



## wwPDB EM Validation Summary Report ⓘ

Feb 1, 2023 – 08:51 pm GMT

PDB ID : 7R46  
EMDB ID : EMD-14277  
Title : Bovine complex I in the presence of IM1761092, deactive class ii (Composite map)  
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.  
Deposited on : 2022-02-08  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

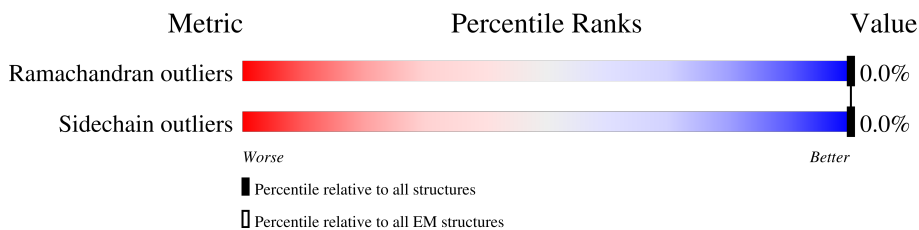
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	88% 12%
2	B	216	71% 28%
3	C	266	77% 23%
4	D	463	91% 9%
5	E	249	86% 14%
6	F	464	93% 7%
7	G	727	95% 5%
8	H	318	98%
9	I	212	83% 17%

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Mol	Chain	Length	Quality of chain
10	J	175	9% 99%
11	K	98	99%
12	L	606	100%
13	M	459	100%
14	N	347	100%
15	O	343	93% 7%
16	P	380	76% 24%
17	Q	175	71% 29%
18	R	124	76% 24%
19	S	99	83% 17%
20	T	156	15% 49% 51%
20	U	156	54% 46%
21	V	116	97%
22	W	128	89% 11%
23	X	172	99%
24	Y	141	38% 98%
25	Z	144	7% 98%
26	a	70	99%
27	b	84	7% 99%
28	c	76	63% 37%
29	d	120	5% 93% 7%
30	e	106	8% 90% 10%
31	f	57	9% 89% 11%
32	g	154	62% 37%
33	h	189	73% 27%

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Mol	Chain	Length	Quality of chain
34	i	127	<p>6% 80% 19%</p>
35	j	108	<p>62% 38%</p>
36	k	98	<p>81% 19%</p>
37	l	186	<p>83% 17%</p>
38	m	129	<p>6% 98%</p>
39	n	179	<p>96%</p>
40	o	137	<p>88% 12%</p>
41	p	176	<p>97%</p>
42	q	145	<p>5% 100%</p>
43	r	113	<p>82% 17%</p>
44	s	109	<p>39% 61%</p>

## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 67614 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
			Total	C	N	O	S		
1	A	101	814	555	118	136	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	155	1241	792	224	211	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1714	1107	295	309	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	421	3395	2168	586	616	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1655	1057	277	311	10	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	430	3310	2085	591	614	20	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	688	5279	3307	920	1013	39	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	312	2462	1651	378	410	23	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	176	1414	889	243	270	12	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	174	1337	902	189	234	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	97	739	483	111	130	15	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	606	4784	3181	736	824	43	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3654	2436	570	609	39	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	347	2733	1817	416	457	43	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2589	1662	429	488	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	289	2298	1469	415	409	5	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	125	1016	641	181	191	3	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	94	Total	C	N	O	S	0	0
			720	442	134	141	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			663	416	124	121	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	84	Total	C	N	O	S	0	0
			681	439	100	137	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			911	589	154	165	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			971	622	180	165	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	140	1030	657	176	191	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	141	1152	740	201	202	9	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	69	561	361	103	92	5	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	83	651	425	109	115	2	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	c	48	405	268	69	68	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	112	934	613	157	161	3	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	95	799	506	150	137	6	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	51	444	291	78	74	1	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	97	813	523	133	153	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	138	1154	759	196	197	2	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	103	884	584	149	150	1	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	67	580	381	95	103	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	79	638	418	107	111	2	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	155	1304	844	213	239	8	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	126	1050	672	186	192		0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	171	1487	952	272	256	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	121	1043	650	200	184	9	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	170	1435	900	265	262	8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	145	1209	778	216	210	5	0	0

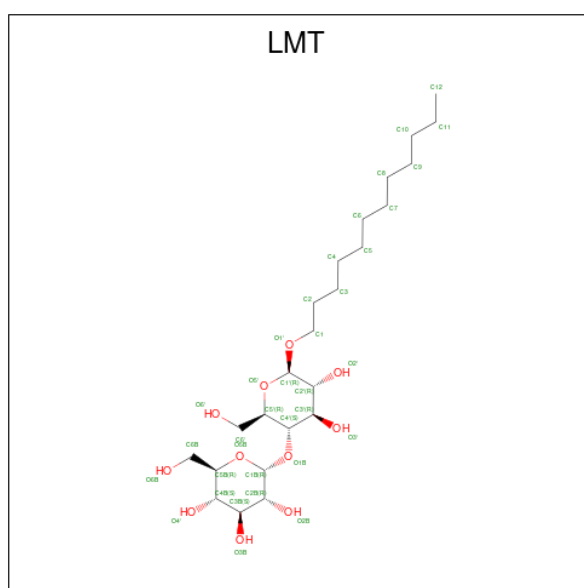
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	94	767	485	143	136	3	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	s	43	364	228	65	70	1	0	0

- Molecule 45 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



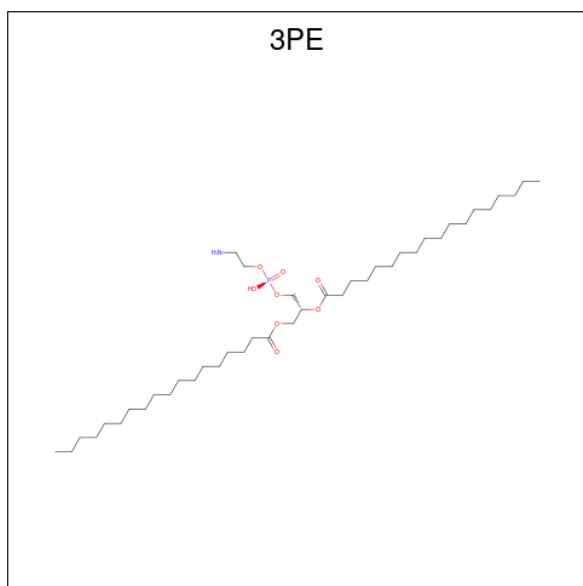
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	A	1	35	24	11	0
45	L	1	35	24	11	0
45	M	1	35	24	11	0
45	M	1	35	24	11	0
45	N	1	35	24	11	0
45	N	1	35	24	11	0
45	Y	1	35	24	11	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	h	1	35	24	11	0
45	h	1	35	24	11	0
45	j	1	35	24	11	0
45	l	1	35	24	11	0

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



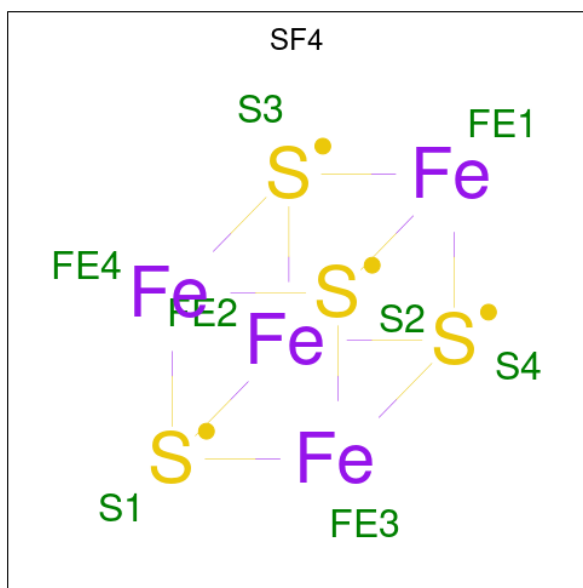
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	40	30	1	8	1	0
46	B	1	36	26	1	8	1	0
46	H	1	24	14	1	8	1	0
46	I	1	51	41	1	8	1	0
46	I	1	31	21	1	8	1	0
46	L	1	49	39	1	8	1	0
46	L	1	45	35	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	L	1	Total 29	C 19	N 1	O 8	P 1	0
46	N	1	Total 43	C 33	N 1	O 8	P 1	0
46	N	1	Total 41	C 31	N 1	O 8	P 1	0
46	Y	1	Total 46	C 36	N 1	O 8	P 1	0
46	Y	1	Total 35	C 25	N 1	O 8	P 1	0
46	Z	1	Total 25	C 15	N 1	O 8	P 1	0
46	d	1	Total 38	C 28	N 1	O 8	P 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



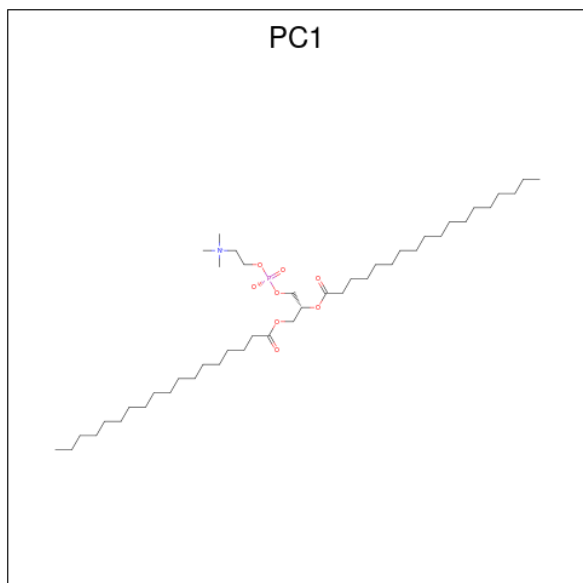
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	Total 8	Fe 4	S 4	0
47	F	1	Total 8	Fe 4	S 4	0
47	G	1	Total 8	Fe 4	S 4	0
47	G	1	Total 8	Fe 4	S 4	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	I	1	8	4	4	0
47	I	1	8	4	4	0

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



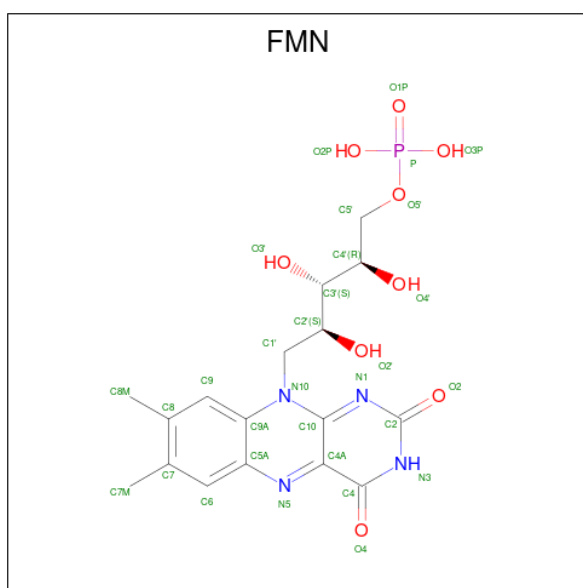
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	35	25	1	8	1	0
48	g	1	49	39	1	8	1	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



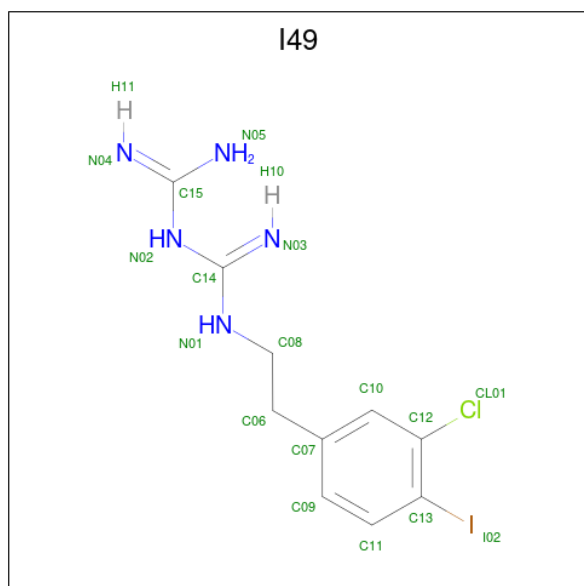
Mol	Chain	Residues	Atoms				AltConf	
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).



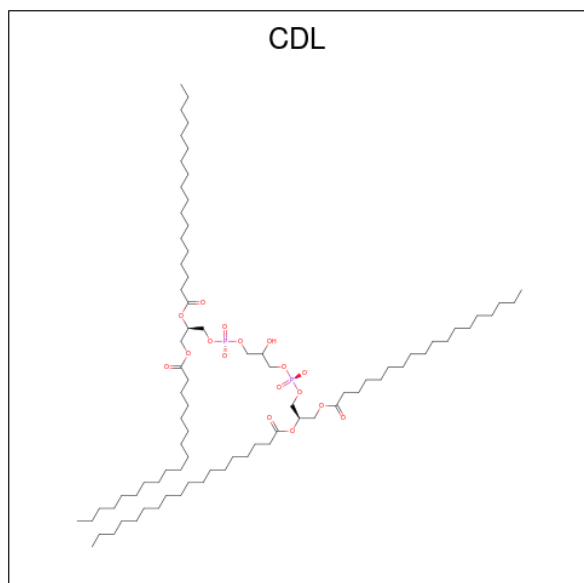
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	K	0
			1	1	

- Molecule 52 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (three-letter code: I49) (formula:  $C_{10}H_{13}ClIN_5$ ) (labeled as "Ligand of Interest" by depositor).



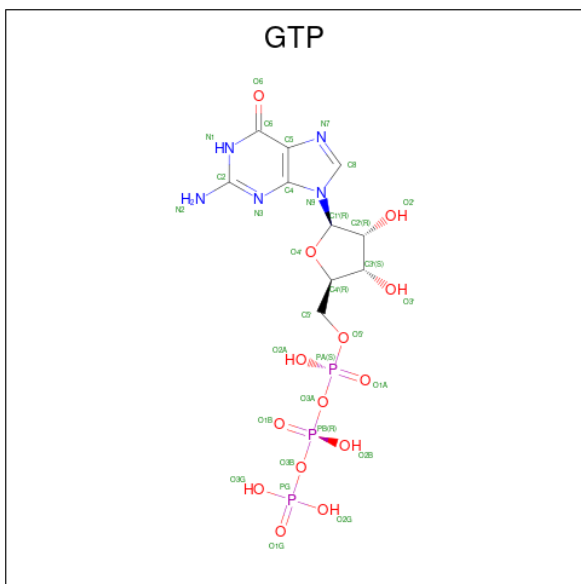
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	I	N	
52	H	1	17	10	1	1	5	0

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
53	K	1	Total	C	O	P	0
			50	35	13	2	
53	L	1	Total	C	O	P	0
			64	45	17	2	
53	X	1	Total	C	O	P	0
			72	53	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			67	48	17	2	
53	q	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



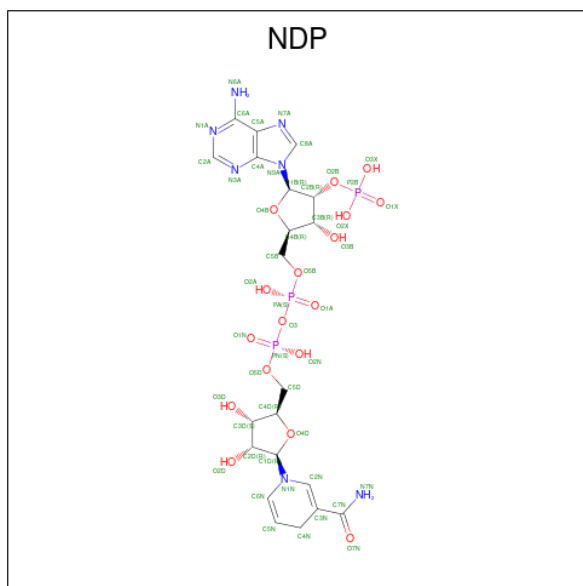
Mol	Chain	Residues	Atoms				AltConf	
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	O	1	Total	Mg	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

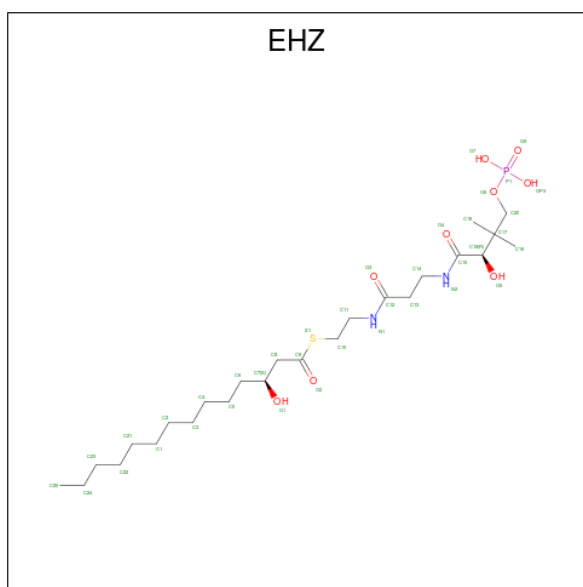


Mol	Chain	Residues	Atoms				AltConf	
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

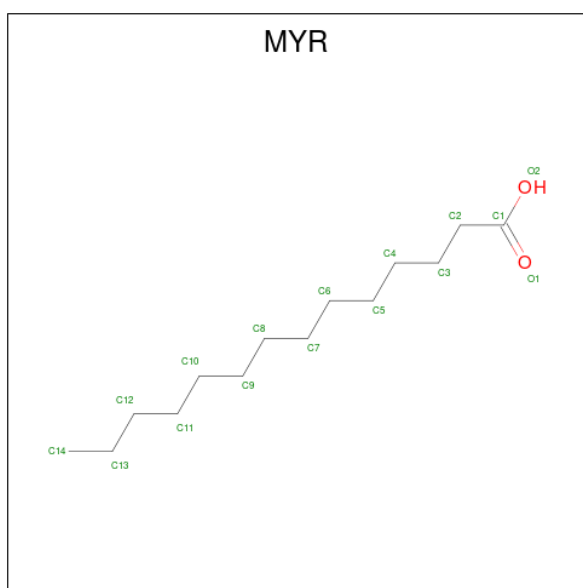
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula:  $C_{25}H_{49}N_2O_9PS$ ).



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

- Molecule 59 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
59	o	1	15	14	1	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	4	Total O 4 4	0
60	B	42	Total O 42 42	0
60	C	61	Total O 61 61	0
60	D	96	Total O 96 96	0
60	E	11	Total O 11 11	0
60	F	44	Total O 44 44	0
60	G	139	Total O 139 139	0
60	H	30	Total O 30 30	0
60	I	76	Total O 76 76	0
60	J	3	Total O 3 3	0
60	K	2	Total O 2 2	0
60	L	25	Total O 25 25	0
60	M	26	Total O 26 26	0
60	N	17	Total O 17 17	0
60	O	5	Total O 5 5	0
60	P	25	Total O 25 25	0
60	Q	51	Total O 51 51	0
60	R	18	Total O 18 18	0
60	U	2	Total O 2 2	0
60	V	10	Total O 10 10	0
60	W	3	Total O 3 3	0
60	X	10	Total O 10 10	0

*Continued on next page...*

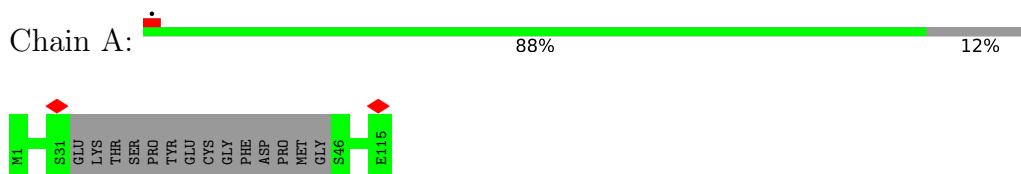
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
60	Y	1	Total 1	O 1	0
60	Z	11	Total 11	O 11	0
60	a	9	Total 9	O 9	0
60	b	3	Total 3	O 3	0
60	d	7	Total 7	O 7	0
60	e	8	Total 8	O 8	0
60	f	3	Total 3	O 3	0
60	g	7	Total 7	O 7	0
60	h	8	Total 8	O 8	0
60	i	4	Total 4	O 4	0
60	j	2	Total 2	O 2	0
60	k	3	Total 3	O 3	0
60	l	13	Total 13	O 13	0
60	m	7	Total 7	O 7	0
60	n	14	Total 14	O 14	0
60	o	7	Total 7	O 7	0
60	p	14	Total 14	O 14	0
60	q	21	Total 21	O 21	0
60	r	14	Total 14	O 14	0
60	s	3	Total 3	O 3	0

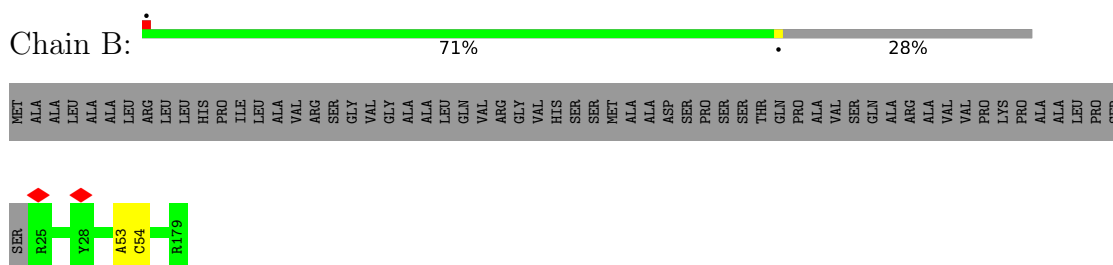
### 3 Residue-property plots [i](#)

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.

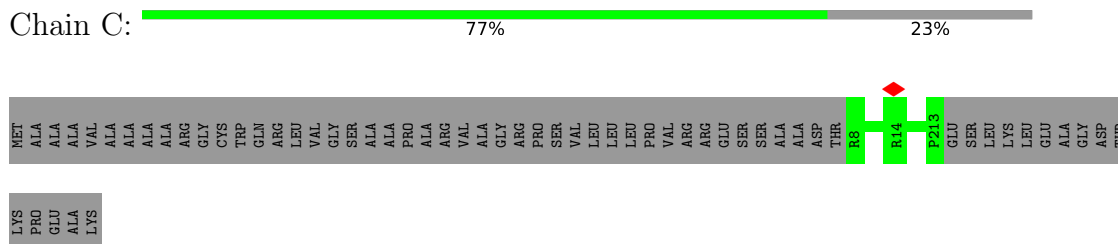
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



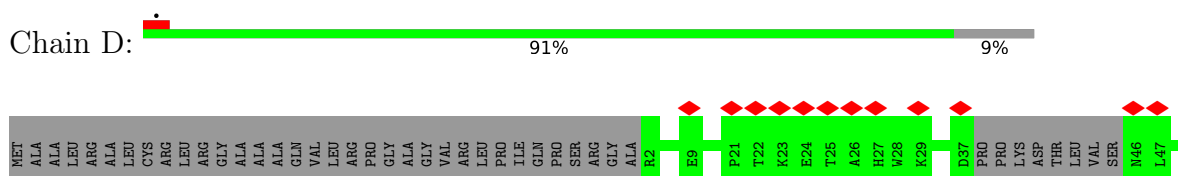
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

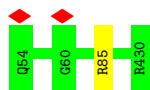


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

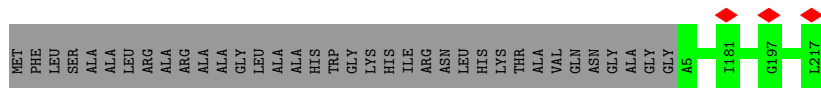
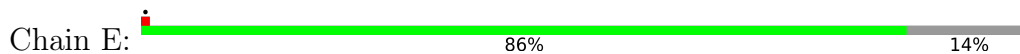


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





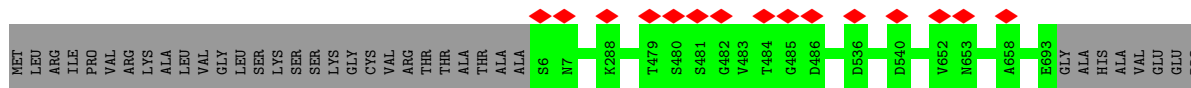
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



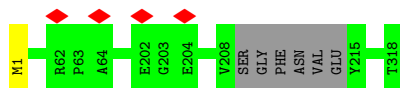
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



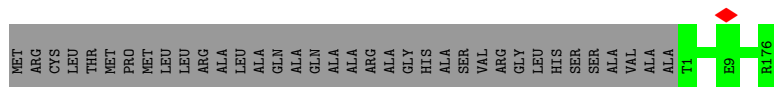
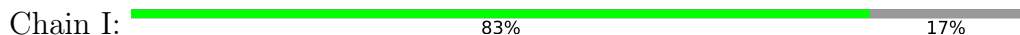
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



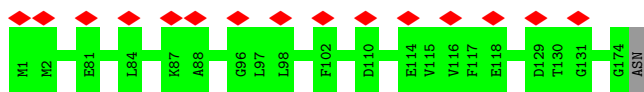
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6







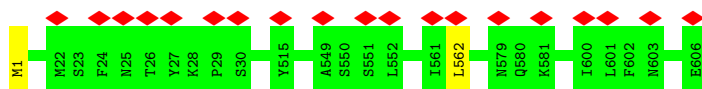
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 99%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 100%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 100%



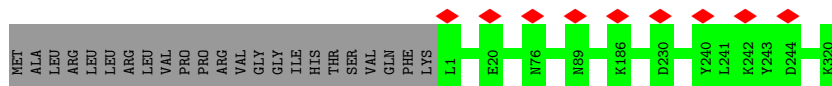
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 100%



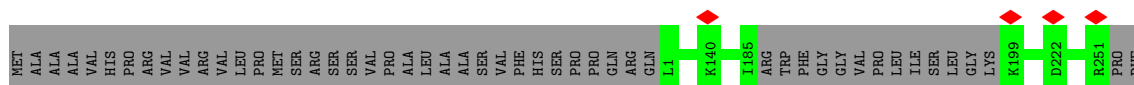
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

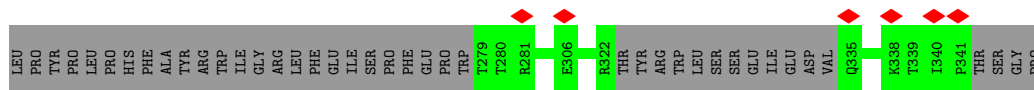
Chain O: 93% 7%



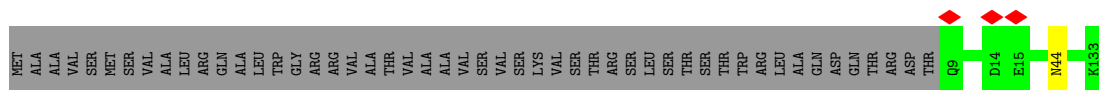
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 76% 24%

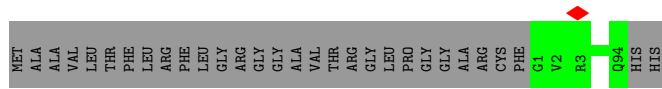
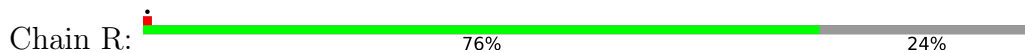




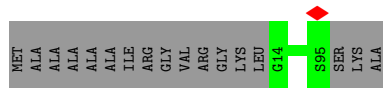
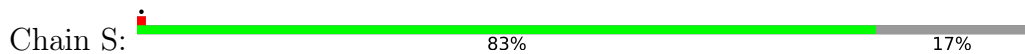
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



• Molecule 20: Acyl carrier protein, mitochondrial

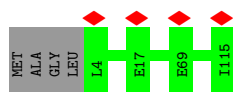


• Molecule 20: Acyl carrier protein, mitochondrial

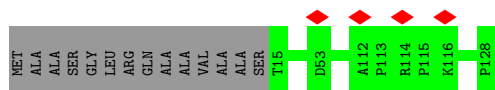
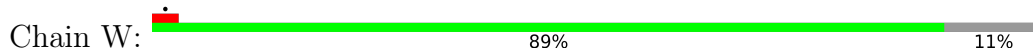


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

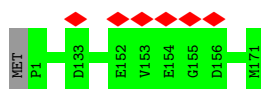




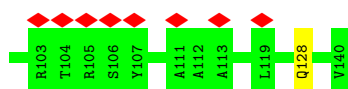
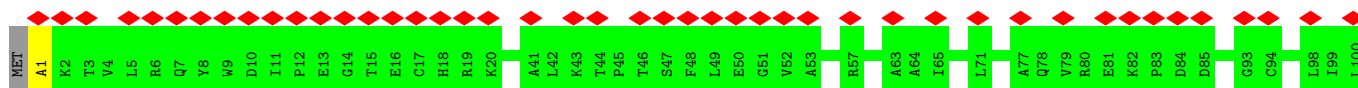
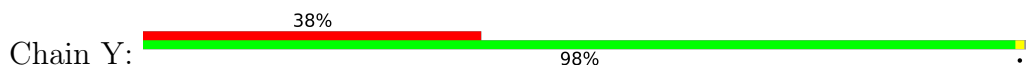
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



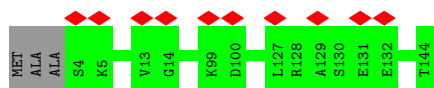
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



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

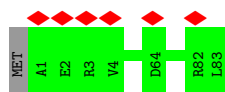


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

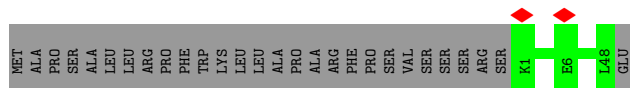


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

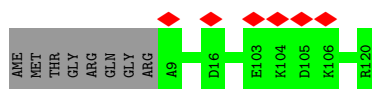
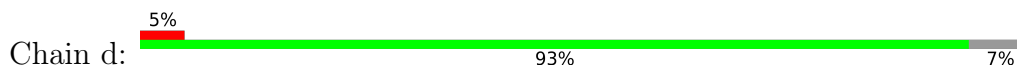




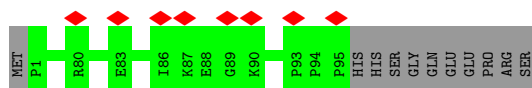
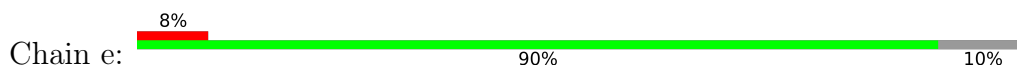
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



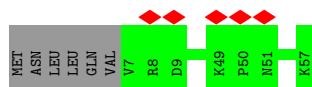
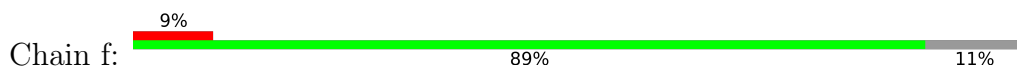
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



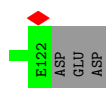
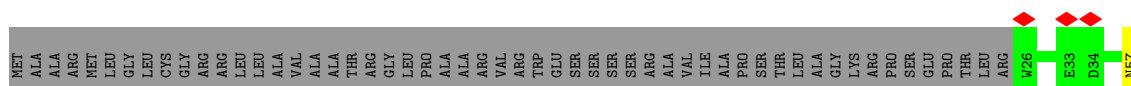
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

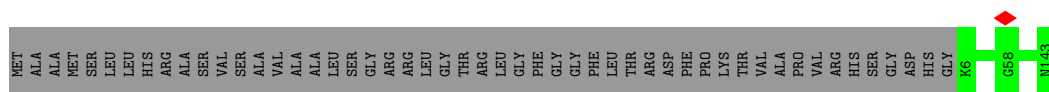


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

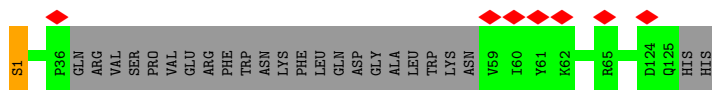
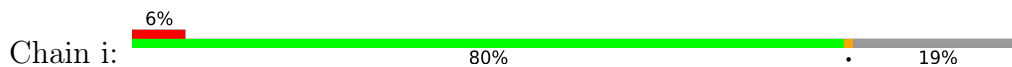


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

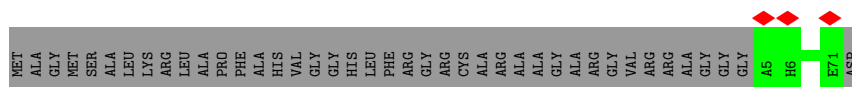




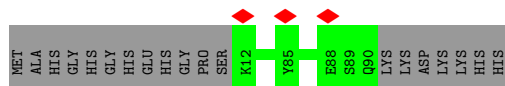
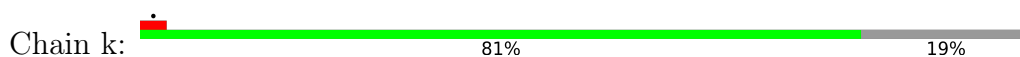
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



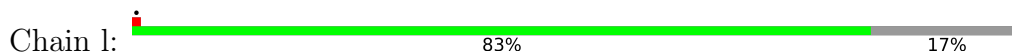
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



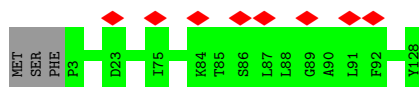
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



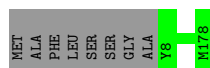
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



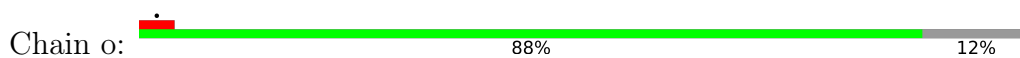
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



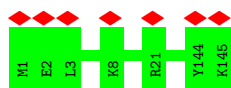
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



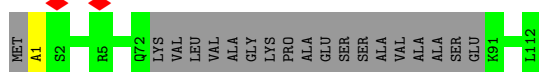
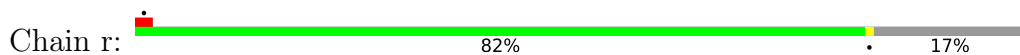
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



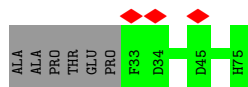
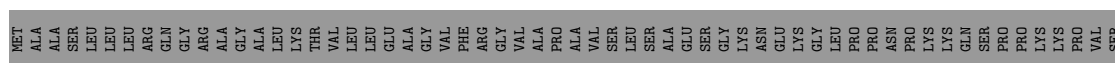
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35448	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	32.083	Depositor
Minimum map value	-12.979	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	5.5	Depositor
Map size ( $\text{\AA}$ )	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.731, 0.731, 0.731	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: MG, FES, LMT, CDL, GTP, 2MR, MYR, K, NDP, SAC, FMN, AYA, PC1, SF4, 3PE, EHZ, ZN, FME, I49

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	0.31	0/824	0.43	0/1128
2	B	0.42	1/1272 (0.1%)	0.48	0/1720
3	C	0.35	0/1765	0.45	0/2403
4	D	0.34	0/3470	0.44	0/4699
5	E	0.33	0/1695	0.44	0/2307
6	F	0.32	0/3384	0.46	0/4573
7	G	0.32	0/5367	0.47	0/7274
8	H	0.34	0/2522	0.44	0/3445
9	I	0.36	0/1445	0.47	0/1956
10	J	0.33	0/1362	0.43	0/1848
11	K	0.32	0/739	0.47	0/1000
12	L	0.33	0/4900	0.42	0/6667
13	M	0.32	0/3738	0.42	0/5097
14	N	0.31	0/2792	0.43	0/3800
15	O	0.34	0/2651	0.41	0/3587
16	P	0.31	0/2348	0.44	0/3172
17	Q	0.32	0/1039	0.45	0/1404
18	R	0.35	0/731	0.46	0/984
19	S	0.30	0/674	0.45	0/908
20	T	0.30	0/621	0.39	0/837
20	U	0.38	0/692	0.41	0/932
21	V	0.29	0/931	0.37	0/1261
22	W	0.31	0/995	0.42	0/1337
23	X	0.33	0/1439	0.41	0/1942
24	Y	0.29	0/1042	0.41	0/1414
25	Z	0.32	0/1181	0.42	0/1592
26	a	0.35	0/576	0.42	0/775
27	b	0.32	0/672	0.41	0/923
28	c	0.30	0/418	0.36	0/567
29	d	0.36	0/964	0.38	0/1305
30	e	0.30	0/818	0.42	0/1093



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	f	0.32	0/457	0.40	0/616
32	g	0.35	0/839	0.38	0/1140
33	h	0.34	0/1188	0.41	0/1607
34	i	0.37	0/904	0.43	0/1230
35	j	0.36	0/607	0.42	0/833
36	k	0.35	0/657	0.41	0/887
37	l	0.39	0/1358	0.41	0/1858
38	m	0.36	0/1076	0.41	0/1455
39	n	0.37	0/1540	0.41	0/2085
40	o	0.39	0/1068	0.41	0/1430
41	p	0.36	0/1468	0.41	0/1979
42	q	0.33	0/1250	0.44	0/1698
43	r	0.33	0/780	0.44	0/1056
44	s	0.32	0/375	0.42	0/507
All	All	0.34	1/66634 (0.0%)	0.43	0/90331

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
34	i	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	CYS	CB-SG	-5.92	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	i	1	SAC	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	A	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
2	B	153/216 (71%)	144 (94%)	8 (5%)	1 (1%)	22	32
3	C	204/266 (77%)	198 (97%)	6 (3%)	0	100	100
4	D	416/463 (90%)	398 (96%)	18 (4%)	0	100	100
5	E	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
6	F	428/464 (92%)	419 (98%)	9 (2%)	0	100	100
7	G	686/727 (94%)	661 (96%)	25 (4%)	0	100	100
8	H	308/318 (97%)	294 (96%)	14 (4%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	172/175 (98%)	157 (91%)	15 (9%)	0	100	100
11	K	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	580 (96%)	23 (4%)	1 (0%)	47	62
13	M	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	311 (98%)	7 (2%)	0	100	100
16	P	281/380 (74%)	275 (98%)	6 (2%)	0	100	100
17	Q	123/175 (70%)	122 (99%)	1 (1%)	0	100	100
18	R	92/124 (74%)	90 (98%)	2 (2%)	0	100	100
19	S	80/99 (81%)	78 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	72 (97%)	2 (3%)	0	100	100
20	U	82/156 (53%)	82 (100%)	0	0	100	100
21	V	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	132 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	139/144 (96%)	131 (94%)	8 (6%)	0	100	100
26	a	67/70 (96%)	67 (100%)	0	0	100	100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	c	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
29	d	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
32	g	95/154 (62%)	89 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
38	m	124/129 (96%)	118 (95%)	6 (5%)	0	100	100
39	n	169/179 (94%)	165 (98%)	4 (2%)	0	100	100
40	o	119/137 (87%)	113 (95%)	6 (5%)	0	100	100
41	p	168/176 (96%)	168 (100%)	0	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	41/109 (38%)	38 (93%)	3 (7%)	0	100	100
All	All	7993/9212 (87%)	7757 (97%)	234 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
2	B	53	ALA

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/100 (88%)	88 (100%)	0	100	100
2	B	131/175 (75%)	131 (100%)	0	100	100
3	C	187/228 (82%)	187 (100%)	0	100	100
4	D	362/392 (92%)	362 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	344/368 (94%)	344 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	268/274 (98%)	268 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	84/85 (99%)	84 (100%)	0	100	100
12	L	529/533 (99%)	529 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	248/327 (76%)	248 (100%)	0	100	100
17	Q	112/153 (73%)	111 (99%)	1 (1%)	78	90
18	R	77/97 (79%)	77 (100%)	0	100	100
19	S	73/82 (89%)	73 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	78/135 (58%)	78 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	100 (99%)	1 (1%)	76	88
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	58/59 (98%)	58 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	f	48/54 (89%)	48 (100%)	0	100	100
32	g	88/131 (67%)	87 (99%)	1 (1%)	73	87
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	98/120 (82%)	98 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	61/76 (80%)	61 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	112/115 (97%)	112 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	131/131 (100%)	131 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	42/92 (46%)	42 (100%)	0	100	100
All	All	7059/7892 (89%)	7056 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	44	ASN
24	Y	128	GLN
32	g	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
38	m	74	ASN
39	n	12	GLN
44	s	44	HIS
15	O	190	HIS
17	Q	44	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

11 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
10	FME	J	1	10	8,9,10	0.93	0	7,9,11	0.83	0
8	FME	H	1	8	8,9,10	0.98	1 (12%)	7,9,11	0.81	0
34	SAC	i	1	34	7,8,9	1.88	1 (14%)	8,9,11	1.78	1 (12%)
1	FME	A	1	1	8,9,10	0.95	0	7,9,11	0.96	0
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	1.21	1 (14%)
11	FME	K	1	11	8,9,10	0.91	0	7,9,11	0.78	0
14	FME	N	1	14	8,9,10	1.02	1 (12%)	7,9,11	0.86	0
43	AYA	r	1	43	6,7,8	1.77	2 (33%)	5,8,10	1.29	1 (20%)
4	2MR	D	85	4	10,12,13	2.65	4 (40%)	5,13,15	0.83	0
12	FME	L	1	12	8,9,10	0.97	0	7,9,11	1.04	1 (14%)
24	AYA	Y	1	24	6,7,8	1.79	1 (16%)	5,8,10	1.18	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FME	J	1	10	-	4/7/9/11	-
8	FME	H	1	8	-	2/7/9/11	-
34	SAC	i	1	34	-	0/7/8/10	-
1	FME	A	1	1	-	2/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
4	2MR	D	85	4	-	0/10/13/15	-
12	FME	L	1	12	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AYA	Y	1	24	-	1/4/6/8	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.97	1.44	1.33
4	D	85	2MR	CZ-NE	4.76	1.44	1.34
34	i	1	SAC	O-C	4.18	1.36	1.19
4	D	85	2MR	O-C	3.93	1.35	1.19
24	Y	1	AYA	CT-N	3.27	1.45	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	O-C-CA	-4.50	112.98	124.78
13	M	1	FME	C-CA-N	2.69	114.59	109.73
43	r	1	AYA	CM-CT-N	2.24	119.90	116.10
12	L	1	FME	C-CA-N	2.19	113.69	109.73
24	Y	1	AYA	CM-CT-N	2.07	119.61	116.10

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 3 are monoatomic - leaving 48 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
53	CDL	X	1701	-	71,71,99	1.02	7 (9%)	77,83,111	1.19	5 (6%)
53	CDL	L	702	-	63,63,99	1.08	6 (9%)	69,75,111	1.11	4 (5%)
45	LMT	M	801	-	36,36,36	1.11	2 (5%)	47,47,47	1.21	4 (8%)
46	3PE	Z	401	-	24,24,50	1.21	4 (16%)	27,29,55	1.16	2 (7%)
45	LMT	h	1003	-	36,36,36	1.16	2 (5%)	47,47,47	0.97	2 (4%)
47	SF4	G	802	7	0,12,12	-	-	-		
46	3PE	L	703	-	44,44,50	0.91	3 (6%)	47,49,55	1.11	2 (4%)
53	CDL	d	1202	-	64,64,99	1.07	7 (10%)	70,76,111	1.14	4 (5%)
46	3PE	L	705	-	28,28,50	1.12	4 (14%)	31,33,55	1.16	2 (6%)
47	SF4	I	202	9	0,12,12	-	-	-		
47	SF4	I	203	9	0,12,12	-	-	-		
49	FES	G	803	7	0,4,4	-	-	-		
45	LMT	A	301	-	36,36,36	1.21	2 (5%)	47,47,47	0.94	1 (2%)
53	CDL	K	401	-	49,49,99	1.01	5 (10%)	54,58,111	1.01	2 (3%)
45	LMT	N	901	-	36,36,36	1.16	3 (8%)	47,47,47	0.79	0
46	3PE	I	201	-	50,50,50	0.86	3 (6%)	53,55,55	1.05	2 (3%)
45	LMT	M	802	-	36,36,36	1.17	3 (8%)	47,47,47	1.37	3 (6%)
47	SF4	G	801	7	0,12,12	-	-	-		
46	3PE	Y	601	-	45,45,50	0.90	3 (6%)	48,50,55	1.16	3 (6%)
58	EHZ	T	101	20	29,36,37	1.66	4 (13%)	35,44,47	1.48	4 (11%)
48	PC1	B	1003	-	34,34,53	1.15	4 (11%)	40,42,61	1.13	2 (5%)
59	MYR	o	201	40	14,14,15	0.81	0	13,13,15	0.66	0
56	NDP	P	501	-	45,52,52	2.10	5 (11%)	53,80,80	1.68	10 (18%)
45	LMT	j	101	-	36,36,36	1.17	2 (5%)	47,47,47	0.81	0
54	GTP	O	401	55	26,34,34	2.92	10 (38%)	32,54,54	1.80	10 (31%)
45	LMT	h	1002	-	36,36,36	1.17	3 (8%)	47,47,47	1.31	5 (10%)
46	3PE	d	1201	-	37,37,50	0.99	4 (10%)	40,42,55	1.10	2 (5%)
48	PC1	g	1501	-	48,48,53	0.99	3 (6%)	54,56,61	0.98	2 (3%)
46	3PE	N	902	-	42,42,50	0.93	3 (7%)	45,47,55	1.13	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	FES	E	301	5	0,4,4	-	-	-	-	-
58	EHZ	U	101	20	29,36,37	1.64	5 (17%)	35,44,47	1.47	4 (11%)
45	LMT	Y	603	-	36,36,36	1.21	2 (5%)	47,47,47	1.01	1 (2%)
46	3PE	N	904	-	40,40,50	0.94	4 (10%)	43,45,55	1.13	2 (4%)
46	3PE	Y	602	-	34,34,50	1.04	4 (11%)	37,39,55	1.17	2 (5%)
45	LMT	l	201	-	36,36,36	1.22	3 (8%)	47,47,47	1.08	3 (6%)
50	FMN	F	501	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
46	3PE	I	204	-	30,30,50	1.08	3 (10%)	33,35,55	1.19	3 (9%)
46	3PE	H	601	-	23,23,50	1.61	4 (17%)	24,27,55	1.15	2 (8%)
53	CDL	h	1001	-	66,66,99	1.06	7 (10%)	72,78,111	1.18	4 (5%)
53	CDL	q	201	-	60,60,99	1.11	8 (13%)	66,72,111	1.11	4 (6%)
52	I49	H	602	-	15,17,17	1.53	2 (13%)	21,22,22	2.50	7 (33%)
46	3PE	B	1001	-	35,35,50	1.02	4 (11%)	38,40,55	1.11	2 (5%)
46	3PE	A	302	-	39,39,50	0.94	4 (10%)	42,44,55	1.23	2 (4%)
45	LMT	N	903	-	36,36,36	1.17	3 (8%)	47,47,47	0.90	1 (2%)
45	LMT	L	704	-	36,36,36	1.18	2 (5%)	47,47,47	0.92	1 (2%)
47	SF4	B	1002	2	0,12,12	-	-	-	-	-
46	3PE	L	701	-	48,48,50	0.87	2 (4%)	51,53,55	1.05	2 (3%)

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
53	CDL	X	1701	-	-	46/82/82/110	-
53	CDL	L	702	-	-	32/74/74/110	-
45	LMT	M	801	-	-	6/21/61/61	0/2/2/2
46	3PE	Z	401	-	-	13/28/28/54	-
45	LMT	h	1003	-	-	6/21/61/61	0/2/2/2
53	CDL	d	1202	-	-	36/75/75/110	-
46	3PE	L	703	-	-	25/48/48/54	-
47	SF4	G	802	7	-	-	0/6/5/5
46	3PE	L	705	-	-	15/32/32/54	-
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	I	203	9	-	-	0/6/5/5
49	FES	G	803	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	A	301	-	-	8/21/61/61	0/2/2/2
53	CDL	K	401	-	-	19/54/54/110	-
45	LMT	N	901	-	-	3/21/61/61	0/2/2/2
46	3PE	I	201	-	-	25/54/54/54	-
45	LMT	M	802	-	-	8/21/61/61	0/2/2/2
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	Y	601	-	-	26/49/49/54	-
58	EHZ	T	101	20	-	14/42/44/45	-
48	PC1	B	1003	-	-	14/38/38/57	-
59	MYR	o	201	40	-	6/11/12/13	-
56	NDP	P	501	-	-	6/30/77/77	0/5/5/5
45	LMT	j	101	-	-	5/21/61/61	0/2/2/2
54	GTP	O	401	55	-	6/18/38/38	0/3/3/3
45	LMT	h	1002	-	-	8/21/61/61	0/2/2/2
46	3PE	d	1201	-	-	22/41/41/54	-
48	PC1	g	1501	-	-	19/52/52/57	-
46	3PE	N	902	-	-	19/46/46/54	-
47	SF4	F	502	6	-	-	0/6/5/5
49	FES	E	301	5	-	-	0/1/1/1
58	EHZ	U	101	20	-	10/42/44/45	-
45	LMT	Y	603	-	-	7/21/61/61	0/2/2/2
46	3PE	N	904	-	-	16/44/44/54	-
46	3PE	Y	602	-	-	18/38/38/54	-
45	LMT	l	201	-	-	7/21/61/61	0/2/2/2
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
46	3PE	I	204	-	-	17/34/34/54	-
46	3PE	H	601	-	-	9/26/26/54	-
53	CDL	h	1001	-	-	35/77/77/110	-
53	CDL	q	201	-	-	36/71/71/110	-
52	I49	H	602	-	-	7/10/10/10	0/1/1/1
46	3PE	B	1001	-	-	17/39/39/54	-
46	3PE	A	302	-	-	24/43/43/54	-
45	LMT	N	903	-	-	10/21/61/61	0/2/2/2
45	LMT	L	704	-	-	8/21/61/61	0/2/2/2
47	SF4	B	1002	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	L	701	-	-	22/52/52/54	-

The worst 5 of 151 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	11.38	1.80	1.59
54	O	401	GTP	O6-C6	8.30	1.40	1.23
58	T	101	EHZ	C15-N2	5.41	1.45	1.33
54	O	401	GTP	O4'-C1'	5.24	1.48	1.41
58	U	101	EHZ	C15-N2	5.24	1.45	1.33

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	H	602	I49	C14-N02-C15	-7.33	113.00	125.21
56	P	501	NDP	PN-O3-PA	-7.00	108.81	132.83
58	U	101	EHZ	C8-C9-S1	5.83	120.84	113.63
58	T	101	EHZ	C8-C9-S1	5.59	120.55	113.63
45	M	802	LMT	C3B-C4B-C5B	5.20	119.51	110.24

There are no chirality outliers.

5 of 632 torsion outliers are listed below:

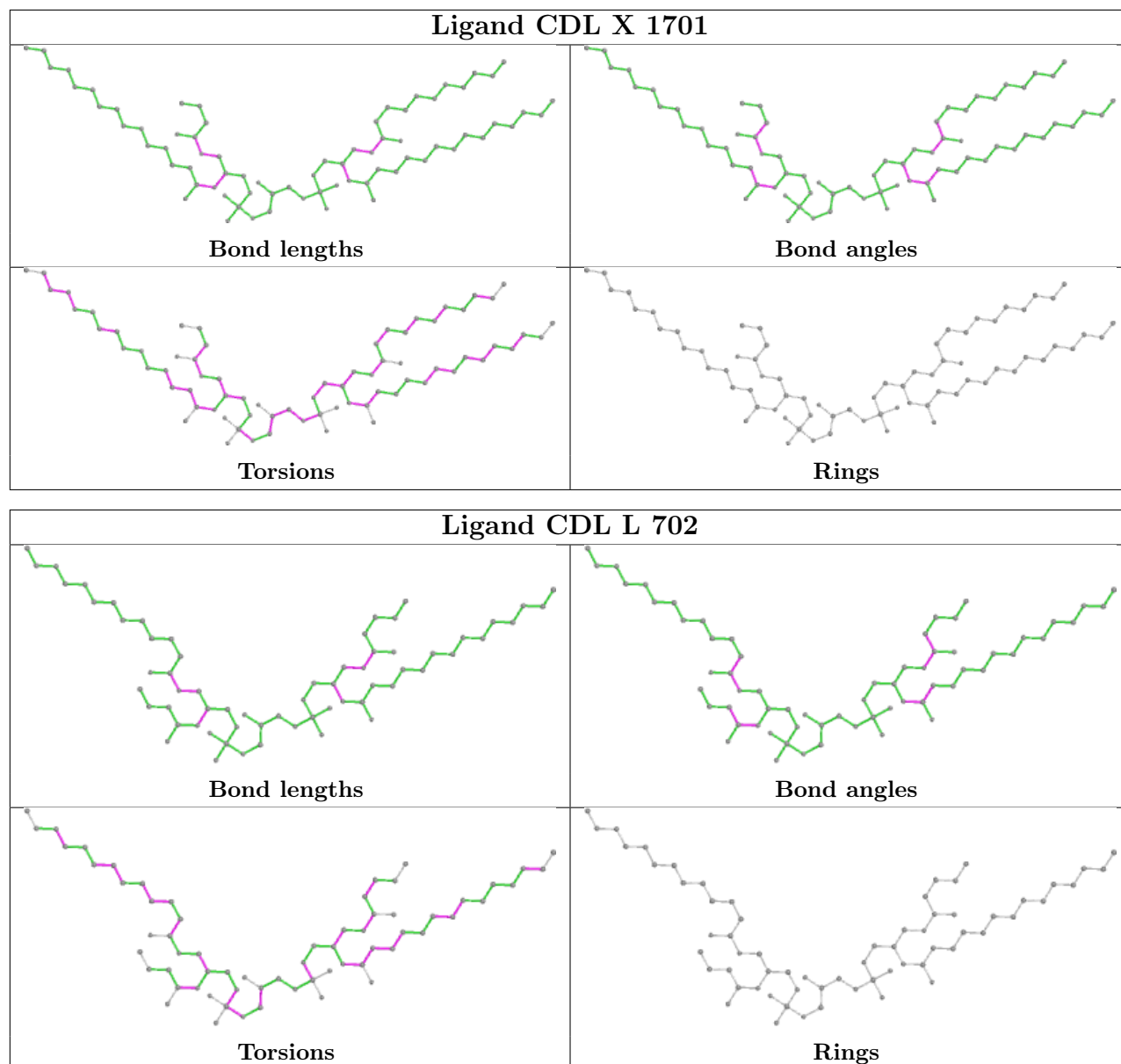
Mol	Chain	Res	Type	Atoms
45	A	301	LMT	C2'-C1'-O1'-C1
45	A	301	LMT	O5'-C1'-O1'-C1
45	h	1002	LMT	C2'-C1'-O1'-C1
45	h	1002	LMT	O5'-C1'-O1'-C1
45	h	1003	LMT	C2-C1-O1'-C1'

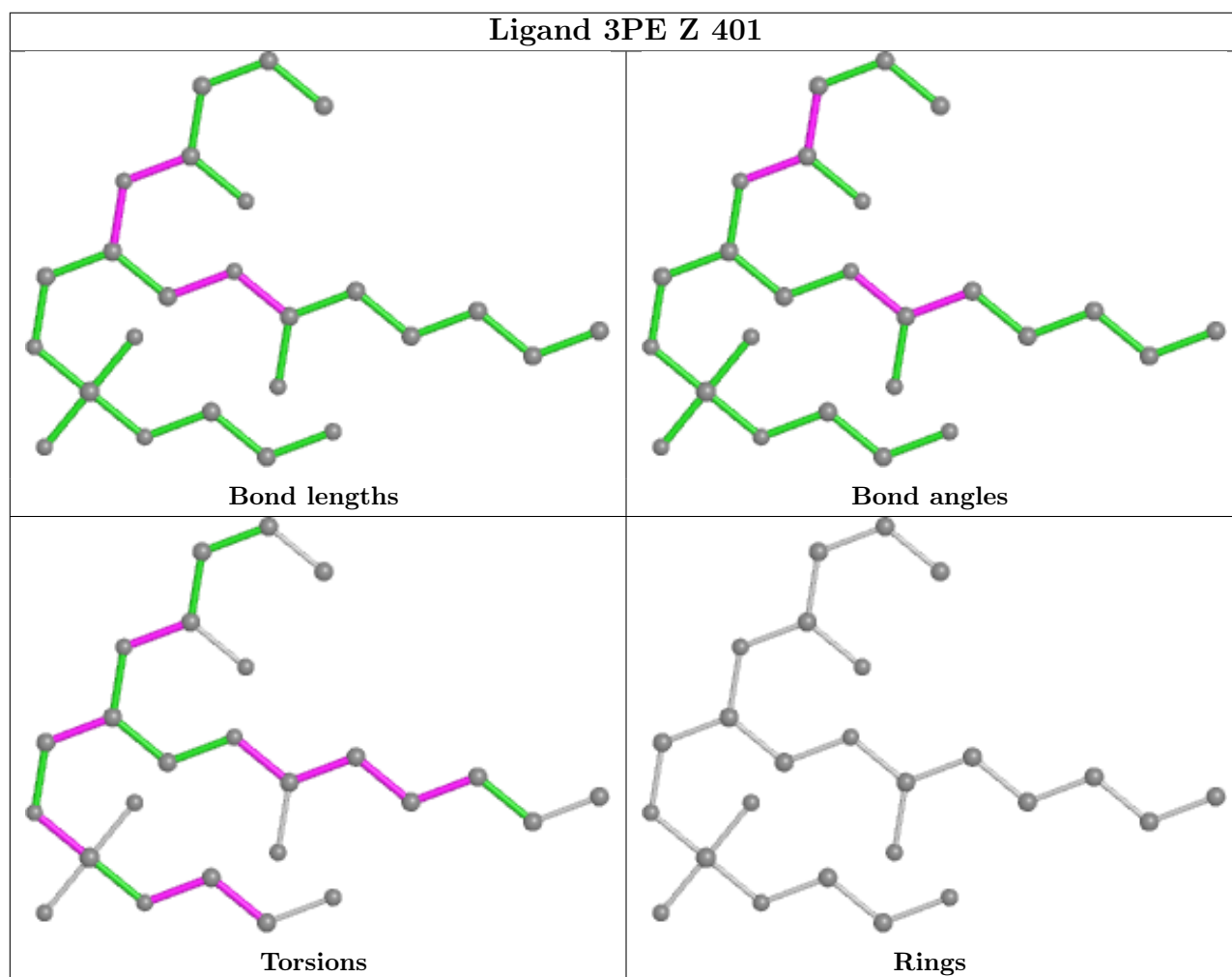
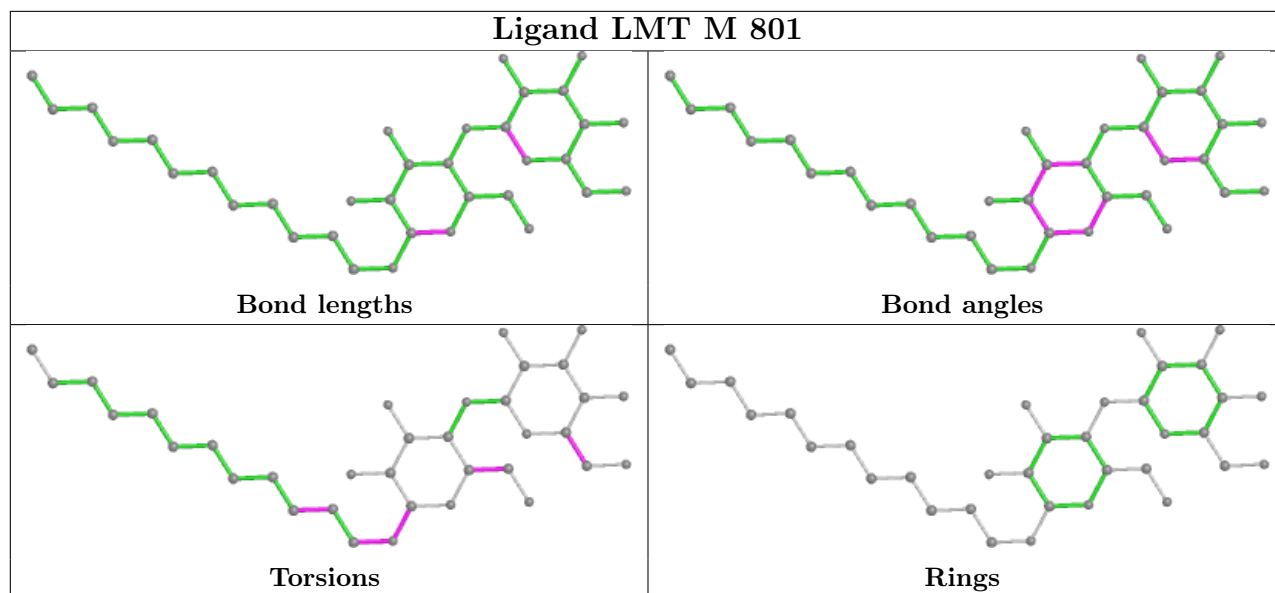
There are no ring outliers.

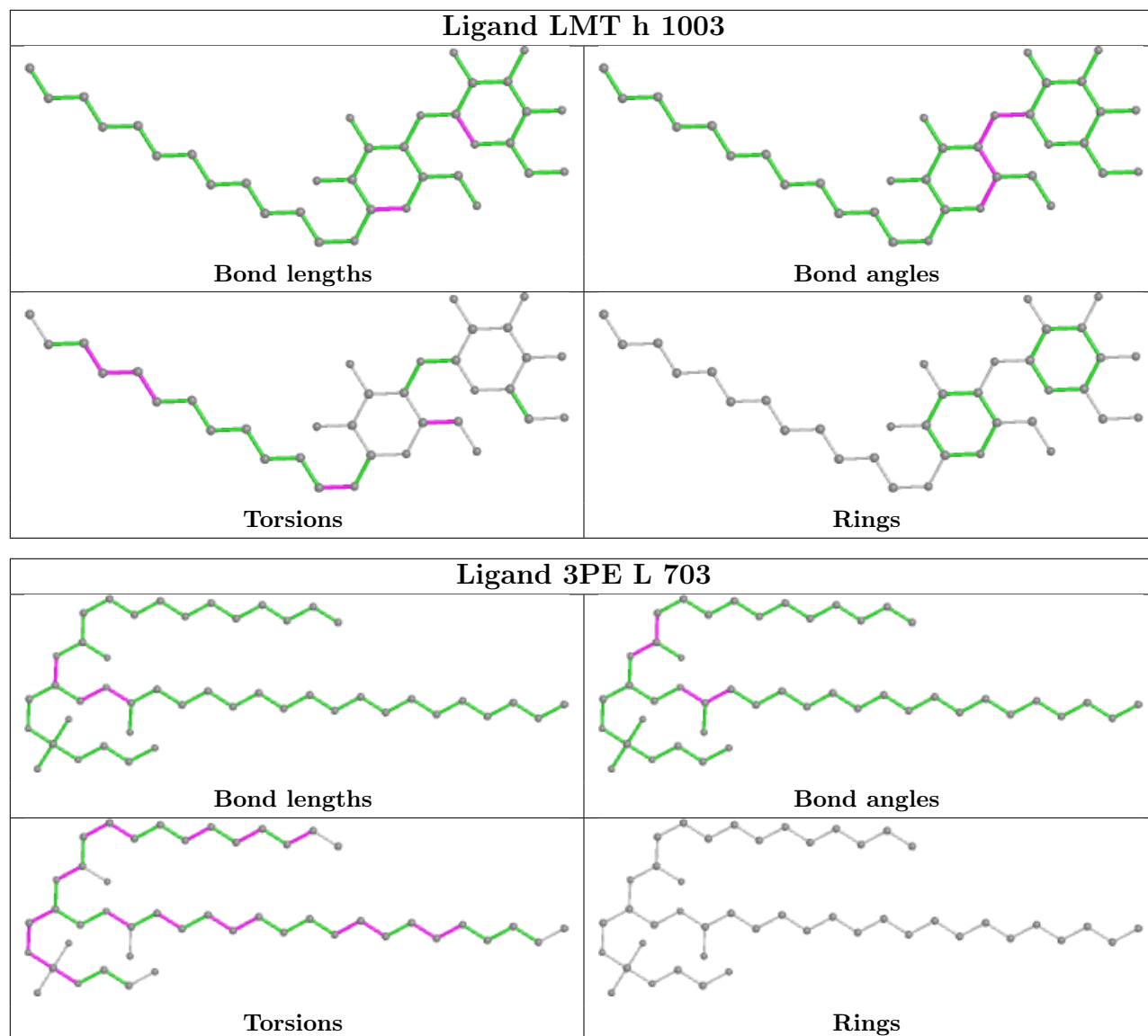
No monomer is involved in short contacts.

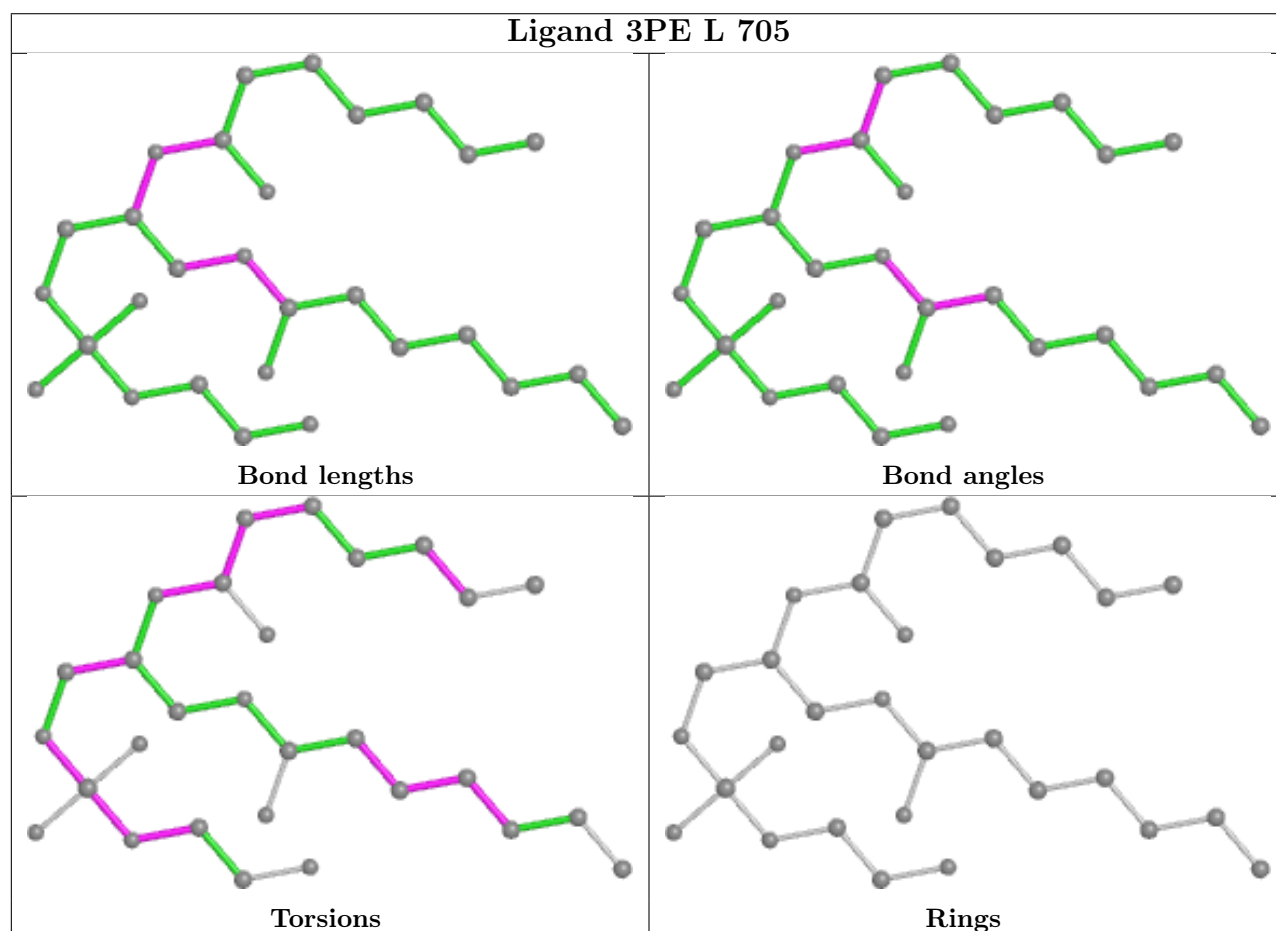
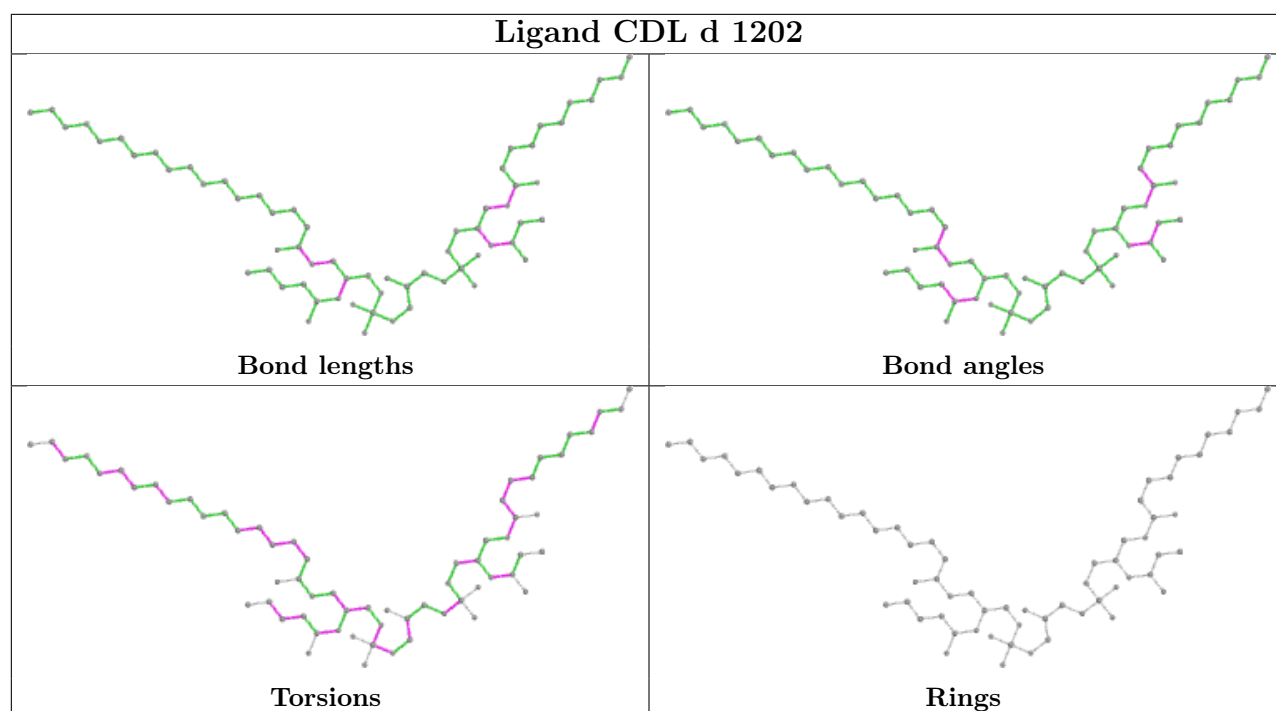
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

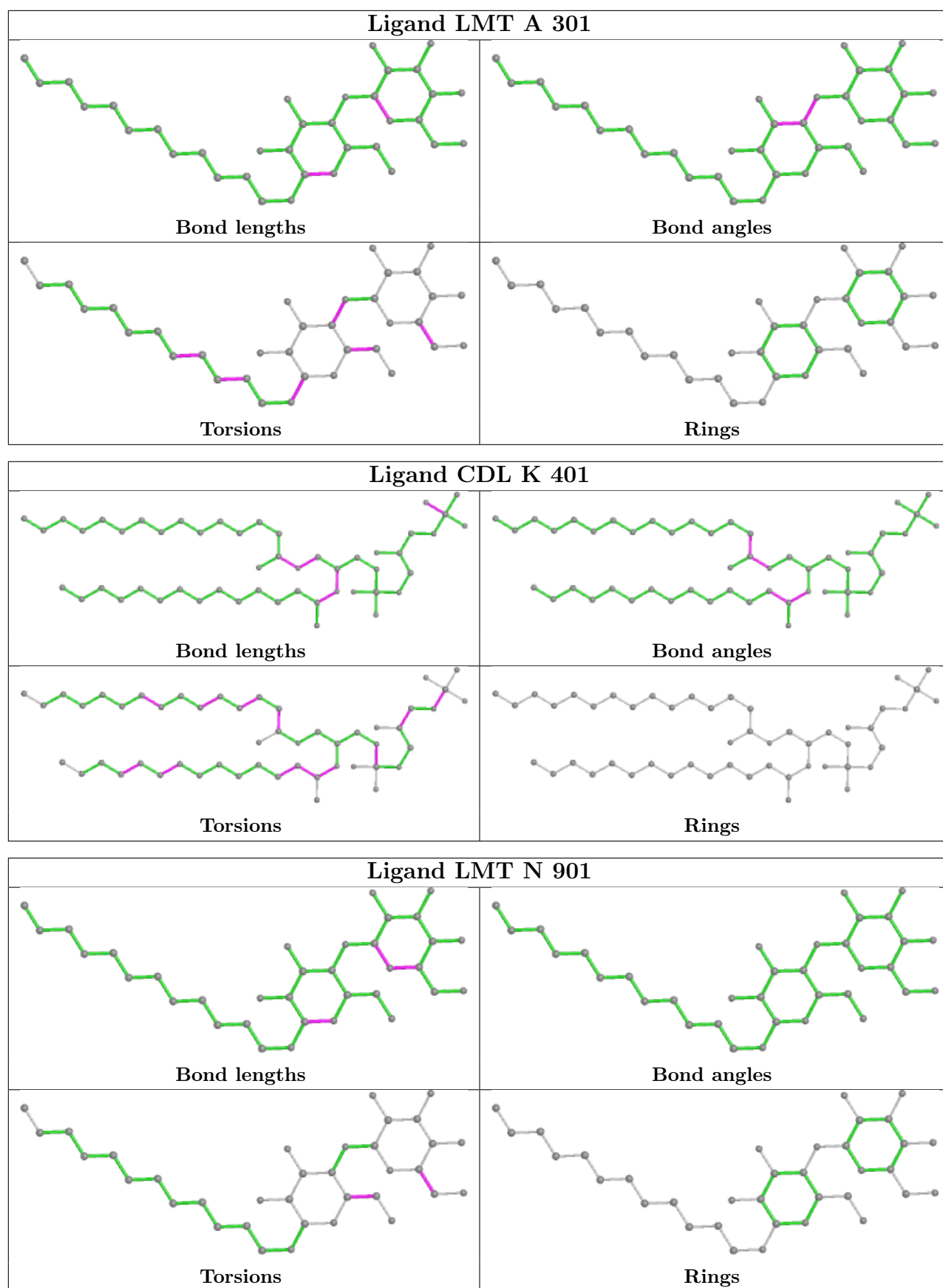
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



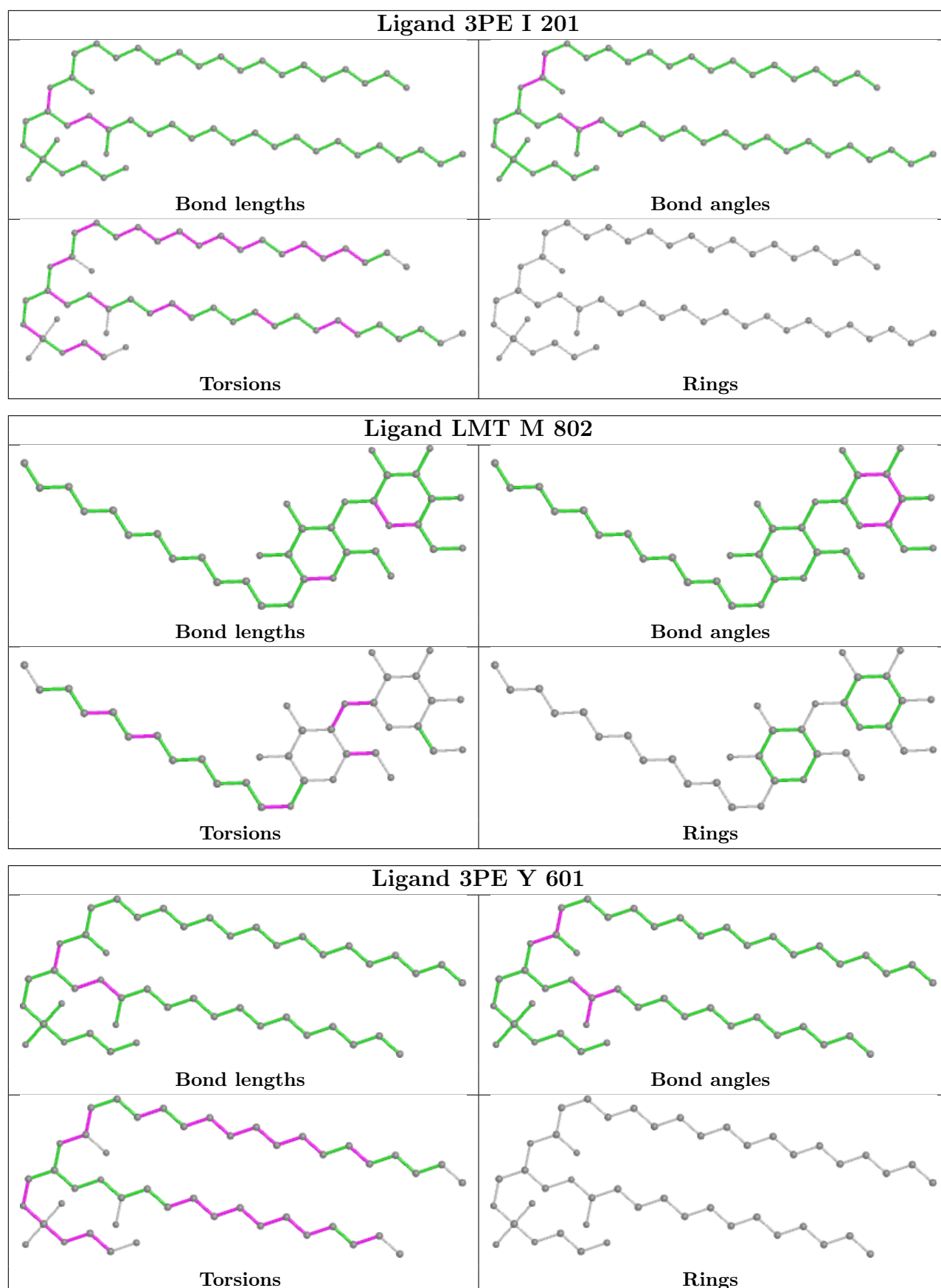


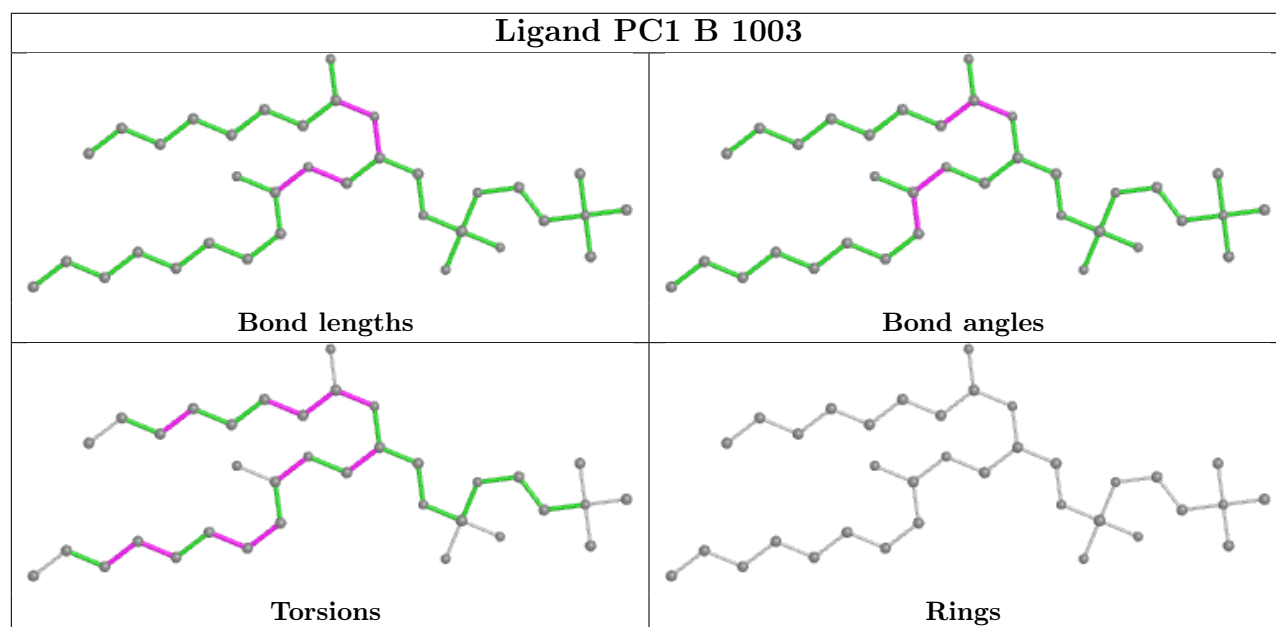
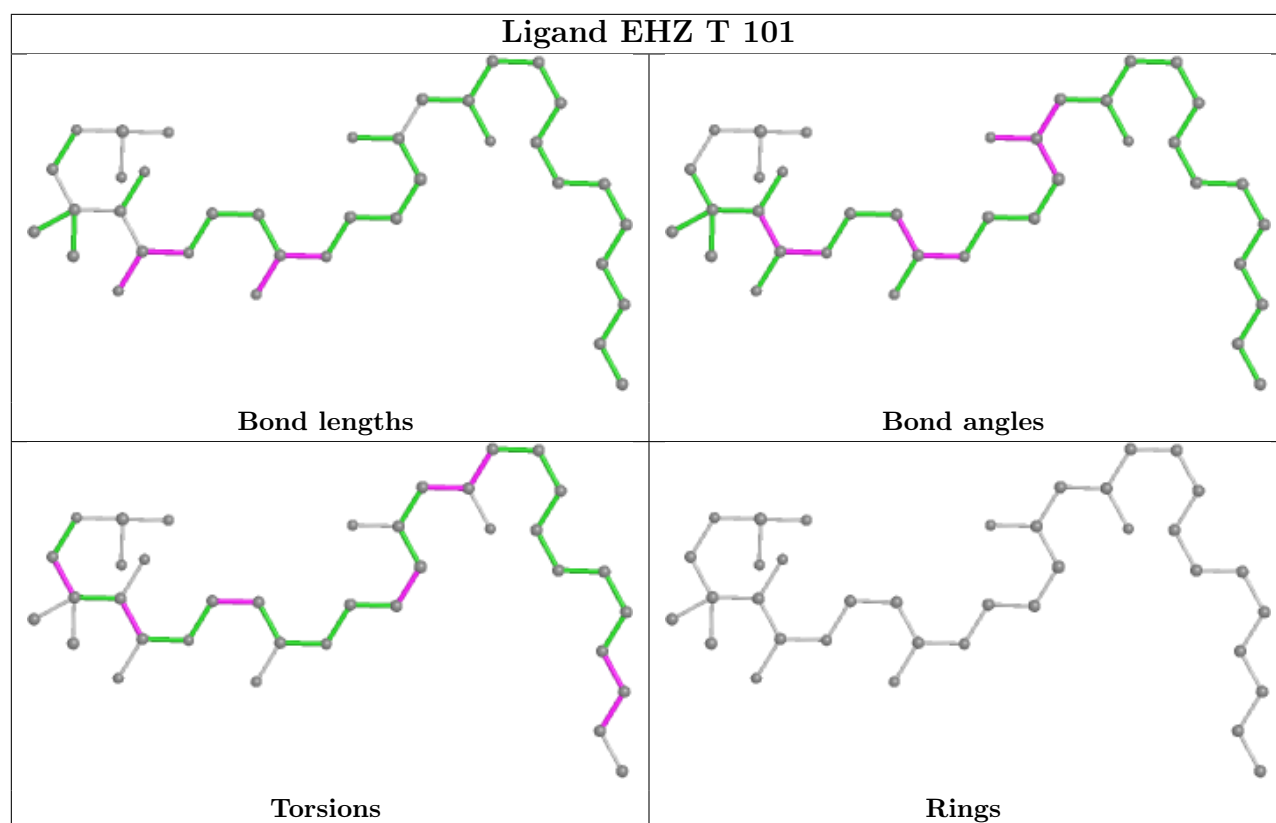


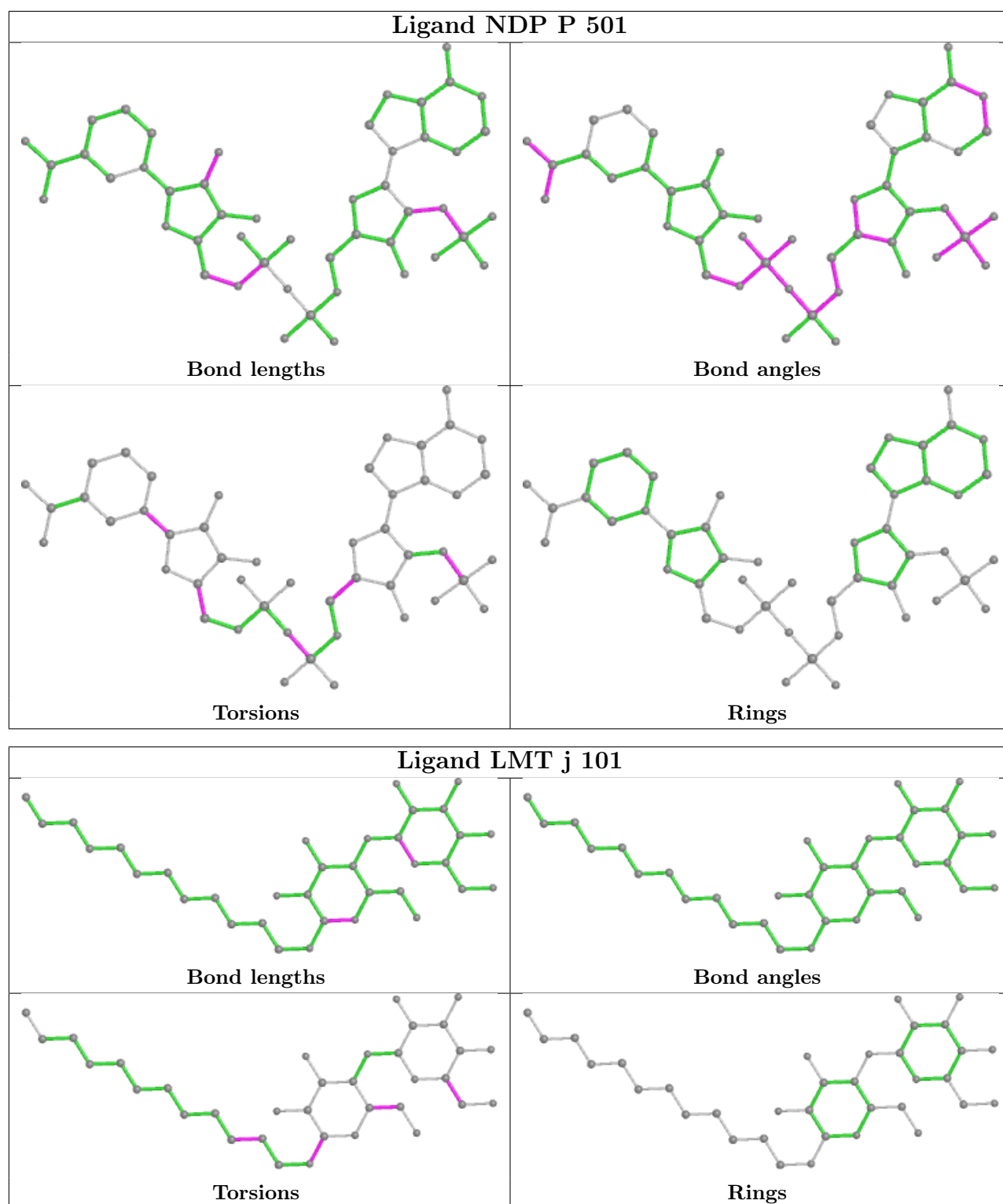


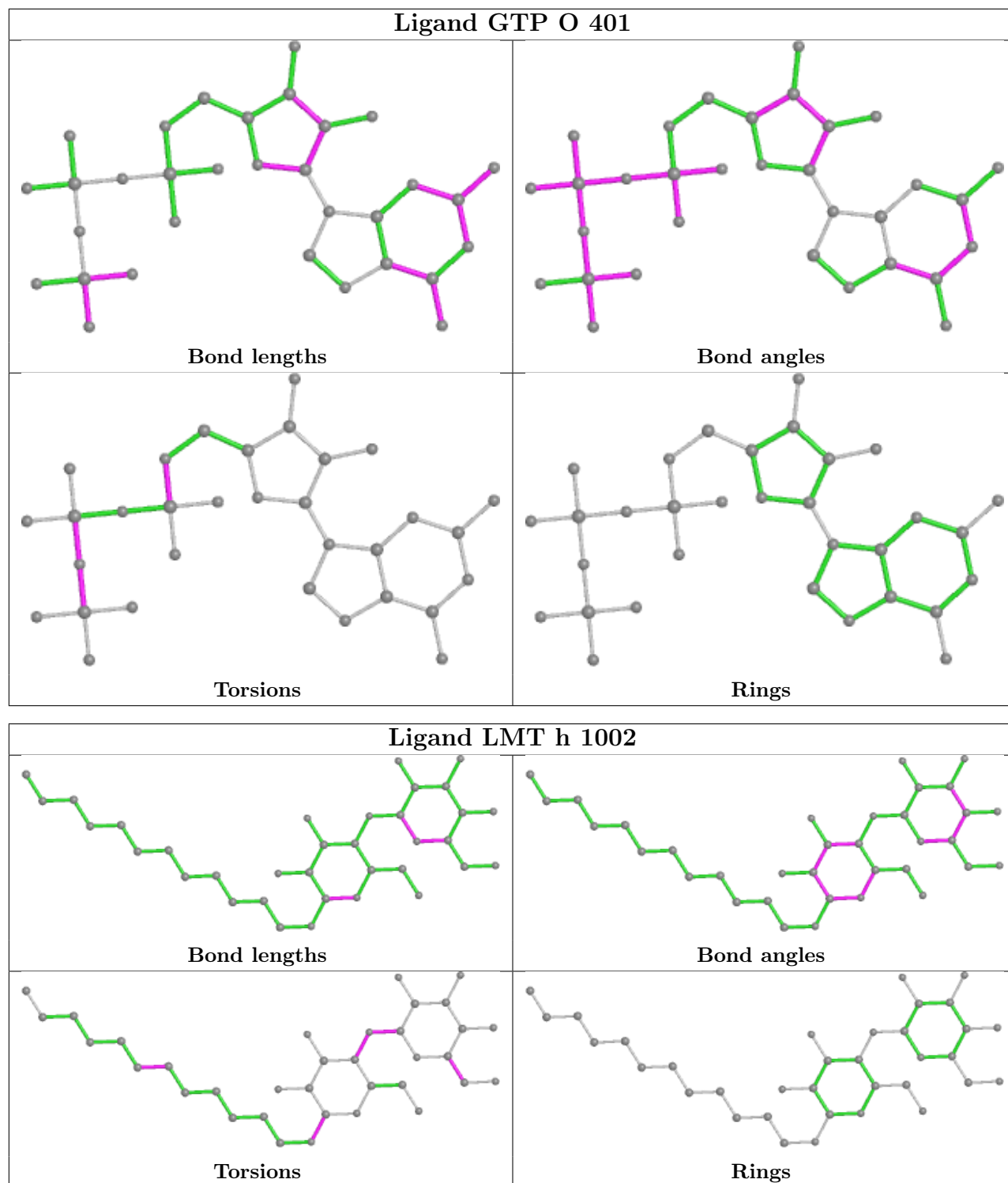


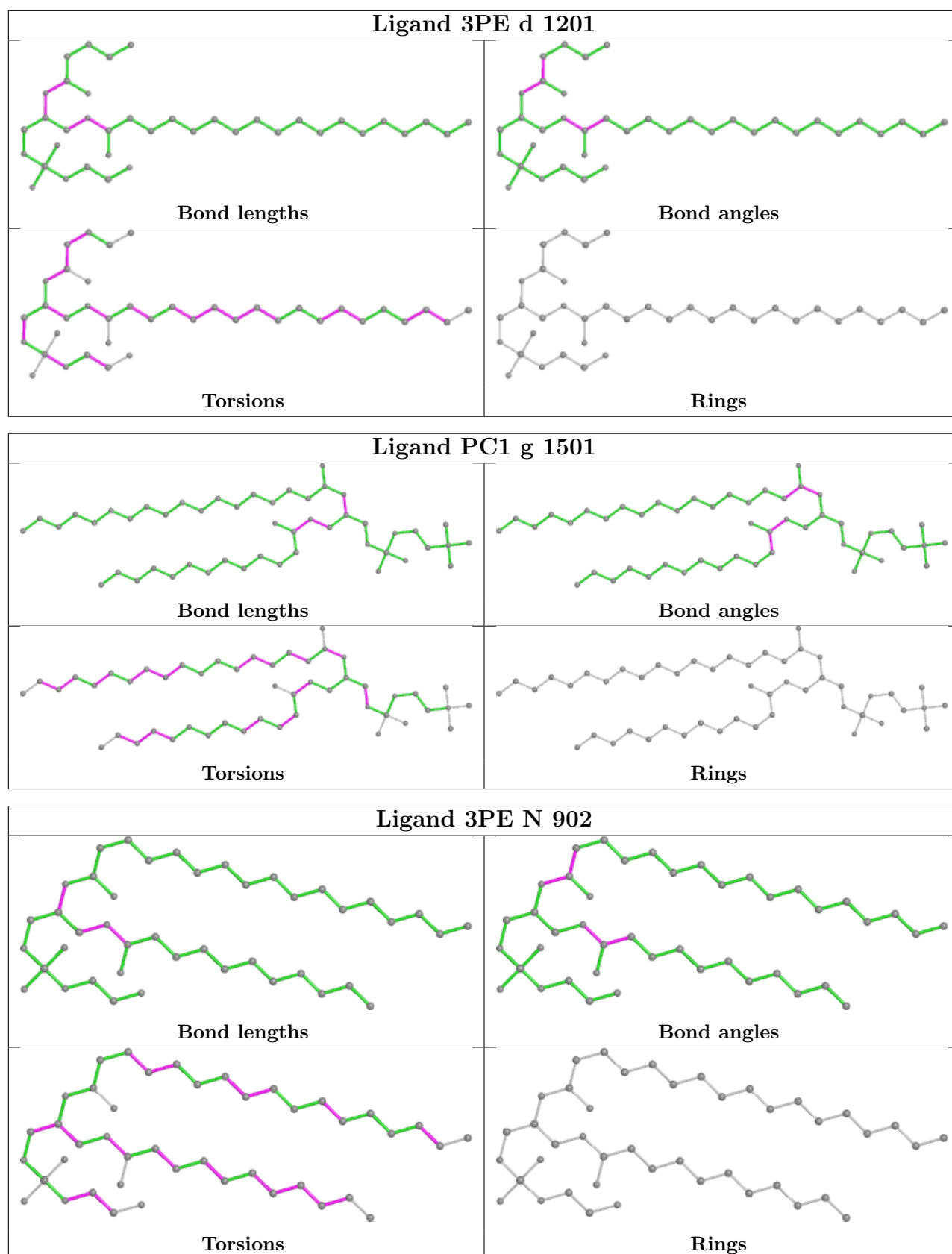


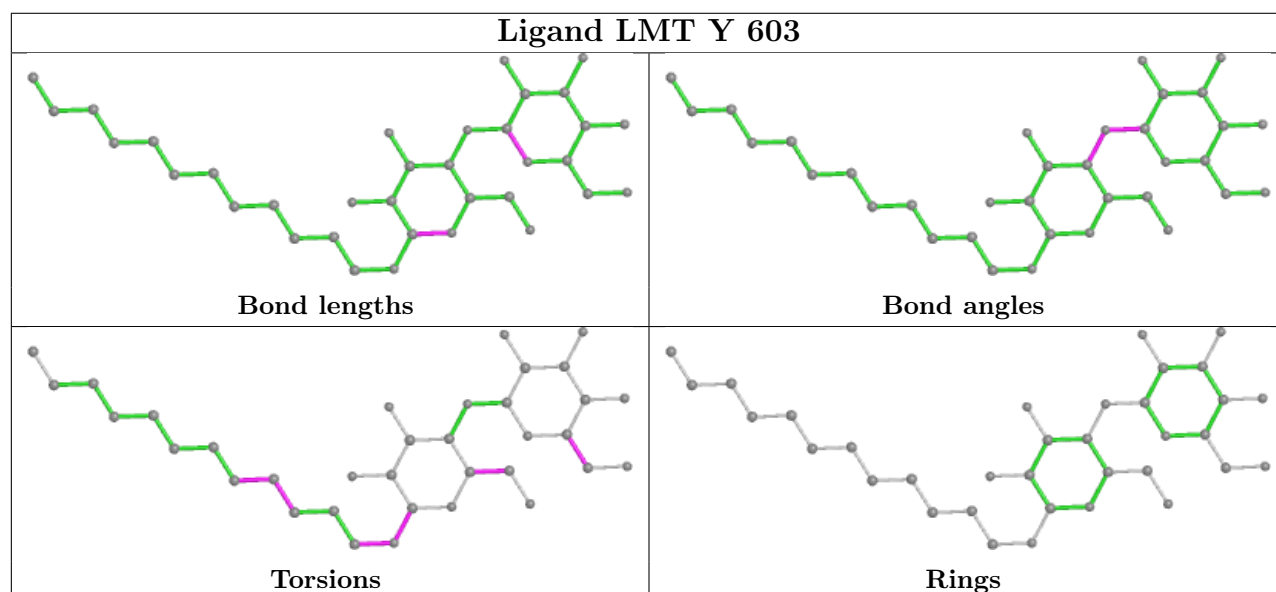
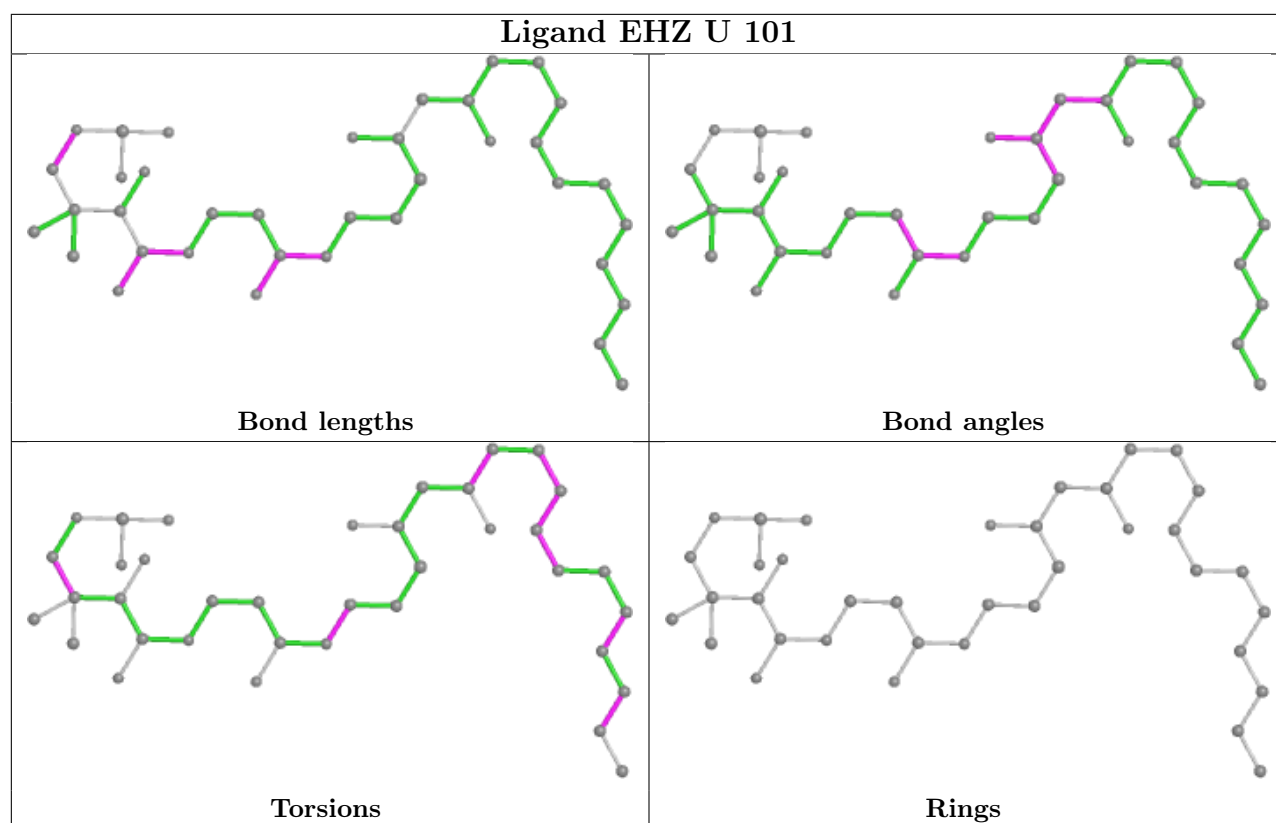


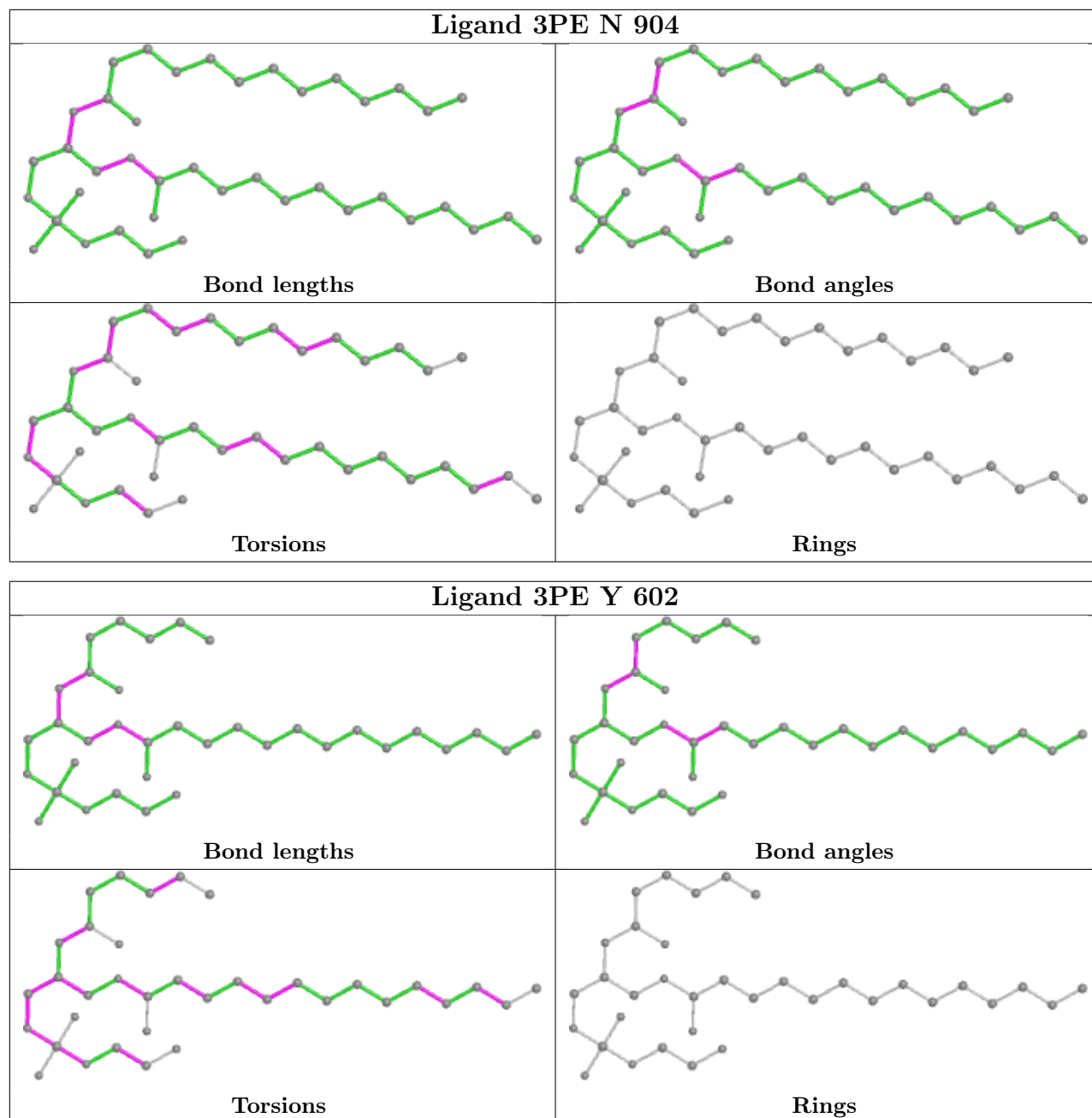


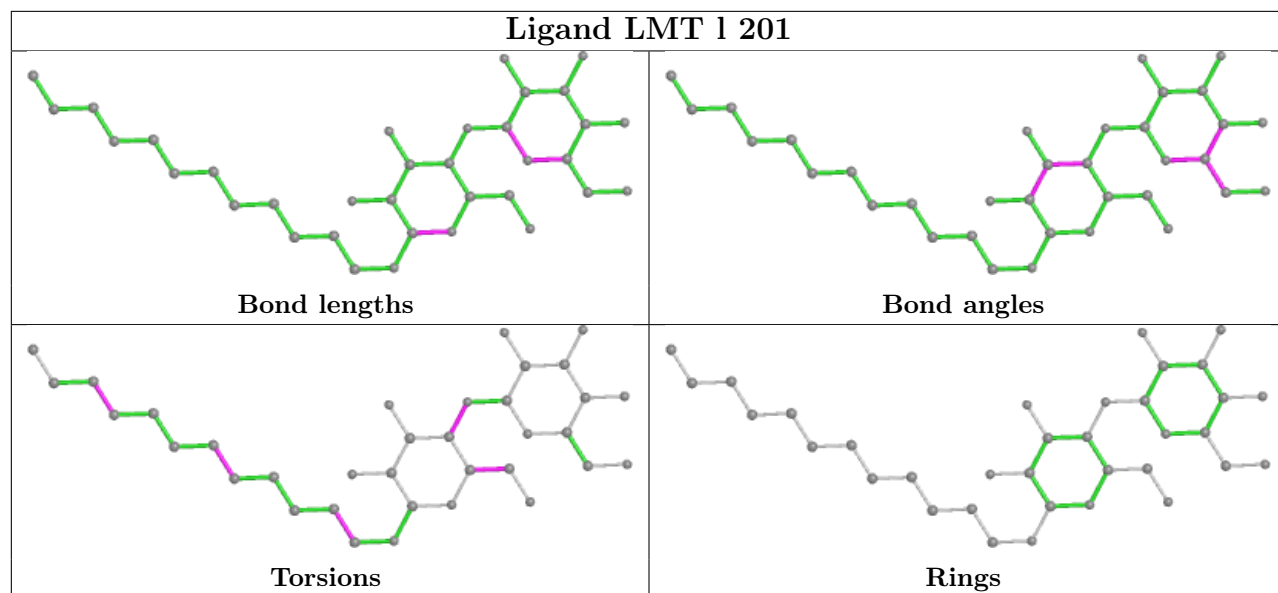




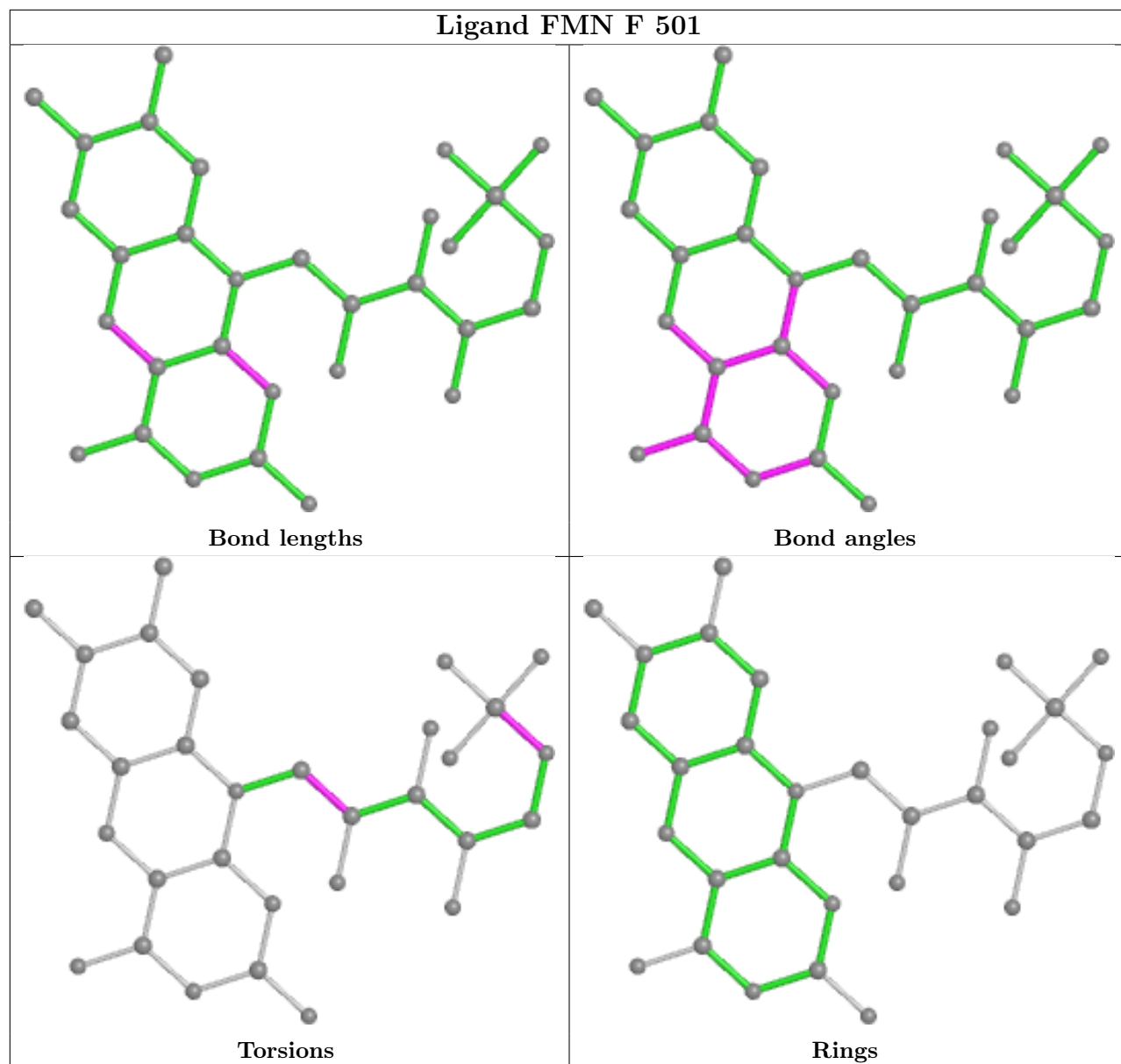


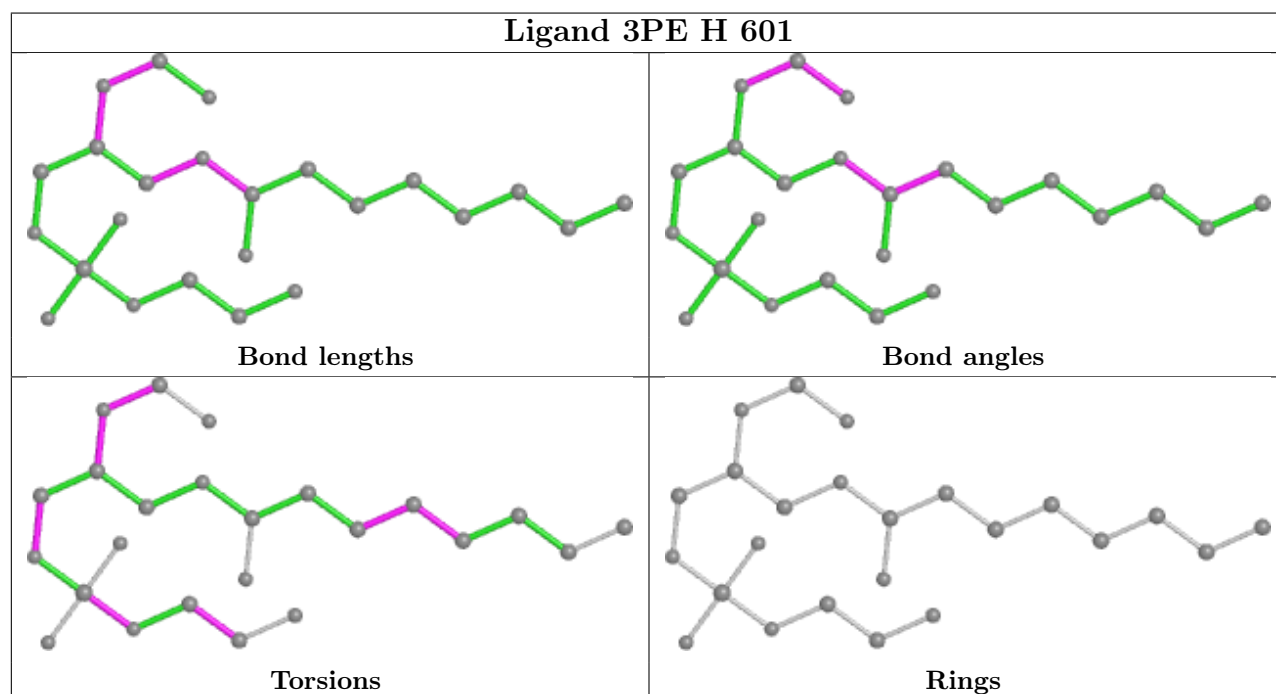
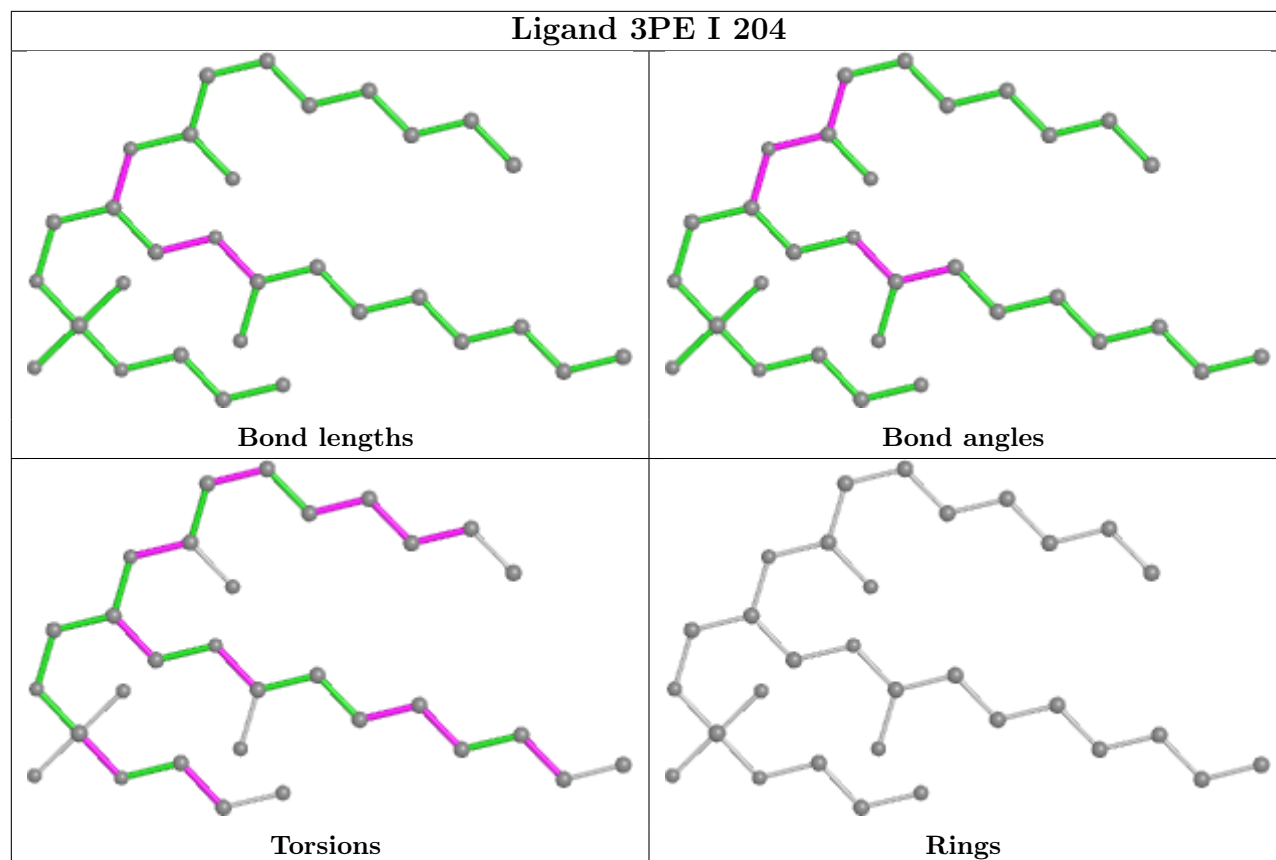


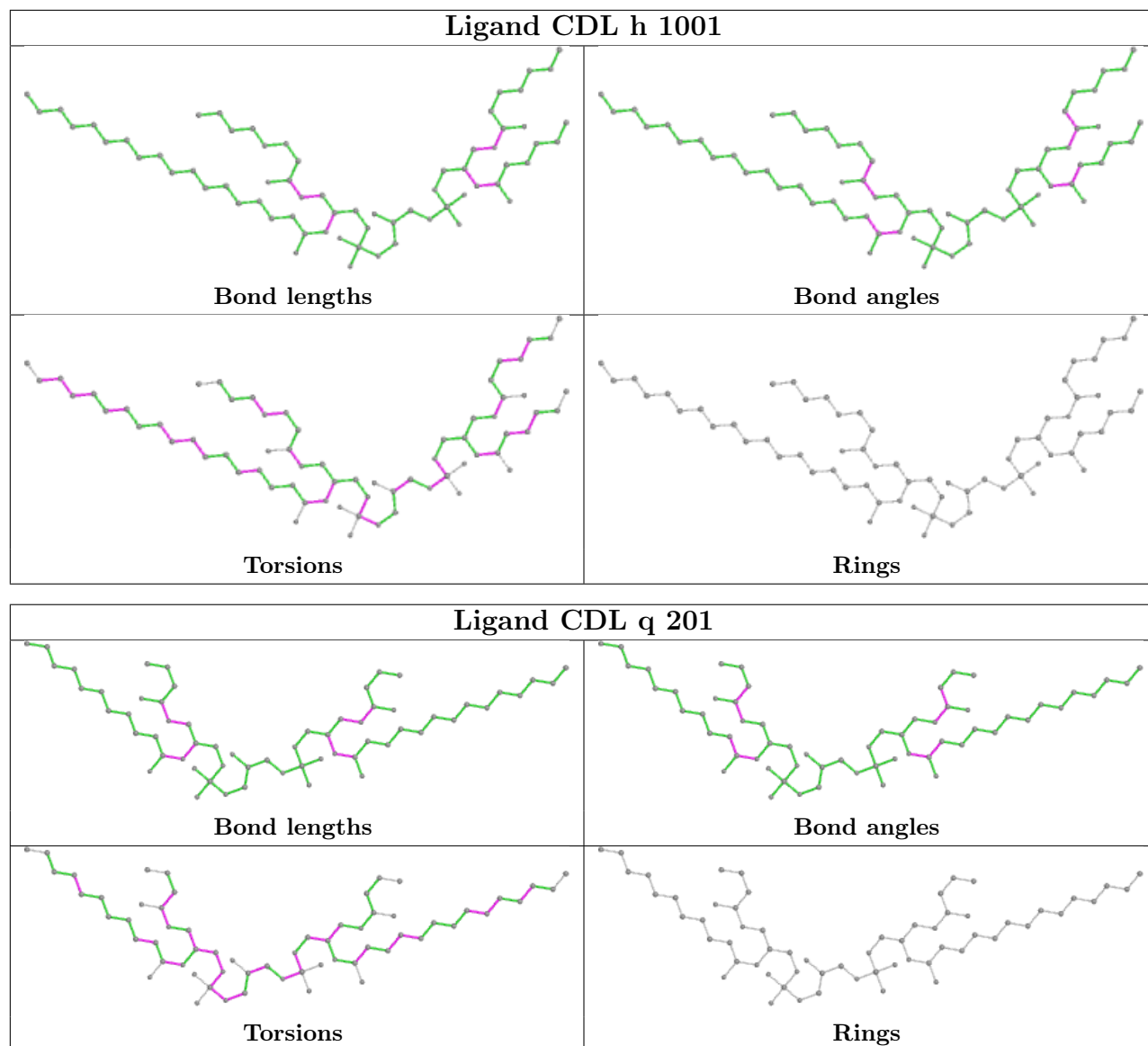


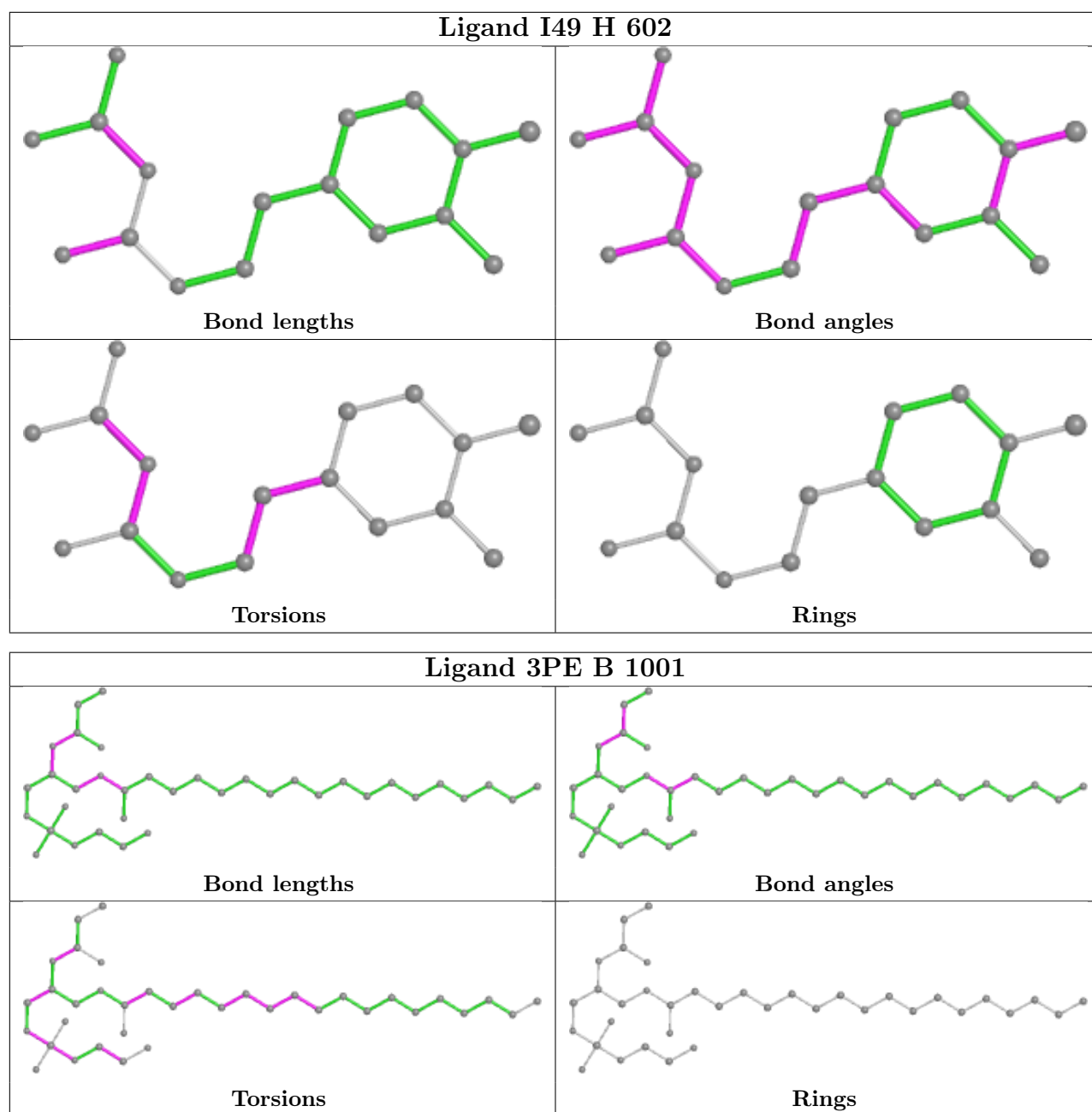


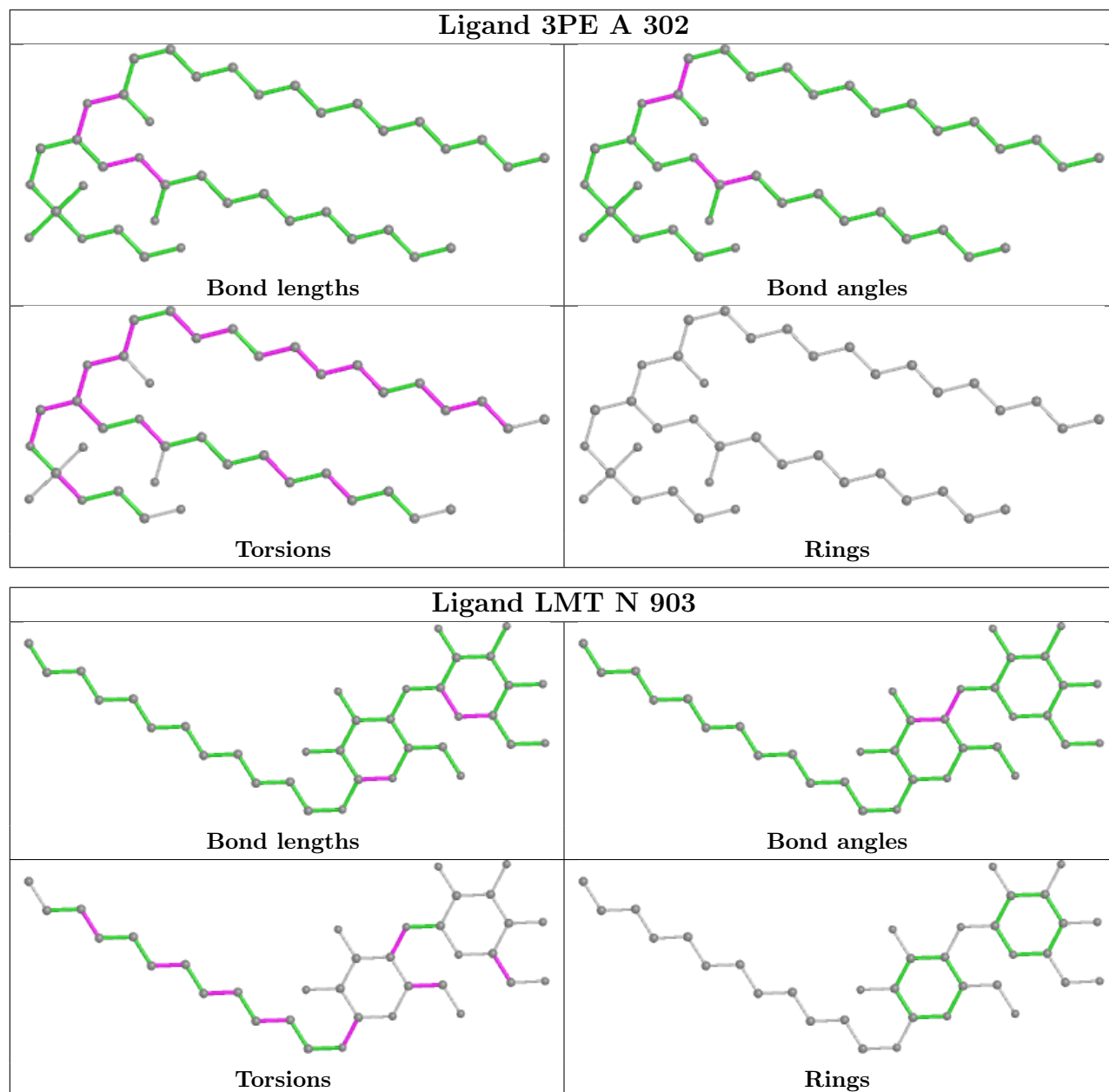


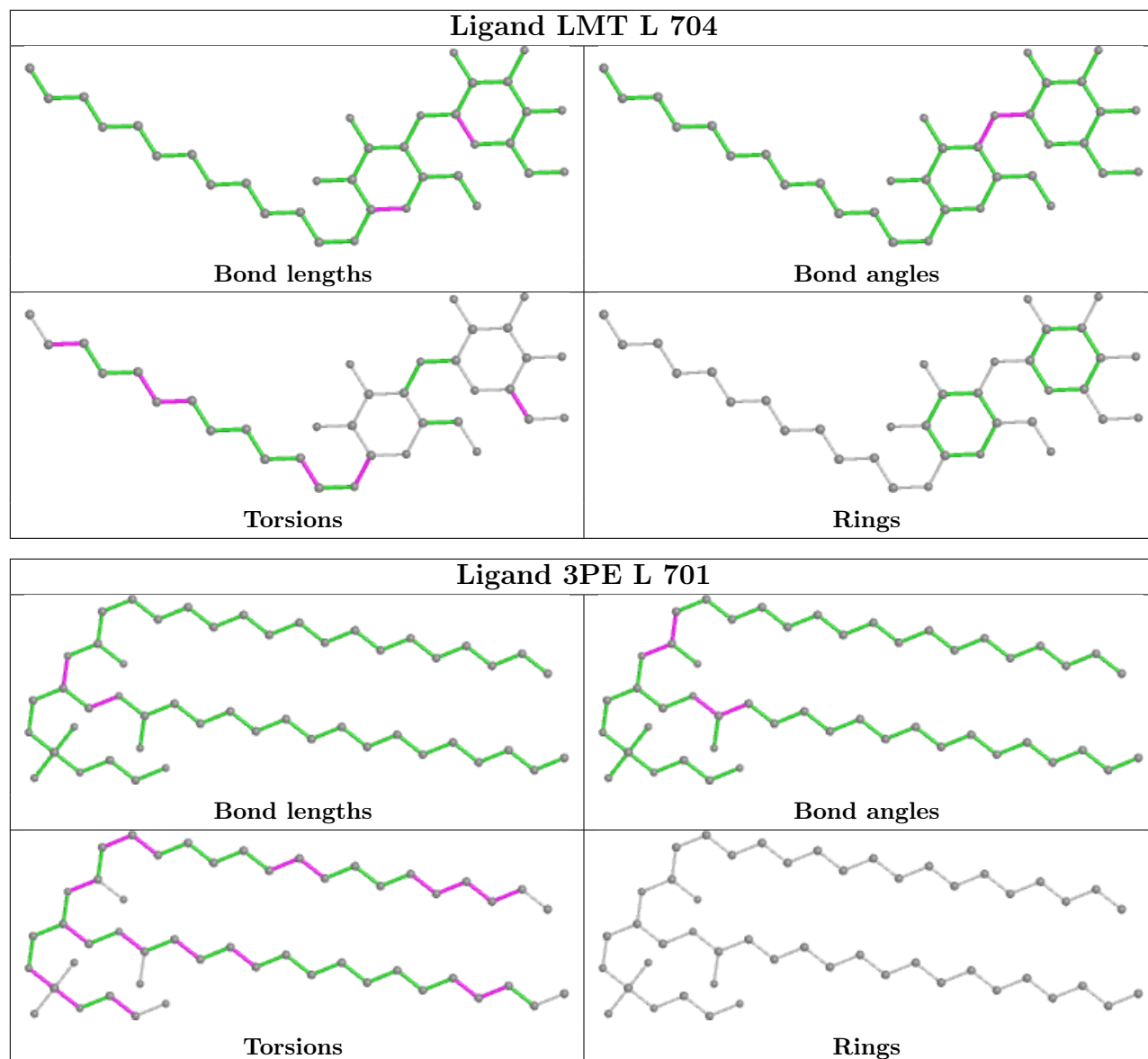












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

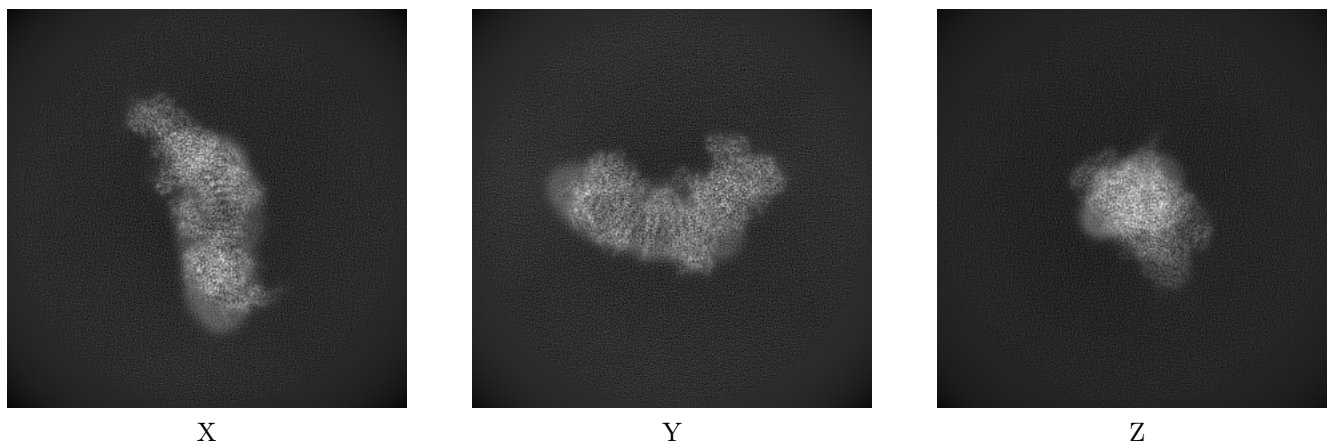
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14277. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

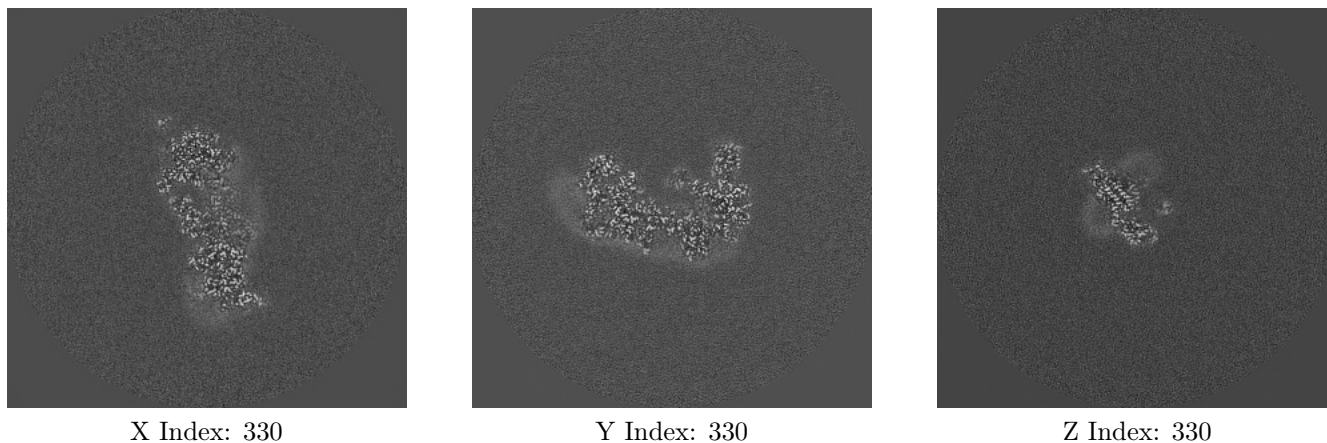
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

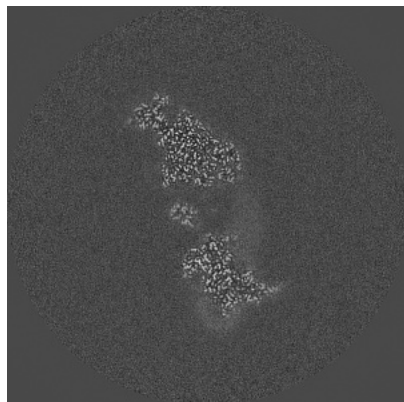
#### 6.2.1 Primary map



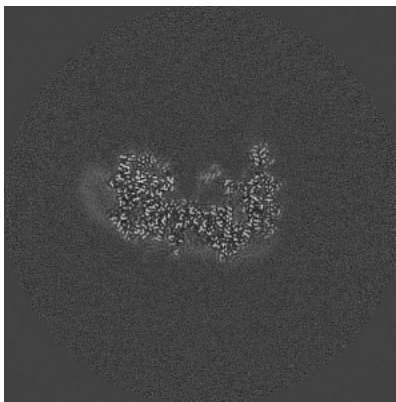
The images above show central slices of the map in three orthogonal directions.

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

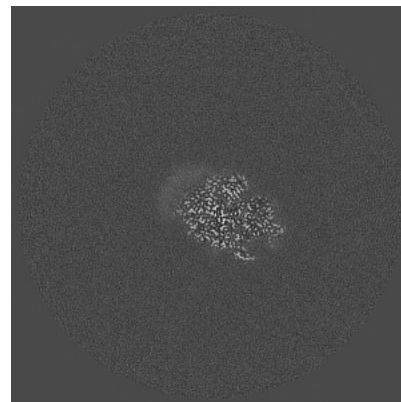
### 6.3.1 Primary map



X Index: 358



Y Index: 337



Z Index: 421

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



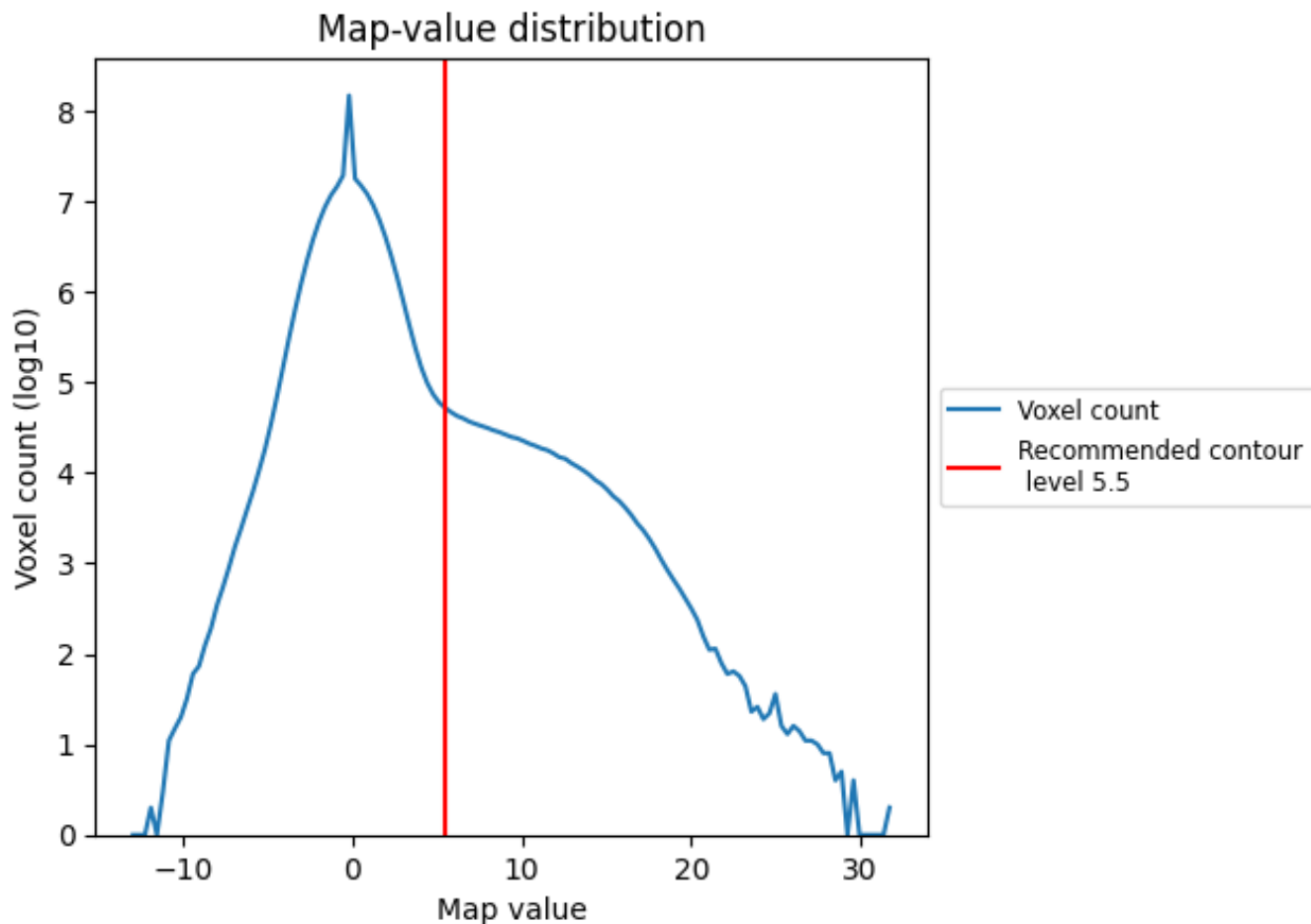
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

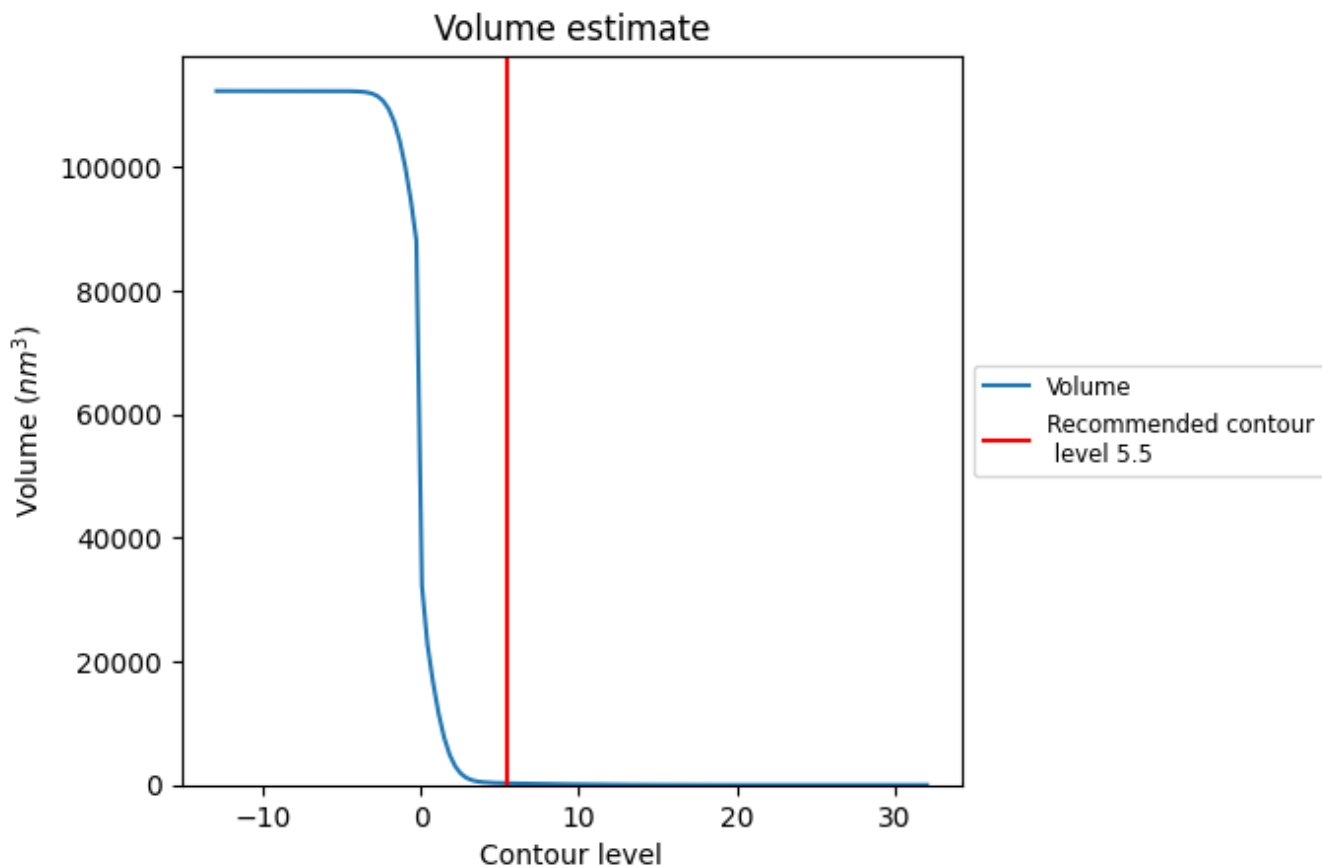
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

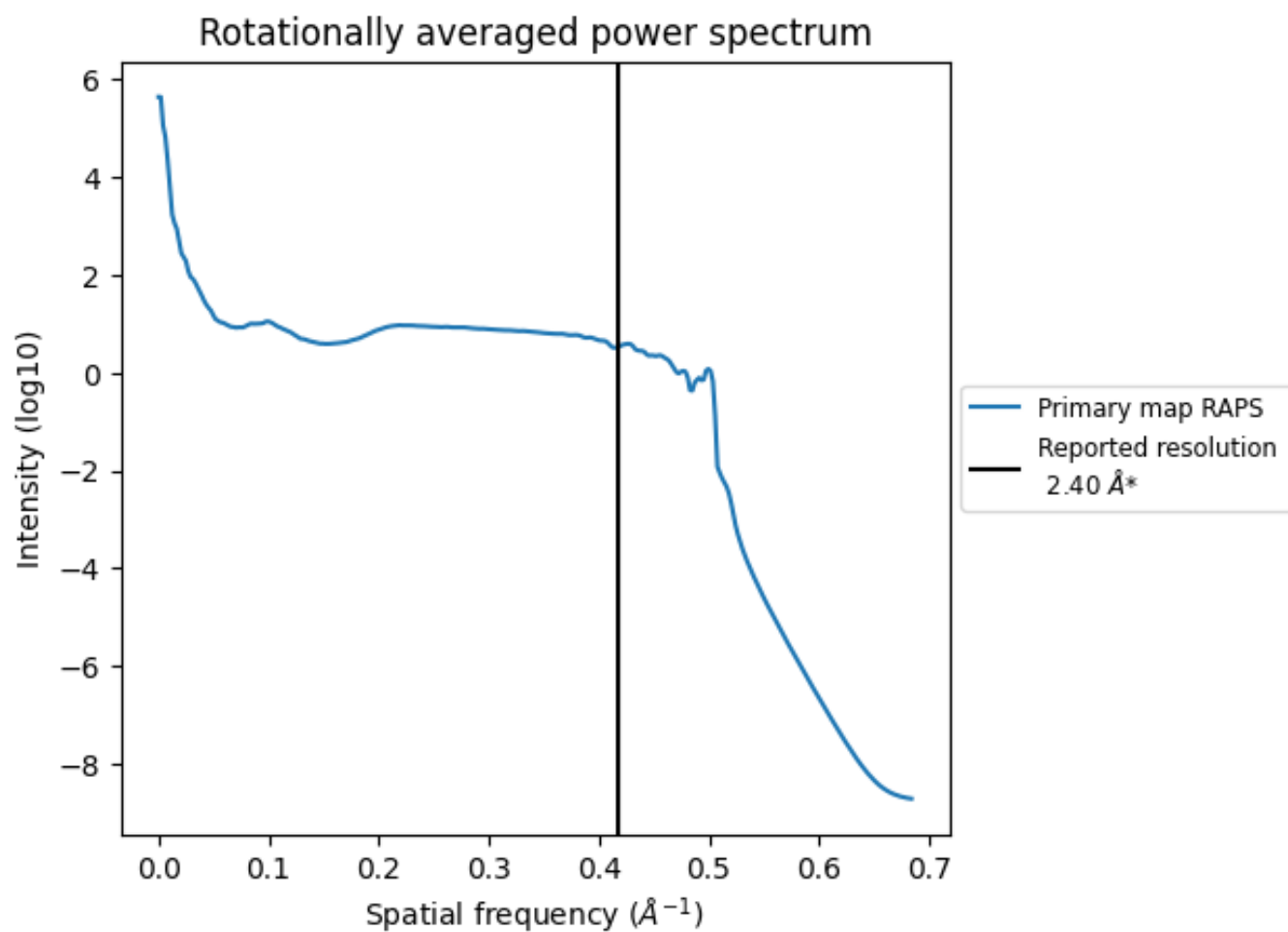
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $270 \text{ nm}^3$ ; this corresponds to an approximate mass of 244 kDa.

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

### 7.3 Rotationally averaged power spectrum i



\*Reported resolution corresponds to spatial frequency of  $0.417 \text{\AA}^{-1}$

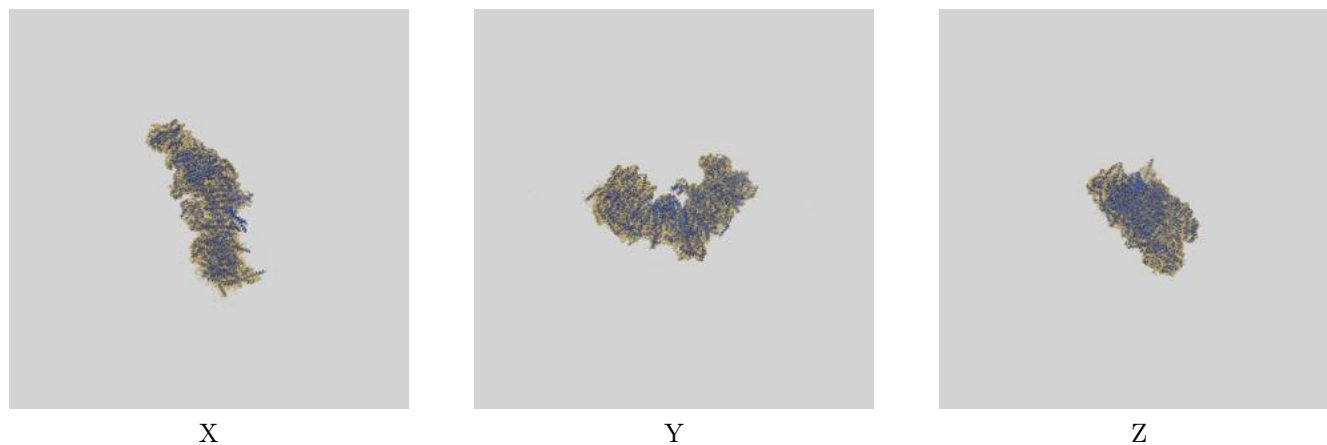
## 8 Fourier-Shell correlation

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

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

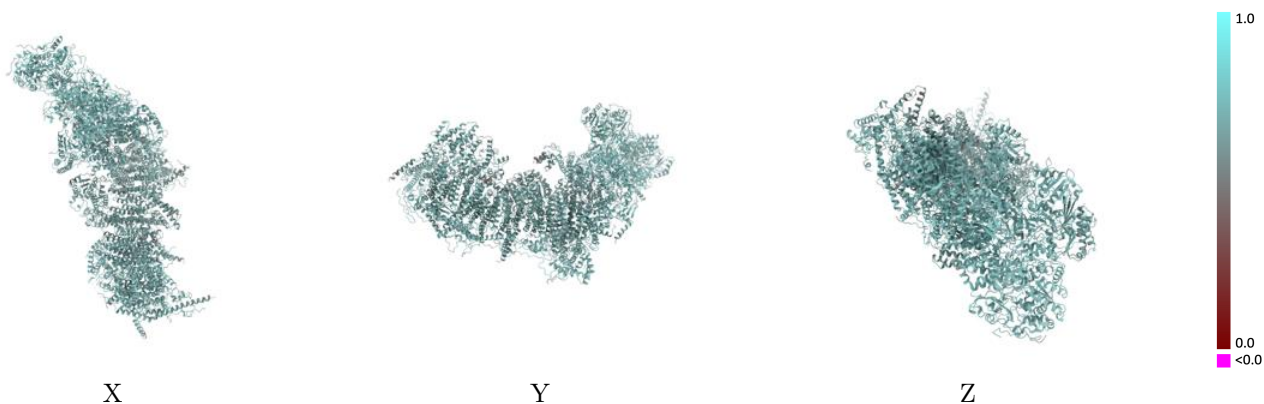
This section contains information regarding the fit between EMDB map EMD-14277 and PDB model 7R46. Per-residue inclusion information can be found in section [3](#) on page [23](#).

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



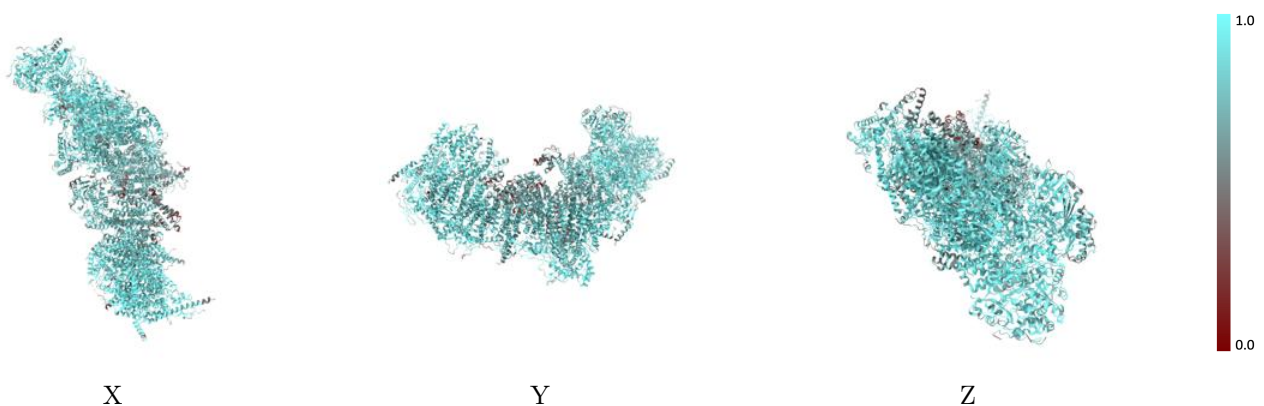
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



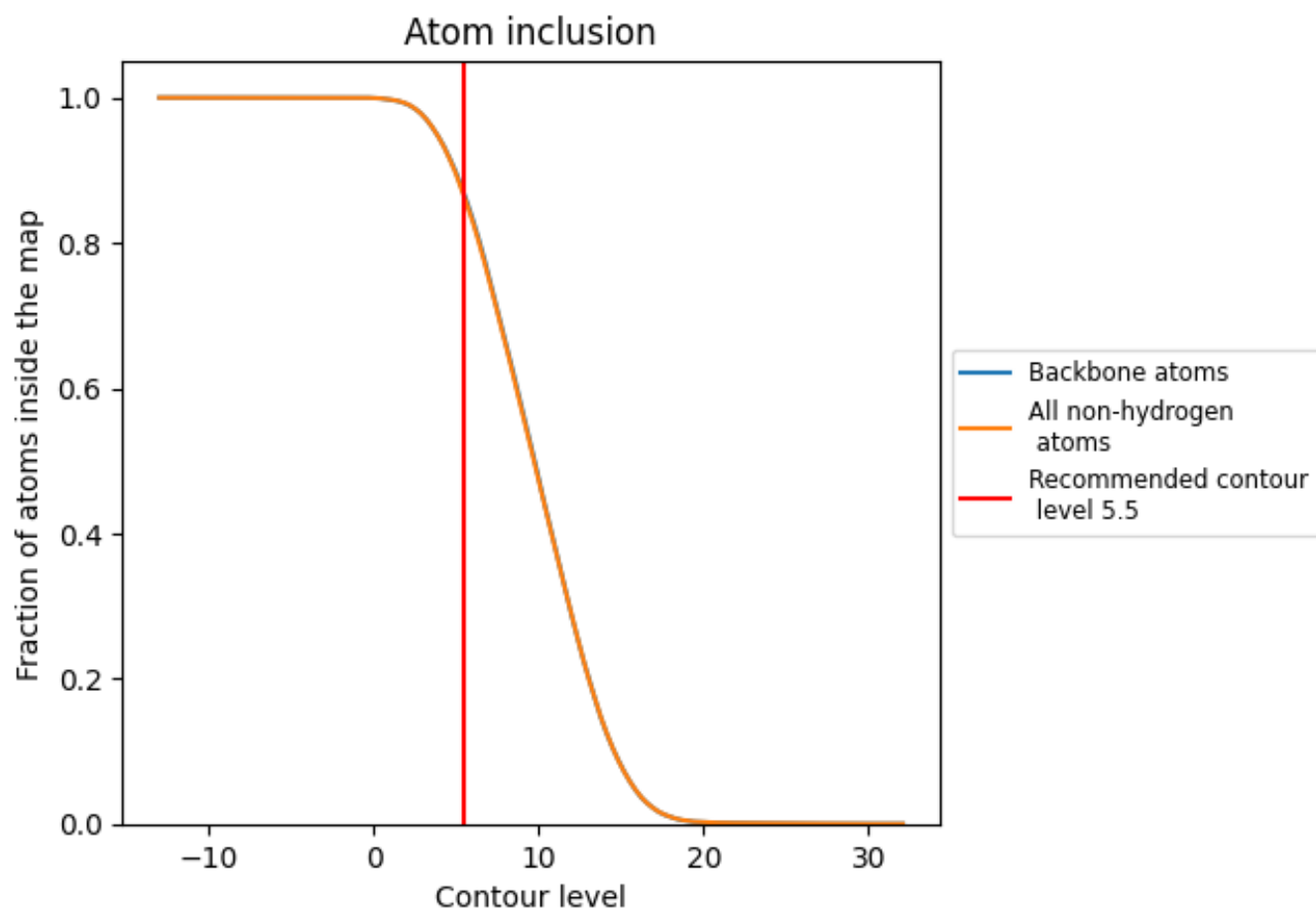
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (5.5).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 87% of all backbone atoms, 86% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8636	 0.6720
A	 0.8218	 0.6570
B	 0.8892	 0.6930
C	 0.9496	 0.7160
D	 0.9076	 0.7050
E	 0.8556	 0.6700
F	 0.9004	 0.6840
G	 0.8947	 0.6920
H	 0.9230	 0.6800
I	 0.9408	 0.7170
J	 0.7926	 0.6490
K	 0.8506	 0.6780
L	 0.8857	 0.6640
M	 0.9464	 0.6890
N	 0.9224	 0.6890
O	 0.8196	 0.6420
P	 0.8444	 0.6720
Q	 0.8943	 0.6970
R	 0.8962	 0.6970
S	 0.8121	 0.6520
T	 0.5699	 0.5870
U	 0.9003	 0.6620
V	 0.8326	 0.6780
W	 0.8386	 0.6730
X	 0.8373	 0.6570
Y	 0.4884	 0.6040
Z	 0.8253	 0.6570
a	 0.9113	 0.6800
b	 0.8320	 0.6530
c	 0.7045	 0.6200
d	 0.8198	 0.6650
e	 0.8054	 0.6480
f	 0.8005	 0.6360
g	 0.8549	 0.6590
h	 0.8611	 0.6670



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Chain	Atom inclusion	Q-score
i	 0.8452	 0.6350
j	 0.8417	 0.6310
k	 0.8473	 0.6310
l	 0.8803	 0.6570
m	 0.8168	 0.6370
n	 0.9044	 0.6580
o	 0.8584	 0.6380
p	 0.8855	 0.6590
q	 0.8309	 0.6810
r	 0.8504	 0.6860
s	 0.8338	 0.6650