



## wwPDB EM Validation Summary Report ⓘ

Aug 3, 2023 – 02:34 pm BST

PDB ID : 8OLT  
EMDB ID : EMD-16962  
Title : Mitochondrial complex I from *Mus musculus* in the active state bound with piericidin A  
Authors : Grba, D.N.; Chung, I.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.  
Deposited on : 2023-03-30  
Resolution : 2.84 Å (reported)  
Based on initial model : 6ZR2

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:

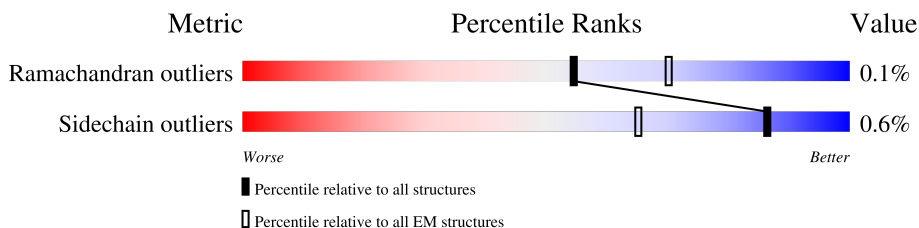
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.34

# 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 2.84 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	100%
2	B	224	68% 30%
3	C	263	79% 21%
4	D	463	92% 7%
5	E	248	7% 86% 14%
6	F	464	92% 7%
7	G	727	94% 5%
8	H	318	98%
9	I	212	83% 16%

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Mol	Chain	Length	Quality of chain
10	J	172	10% 99%
11	K	98	98%
12	L	607	99%
13	M	459	100%
14	N	345	100%
15	O	355	90% 10%
16	P	377	90% 9%
17	Q	175	71% 29%
18	R	116	82% 18%
19	S	99	83% 16%
20	T	156	27% 49% 50%
20	U	156	55% 45%
21	V	116	97%
22	W	131	87% 13%
23	X	172	99%
24	Y	143	8% 99%
25	Z	144	97%
26	a	70	99%
27	b	84	12% 99%
28	c	76	9% 63% 37%
29	d	120	100%
30	e	106	99%
31	f	57	18% 86% 11%
32	g	151	64% 34%
33	h	189	73% 27%

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Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

## 2 Entry composition i

There are 60 unique types of molecules in this entry. The entry contains 68075 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	115	933	633	133	160	7	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	156	1247	796	223	214	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	208	1730	1116	297	314	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	430	3464	2215	595	630	24	0	0

- 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	214	1660	1056	279	314	11	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	3321	2092	596	611	22	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	5296	3321	919	1015	41	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	318	2540	1706	384	428	22	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	178	1431	898	245	276	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	172	1308	878	186	229	15	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	98	737	477	112	137	11	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	4800	3182	746	827	45	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	3632	2408	567	617	40	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	345	2703	1795	417	454	37	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	2607	1674	431	492	10	0	0

- 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	342	2748	1777	483	481	7	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	1015	642	179	190	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	95	748	464	138	143	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	83	663	415	126	119	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	78	628	404	93	126	5	0	0
20	U	86	692	446	102	139	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	112	915	596	152	164	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	114	970	619	180	165	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	171	1396	889	250	247	10	0	0

- 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	142	1050	670	177	194	9	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	140	1161	747	206	200	8	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	564	366	100	94	4	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	648	425	105	114	4	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	S		
28	c	48	398	261	69	67	1	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	120	996	651	171	165	9	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	105	877	555	162	152	8	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	439	284	79	74	2	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	100	842	545	135	158	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	1162	762	194	203	3	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	104	869	565	152	149	3	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	65	562	370	93	98	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	78	630	416	107	105	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	1302	840	216	235	11	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		
38	m	126	1050	676	189	185	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	177	1534	981	275	267	11	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7, METHYLGLYOXAL BIS-(GUANYLHYDRAZONE), NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	117	1005	634	189	174	8	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	1439	904	258	269	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	144	1203	773	213	212	5	0	0

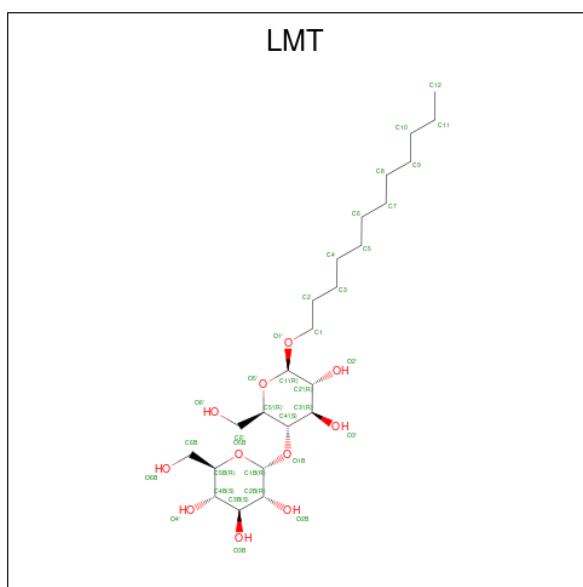
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	95	767	484	143	137	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		
44	s	43	361	225	65	71	0	0

- Molecule 45 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



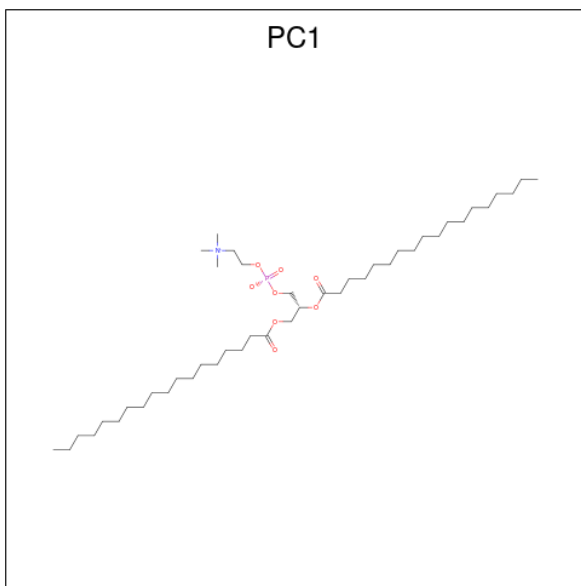
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	K	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	O	1	Total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

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

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



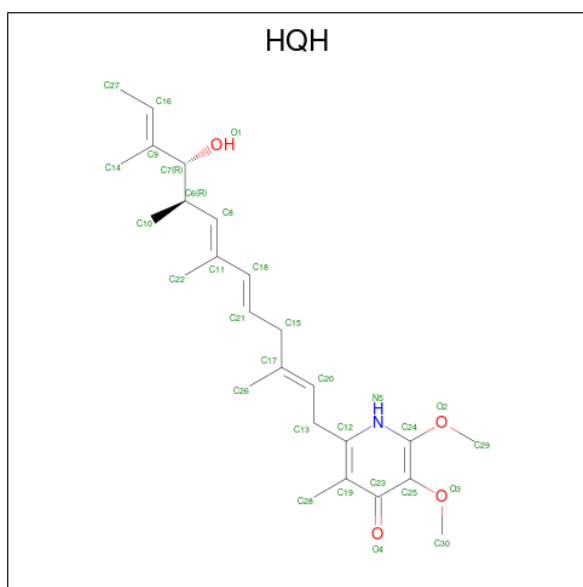
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	29	19	1	8	1	0
46	B	1	38	28	1	8	1	0
46	B	1	41	31	1	8	1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



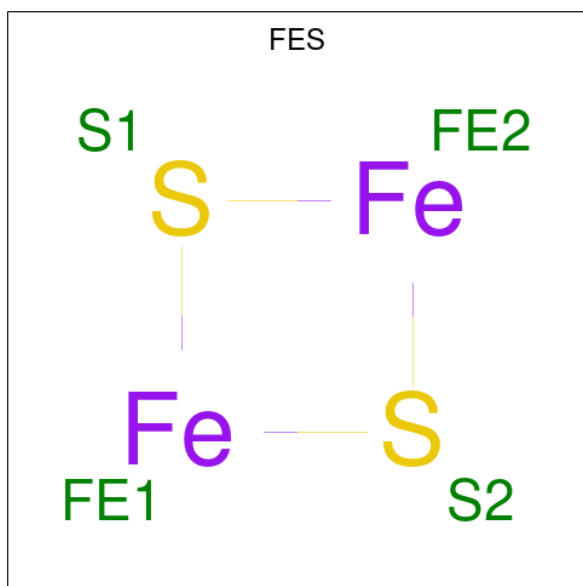
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is Piericidin A (three-letter code: HQH) (formula: C<sub>25</sub>H<sub>37</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



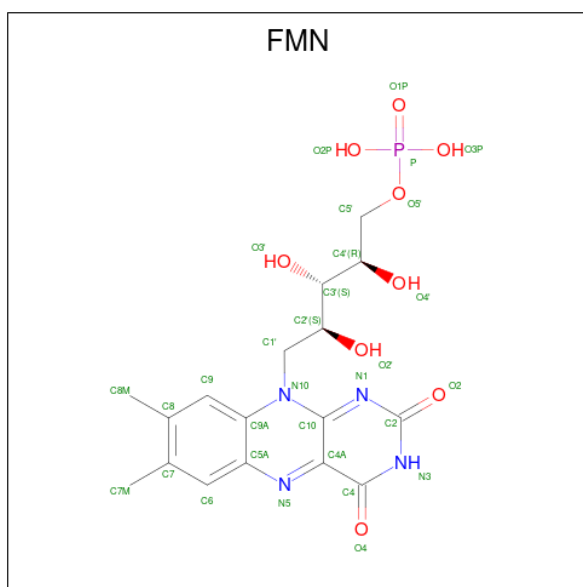
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
48	D	1	30	25	1	4	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- 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).

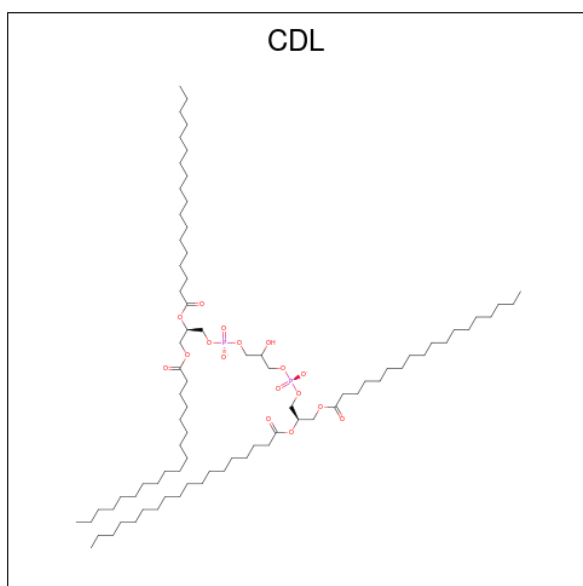


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is SODIUM ION (three-letter code: NA) (formula: Na).

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

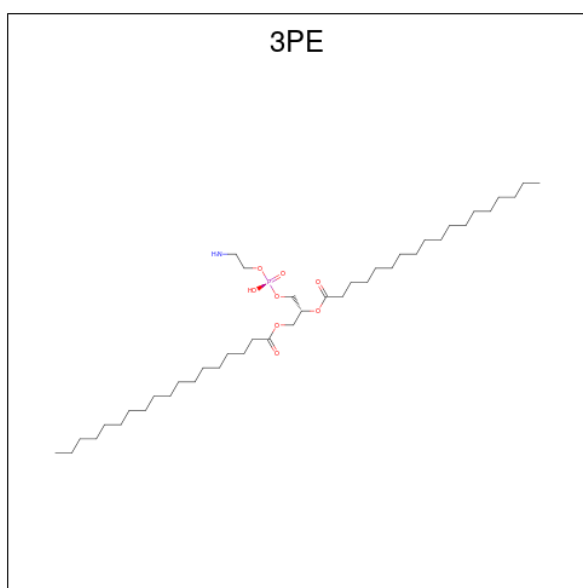
- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms				AltConf
52	H	1	Total	C	O	P	0
			48	29	17	2	
52	L	1	Total	C	O	P	0
			64	45	17	2	
52	h	1	Total	C	O	P	0
			57	39	16	2	
52	h	1	Total	C	O	P	0
			48	29	17	2	
52	q	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 53 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
53	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
53	L	1	Total	C	N	O	P	0
			41	31	1	8	1	
53	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
53	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	N	1	Total	C	N	O	P	0
			34	24	1	8	1	

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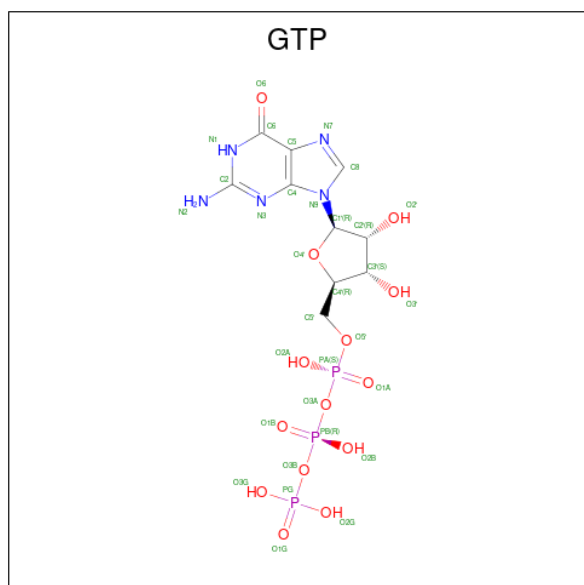
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	N	1	Total 33	C 23	N 1	O 8	P 1	0
53	O	1	Total 30	C 20	N 1	O 8	P 1	0
53	X	1	Total 36	C 26	N 1	O 8	P 1	0
53	Z	1	Total 31	C 21	N 1	O 8	P 1	0
53	Z	1	Total 41	C 31	N 1	O 8	P 1	0
53	d	1	Total 33	C 23	N 1	O 8	P 1	0
53	i	1	Total 30	C 20	N 1	O 8	P 1	0
53	r	1	Total 45	C 35	N 1	O 8	P 1	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

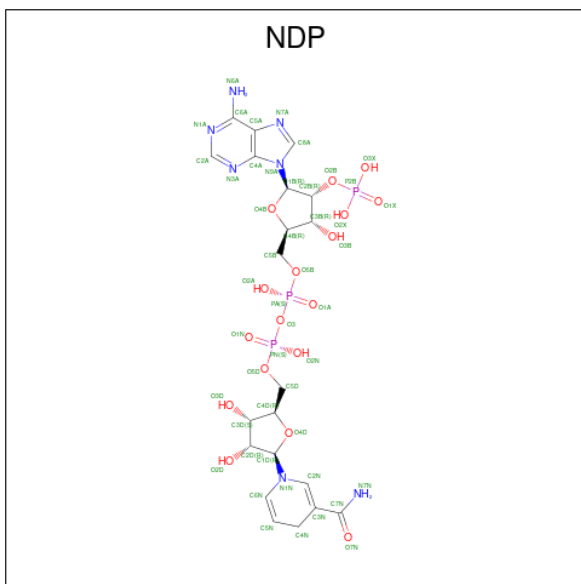
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	O	1	Total 1	Mg 1	0

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

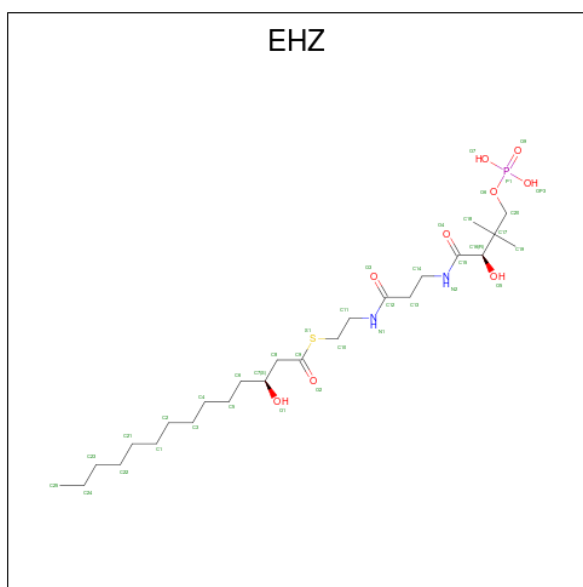


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
56	P	1	48	21	7	17	3	0

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

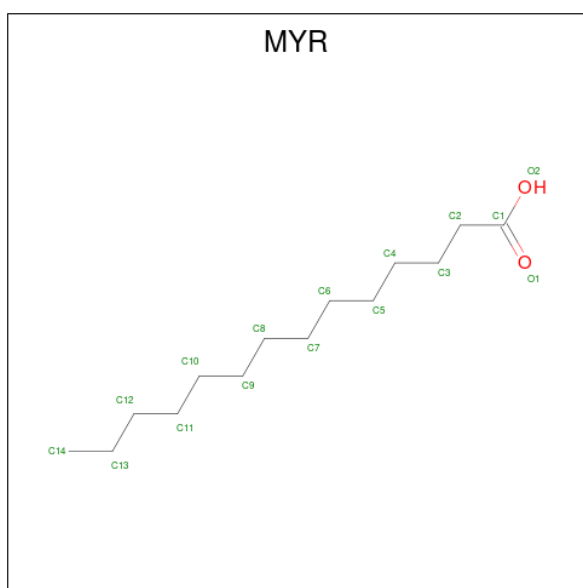
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	R	1	1	1	0

- 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	1	Total O 1 1	0
60	B	33	Total O 33 33	0
60	C	25	Total O 25 25	0
60	D	46	Total O 46 46	0
60	E	1	Total O 1 1	0
60	F	3	Total O 3 3	0
60	G	43	Total O 43 43	0
60	H	8	Total O 8 8	0
60	I	40	Total O 40 40	0
60	J	3	Total O 3 3	0
60	K	1	Total O 1 1	0
60	L	3	Total O 3 3	0
60	M	3	Total O 3 3	0
60	N	4	Total O 4 4	0
60	O	5	Total O 5 5	0
60	P	13	Total O 13 13	0
60	Q	9	Total O 9 9	0
60	R	5	Total O 5 5	0
60	W	1	Total O 1 1	0
60	X	4	Total O 4 4	0
60	Z	5	Total O 5 5	0
60	a	2	Total O 2 2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
60	d	1	Total 1	O 1	0
60	e	2	Total 2	O 2	0
60	g	1	Total 1	O 1	0
60	h	3	Total 3	O 3	0
60	i	1	Total 1	O 1	0
60	l	3	Total 3	O 3	0
60	m	1	Total 1	O 1	0
60	n	1	Total 1	O 1	0
60	p	1	Total 1	O 1	0
60	q	5	Total 5	O 5	0
60	r	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.

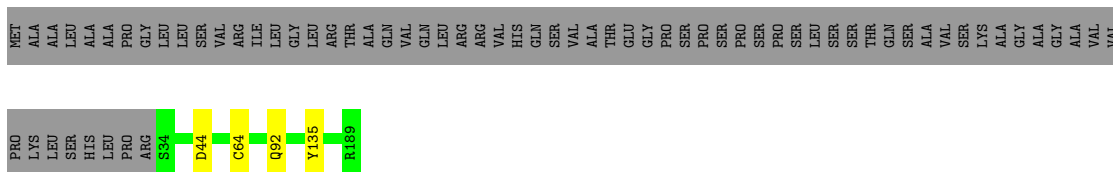
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:  100%




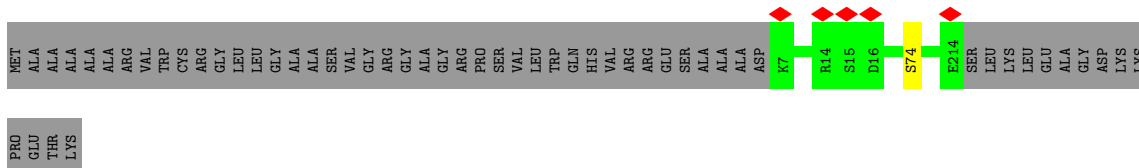
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:  68% 30%



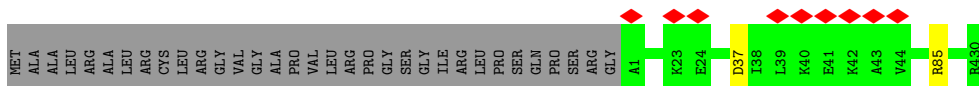
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:  79% 21%

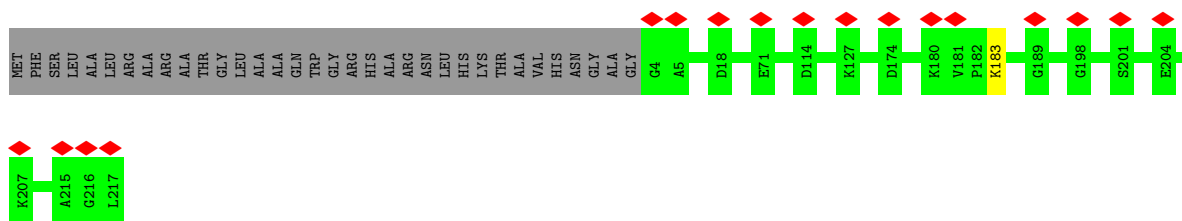
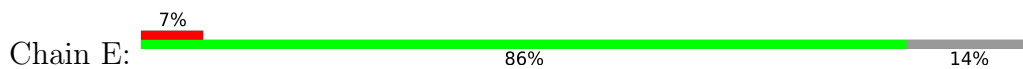


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

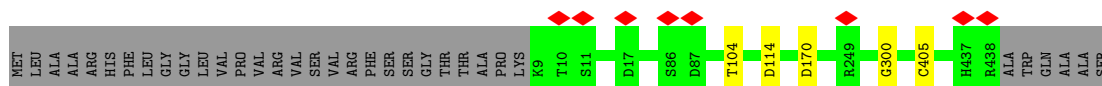
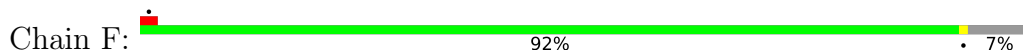
Chain D:  92% 7%



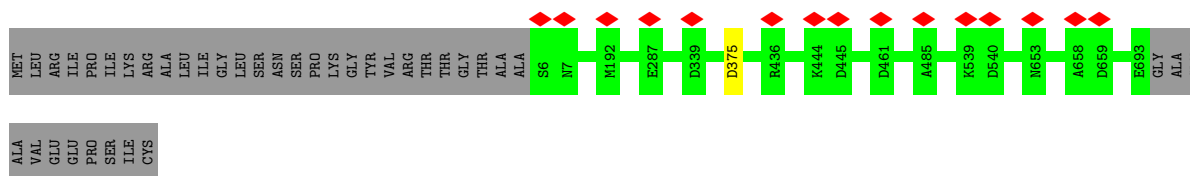
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



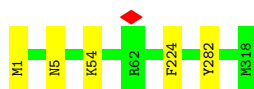
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



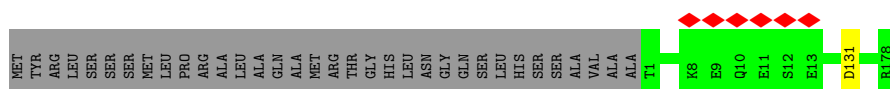
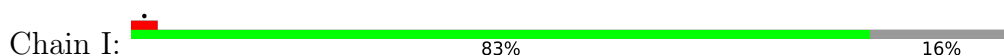
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



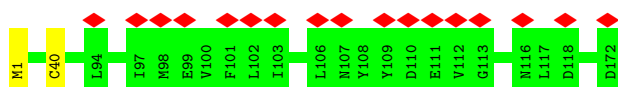
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



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

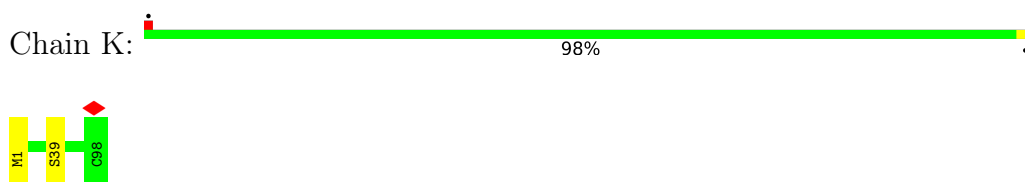


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

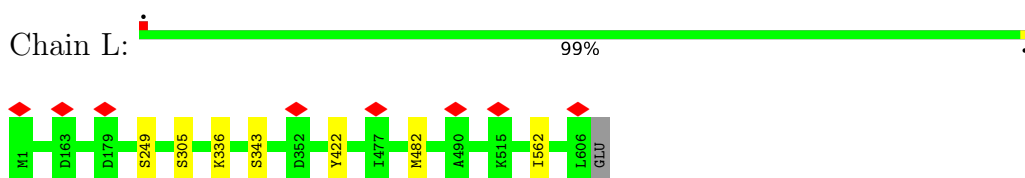




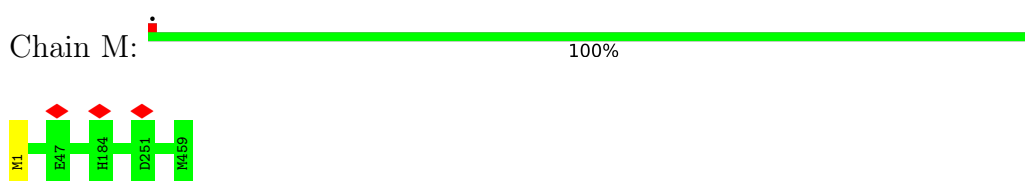
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



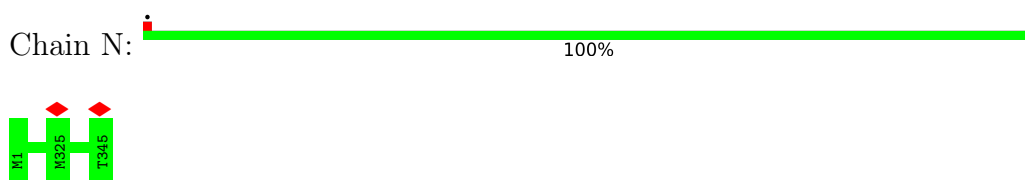
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



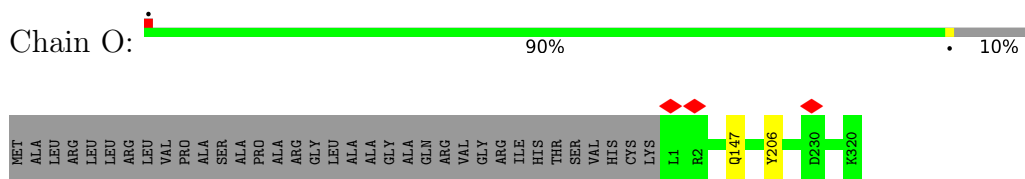
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



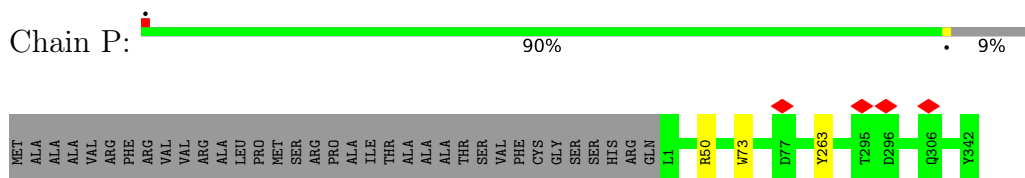
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



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

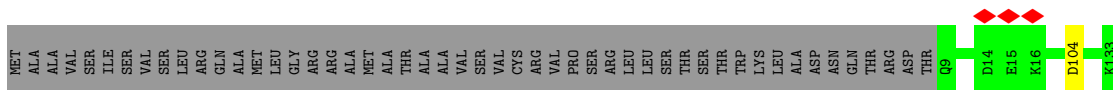


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

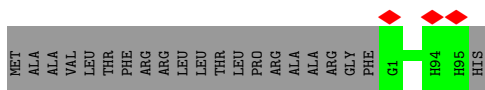
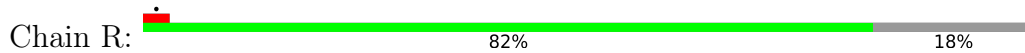


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

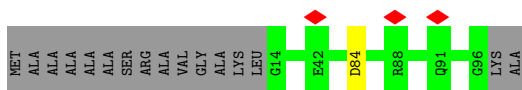
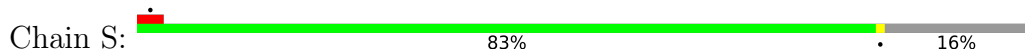




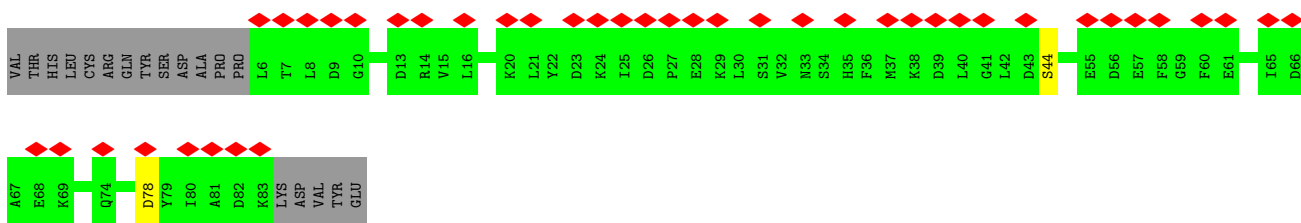
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



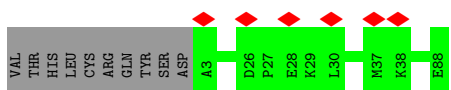
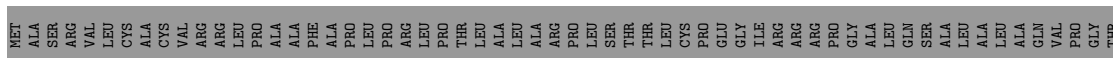
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



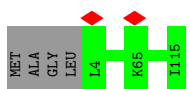
• Molecule 20: Acyl carrier protein, mitochondrial



• Molecule 20: Acyl carrier protein, mitochondrial

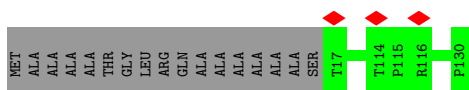


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



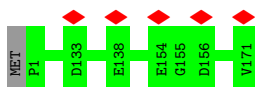
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:  87% 13%



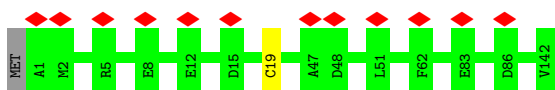
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  99%



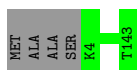
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  8% 99%



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

Chain Z:  97%



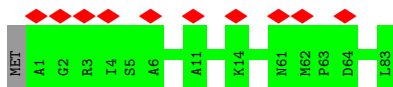
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  99%



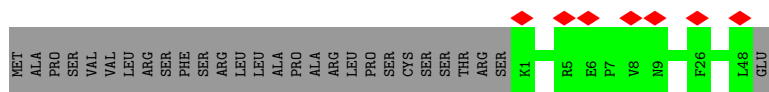
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  12% 99%

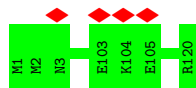


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

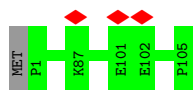
Chain c:  9% 63% 37%



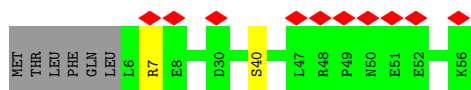
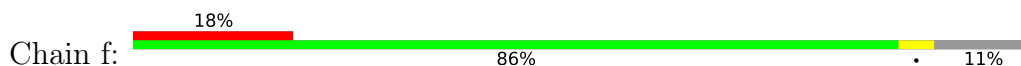
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



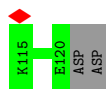
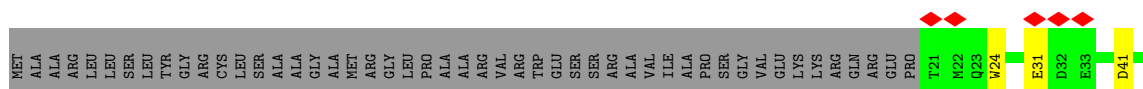
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



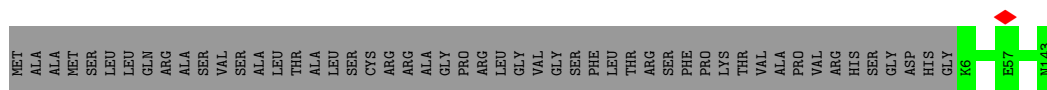
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



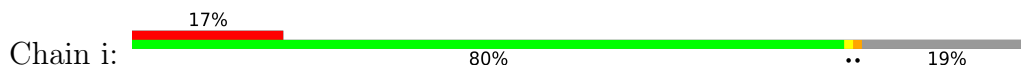
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

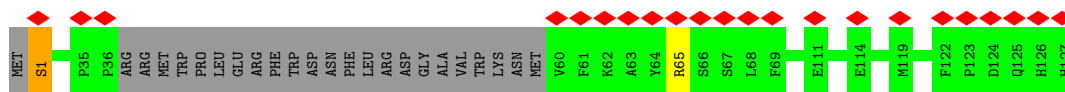


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

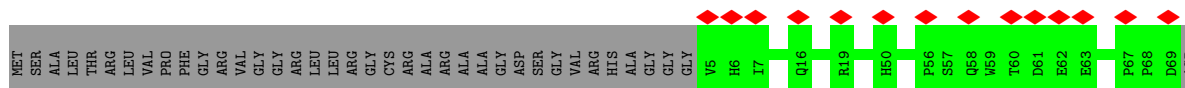


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

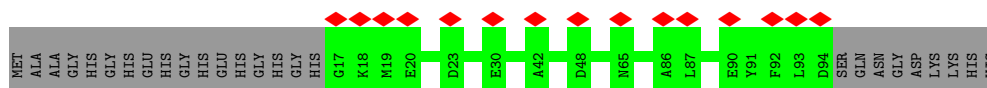
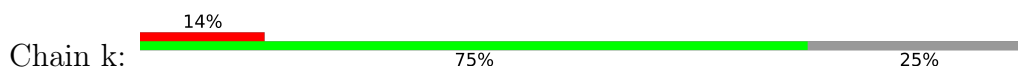




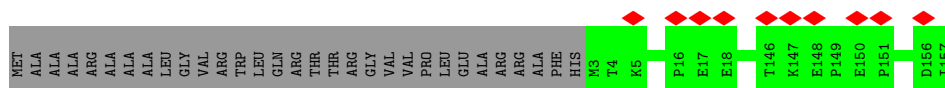
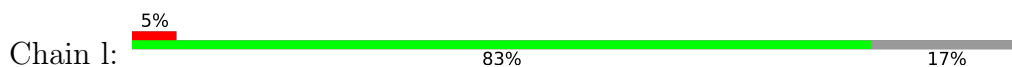
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



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



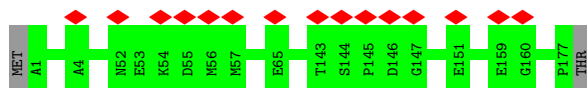
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



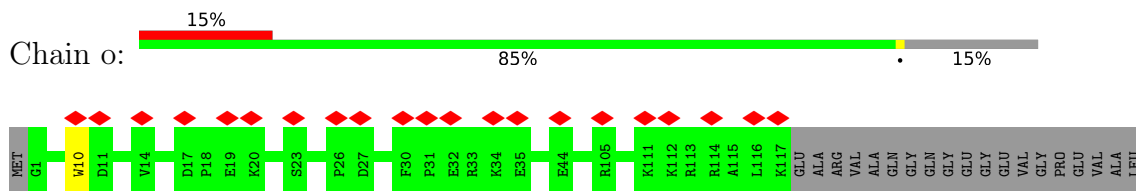
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



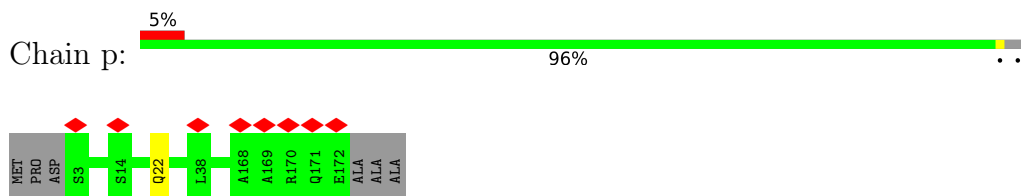
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



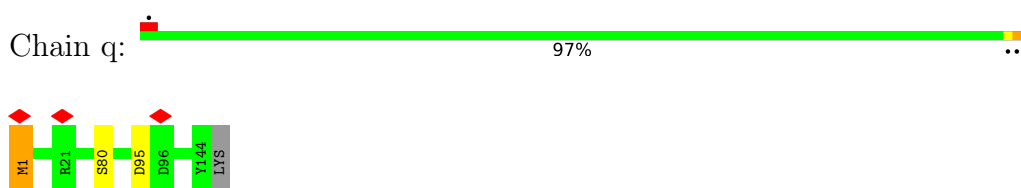
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7, METHYLGLY-OXAL BIS-(GUANYLHYDRAZONE), NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



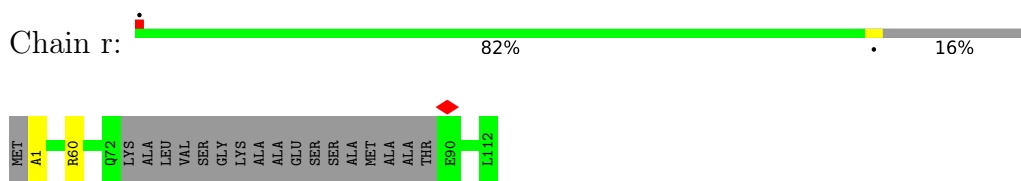
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



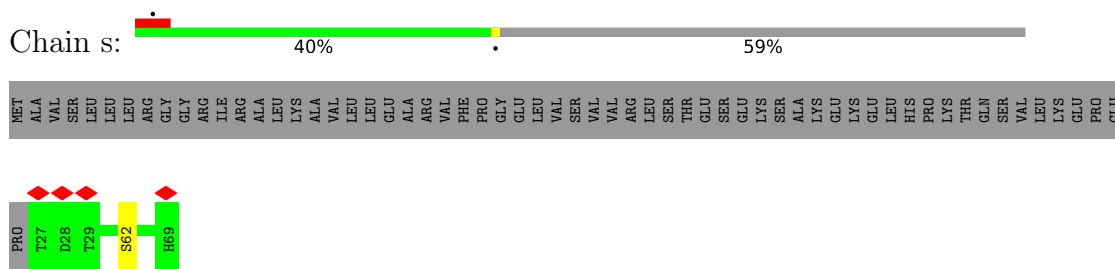
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



• 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	41670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50, 46	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.386	Depositor
Minimum map value	-0.195	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size ( $\text{\AA}$ )	535.5, 535.5, 535.5	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0625, 1.0625, 1.0625	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: 3PE, MYR, AME, MG, GTP, HQH, FMN, ZN, FME, FES, AYA, EHZ, 2MR, NA, SF4, CDL, NDP, LMT, SAC, PC1

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	0.41	0/949	0.46	0/1297
2	B	0.56	0/1278	0.47	0/1730
3	C	0.49	0/1780	0.48	0/2424
4	D	0.47	0/3540	0.47	0/4795
5	E	0.43	0/1700	0.47	0/2316
6	F	0.44	0/3396	0.48	0/4586
7	G	0.43	0/5383	0.48	0/7293
8	H	0.44	0/2607	0.45	0/3564
9	I	0.54	0/1461	0.50	0/1974
10	J	0.44	0/1330	0.45	0/1810
11	K	0.41	0/738	0.44	0/1002
12	L	0.40	0/4913	0.45	0/6686
13	M	0.41	0/3709	0.46	0/5052
14	N	0.40	0/2755	0.45	0/3751
15	O	0.49	0/2674	0.46	0/3626
16	P	0.44	0/2823	0.47	0/3828
17	Q	0.42	0/1038	0.48	0/1401
18	R	0.48	0/762	0.46	0/1026
19	S	0.39	0/674	0.47	0/909
20	T	0.37	0/637	0.42	0/858
20	U	0.46	0/704	0.44	0/951
21	V	0.43	0/937	0.41	0/1270
22	W	0.45	0/993	0.45	0/1335
23	X	0.44	0/1434	0.44	0/1937
24	Y	0.42	0/1074	0.45	0/1456
25	Z	0.44	0/1192	0.46	0/1608
26	a	0.50	0/577	0.45	0/777
27	b	0.42	0/671	0.43	0/921
28	c	0.47	0/409	0.42	0/555
29	d	0.47	0/1028	0.43	0/1387
30	e	0.43	0/900	0.43	0/1199



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	f	0.38	0/451	0.44	0/607
32	g	0.50	0/870	0.44	0/1185
33	h	0.49	0/1197	0.42	0/1621
34	i	0.45	0/889	0.46	0/1210
35	j	0.44	0/587	0.42	0/804
36	k	0.41	0/650	0.46	0/878
37	l	0.49	0/1356	0.44	0/1851
38	m	0.46	0/1079	0.45	0/1463
39	n	0.47	0/1589	0.43	0/2152
40	o	0.41	0/1030	0.43	0/1382
41	p	0.46	0/1472	0.42	0/1989
42	q	0.47	0/1234	0.48	0/1681
43	r	0.45	0/777	0.47	0/1051
44	s	0.40	0/371	0.48	0/504
All	All	0.45	0/67618	0.46	0/91702

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
42	q	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	i	1	SAC	Mainchain
42	q	1	AME	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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	B	154/224 (69%)	147 (96%)	7 (4%)	0	100	100
3	C	206/263 (78%)	196 (95%)	10 (5%)	0	100	100
4	D	427/463 (92%)	410 (96%)	17 (4%)	0	100	100
5	E	212/248 (86%)	192 (91%)	19 (9%)	1 (0%)	29	51
6	F	428/464 (92%)	410 (96%)	16 (4%)	2 (0%)	29	51
7	G	686/727 (94%)	652 (95%)	34 (5%)	0	100	100
8	H	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
9	I	176/212 (83%)	169 (96%)	7 (4%)	0	100	100
10	J	170/172 (99%)	153 (90%)	17 (10%)	0	100	100
11	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
12	L	604/607 (100%)	568 (94%)	34 (6%)	2 (0%)	41	61
13	M	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
14	N	343/345 (99%)	332 (97%)	11 (3%)	0	100	100
15	O	318/355 (90%)	310 (98%)	8 (2%)	0	100	100
16	P	340/377 (90%)	328 (96%)	12 (4%)	0	100	100
17	Q	123/175 (70%)	117 (95%)	6 (5%)	0	100	100
18	R	93/116 (80%)	84 (90%)	9 (10%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	76/156 (49%)	64 (84%)	12 (16%)	0	100	100
20	U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
23	X	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
24	Y	140/143 (98%)	138 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	72 (89%)	9 (11%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	e	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
31	f	49/57 (86%)	45 (92%)	4 (8%)	0	100	100
32	g	98/151 (65%)	98 (100%)	0	0	100	100
33	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
34	i	100/128 (78%)	90 (90%)	10 (10%)	0	100	100
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	76/104 (73%)	74 (97%)	2 (3%)	0	100	100
37	l	153/186 (82%)	145 (95%)	8 (5%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
40	o	115/137 (84%)	105 (91%)	9 (8%)	1 (1%)	17	34
41	p	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
42	q	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
43	r	91/113 (80%)	84 (92%)	7 (8%)	0	100	100
44	s	41/104 (39%)	38 (93%)	3 (7%)	0	100	100
All	All	8118/9214 (88%)	7731 (95%)	381 (5%)	6 (0%)	54	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	170	ASP
12	L	562	ILE
40	o	10	TRP
12	L	249	SER
5	E	183	LYS

### 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	103/103 (100%)	103 (100%)	0	100	100
2	B	132/185 (71%)	128 (97%)	4 (3%)	41	65
3	C	190/227 (84%)	189 (100%)	1 (0%)	88	94
4	D	370/394 (94%)	369 (100%)	1 (0%)	92	96
5	E	184/206 (89%)	184 (100%)	0	100	100
6	F	345/370 (93%)	342 (99%)	3 (1%)	78	89
7	G	580/610 (95%)	579 (100%)	1 (0%)	93	97
8	H	279/279 (100%)	275 (99%)	4 (1%)	67	83
9	I	152/178 (85%)	151 (99%)	1 (1%)	84	91
10	J	137/137 (100%)	136 (99%)	1 (1%)	84	91
11	K	87/87 (100%)	86 (99%)	1 (1%)	73	86
12	L	548/549 (100%)	543 (99%)	5 (1%)	78	89
13	M	414/414 (100%)	414 (100%)	0	100	100
14	N	307/307 (100%)	307 (100%)	0	100	100
15	O	284/309 (92%)	282 (99%)	2 (1%)	84	91
16	P	299/325 (92%)	296 (99%)	3 (1%)	76	88
17	Q	112/153 (73%)	111 (99%)	1 (1%)	78	89
18	R	80/96 (83%)	80 (100%)	0	100	100
19	S	73/80 (91%)	72 (99%)	1 (1%)	67	83
20	T	72/135 (53%)	70 (97%)	2 (3%)	43	68
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	106/107 (99%)	105 (99%)	1 (1%)	78	89
25	Z	121/123 (98%)	121 (100%)	0	100	100
26	a	59/60 (98%)	59 (100%)	0	100	100
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	42/67 (63%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	93 (100%)	0	100	100
31	f	47/53 (89%)	45 (96%)	2 (4%)	29	54
32	g	91/129 (70%)	88 (97%)	3 (3%)	38	63
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	95/119 (80%)	94 (99%)	1 (1%)	73	86
35	j	61/87 (70%)	61 (100%)	0	100	100
36	k	60/78 (77%)	60 (100%)	0	100	100
37	l	140/161 (87%)	140 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	162/164 (99%)	162 (100%)	0	100	100
40	o	108/121 (89%)	108 (100%)	0	100	100
41	p	155/158 (98%)	154 (99%)	1 (1%)	86	93
42	q	129/130 (99%)	127 (98%)	2 (2%)	62	81
43	r	85/96 (88%)	84 (99%)	1 (1%)	71	85
44	s	42/95 (44%)	41 (98%)	1 (2%)	49	72
All	All	7198/7947 (91%)	7155 (99%)	43 (1%)	86	93

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	84	ASP
32	g	31	GLU
20	T	44	SER
31	f	7	ARG
34	i	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	184	HIS
30	e	97	HIS
38	m	85	ASN
32	g	55	ASN
12	L	109	HIS

### 5.3.3 RNA [i](#)

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
1	FME	A	1	1	8,9,10	0.92	0	7,9,11	0.86	0
34	SAC	i	1	34	7,8,9	1.83	1 (14%)	8,9,11	1.88	2 (25%)
42	AME	q	1	42	9,10,11	1.50	1 (11%)	9,11,13	1.88	2 (22%)
8	FME	H	1	8	8,9,10	1.02	1 (12%)	7,9,11	1.08	0
4	2MR	D	85	4	10,12,13	2.25	2 (20%)	5,13,15	1.23	1 (20%)
12	FME	L	1	12	8,9,10	0.97	0	7,9,11	0.65	0
11	FME	K	1	11	8,9,10	1.02	1 (12%)	7,9,11	1.21	1 (14%)
13	FME	M	1	13	8,9,10	1.10	1 (12%)	7,9,11	0.71	0
43	AYA	r	1	43	6,7,8	1.41	1 (16%)	5,8,10	1.17	1 (20%)
10	FME	J	1	10	8,9,10	0.97	1 (12%)	7,9,11	0.91	0
14	FME	N	1	14	8,9,10	0.88	0	7,9,11	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/7/9/11	-
34	SAC	i	1	34	-	2/7/8/10	-
42	AME	q	1	42	-	5/9/10/12	-
8	FME	H	1	8	-	3/7/9/11	-
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
11	FME	K	1	11	-	2/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
10	FME	J	1	10	-	3/7/9/11	-
14	FME	N	1	14	-	4/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.62	1.43	1.33
4	D	85	2MR	CZ-NE	4.48	1.43	1.34
34	i	1	SAC	O-C	4.21	1.36	1.19
42	q	1	AME	CT1-N	3.41	1.46	1.34
43	r	1	AYA	CA-N	-3.03	1.43	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	O-C-CA	-4.52	112.94	124.78
42	q	1	AME	CT2-CT1-N	3.67	122.31	116.10
42	q	1	AME	CE-SD-CG	2.74	109.81	100.40
34	i	1	SAC	OG-CB-CA	-2.57	104.41	110.97
11	K	1	FME	C-CA-N	2.34	113.95	109.73

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CA-N-CN
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 56 ligands modelled in this entry, 3 are monoatomic - leaving 53 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
45	LMT	Y	202	-	36,36,36	1.22	6 (16%)	47,47,47	0.96	2 (4%)
45	LMT	h	203	-	36,36,36	1.22	5 (13%)	47,47,47	1.02	2 (4%)
53	3PE	L	702	-	40,40,50	0.96	3 (7%)	43,45,55	1.12	2 (4%)
45	LMT	J	202	-	36,36,36	1.19	6 (16%)	47,47,47	1.00	0
53	3PE	N	401	-	33,33,50	1.07	4 (12%)	36,38,55	1.05	2 (5%)
53	3PE	L	703	-	43,43,50	0.91	4 (9%)	46,48,55	1.07	3 (6%)
45	LMT	j	101	-	36,36,36	1.15	4 (11%)	47,47,47	0.95	1 (2%)
46	PC1	B	202	-	37,37,53	1.12	4 (10%)	43,45,61	1.15	2 (4%)
58	EHZ	U	201	20	29,36,37	1.62	5 (17%)	35,44,47	1.72	8 (22%)
59	MYR	o	201	40	14,14,15	0.75	0	13,13,15	0.63	0
52	CDL	h	201	-	56,56,99	1.05	5 (8%)	61,67,111	1.18	4 (6%)
45	LMT	M	501	-	36,36,36	1.27	7 (19%)	47,47,47	1.19	3 (6%)
52	CDL	L	705	-	63,63,99	1.08	7 (11%)	69,75,111	1.20	4 (5%)
45	LMT	L	701	-	36,36,36	1.25	6 (16%)	47,47,47	0.94	1 (2%)
53	3PE	r	201	-	44,44,50	0.93	4 (9%)	47,49,55	1.08	2 (4%)
53	3PE	M	502	-	35,35,50	1.00	3 (8%)	38,40,55	1.13	2 (5%)
45	LMT	P	502	-	36,36,36	1.18	5 (13%)	47,47,47	1.19	4 (8%)
47	SF4	F	501	6	0,12,12	-	-	-	-	-
53	3PE	Z	201	-	30,30,50	1.09	3 (10%)	33,35,55	1.10	2 (6%)
45	LMT	Y	204	-	36,36,36	1.22	6 (16%)	47,47,47	1.05	3 (6%)
52	CDL	H	401	-	47,47,99	1.16	6 (12%)	51,58,111	1.26	3 (5%)
53	3PE	N	402	-	32,32,50	1.06	4 (12%)	35,37,55	1.11	2 (5%)
53	3PE	i	201	34	29,29,50	1.14	3 (10%)	32,34,55	1.25	2 (6%)
56	NDP	P	501	-	45,52,52	2.07	8 (17%)	53,80,80	1.68	9 (16%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
53	3PE	Z	202	-	40,40,50	0.97	4 (10%)	43,45,55	1.05	2 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	LMT	A	401	-	36,36,36	1.23	6 (16%)	47,47,47	1.01	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-		
47	SF4	I	202	9	0,12,12	-	-	-		
45	LMT	J	201	-	36,36,36	1.22	5 (13%)	47,47,47	1.15	2 (4%)
45	LMT	Y	203	-	36,36,36	1.15	5 (13%)	47,47,47	1.07	2 (4%)
58	EHZ	T	201	20	29,36,37	1.67	5 (17%)	35,44,47	1.63	9 (25%)
47	SF4	G	802	7	0,12,12	-	-	-		
52	CDL	h	202	-	46,46,99	1.53	8 (17%)	50,57,111	1.36	4 (8%)
53	3PE	d	201	-	32,32,50	1.06	3 (9%)	35,37,55	1.11	2 (5%)
45	LMT	L	704	-	36,36,36	1.23	7 (19%)	47,47,47	1.12	4 (8%)
50	FMN	F	502	-	33,33,33	2.51	6 (18%)	48,50,50	1.51	10 (20%)
49	FES	E	301	5	0,4,4	-	-	-		
47	SF4	B	201	2	0,12,12	-	-	-		
53	3PE	O	504	-	29,29,50	1.10	4 (13%)	32,34,55	1.04	2 (6%)
55	GTP	O	502	-	26,34,34	2.95	11 (42%)	32,54,54	1.91	10 (31%)
45	LMT	O	503	-	36,36,36	1.15	5 (13%)	47,47,47	1.48	4 (8%)
45	LMT	A	403	-	36,36,36	1.18	4 (11%)	47,47,47	1.06	2 (4%)
47	SF4	I	201	9	0,12,12	-	-	-		
46	PC1	B	203	-	40,40,53	1.09	2 (5%)	46,48,61	1.14	2 (4%)
53	3PE	X	201	-	35,35,50	1.00	4 (11%)	38,40,55	1.22	2 (5%)
52	CDL	q	501	-	63,63,99	1.06	5 (7%)	69,75,111	1.03	4 (5%)
45	LMT	K	201	-	36,36,36	1.33	7 (19%)	47,47,47	1.07	2 (4%)
45	LMT	Y	201	-	36,36,36	1.29	6 (16%)	47,47,47	1.02	1 (2%)
53	3PE	I	203	-	43,43,50	0.92	3 (6%)	46,48,55	1.08	2 (4%)
46	PC1	A	402	-	28,28,53	1.29	3 (10%)	34,36,61	0.98	2 (5%)
53	3PE	M	503	-	35,35,50	1.01	4 (11%)	38,40,55	1.11	2 (5%)
48	HQH	D	601	-	29,30,30	0.83	2 (6%)	28,40,40	1.40	4 (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
45	LMT	Y	202	-	-	9/21/61/61	0/2/2/2
45	LMT	h	203	-	-	7/21/61/61	0/2/2/2
53	3PE	L	702	-	-	20/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	J	202	-	-	8/21/61/61	0/2/2/2
53	3PE	N	401	-	-	19/37/37/54	-
53	3PE	L	703	-	-	24/47/47/54	-
45	LMT	j	101	-	-	11/21/61/61	0/2/2/2
46	PC1	B	202	-	-	19/41/41/57	-
58	EHZ	U	201	20	-	16/42/44/45	-
59	MYR	o	201	40	-	6/11/12/13	-
52	CDL	h	201	-	-	31/65/65/110	-
45	LMT	M	501	-	-	14/21/61/61	0/2/2/2
52	CDL	L	705	-	-	36/74/74/110	-
45	LMT	L	701	-	-	7/21/61/61	0/2/2/2
53	3PE	r	201	-	-	16/48/48/54	-
53	3PE	M	502	-	-	19/39/39/54	-
45	LMT	P	502	-	-	13/21/61/61	0/2/2/2
47	SF4	F	501	6	-	-	0/6/5/5
53	3PE	Z	201	-	-	21/34/34/54	-
45	LMT	Y	204	-	-	11/21/61/61	0/2/2/2
52	CDL	H	401	-	-	24/57/57/110	-
53	3PE	N	402	-	-	16/36/36/54	-
53	3PE	i	201	34	-	19/33/33/54	-
56	NDP	P	501	-	-	3/30/77/77	0/5/5/5
49	FES	G	803	7	-	-	0/1/1/1
53	3PE	Z	202	-	-	20/44/44/54	-
45	LMT	A	401	-	-	10/21/61/61	0/2/2/2
47	SF4	G	801	7	-	-	0/6/5/5
47	SF4	I	202	9	-	-	0/6/5/5
45	LMT	J	201	-	-	10/21/61/61	0/2/2/2
45	LMT	Y	203	-	-	15/21/61/61	0/2/2/2
58	EHZ	T	201	20	-	17/42/44/45	-
47	SF4	G	802	7	-	-	0/6/5/5
52	CDL	h	202	-	-	32/56/56/110	-
53	3PE	d	201	-	-	18/36/36/54	-
45	LMT	L	704	-	-	11/21/61/61	0/2/2/2
50	FMN	F	502	-	-	9/18/18/18	0/3/3/3
55	GTP	O	502	-	-	7/18/38/38	0/3/3/3

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	3PE	O	504	-	-	14/33/33/54	-
47	SF4	B	201	2	-	-	0/6/5/5
49	FES	E	301	5	-	-	0/1/1/1
45	LMT	O	503	-	-	9/21/61/61	0/2/2/2
45	LMT	A	403	-	-	10/21/61/61	0/2/2/2
47	SF4	I	201	9	-	-	0/6/5/5
46	PC1	B	203	-	-	20/44/44/57	-
53	3PE	X	201	-	-	16/39/39/54	-
52	CDL	q	501	-	-	36/73/73/110	-
45	LMT	K	201	-	-	6/21/61/61	0/2/2/2
45	LMT	Y	201	-	-	12/21/61/61	0/2/2/2
53	3PE	I	203	-	-	16/47/47/54	-
46	PC1	A	402	-	-	15/32/32/57	-
53	3PE	M	503	-	-	17/39/39/54	-
48	HQH	D	601	-	-	10/27/29/29	0/1/1/1

The worst 5 of 217 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	10.62	1.79	1.59
50	F	502	FMN	O4-C4	8.42	1.39	1.23
55	O	502	GTP	O6-C6	8.17	1.39	1.23
50	F	502	FMN	O2-C2	8.16	1.39	1.24
52	h	202	CDL	OA6-CA4	-6.08	1.39	1.46

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	501	NDP	PN-O3-PA	-6.41	110.84	132.83
45	O	503	LMT	C1-O1'-C1'	5.12	122.33	113.84
45	O	503	LMT	O1'-C1'-C2'	4.97	116.06	108.30
52	H	401	CDL	OB6-CB5-C51	4.79	121.83	111.50
52	L	705	CDL	OA6-CA5-C11	4.57	121.35	111.50

There are no chirality outliers.

5 of 699 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	401	LMT	O5'-C1'-O1'-C1

Continued on next page...

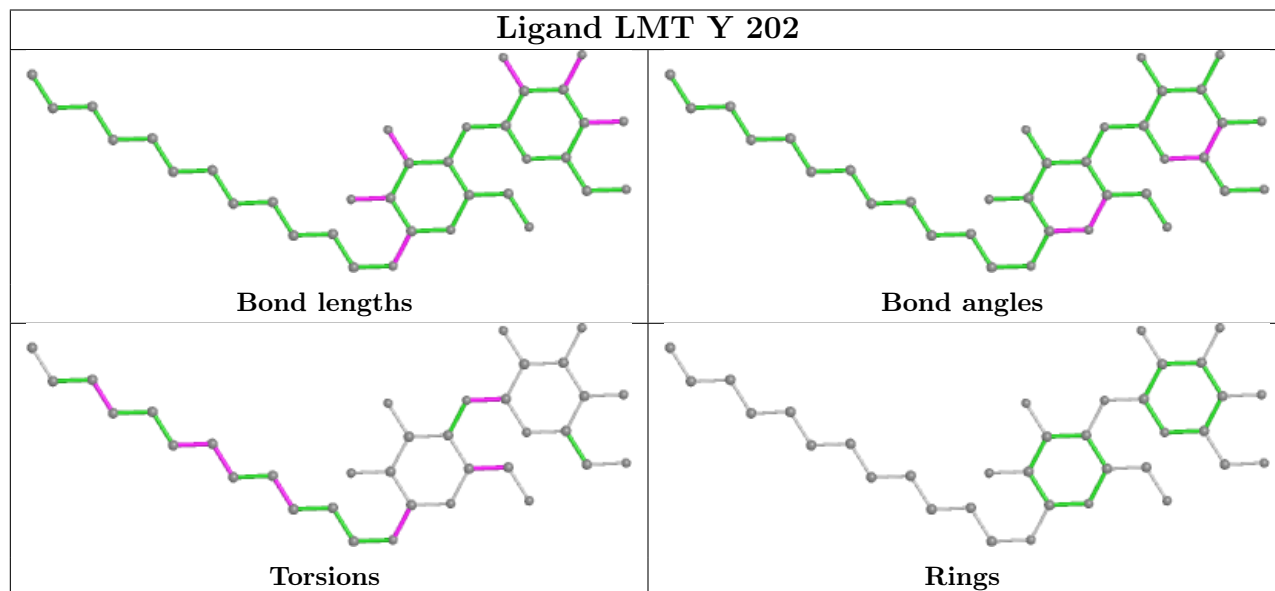
Continued from previous page...

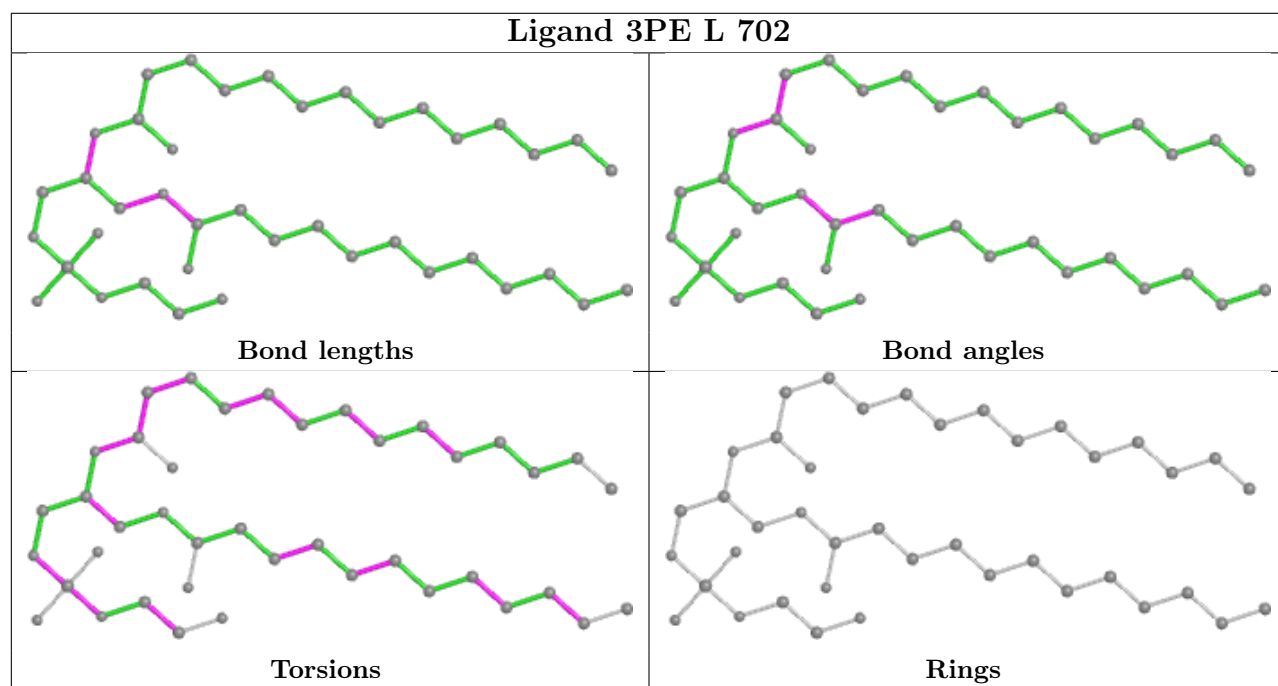
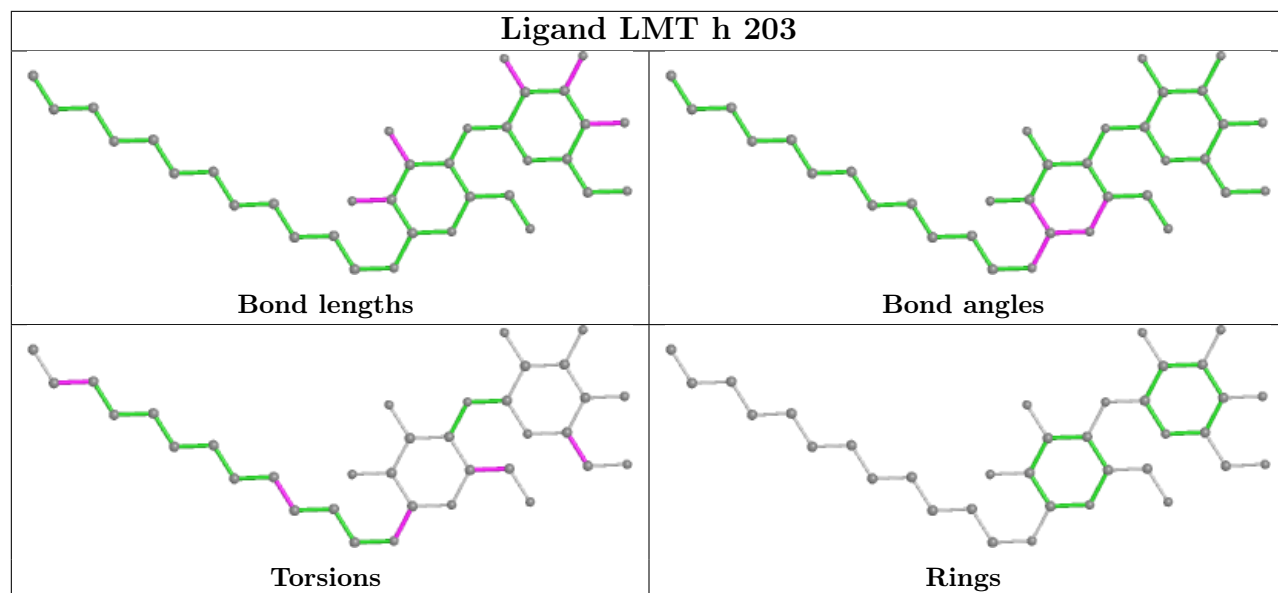
Mol	Chain	Res	Type	Atoms
45	A	401	LMT	C2-C1-O1'-C1'
45	K	201	LMT	O5'-C1'-O1'-C1
45	L	701	LMT	C2'-C1'-O1'-C1
45	L	701	LMT	O5'-C1'-O1'-C1

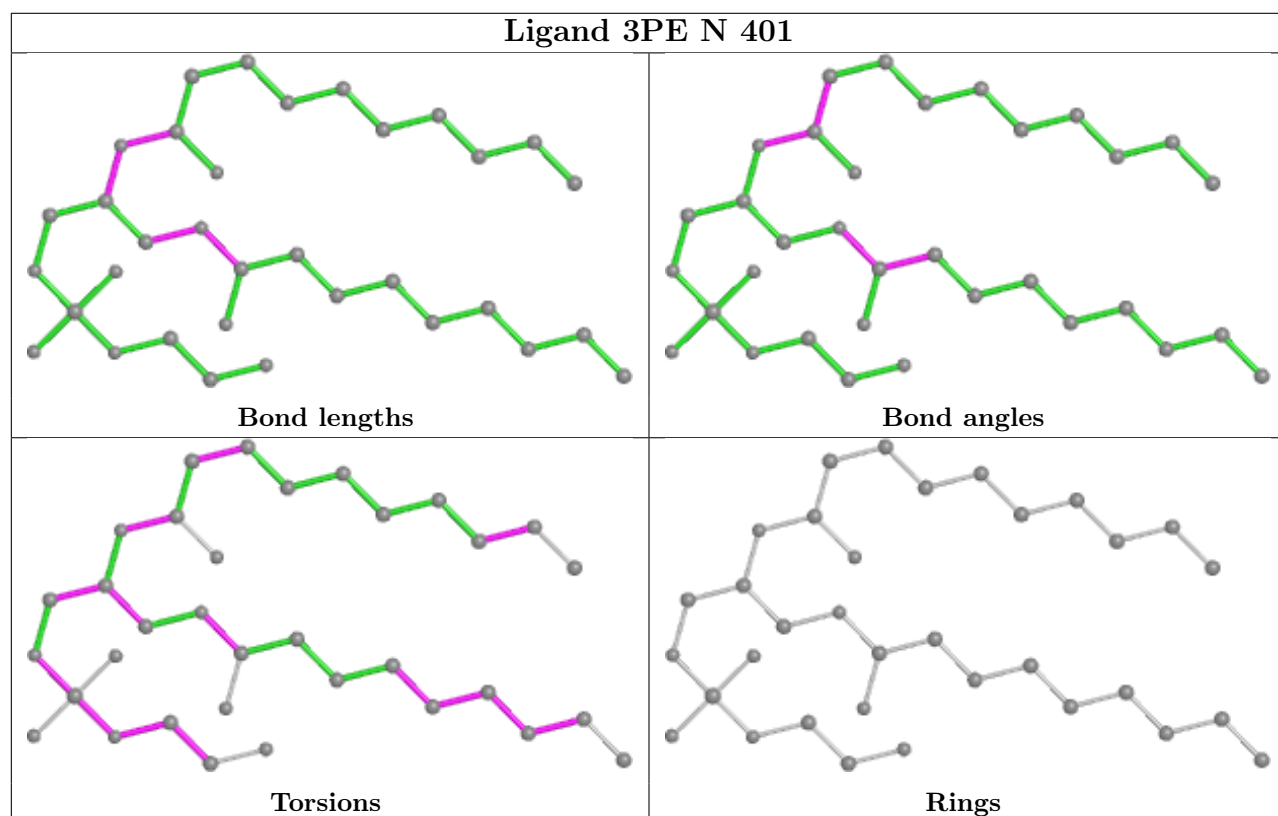
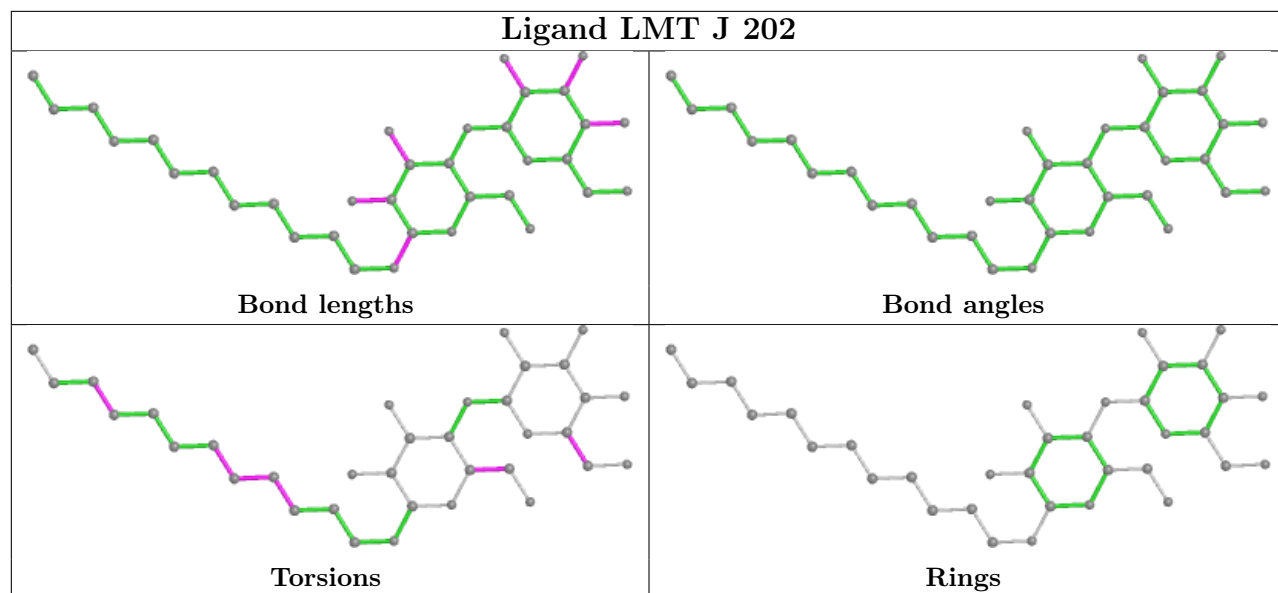
There are no ring outliers.

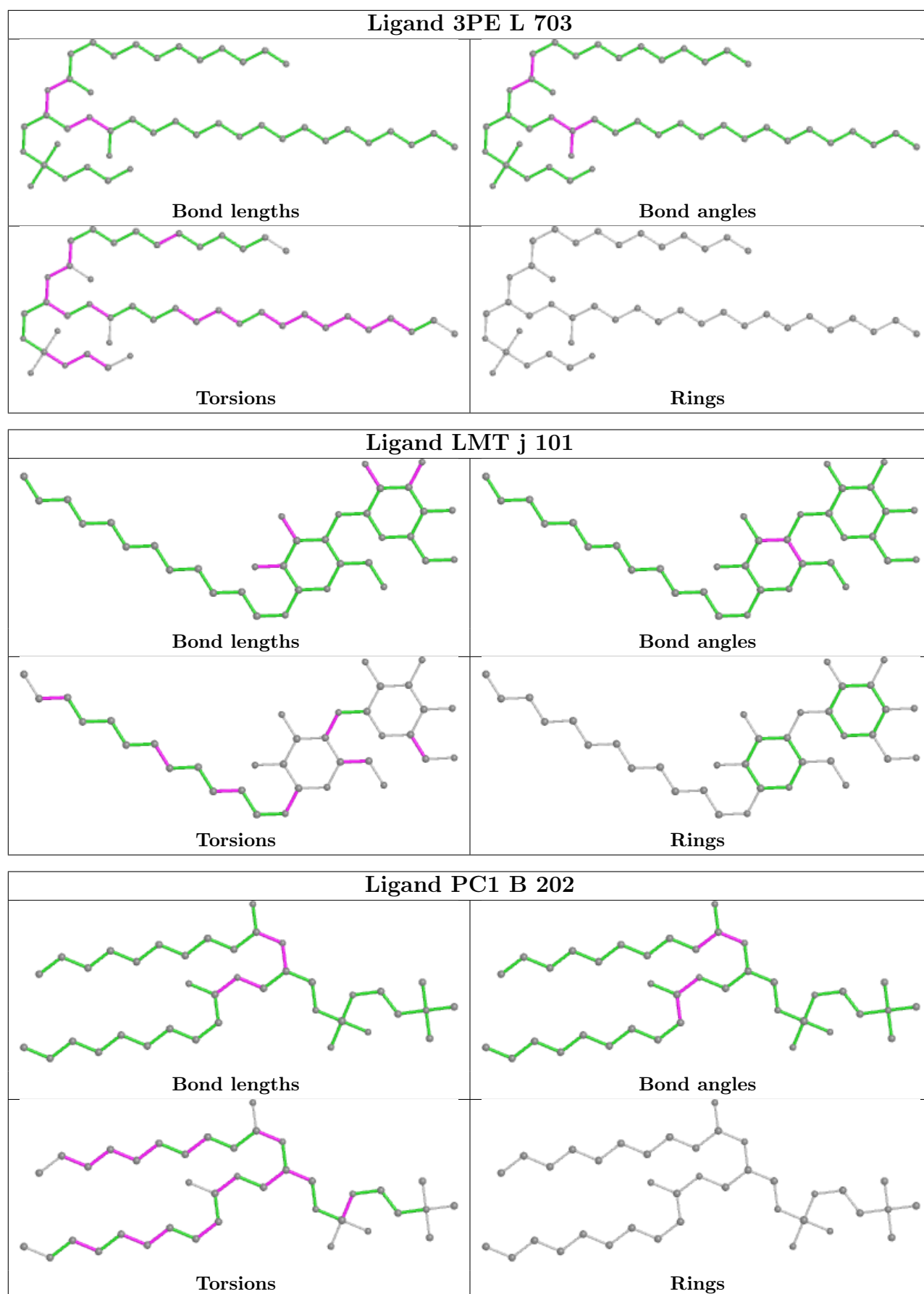
No monomer is involved in short contacts.

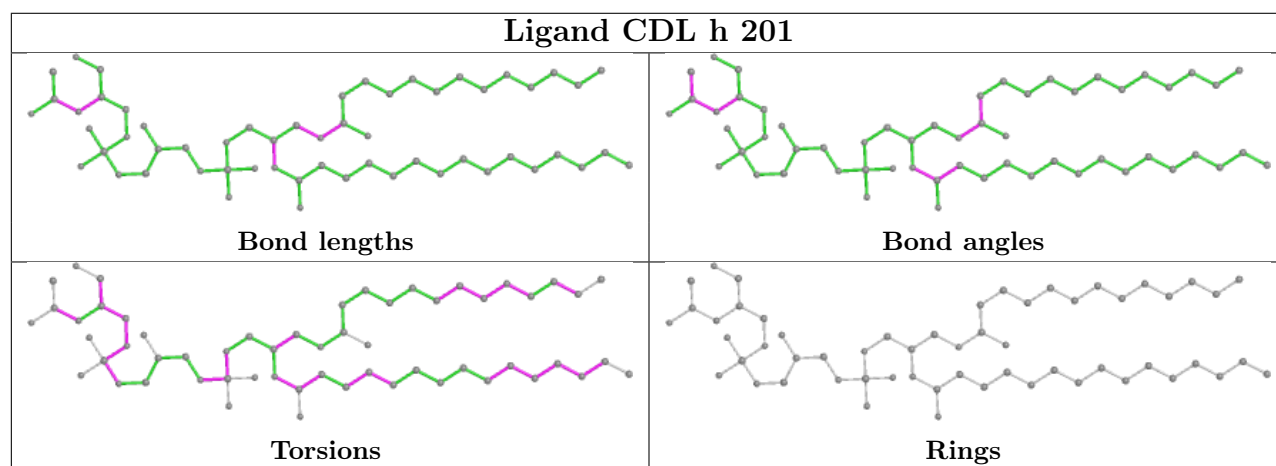
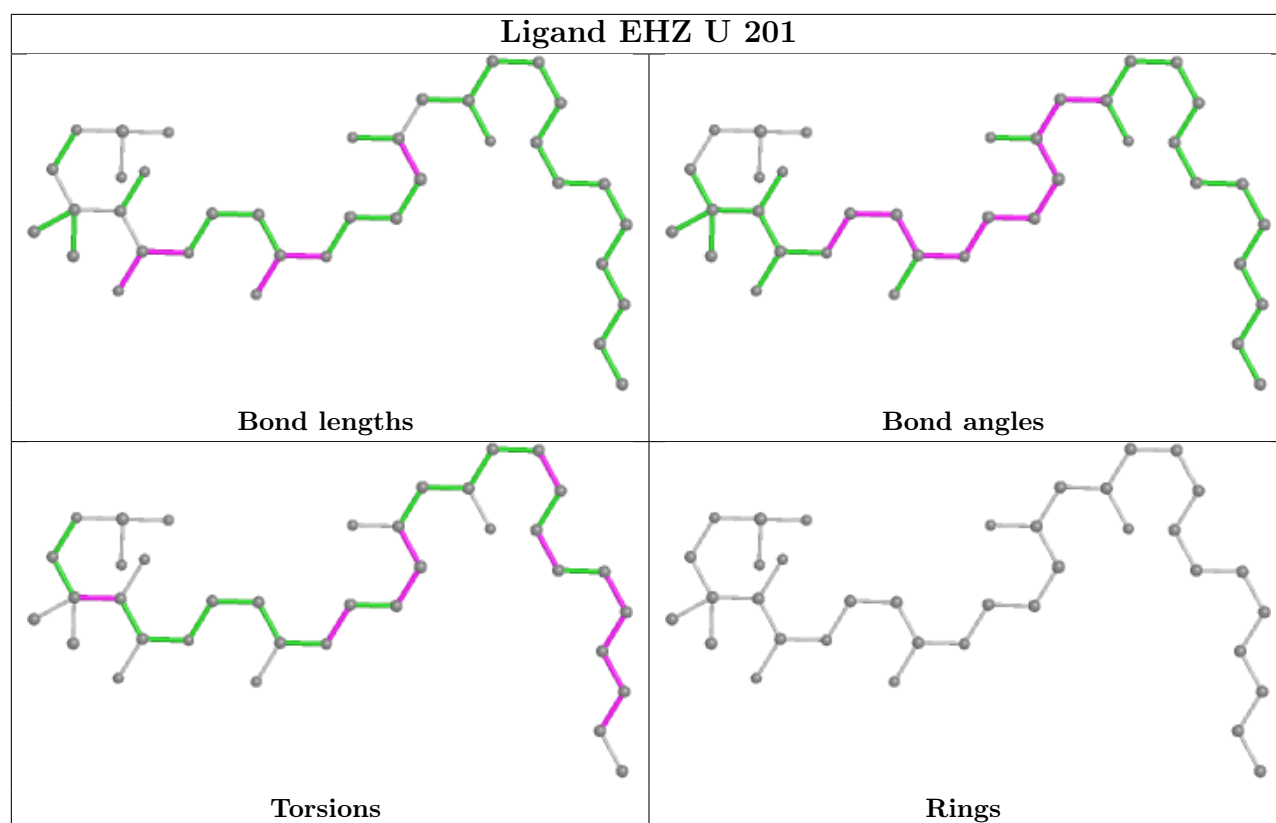
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



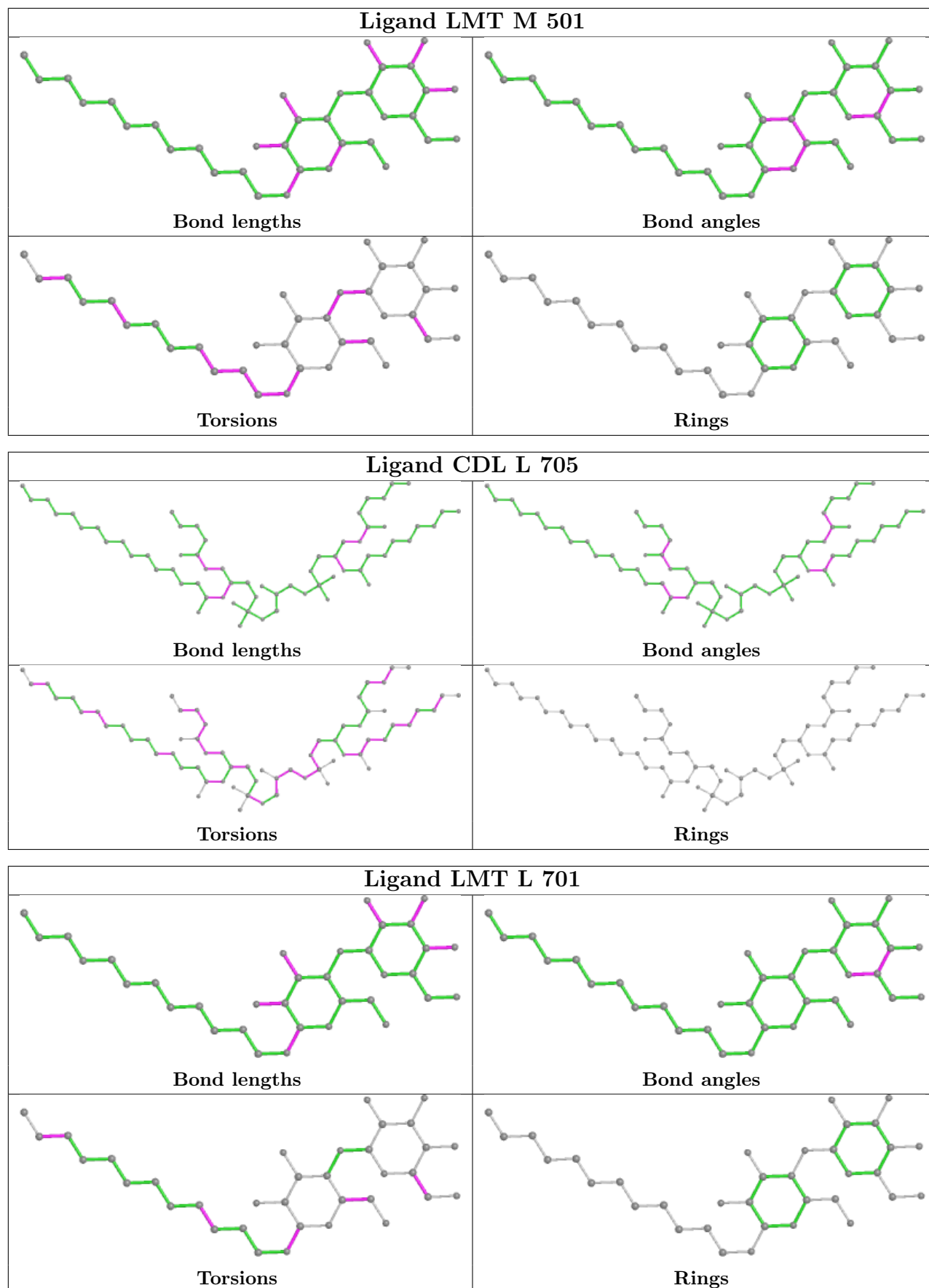


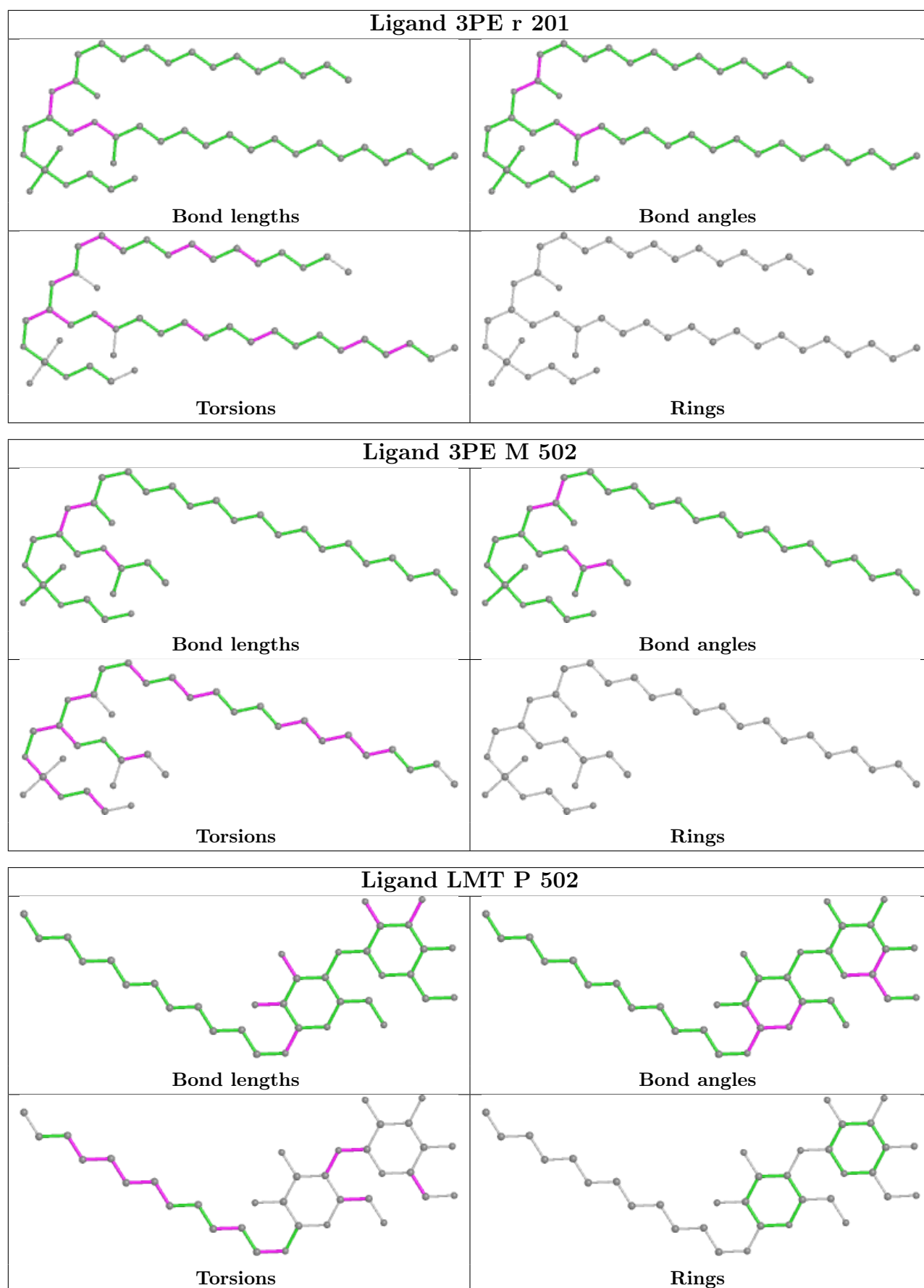


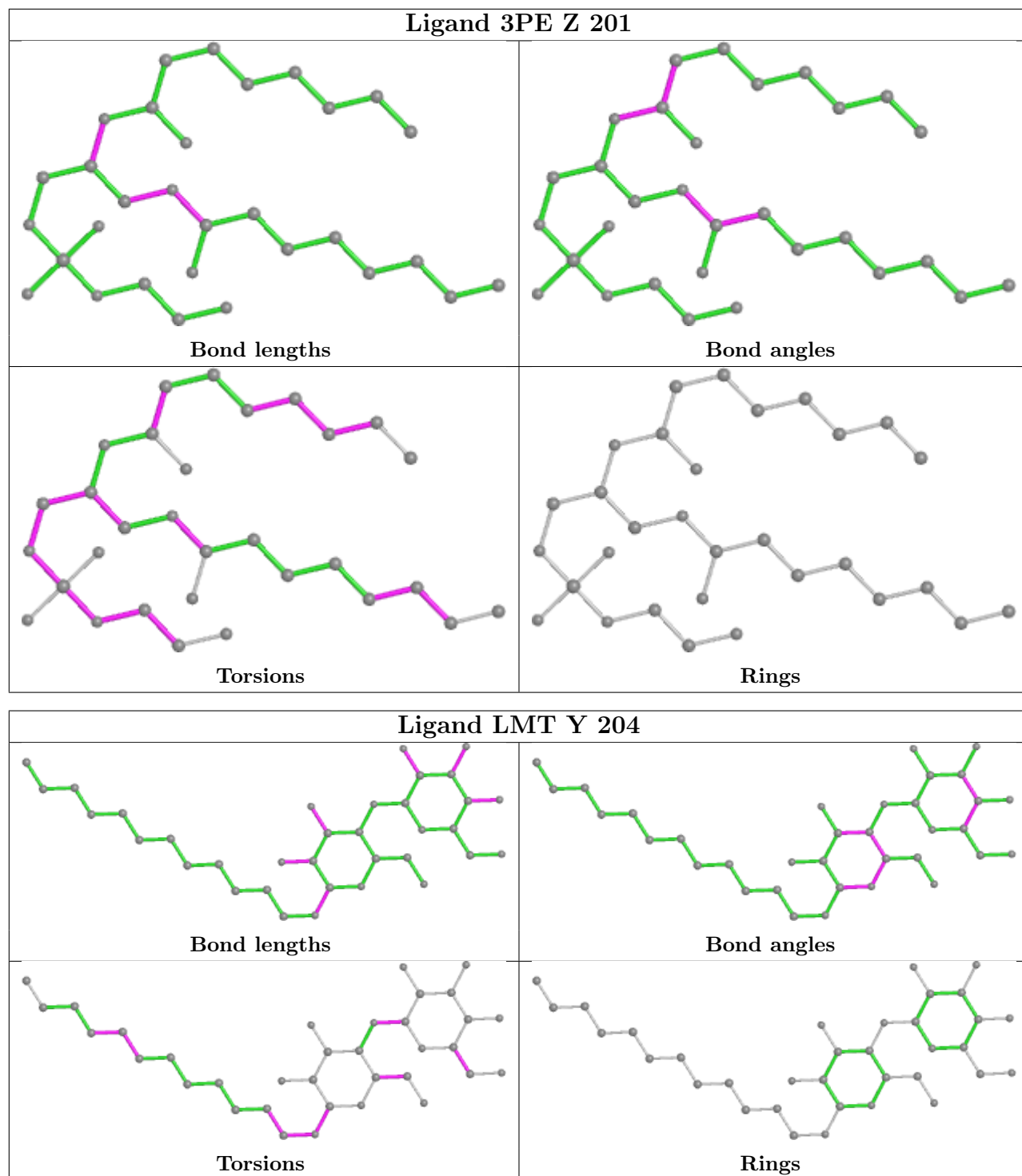


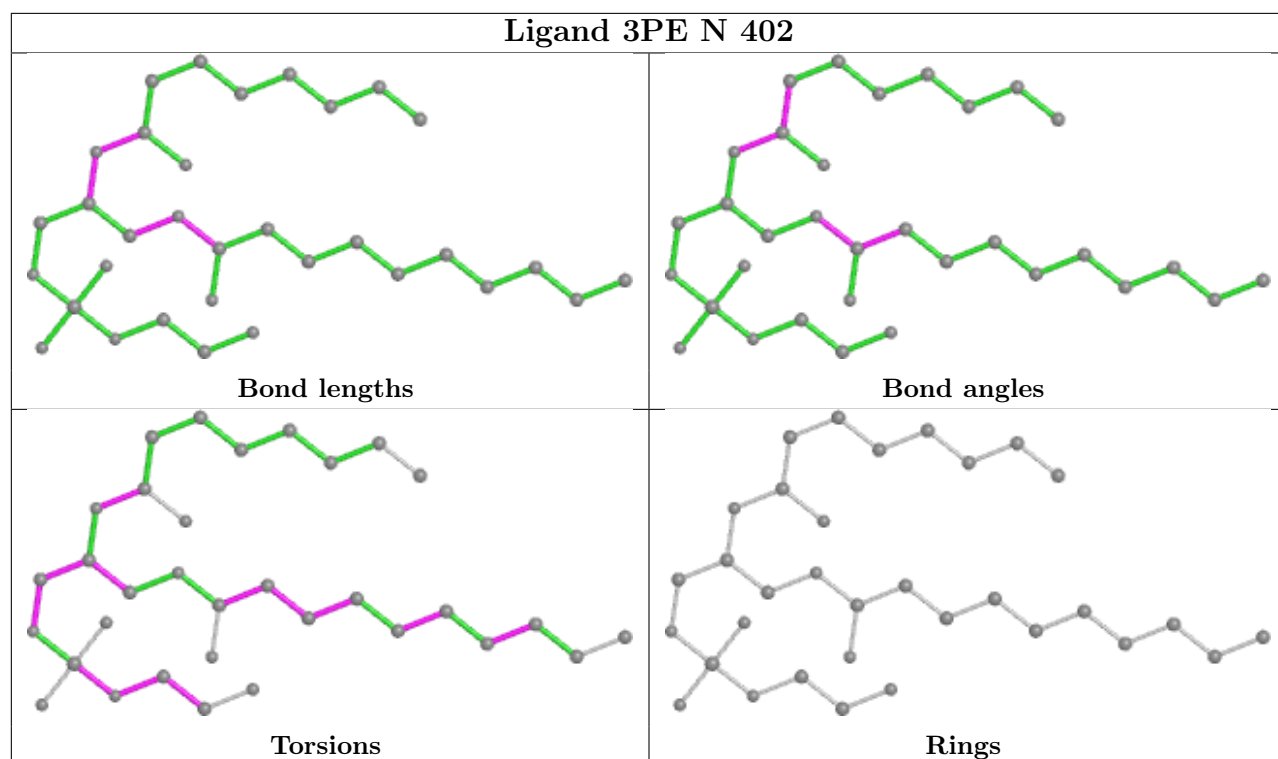
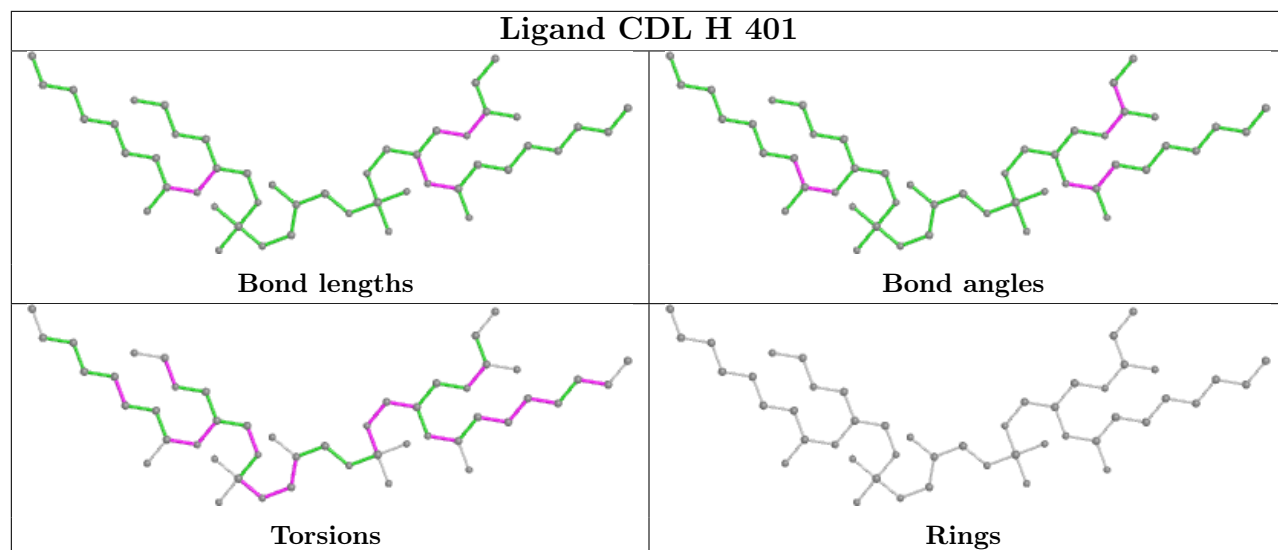


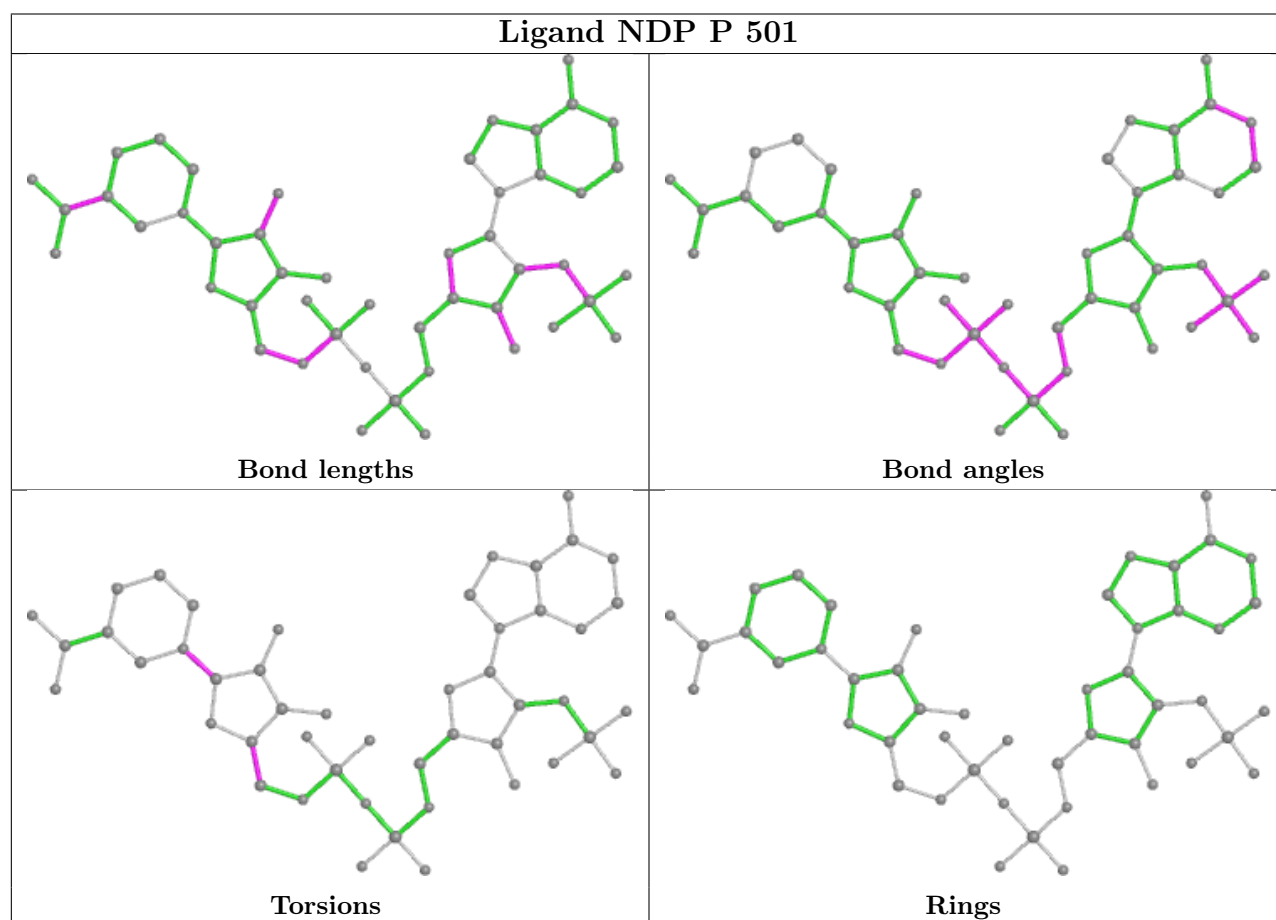
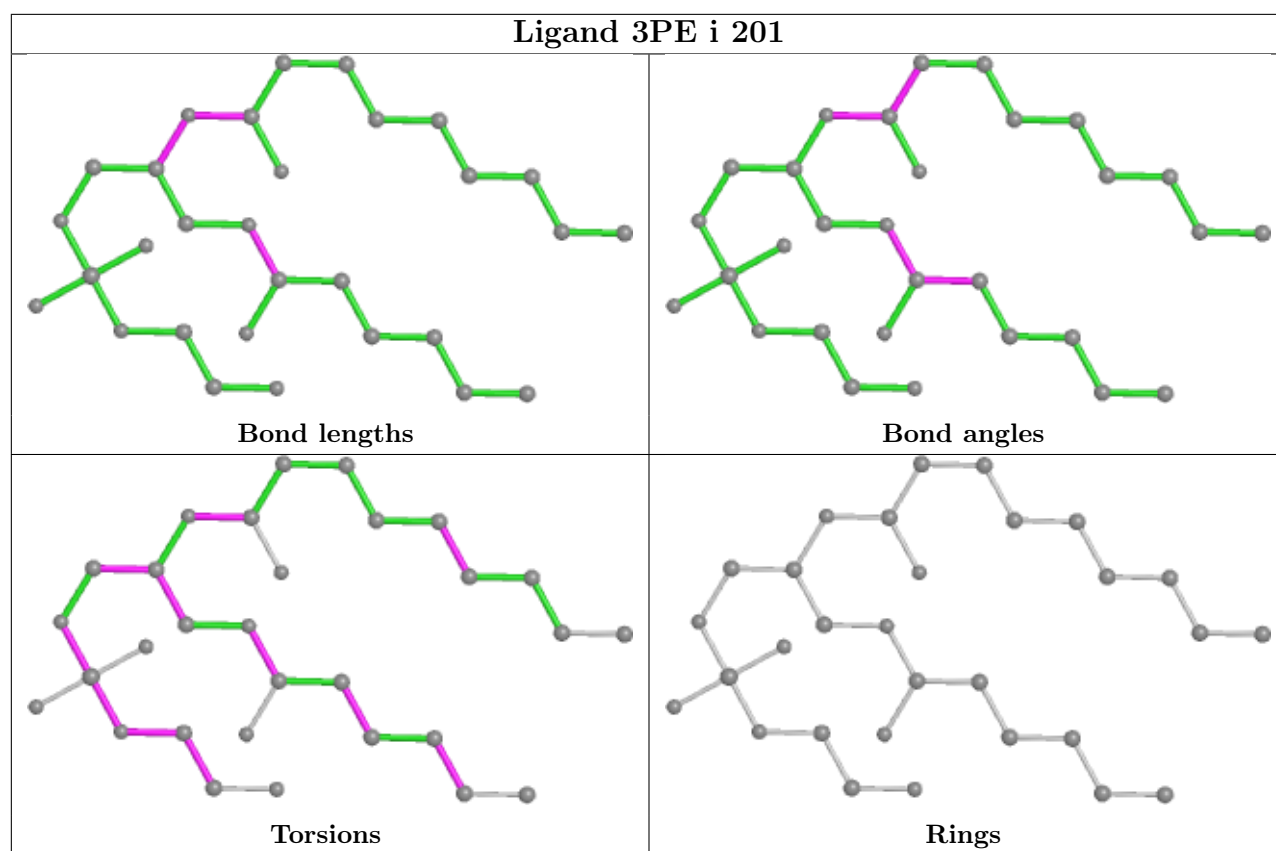


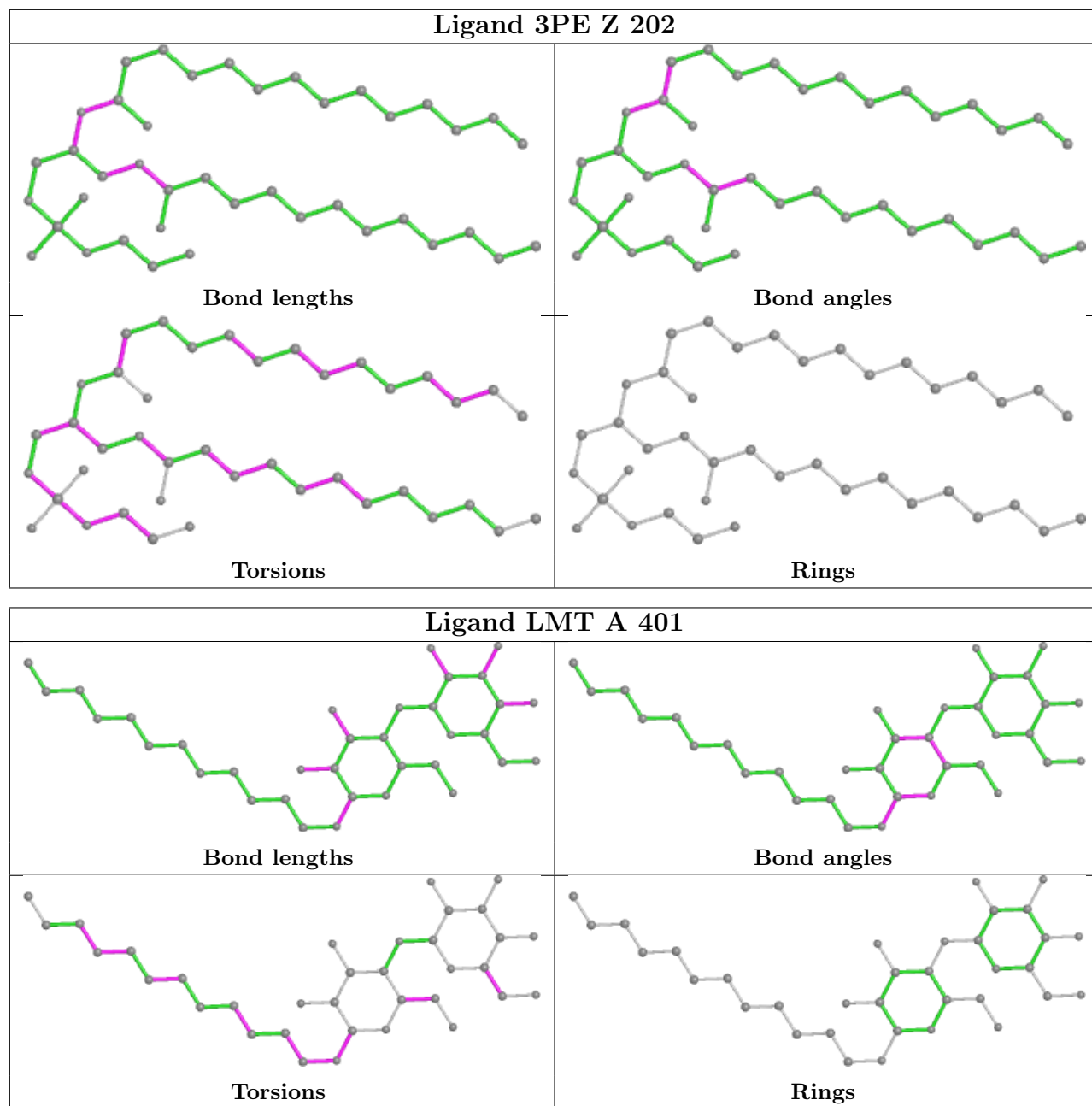


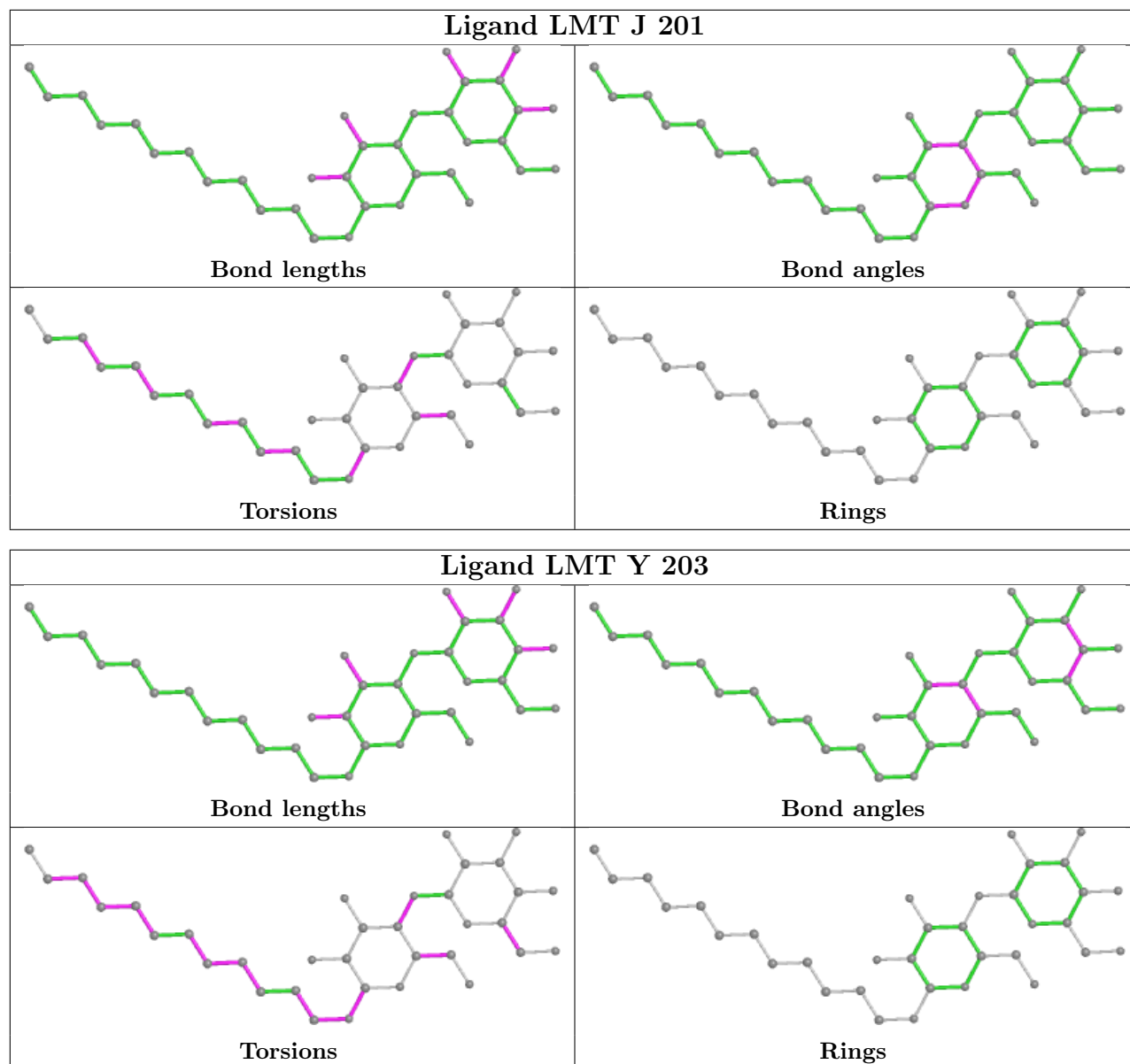


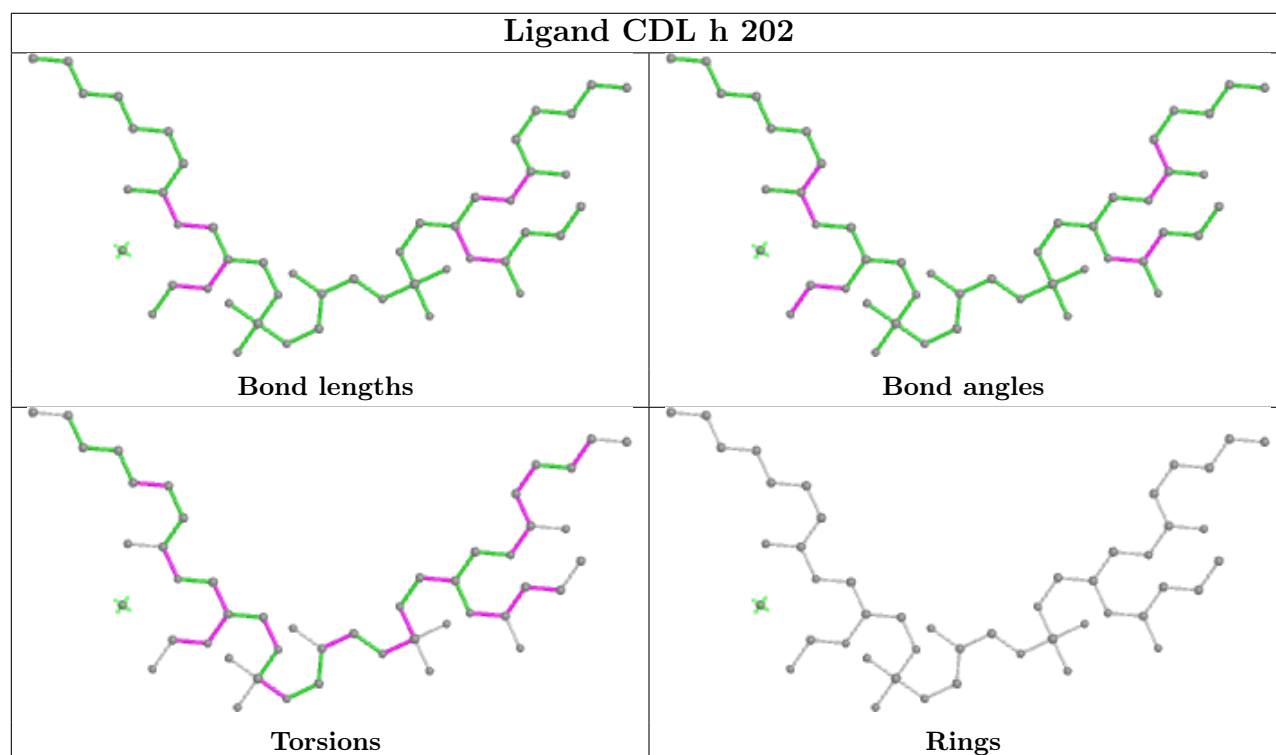
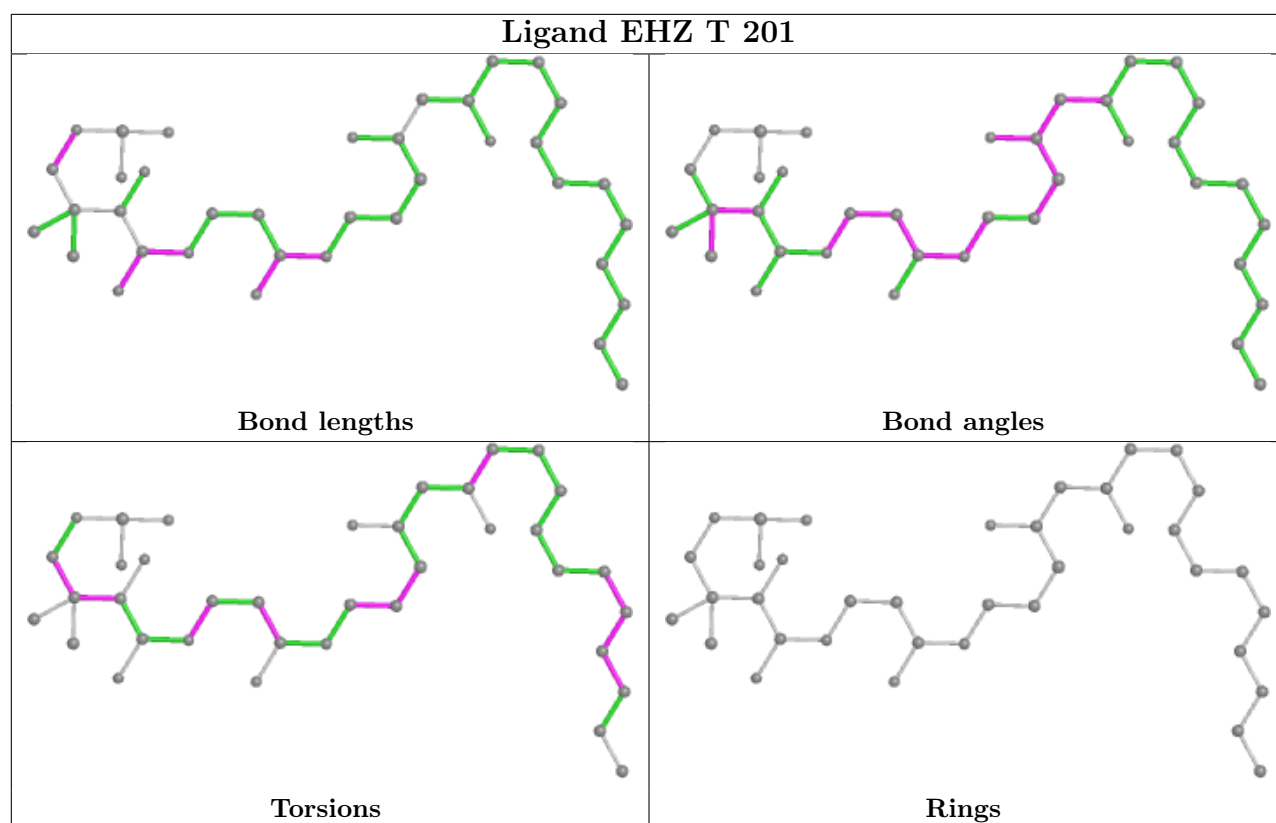




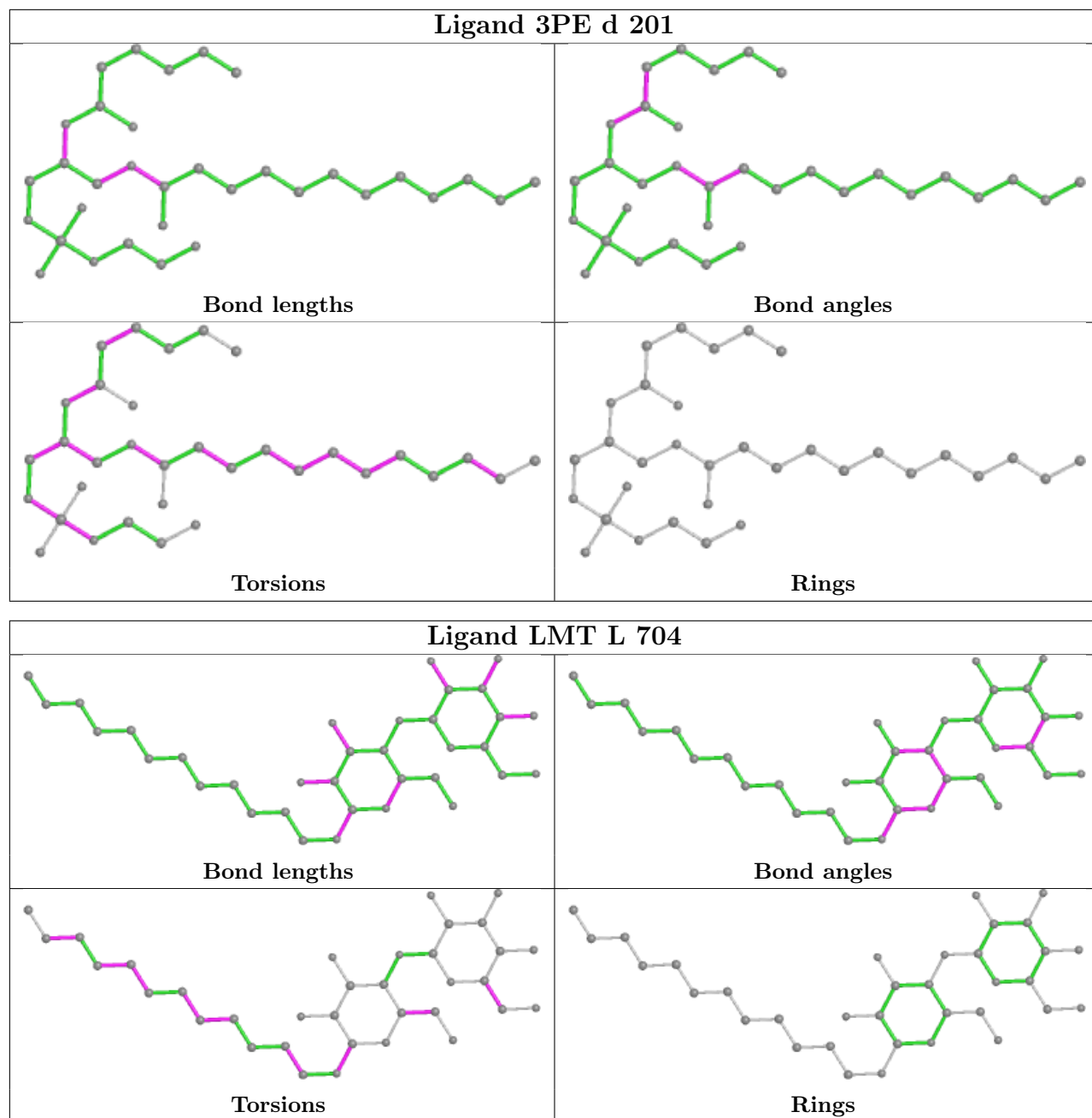


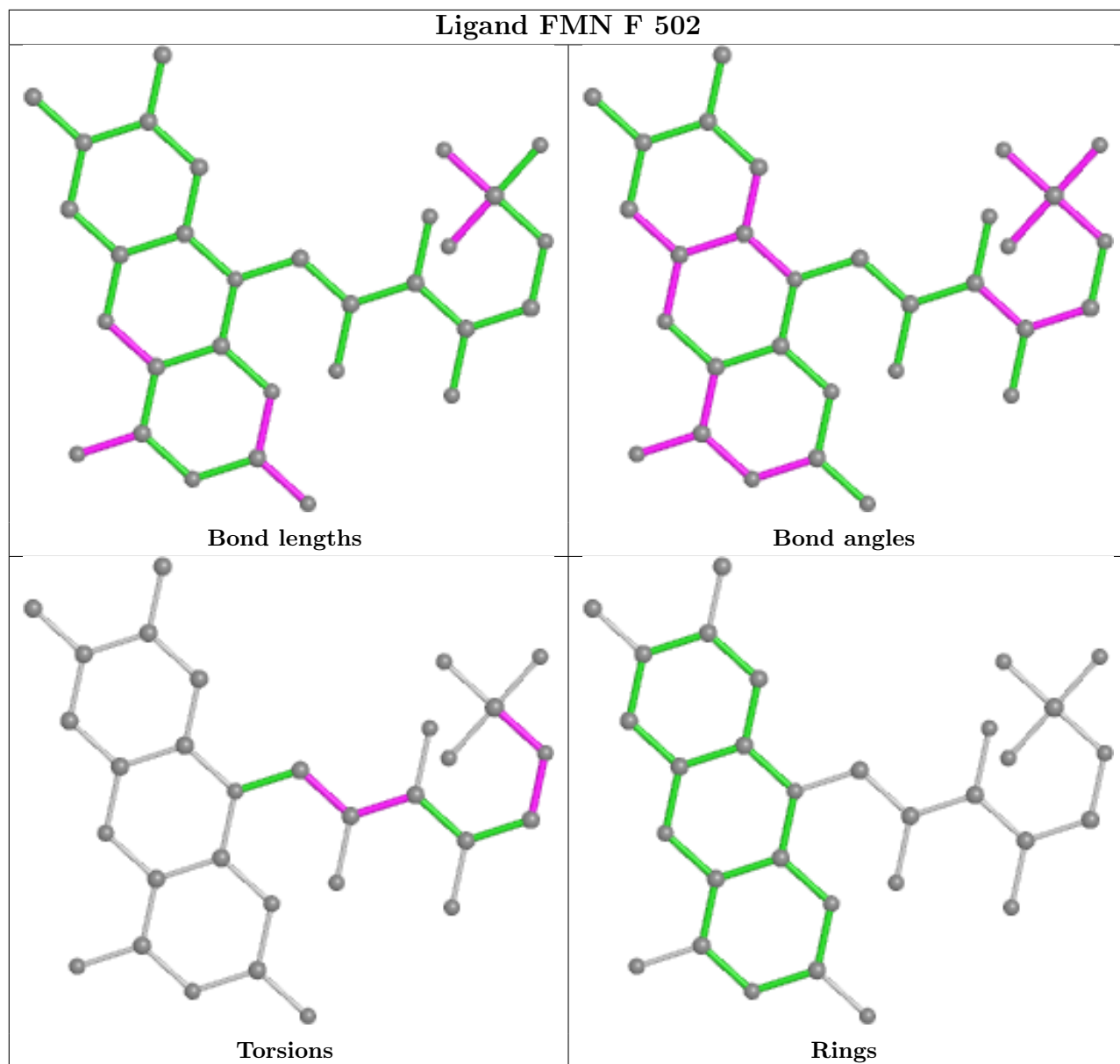


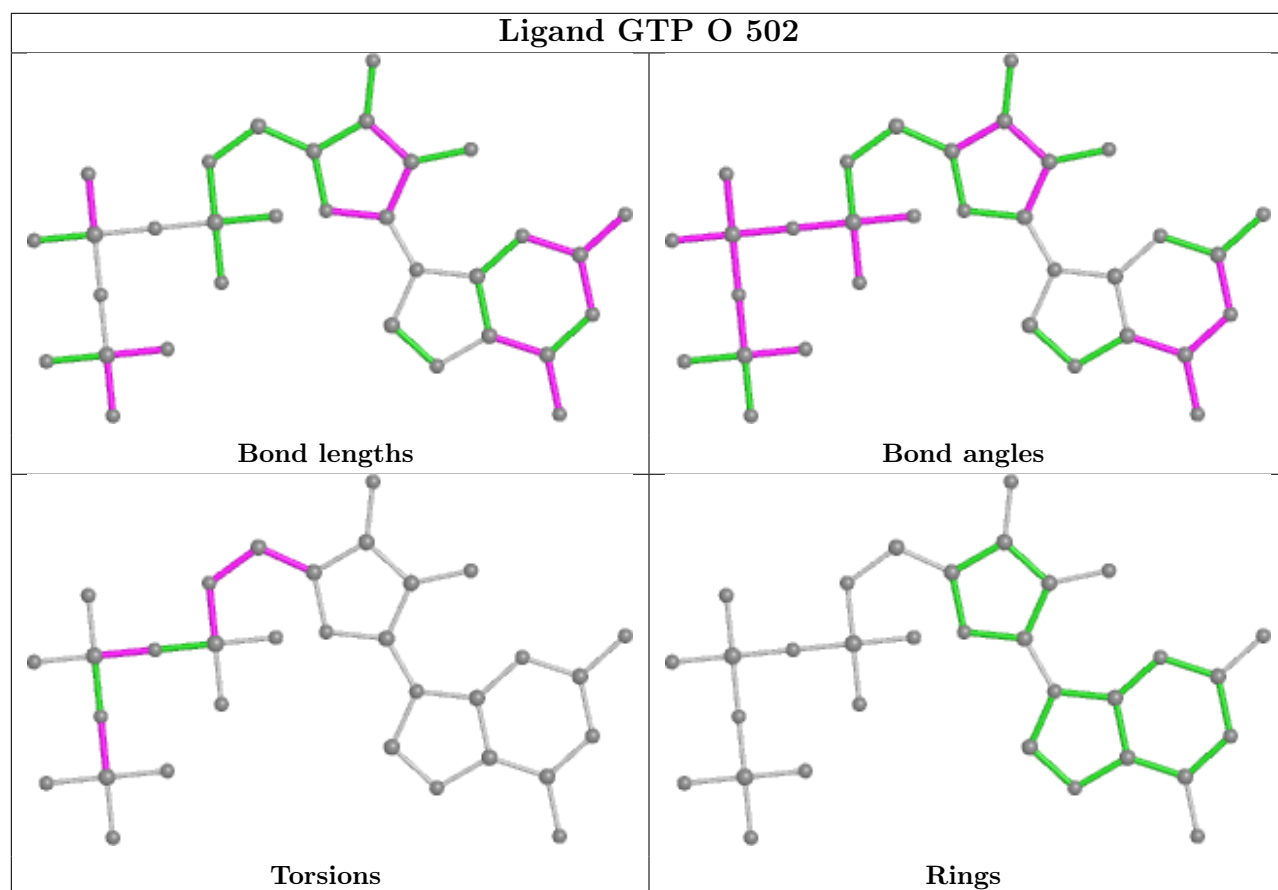
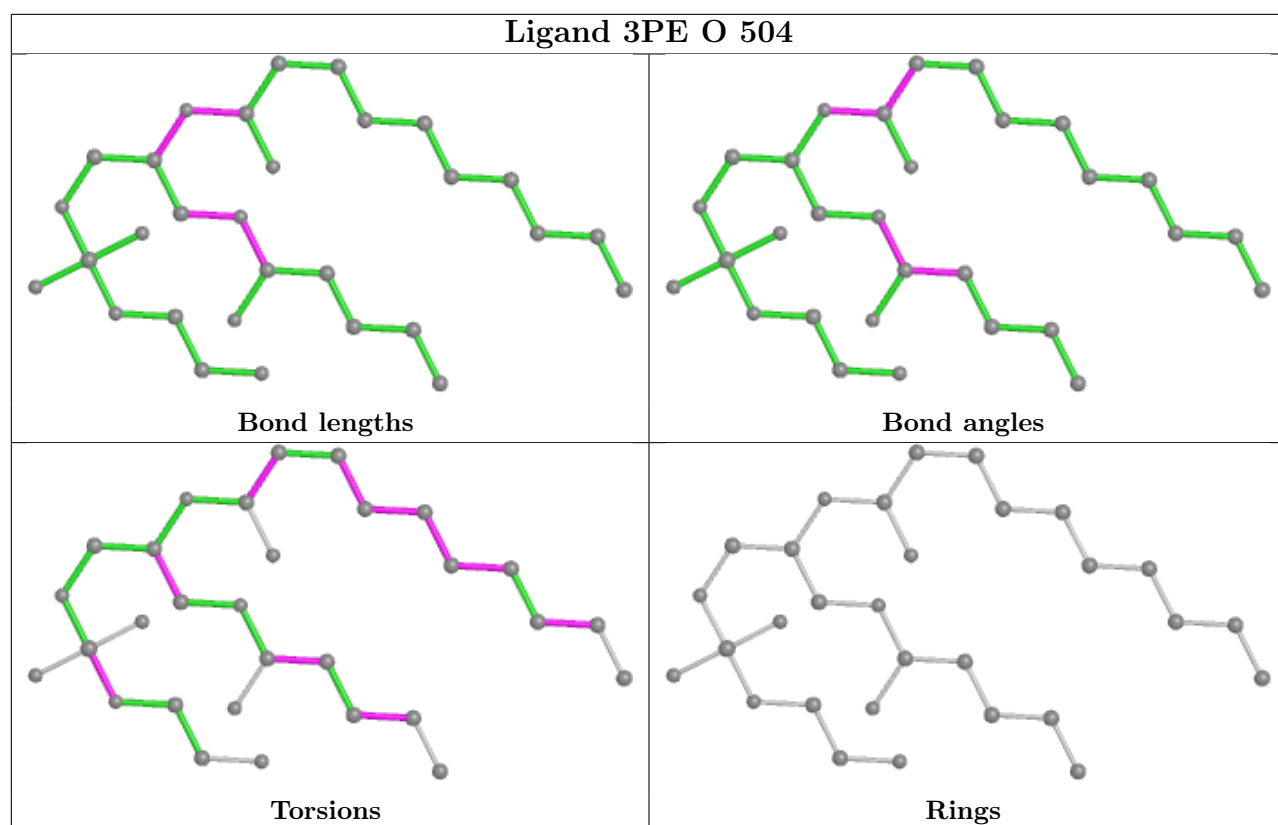


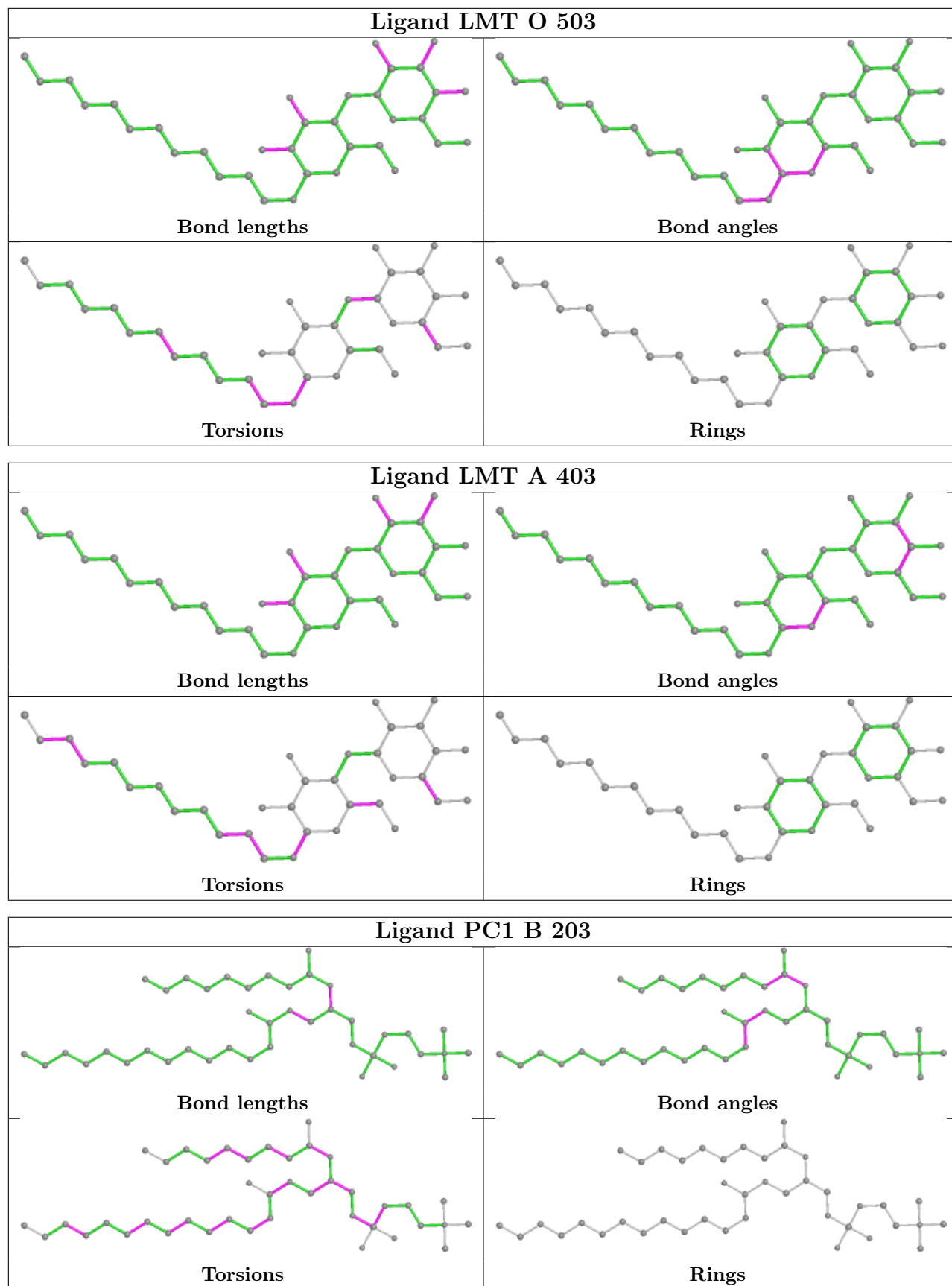


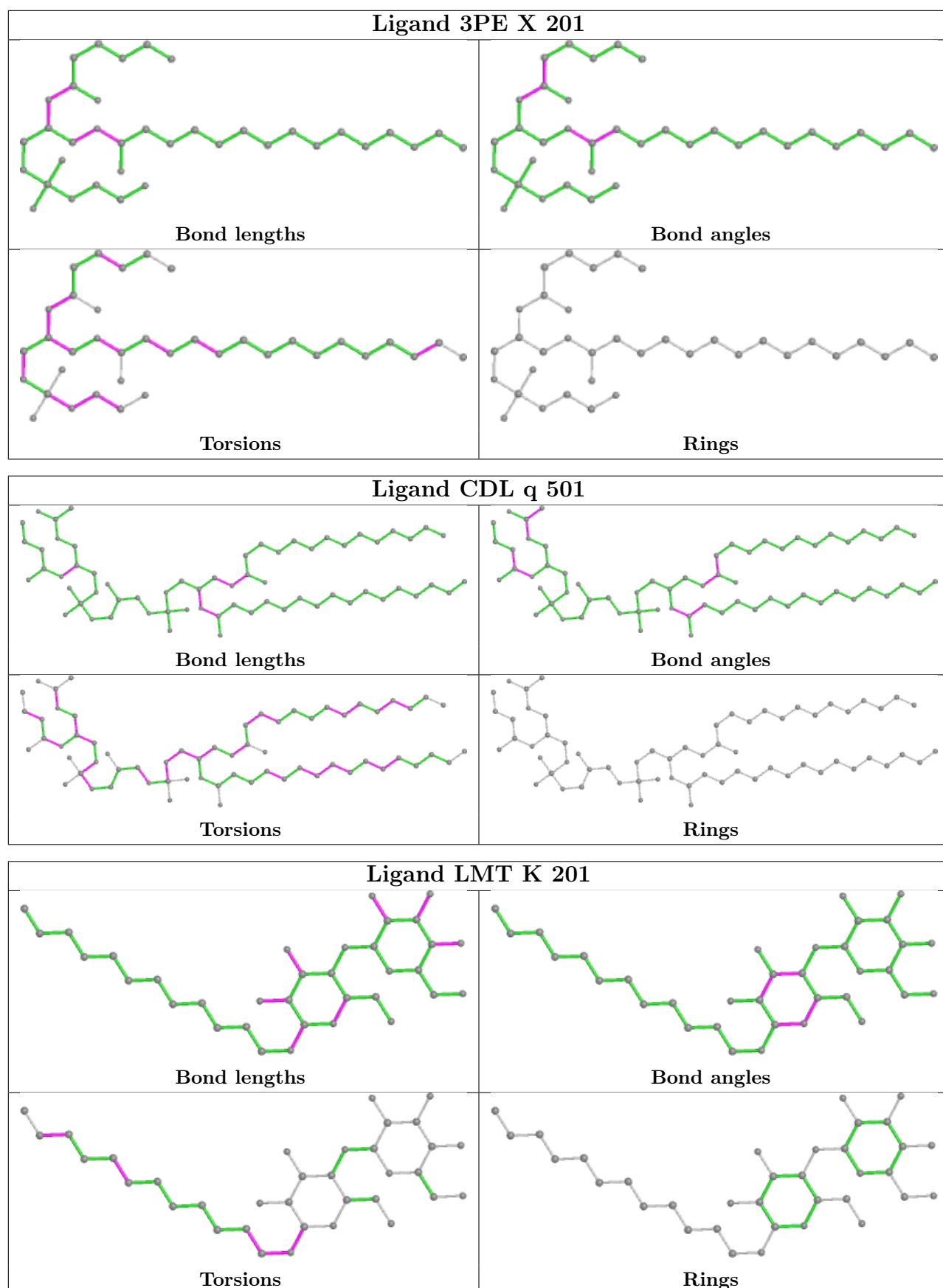


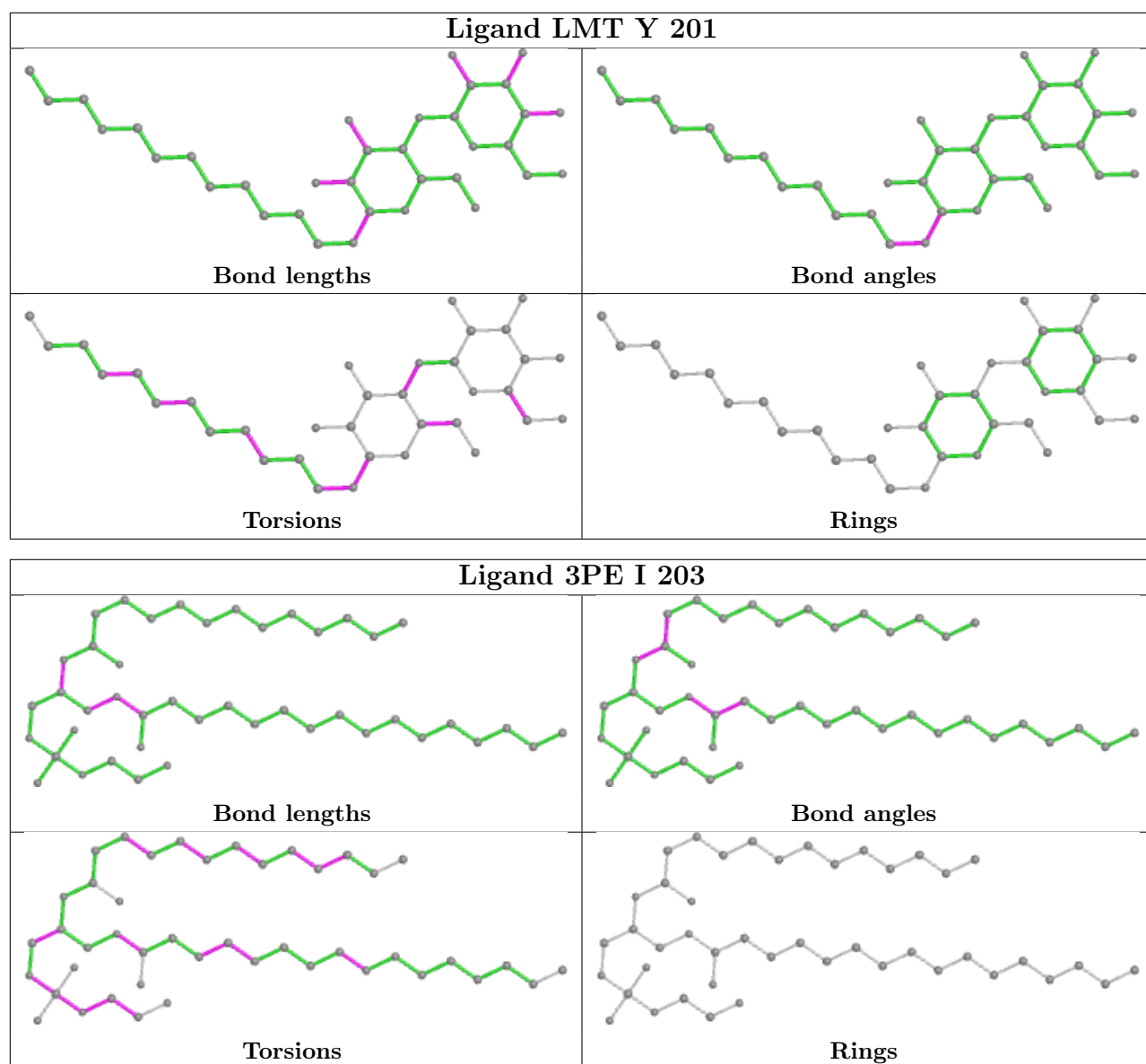


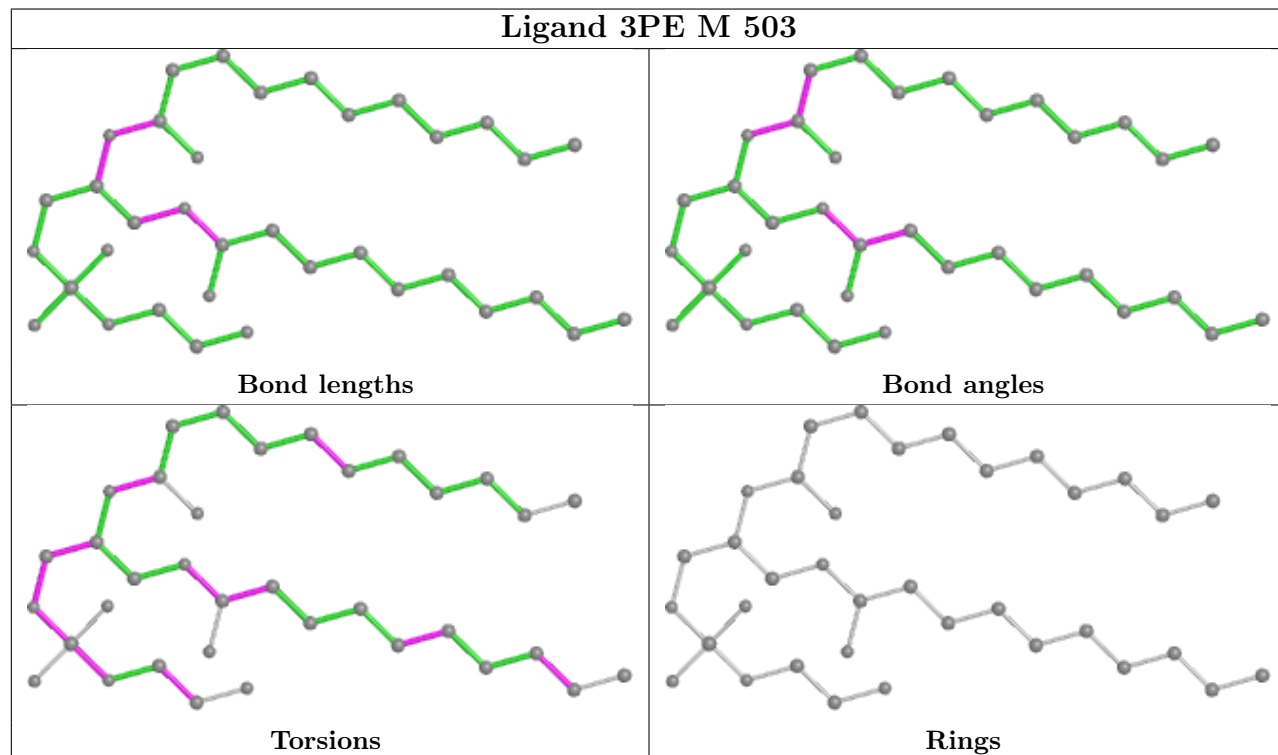
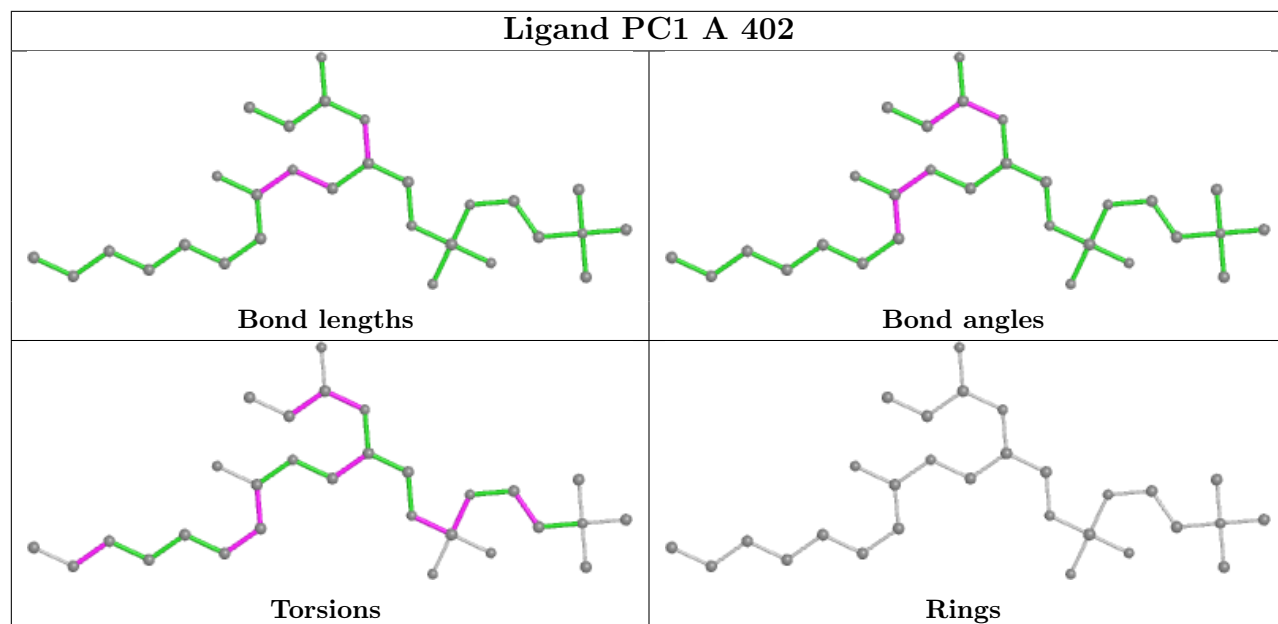


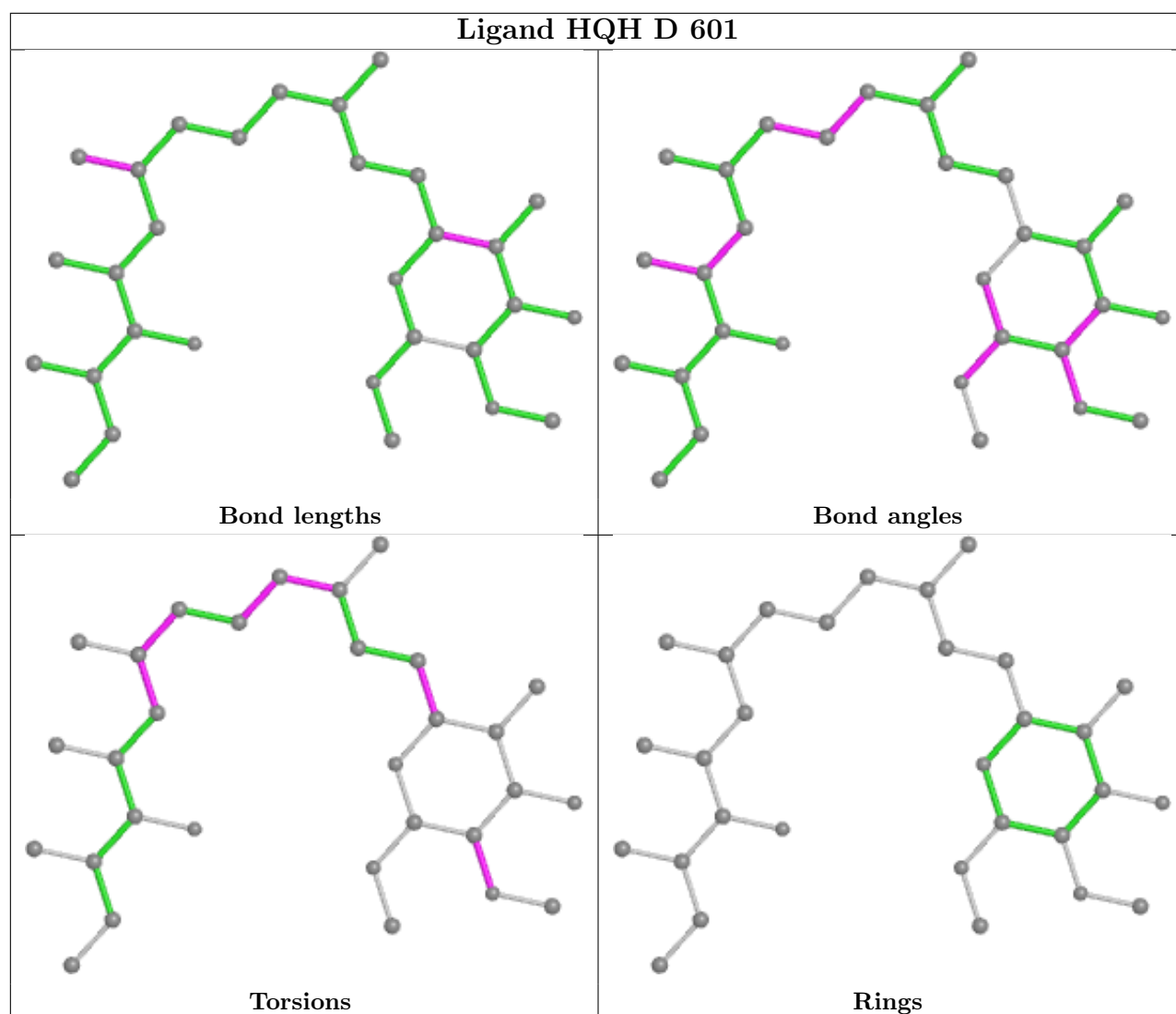












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



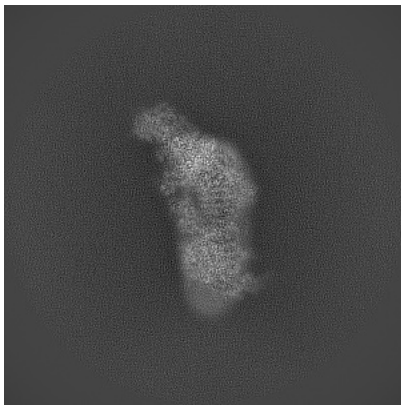
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16962. These allow visual inspection of the internal detail of the map and identification of artifacts.

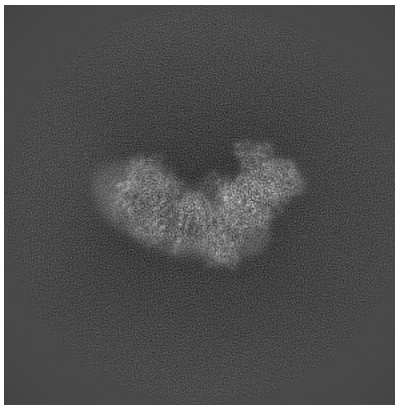
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

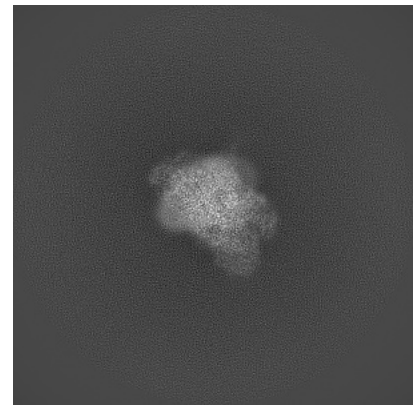
#### 6.1.1 Primary map



X

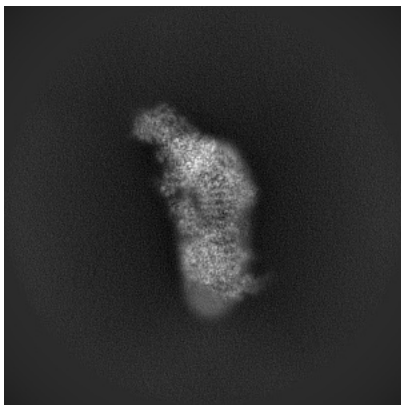


Y

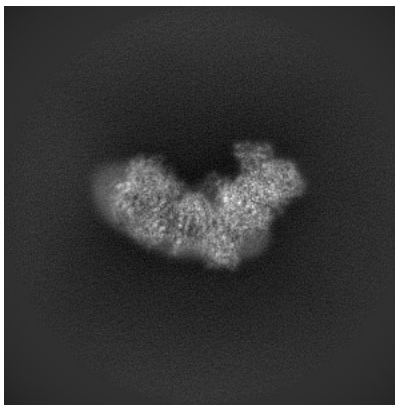


Z

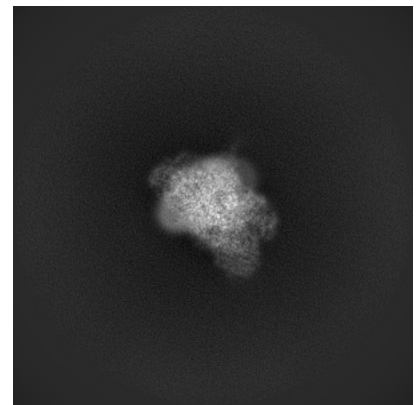
#### 6.1.2 Raw map



X



Y

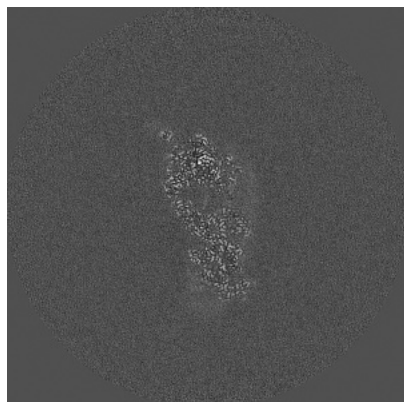


Z

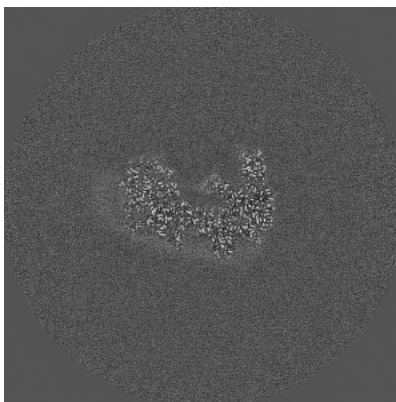
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

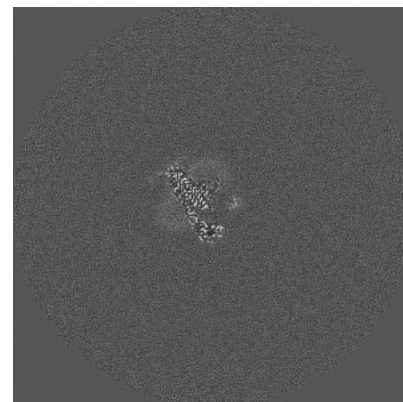
### 6.2.1 Primary map



X Index: 252

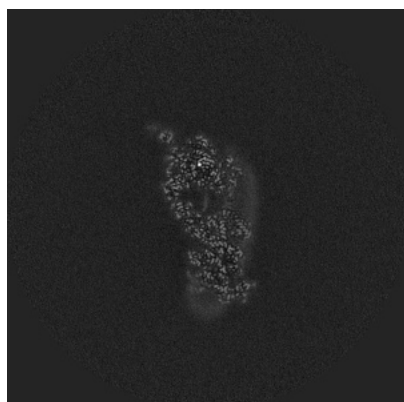


Y Index: 252

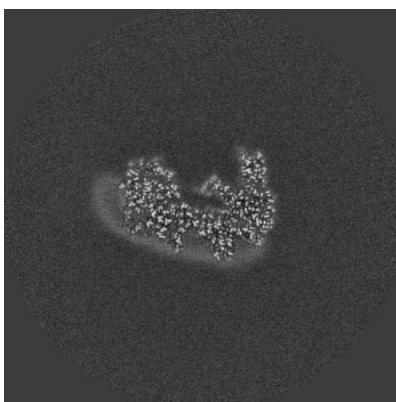


Z Index: 252

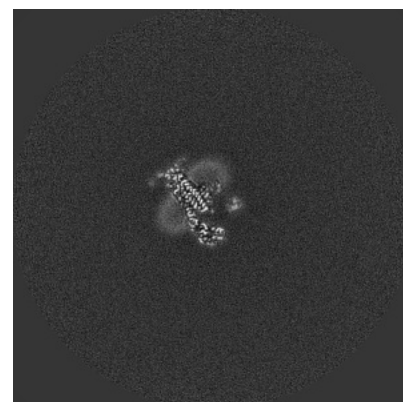
### 6.2.2 Raw map



X Index: 252



Y Index: 252

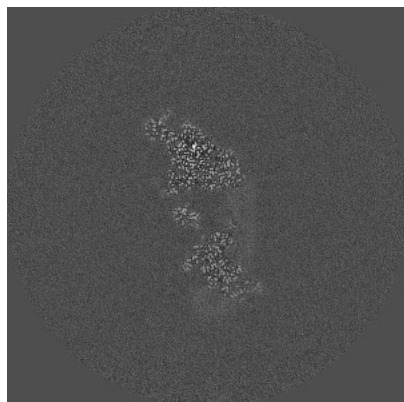


Z Index: 252

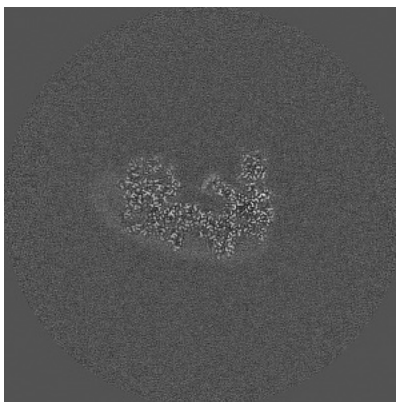
The images above show central slices of the map in three orthogonal directions.

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

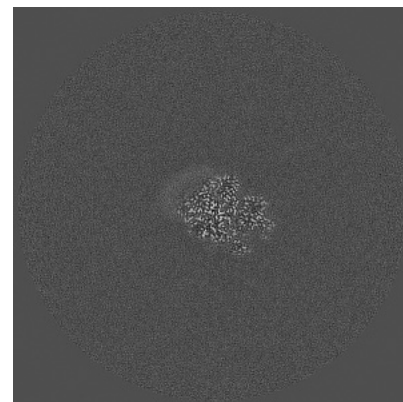
### 6.3.1 Primary map



X Index: 264



Y Index: 254

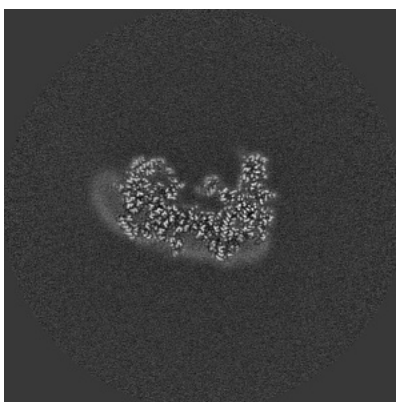


Z Index: 313

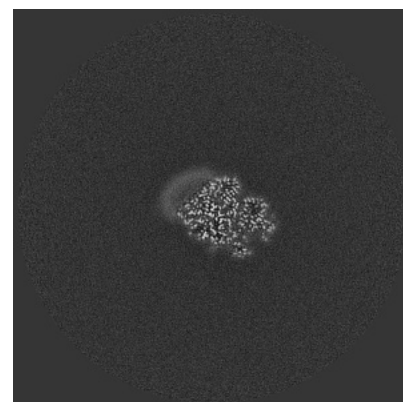
### 6.3.2 Raw map



X Index: 264



Y Index: 257

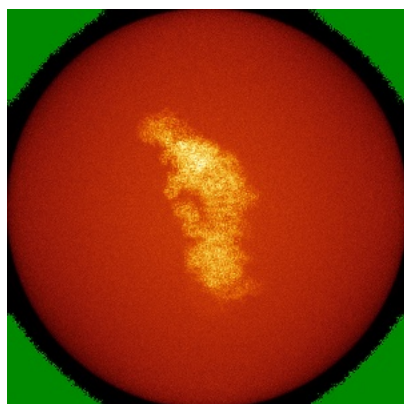


Z Index: 313

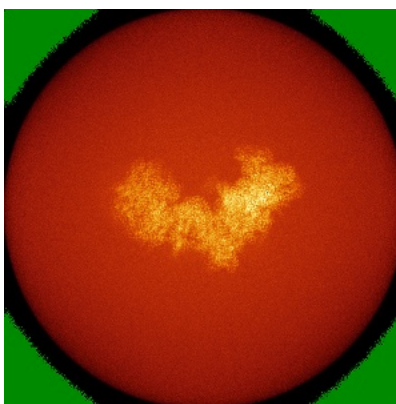
The images above show the largest variance slices of the map in three orthogonal directions.

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

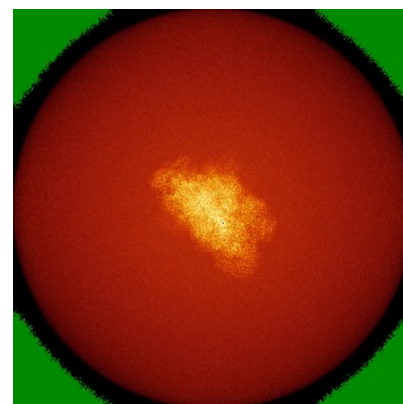
### 6.4.1 Primary map



X

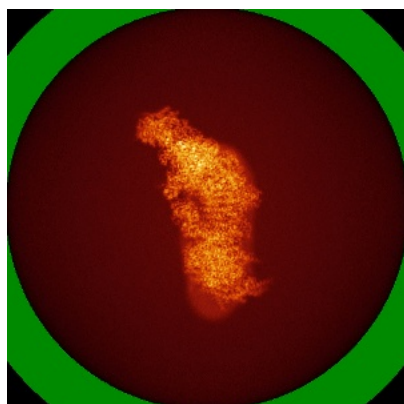


Y

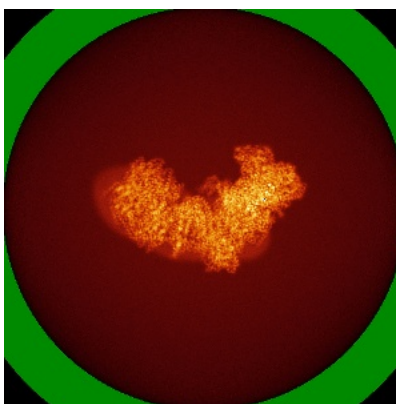


Z

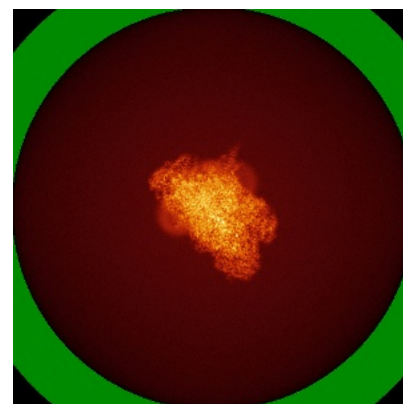
### 6.4.2 Raw map



X



Y

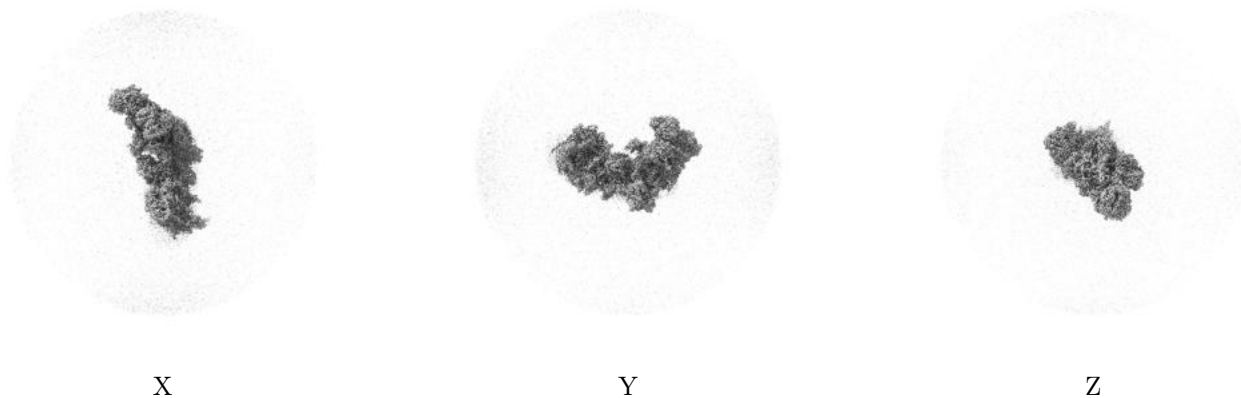


Z

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.

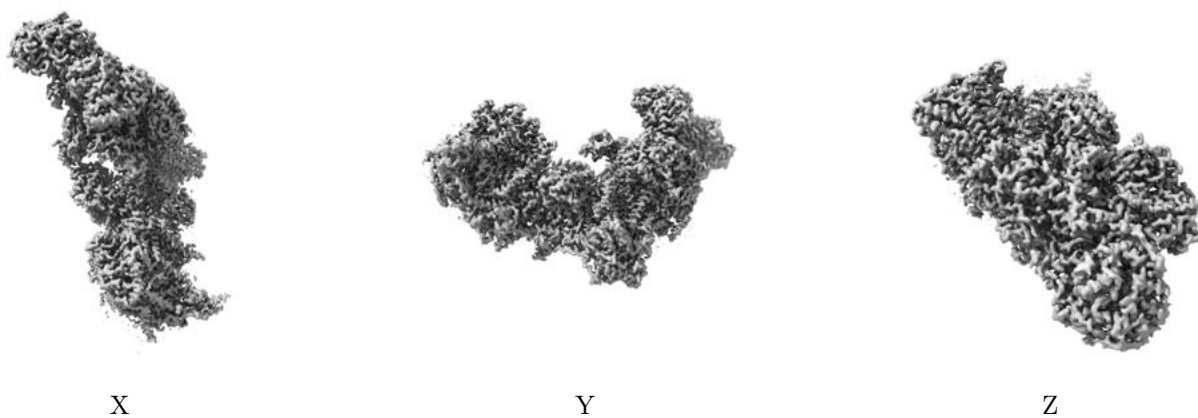
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

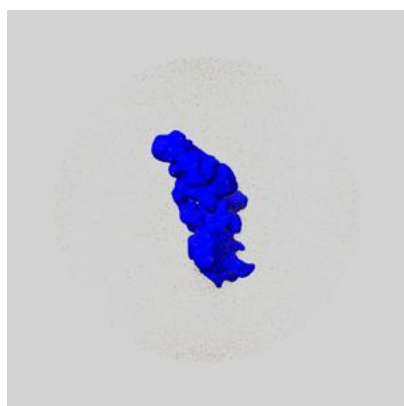
## 6.6 Mask visualisation [i](#)

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

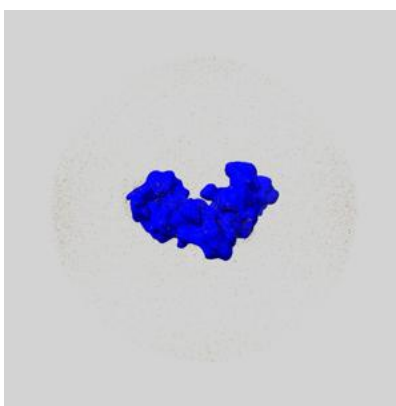
A mask typically either:

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

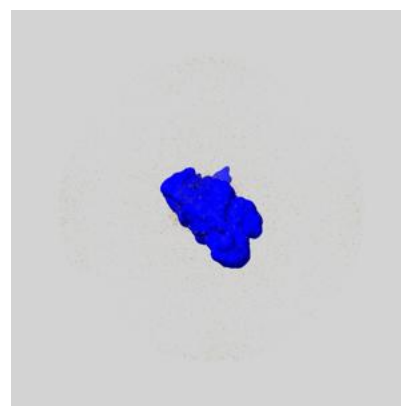
### 6.6.1 emd\_16962\_msk\_1.map [i](#)



X



Y

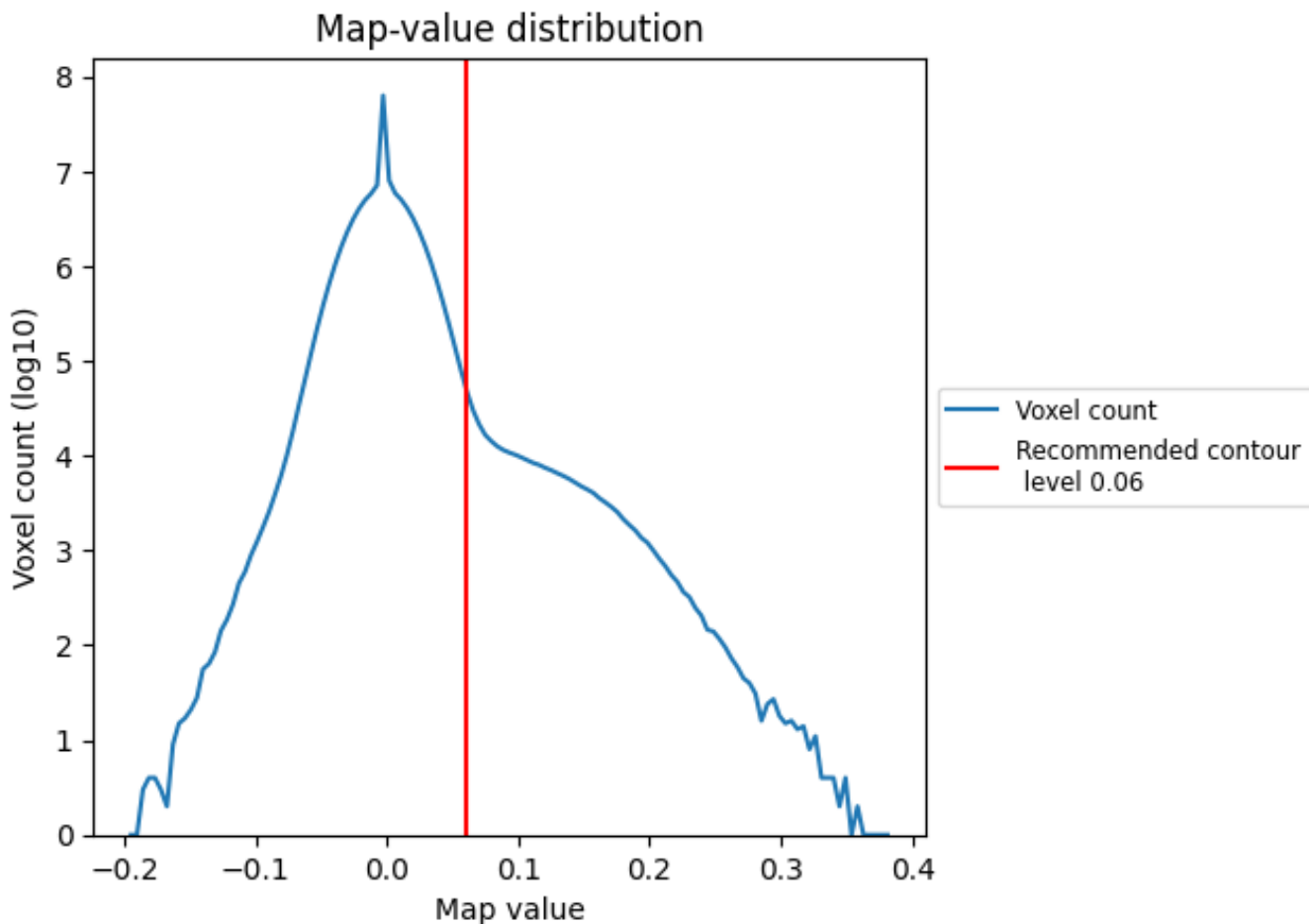


Z

## 7 Map analysis [i](#)

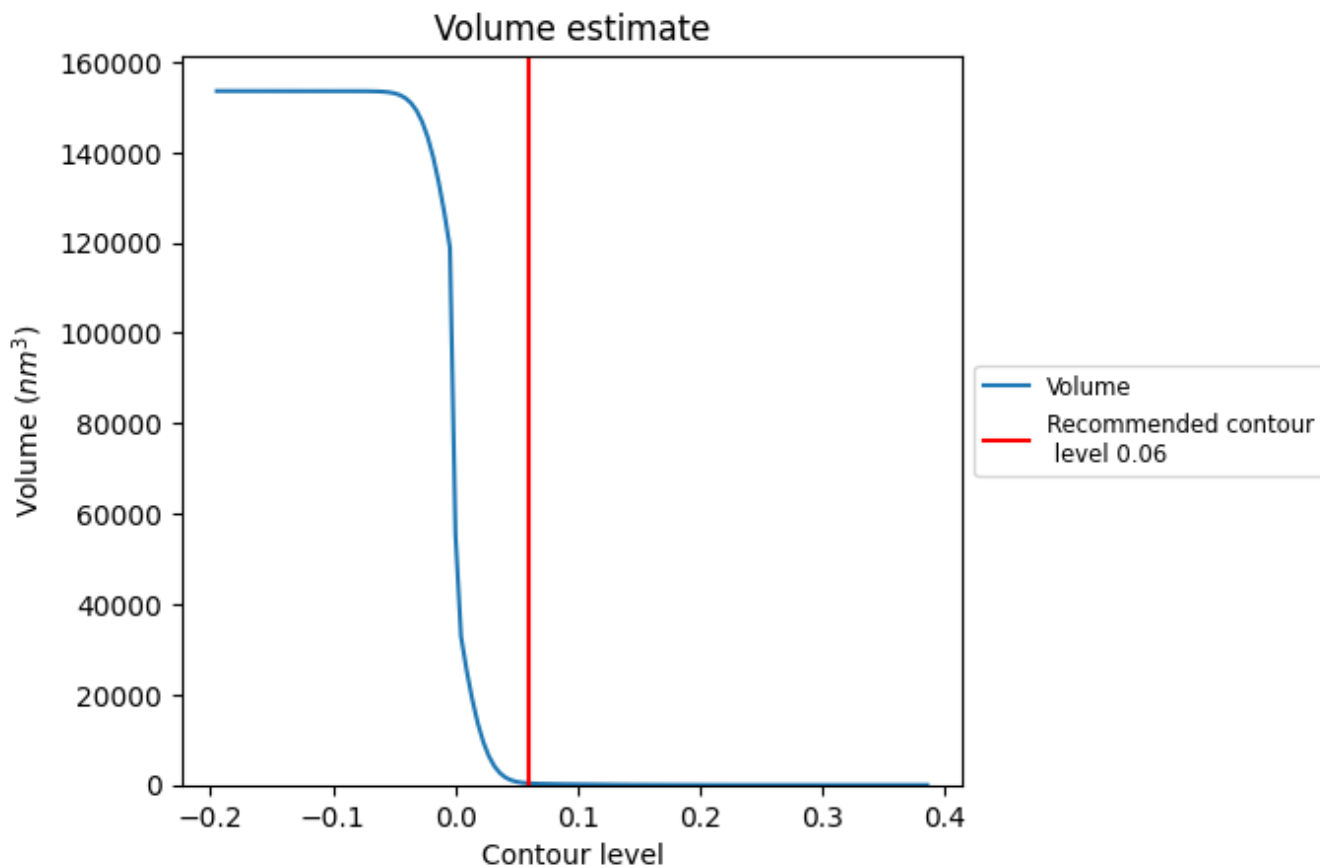
This section contains the results of statistical analysis of the map.

### 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](#)

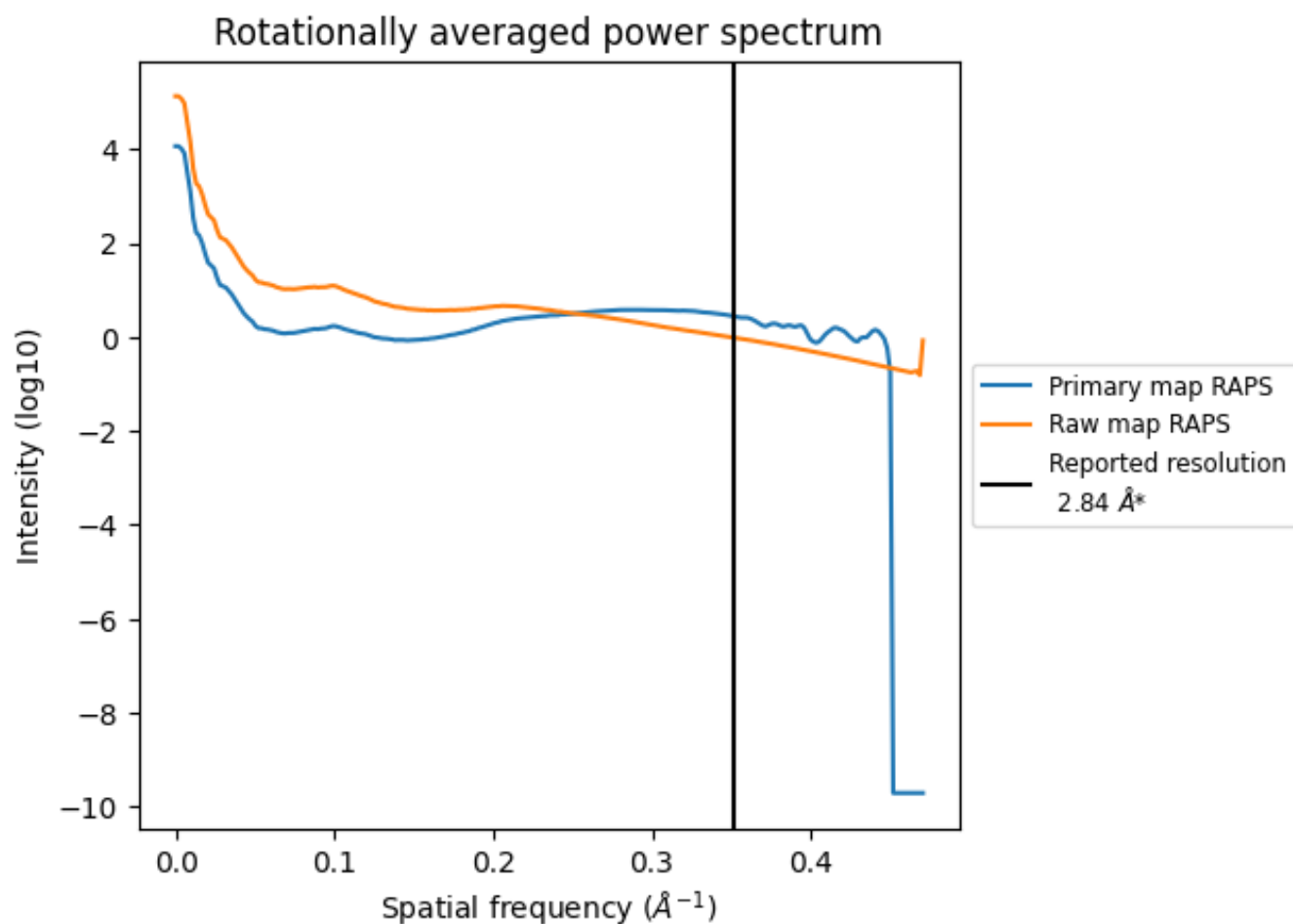


The volume at the recommended contour level is 366 nm<sup>3</sup>; this corresponds to an approximate mass of 331 kDa.

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

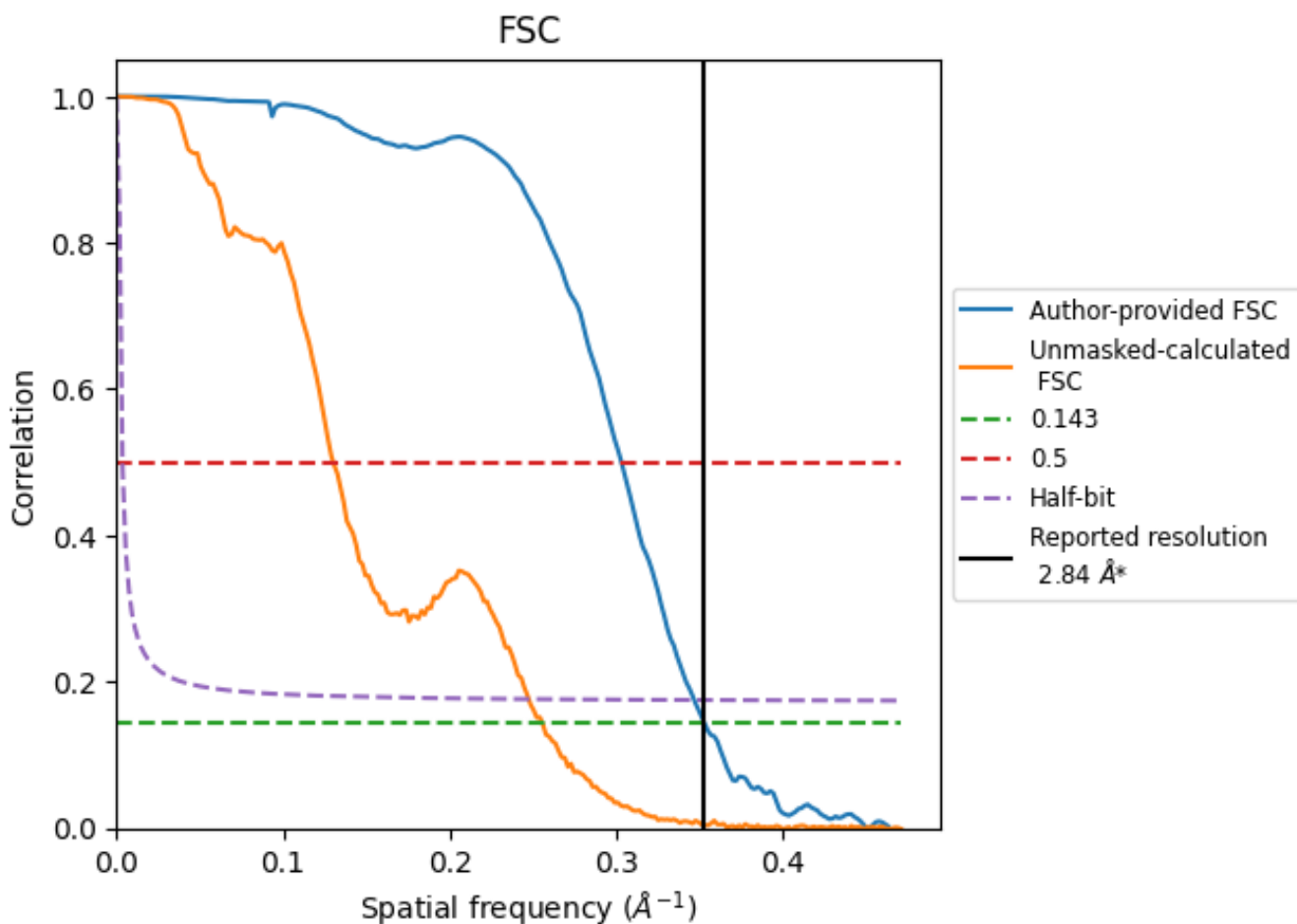


\*Reported resolution corresponds to spatial frequency of 0.352 Å<sup>-1</sup>

## 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 0.352 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

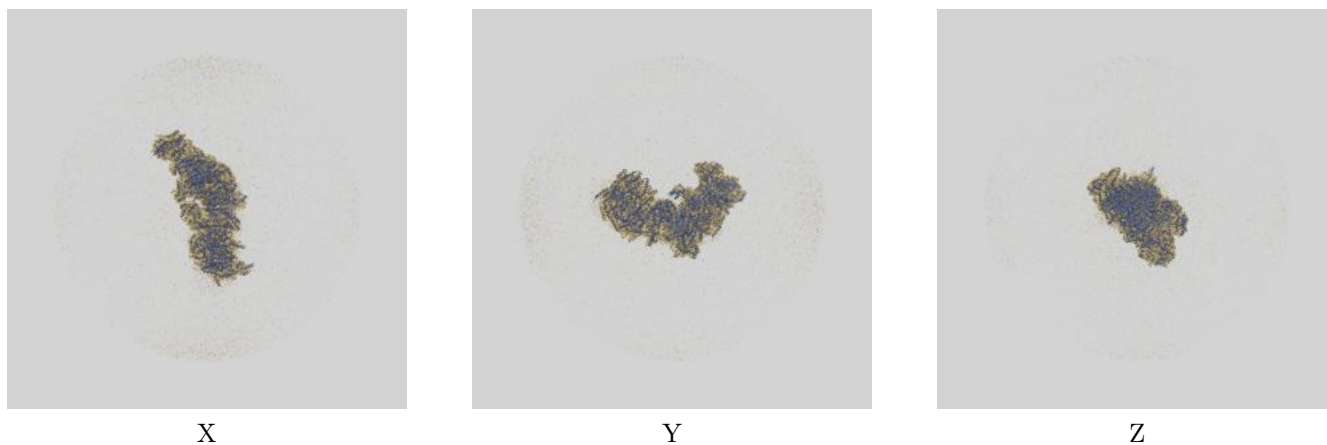
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.30	2.89
Unmasked-calculated*	3.91	7.69	4.04

\*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 3.91 differs from the reported value 2.84 by more than 10 %

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

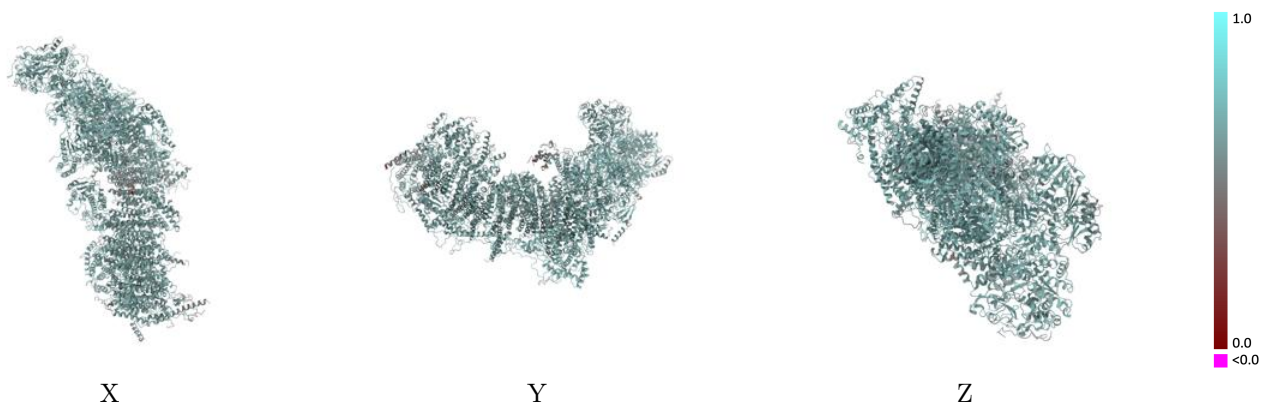
This section contains information regarding the fit between EMDB map EMD-16962 and PDB model 8OLT. Per-residue inclusion information can be found in section 3 on page 23.

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



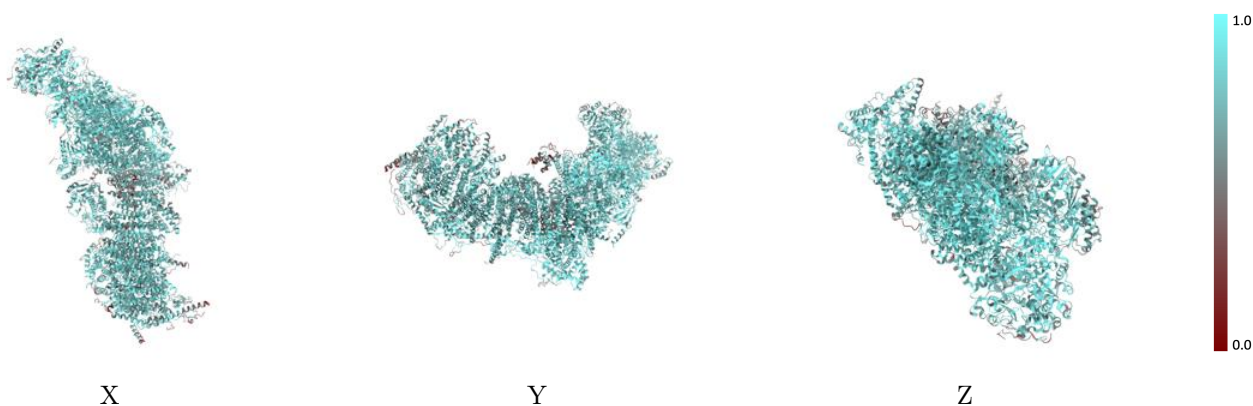
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



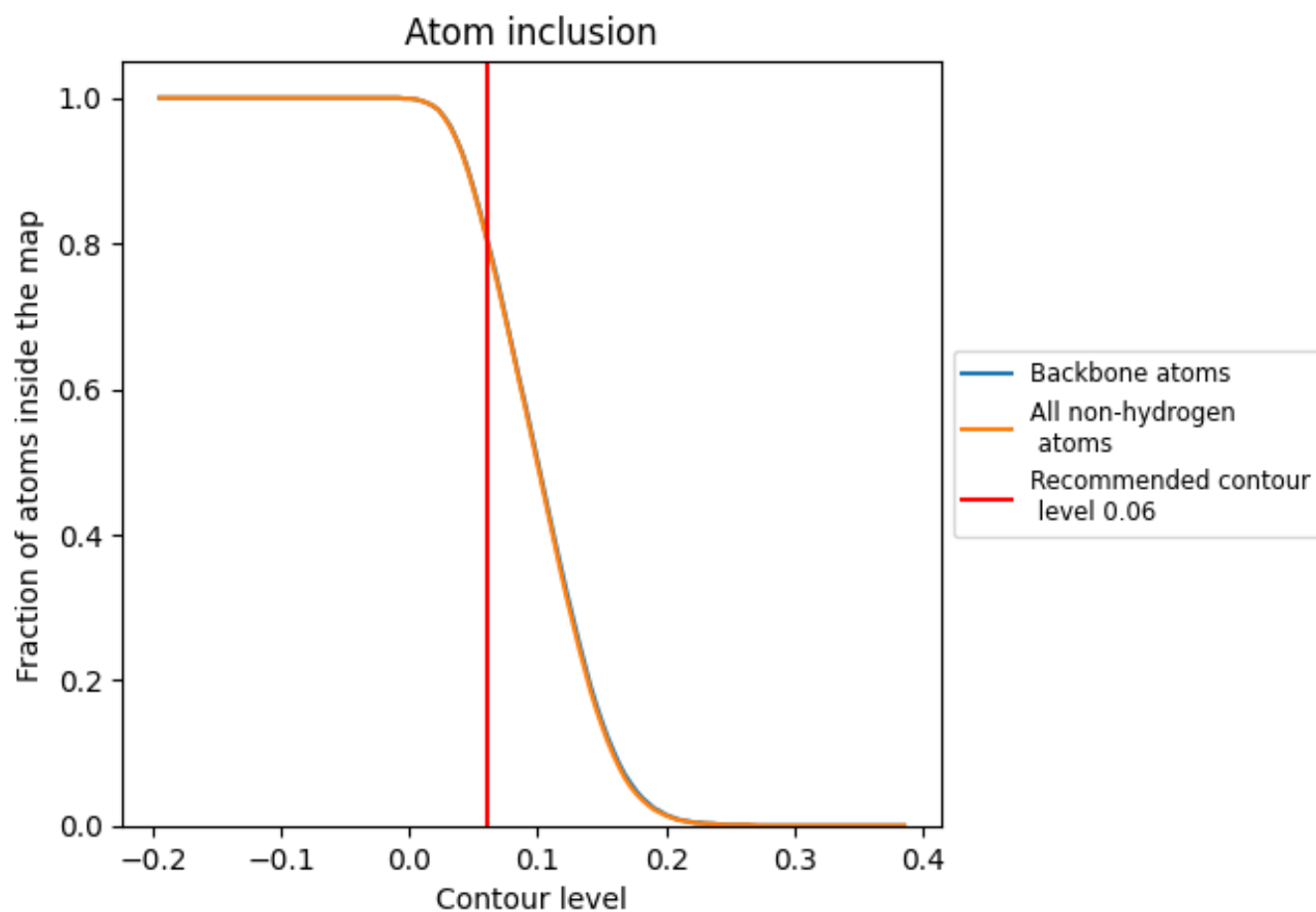
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.6280
A	 0.7870	 0.6350
B	 0.9050	 0.6610
C	 0.9000	 0.6610
D	 0.8880	 0.6560
E	 0.7650	 0.6010
F	 0.8080	 0.6180
G	 0.8310	 0.6320
H	 0.8680	 0.6510
I	 0.8960	 0.6550
J	 0.7490	 0.6110
K	 0.8410	 0.6450
L	 0.8020	 0.6270
M	 0.8610	 0.6470
N	 0.8660	 0.6520
O	 0.8270	 0.6390
P	 0.8480	 0.6380
Q	 0.8560	 0.6450
R	 0.8460	 0.6370
S	 0.7190	 0.5950
T	 0.4240	 0.4780
U	 0.7080	 0.6040
V	 0.8160	 0.6390
W	 0.8190	 0.6290
X	 0.8150	 0.6280
Y	 0.6600	 0.5890
Z	 0.8270	 0.6370
a	 0.8790	 0.6460
b	 0.7520	 0.6120
c	 0.6980	 0.5950
d	 0.8170	 0.6300
e	 0.8260	 0.6310
f	 0.7140	 0.5950
g	 0.8060	 0.6230
h	 0.7960	 0.6290



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Chain	Atom inclusion	Q-score
i	 0.6630	 0.5830
j	 0.6320	 0.5570
k	 0.6220	 0.5620
l	 0.7790	 0.6140
m	 0.7690	 0.6120
n	 0.7680	 0.6090
o	 0.6330	 0.5550
p	 0.7710	 0.6090
q	 0.8410	 0.6370
r	 0.8130	 0.6310
s	 0.7440	 0.5980