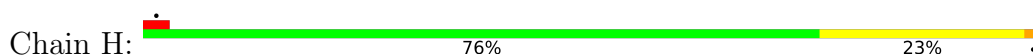
- Molecule 6: NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain G: 26% 62% 19% 18%

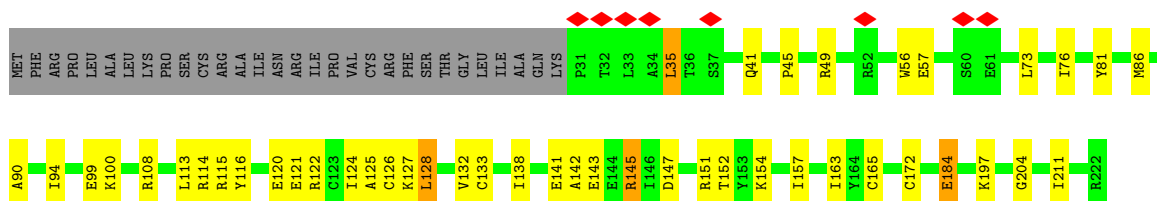




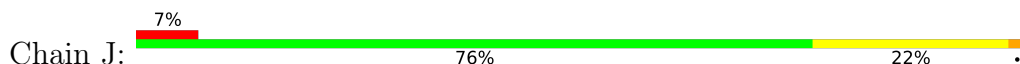
• Molecule 7: NADH-ubiquinone oxidoreductase chain 1

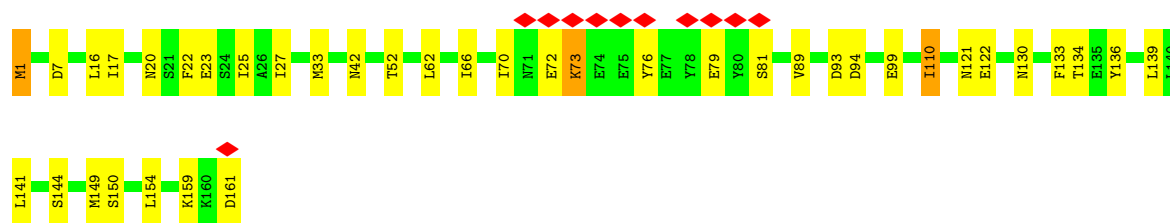


• Molecule 8: NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

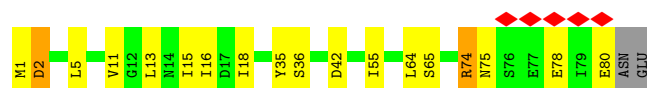
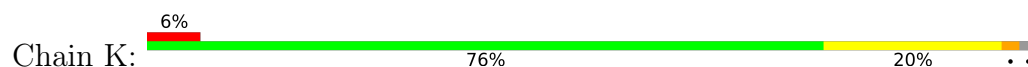


• Molecule 9: NADH-ubiquinone oxidoreductase chain 6

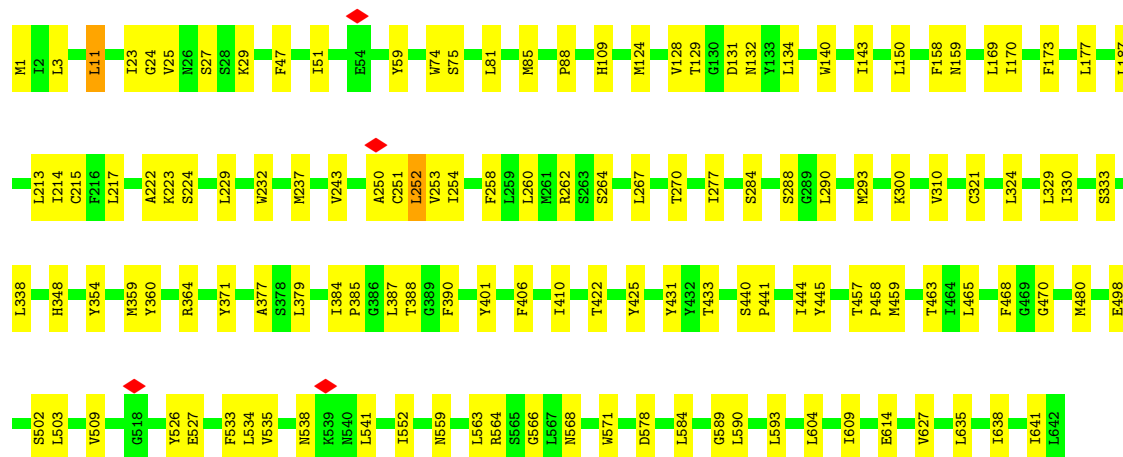
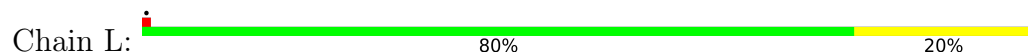




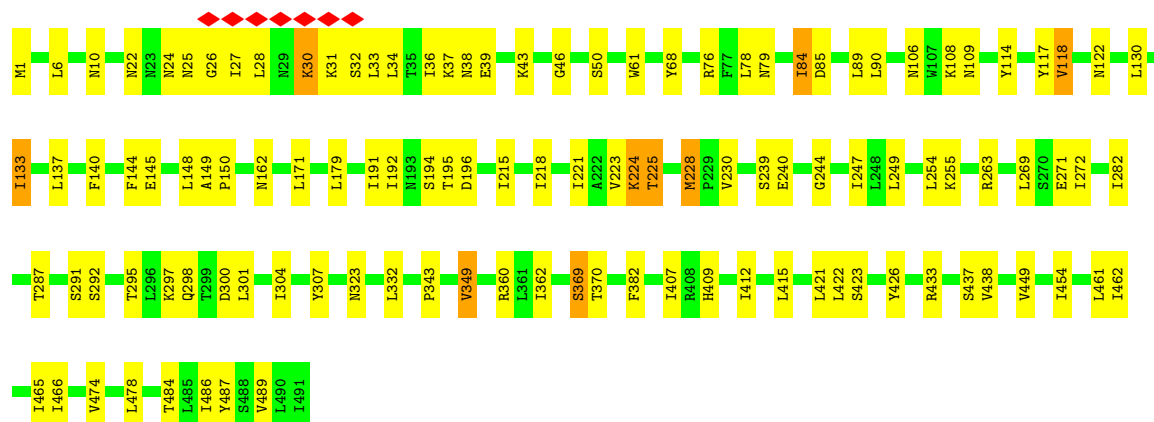
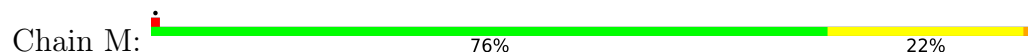
- Molecule 10: NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



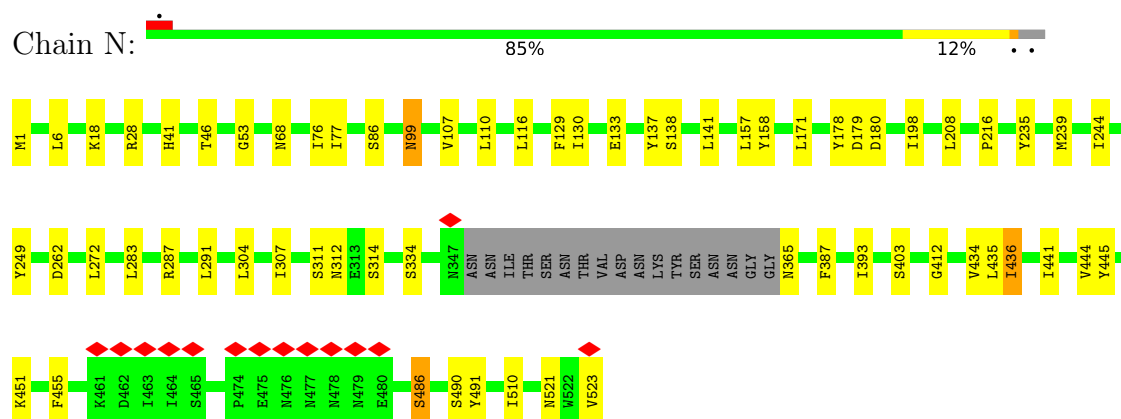
- Molecule 11: NADH-ubiquinone oxidoreductase chain 5



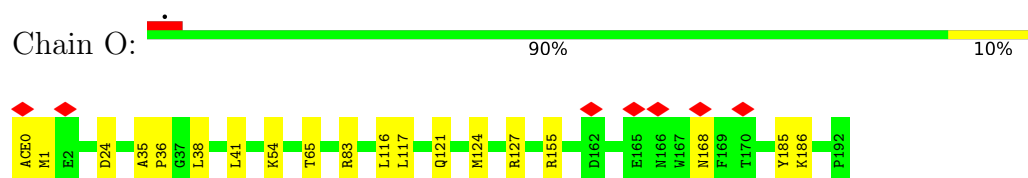
- Molecule 12: NADH-ubiquinone oxidoreductase chain 4



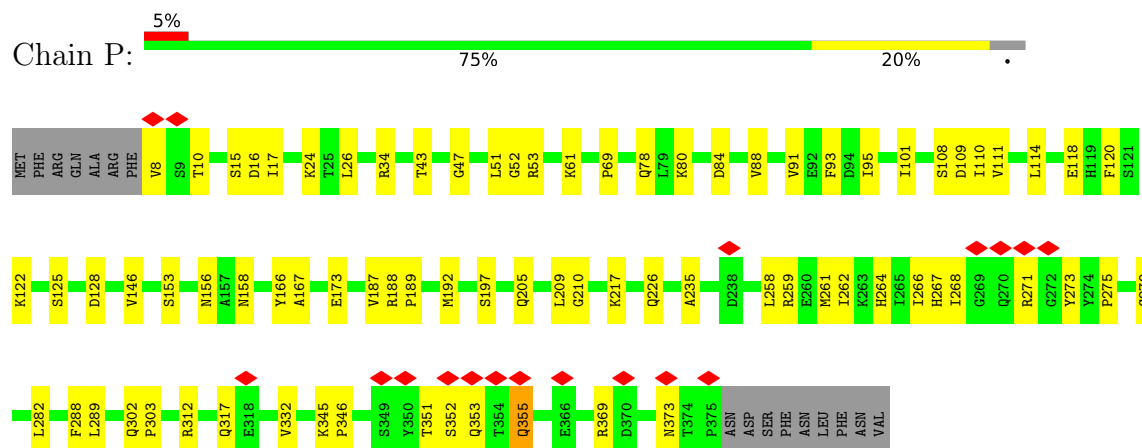
- Molecule 13: NADH-ubiquinone oxidoreductase chain 2



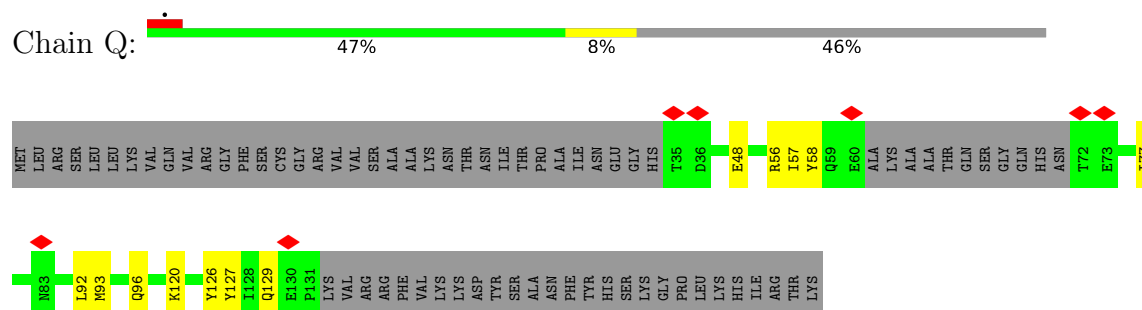
- Molecule 14: NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)




- Molecule 15: NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

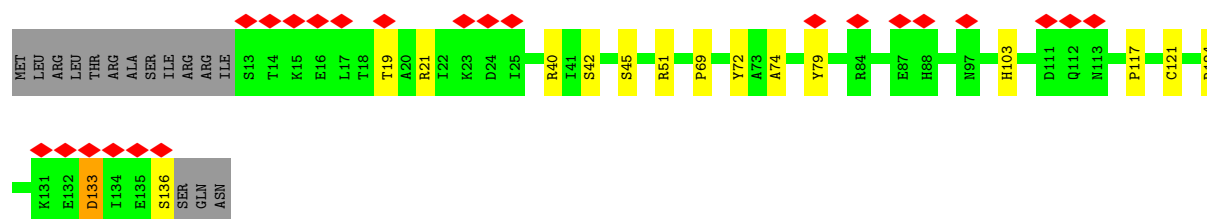


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial




- Molecule 17: NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain R: 



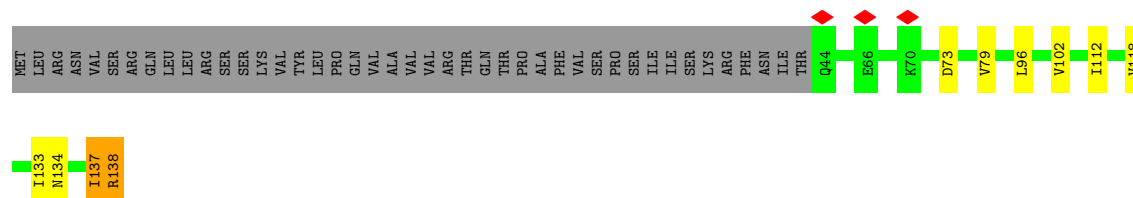
- Molecule 18: NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain S: 



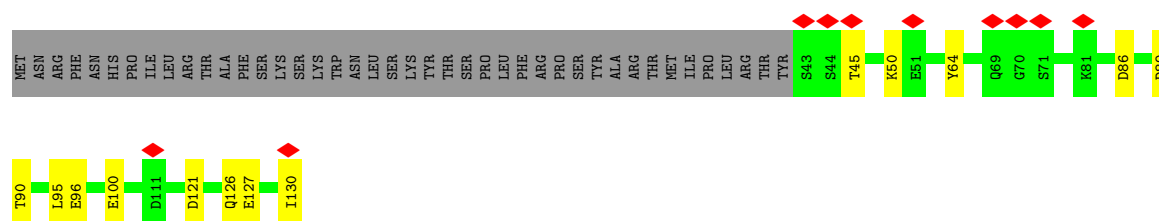
- Molecule 19: Acyl carrier protein

Chain T: 




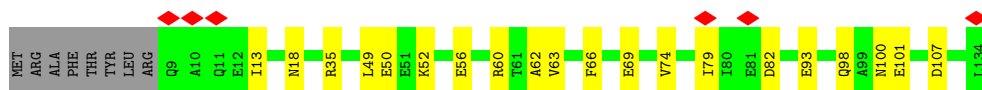
- Molecule 20: Acyl carrier protein

Chain U: 

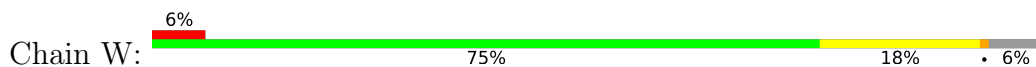


- Molecule 21: NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain V: 



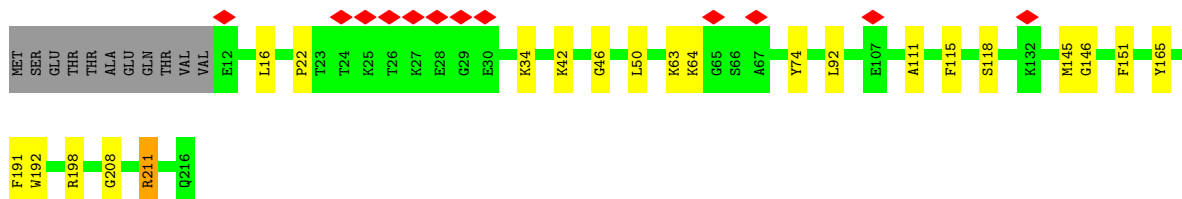
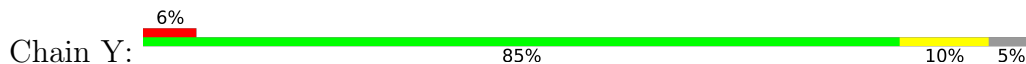
- Molecule 22: BA75_04796T0



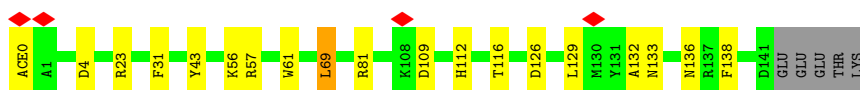
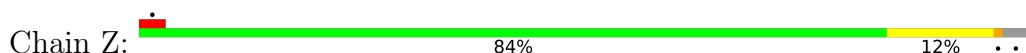
- Molecule 23: NADH-ubiquinone oxidoreductase



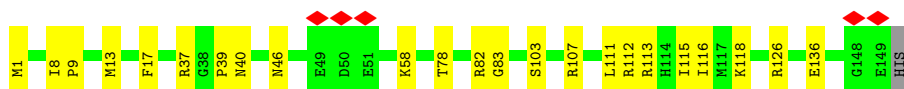
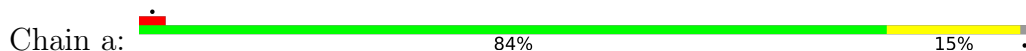
- Molecule 24: NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



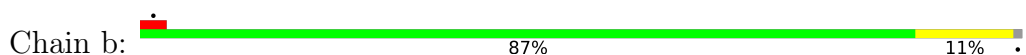
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

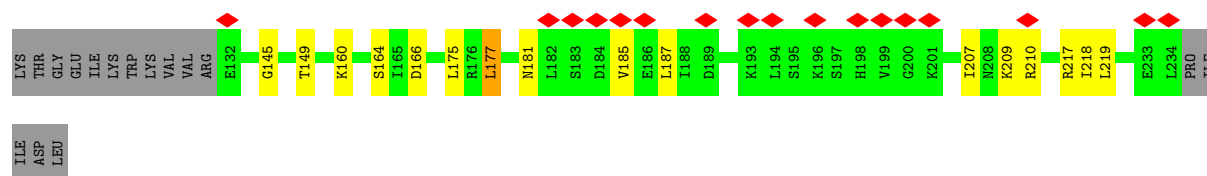


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

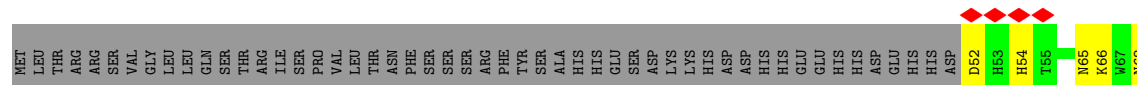


- Molecule 27: NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

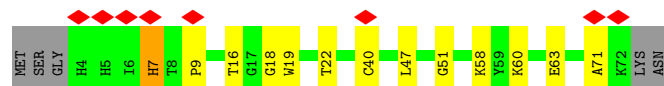
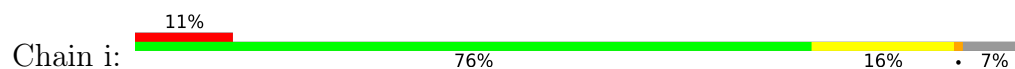




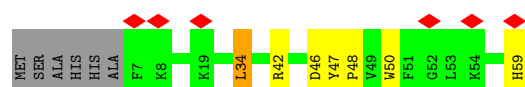
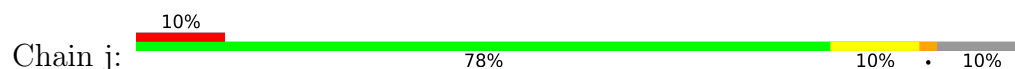
- Molecule 33: NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



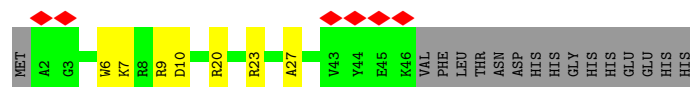
- Molecule 34: NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



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



- Molecule 36: NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

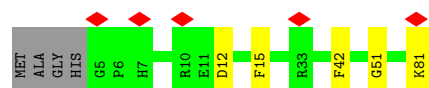
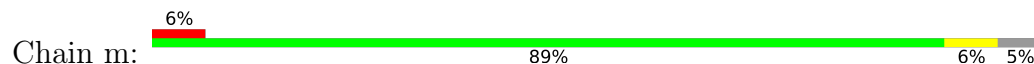


- Molecule 37: NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

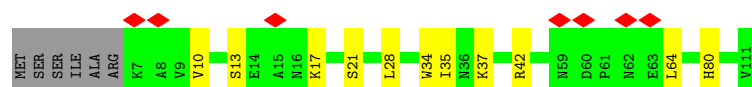
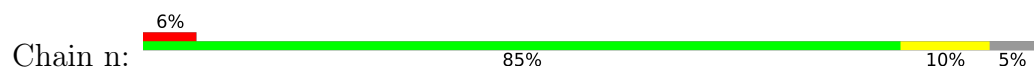




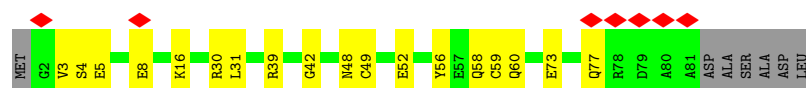
- Molecule 38: NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



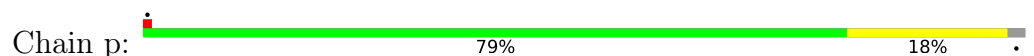
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



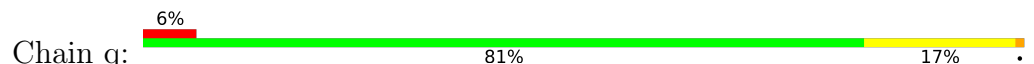
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 41: NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 42: 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	61256	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	0.079	Depositor
Minimum map value	-0.036	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0127	Depositor
Map size (\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 (\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: SF4, K, CDL, 3PE, PLC, FME, EHZ, NDP, ACE, ZN, FES, 2MR

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	0.11	0/1405	0.25	0/1896
2	A	0.13	0/1151	0.23	0/1564
3	B	0.16	0/1450	0.27	0/1969
4	C	0.14	0/2033	0.26	0/2770
5	D	0.14	0/3698	0.26	0/5007
6	G	0.11	0/4642	0.27	0/6299
7	H	0.15	0/2880	0.27	0/3939
8	I	0.15	0/1596	0.28	0/2164
9	J	0.14	0/1329	0.28	0/1816
10	K	0.13	0/610	0.24	0/828
11	L	0.14	0/5236	0.26	0/7128
12	M	0.15	0/3940	0.27	0/5379
13	N	0.14	0/4110	0.26	0/5609
14	O	0.21	1/1621 (0.1%)	0.28	0/2199
15	P	0.13	0/2985	0.26	0/4035
16	Q	0.13	0/726	0.24	0/979
17	R	0.11	0/998	0.25	0/1350
18	S	0.26	1/710 (0.1%)	0.32	1/961 (0.1%)
19	T	0.10	0/752	0.23	0/1021
20	U	0.11	0/688	0.22	0/936
21	V	0.12	0/1044	0.24	0/1411
22	W	0.12	0/999	0.21	0/1340
23	X	0.20	1/1475 (0.1%)	0.25	0/1990
24	Y	0.12	0/1615	0.24	0/2175
25	Z	0.22	1/1210 (0.1%)	0.24	0/1639
26	a	0.13	0/1241	0.25	0/1670
27	b	0.13	0/666	0.25	0/911
28	c	0.21	1/1282 (0.1%)	0.25	0/1736
29	d	0.12	0/633	0.21	0/854
30	e	0.13	0/865	0.24	0/1158
31	f	0.12	0/663	0.20	0/896
32	g	0.11	0/1293	0.24	0/1735

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.13	0/1114	0.27	0/1516
34	i	0.14	0/571	0.31	0/777
35	j	0.11	0/484	0.25	0/658
36	k	0.12	0/382	0.23	0/514
37	l	0.13	0/1119	0.27	0/1520
38	m	0.12	0/661	0.23	0/893
39	n	0.12	0/884	0.23	0/1197
40	o	0.11	0/696	0.22	0/933
41	p	0.13	0/756	0.25	0/1020
42	q	0.22	1/1192 (0.1%)	0.29	0/1620
All	All	0.14	6/63405 (0.0%)	0.26	1/86012 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	S	0	ACE	C-N	6.21	1.45	1.33
14	O	0	ACE	C-N	6.15	1.45	1.33
28	c	0	ACE	C-N	6.14	1.45	1.33
25	Z	0	ACE	C-N	6.13	1.45	1.33
42	q	0	ACE	C-N	6.08	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	S	2	SER	CB-CA-C	-5.28	109.51	115.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1383	0	1390	24	0
2	A	1133	0	1167	32	0
3	B	1407	0	1372	28	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1970	0	1905	26	0
5	D	3621	0	3531	62	0
6	G	4563	0	4527	89	0
7	H	2809	0	2880	60	0
8	I	1556	0	1499	31	0
9	J	1313	0	1320	36	0
10	K	617	0	657	18	0
11	L	5115	0	5338	90	0
12	M	3868	0	4127	75	0
13	N	4045	0	4327	42	0
14	O	1575	0	1523	11	0
15	P	2922	0	2915	53	0
16	Q	711	0	679	9	0
17	R	978	0	964	11	0
18	S	697	0	736	12	0
19	T	745	0	734	7	0
20	U	681	0	664	7	0
21	V	1025	0	1035	14	0
22	W	979	0	980	15	0
23	X	1450	0	1422	10	0
24	Y	1578	0	1567	16	0
25	Z	1176	0	1165	15	0
26	a	1215	0	1197	19	0
27	b	641	0	620	7	0
28	c	1256	0	1281	20	0
29	d	616	0	624	6	0
30	e	848	0	830	9	0
31	f	642	0	640	7	0
32	g	1280	0	1302	19	0
33	h	1078	0	1036	16	0
34	i	552	0	540	11	0
35	j	460	0	455	5	0
36	k	368	0	348	6	0
37	l	1082	0	1033	9	0
38	m	642	0	635	5	0
39	n	861	0	866	8	0
40	o	682	0	677	9	0
41	p	740	0	700	13	0
42	q	1156	0	1115	20	0
43	A	31	0	36	2	0
43	B	31	0	36	0	0
43	D	42	0	64	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	H	24	0	22	1	0
43	L	109	0	146	9	0
43	M	84	0	128	5	0
43	P	31	0	36	4	0
43	Y	72	0	98	5	0
43	Z	42	0	64	0	0
43	a	22	0	18	2	0
43	b	39	0	55	1	0
43	d	84	0	128	4	0
43	g	39	0	55	3	0
43	h	42	0	64	2	0
43	q	78	0	113	4	0
44	B	8	0	0	0	0
44	G	16	0	0	1	0
44	I	16	0	0	4	0
45	G	4	0	0	0	0
46	G	1	0	0	0	0
47	H	31	0	36	0	0
47	L	400	0	596	36	0
47	M	35	0	44	1	0
47	N	40	0	57	1	0
47	O	66	0	80	2	0
47	Y	26	0	26	2	0
47	Z	36	0	46	3	0
47	b	40	0	57	1	0
47	f	51	0	82	6	0
47	j	27	0	28	1	0
47	m	60	0	68	2	0
48	O	75	0	97	4	0
48	P	42	0	28	1	0
48	Z	49	0	42	0	0
48	b	59	0	62	3	0
48	c	60	0	64	3	0
49	P	48	0	25	0	0
50	R	1	0	0	0	0
51	T	37	0	0	0	0
51	U	37	0	0	1	0
All	All	64071	0	64824	826	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 826 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)
17:R:103:HIS:CD2	17:R:121:CYS:SG	2.68	0.87
12:M:24:ASN:HB3	12:M:30:LYS:HD2	1.65	0.78
43:L:705:PLC:H42	34:i:18:GLY:HA2	1.64	0.78
5:D:380:PHE:HB2	6:G:144:ASP:HB2	1.69	0.73
5:D:121:HIS:HB2	5:D:126:LEU:HD11	1.71	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%)	135 (97%)	4 (3%)	0	100	100
3	B	173/204 (85%)	168 (97%)	5 (3%)	0	100	100
4	C	238/289 (82%)	231 (97%)	7 (3%)	0	100	100
5	D	448/482 (93%)	432 (96%)	15 (3%)	1 (0%)	44	73
6	G	580/726 (80%)	562 (97%)	18 (3%)	0	100	100
7	H	351/353 (99%)	338 (96%)	11 (3%)	2 (1%)	22	52
8	I	190/222 (86%)	186 (98%)	4 (2%)	0	100	100
9	J	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
10	K	78/82 (95%)	78 (100%)	0	0	100	100
11	L	640/642 (100%)	626 (98%)	13 (2%)	1 (0%)	44	73
12	M	489/491 (100%)	475 (97%)	14 (3%)	0	100	100
13	N	502/523 (96%)	490 (98%)	12 (2%)	0	100	100
14	O	191/193 (99%)	186 (97%)	5 (3%)	0	100	100
15	P	366/384 (95%)	355 (97%)	11 (3%)	0	100	100
16	Q	82/159 (52%)	82 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	122/139 (88%)	120 (98%)	2 (2%)	0	100	100
18	S	88/90 (98%)	85 (97%)	3 (3%)	0	100	100
19	T	93/138 (67%)	91 (98%)	2 (2%)	0	100	100
20	U	86/130 (66%)	81 (94%)	5 (6%)	0	100	100
21	V	124/134 (92%)	121 (98%)	3 (2%)	0	100	100
22	W	111/122 (91%)	110 (99%)	1 (1%)	0	100	100
23	X	182/184 (99%)	182 (100%)	0	0	100	100
24	Y	203/216 (94%)	194 (96%)	9 (4%)	0	100	100
25	Z	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
26	a	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
27	b	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
28	c	157/182 (86%)	153 (98%)	4 (2%)	0	100	100
29	d	73/78 (94%)	72 (99%)	1 (1%)	0	100	100
30	e	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
31	f	76/86 (88%)	76 (100%)	0	0	100	100
32	g	152/239 (64%)	146 (96%)	6 (4%)	0	100	100
33	h	129/182 (71%)	124 (96%)	5 (4%)	0	100	100
34	i	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
35	j	51/59 (86%)	49 (96%)	2 (4%)	0	100	100
36	k	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
37	l	130/156 (83%)	127 (98%)	3 (2%)	0	100	100
38	m	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
39	n	103/111 (93%)	103 (100%)	0	0	100	100
40	o	78/87 (90%)	75 (96%)	3 (4%)	0	100	100
41	p	88/92 (96%)	86 (98%)	2 (2%)	0	100	100
42	q	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
All	All	7628/8505 (90%)	7420 (97%)	204 (3%)	4 (0%)	50	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	222	VAL
7	H	2	LEU

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Mol	Chain	Res	Type
5	D	33	ALA
11	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	62
2	A	128/128 (100%)	124 (97%)	4 (3%)	35	70
3	B	154/180 (86%)	151 (98%)	3 (2%)	52	81
4	C	214/254 (84%)	210 (98%)	4 (2%)	52	81
5	D	384/408 (94%)	378 (98%)	6 (2%)	58	84
6	G	498/610 (82%)	490 (98%)	8 (2%)	58	84
7	H	307/307 (100%)	298 (97%)	9 (3%)	37	72
8	I	166/192 (86%)	158 (95%)	8 (5%)	21	54
9	J	149/149 (100%)	143 (96%)	6 (4%)	27	61
10	K	70/72 (97%)	65 (93%)	5 (7%)	12	36
11	L	576/576 (100%)	564 (98%)	12 (2%)	48	78
12	M	439/439 (100%)	425 (97%)	14 (3%)	34	69
13	N	474/489 (97%)	462 (98%)	12 (2%)	42	75
14	O	169/169 (100%)	164 (97%)	5 (3%)	36	71
15	P	317/332 (96%)	313 (99%)	4 (1%)	65	88
16	Q	74/135 (55%)	74 (100%)	0	100	100
17	R	104/118 (88%)	103 (99%)	1 (1%)	73	91
18	S	77/77 (100%)	74 (96%)	3 (4%)	27	62
19	T	87/128 (68%)	82 (94%)	5 (6%)	17	47
20	U	80/120 (67%)	76 (95%)	4 (5%)	20	52
21	V	112/119 (94%)	111 (99%)	1 (1%)	75	92
22	W	107/114 (94%)	105 (98%)	2 (2%)	52	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	X	165/165 (100%)	163 (99%)	2 (1%)	67	89
24	Y	163/173 (94%)	160 (98%)	3 (2%)	54	82
25	Z	123/128 (96%)	120 (98%)	3 (2%)	44	76
26	a	128/129 (99%)	127 (99%)	1 (1%)	79	93
27	b	66/67 (98%)	65 (98%)	1 (2%)	60	85
28	c	140/159 (88%)	137 (98%)	3 (2%)	48	78
29	d	62/65 (95%)	61 (98%)	1 (2%)	58	84
30	e	91/92 (99%)	91 (100%)	0	100	100
31	f	64/71 (90%)	64 (100%)	0	100	100
32	g	143/215 (66%)	139 (97%)	4 (3%)	38	73
33	h	118/167 (71%)	117 (99%)	1 (1%)	79	93
34	i	59/63 (94%)	58 (98%)	1 (2%)	56	83
35	j	46/50 (92%)	44 (96%)	2 (4%)	25	57
36	k	32/47 (68%)	31 (97%)	1 (3%)	35	70
37	l	116/137 (85%)	111 (96%)	5 (4%)	25	57
38	m	64/66 (97%)	64 (100%)	0	100	100
39	n	95/100 (95%)	95 (100%)	0	100	100
40	o	74/79 (94%)	72 (97%)	2 (3%)	40	73
41	p	83/85 (98%)	83 (100%)	0	100	100
42	q	125/125 (100%)	122 (98%)	3 (2%)	44	76
All	All	6795/7467 (91%)	6640 (98%)	155 (2%)	46	77

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	U	45	THR
35	j	59	HIS
21	V	56	GLU
26	a	111	LEU
40	o	16	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
14	O	184	GLN
37	l	63	ASN
18	S	80	GLN
34	i	4	HIS
40	o	77	GLN

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
2	FME	A	1	2	8,9,10	1.53	1 (12%)	7,9,11	1.76	2 (28%)
7	FME	H	1	7	8,9,10	1.53	1 (12%)	7,9,11	1.56	1 (14%)
12	FME	M	1	12	8,9,10	1.51	1 (12%)	7,9,11	1.55	1 (14%)
10	FME	K	1	10	8,9,10	1.50	1 (12%)	7,9,11	1.56	1 (14%)
9	FME	J	1	9	8,9,10	1.49	1 (12%)	7,9,11	1.64	2 (28%)
5	2MR	D	137	5	10,12,13	2.36	2 (20%)	5,13,15	1.91	1 (20%)
11	FME	L	1	11	8,9,10	1.49	1 (12%)	7,9,11	1.62	2 (28%)
13	FME	N	1	13	8,9,10	1.49	1 (12%)	7,9,11	1.52	1 (14%)

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
2	FME	A	1	2	-	5/7/9/11	-
7	FME	H	1	7	-	5/7/9/11	-

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

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	5.24	1.45	1.33
5	D	137	2MR	CZ-NE	4.87	1.44	1.34
7	H	1	FME	CN-N	3.74	1.45	1.33
2	A	1	FME	CN-N	3.71	1.45	1.33
12	M	1	FME	CN-N	3.71	1.45	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	137	2MR	CD-NE-CZ	-3.50	116.86	123.41
2	A	1	FME	CE-SD-CG	2.99	110.67	100.40
12	M	1	FME	CE-SD-CG	2.77	109.93	100.40
7	H	1	FME	CE-SD-CG	2.66	109.55	100.40
10	K	1	FME	CE-SD-CG	2.66	109.53	100.40

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	FME	O1-CN-N-CA
2	A	1	FME	CB-CA-N-CN
2	A	1	FME	N-CA-CB-CG
2	A	1	FME	C-CA-CB-CG
7	H	1	FME	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	FME	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	1	FME	1	0
9	J	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 2 are monoatomic - leaving 56 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	PLC	D	501	-	41,41,41	0.50	0	47,49,49	0.57	1 (2%)
47	3PE	L	707	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
47	3PE	j	101	-	26,26,50	1.16	4 (15%)	29,31,55	1.17	2 (6%)
48	CDL	b	102	-	58,58,99	1.11	8 (13%)	64,70,111	1.22	4 (6%)
48	CDL	Z	202	-	48,48,99	1.22	8 (16%)	54,60,111	1.27	4 (7%)
48	CDL	c	201	-	59,59,99	1.10	8 (13%)	65,71,111	1.17	4 (6%)
47	3PE	Z	203	-	35,35,50	1.01	4 (11%)	38,40,55	1.13	2 (5%)
47	3PE	m	102	-	34,34,50	1.03	4 (11%)	37,39,55	1.10	2 (5%)
43	PLC	q	202	-	35,35,41	0.55	0	41,43,49	0.63	0
47	3PE	f	101	-	50,50,50	0.86	4 (8%)	53,55,55	1.11	2 (3%)
47	3PE	m	101	-	24,24,50	1.21	4 (16%)	27,29,55	1.38	2 (7%)
47	3PE	L	711	-	45,45,50	0.90	4 (8%)	48,50,55	1.11	2 (4%)
47	3PE	N	601	-	39,39,50	0.97	4 (10%)	42,44,55	1.16	2 (4%)
44	SF4	I	302	8	0,12,12	-	-	-	-	-
47	3PE	L	703	-	41,41,50	0.95	3 (7%)	44,46,55	1.15	2 (4%)
43	PLC	L	702	-	34,34,41	0.56	0	40,42,49	0.63	1 (2%)
43	PLC	d	102	-	41,41,41	0.52	0	47,49,49	0.51	0
44	SF4	B	301	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	SF4	G	802	6	0,12,12	-	-	-		
43	PLC	h	201	-	41,41,41	0.51	0	47,49,49	0.52	0
43	PLC	d	101	-	41,41,41	0.52	0	47,49,49	0.54	0
51	EHZ	T	201	19	29,36,37	1.68	5 (17%)	35,44,47	1.58	7 (20%)
43	PLC	Y	301	-	35,35,41	0.55	0	41,43,49	0.51	0
44	SF4	I	301	8	0,12,12	-	-	-		
47	3PE	L	708	-	50,50,50	0.85	4 (8%)	53,55,55	1.11	2 (3%)
47	3PE	L	710	-	50,50,50	0.86	4 (8%)	53,55,55	1.11	2 (3%)
47	3PE	L	712	-	50,50,50	0.86	4 (8%)	53,55,55	1.12	2 (3%)
43	PLC	P	502	-	30,30,41	0.58	0	36,38,49	0.60	0
47	3PE	Y	302	-	25,25,50	1.18	4 (16%)	28,30,55	1.29	3 (10%)
47	3PE	L	709	-	45,45,50	0.90	4 (8%)	48,50,55	1.10	2 (4%)
51	EHZ	U	201	20	29,36,37	1.68	5 (17%)	35,44,47	1.61	8 (22%)
43	PLC	a	201	-	21,21,41	0.68	0	27,29,49	0.65	0
47	3PE	H	402	-	30,30,50	1.08	4 (13%)	33,35,55	1.16	2 (6%)
43	PLC	L	705	-	41,41,41	0.52	0	47,49,49	0.65	1 (2%)
48	CDL	O	201	-	74,74,99	0.99	7 (9%)	80,86,111	1.13	5 (6%)
43	PLC	M	1002	-	41,41,41	0.52	0	47,49,49	0.50	0
43	PLC	b	101	-	38,38,41	0.53	0	44,46,49	0.54	0
43	PLC	H	401	-	23,23,41	0.68	0	29,31,49	0.61	1 (3%)
43	PLC	M	1001	-	41,41,41	0.52	0	47,49,49	0.52	0
43	PLC	q	201	-	41,41,41	0.52	0	47,49,49	0.52	0
48	CDL	P	503	-	41,41,99	1.27	7 (17%)	47,53,111	1.32	4 (8%)
49	NDP	P	501	-	45,52,52	4.28	23 (51%)	53,80,80	2.11	5 (9%)
43	PLC	A	201	-	30,30,41	0.60	0	36,38,49	0.53	0
43	PLC	L	704	-	31,31,41	0.55	0	37,39,49	0.57	0
43	PLC	B	302	-	30,30,41	0.59	0	36,38,49	0.55	0
47	3PE	M	1003	-	34,34,50	1.02	4 (11%)	37,39,55	1.16	2 (5%)
44	SF4	G	801	6	0,12,12	-	-	-		
47	3PE	L	706	-	32,32,50	1.06	4 (12%)	35,37,55	1.18	2 (5%)
47	3PE	O	202	-	30,30,50	1.08	4 (13%)	33,35,55	1.12	2 (6%)
43	PLC	g	301	-	38,38,41	0.53	0	44,46,49	0.53	0
47	3PE	b	103	-	39,39,50	0.96	4 (10%)	42,44,55	1.12	2 (4%)
47	3PE	O	203	-	34,34,50	1.04	4 (11%)	37,39,55	1.17	2 (5%)
43	PLC	Z	201	-	41,41,41	0.52	0	47,49,49	0.53	0
47	3PE	L	701	-	28,28,50	1.13	4 (14%)	31,33,55	1.15	2 (6%)
43	PLC	Y	303	-	35,35,41	0.53	0	41,43,49	0.58	0
45	FES	G	803	6	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
43	PLC	D	501	-	-	18/45/45/45	-
47	3PE	L	707	-	-	33/54/54/54	-
47	3PE	j	101	-	-	12/30/30/54	-
48	CDL	b	102	-	-	32/69/69/110	-
48	CDL	Z	202	-	-	27/58/58/110	-
48	CDL	c	201	-	-	35/70/70/110	-
47	3PE	Z	203	-	-	22/39/39/54	-
47	3PE	m	102	-	-	12/38/38/54	-
43	PLC	q	202	-	-	13/39/39/45	-
47	3PE	f	101	-	-	26/54/54/54	-
47	3PE	m	101	-	-	15/27/27/54	-
47	3PE	L	711	-	-	28/49/49/54	-
47	3PE	N	601	-	-	20/43/43/54	-
44	SF4	I	302	8	-	-	0/6/5/5
47	3PE	L	703	-	-	22/45/45/54	-
43	PLC	L	702	-	-	18/38/38/45	-
43	PLC	d	102	-	-	19/45/45/45	-
44	SF4	B	301	3	-	-	0/6/5/5
44	SF4	G	802	6	-	-	0/6/5/5
43	PLC	h	201	-	-	21/45/45/45	-
43	PLC	d	101	-	-	14/45/45/45	-
51	EHZ	T	201	19	-	22/42/44/45	-
43	PLC	Y	301	-	-	8/39/39/45	-
47	3PE	L	708	-	-	20/54/54/54	-
44	SF4	I	301	8	-	-	0/6/5/5
47	3PE	L	710	-	-	23/54/54/54	-
47	3PE	L	712	-	-	29/54/54/54	-
43	PLC	P	502	-	-	11/34/34/45	-
47	3PE	Y	302	-	-	12/28/28/54	-
47	3PE	L	709	-	-	23/49/49/54	-
51	EHZ	U	201	20	-	15/42/44/45	-
43	PLC	a	201	-	-	7/23/23/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	3PE	H	402	-	-	18/34/34/54	-
43	PLC	L	705	-	-	21/45/45/45	-
48	CDL	O	201	-	-	45/85/85/110	-
43	PLC	M	1002	-	-	15/45/45/45	-
43	PLC	b	101	-	-	14/42/42/45	-
43	PLC	H	401	-	-	8/26/26/45	-
43	PLC	M	1001	-	-	14/45/45/45	-
43	PLC	q	201	-	-	20/45/45/45	-
48	CDL	P	503	-	-	21/50/50/110	-
49	NDP	P	501	-	-	11/30/77/77	0/5/5/5
43	PLC	A	201	-	-	9/34/34/45	-
43	PLC	L	704	-	-	17/35/35/45	-
43	PLC	B	302	-	-	14/34/34/45	-
47	3PE	M	1003	-	-	15/38/38/54	-
44	SF4	G	801	6	-	-	0/6/5/5
47	3PE	L	706	-	-	16/36/36/54	-
47	3PE	O	202	-	-	21/34/34/54	-
43	PLC	g	301	-	-	16/42/42/45	-
47	3PE	b	103	-	-	29/43/43/54	-
47	3PE	O	203	-	-	21/38/38/54	-
43	PLC	Z	201	-	-	16/45/45/45	-
47	3PE	L	701	-	-	14/32/32/54	-
43	PLC	Y	303	-	-	17/39/39/45	-
45	FES	G	803	6	-	-	0/1/1/1

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	P	501	NDP	O4B-C1B	14.86	1.61	1.41
49	P	501	NDP	C6N-C5N	12.21	1.55	1.33
49	P	501	NDP	C7N-N7N	8.27	1.55	1.33
49	P	501	NDP	O4D-C1D	8.02	1.61	1.42
49	P	501	NDP	C2D-C1D	-7.21	1.30	1.53

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	P	501	NDP	C5A-C6A-N6A	8.56	133.36	120.35
49	P	501	NDP	C1B-N9A-C4A	-7.78	112.97	126.64
49	P	501	NDP	N6A-C6A-N1A	-6.02	106.09	118.57
49	P	501	NDP	N3A-C2A-N1A	-5.57	119.97	128.68
51	U	201	EHZ	C8-C9-S1	5.34	120.24	113.63

There are no chirality outliers.

5 of 949 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	A	201	PLC	O4P-C4-C5-N
43	A	201	PLC	C1'-C'-O2-C2
43	A	201	PLC	O'-C'-O2-C2
43	A	201	PLC	C4-O4P-P-O3P
43	B	302	PLC	O4P-C4-C5-N

There are no ring outliers.

46 monomers are involved in 112 short contacts:

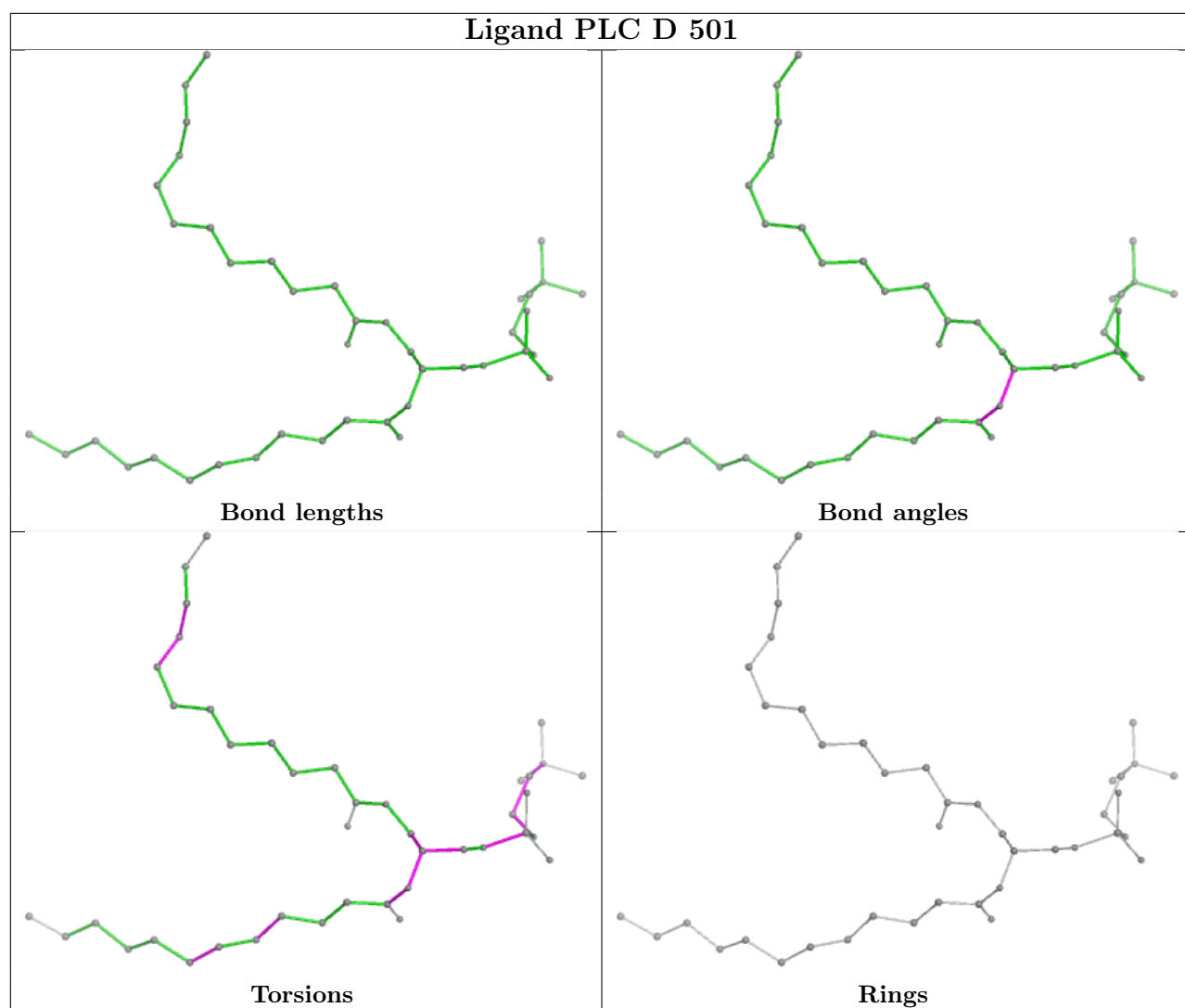
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	D	501	PLC	2	0
47	L	707	3PE	8	0
47	j	101	3PE	1	0
48	b	102	CDL	3	0
48	c	201	CDL	3	0
47	Z	203	3PE	3	0
47	m	102	3PE	2	0
43	q	202	PLC	3	0
47	f	101	3PE	6	0
47	m	101	3PE	1	0
47	L	711	3PE	8	0
47	N	601	3PE	1	0
44	I	302	SF4	2	0
47	L	703	3PE	6	0
43	L	702	PLC	3	0
43	d	102	PLC	2	0
43	h	201	PLC	2	0
43	d	101	PLC	2	0
43	Y	301	PLC	1	0
44	I	301	SF4	2	0
47	L	708	3PE	4	0
47	L	710	3PE	2	0

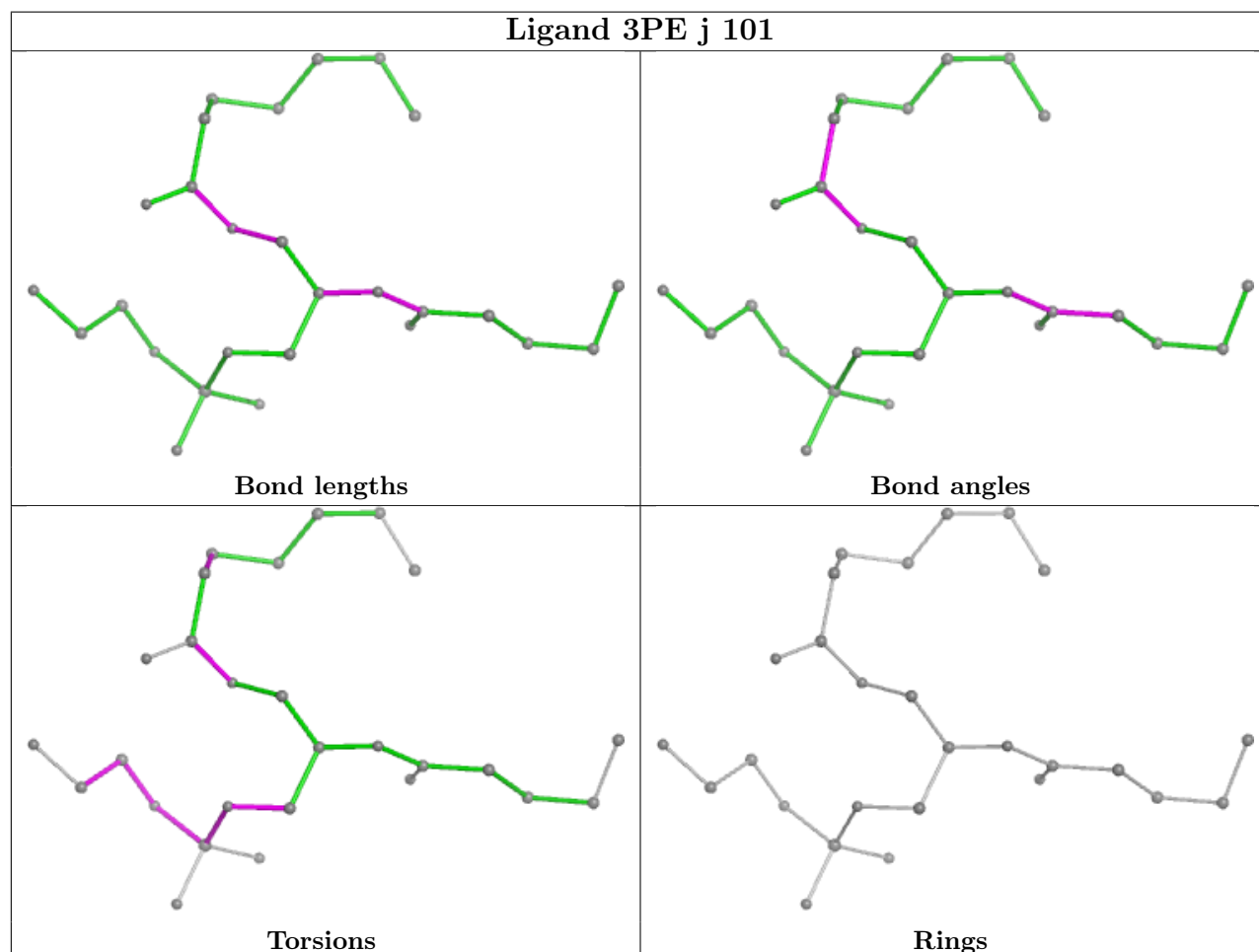
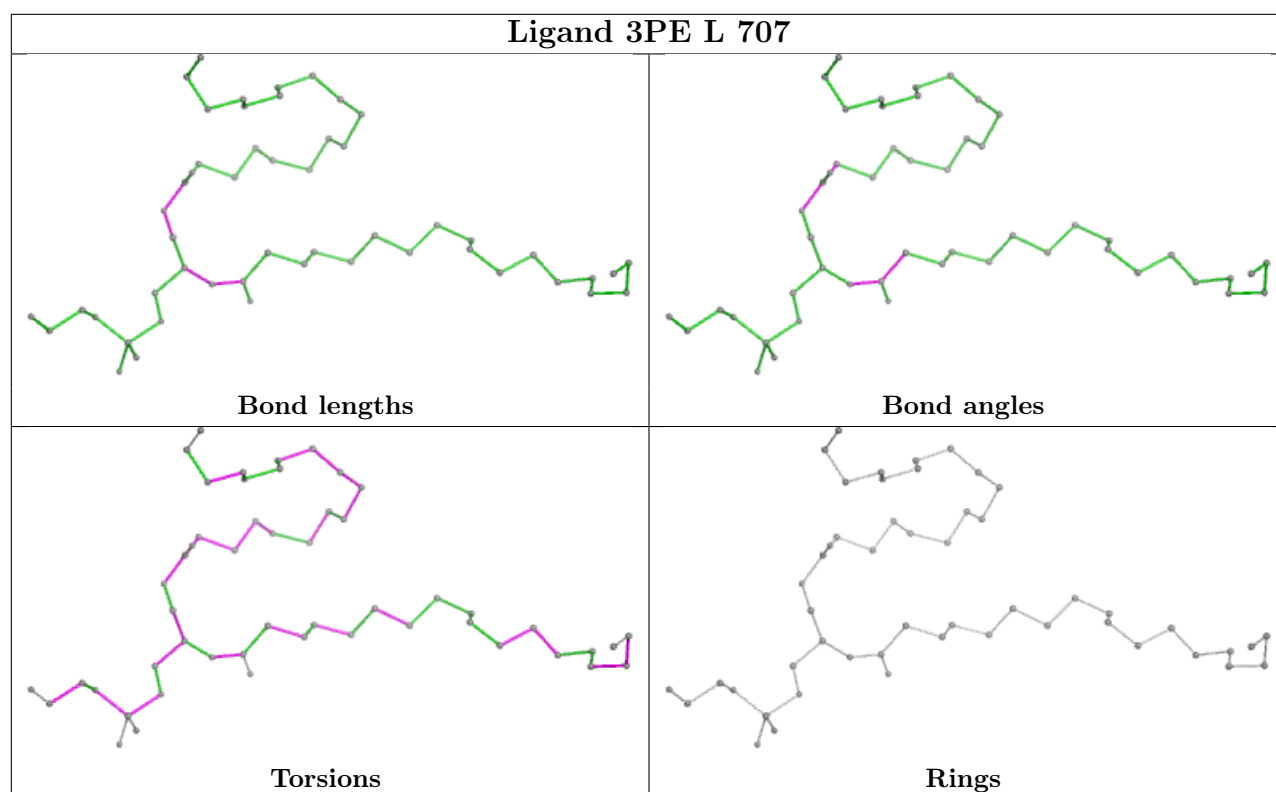
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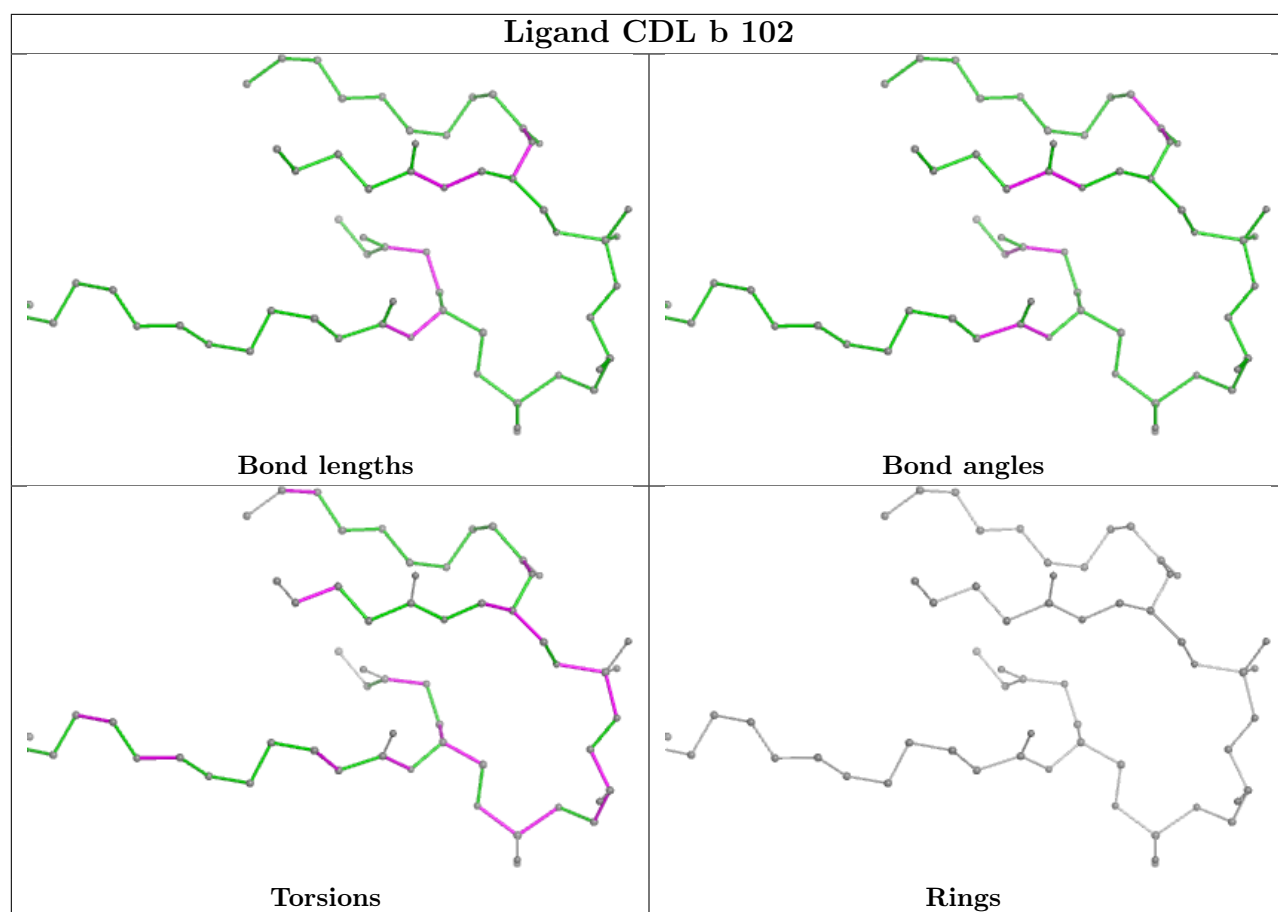
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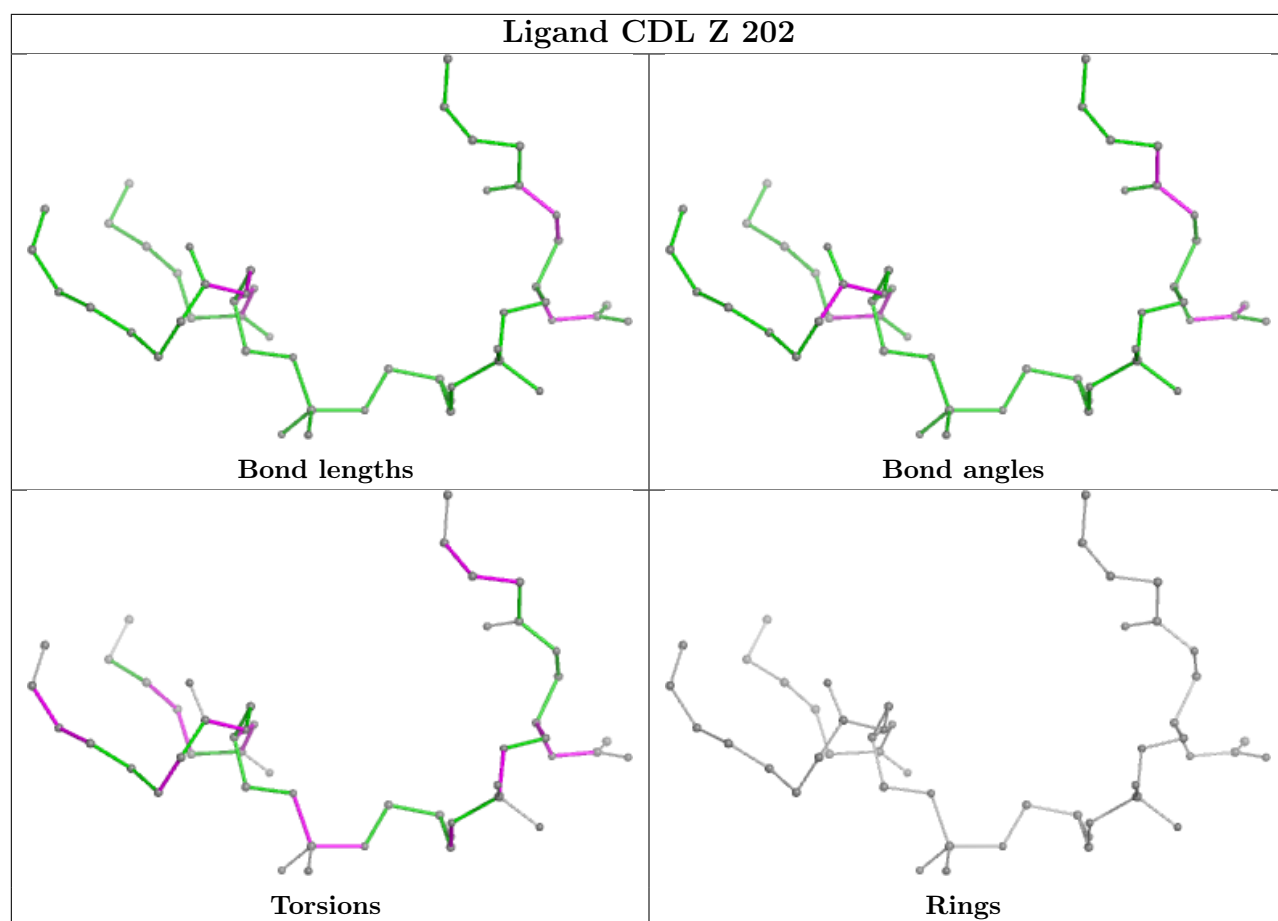
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	L	712	3PE	6	0
43	P	502	PLC	4	0
47	Y	302	3PE	2	0
47	L	709	3PE	1	0
51	U	201	EHZ	1	0
43	a	201	PLC	2	0
43	L	705	PLC	6	0
48	O	201	CDL	4	0
43	M	1002	PLC	1	0
43	b	101	PLC	1	0
43	H	401	PLC	1	0
43	M	1001	PLC	4	0
43	q	201	PLC	1	0
48	P	503	CDL	1	0
43	A	201	PLC	2	0
47	M	1003	3PE	1	0
44	G	801	SF4	1	0
47	L	706	3PE	1	0
47	O	202	3PE	1	0
43	g	301	PLC	3	0
47	b	103	3PE	1	0
47	O	203	3PE	1	0
47	L	701	3PE	2	0
43	Y	303	PLC	4	0

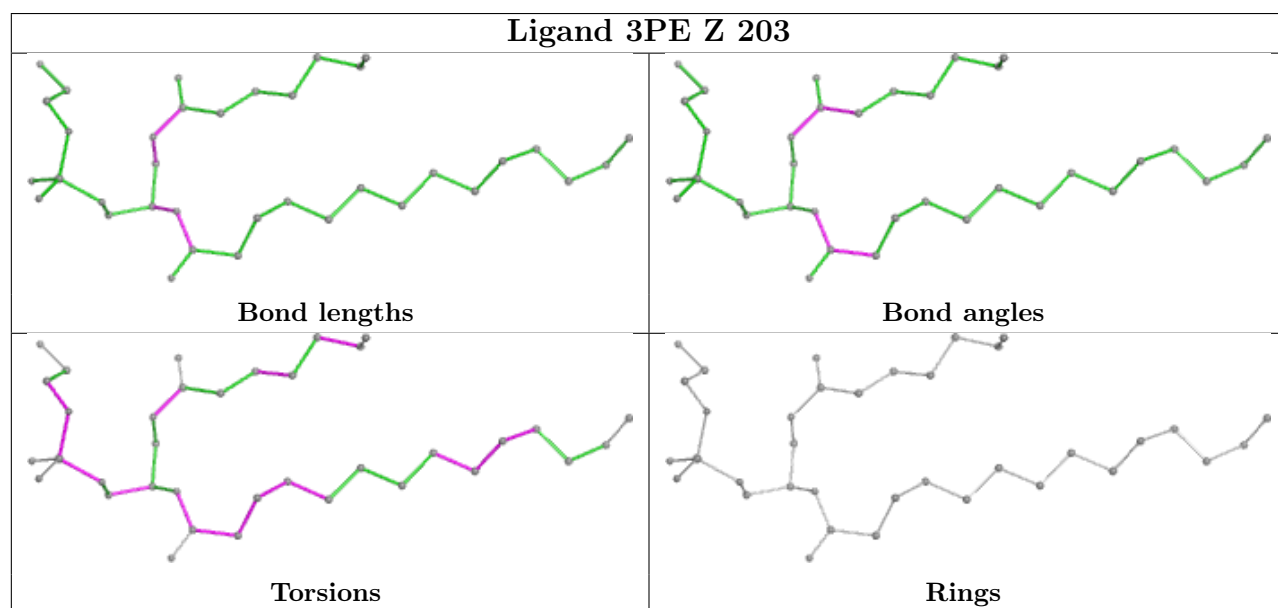
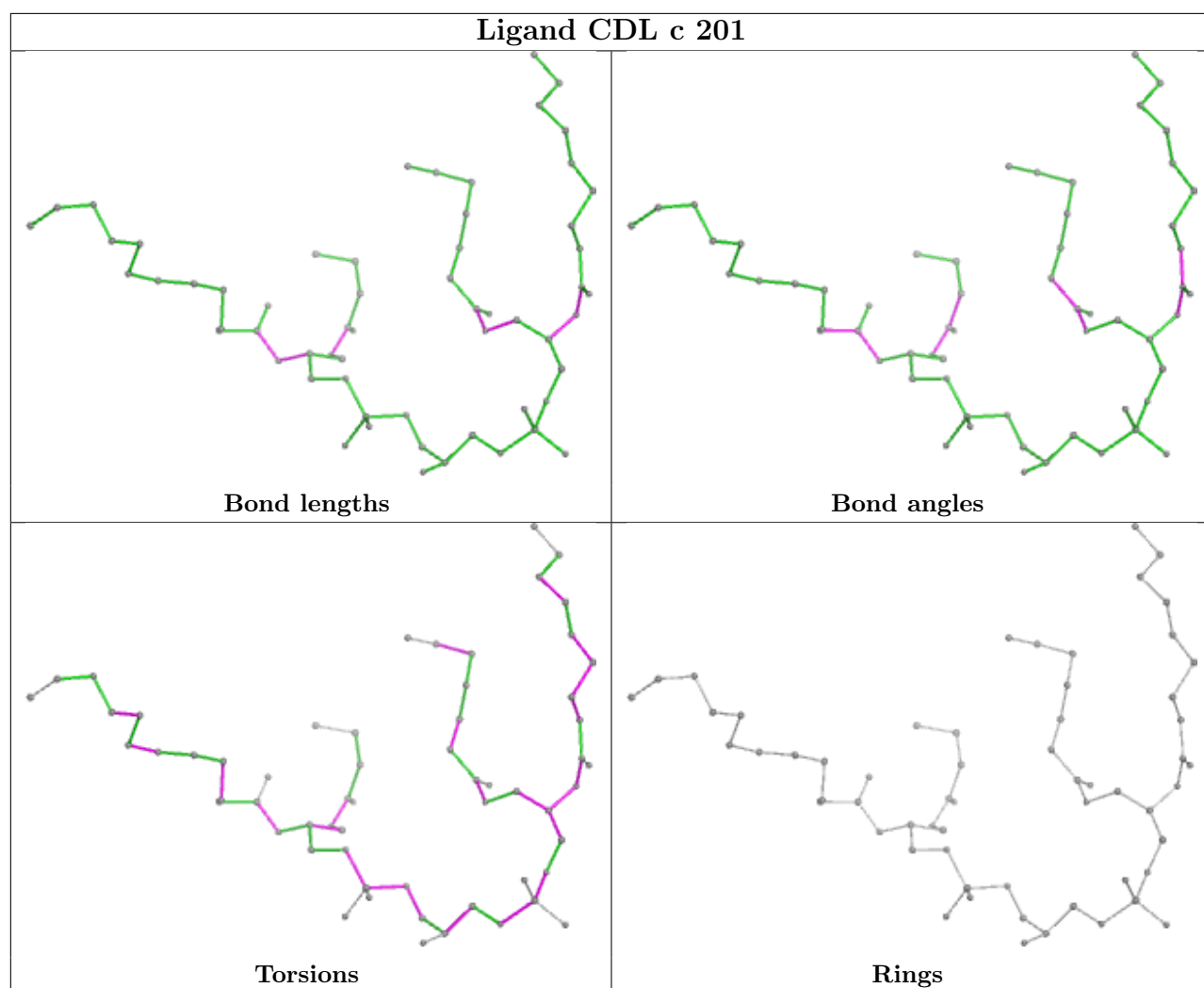
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

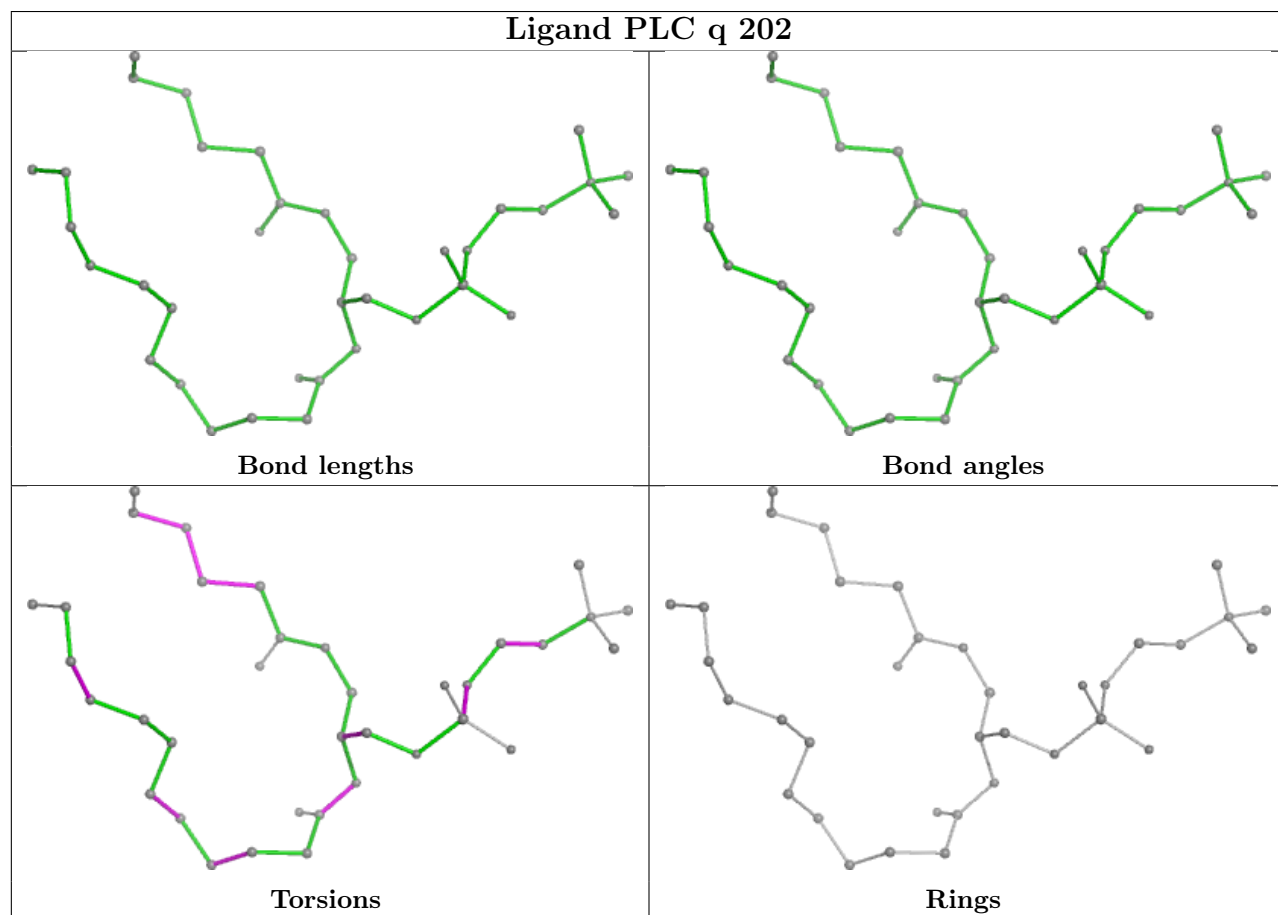
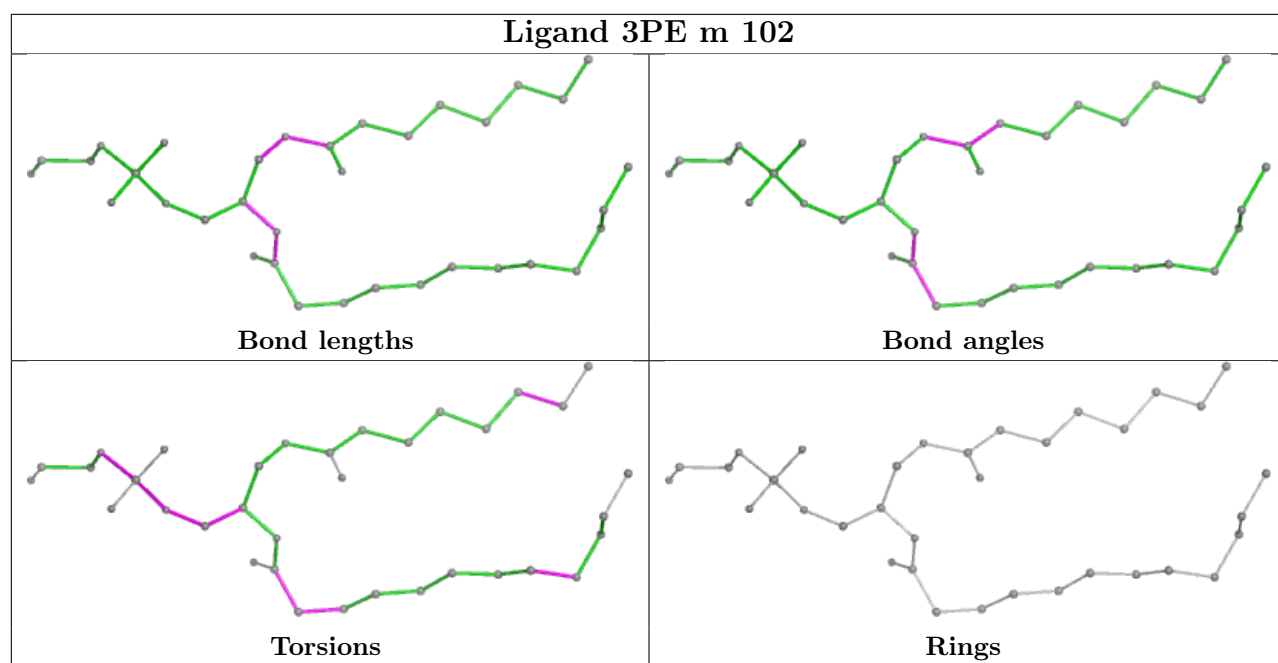


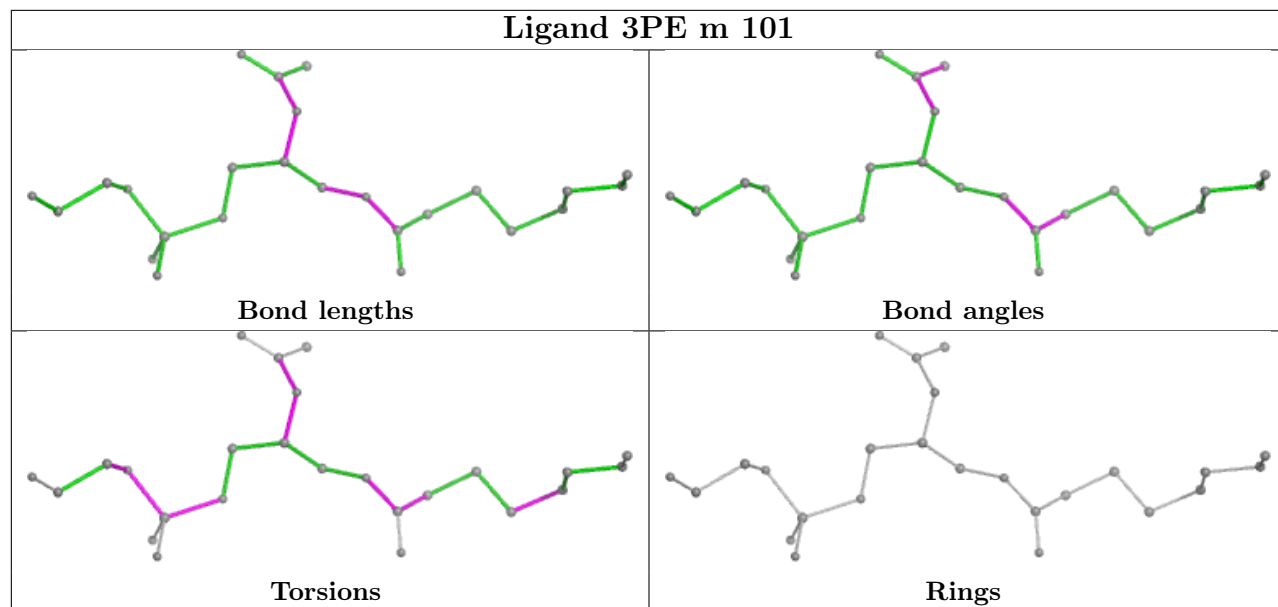
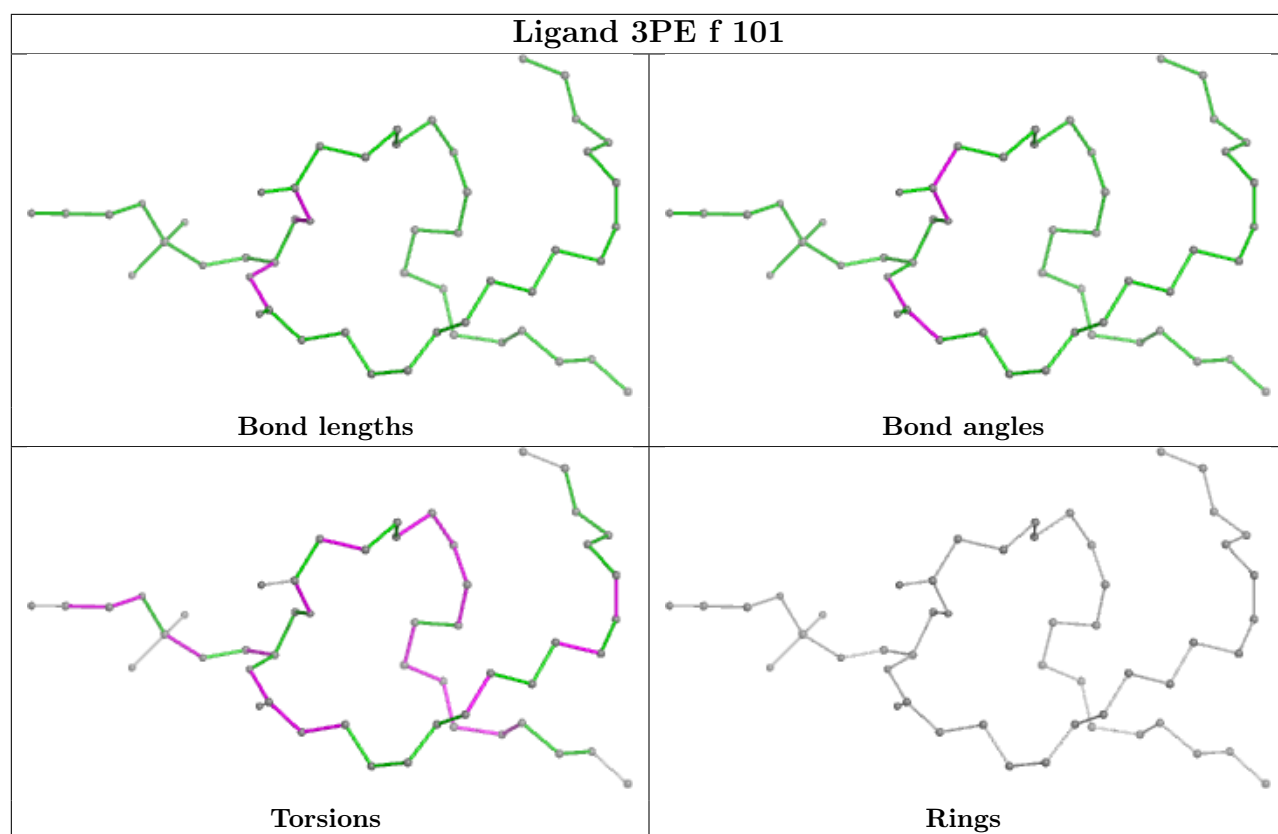




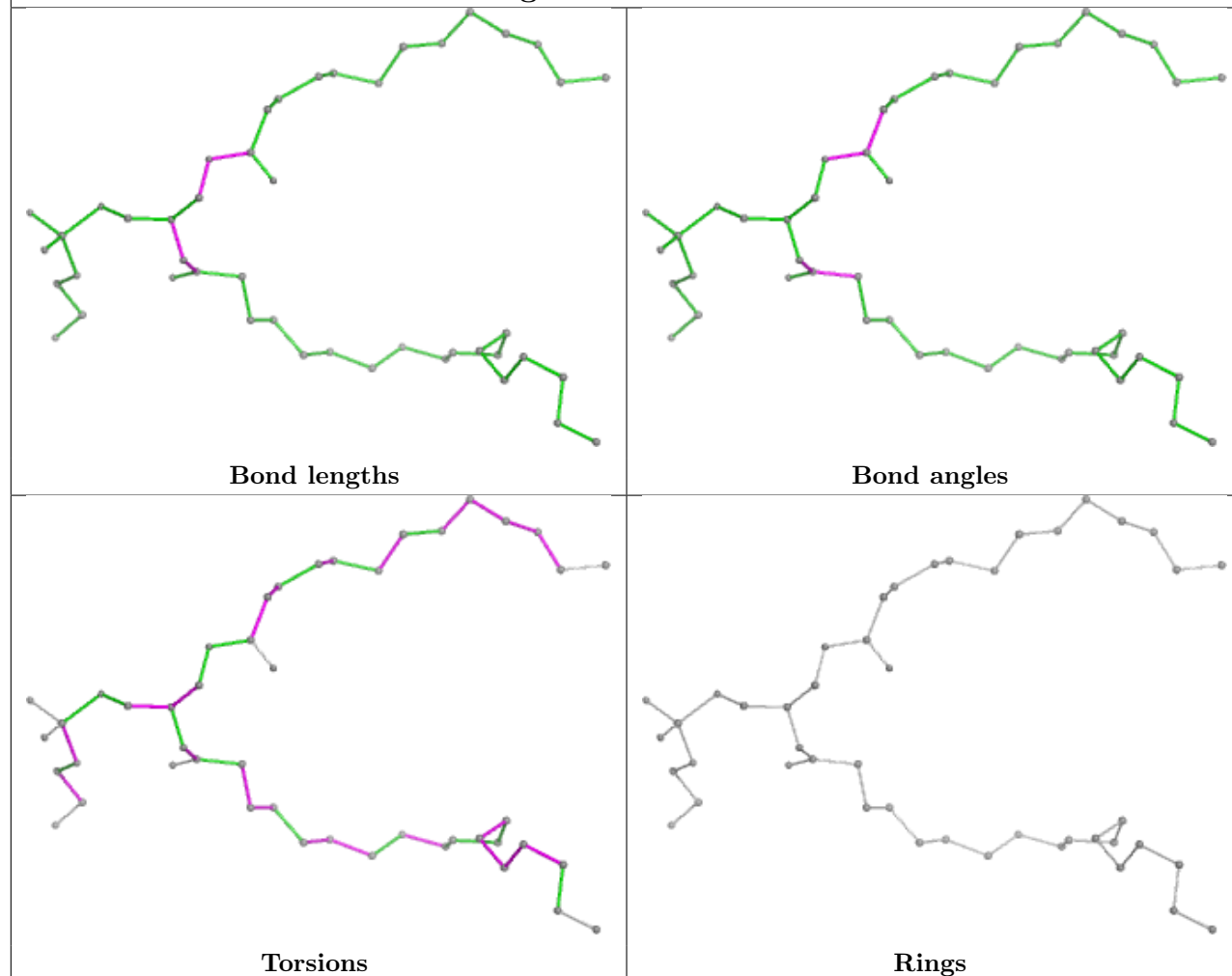




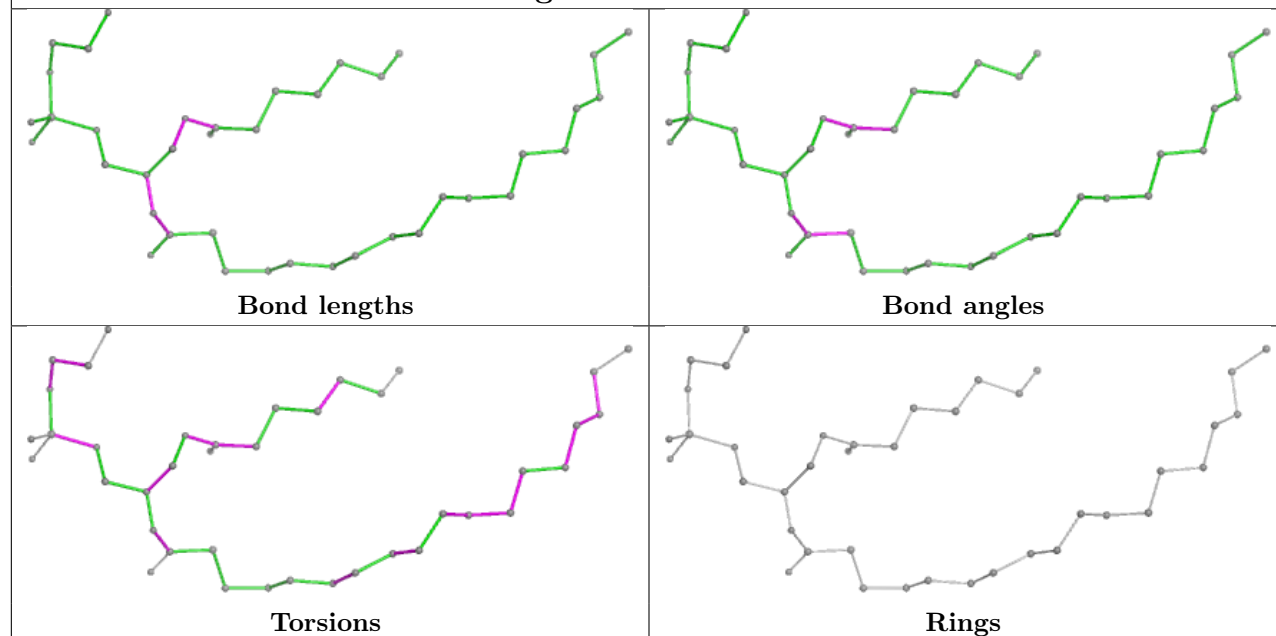


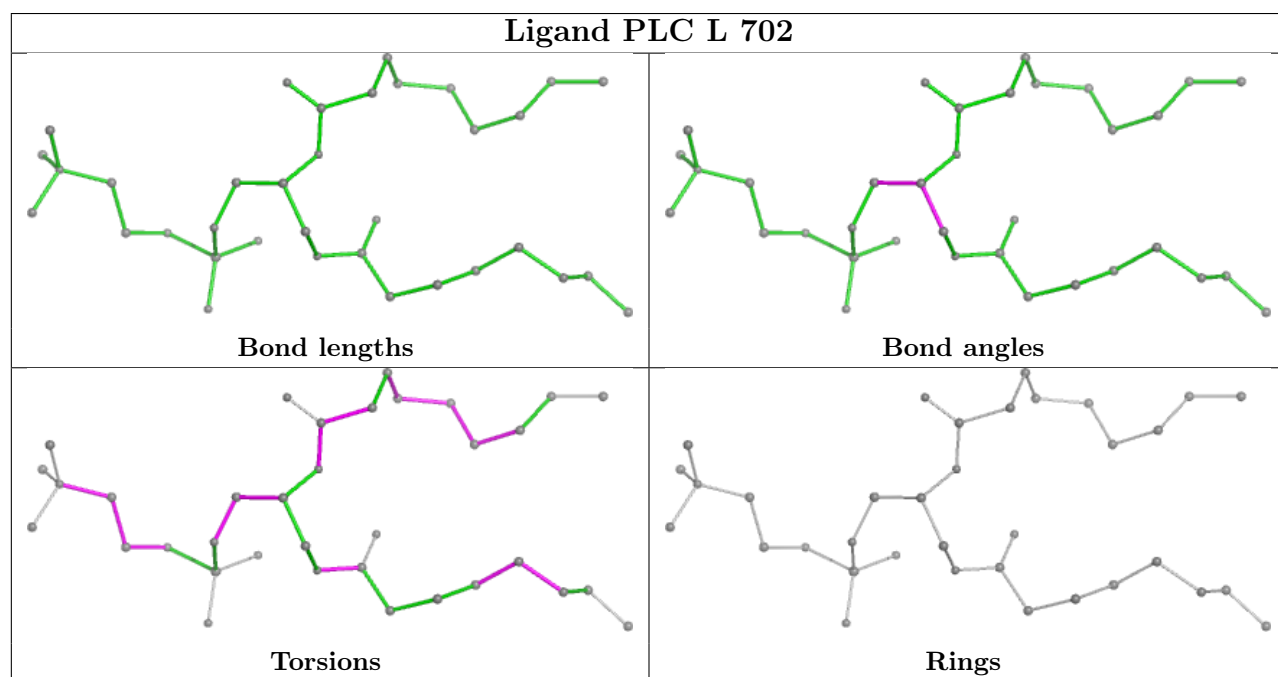
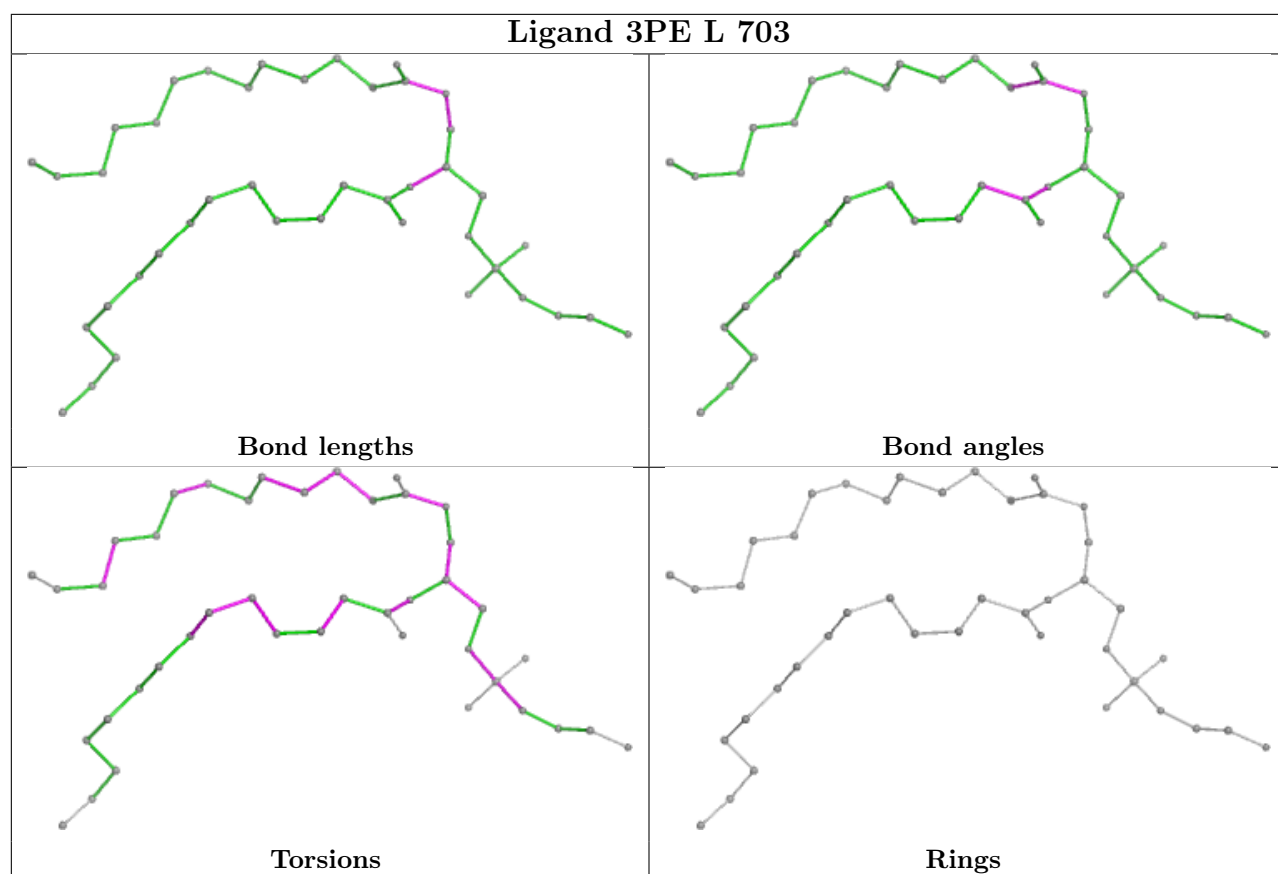


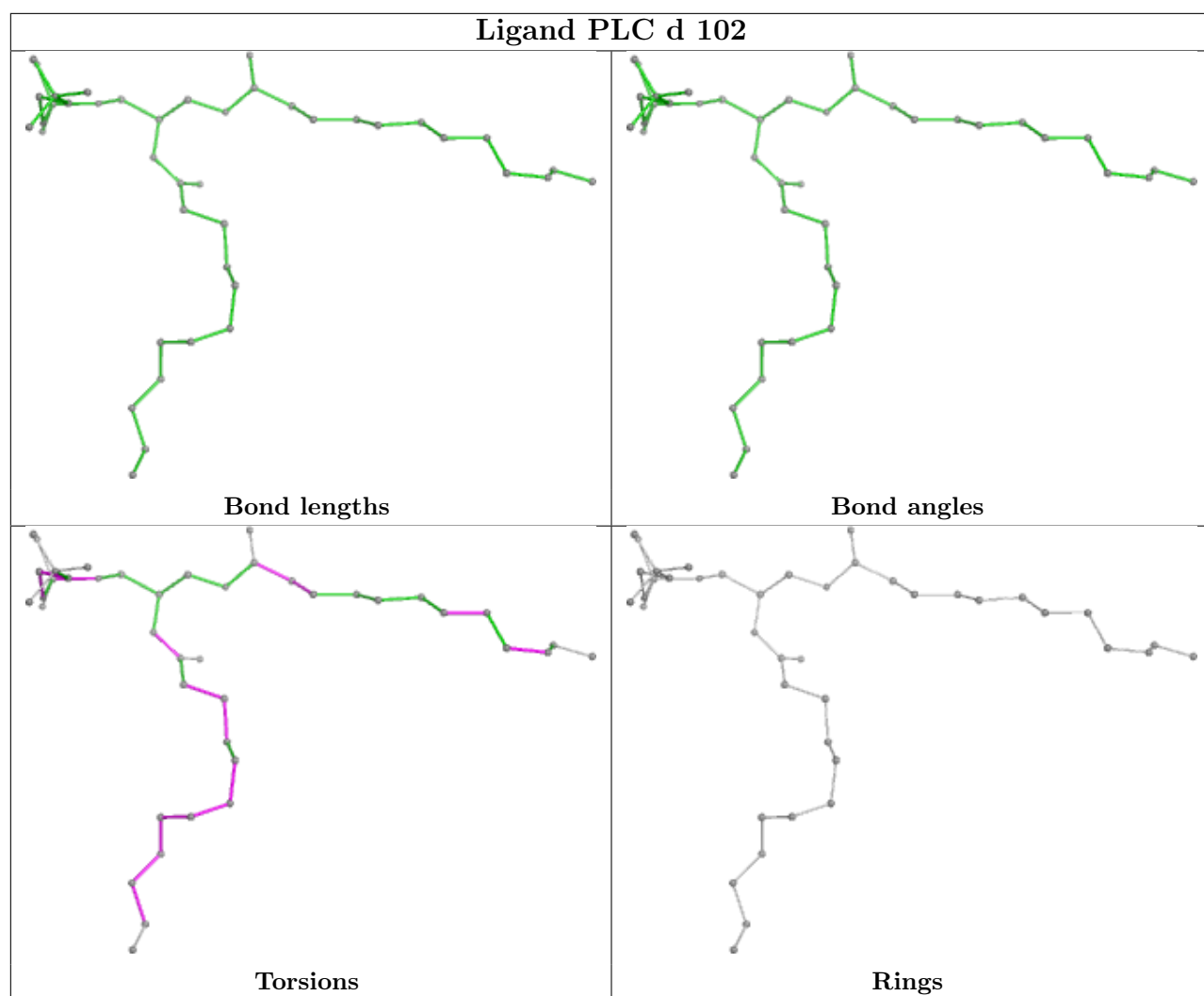
Ligand 3PE L 711

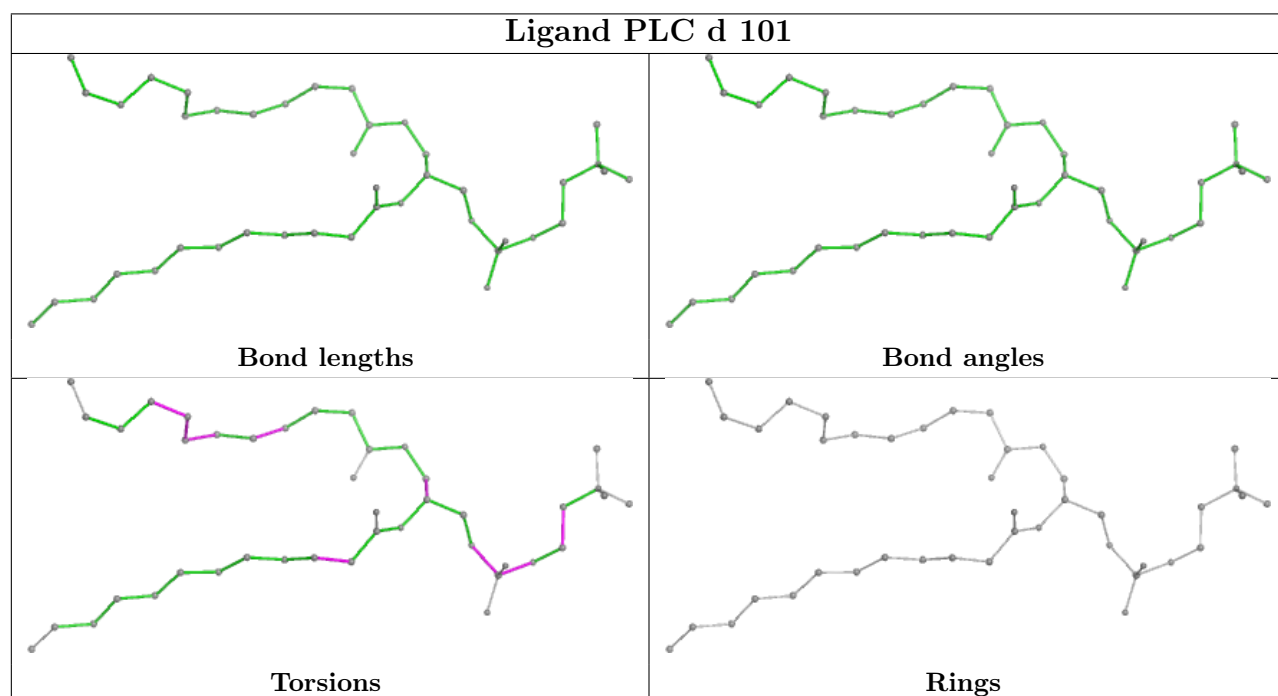
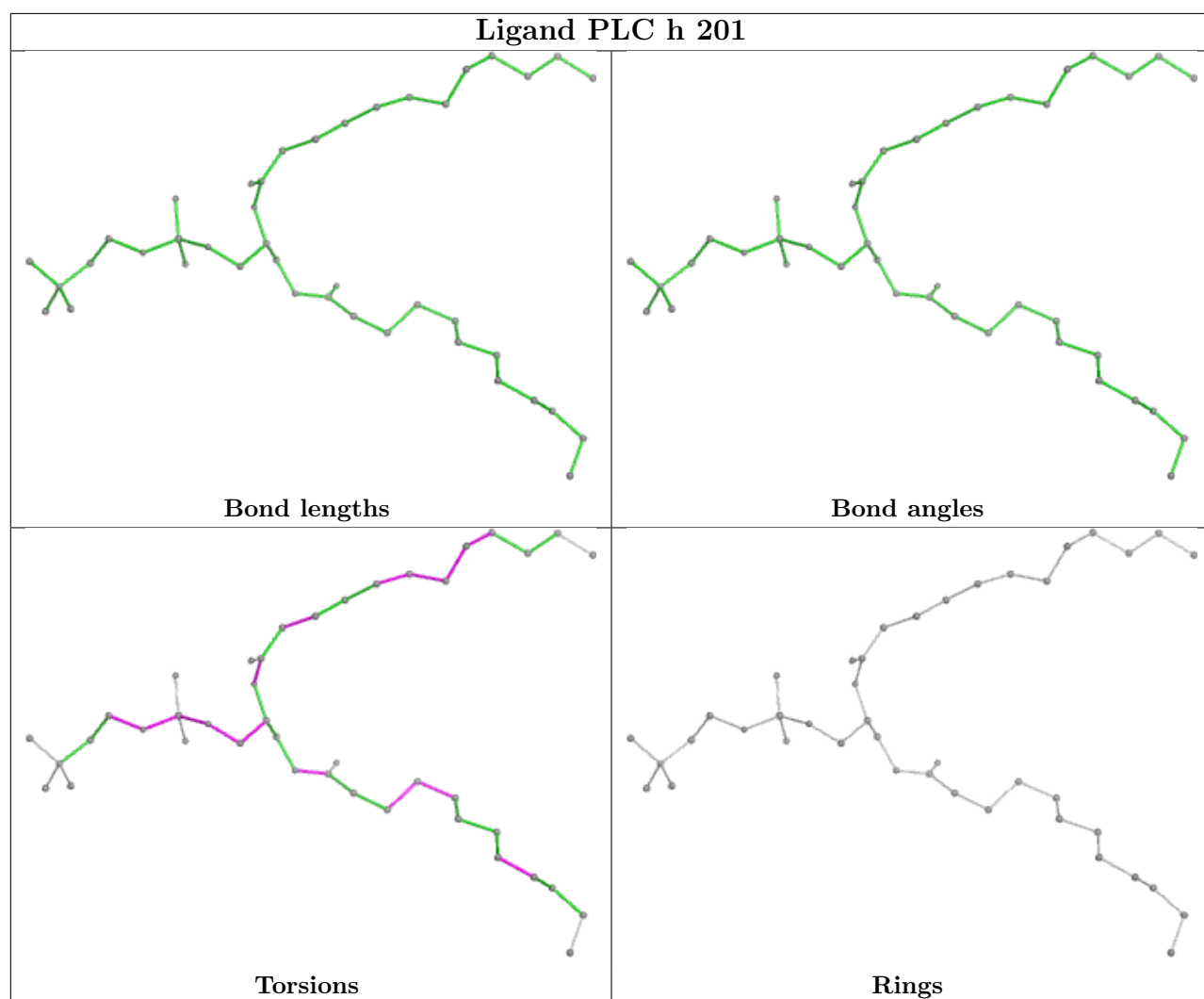


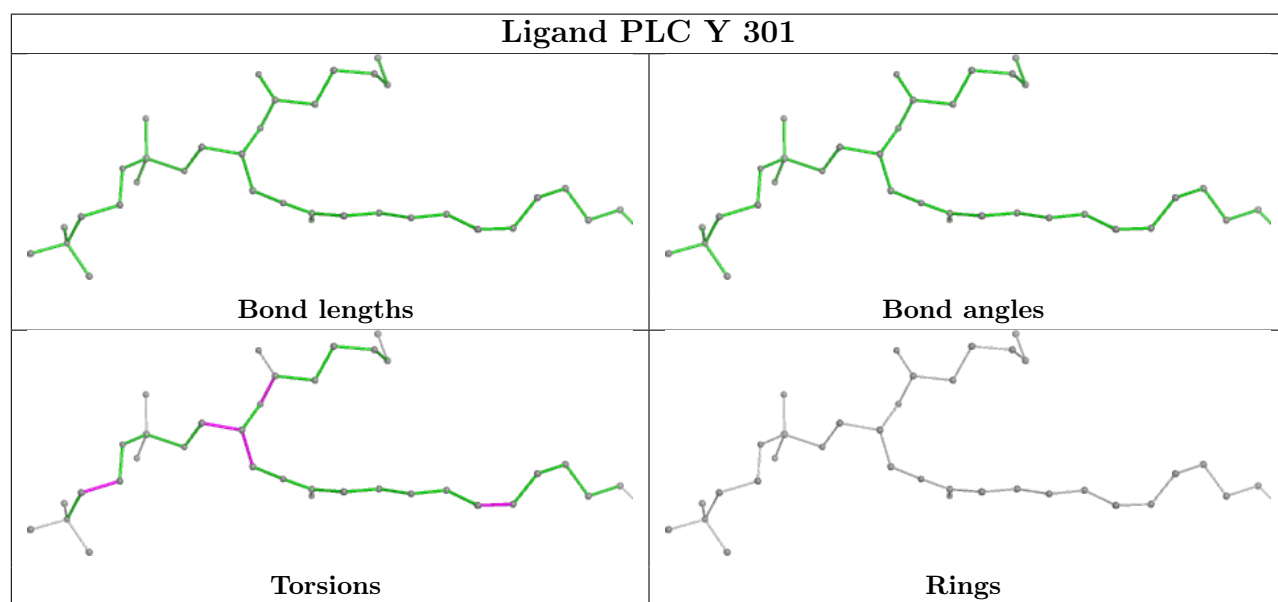
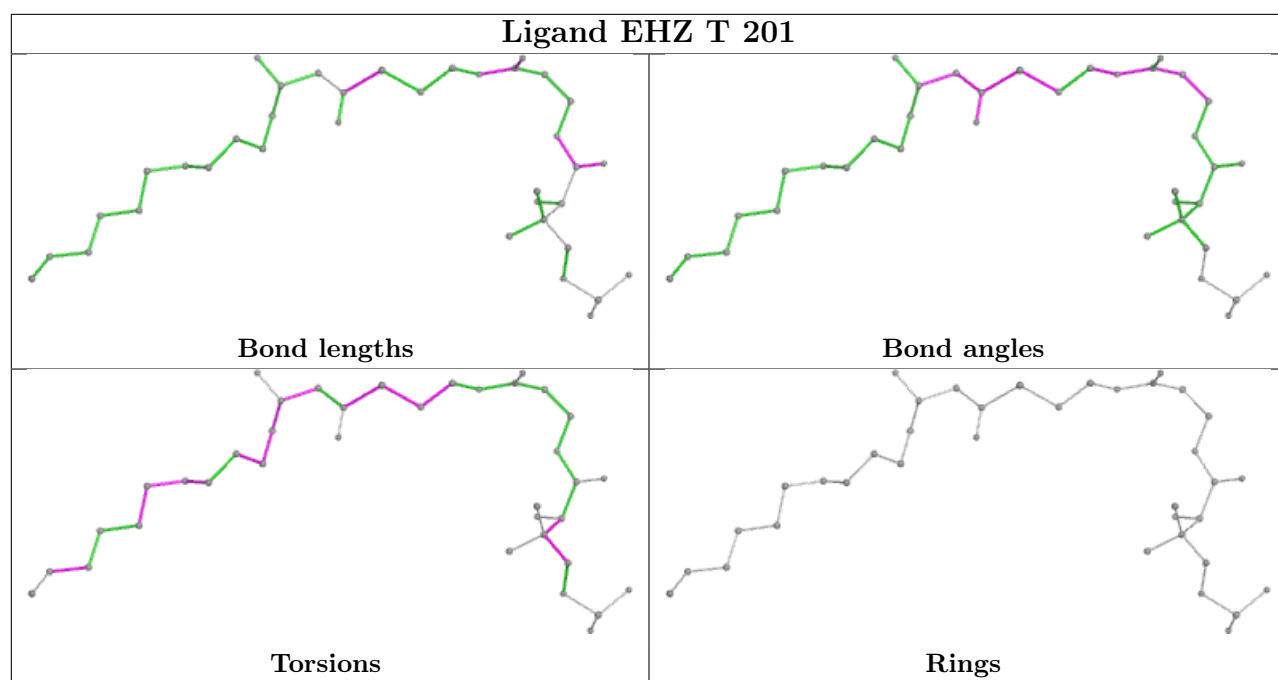
Ligand 3PE N 601

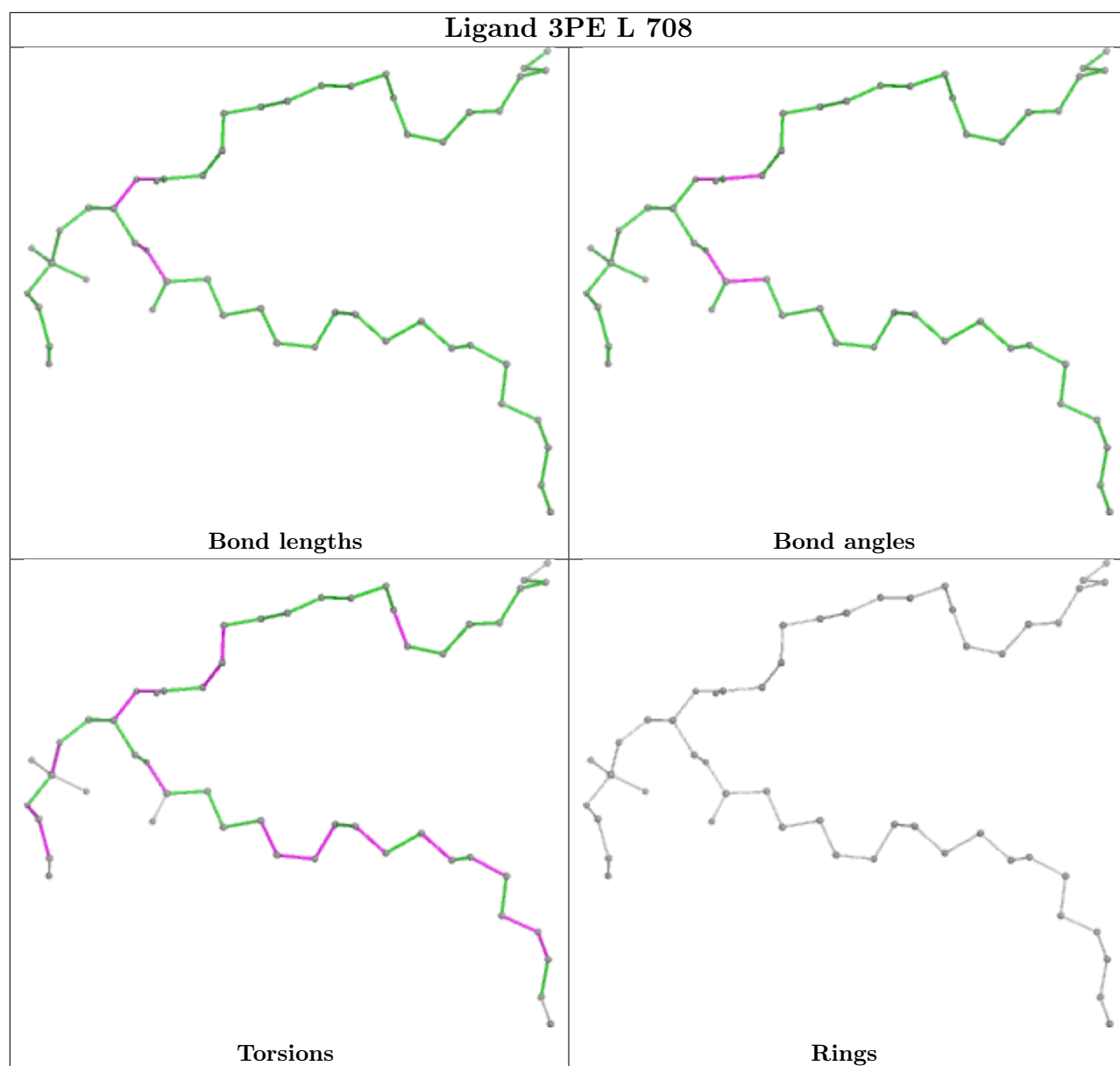


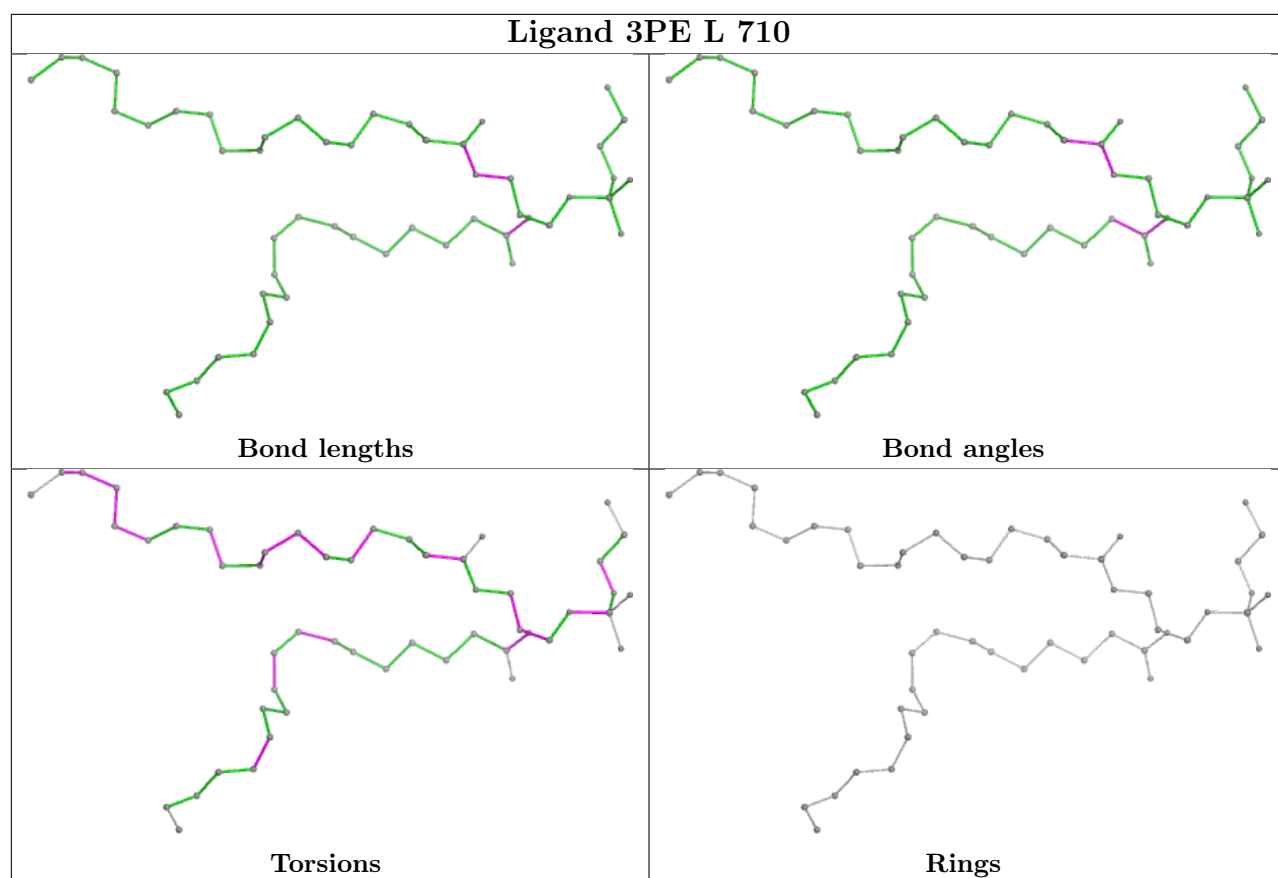


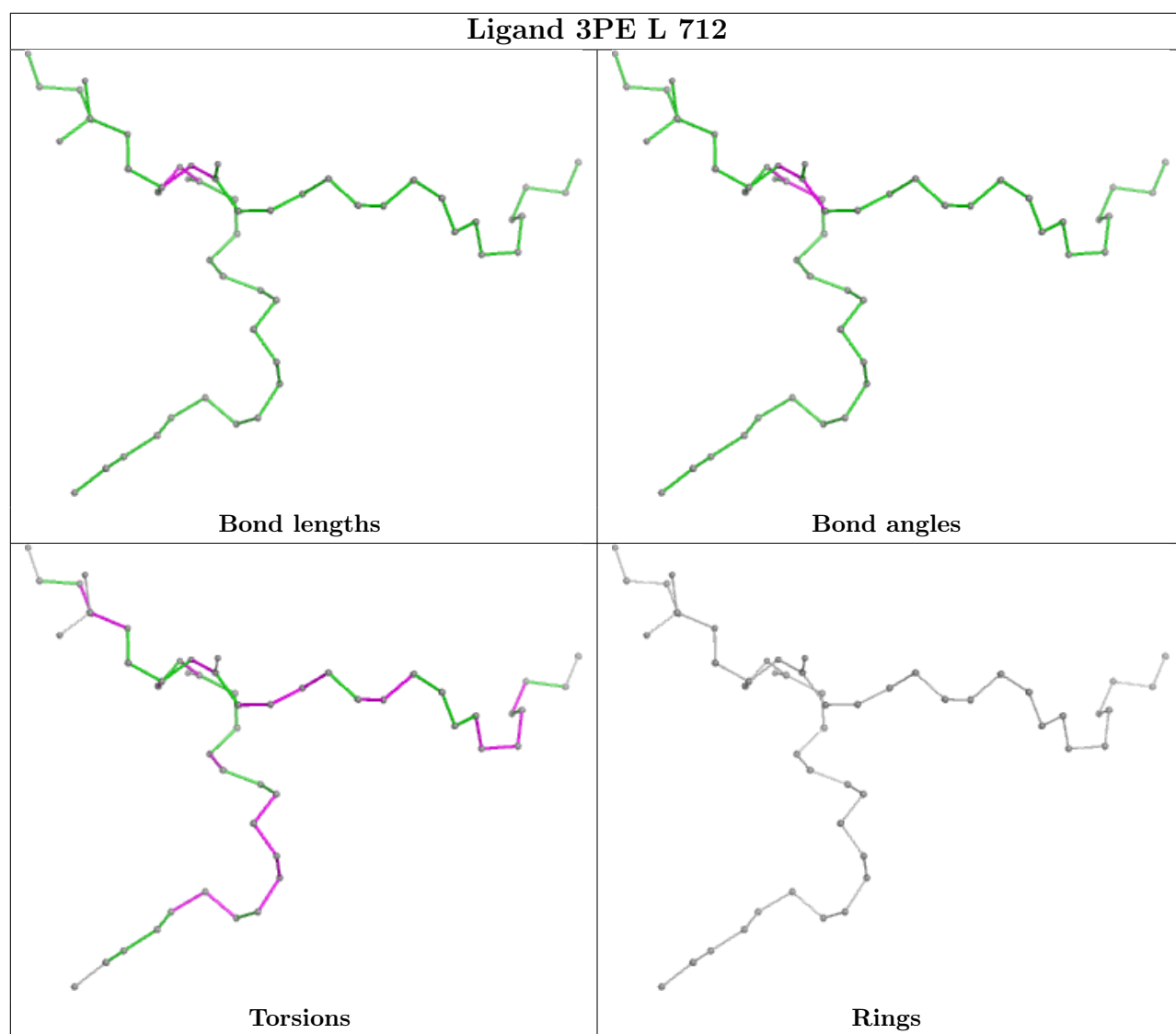




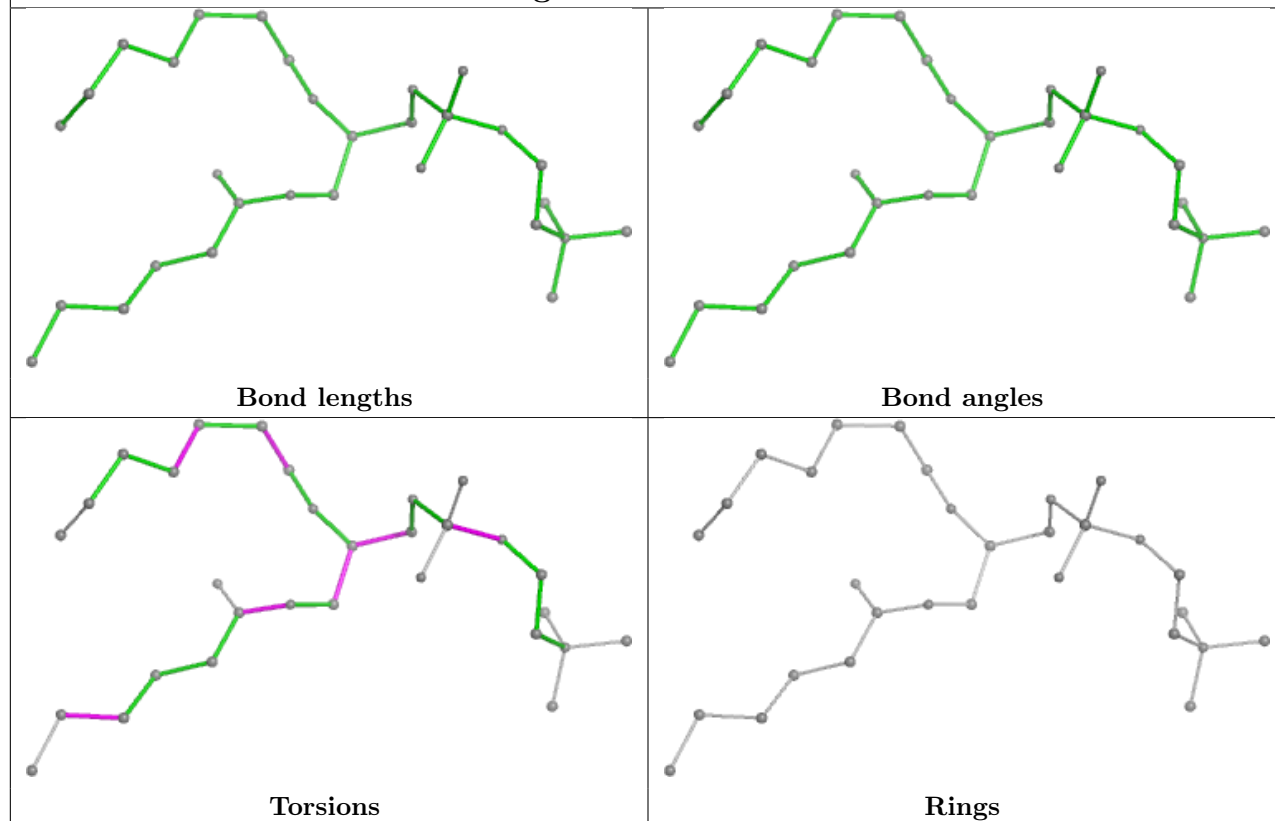




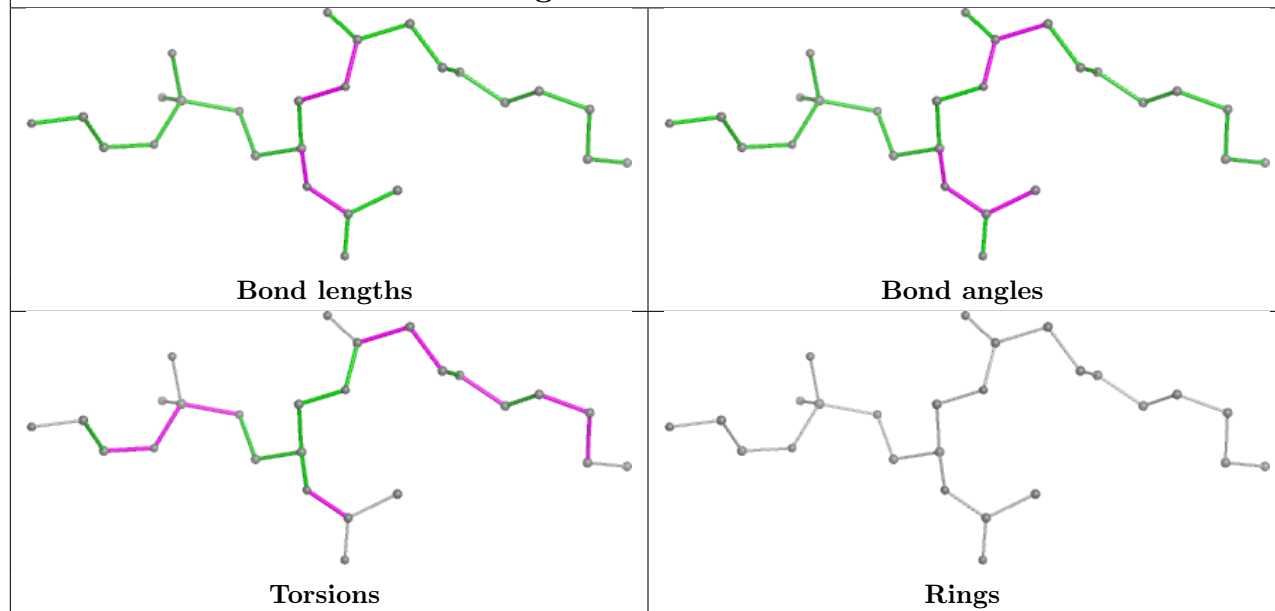


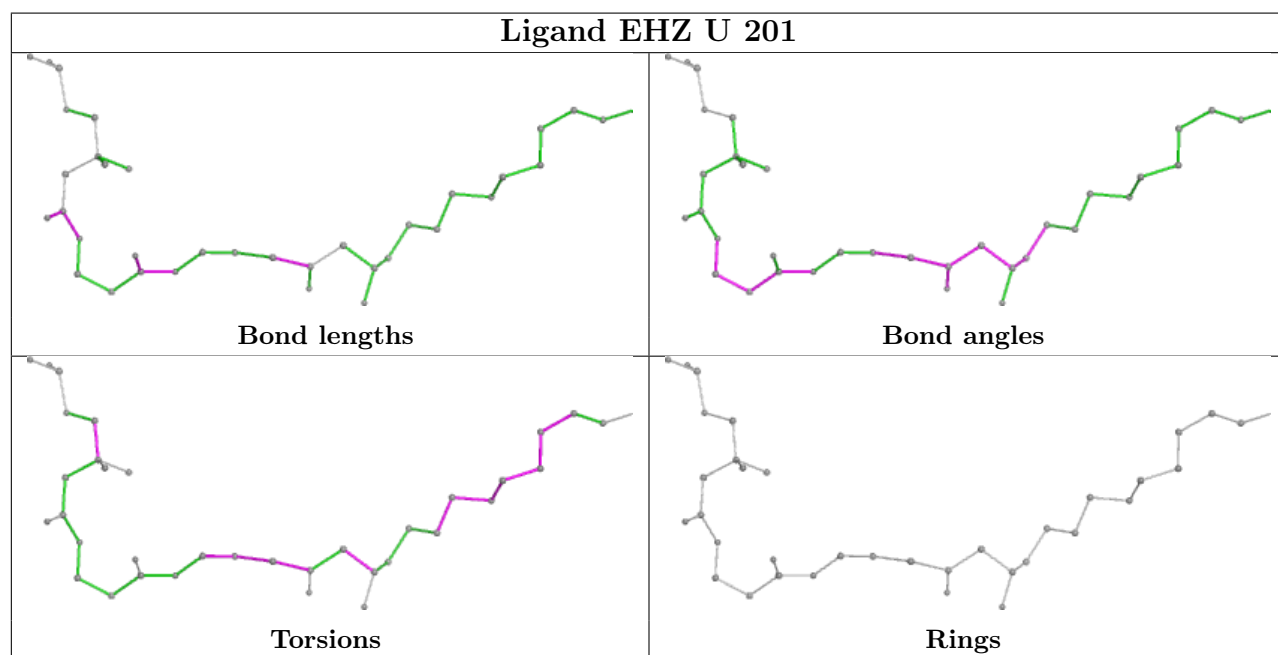
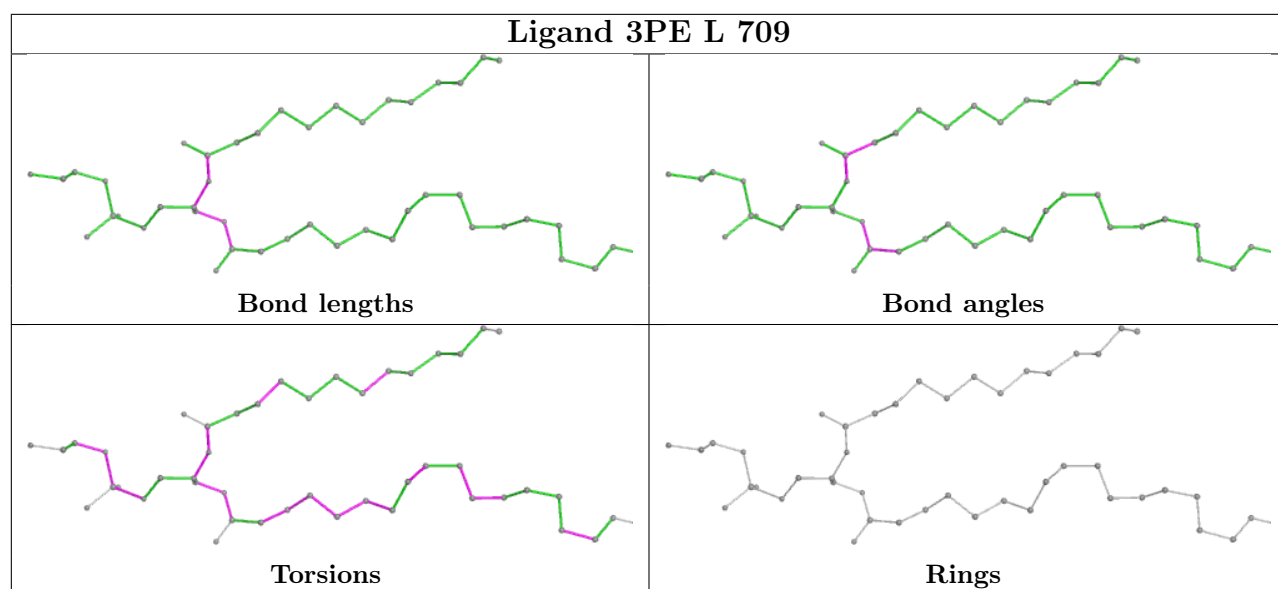


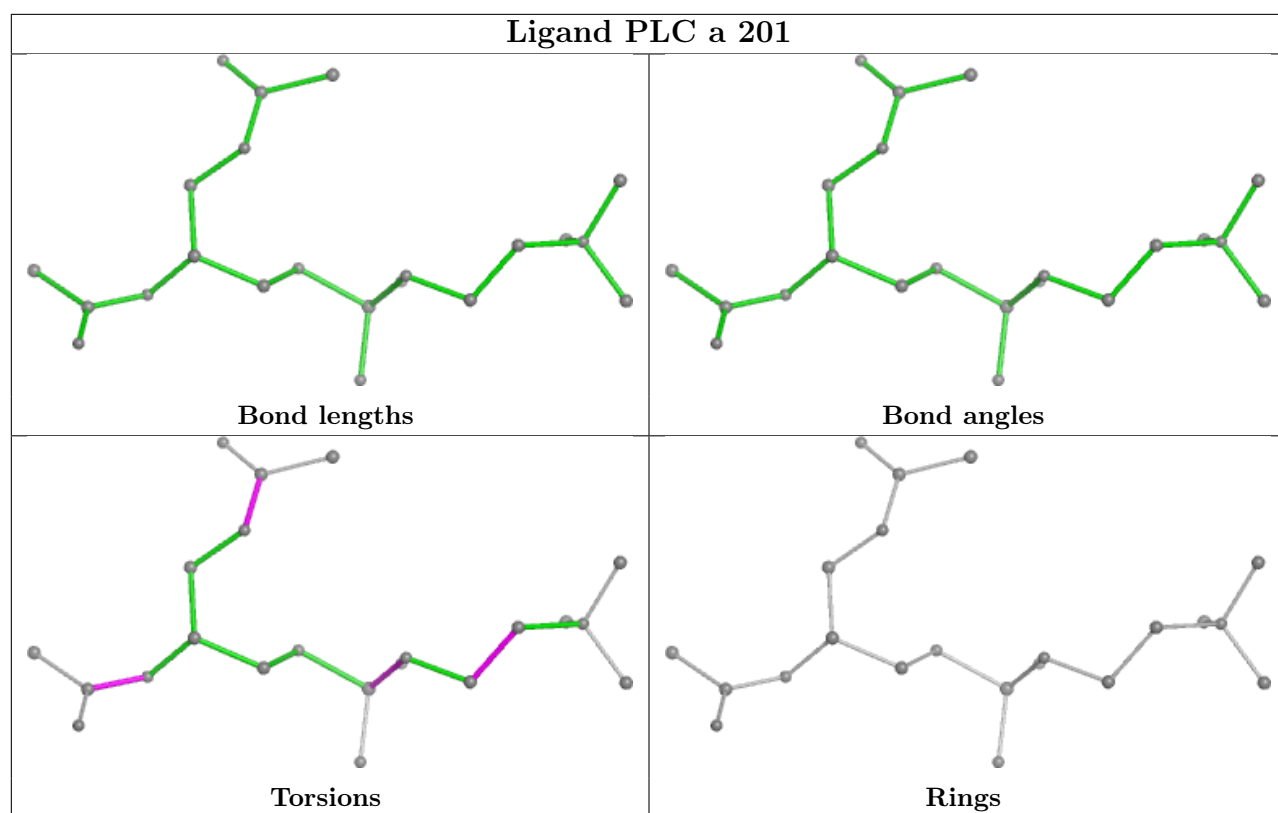
Ligand PLC P 502

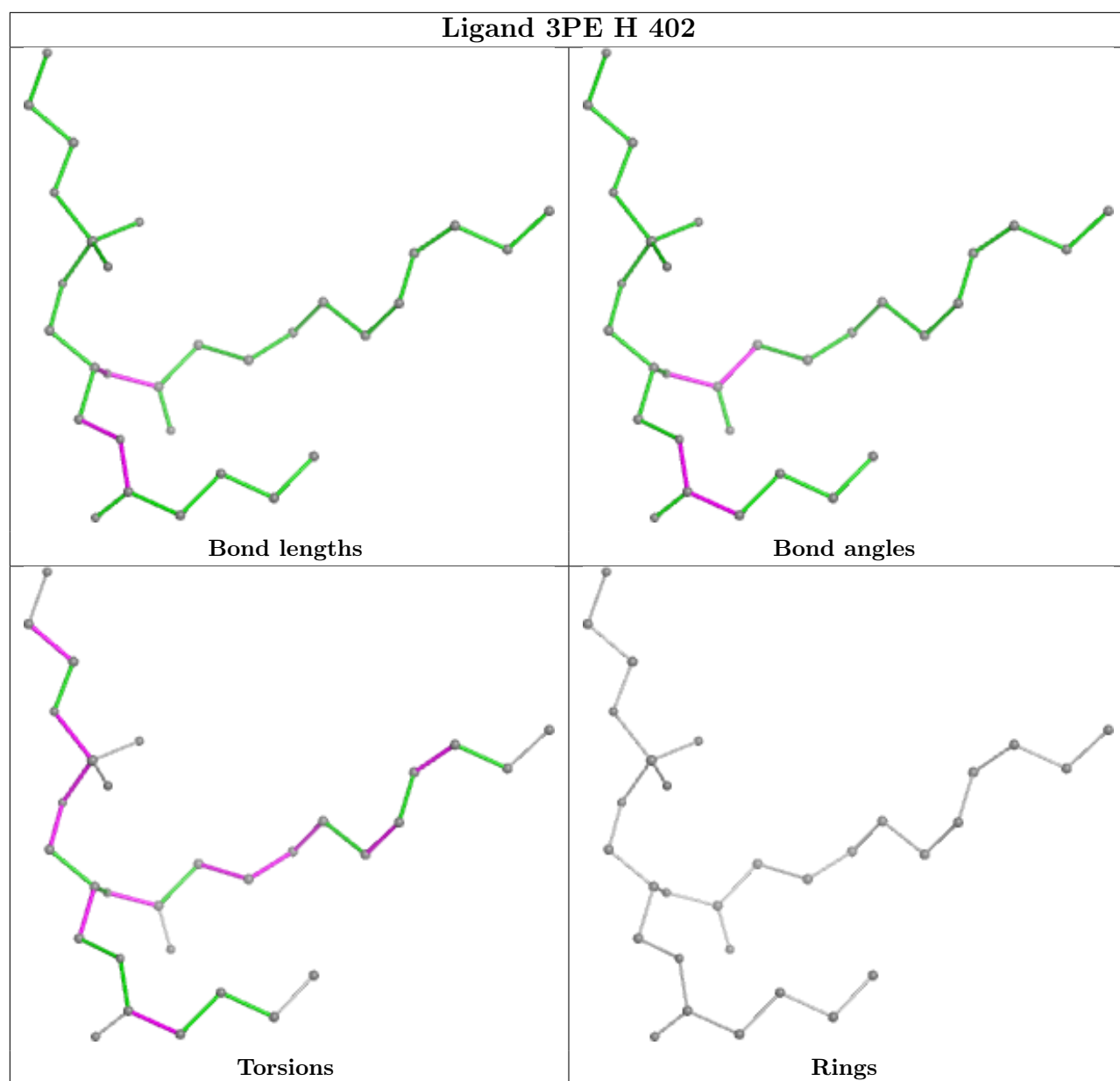


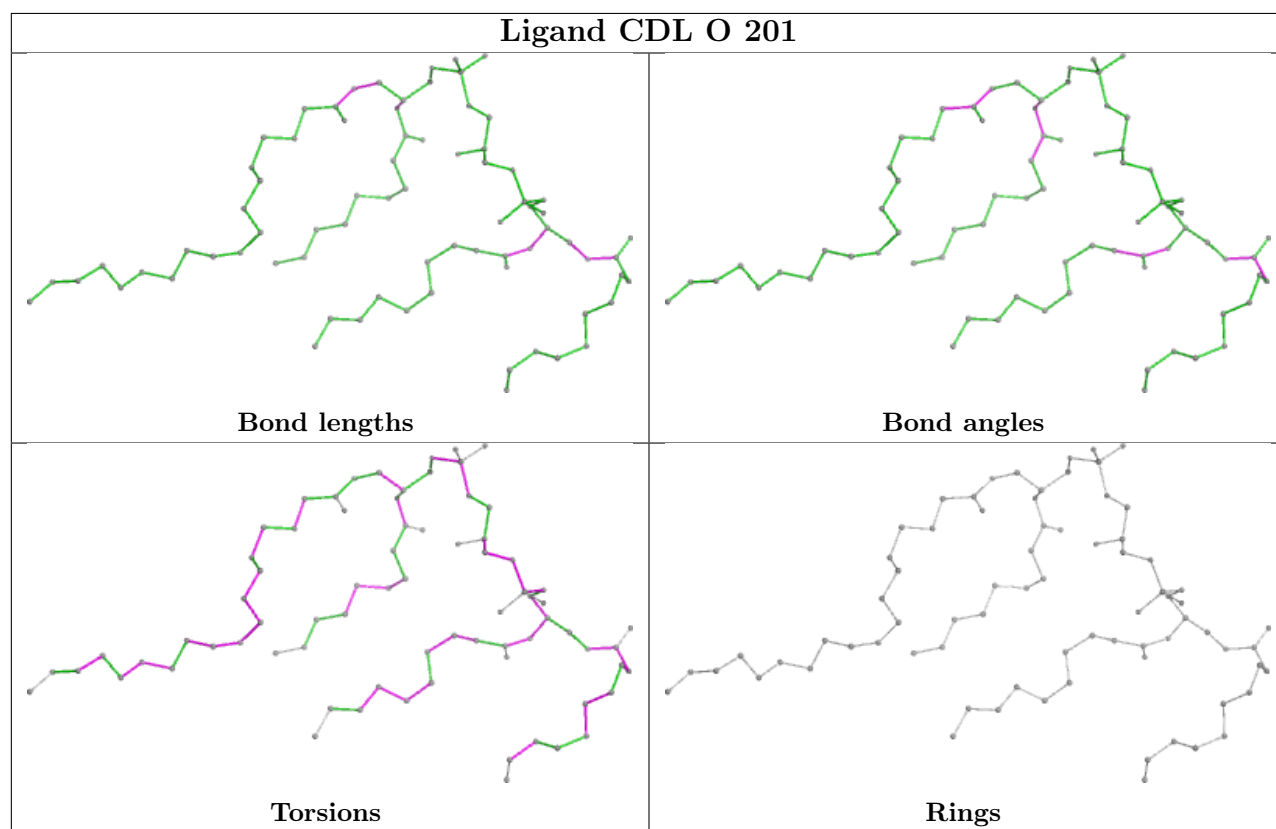
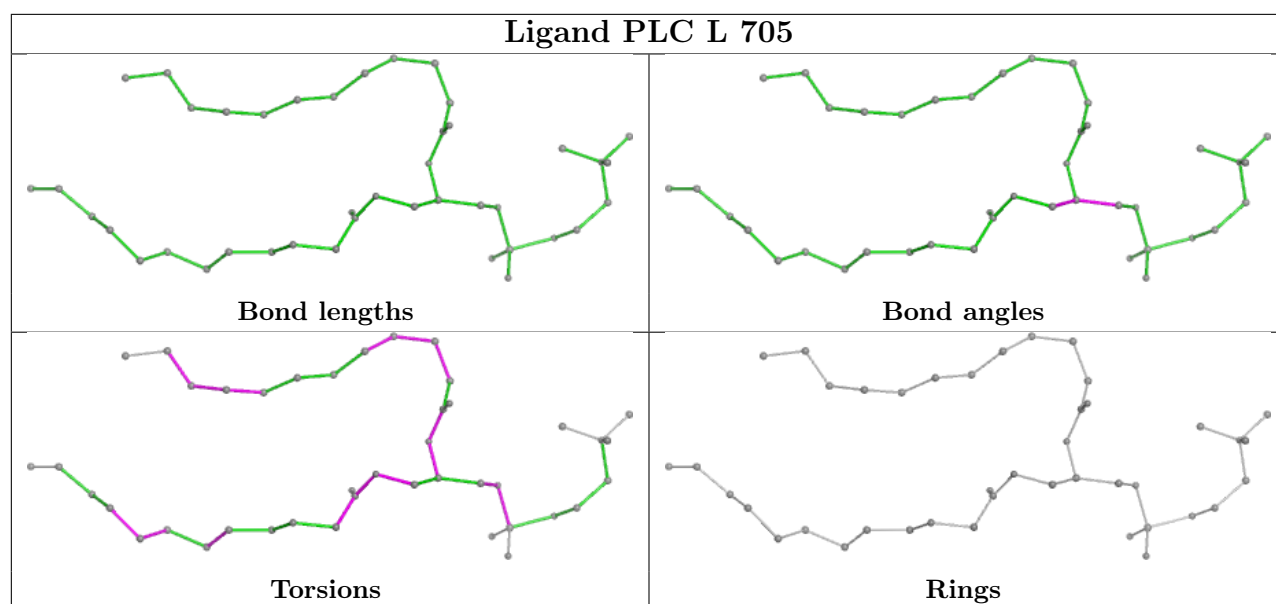
Ligand 3PE Y 302

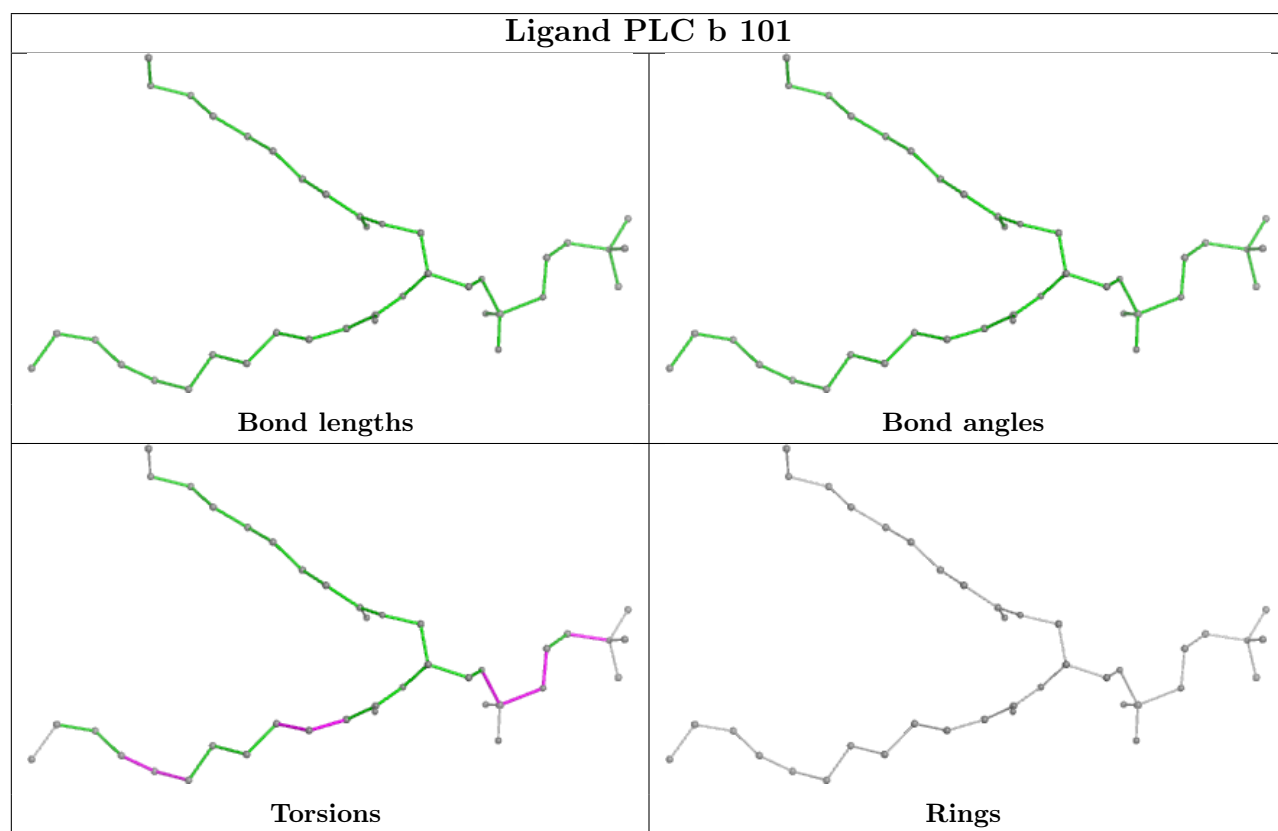
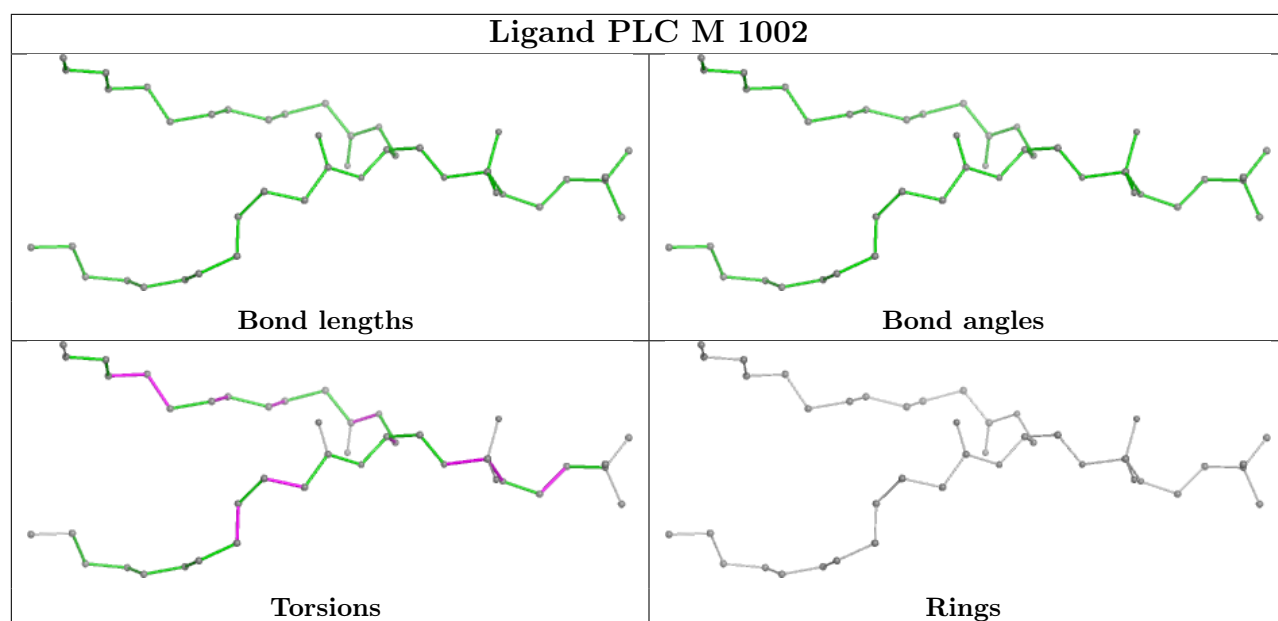


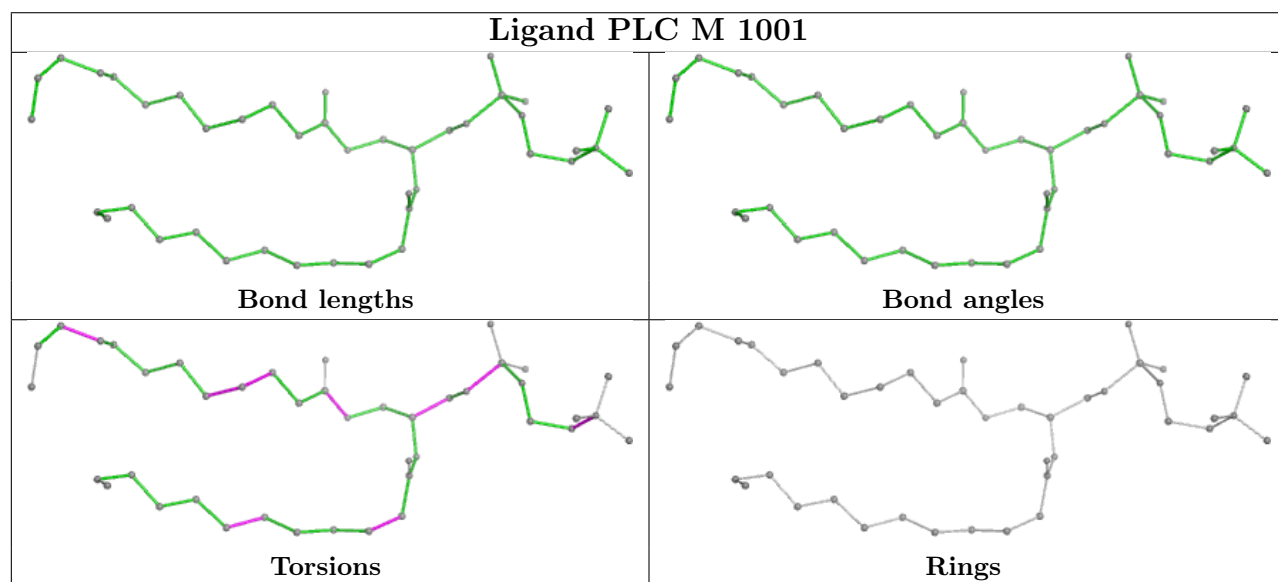
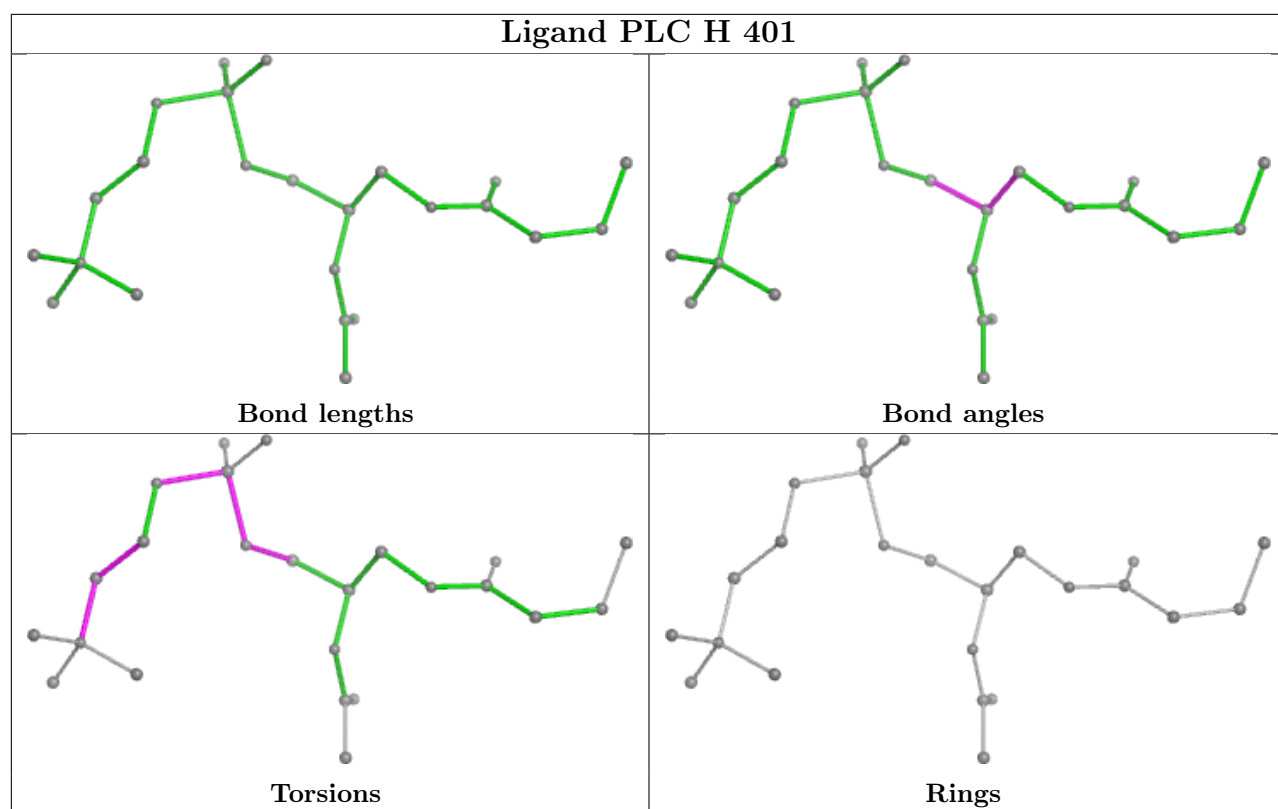


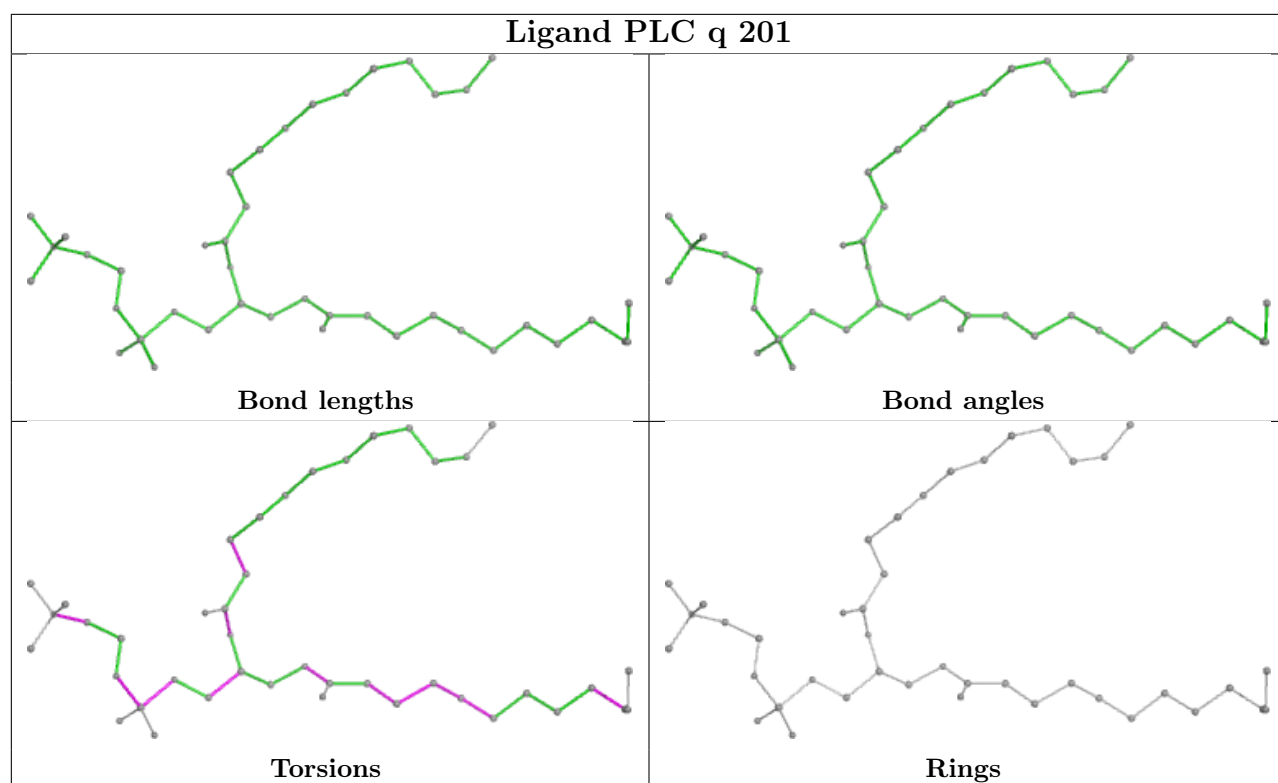


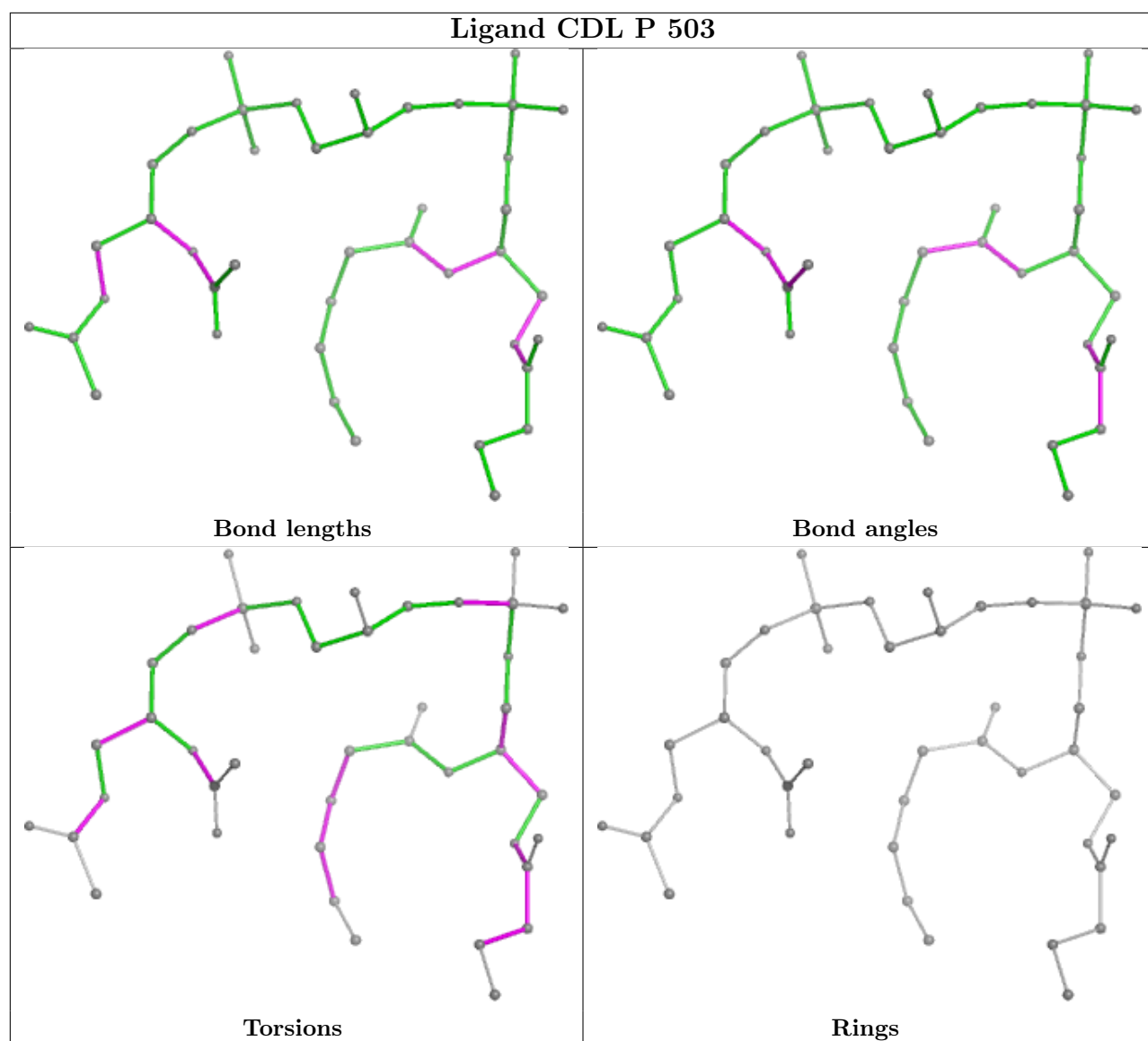


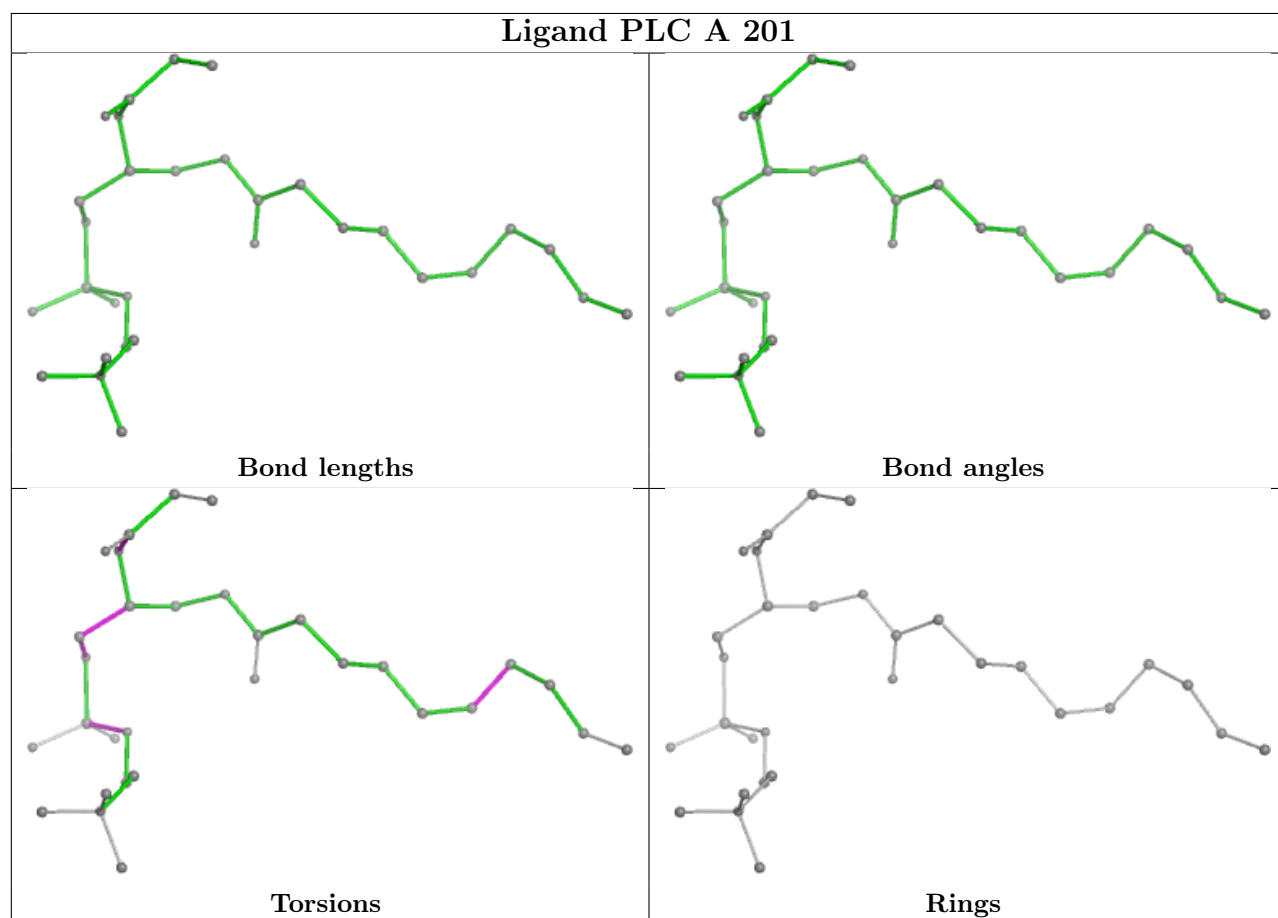
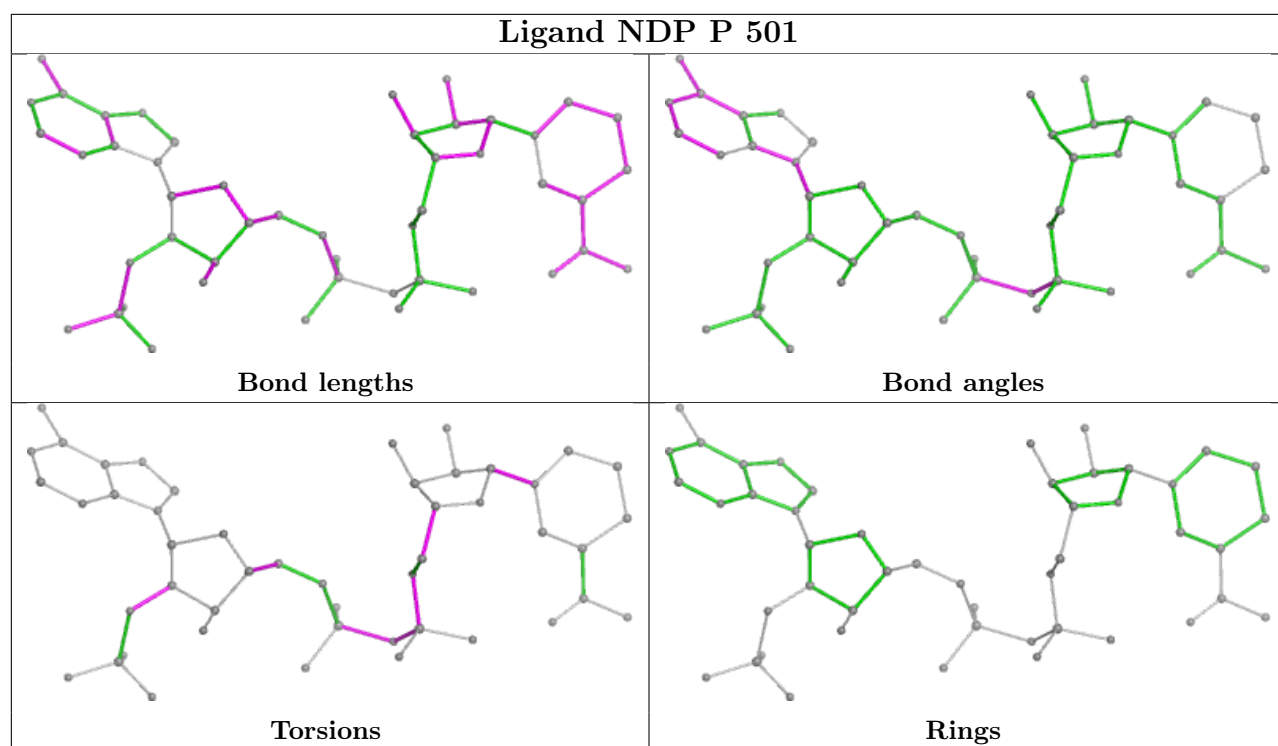




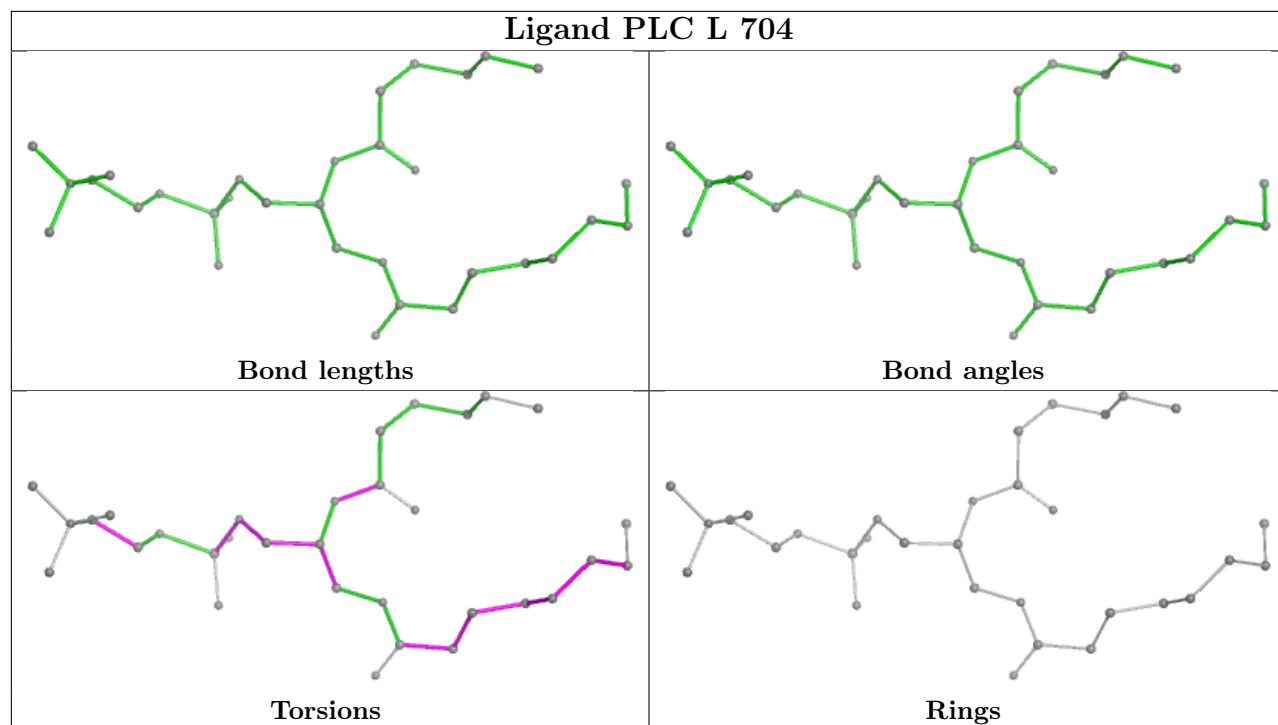




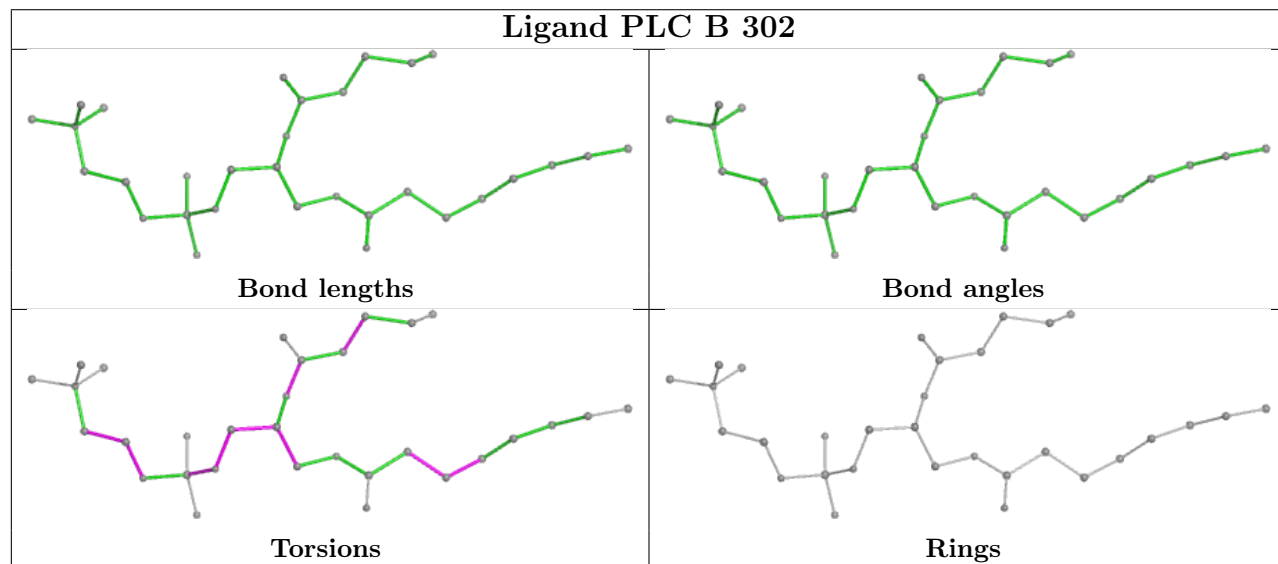


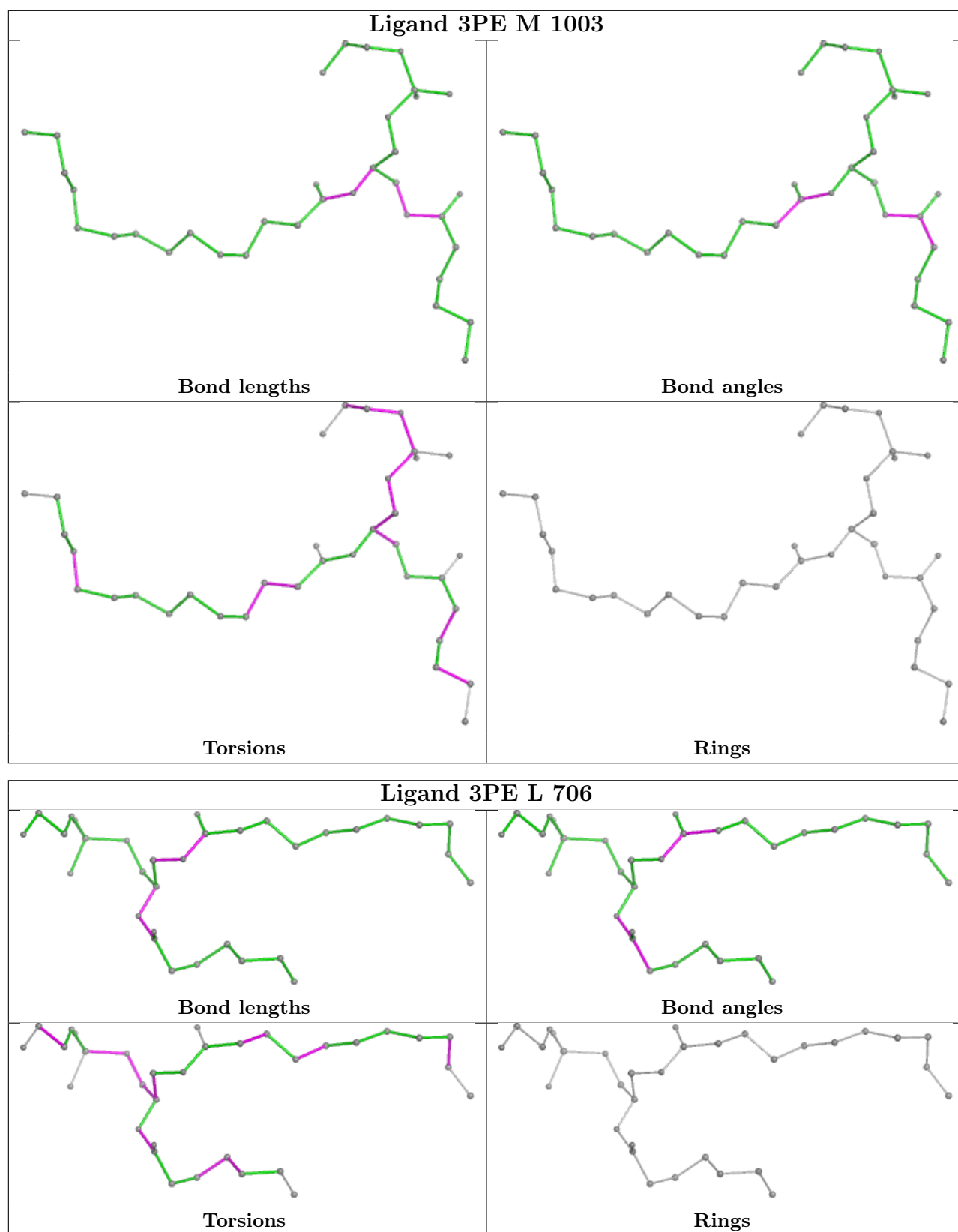


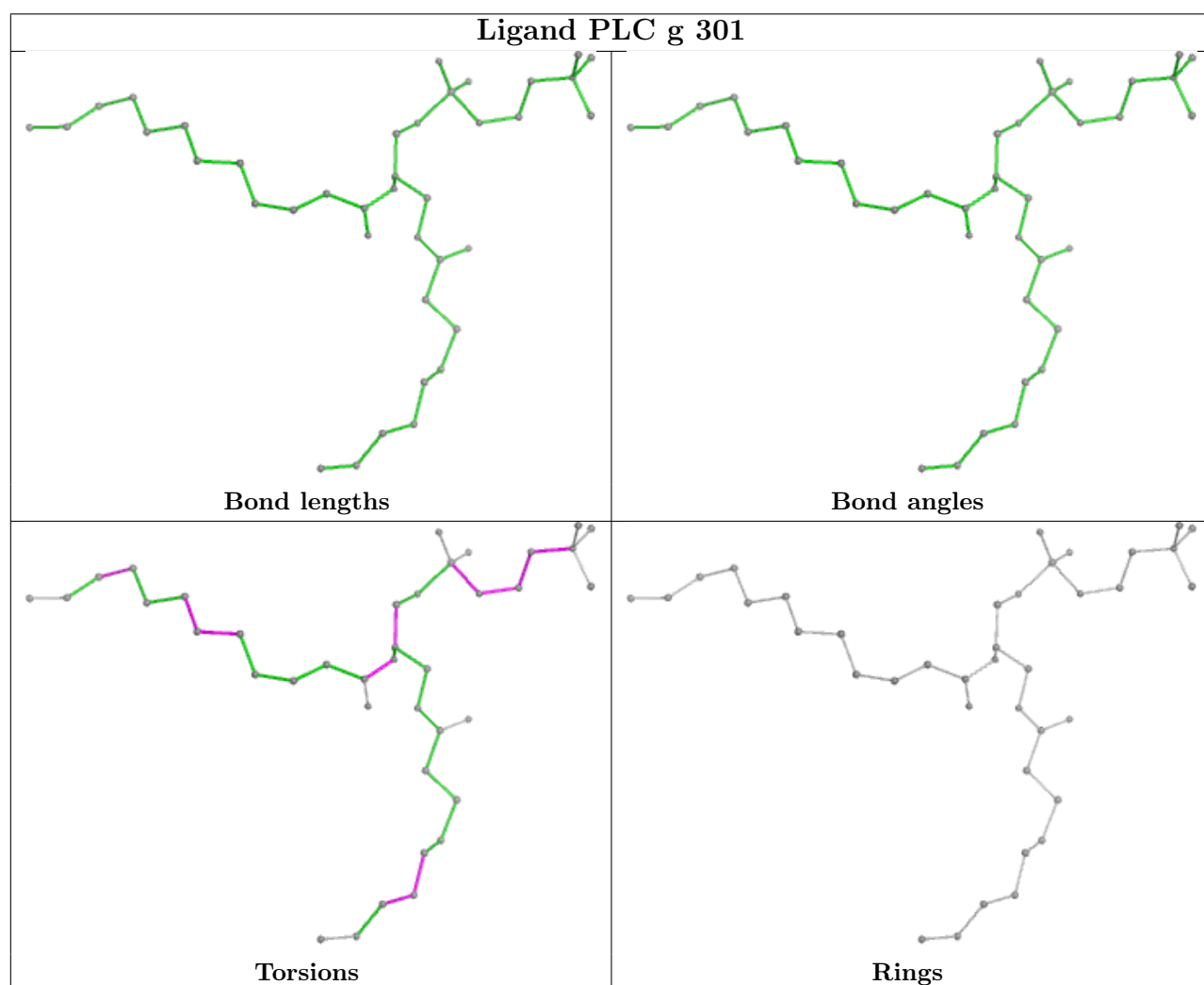
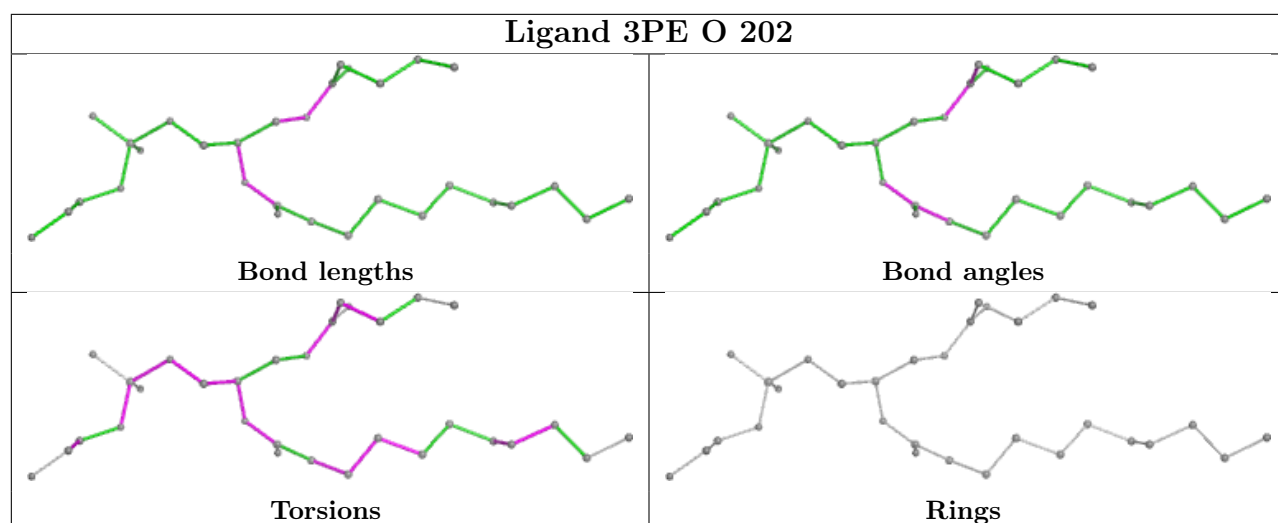
Ligand PLC L 704

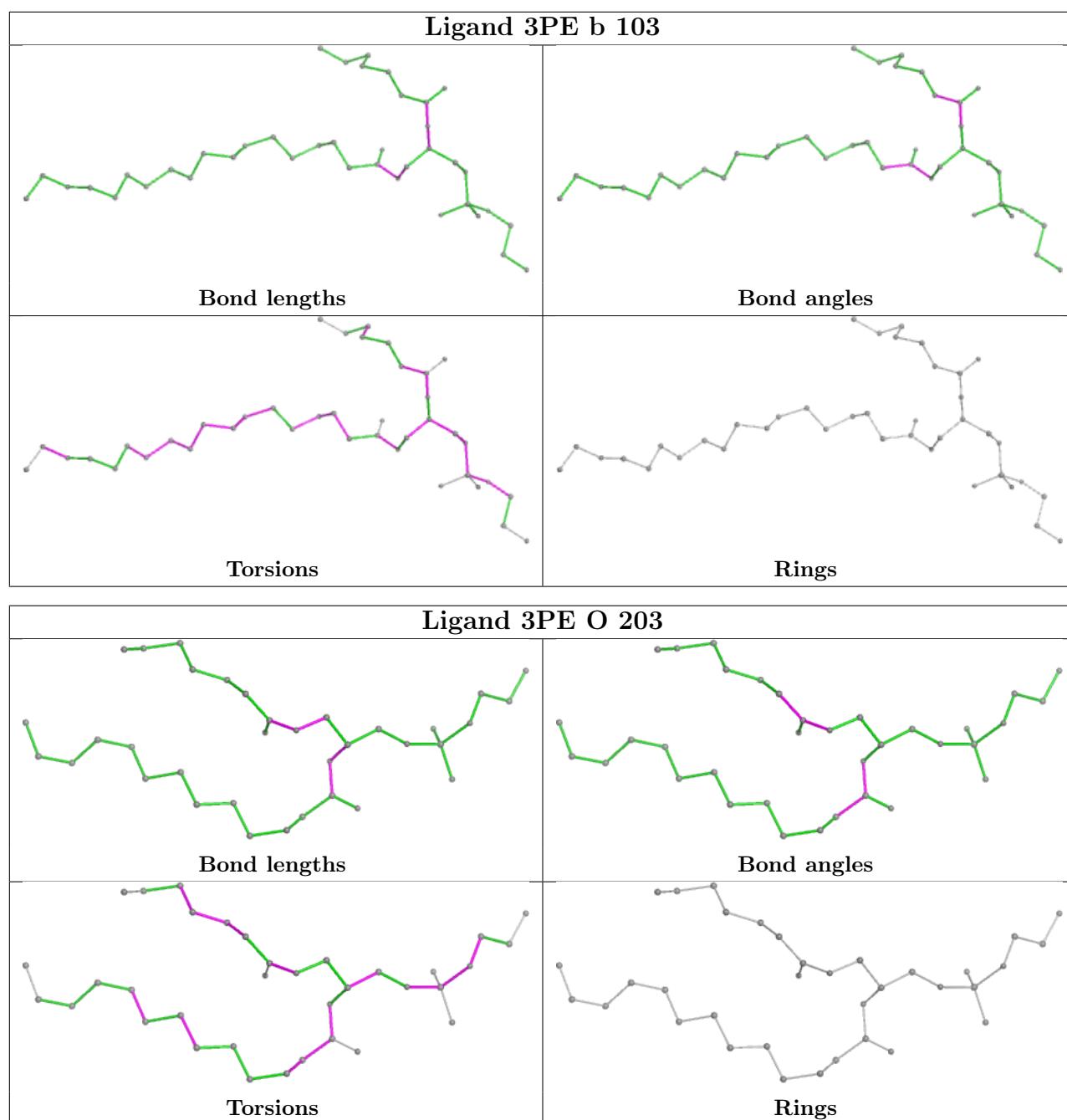


Ligand PLC B 302

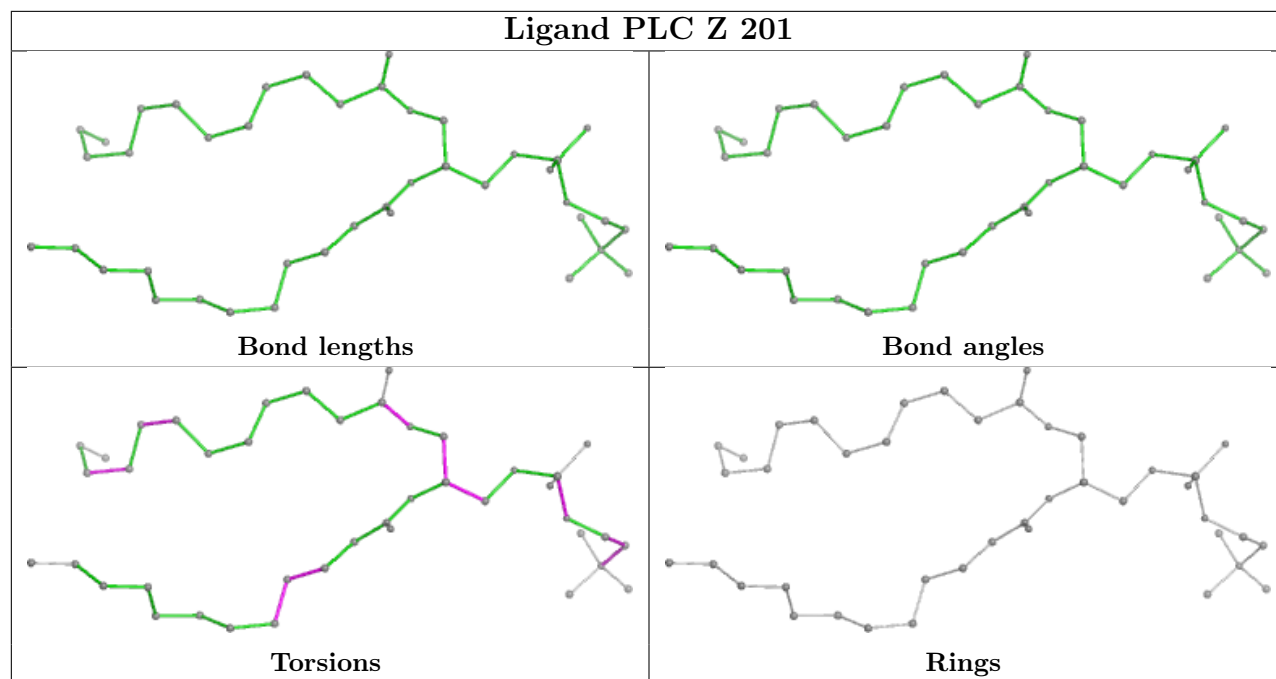




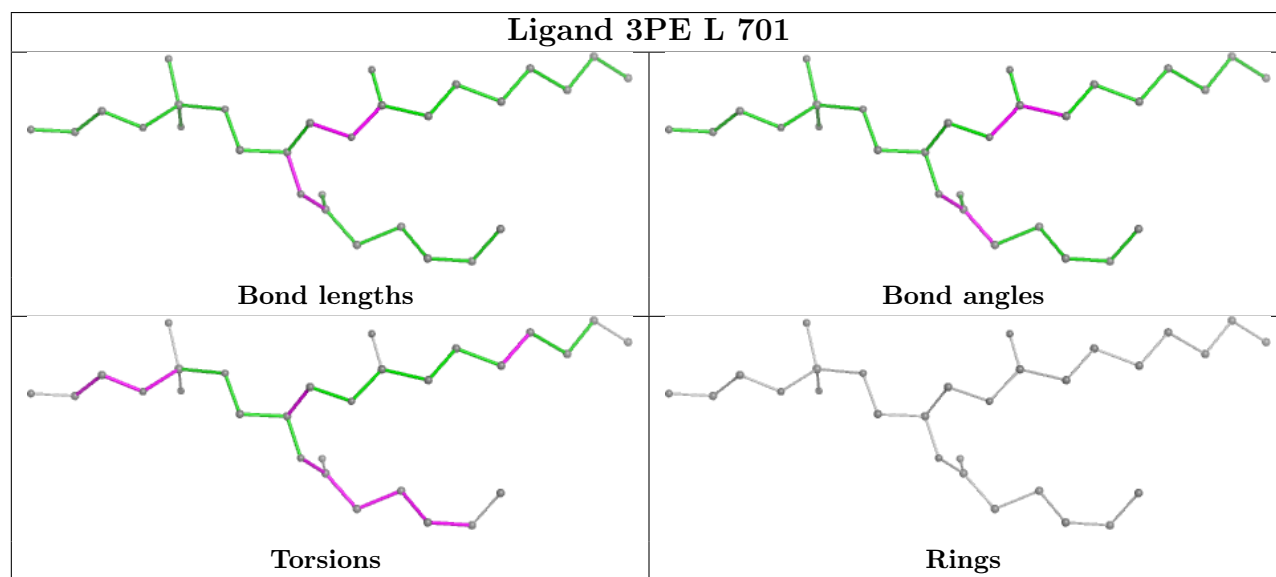


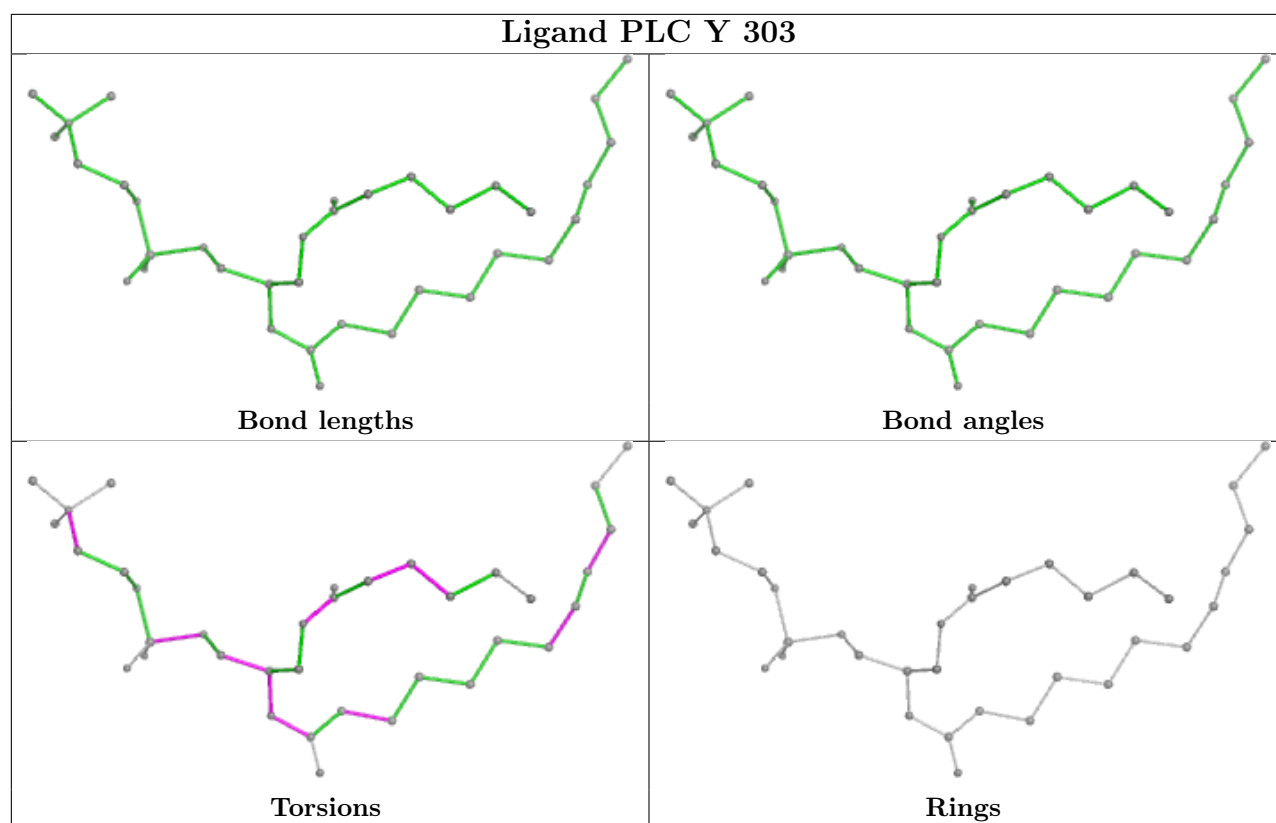


Ligand PLC Z 201



Ligand 3PE L 701





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.

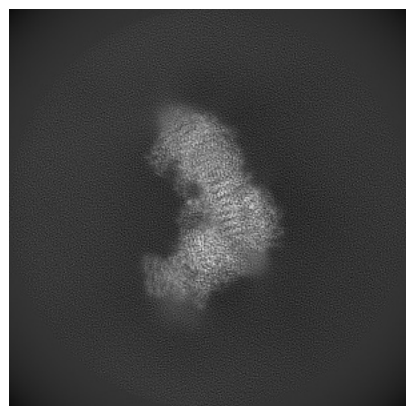
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52877. These allow visual inspection of the internal detail of the map and identification of artifacts.

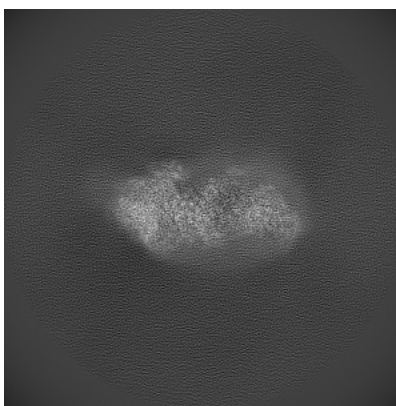
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

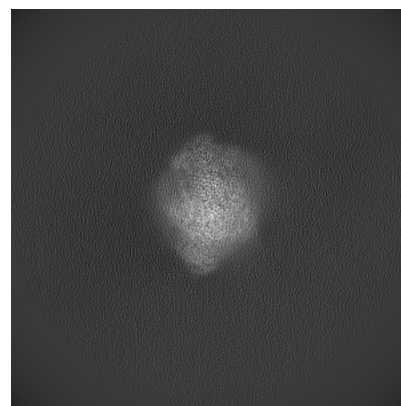
6.1.1 Primary map



X

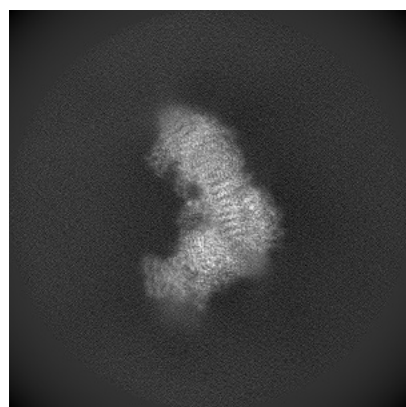


Y

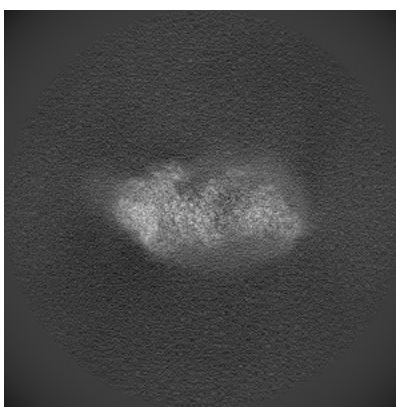


Z

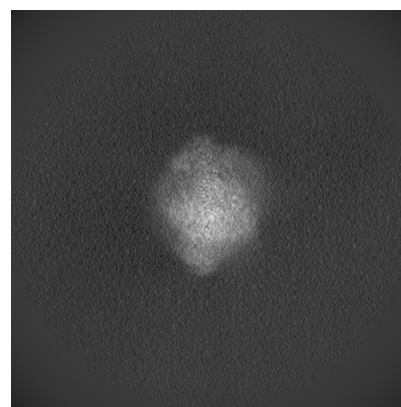
6.1.2 Raw map



X



Y

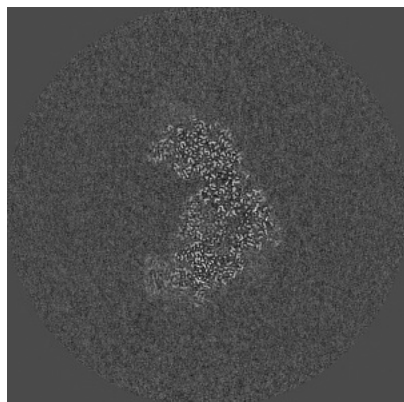


Z

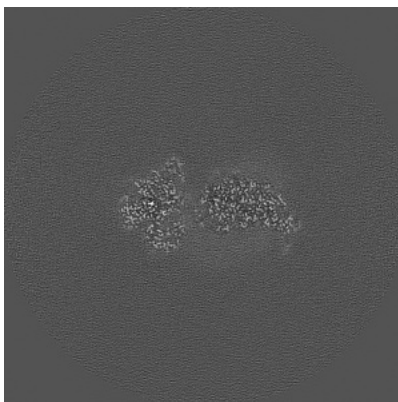
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

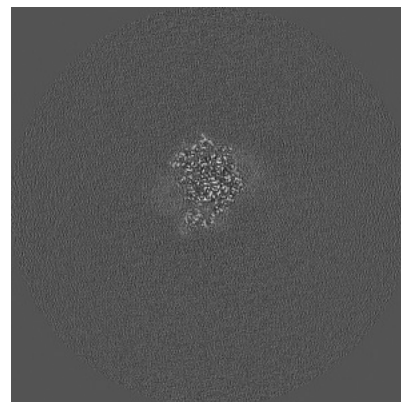
6.2.1 Primary map



X Index: 270

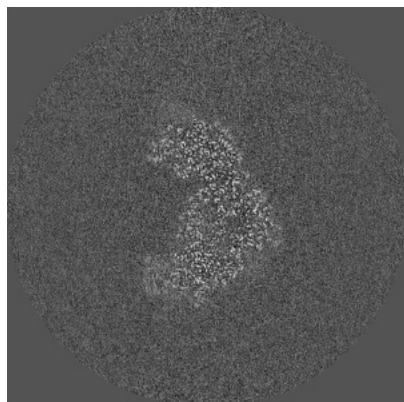


Y Index: 270

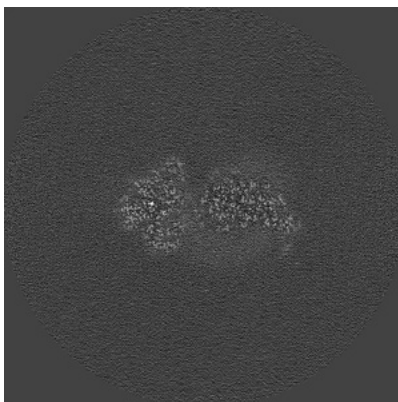


Z Index: 270

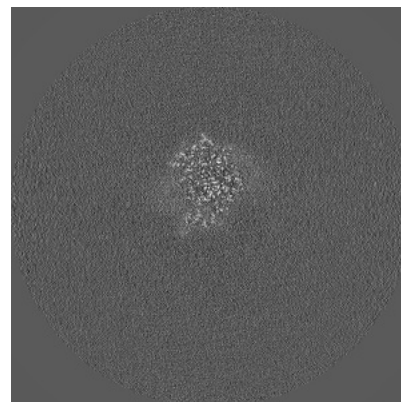
6.2.2 Raw map



X Index: 270



Y Index: 270

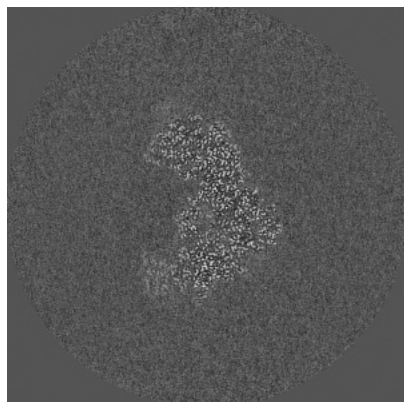


Z Index: 270

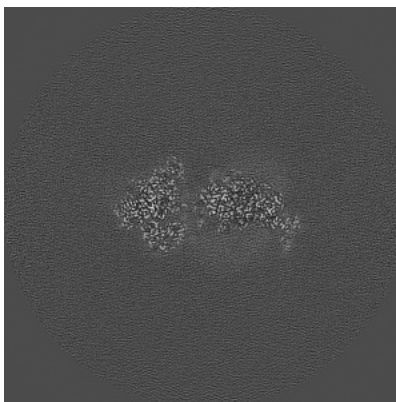
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

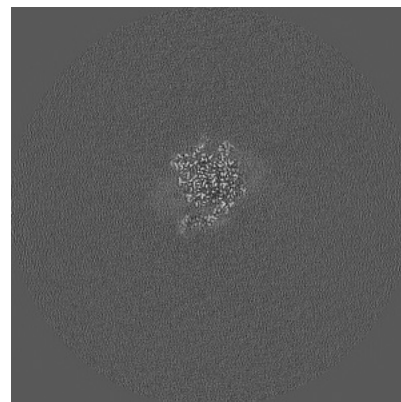
6.3.1 Primary map



X Index: 265

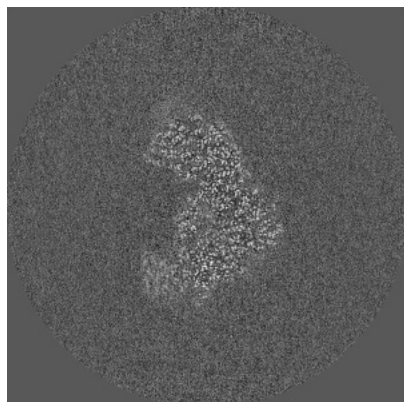


Y Index: 268

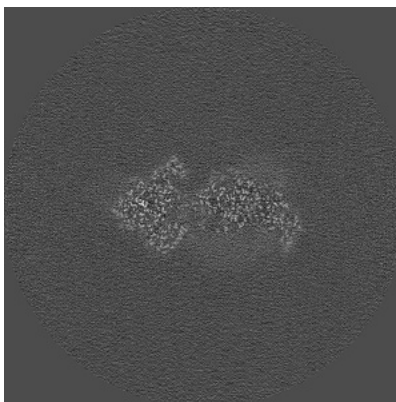


Z Index: 273

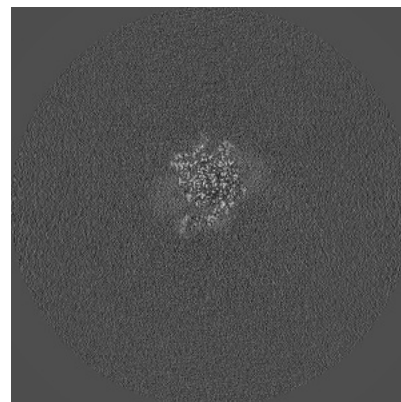
6.3.2 Raw map



X Index: 265



Y Index: 266

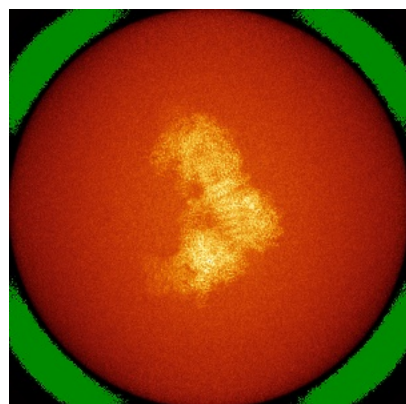


Z Index: 273

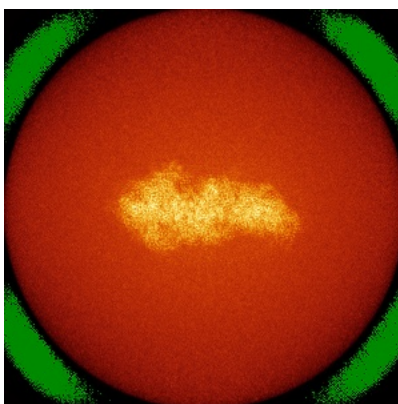
The images above show the largest variance slices of the map in three orthogonal directions.

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

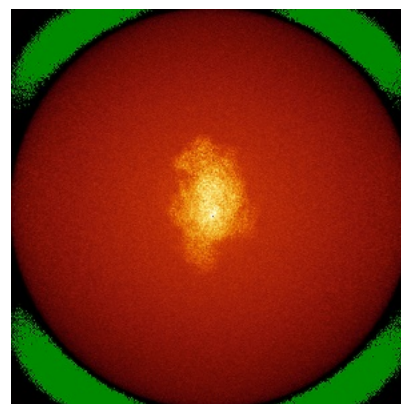
6.4.1 Primary map



X

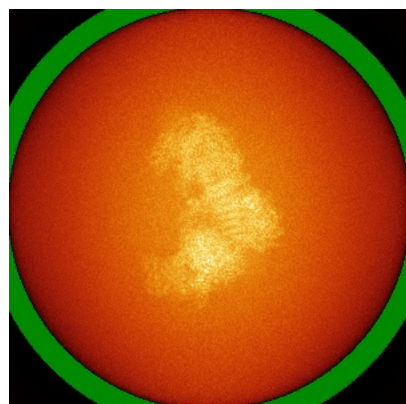


Y

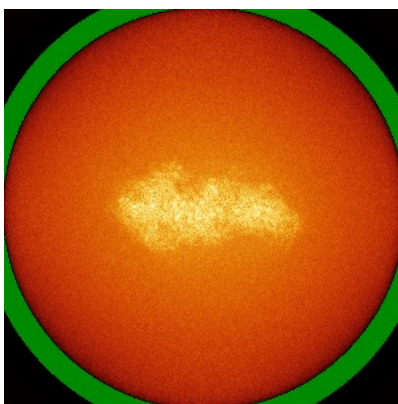


Z

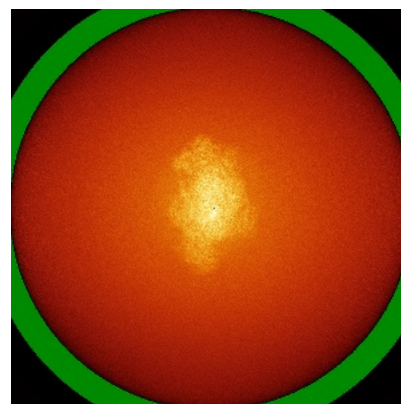
6.4.2 Raw map



X



Y

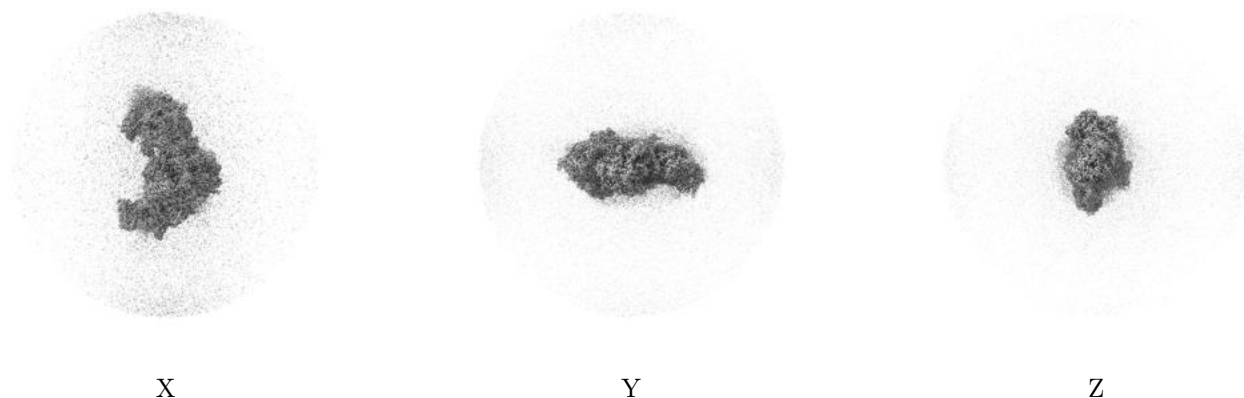


Z

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.

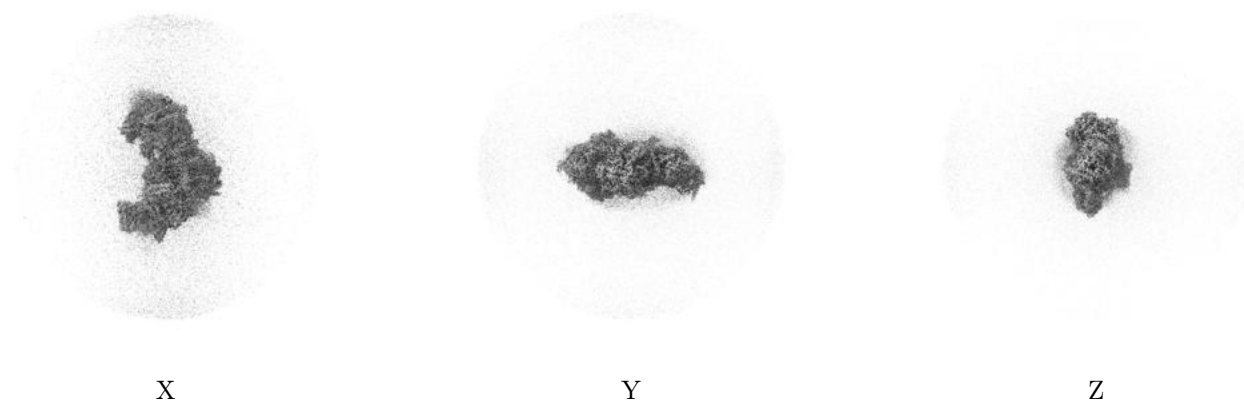
6.5 Orthogonal surface views [i](#)

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.

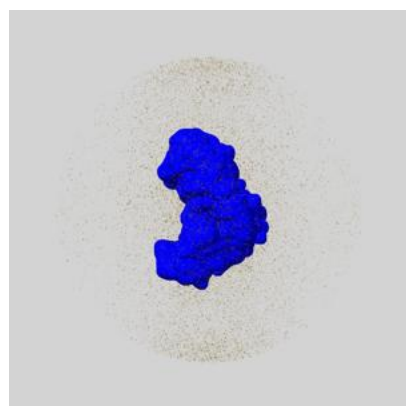
6.6 Mask visualisation [i](#)

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

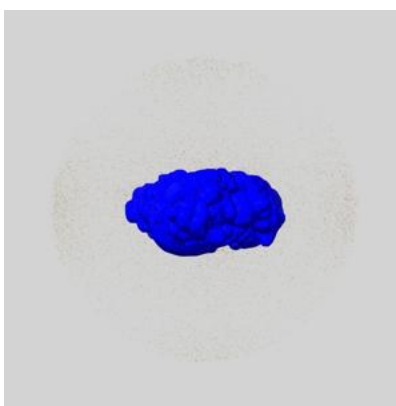
A mask typically either:

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

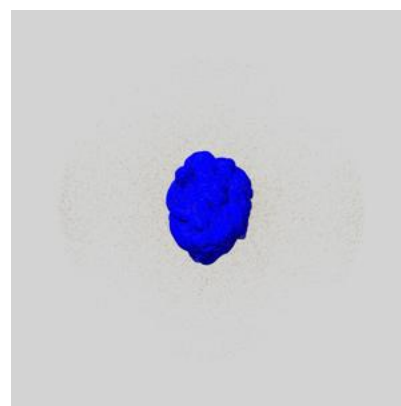
6.6.1 emd_52877_msk_1.map [i](#)



X



Y

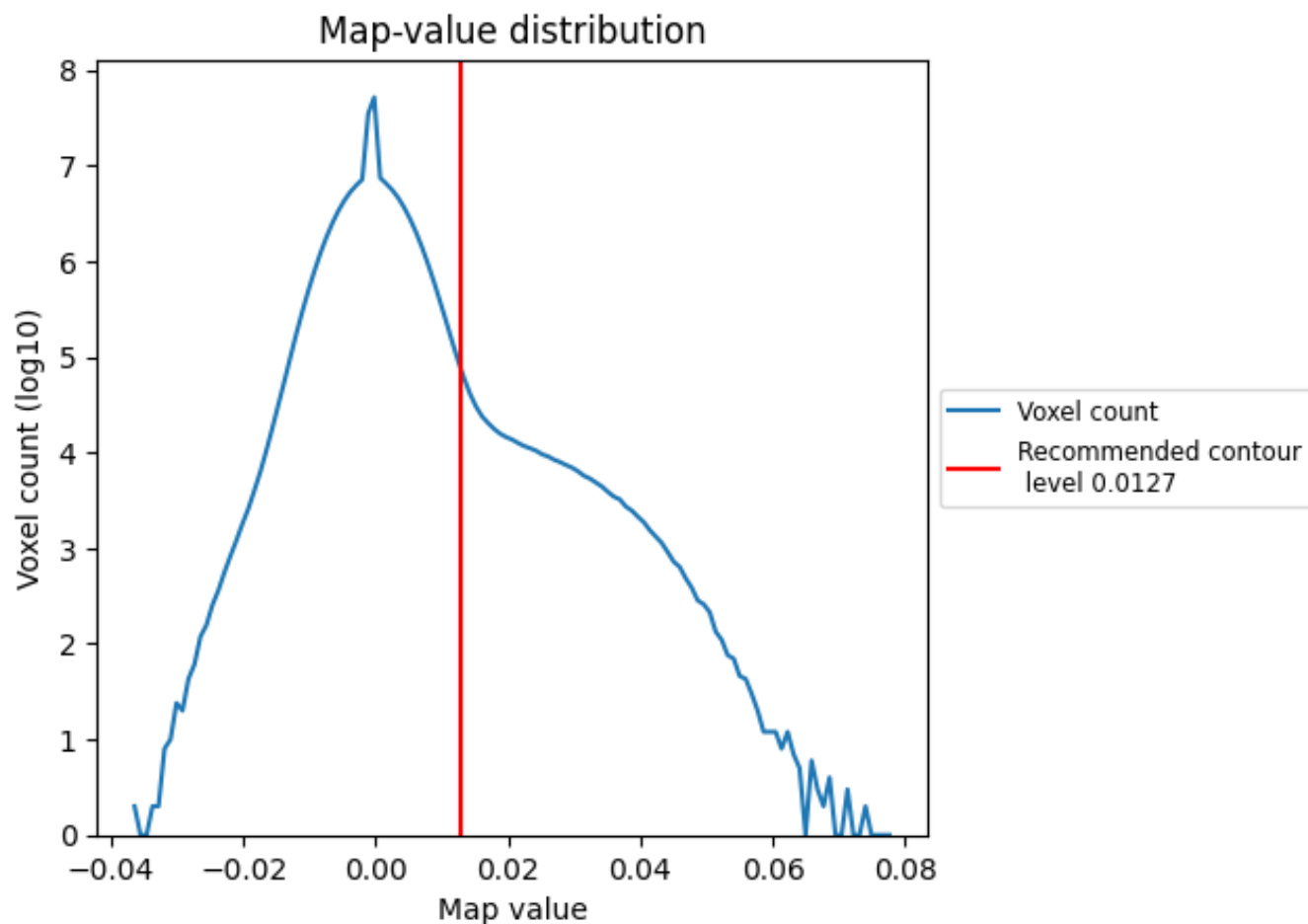


Z

7 Map analysis [i](#)

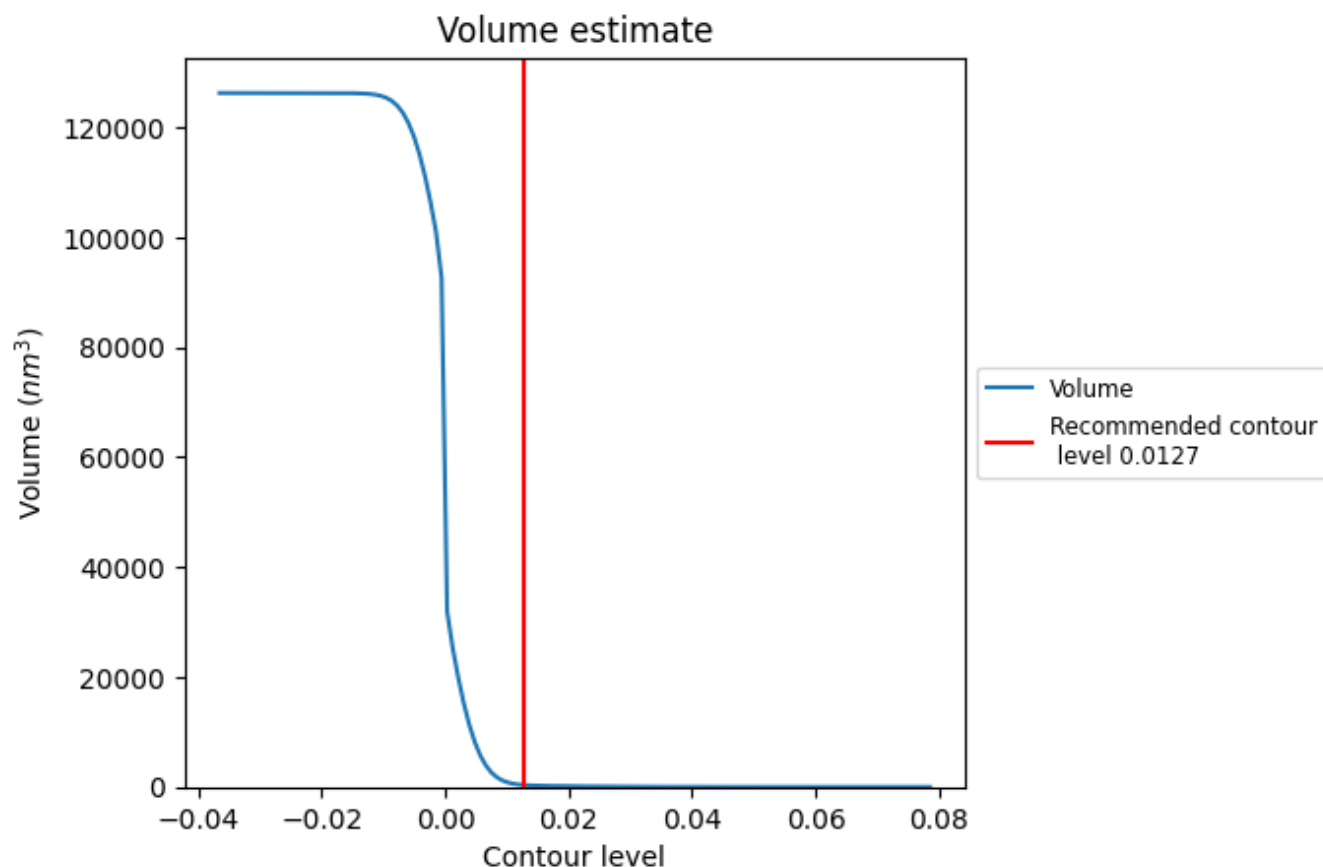
This section contains the results of statistical analysis of the map.

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.

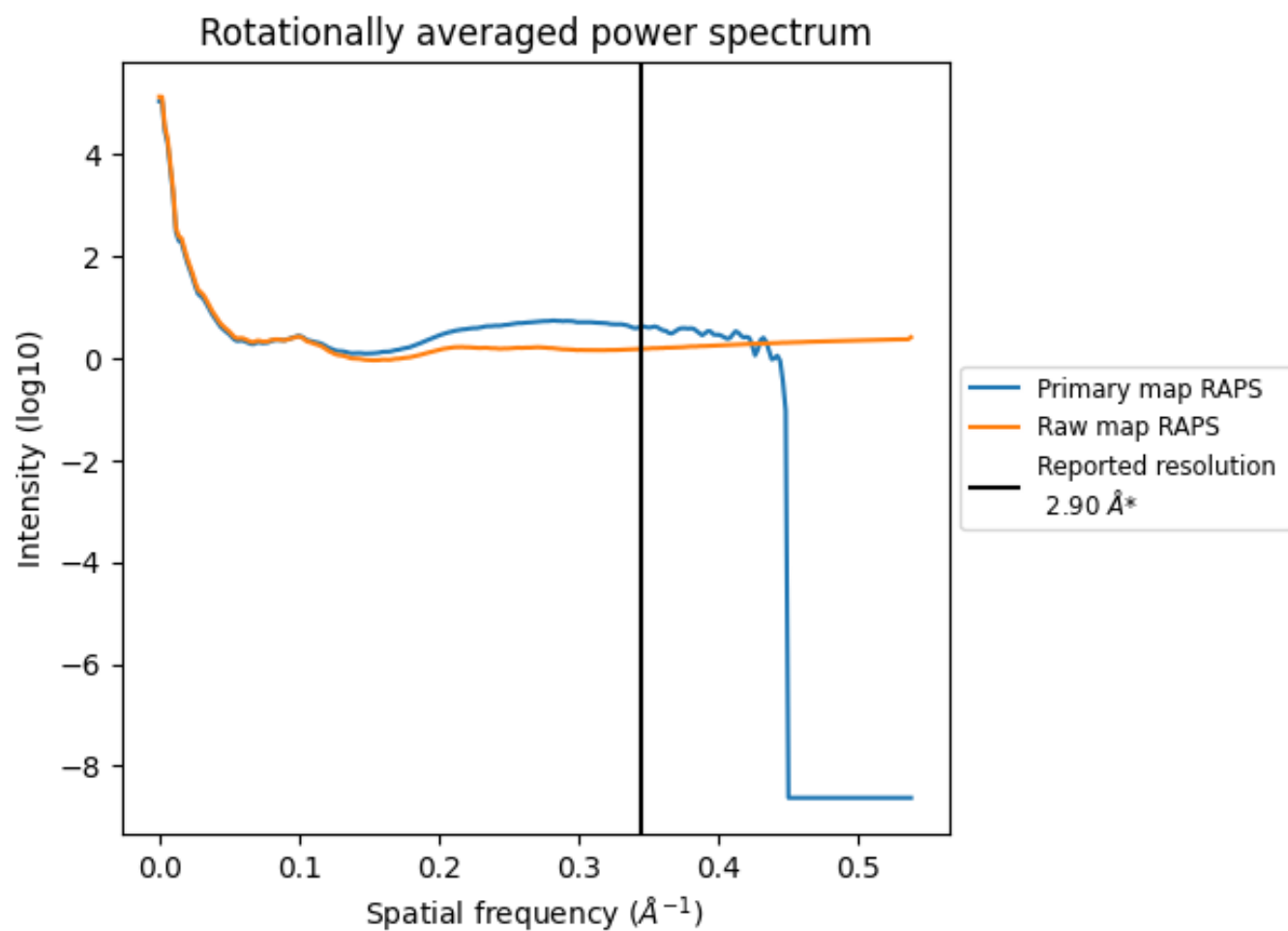
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm^3 ; this corresponds to an approximate mass of 327 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 ⓘ

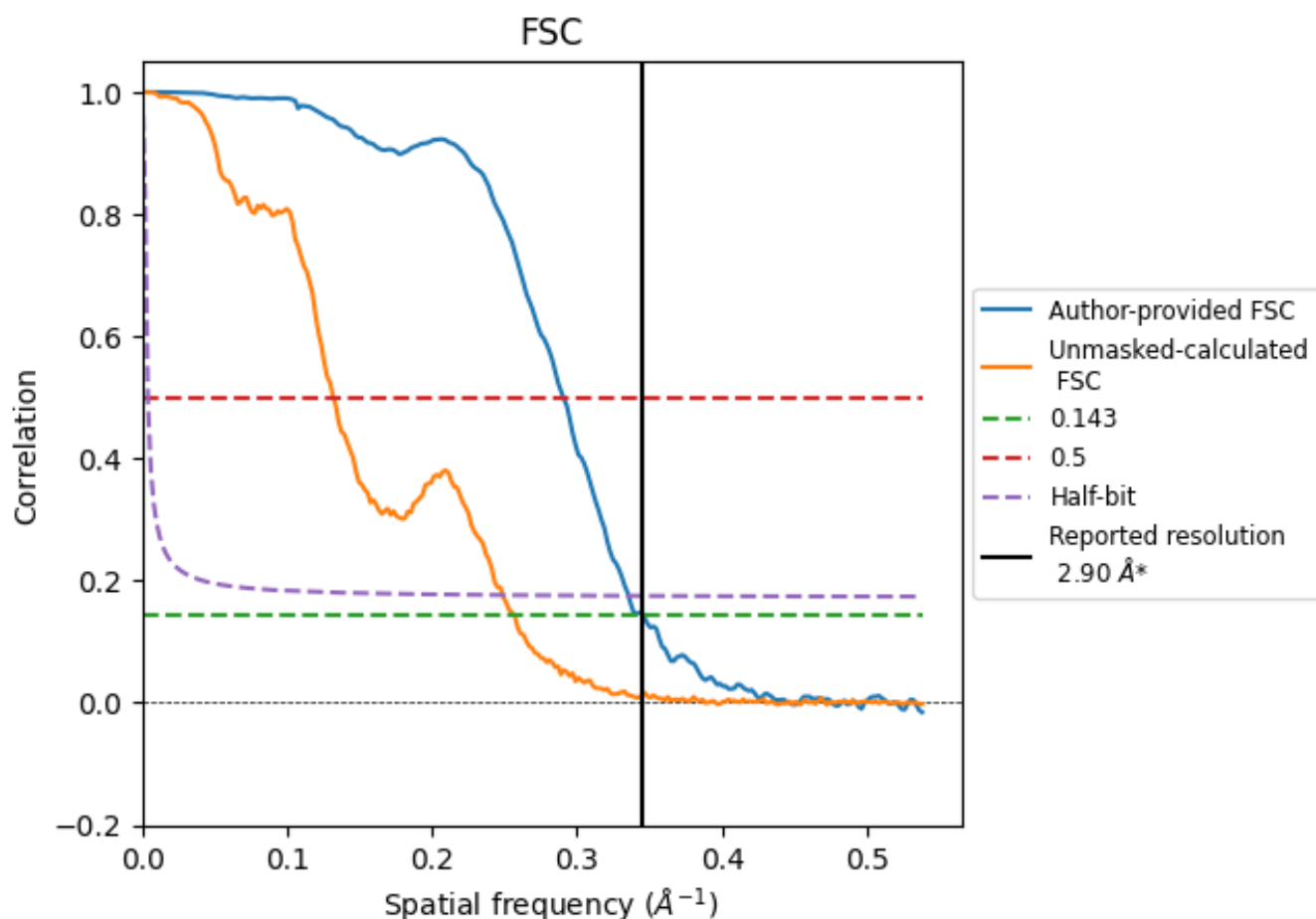


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

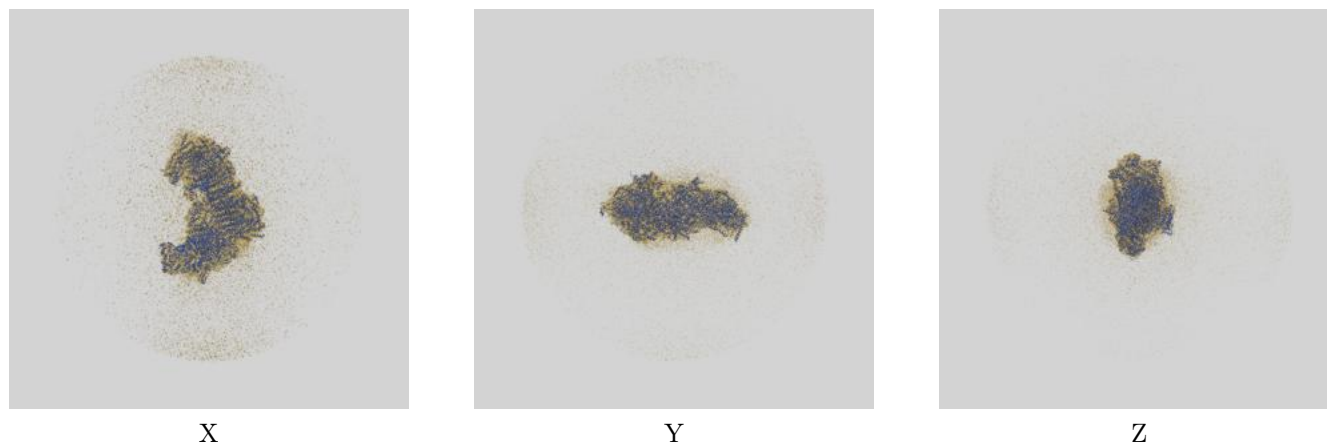
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.44	2.98
Unmasked-calculated*	3.89	7.58	4.02

*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 3.89 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

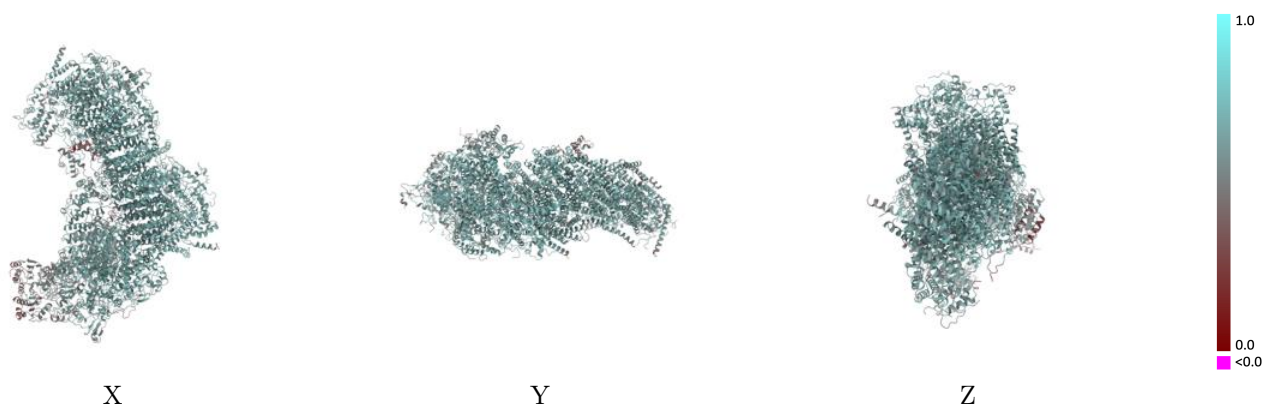
This section contains information regarding the fit between EMDB map EMD-52877 and PDB model 9IHQ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



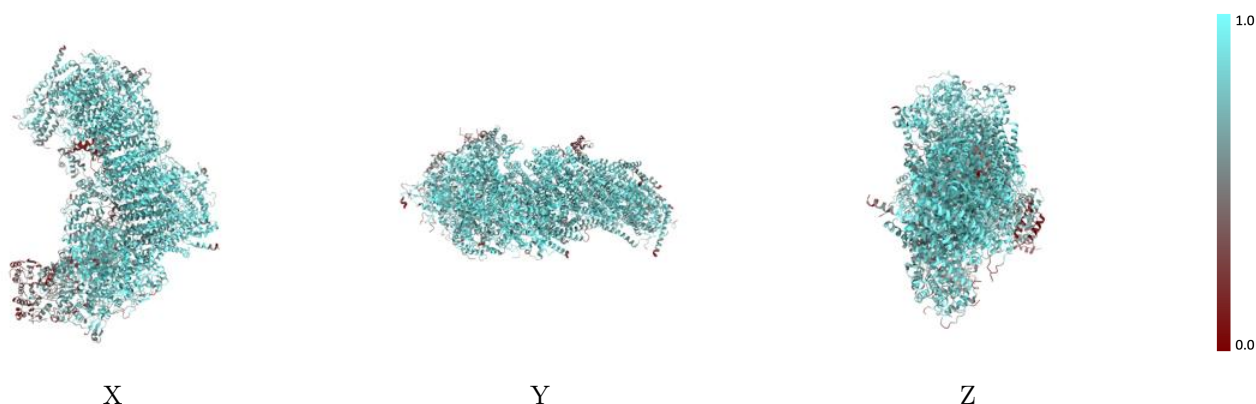
The images above show the 3D surface view of the map at the recommended contour level 0.0127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



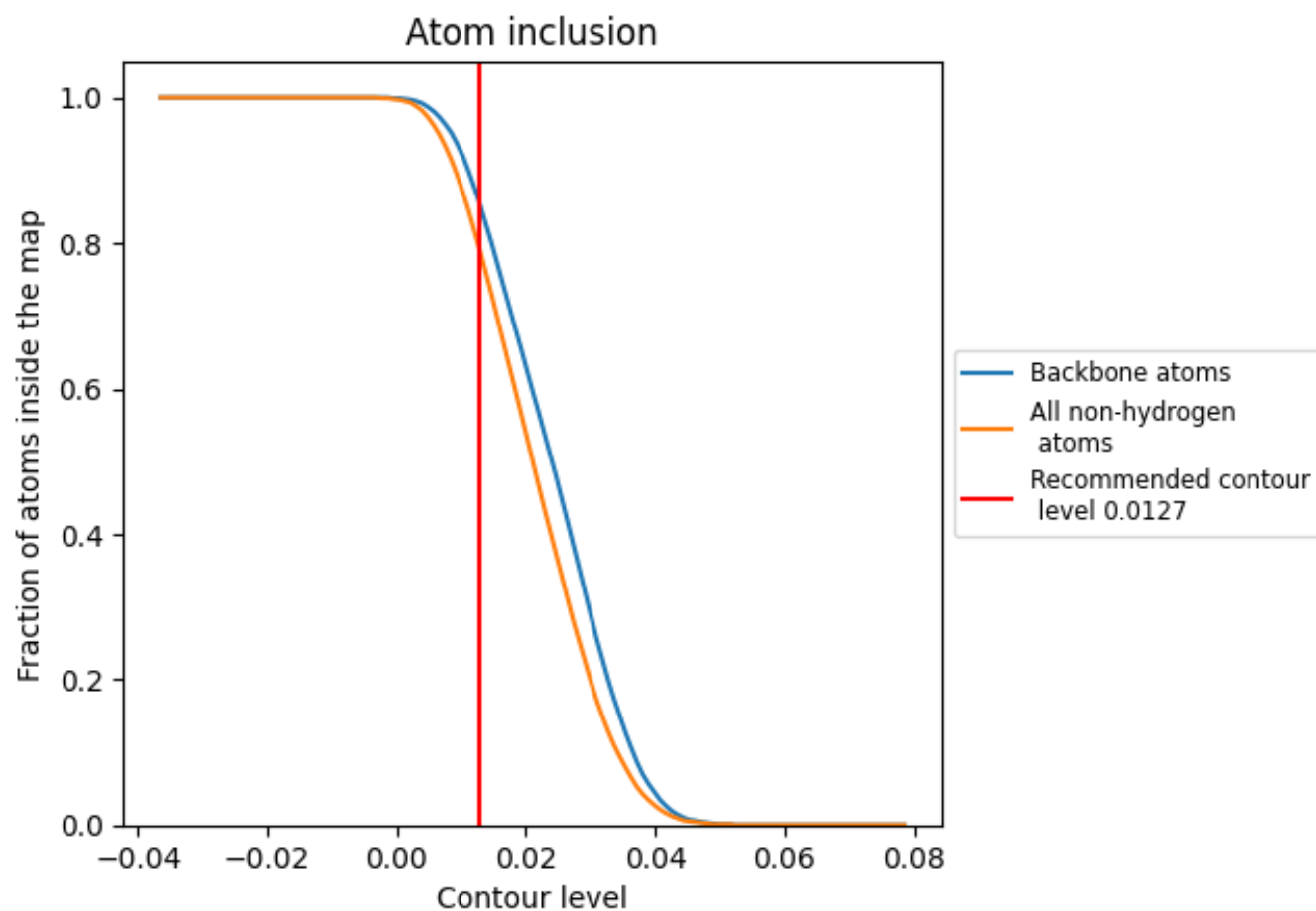
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 80% 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	 0.7970	 0.6120
1	 0.6520	 0.5430
A	 0.8100	 0.6270
B	 0.9030	 0.6560
C	 0.7930	 0.6130
D	 0.8920	 0.6470
G	 0.5550	 0.5120
H	 0.8610	 0.6410
I	 0.8850	 0.6480
J	 0.8140	 0.6110
K	 0.8420	 0.6450
L	 0.8630	 0.6400
M	 0.9140	 0.6600
N	 0.9080	 0.6560
O	 0.8180	 0.6270
P	 0.8140	 0.6120
Q	 0.7960	 0.6070
R	 0.6990	 0.5680
S	 0.2940	 0.4080
T	 0.7420	 0.5970
U	 0.6550	 0.5540
V	 0.7450	 0.5850
W	 0.8380	 0.6240
X	 0.8630	 0.6360
Y	 0.8080	 0.6260
Z	 0.8530	 0.6320
a	 0.8670	 0.6420
b	 0.8040	 0.6300
c	 0.6010	 0.5480
d	 0.8540	 0.6430
e	 0.8660	 0.6450
f	 0.7960	 0.6140
g	 0.5330	 0.5200
h	 0.7790	 0.6030
i	 0.7290	 0.5810



Continued on next page...

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Chain	Atom inclusion	Q-score
j	 0.6740	 0.5720
k	 0.7290	 0.5730
l	 0.8180	 0.6140
m	 0.7920	 0.6150
n	 0.7450	 0.5780
o	 0.7640	 0.5900
p	 0.8770	 0.6420
q	 0.8210	 0.6170