



wwPDB EM Validation Summary Report ⓘ

Aug 8, 2023 – 05:09 pm BST

PDB ID : 8OM1
EMDB ID : EMD-16965
Title : Mitochondrial complex I from *Mus musculus* in the active state
Authors : Grba, D.N.; Chung, I.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.
Deposited on : 2023-03-31
Resolution : 2.39 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

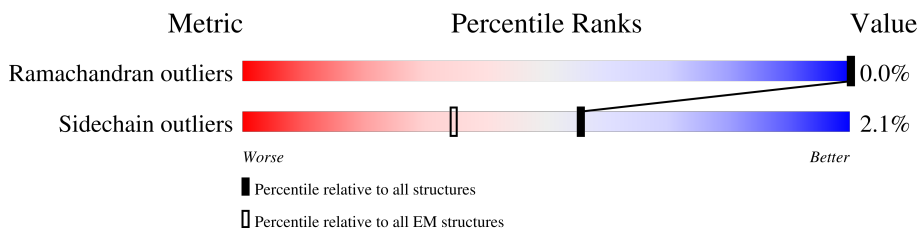
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.39 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 ≥ 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	98% .
2	B	224	66% . 30%
3	C	263	79% 21%
4	D	463	92% 7%
5	E	248	85% . 14%
6	F	464	91% . 7%
7	G	727	93% . 5%
8	H	318	97% .
9	I	212	83% . 16%





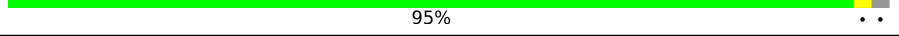
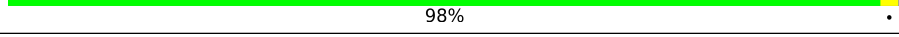

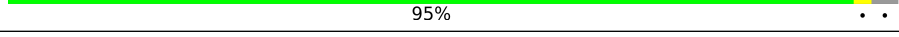
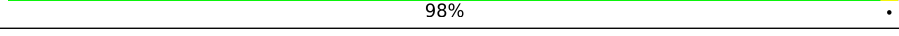

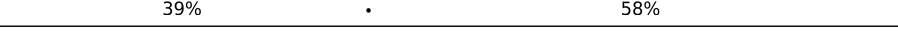
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Mol	Chain	Length	Quality of chain
10	J	172	99%
11	K	98	95% 5%
12	L	607	98%
13	M	459	97%
14	N	345	98%
15	O	355	89% 10%
16	P	377	89% 9%
17	Q	175	71% 28%
18	R	116	82% 18%
19	S	99	82% 5% 13%
20	T	156	45% 5% 50%
20	U	156	55% 44%
21	V	116	98%
22	W	131	85% 13%
23	X	172	97%
24	Y	142	97%
25	Z	144	95%
26	a	70	97%
27	b	84	99%
28	c	76	64% 36%
29	d	120	99%
30	e	106	97%
31	f	57	96%
32	g	151	64% 33%
33	h	189	74% 26%

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Mol	Chain	Length	Quality of chain
34	i	127	 80% 18%
35	j	105	 62% 37%
36	k	104	 73% 25%
37	l	186	 83% 16%
38	m	129	 95%
39	n	179	 98%
40	o	136	 85% 12%
41	p	176	 95%
42	q	145	 98%
43	r	112	 88% 10%
44	s	104	 39% 58%

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 71256 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	157	1259	802	227	216	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	689	5301	3324	920	1016	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	607	4809	3187	747	830	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	126	1021	646	179	192	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	86	685	430	130	122	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	88	706	453	104	144	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	114	927	604	154	166	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	49	407	266	70	70	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	56	482	314	85	81	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	101	850	549	136	161	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	139	1166	764	195	204	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	66	566	372	94	99	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	157	1323	855	220	237	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	178	1541	985	276	269	11	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	119	1019	642	191	178	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	145	1212	779	215	213	5	0	0

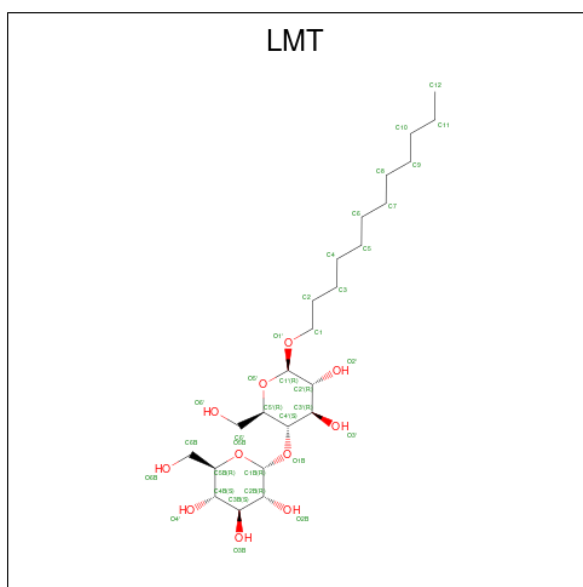
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	101	809	511	150	145	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	44	368	230	66	72	0	0

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



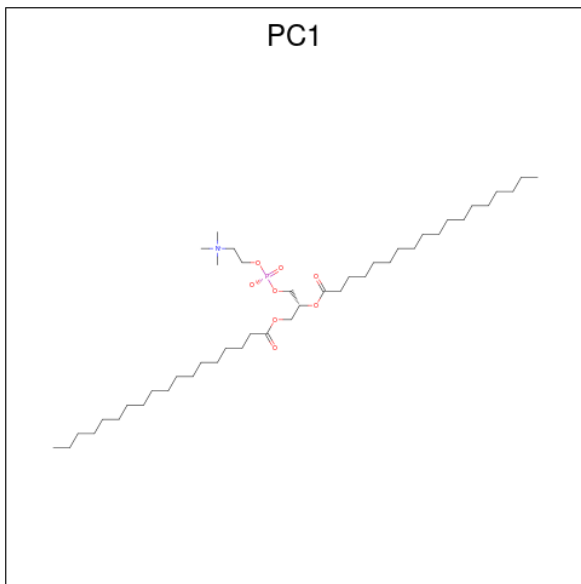
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	H	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	N	1	Total	C	O	0
			35	24	11	
45	N	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	34	24	1	8	1	0
46	B	1	43	33	1	8	1	0
46	B	1	52	42	1	8	1	0
46	L	1	27	17	1	8	1	0
46	p	1	36	26	1	8	1	0

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



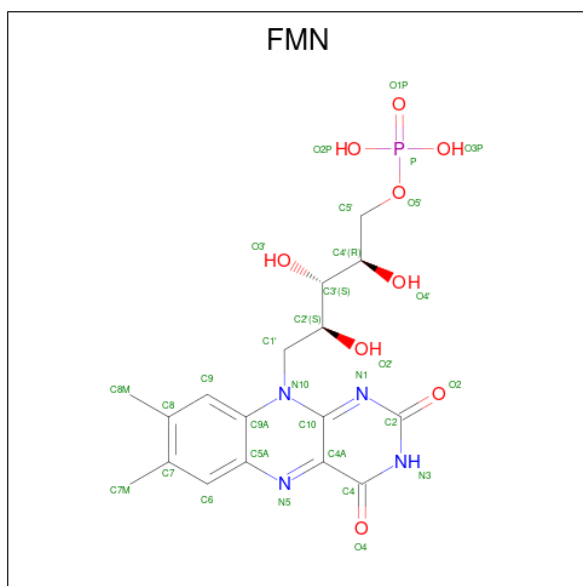
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	8	4	4	0
47	F	1	8	4	4	0
47	G	1	8	4	4	0
47	G	1	8	4	4	0
47	I	1	8	4	4	0
47	I	1	8	4	4	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

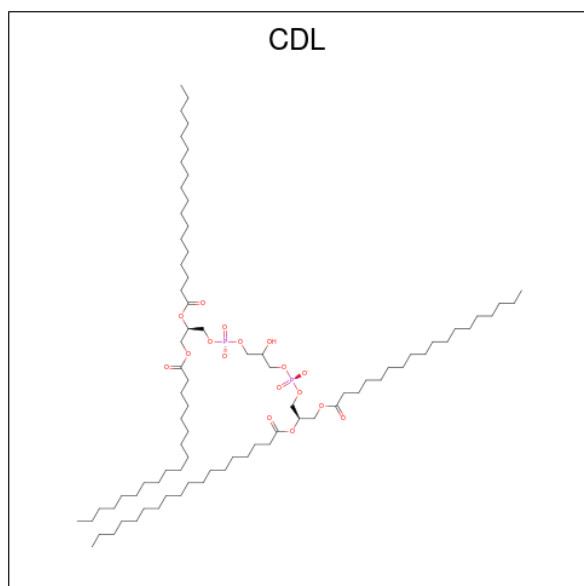


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is SODIUM ION (three-letter code: NA) (formula: Na).

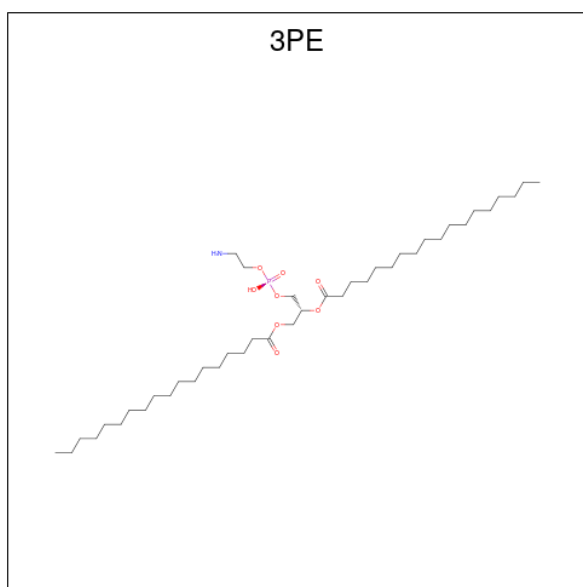
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	Na	0
			1	1	

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	H	1	51	33	16	2	0
51	K	1	71	52	17	2	0
51	L	1	68	49	17	2	0
51	h	1	58	39	17	2	0
51	h	1	78	60	16	2	0
51	q	1	62	43	17	2	0

- Molecule 52 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	
52	I	1	36	26	1	8	1	0
52	I	1	44	34	1	8	1	0
52	L	1	43	33	1	8	1	0
52	L	1	45	35	1	8	1	0
52	M	1	41	31	1	8	1	0
52	N	1	34	24	1	8	1	0
52	N	1	38	28	1	8	1	0
52	O	1	30	20	1	8	1	0
52	X	1	37	27	1	8	1	0
52	Y	1	38	28	1	8	1	0
52	Z	1	43	33	1	8	1	0
52	d	1	43	33	1	8	1	0
52	d	1	32	22	1	8	1	0
52	f	1	42	32	1	8	1	0

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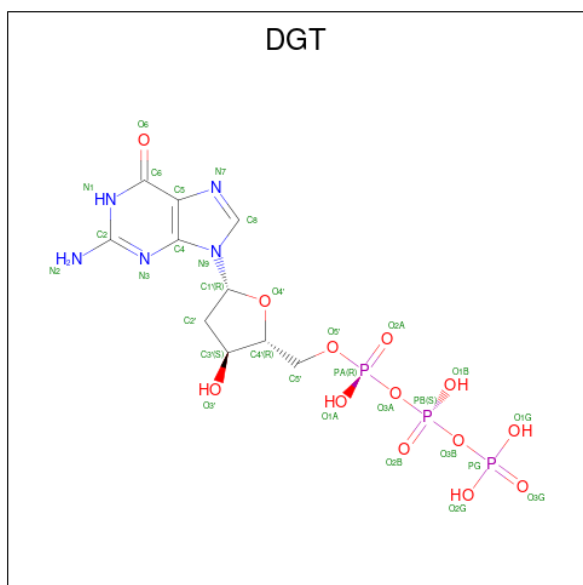
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Mol	Chain	Residues	Atoms					AltConf
52	i	1	Total	C	N	O	P	0
			30	20	1	8	1	
52	r	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

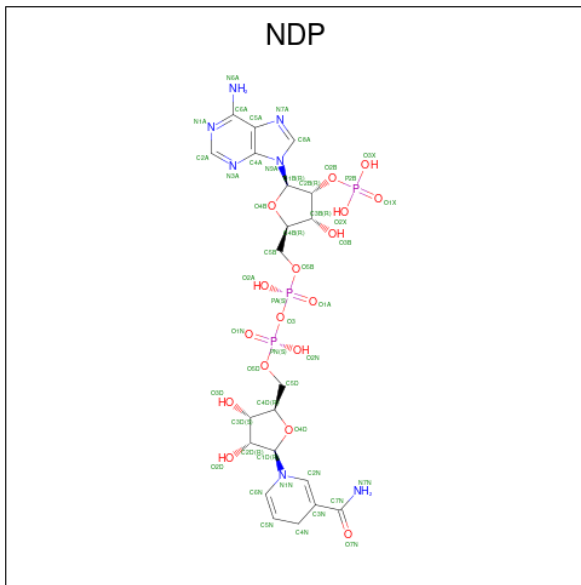
Mol	Chain	Residues	Atoms		AltConf
53	O	1	Total	Mg	0
			1	1	

- Molecule 54 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

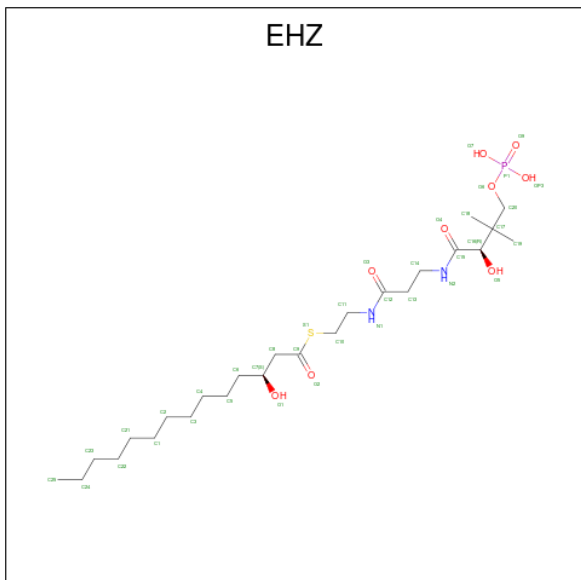


Mol	Chain	Residues	Atoms					AltConf
55	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

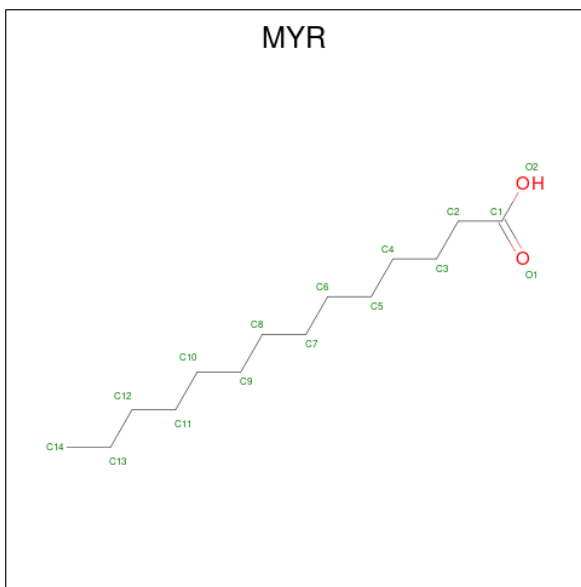
Mol	Chain	Residues	Atoms		AltConf
56	R	1	Total	Zn	0
			1	1	

- Molecule 57 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: C₂₅H₄₉N₂O₉PS).



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

- Molecule 58 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	A	59	Total	O	0
			59	59	
59	B	96	Total	O	0
			96	96	
59	C	160	Total	O	0
			160	160	
59	D	257	Total	O	0
			257	257	
59	E	43	Total	O	0
			43	43	
59	F	85	Total	O	0
			85	85	
59	G	300	Total	O	0
			300	300	

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Mol	Chain	Residues	Atoms		AltConf
59	H	120	Total 120	O 120	0
59	I	124	Total 124	O 124	0
59	J	60	Total 60	O 60	0
59	K	41	Total 41	O 41	0
59	L	105	Total 105	O 105	0
59	M	190	Total 190	O 190	0
59	N	123	Total 123	O 123	0
59	O	108	Total 108	O 108	0
59	P	149	Total 149	O 149	0
59	Q	120	Total 120	O 120	0
59	R	52	Total 52	O 52	0
59	S	2	Total 2	O 2	0
59	T	1	Total 1	O 1	0
59	U	3	Total 3	O 3	0
59	V	35	Total 35	O 35	0
59	W	58	Total 58	O 58	0
59	X	64	Total 64	O 64	0
59	Y	2	Total 2	O 2	0
59	Z	73	Total 73	O 73	0
59	a	37	Total 37	O 37	0
59	b	15	Total 15	O 15	0

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Mol	Chain	Residues	Atoms		AltConf
59	c	4	Total 4	O 4	0
59	d	31	Total 31	O 31	0
59	e	44	Total 44	O 44	0
59	f	11	Total 11	O 11	0
59	g	27	Total 27	O 27	0
59	h	45	Total 45	O 45	0
59	i	6	Total 6	O 6	0
59	j	2	Total 2	O 2	0
59	k	3	Total 3	O 3	0
59	l	37	Total 37	O 37	0
59	m	34	Total 34	O 34	0
59	n	31	Total 31	O 31	0
59	p	45	Total 45	O 45	0
59	q	84	Total 84	O 84	0
59	r	51	Total 51	O 51	0
59	s	8	Total 8	O 8	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.

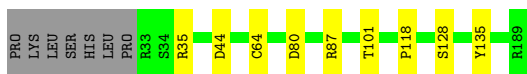
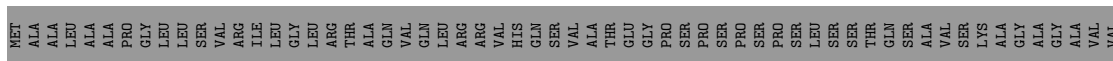
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:  98%




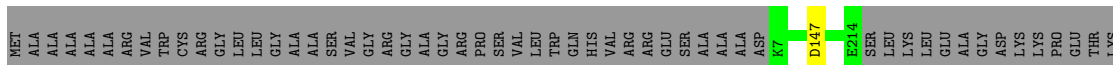
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:  66% 30%



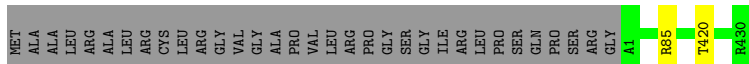
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:  79% 21%




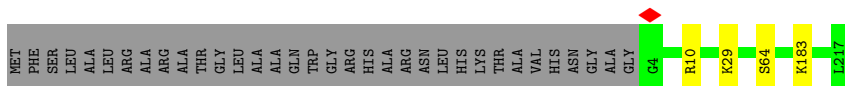
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:  92% 7%




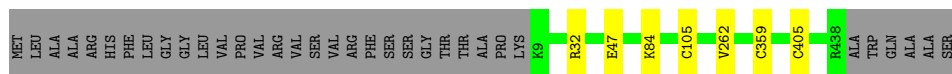
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  85% 14%



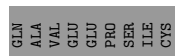
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  91% 7%



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

Chain G:  93% 5%




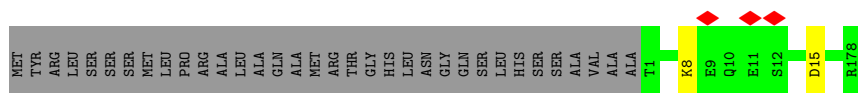
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  97%



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

Chain I:  83% 16%



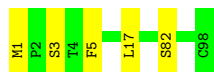
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  99%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  95% 5%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  98%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 97%



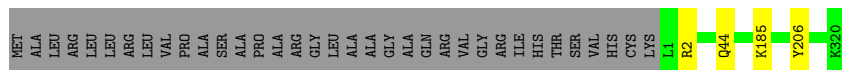
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 98%



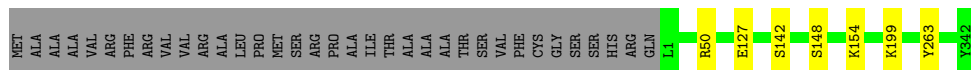
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 89% 10%



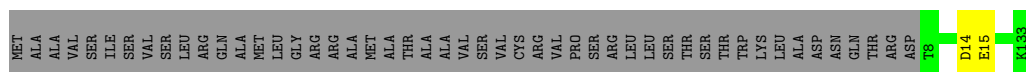
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 89% 9%



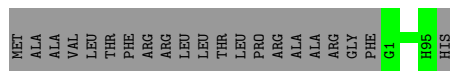
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 71% 28%




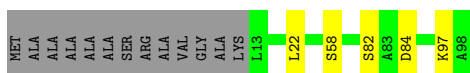
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 82% 18%



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

Chain S:  82% 5% 13%



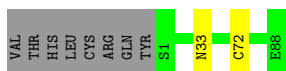
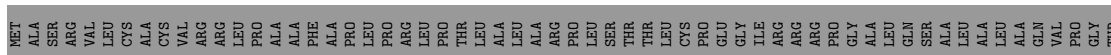
- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:  45% 5% 50%



- Molecule 20: Acyl carrier protein, mitochondrial

Chain U:  55% 44%




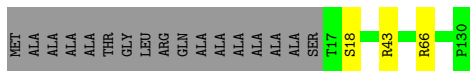
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:  98%



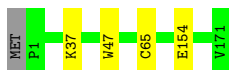
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:  85% 13%



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

Chain X:  97%



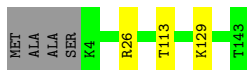
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  97%



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

Chain Z: 95%



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

Chain a: 97%



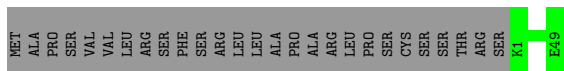
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b: 99%



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

Chain c: 64% 36%



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

Chain d: 99%



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

Chain e: 97%



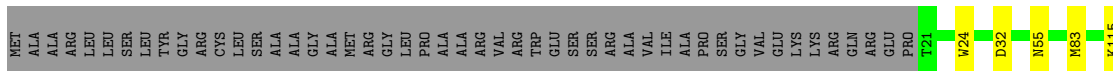
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 96%



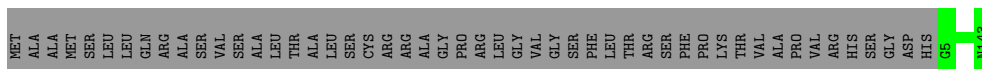
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 64% 33%



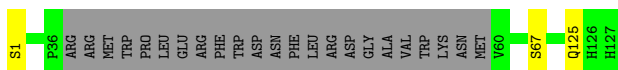
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 74% 26%



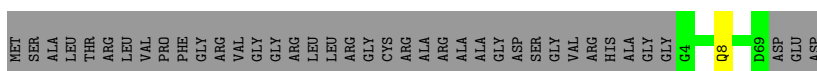
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 80% 18%



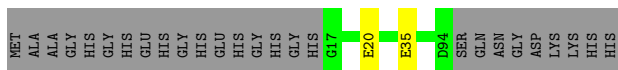
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j: 62% 37%



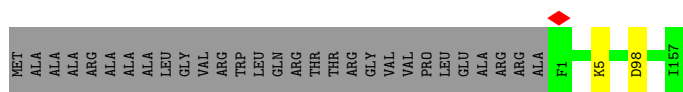
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k: 73% 25%

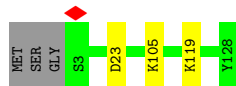


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l: 83% 16%



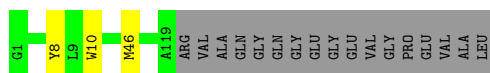
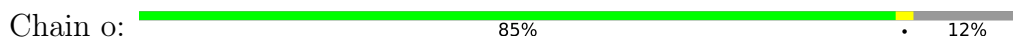
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



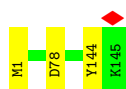
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



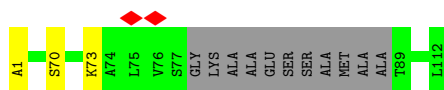
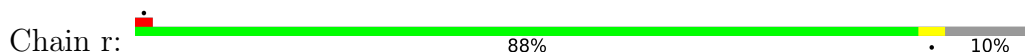
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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



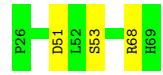
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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



MET
ALA
VAL
SER
LEU
LEU
LEU
ARG
GLY
GLY
ARG
ILE
ARG
ALA
LYS
LYS
VAL
LEU
LEU
GLU
ALA
ARG
VAL
PHE
PRO
GLY
GLU
LEU
VAL
SER
VAL
VAL
ARG
LEU
SER
THR
GLU
SER
GLU
LYS
SER
ALA
LYS
GLU
LYS
GLU
LEU
LEU
HIS
PRO
LYS
THR
GLN
SER
VAL
LEU
LYS
GLU
PRO
GLU



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109866	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 ($e^-/\text{\AA}^2$)	39.94	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	44.320	Depositor
Minimum map value	-20.720	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.927	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	480.62003, 480.62003, 480.62003	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6866, 0.6866, 0.6866	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGT, MYR, 3PE, NDP, PC1, AME, FES, FMN, WYK, FME, 2MR, MG, LMT, ZN, AYA, NA, EHZ, SAC, CDL, SF4

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	0.33	0/949	0.50	0/1297
2	B	0.43	1/1277 (0.1%)	0.55	0/1727
3	C	0.38	0/1780	0.54	0/2424
4	D	0.37	0/3540	0.53	0/4795
5	E	0.35	0/1700	0.52	0/2316
6	F	0.37	0/3396	0.51	0/4586
7	G	0.36	0/5388	0.52	0/7300
8	H	0.36	0/2607	0.52	0/3564
9	I	0.39	0/1461	0.56	0/1974
10	J	0.35	0/1330	0.48	0/1810
11	K	0.32	0/738	0.45	0/1002
12	L	0.34	0/4922	0.47	0/6698
13	M	0.33	0/3709	0.50	0/5052
14	N	0.33	0/2755	0.50	0/3751
15	O	0.38	0/2674	0.49	0/3626
16	P	0.36	0/2823	0.52	0/3828
17	Q	0.35	0/1044	0.53	0/1409
18	R	0.37	0/762	0.51	0/1026
19	S	0.36	0/696	0.51	0/938
20	T	0.32	0/637	0.50	0/858
20	U	0.41	0/718	0.44	0/970
21	V	0.32	0/949	0.41	0/1286
22	W	0.32	0/993	0.50	0/1335
23	X	0.34	0/1434	0.49	0/1937
24	Y	0.35	0/1074	0.45	0/1456
25	Z	0.37	0/1192	0.51	0/1608
26	a	0.36	0/577	0.50	0/777
27	b	0.35	0/671	0.45	0/921
28	c	0.38	0/418	0.52	0/567
29	d	0.39	0/1028	0.51	0/1387
30	e	0.35	0/900	0.50	0/1199

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.34	0/495	0.47	0/667
32	g	0.39	0/878	0.50	0/1196
33	h	0.39	0/1201	0.50	0/1626
34	i	0.38	0/889	0.52	0/1210
35	j	0.38	0/591	0.46	0/809
36	k	0.39	0/650	0.48	0/878
37	l	0.40	0/1379	0.50	0/1882
38	m	0.40	0/1079	0.53	0/1463
39	n	0.40	0/1596	0.46	0/2162
40	o	0.37	0/1044	0.50	0/1401
41	p	0.38	0/1472	0.49	0/1989
42	q	0.37	0/1243	0.52	0/1692
43	r	0.38	0/819	0.53	0/1108
44	s	0.35	0/379	0.59	1/515 (0.2%)
All	All	0.36	1/67857 (0.0%)	0.50	1/92022 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	118	PRO	C-N	-5.09	1.22	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	s	51	ASP	CB-CG-OD2	5.58	123.32	118.30

There are no chirality outliers.

There are no planarity outliers.

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	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%)	201 (98%)	5 (2%)	0	100	100
4	D	427/463 (92%)	413 (97%)	14 (3%)	0	100	100
5	E	212/248 (86%)	205 (97%)	6 (3%)	1 (0%)	29	41
6	F	428/464 (92%)	417 (97%)	11 (3%)	0	100	100
7	G	687/727 (94%)	667 (97%)	20 (3%)	0	100	100
8	H	316/318 (99%)	305 (96%)	9 (3%)	2 (1%)	25	36
9	I	176/212 (83%)	171 (97%)	5 (3%)	0	100	100
10	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	605/607 (100%)	583 (96%)	21 (4%)	1 (0%)	47	62
13	M	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
14	N	343/345 (99%)	340 (99%)	3 (1%)	0	100	100
15	O	318/355 (90%)	313 (98%)	5 (2%)	0	100	100
16	P	340/377 (90%)	332 (98%)	8 (2%)	0	100	100
17	Q	124/175 (71%)	123 (99%)	1 (1%)	0	100	100
18	R	93/116 (80%)	90 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
20	T	76/156 (49%)	71 (93%)	5 (7%)	0	100	100
20	U	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
21	V	112/116 (97%)	112 (100%)	0	0	100	100
22	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
24	Y	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
25	Z	138/144 (96%)	136 (99%)	2 (1%)	0	100	100
26	a	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	118 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	e	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
31	f	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
32	g	99/151 (66%)	98 (99%)	1 (1%)	0	100	100
33	h	137/189 (72%)	134 (98%)	3 (2%)	0	100	100
34	i	100/127 (79%)	94 (94%)	6 (6%)	0	100	100
35	j	64/105 (61%)	62 (97%)	2 (3%)	0	100	100
36	k	76/104 (73%)	73 (96%)	3 (4%)	0	100	100
37	l	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
38	m	124/129 (96%)	121 (98%)	3 (2%)	0	100	100
39	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
40	o	117/136 (86%)	112 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	165 (98%)	3 (2%)	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	97/112 (87%)	90 (93%)	7 (7%)	0	100	100
44	s	42/104 (40%)	39 (93%)	3 (7%)	0	100	100
All	All	8150/9210 (88%)	7934 (97%)	212 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	183	LYS
8	H	203	GLY
8	H	244	GLY
12	L	562	ILE

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%)	102 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	132/184 (72%)	125 (95%)	7 (5%)	22	37
3	C	190/227 (84%)	189 (100%)	1 (0%)	88	95
4	D	370/394 (94%)	369 (100%)	1 (0%)	92	97
5	E	184/206 (89%)	181 (98%)	3 (2%)	62	79
6	F	345/370 (93%)	338 (98%)	7 (2%)	55	74
7	G	580/610 (95%)	566 (98%)	14 (2%)	49	68
8	H	279/279 (100%)	272 (98%)	7 (2%)	47	67
9	I	152/178 (85%)	150 (99%)	2 (1%)	69	84
10	J	137/137 (100%)	136 (99%)	1 (1%)	84	92
11	K	87/87 (100%)	83 (95%)	4 (5%)	27	43
12	L	549/549 (100%)	538 (98%)	11 (2%)	55	74
13	M	414/414 (100%)	403 (97%)	11 (3%)	44	65
14	N	307/307 (100%)	302 (98%)	5 (2%)	62	79
15	O	284/309 (92%)	280 (99%)	4 (1%)	67	82
16	P	299/325 (92%)	292 (98%)	7 (2%)	50	70
17	Q	112/153 (73%)	110 (98%)	2 (2%)	59	76
18	R	80/96 (83%)	80 (100%)	0	100	100
19	S	75/80 (94%)	70 (93%)	5 (7%)	16	26
20	T	72/135 (53%)	64 (89%)	8 (11%)	6	8
20	U	81/135 (60%)	79 (98%)	2 (2%)	47	67
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	105 (97%)	3 (3%)	43	63
23	X	153/154 (99%)	149 (97%)	4 (3%)	46	66
24	Y	106/106 (100%)	102 (96%)	4 (4%)	33	51
25	Z	121/123 (98%)	118 (98%)	3 (2%)	47	67
26	a	59/60 (98%)	58 (98%)	1 (2%)	60	78
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	43/67 (64%)	43 (100%)	0	100	100
29	d	107/107 (100%)	106 (99%)	1 (1%)	78	90
30	e	93/94 (99%)	91 (98%)	2 (2%)	52	71
31	f	52/53 (98%)	51 (98%)	1 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	92/129 (71%)	87 (95%)	5 (5%)	22	36
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	95/118 (80%)	93 (98%)	2 (2%)	53	72
35	j	61/87 (70%)	60 (98%)	1 (2%)	62	79
36	k	60/78 (77%)	58 (97%)	2 (3%)	38	57
37	l	142/161 (88%)	140 (99%)	2 (1%)	67	82
38	m	112/114 (98%)	109 (97%)	3 (3%)	44	65
39	n	163/164 (99%)	160 (98%)	3 (2%)	59	76
40	o	109/120 (91%)	106 (97%)	3 (3%)	43	63
41	p	155/158 (98%)	152 (98%)	3 (2%)	57	75
42	q	130/130 (100%)	128 (98%)	2 (2%)	65	80
43	r	90/95 (95%)	88 (98%)	2 (2%)	52	71
44	s	43/95 (45%)	41 (95%)	2 (5%)	26	42
All	All	7222/7942 (91%)	7070 (98%)	152 (2%)	56	72

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Z	113	THR
41	p	5	ASP
30	e	4	ASP
36	k	20	GLU
44	s	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
39	n	25	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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	WYK	B	87	2	9,11,12	2.48	2 (22%)	7,13,15	1.36	1 (14%)
11	FME	K	1	11	8,9,10	0.98	1 (12%)	7,9,11	1.21	1 (14%)
8	FME	H	1	8	8,9,10	0.97	1 (12%)	7,9,11	1.14	0
1	FME	A	1	1	8,9,10	0.97	1 (12%)	7,9,11	0.82	0
34	SAC	i	1	34	7,8,9	0.50	0	8,9,11	0.78	1 (12%)
14	FME	N	1	14	8,9,10	1.02	1 (12%)	7,9,11	0.82	0
42	AME	q	1	42	9,10,11	1.46	1 (11%)	9,11,13	1.83	3 (33%)
13	FME	M	1	13	8,9,10	0.91	0	7,9,11	1.40	1 (14%)
43	AYA	r	1	43	6,7,8	1.16	1 (16%)	5,8,10	1.13	0
12	FME	L	1	12	8,9,10	0.93	0	7,9,11	1.09	0
10	FME	J	1	10	8,9,10	0.94	0	7,9,11	0.96	0
4	2MR	D	85	4	10,12,13	2.37	3 (30%)	5,13,15	1.14	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
2	WYK	B	87	2	-	0/10/11/13	-
11	FME	K	1	11	-	4/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
34	SAC	i	1	34	-	5/7/8/10	-
14	FME	N	1	14	-	0/7/9/11	-
42	AME	q	1	42	-	3/9/10/12	-
13	FME	M	1	13	-	1/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	L	1	12	-	1/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	WYK	CZ-NE	6.37	1.45	1.33
4	D	85	2MR	CZ-NH2	4.82	1.44	1.33
4	D	85	2MR	CZ-NE	4.75	1.44	1.34
42	q	1	AME	CT1-N	3.37	1.45	1.34
2	B	87	WYK	CZ-NH2	-2.47	1.24	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1	FME	C-CA-N	3.17	115.45	109.73
42	q	1	AME	CE-SD-CG	3.08	110.99	100.40
2	B	87	WYK	CB-CA-N	2.93	116.84	110.32
42	q	1	AME	CT2-CT1-N	2.58	120.47	116.10
42	q	1	AME	O-C-CA	-2.47	118.31	124.78

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1	FME	C-CA-CB-CG
10	J	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
11	K	1	FME	CA-CB-CG-SD

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 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 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	J	202	-	36,36,36	1.12	5 (13%)	47,47,47	1.15	5 (10%)
45	LMT	Y	202	-	36,36,36	1.19	6 (16%)	47,47,47	0.94	0
45	LMT	Y	204	-	36,36,36	1.22	6 (16%)	47,47,47	0.97	1 (2%)
45	LMT	M	502	-	36,36,36	1.33	6 (16%)	47,47,47	1.03	1 (2%)
45	LMT	N	401	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	3 (6%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
54	DGT	O	502	53	26,33,33	2.62	10 (38%)	32,52,52	1.71	10 (31%)
47	SF4	F	501	6	0,12,12	-	-	-	-	-
57	EHZ	T	201	20	29,36,37	1.73	5 (17%)	35,44,47	1.63	7 (20%)
45	LMT	A	201	-	36,36,36	1.12	5 (13%)	47,47,47	1.28	3 (6%)
51	CDL	h	202	-	77,77,99	0.91	6 (7%)	82,88,111	1.07	3 (3%)
52	3PE	L	702	-	42,42,50	0.98	4 (9%)	45,47,55	0.93	1 (2%)
46	PC1	A	203	-	33,33,53	1.20	4 (12%)	39,41,61	1.00	2 (5%)
52	3PE	d	201	-	42,42,50	0.95	3 (7%)	45,47,55	1.09	2 (4%)
47	SF4	I	201	9	0,12,12	-	-	-	-	-
51	CDL	K	101	-	70,70,99	1.05	6 (8%)	76,82,111	1.09	4 (5%)
45	LMT	L	704	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	1 (2%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
45	LMT	j	101	-	36,36,36	1.20	6 (16%)	47,47,47	0.90	0
57	EHZ	U	201	20	29,36,37	1.65	5 (17%)	35,44,47	1.71	8 (22%)
45	LMT	J	201	-	36,36,36	1.20	5 (13%)	47,47,47	0.93	1 (2%)
52	3PE	N	402	-	33,33,50	0.94	2 (6%)	34,37,55	0.98	1 (2%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
52	3PE	M	501	-	40,40,50	0.98	3 (7%)	43,45,55	0.97	2 (4%)
46	PC1	L	707	-	26,26,53	1.28	4 (15%)	32,34,61	1.04	2 (6%)
52	3PE	I	204	-	43,43,50	0.91	4 (9%)	46,48,55	1.04	2 (4%)
52	3PE	i	201	-	29,29,50	1.16	4 (13%)	32,34,55	1.23	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	3PE	I	203	-	35,35,50	1.03	4 (11%)	38,40,55	1.02	2 (5%)
45	LMT	N	404	-	36,36,36	1.16	5 (13%)	47,47,47	0.89	0
52	3PE	L	706	-	44,44,50	0.89	4 (9%)	47,49,55	1.02	2 (4%)
52	3PE	O	503	-	29,29,50	1.10	4 (13%)	32,34,55	1.08	2 (6%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
52	3PE	r	201	-	45,45,50	0.92	4 (8%)	48,50,55	1.09	2 (4%)
45	LMT	L	705	-	36,36,36	1.20	6 (16%)	47,47,47	0.97	2 (4%)
46	PC1	B	204	-	51,51,53	0.95	4 (7%)	57,59,61	0.92	2 (3%)
51	CDL	L	703	-	67,67,99	1.07	7 (10%)	73,79,111	1.12	4 (5%)
45	LMT	H	402	-	36,36,36	1.23	6 (16%)	47,47,47	1.07	5 (10%)
51	CDL	h	201	-	57,57,99	1.36	8 (14%)	61,68,111	1.19	4 (6%)
52	3PE	Y	203	-	37,37,50	0.99	4 (10%)	40,42,55	1.14	2 (5%)
52	3PE	X	201	-	36,36,50	1.02	4 (11%)	39,41,55	1.09	2 (5%)
51	CDL	q	201	-	61,61,99	1.10	6 (9%)	67,73,111	1.13	4 (5%)
58	MYR	o	201	40	14,14,15	0.76	0	13,13,15	0.63	0
52	3PE	f	101	-	41,41,50	0.96	4 (9%)	44,46,55	1.11	2 (4%)
45	LMT	h	203	-	36,36,36	1.17	4 (11%)	47,47,47	0.96	1 (2%)
46	PC1	B	203	-	42,42,53	1.07	4 (9%)	48,50,61	1.15	2 (4%)
52	3PE	N	403	-	37,37,50	1.00	4 (10%)	40,42,55	1.09	2 (5%)
49	FMN	F	502	-	33,33,33	2.43	7 (21%)	48,50,50	1.67	13 (27%)
45	LMT	A	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.90	1 (2%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
45	LMT	L	701	-	36,36,36	1.28	5 (13%)	47,47,47	0.96	1 (2%)
55	NDP	P	501	-	45,52,52	2.15	7 (15%)	53,80,80	1.59	11 (20%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
46	PC1	p	302	-	35,35,53	1.14	3 (8%)	41,43,61	1.11	2 (4%)
45	LMT	Y	201	-	36,36,36	1.17	6 (16%)	47,47,47	1.11	3 (6%)
52	3PE	Z	201	-	42,42,50	0.95	3 (7%)	45,47,55	1.00	2 (4%)
52	3PE	d	202	-	31,31,50	1.11	4 (12%)	34,36,55	1.09	2 (5%)
51	CDL	H	401	-	50,50,99	1.10	6 (12%)	55,61,111	1.04	3 (5%)

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	J	202	-	-	7/21/61/61	0/2/2/2
45	LMT	Y	202	-	-	7/21/61/61	0/2/2/2
45	LMT	Y	204	-	-	11/21/61/61	0/2/2/2
45	LMT	M	502	-	-	11/21/61/61	0/2/2/2
45	LMT	N	401	-	-	8/21/61/61	0/2/2/2
54	DGT	O	502	53	-	10/18/34/34	0/3/3/3
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	F	501	6	-	-	0/6/5/5
57	EHZ	T	201	20	-	20/42/44/45	-
45	LMT	A	201	-	-	8/21/61/61	0/2/2/2
51	CDL	h	202	-	-	42/87/87/110	-
52	3PE	L	702	-	-	23/46/46/54	-
46	PC1	A	203	-	-	10/37/37/57	-
52	3PE	d	201	-	-	21/46/46/54	-
47	SF4	I	201	9	-	-	0/6/5/5
51	CDL	K	101	-	-	32/81/81/110	-
45	LMT	L	704	-	-	7/21/61/61	0/2/2/2
57	EHZ	U	201	20	-	15/42/44/45	-
45	LMT	j	101	-	-	9/21/61/61	0/2/2/2
47	SF4	G	801	7	-	-	0/6/5/5
45	LMT	J	201	-	-	5/21/61/61	0/2/2/2
52	3PE	N	402	-	-	11/36/36/54	-
47	SF4	G	802	7	-	-	0/6/5/5
52	3PE	M	501	-	-	26/44/44/54	-
46	PC1	L	707	-	-	16/30/30/57	-
52	3PE	I	204	-	-	15/47/47/54	-
52	3PE	i	201	-	-	14/33/33/54	-
52	3PE	I	203	-	-	19/39/39/54	-
45	LMT	N	404	-	-	12/21/61/61	0/2/2/2
52	3PE	L	706	-	-	20/48/48/54	-
52	3PE	O	503	-	-	14/33/33/54	-
47	SF4	B	201	2	-	-	0/6/5/5
52	3PE	r	201	-	-	22/49/49/54	-
45	LMT	L	705	-	-	7/21/61/61	0/2/2/2
46	PC1	B	204	-	-	28/55/55/57	-
51	CDL	L	703	-	-	29/78/78/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	H	402	-	-	10/21/61/61	0/2/2/2
51	CDL	h	201	-	-	30/67/67/110	-
52	3PE	Y	203	-	-	24/41/41/54	-
52	3PE	X	201	-	-	21/40/40/54	-
51	CDL	q	201	-	-	35/72/72/110	-
58	MYR	o	201	40	-	6/11/12/13	-
52	3PE	f	101	-	-	14/45/45/54	-
45	LMT	h	203	-	-	7/21/61/61	0/2/2/2
46	PC1	B	203	-	-	19/46/46/57	-
52	3PE	N	403	-	-	13/41/41/54	-
49	FMN	F	502	-	-	8/18/18/18	0/3/3/3
45	LMT	A	202	-	-	8/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1
45	LMT	L	701	-	-	12/21/61/61	0/2/2/2
55	NDP	P	501	-	-	5/30/77/77	0/5/5/5
48	FES	G	803	7	-	-	0/1/1/1
46	PC1	p	302	-	-	11/39/39/57	-
45	LMT	Y	201	-	-	12/21/61/61	0/2/2/2
52	3PE	Z	201	-	-	16/46/46/54	-
52	3PE	d	202	-	-	20/35/35/54	-
51	CDL	H	401	-	-	33/59/59/110	-

The worst 5 of 239 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	501	NDP	P2B-O2B	11.60	1.81	1.59
49	F	502	FMN	O4-C4	8.35	1.39	1.23
54	O	502	DGT	O6-C6	8.10	1.39	1.23
49	F	502	FMN	O2-C2	7.80	1.38	1.24
51	h	201	CDL	OA6-CA4	-5.86	1.40	1.46

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	P	501	NDP	PN-O3-PA	-6.09	111.94	132.83
57	U	201	EHZ	C8-C9-S1	5.76	120.75	113.63
46	B	203	PC1	O21-C21-C22	5.29	122.90	111.50
57	T	201	EHZ	C8-C9-S1	5.24	120.11	113.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	i	201	3PE	O21-C21-C22	4.72	121.67	111.50

There are no chirality outliers.

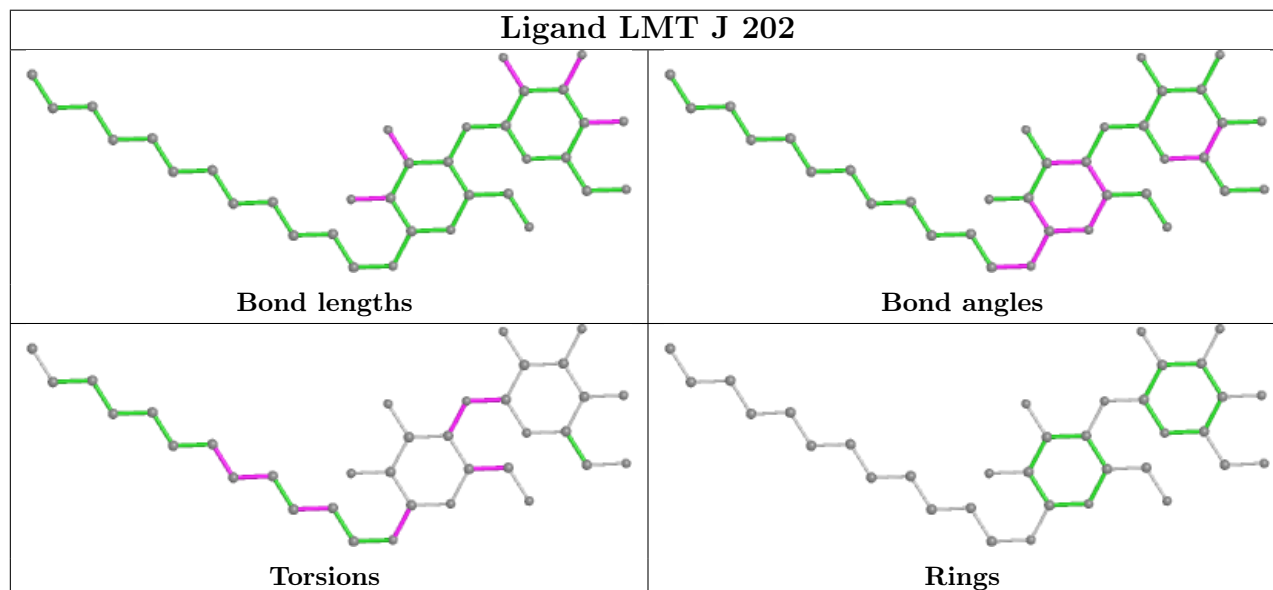
5 of 783 torsion outliers are listed below:

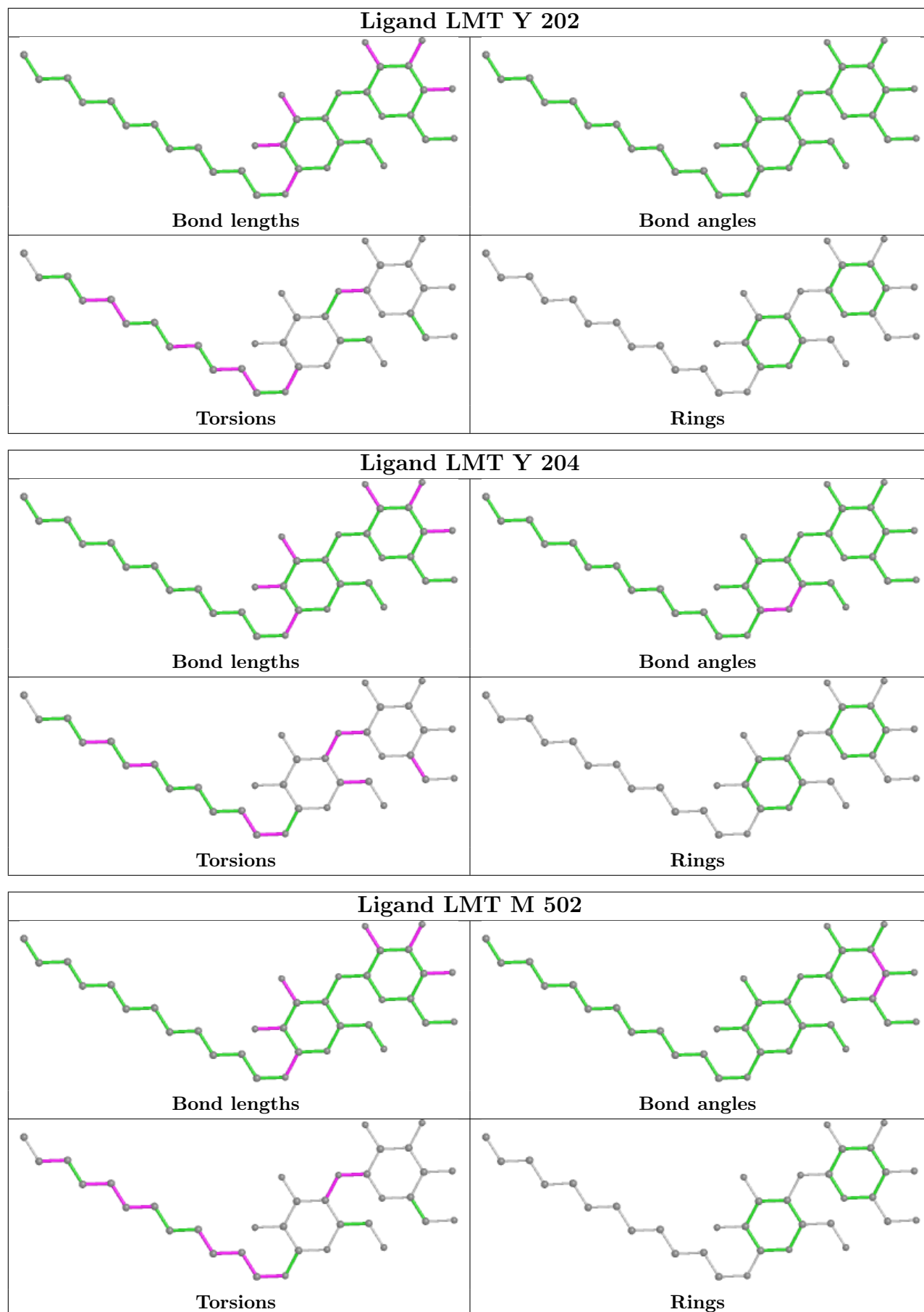
Mol	Chain	Res	Type	Atoms
45	H	402	LMT	C2'-C1'-O1'-C1
45	H	402	LMT	O5'-C1'-O1'-C1
45	L	701	LMT	C2'-C1'-O1'-C1
45	L	701	LMT	O5'-C1'-O1'-C1
45	Y	204	LMT	C2-C1-O1'-C1'

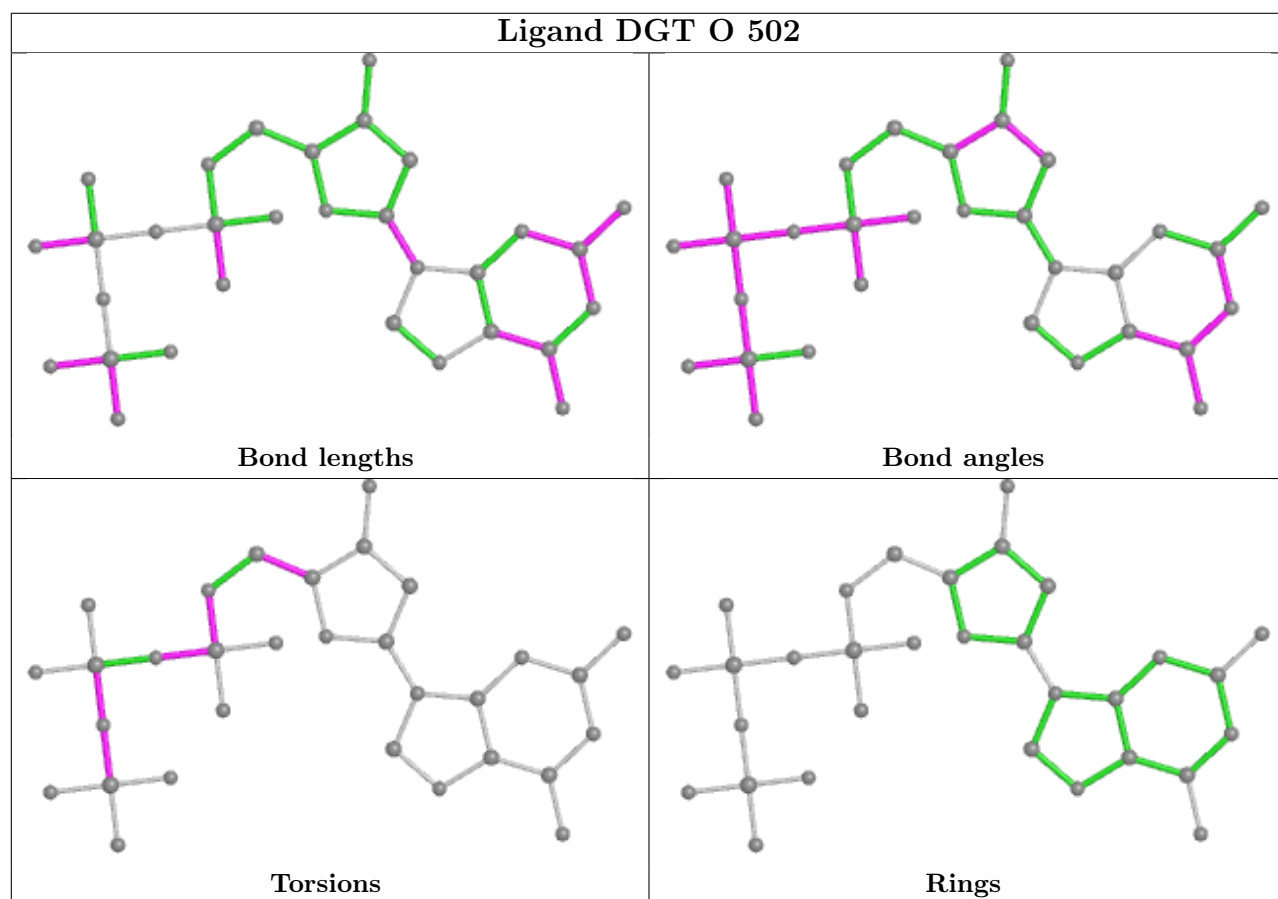
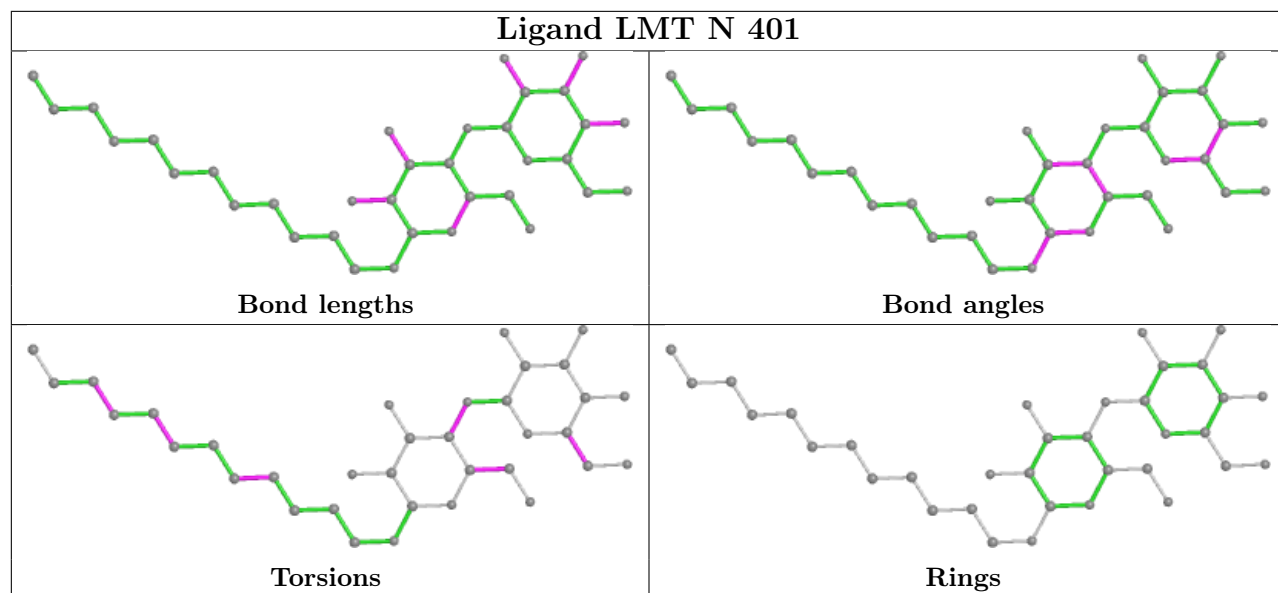
There are no ring outliers.

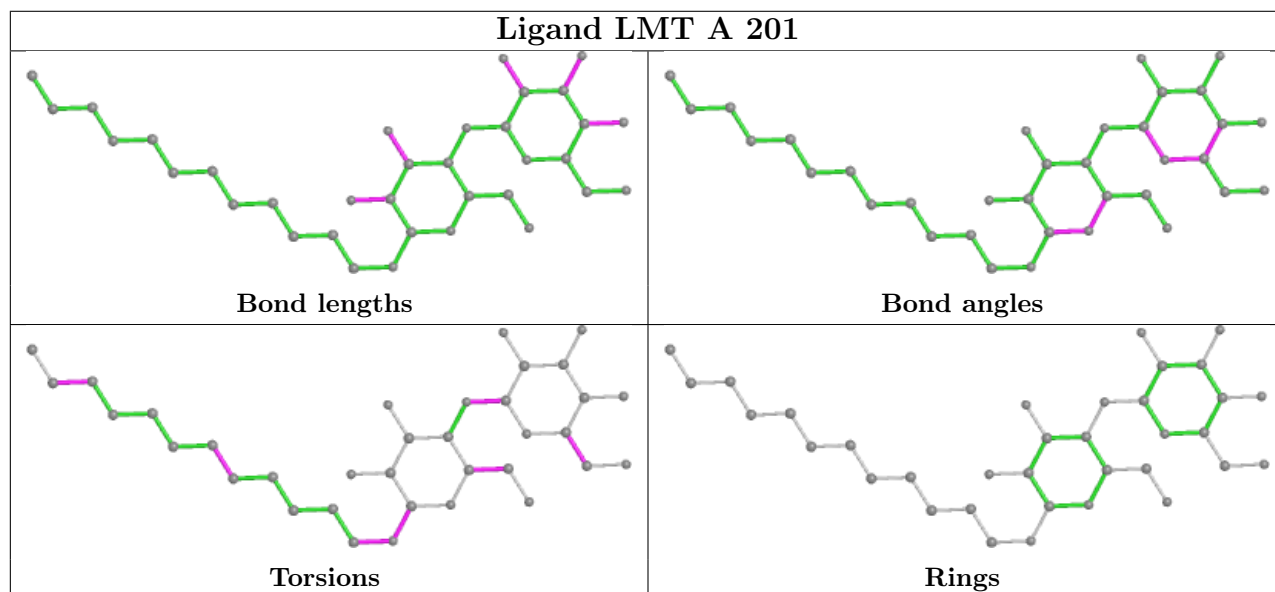
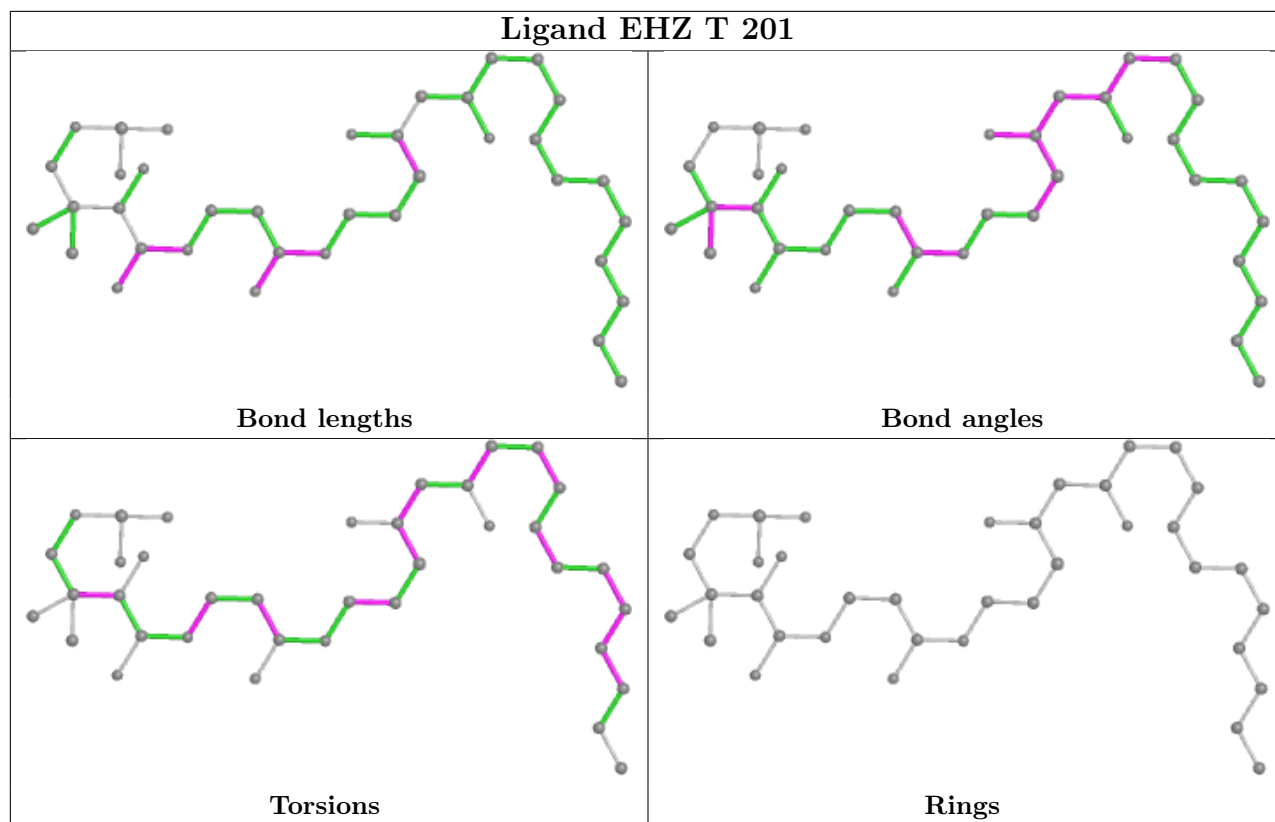
No monomer is involved in short contacts.

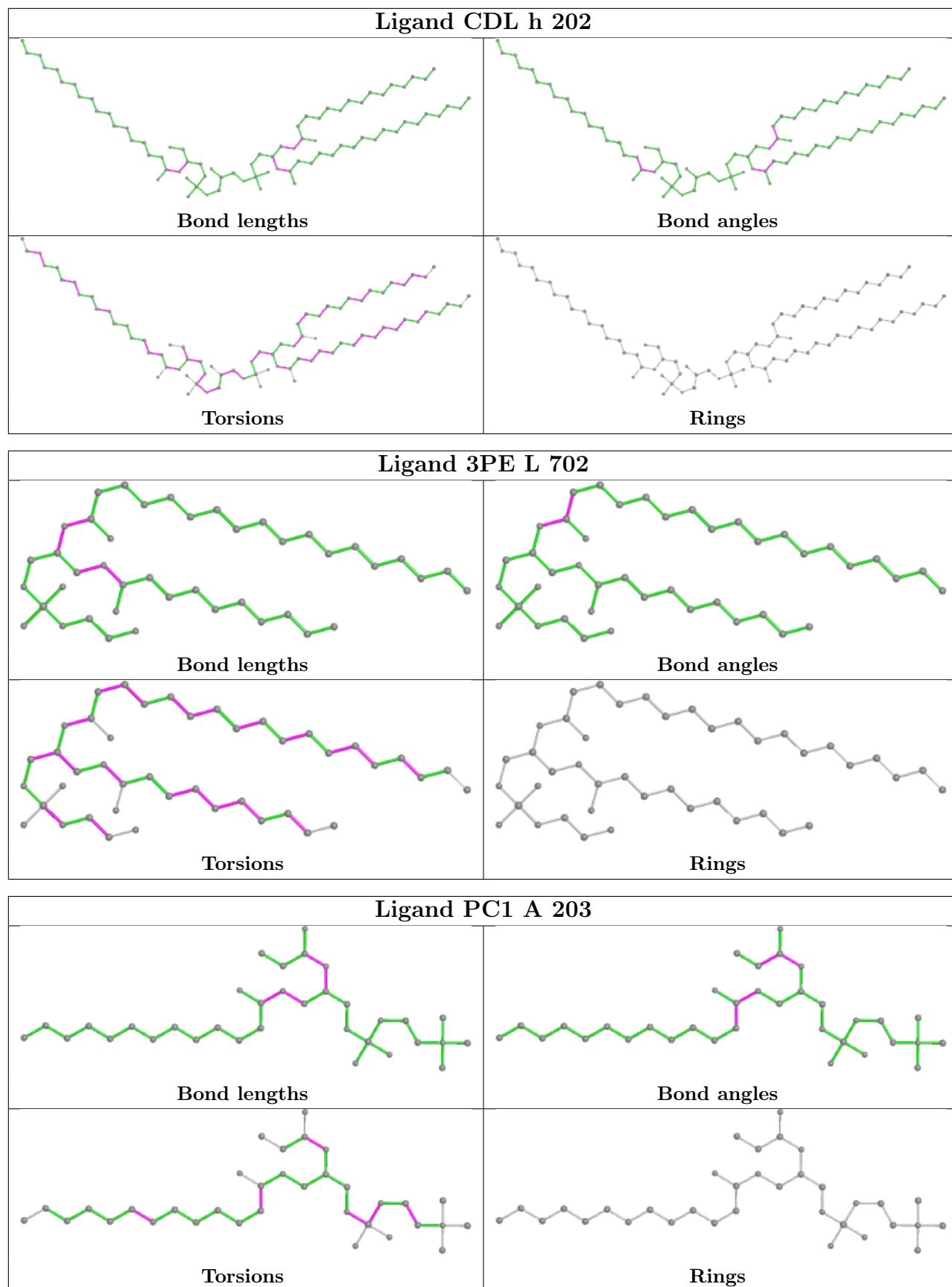
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

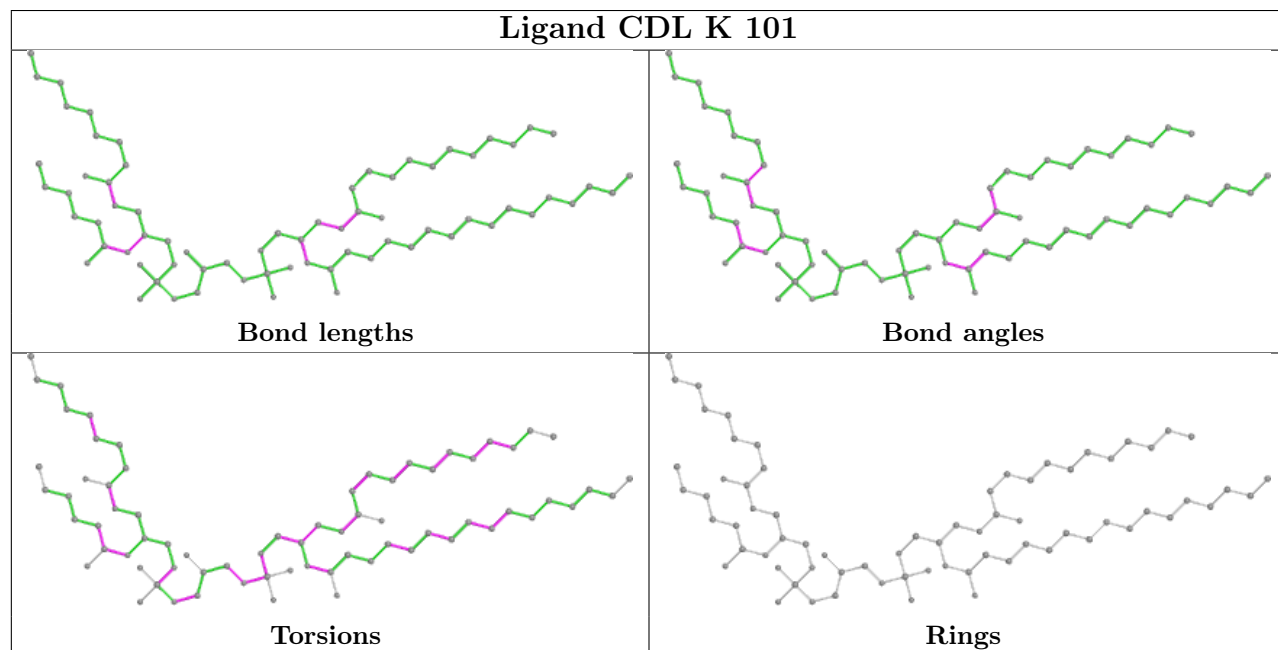
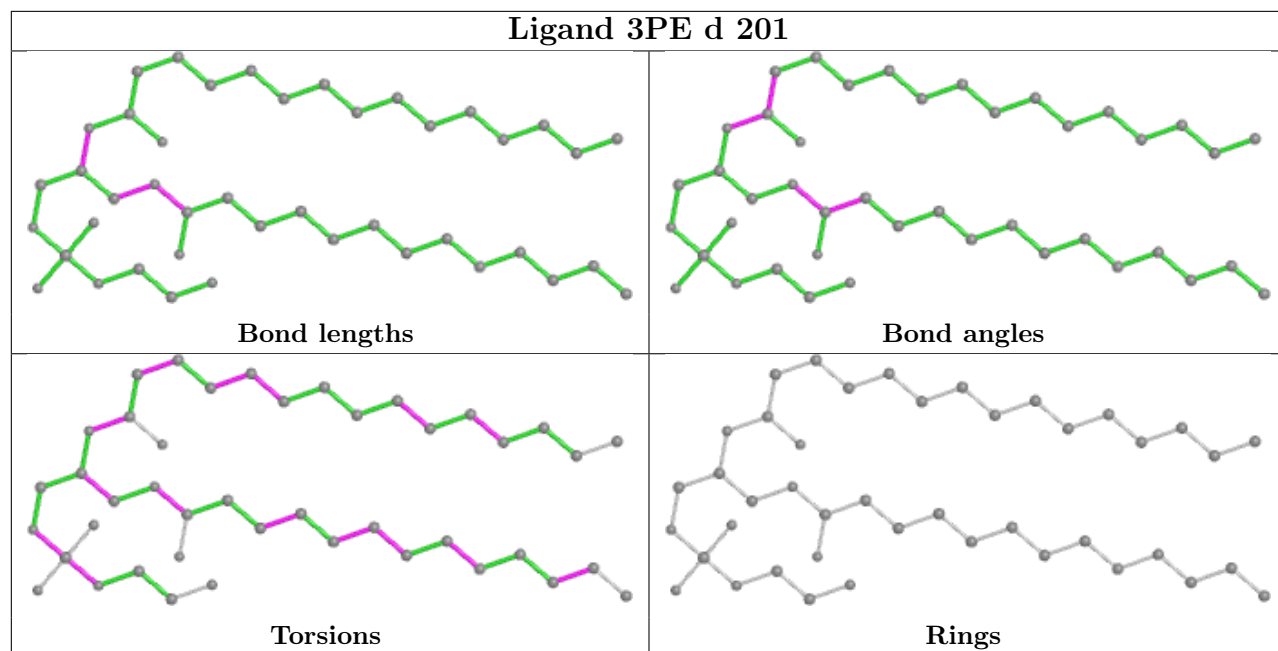


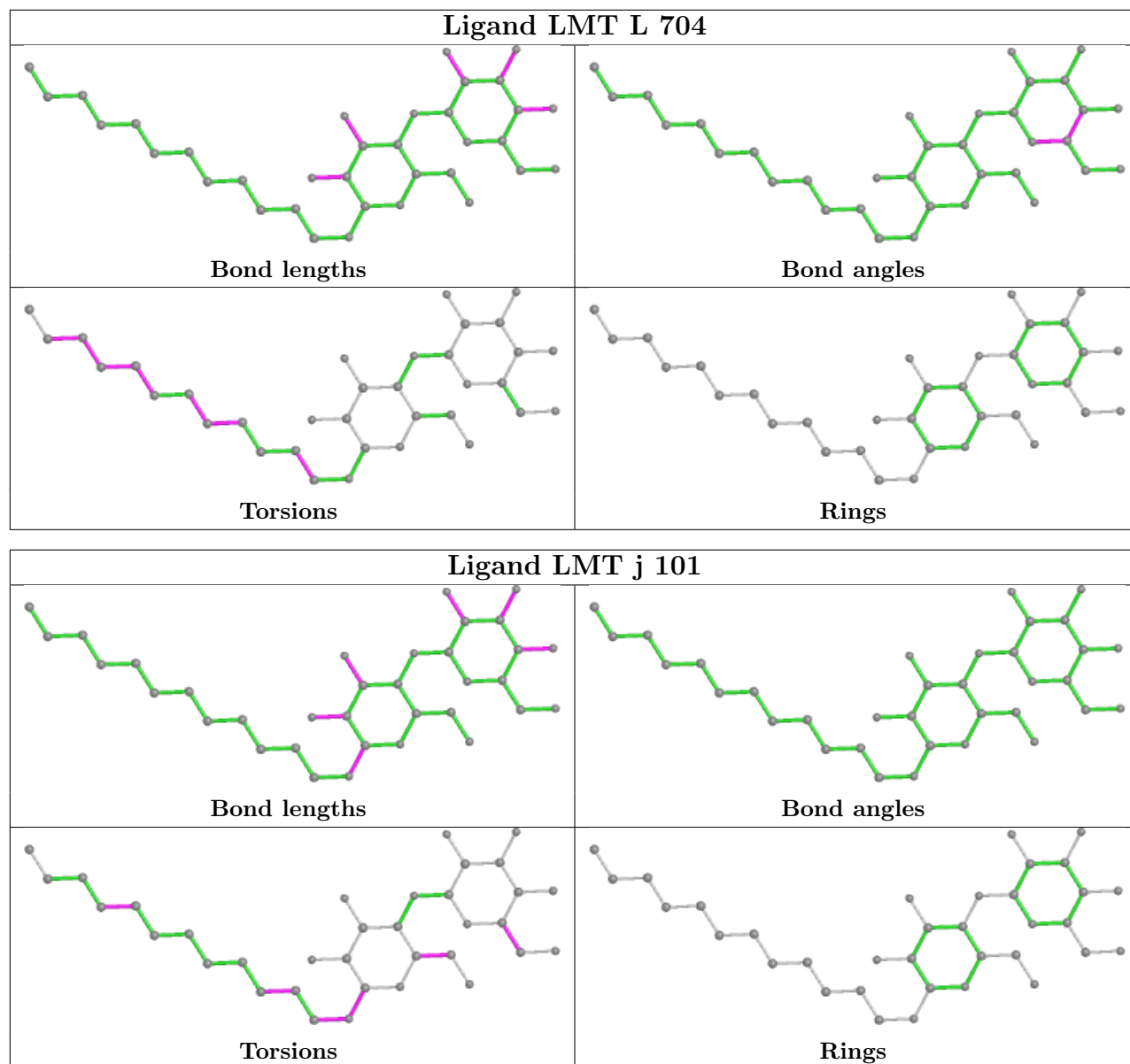


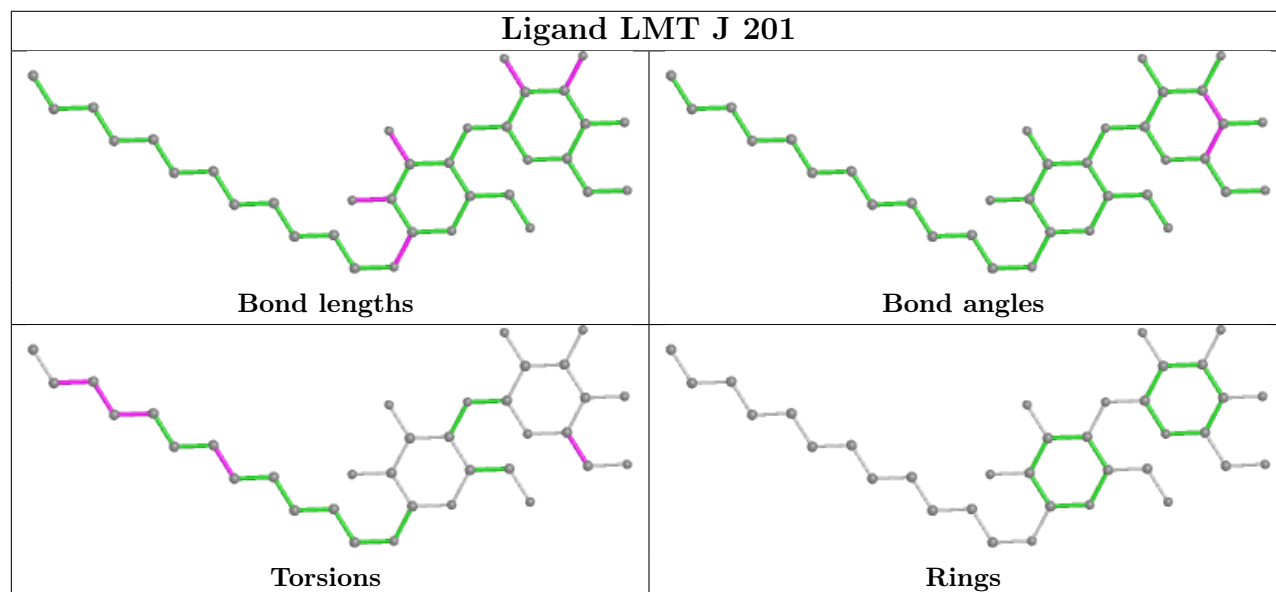
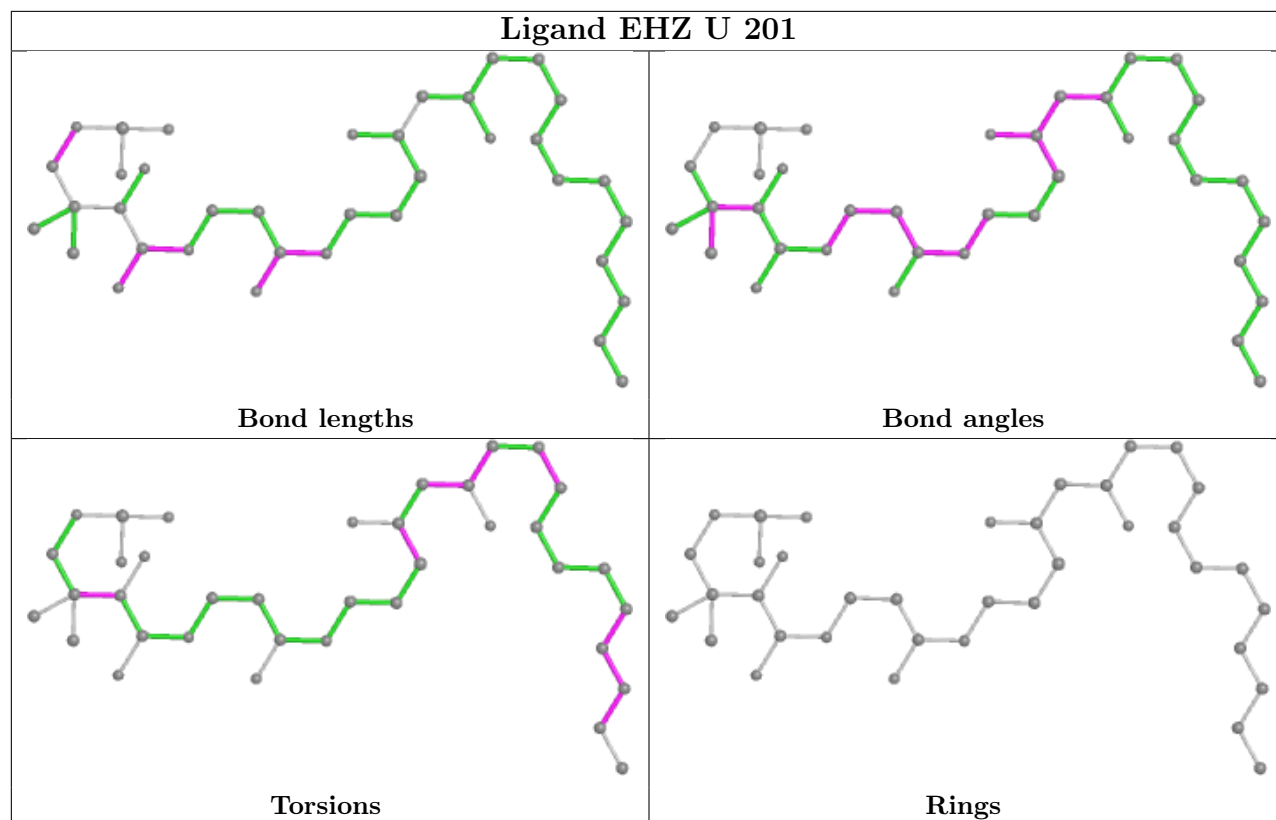


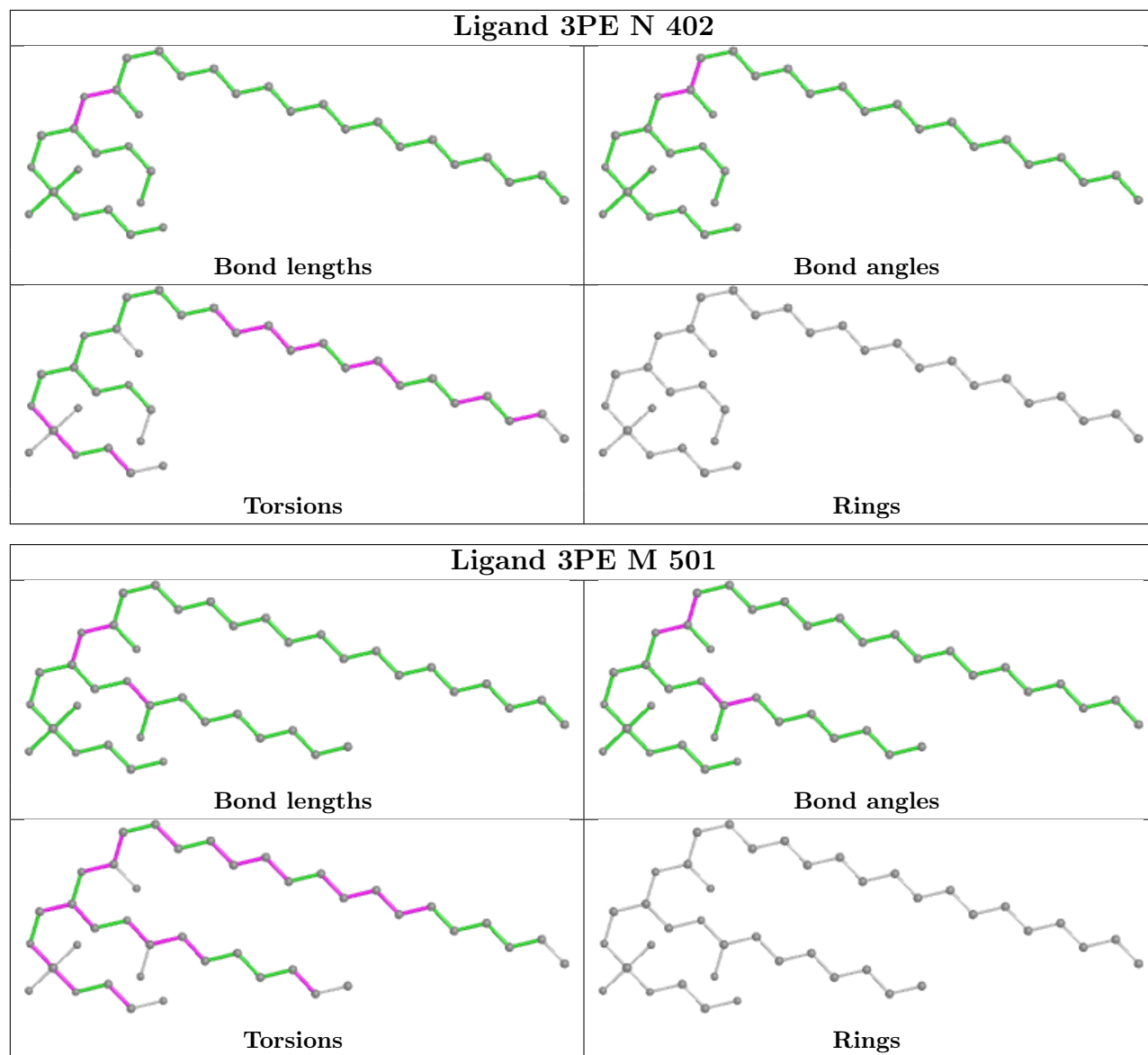


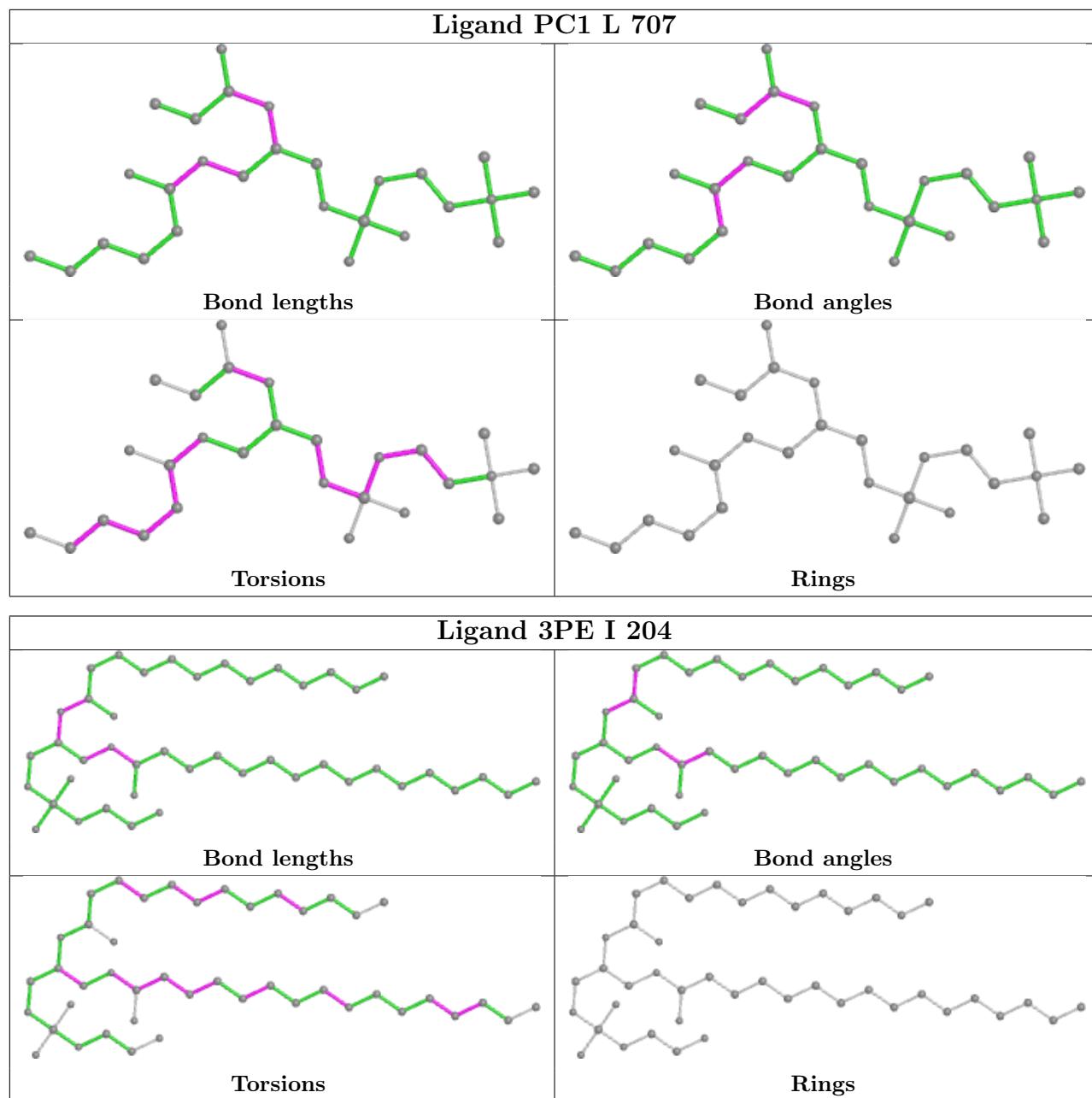


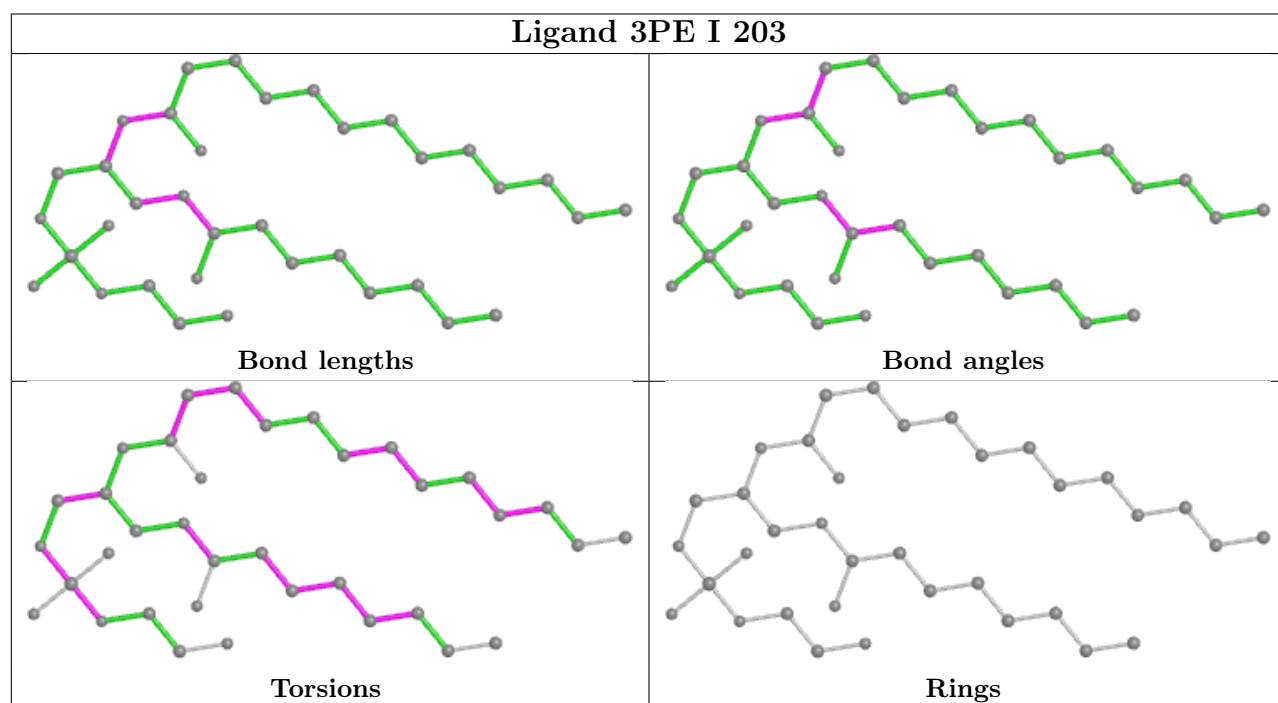
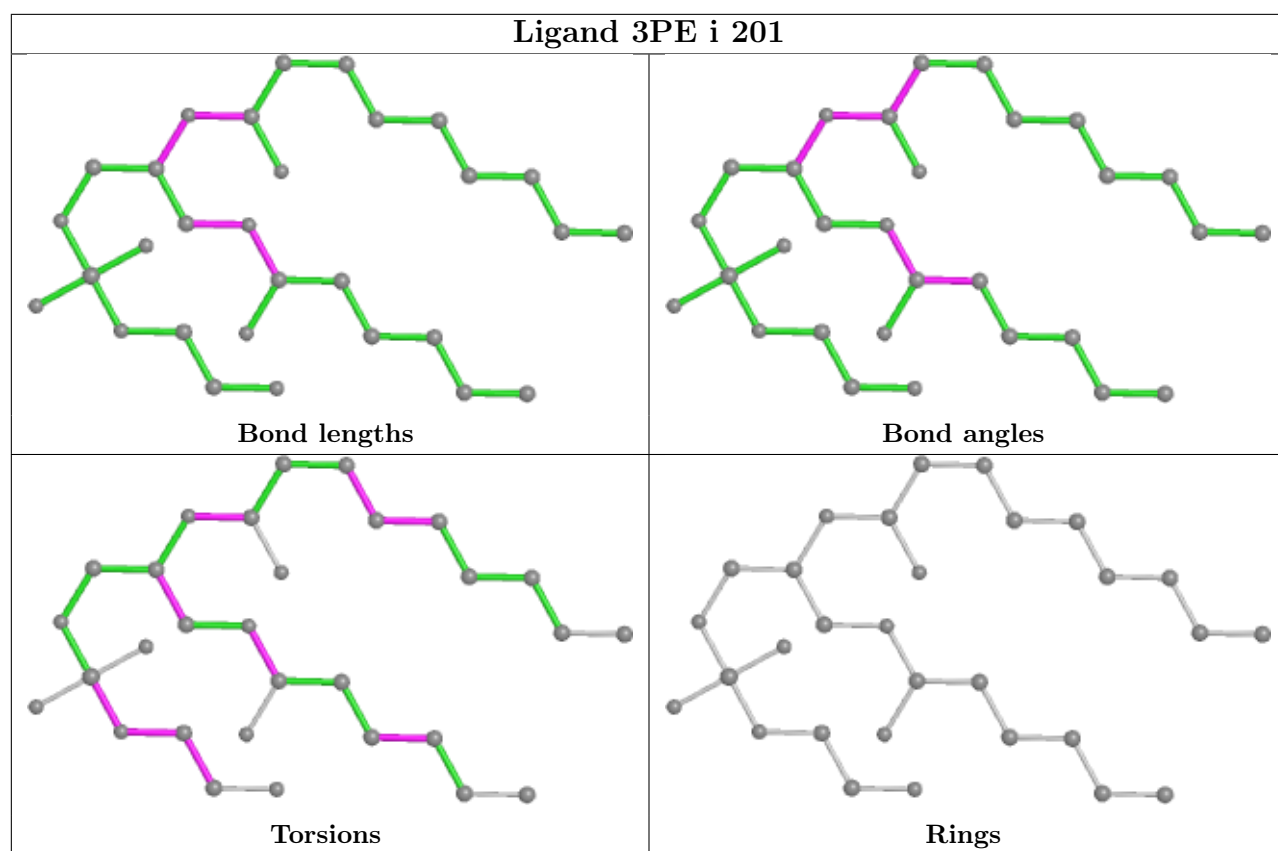


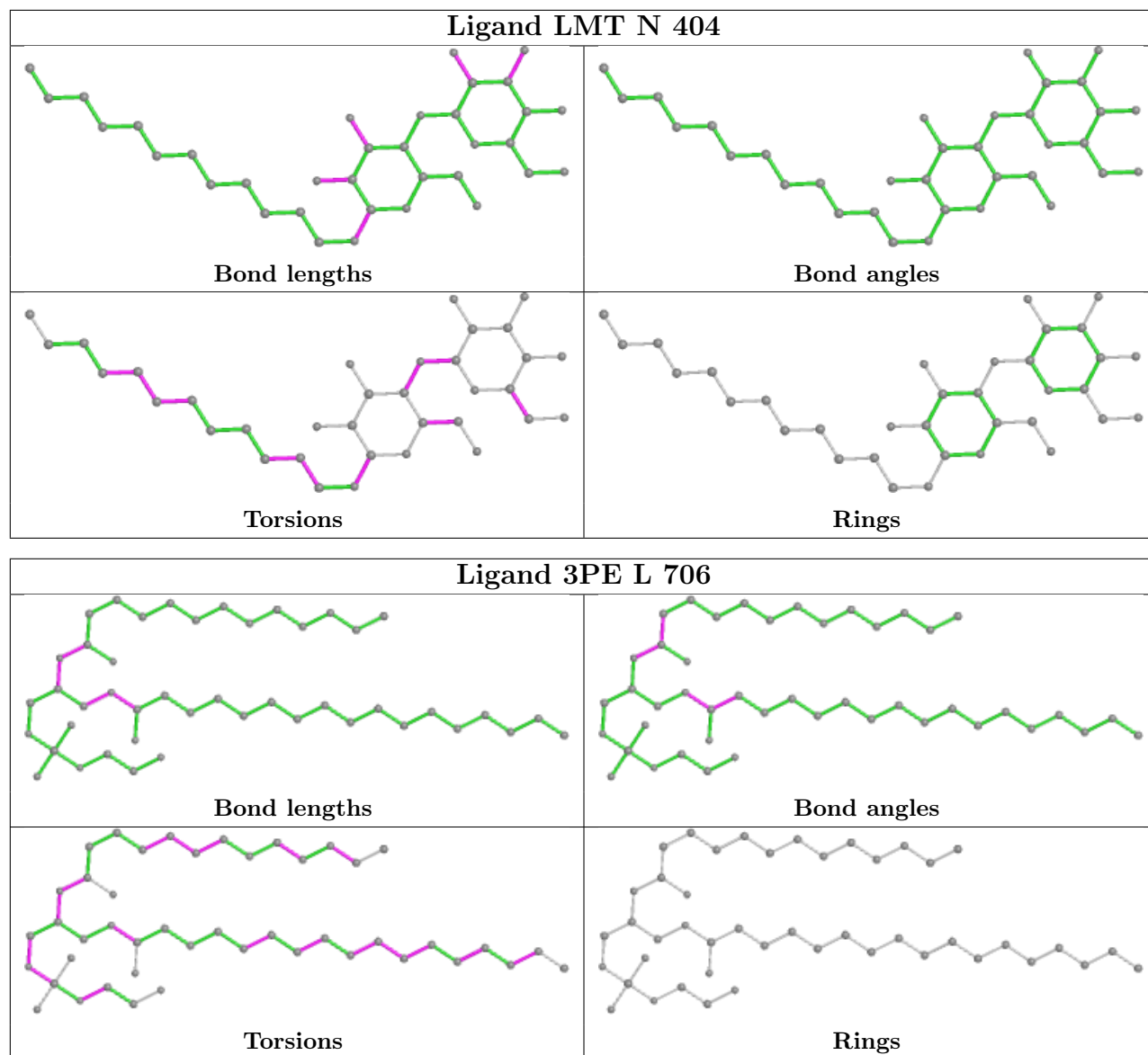


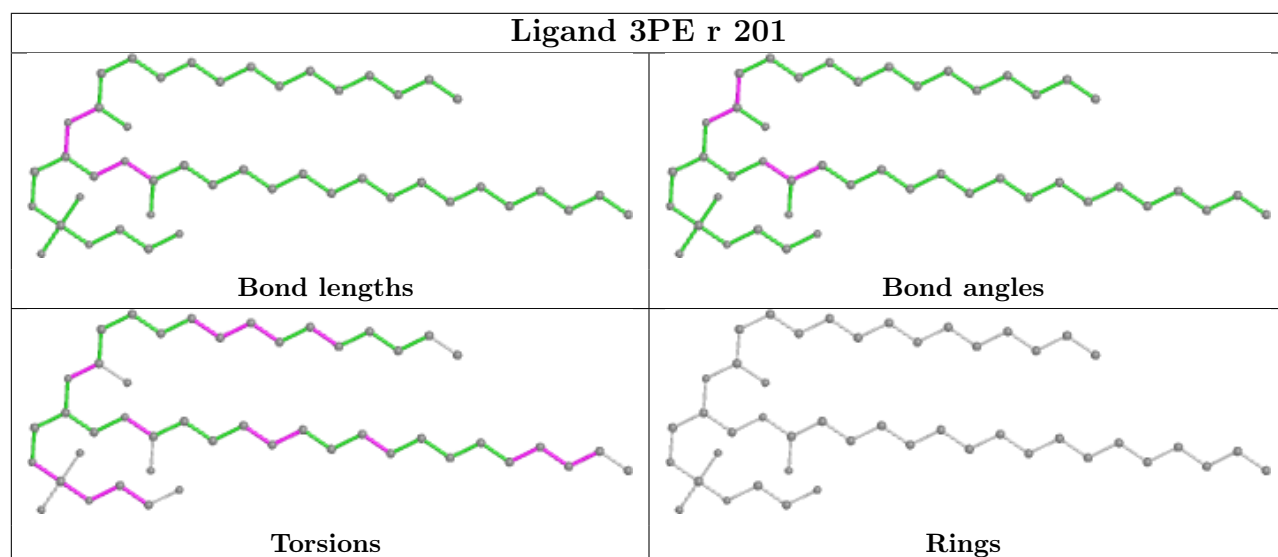
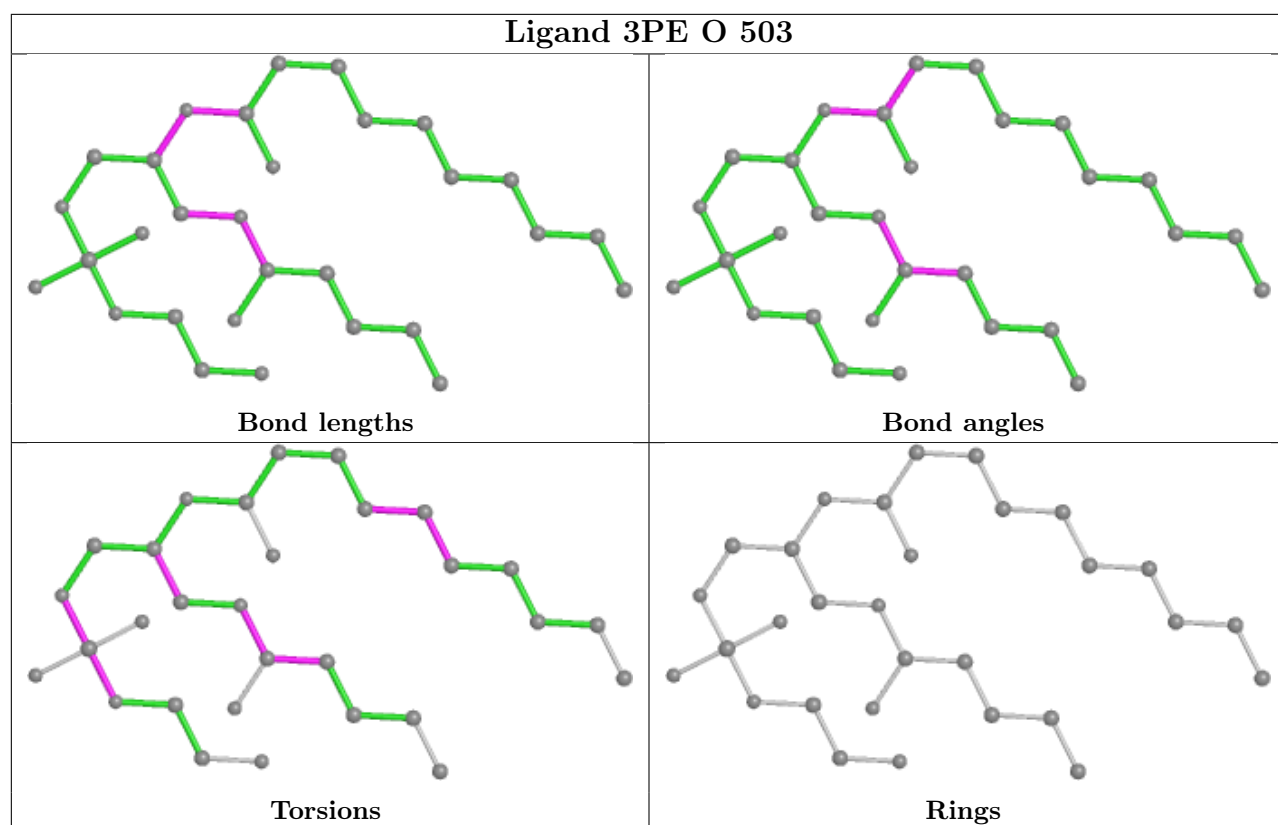


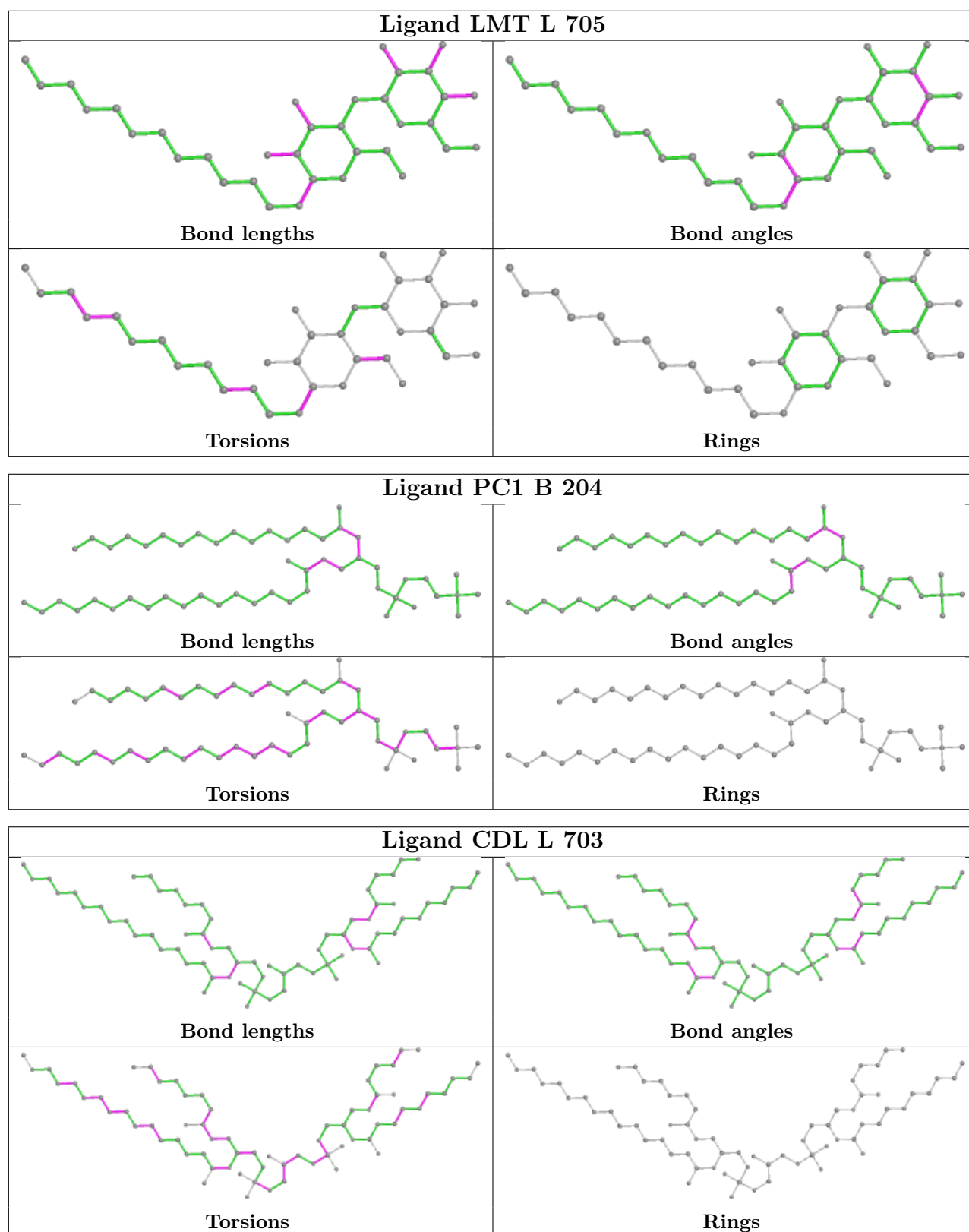


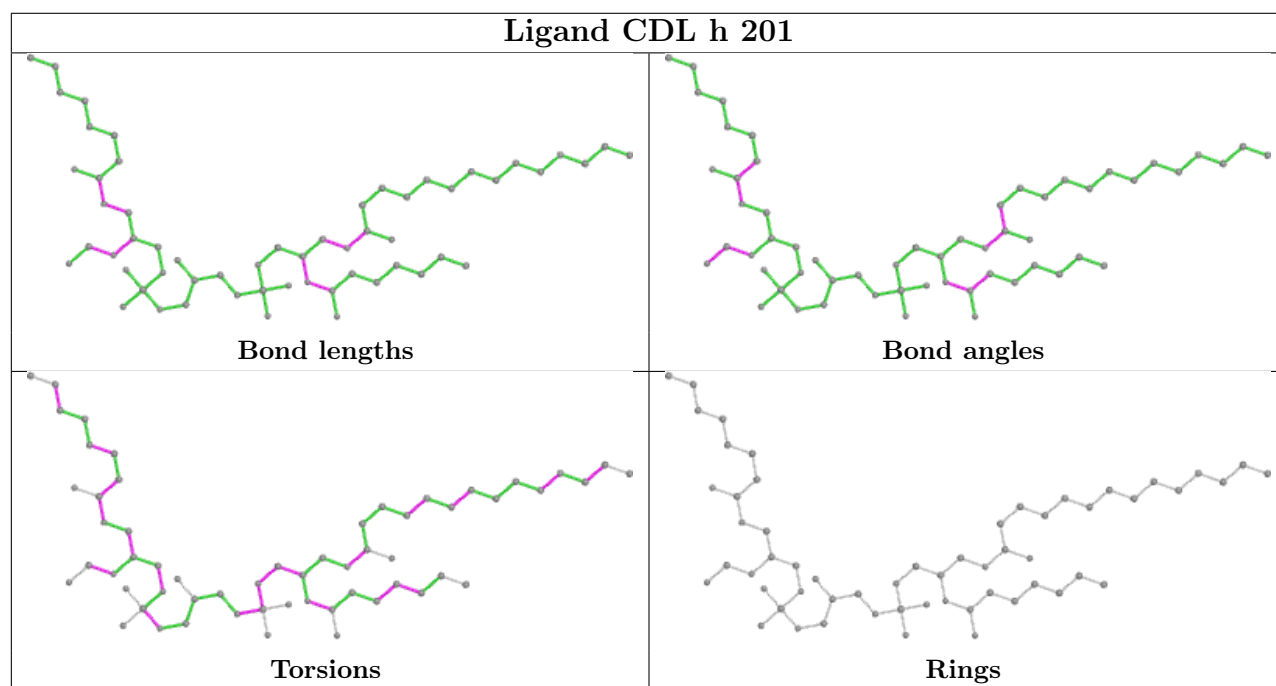
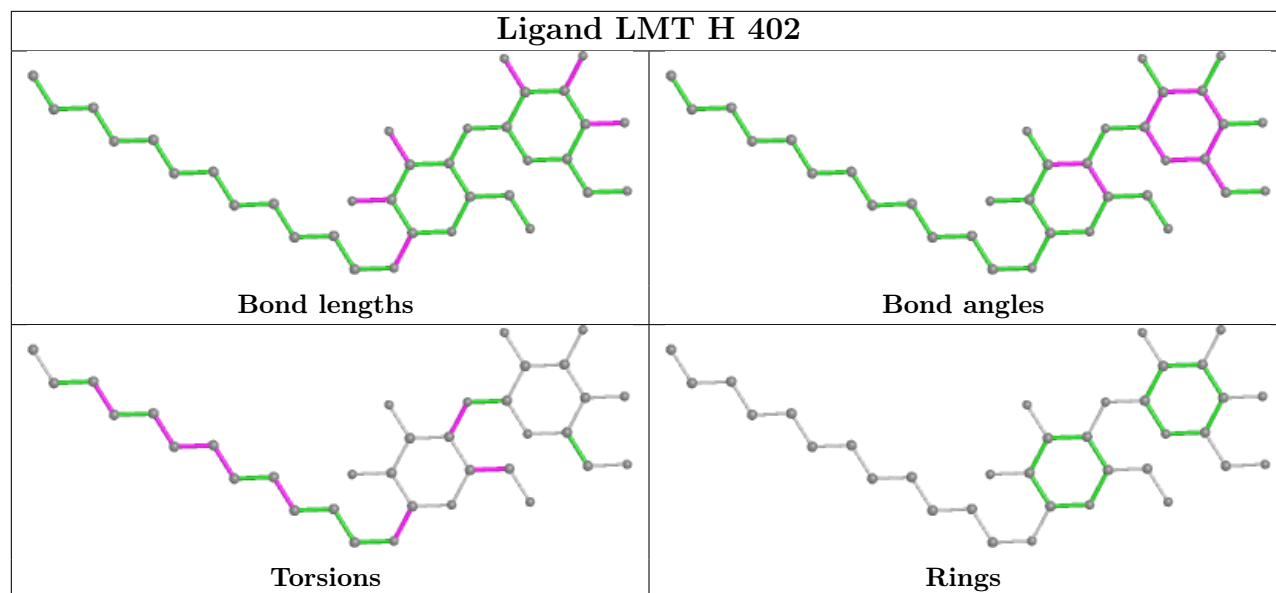


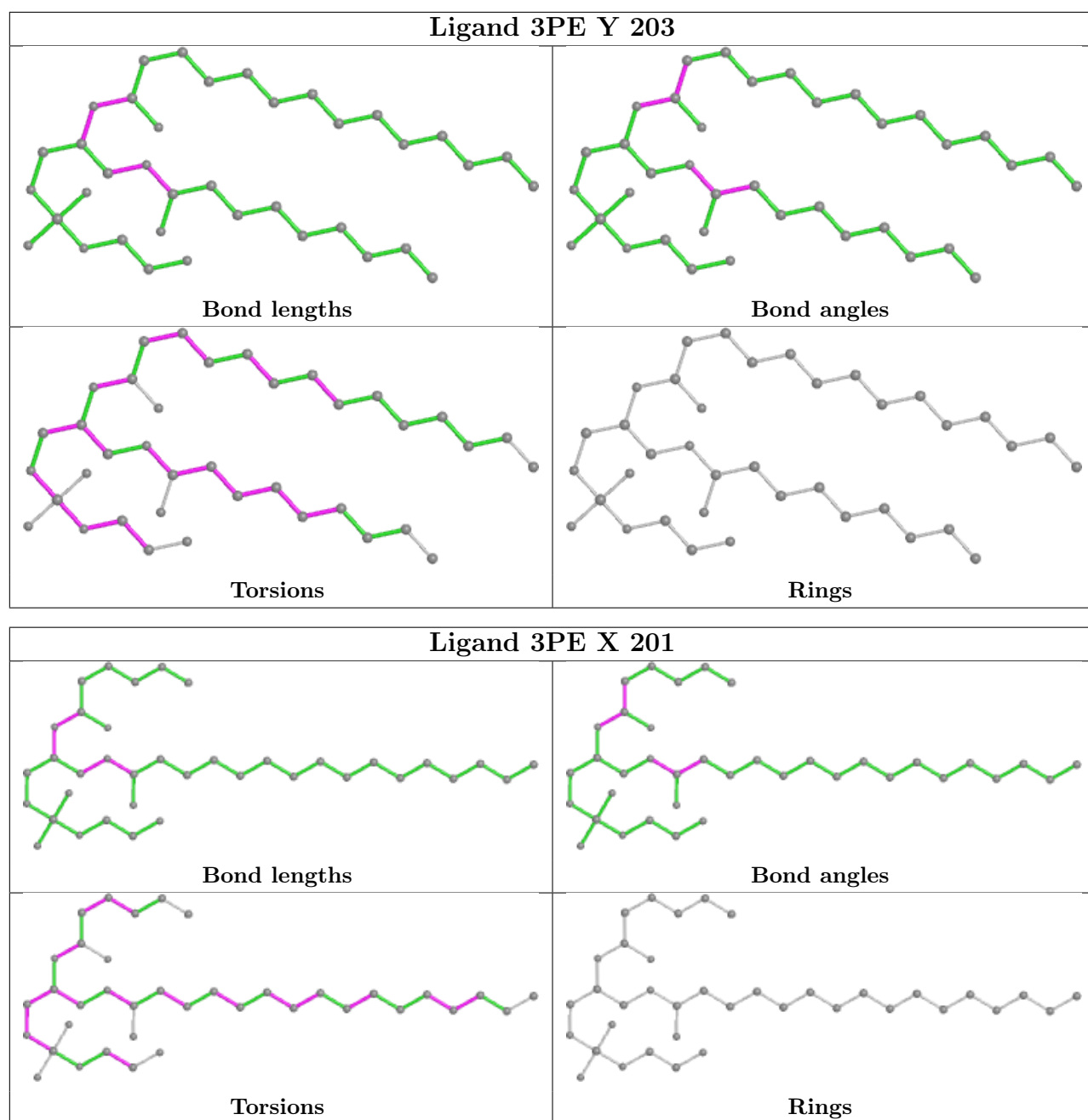


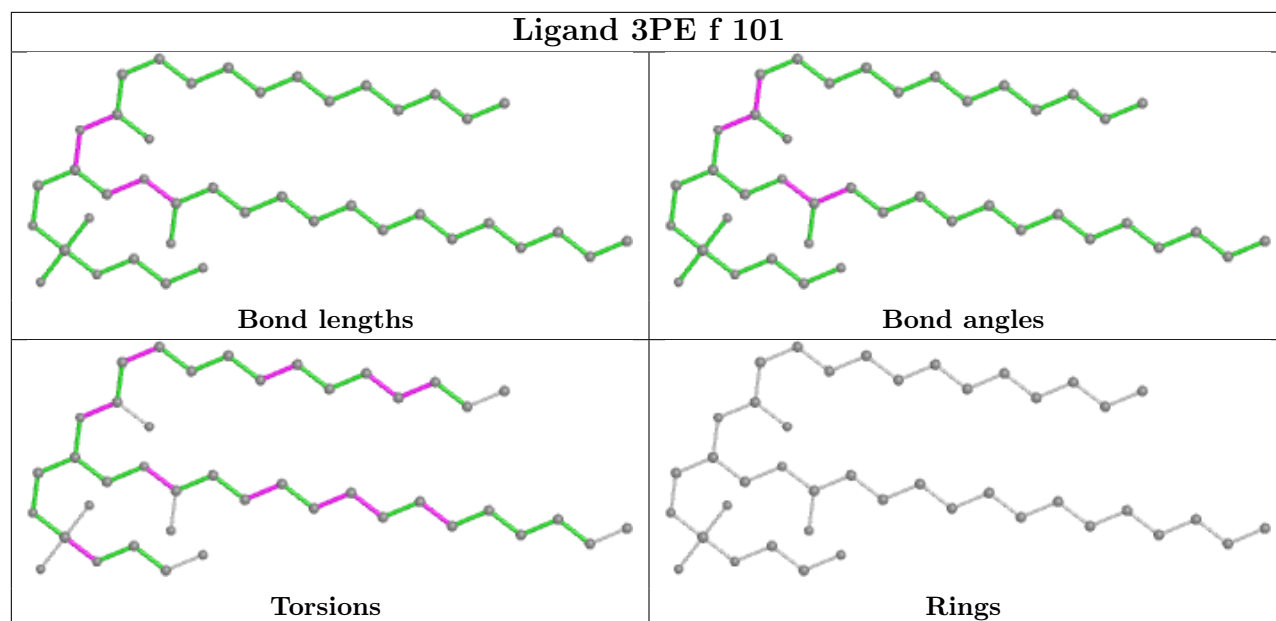
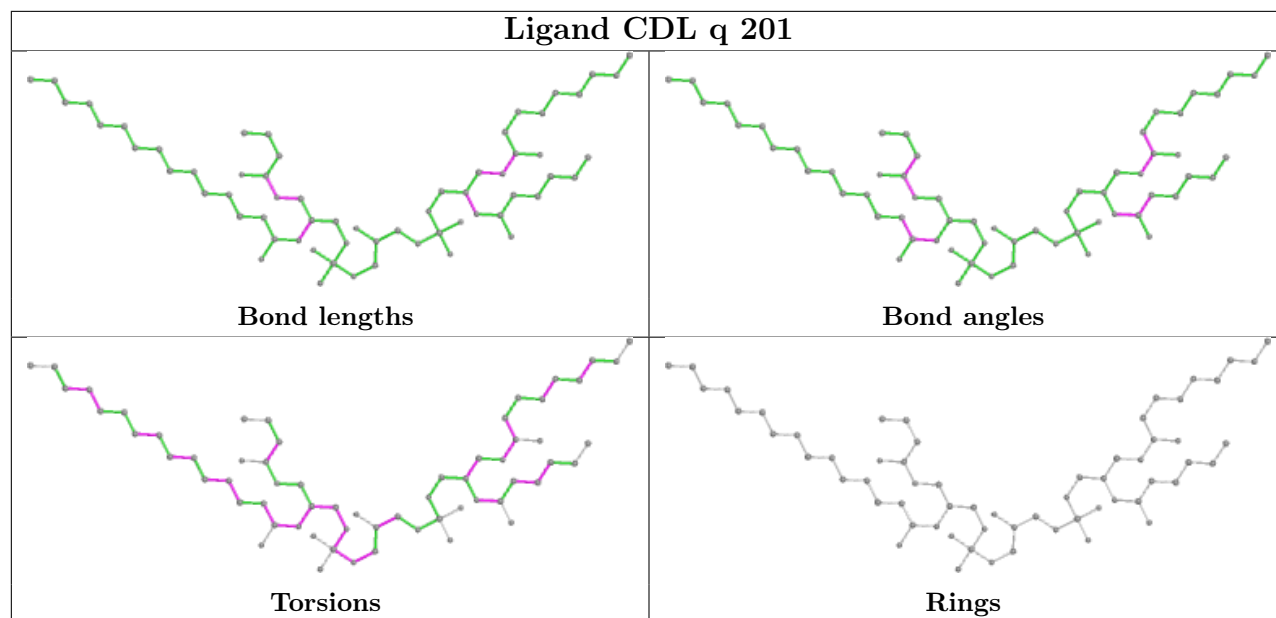


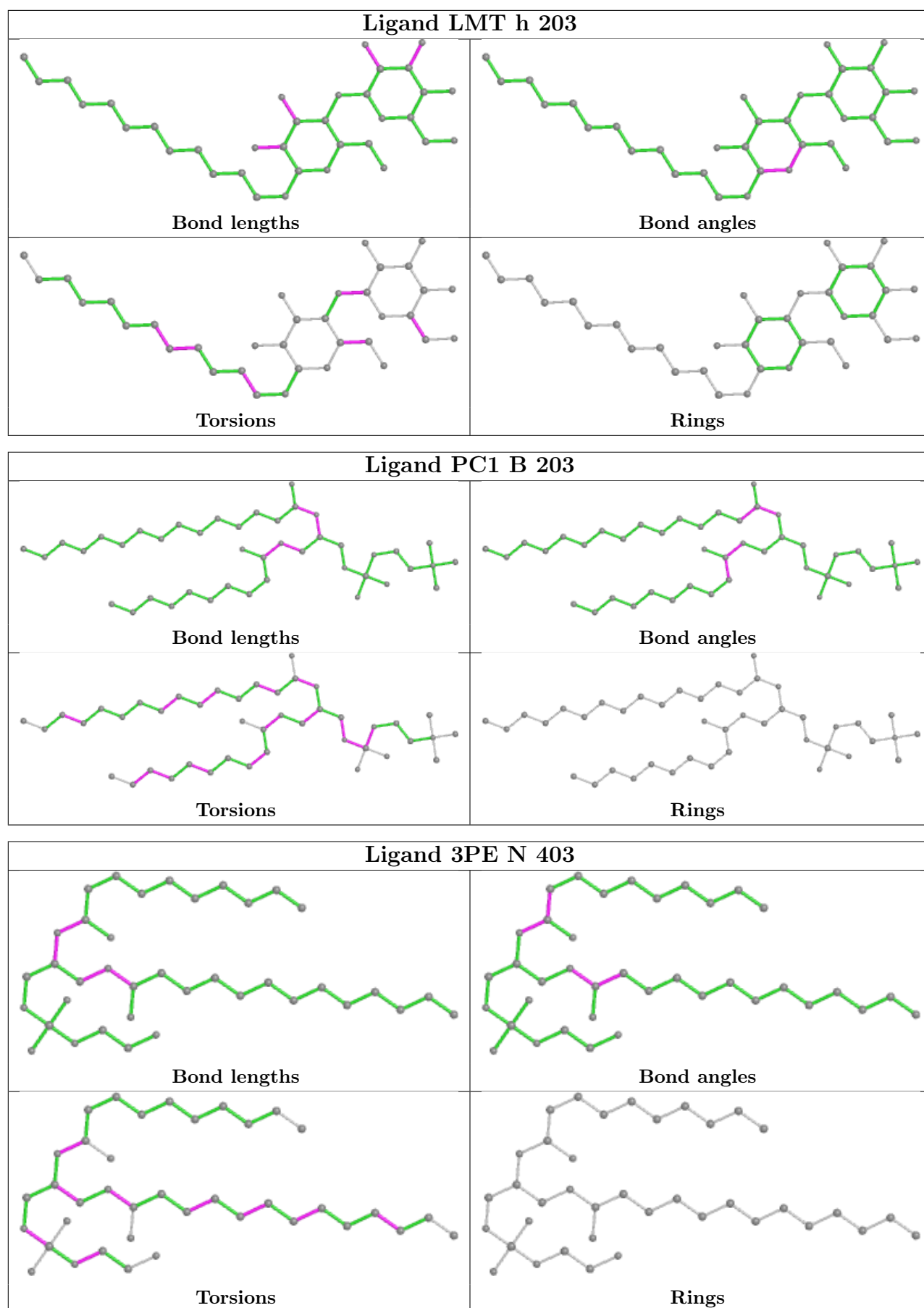


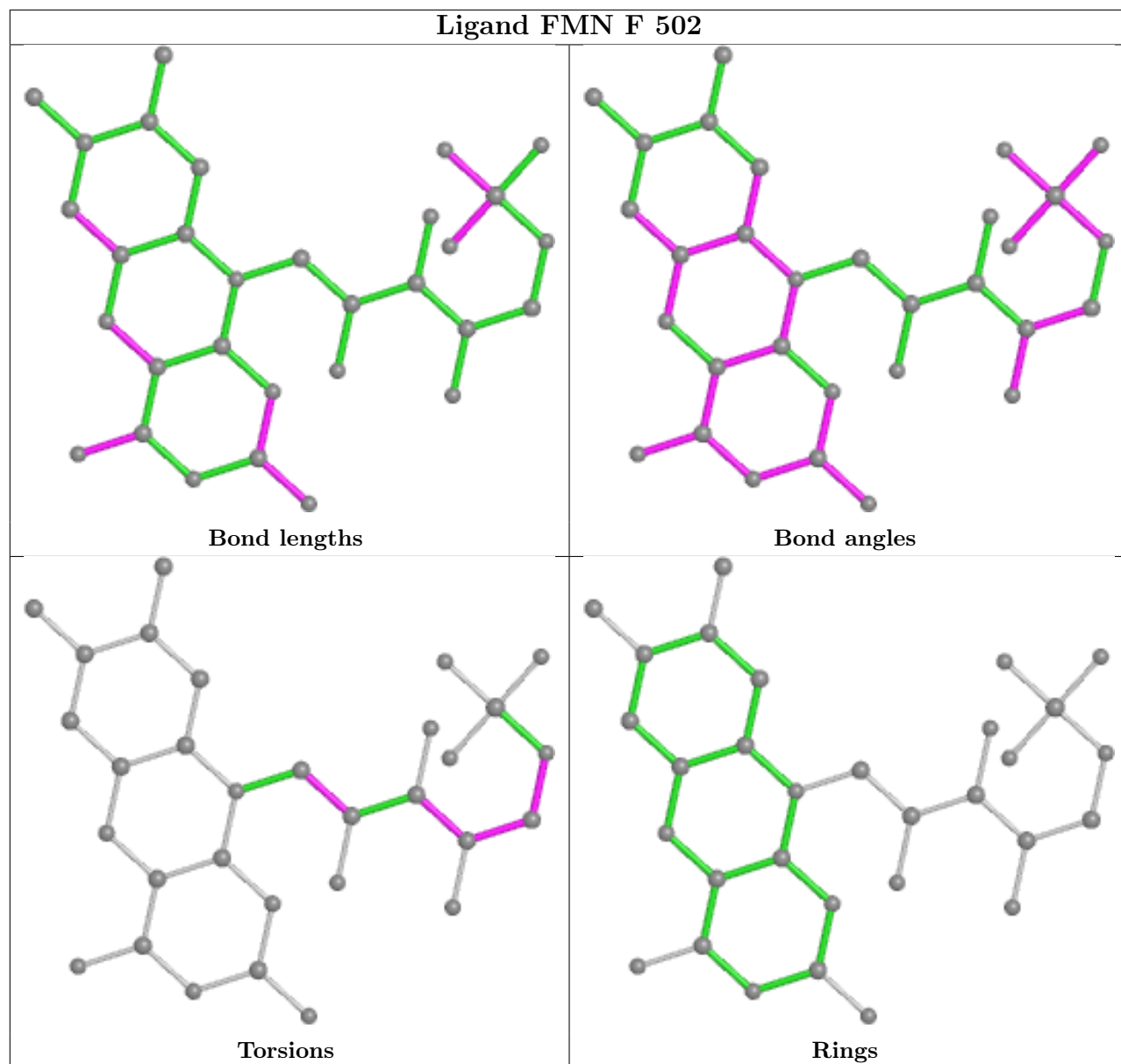


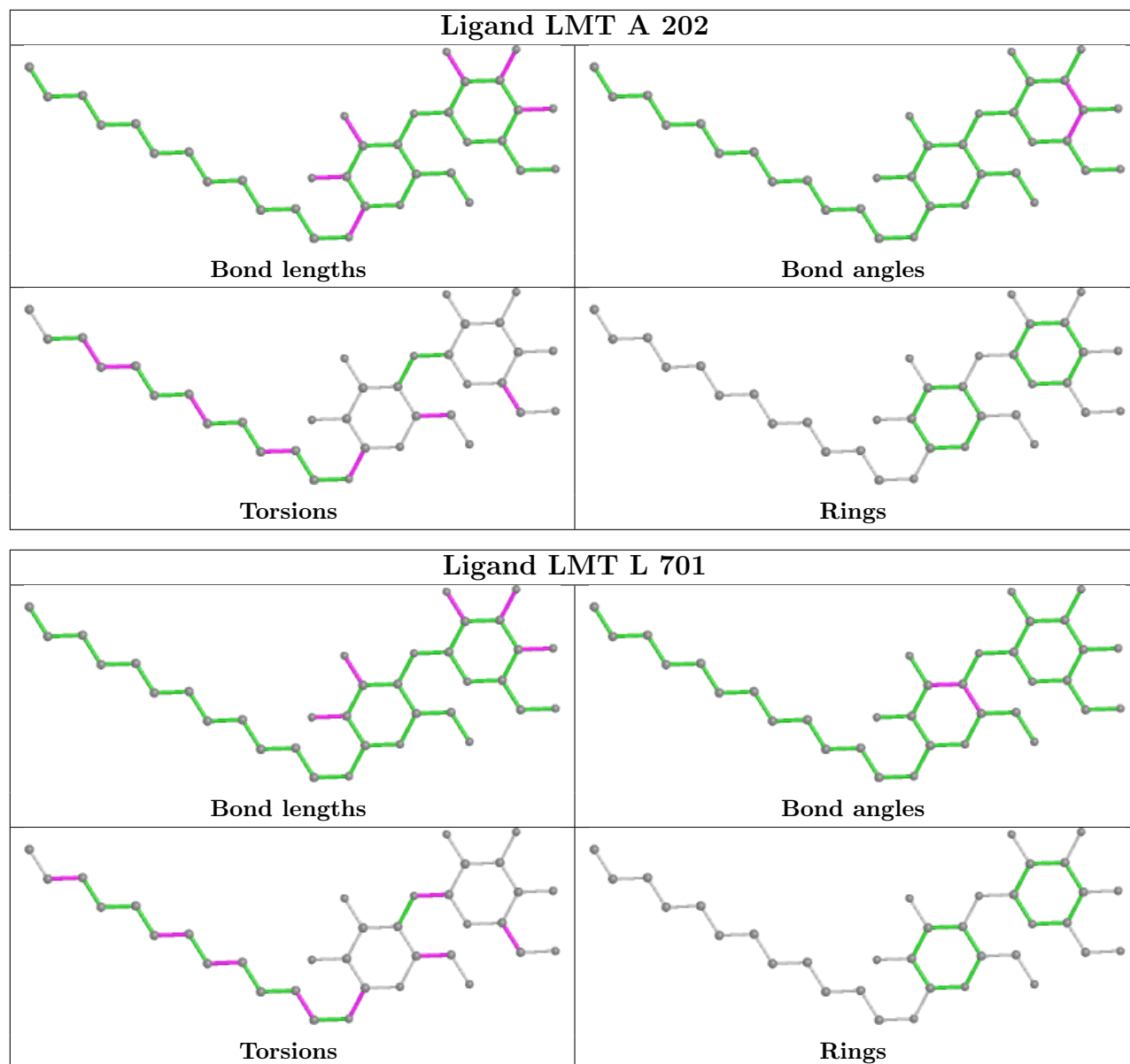


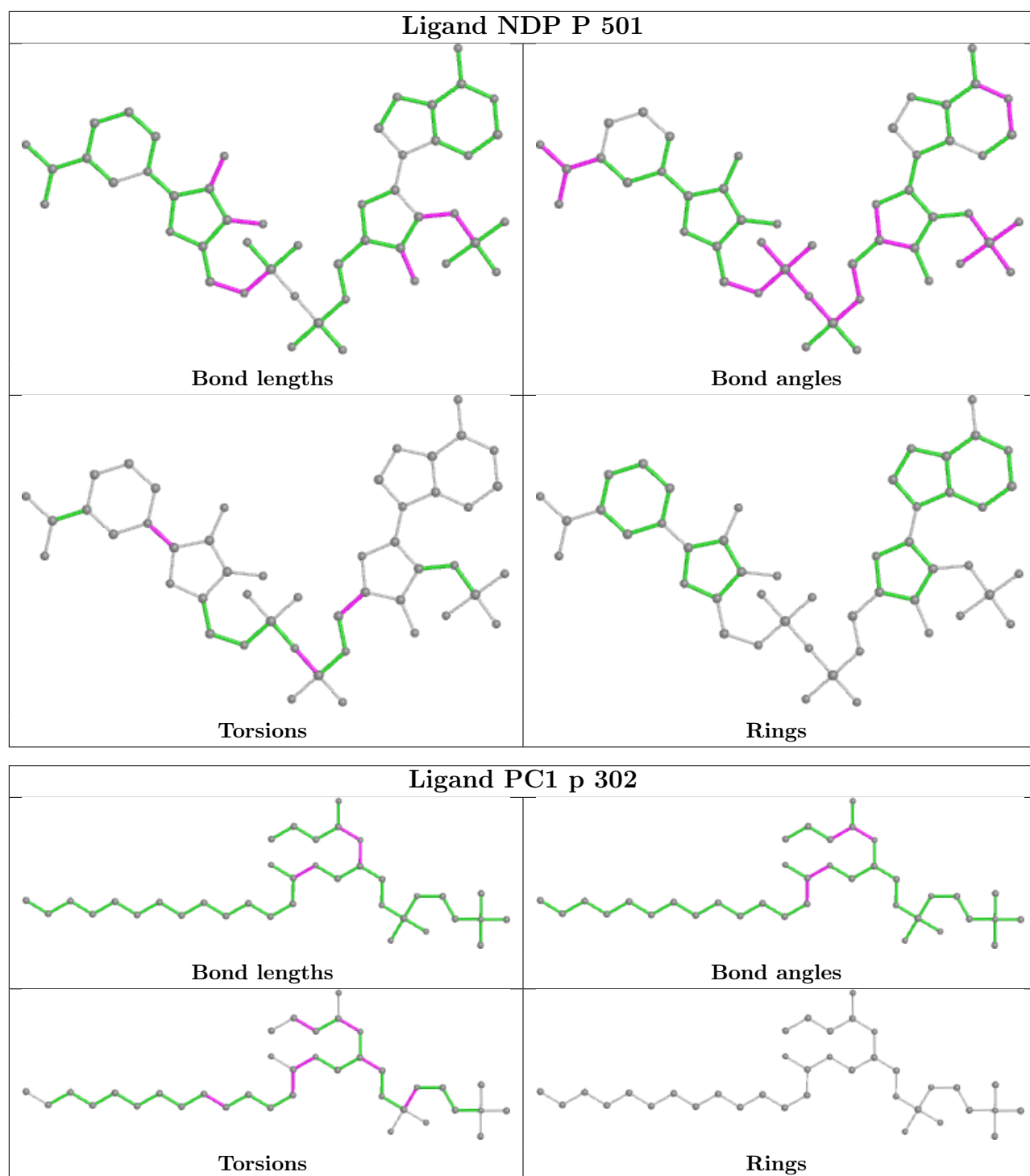


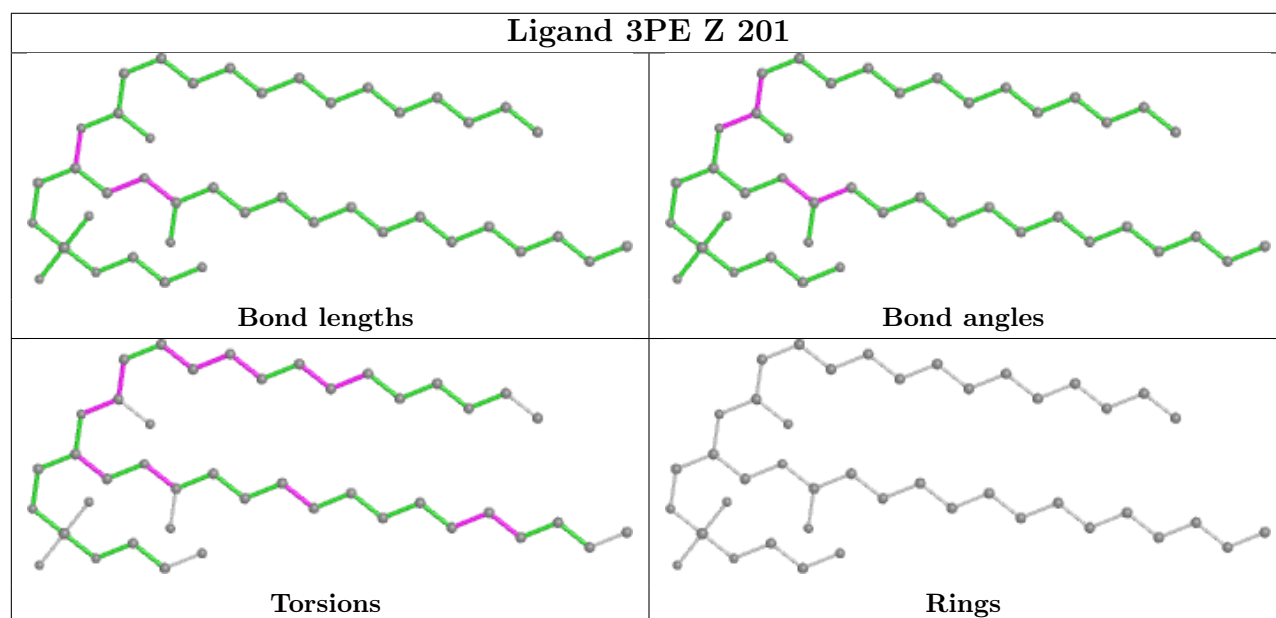
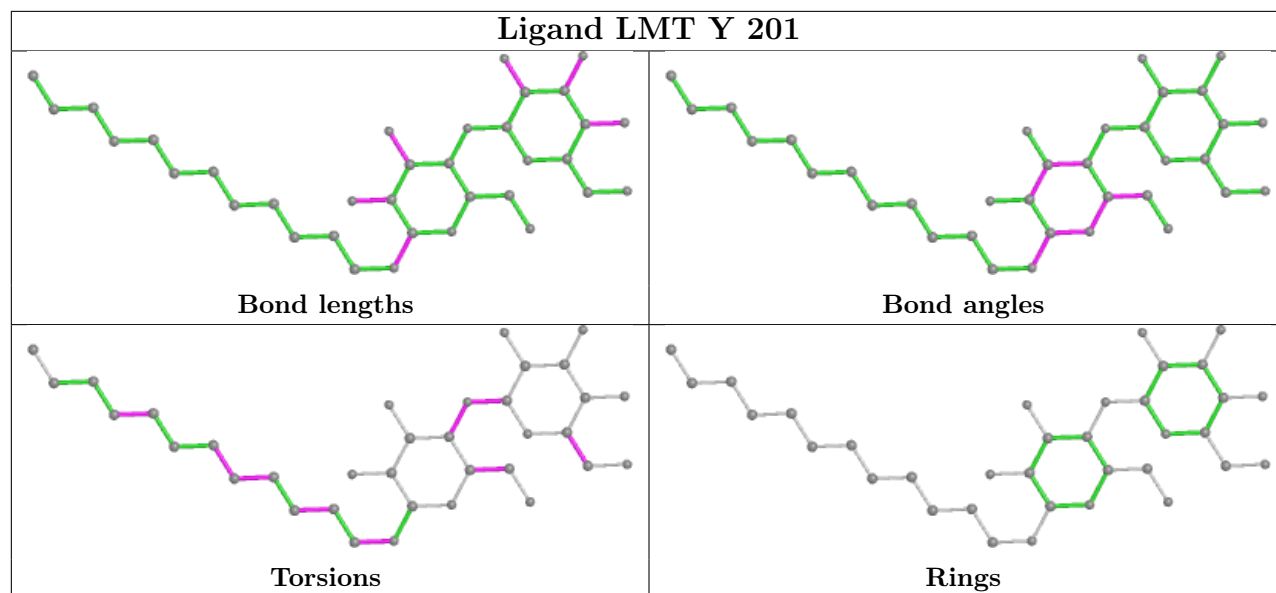


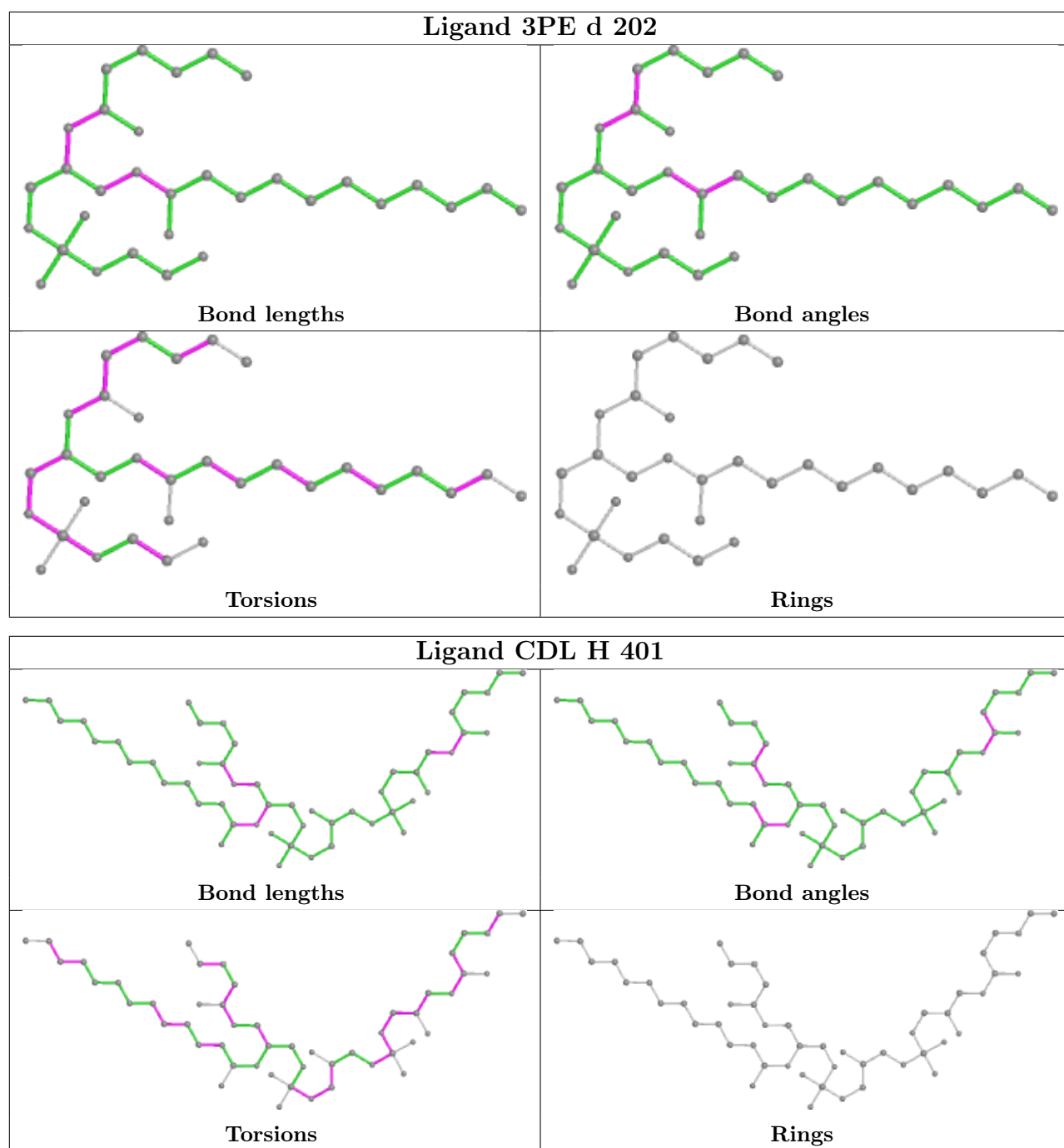












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

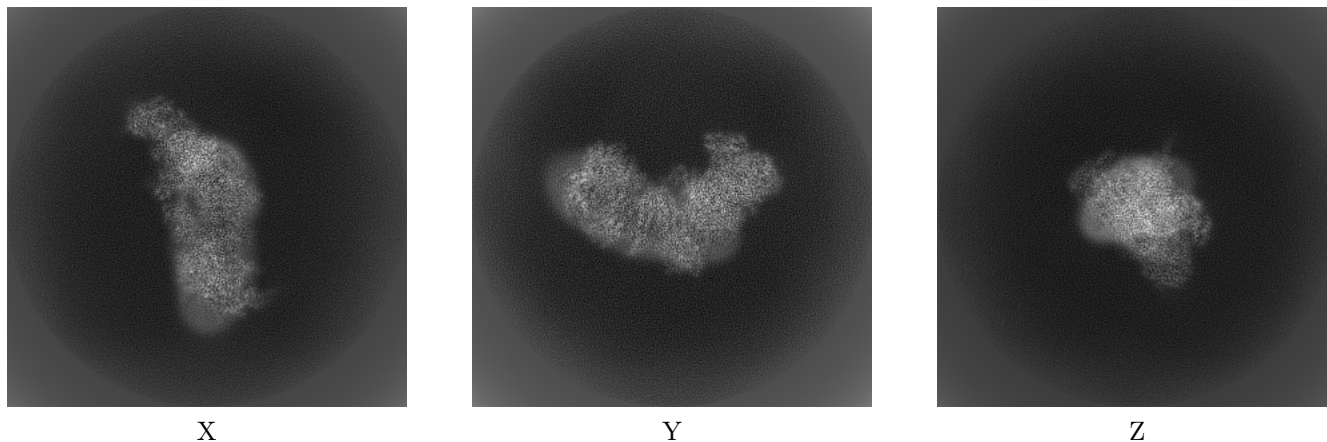
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16965. These allow visual inspection of the internal detail of the map and identification of artifacts.

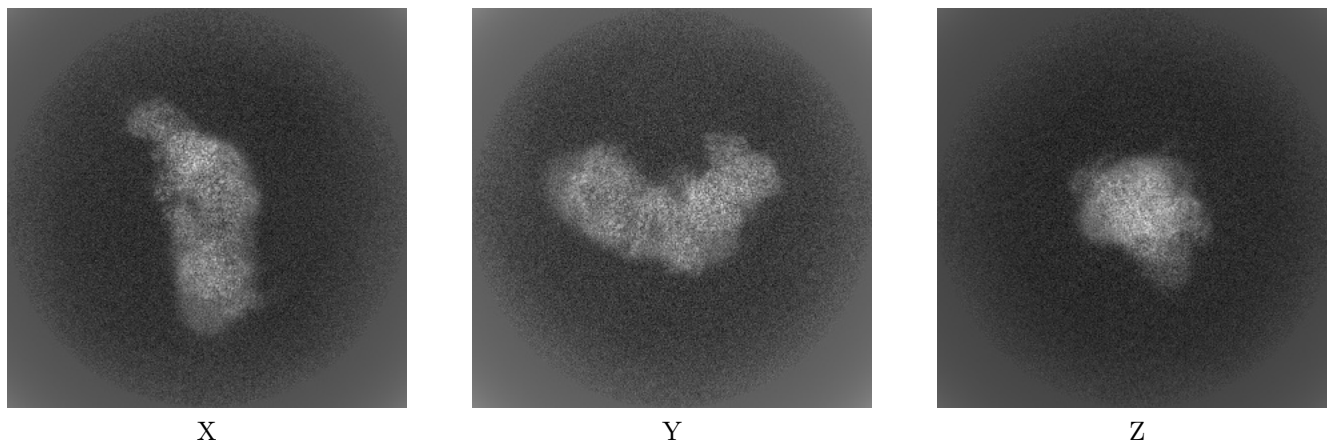
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



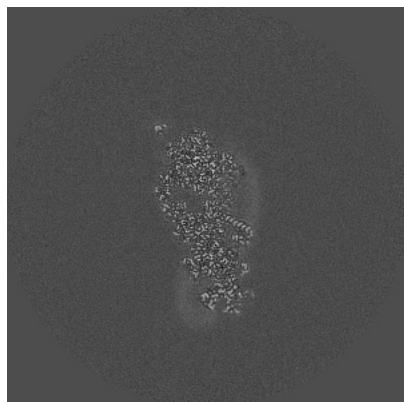
6.1.2 Raw map



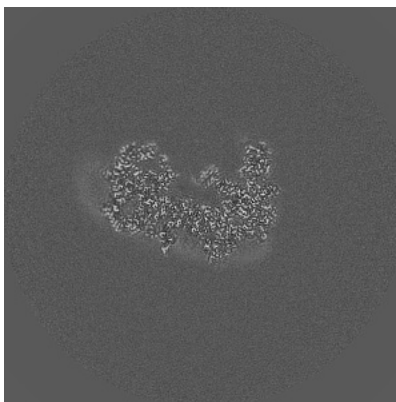
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

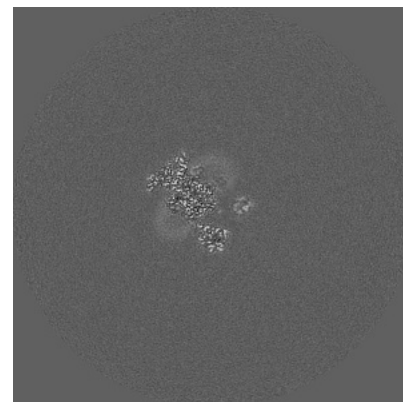
6.2.1 Primary map



X Index: 350

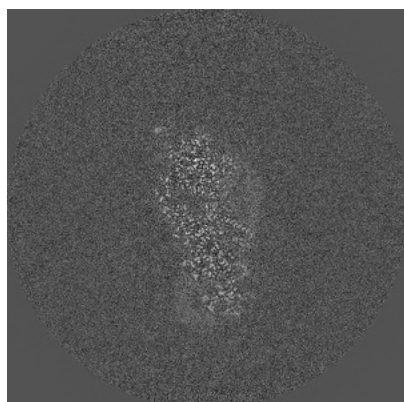


Y Index: 350

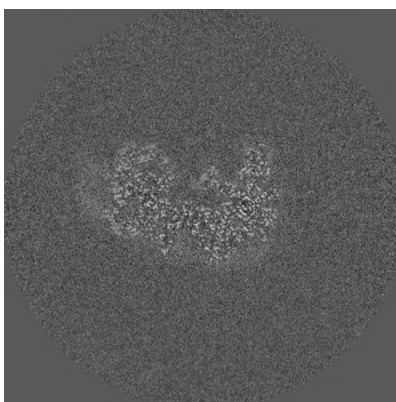


Z Index: 350

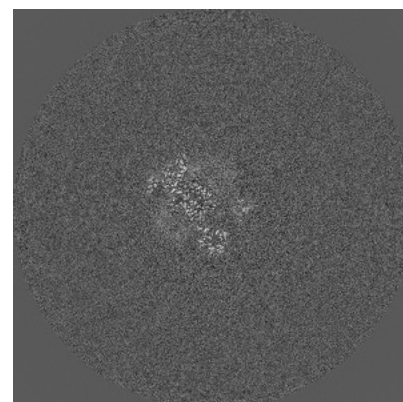
6.2.2 Raw map



X Index: 350



Y Index: 350



Z Index: 350

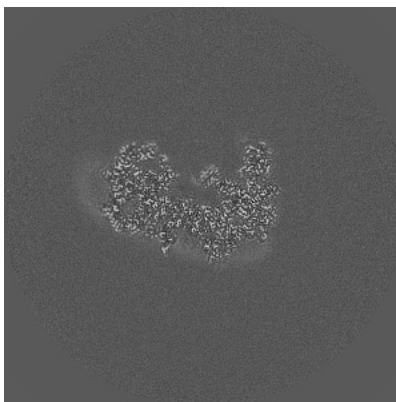
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

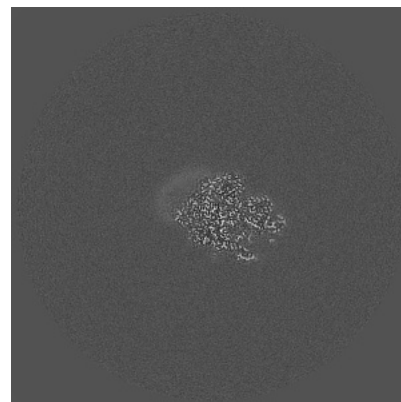
6.3.1 Primary map



X Index: 370

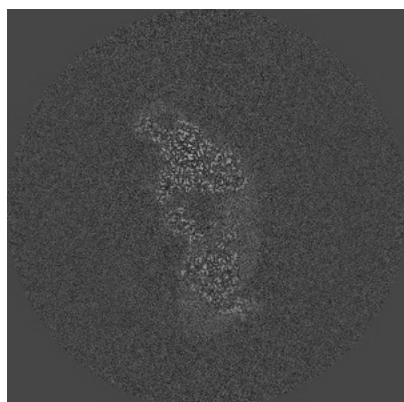


Y Index: 350

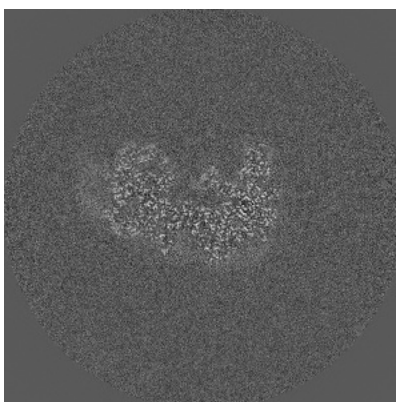


Z Index: 438

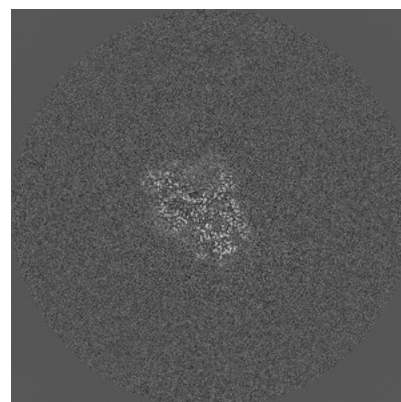
6.3.2 Raw map



X Index: 370



Y Index: 350

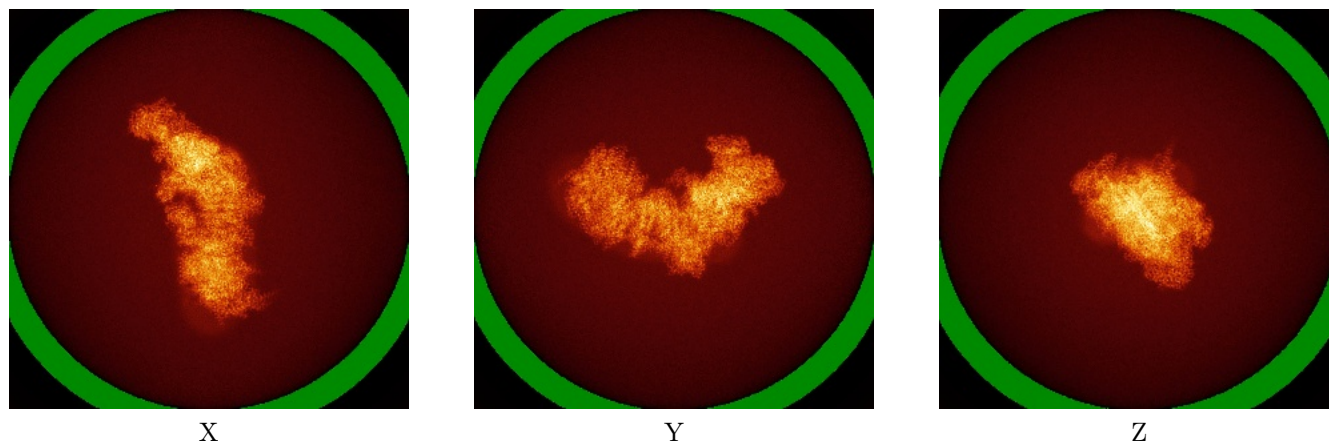


Z Index: 386

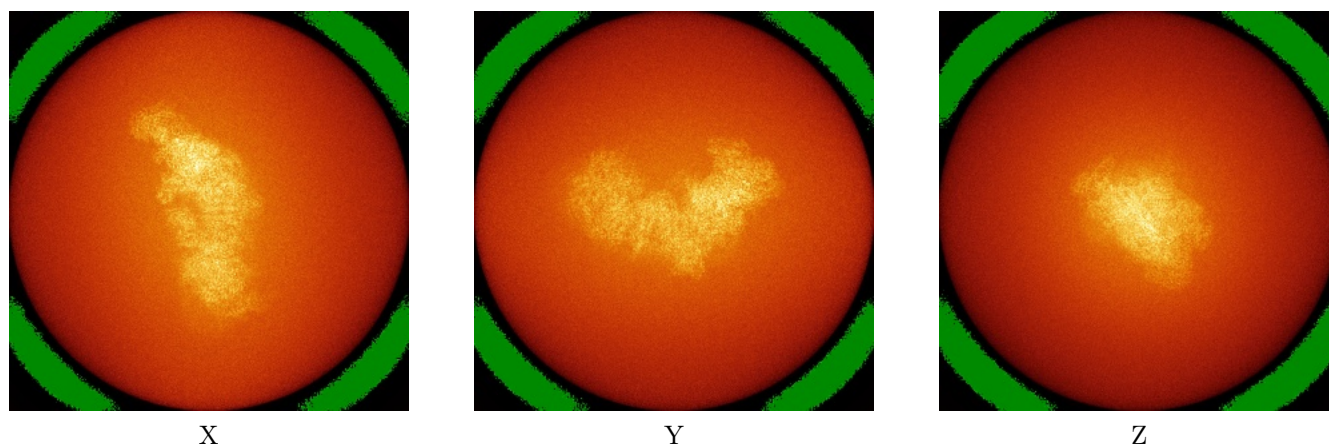
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



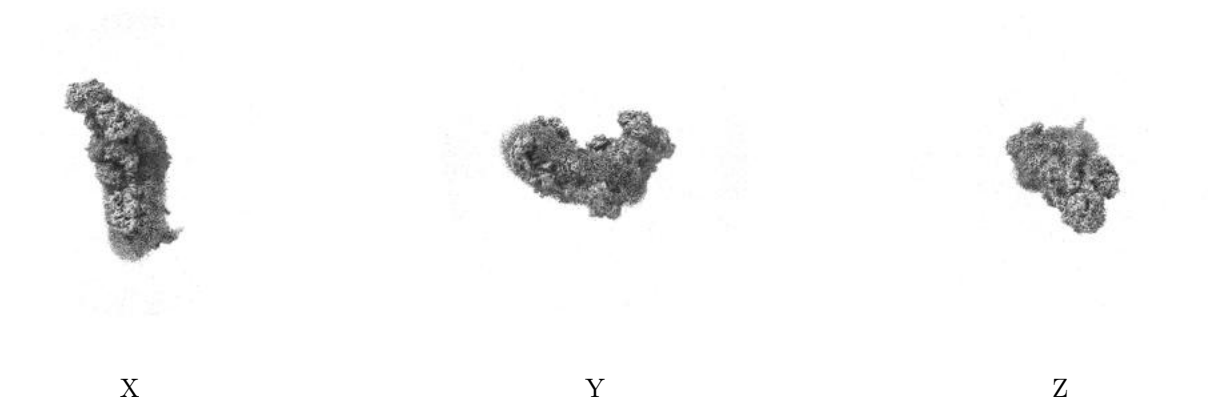
6.4.2 Raw map



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.

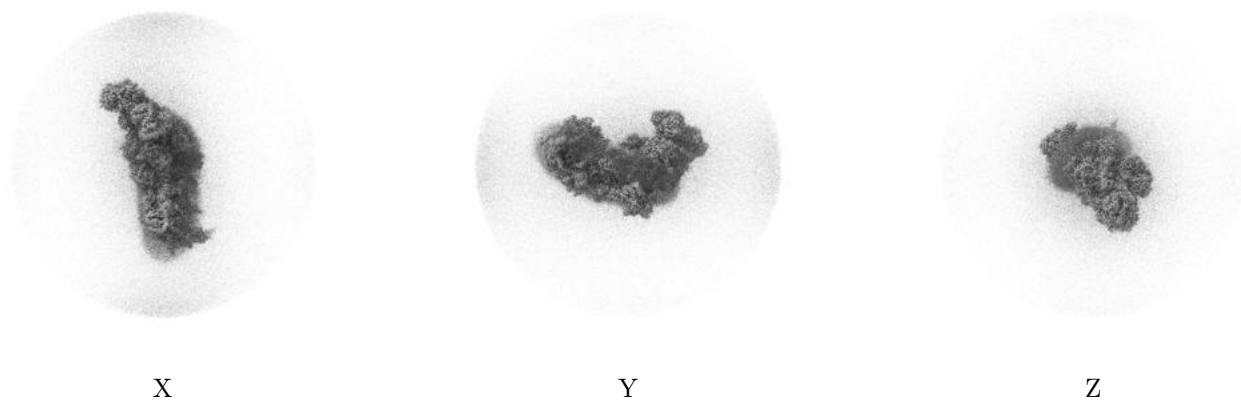
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. 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.

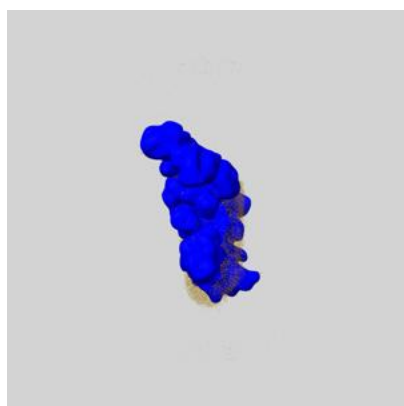
6.6 Mask visualisation [i](#)

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

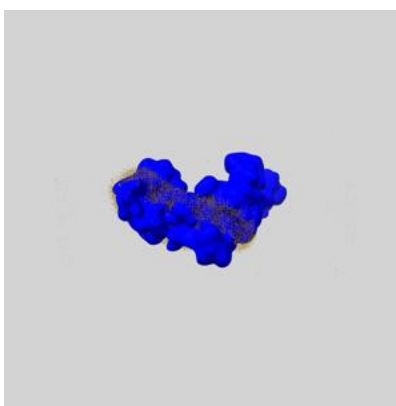
A mask typically either:

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

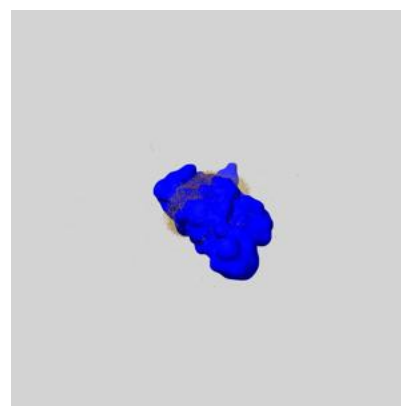
6.6.1 emd_16965_msk_1.map [i](#)



X



Y

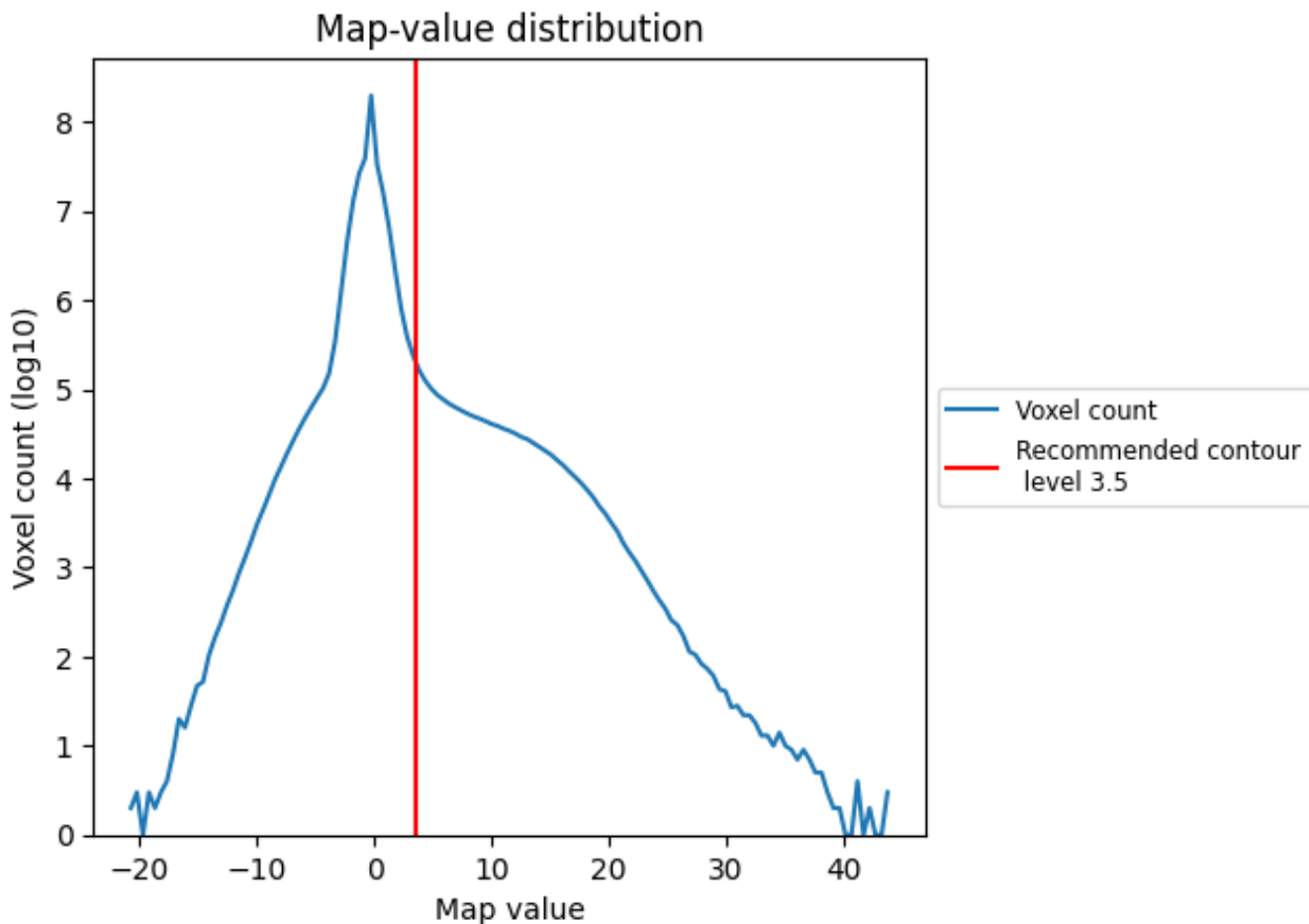


Z

7 Map analysis [i](#)

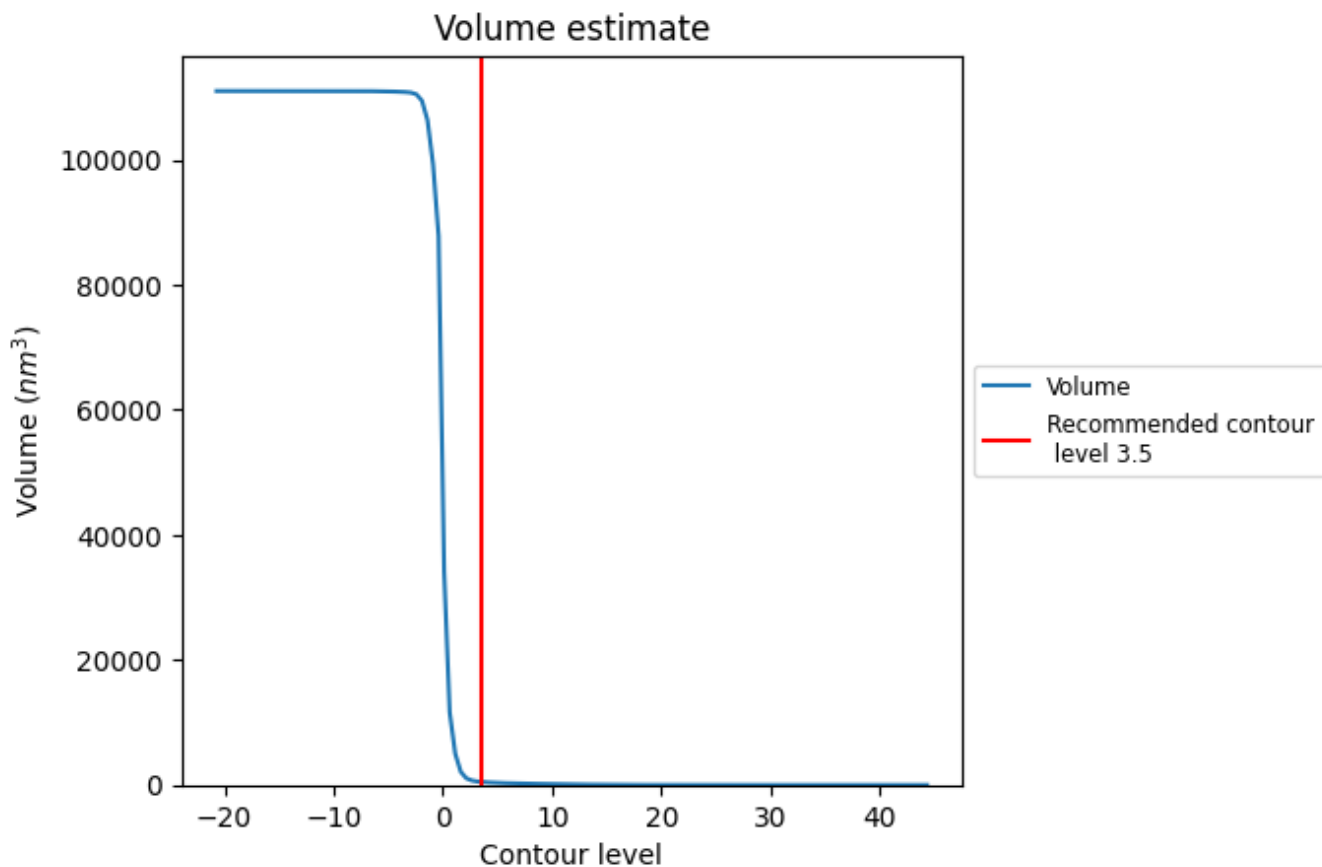
This section contains the results of statistical analysis of the map.

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.

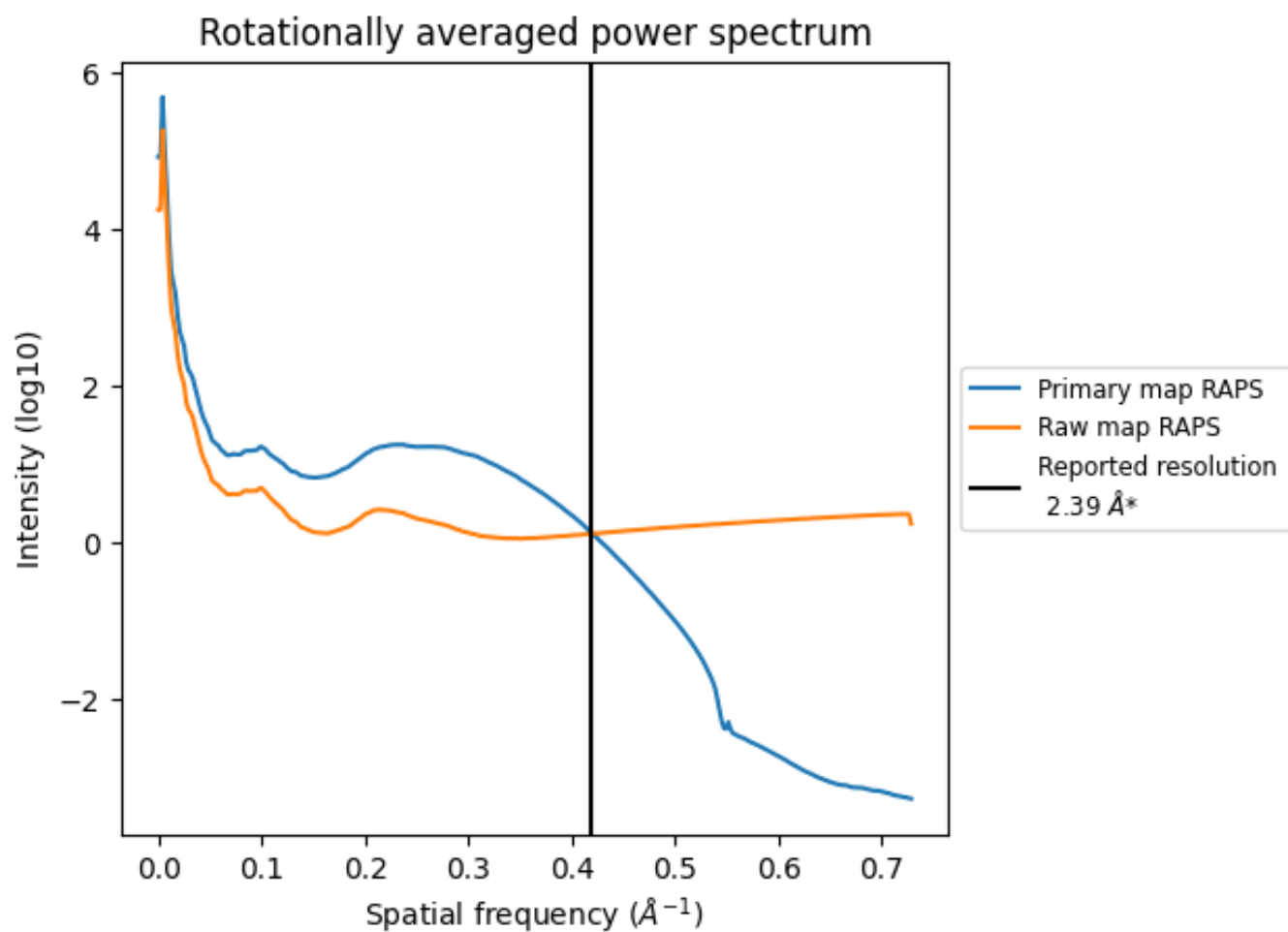
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 496 nm^3 ; this corresponds to an approximate mass of 448 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

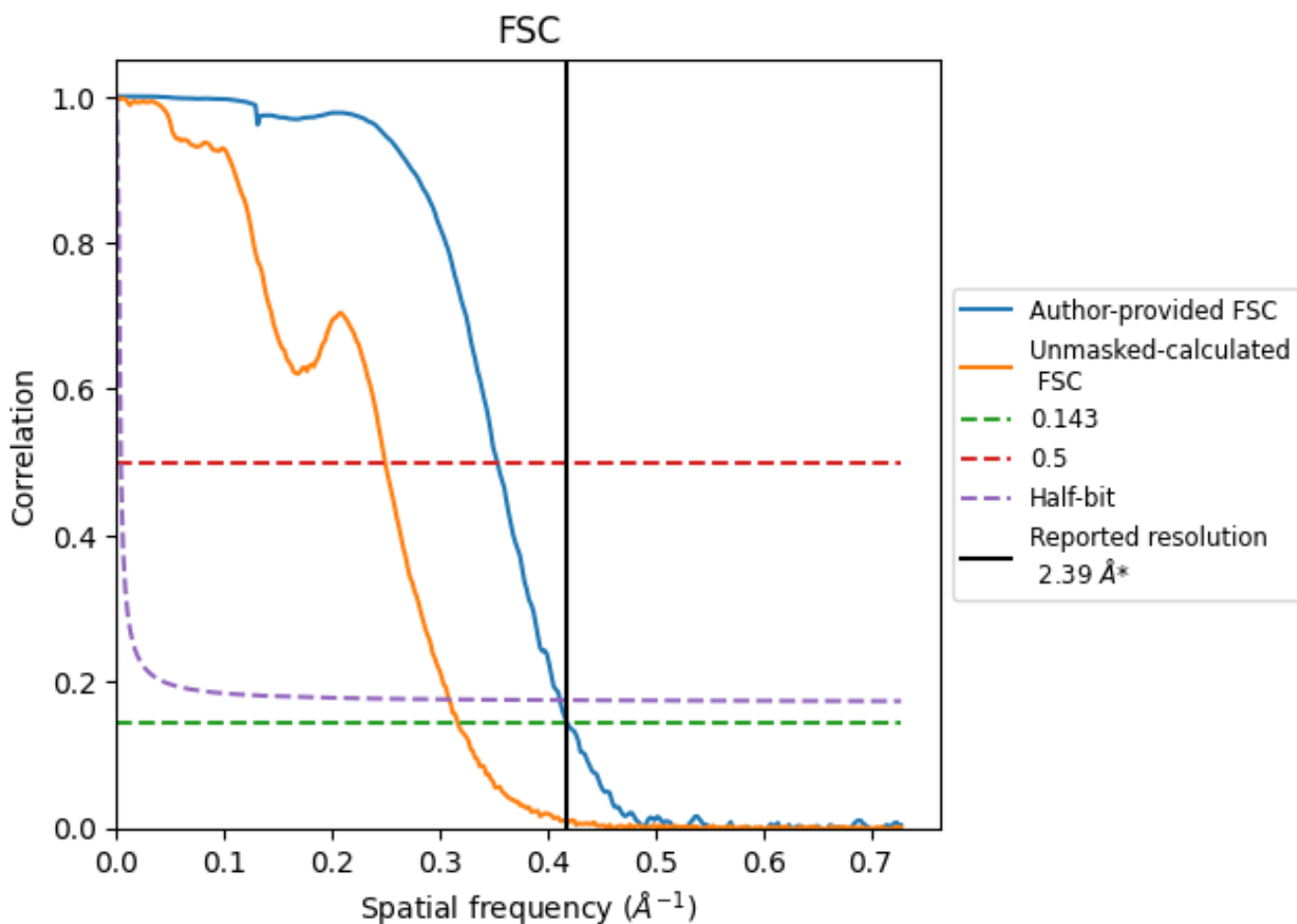


*Reported resolution corresponds to spatial frequency of 0.418 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.418 Å⁻¹

8.2 Resolution estimates [i](#)

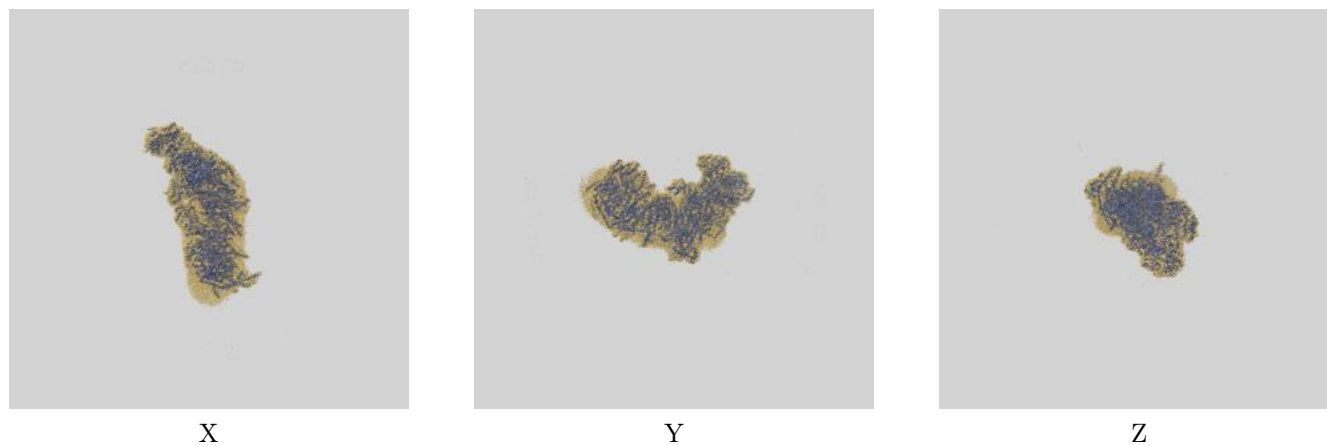
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.39	2.83	2.43
Unmasked-calculated*	3.15	4.01	3.24

*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 3.15 differs from the reported value 2.39 by more than 10 %

9 Map-model fit [i](#)

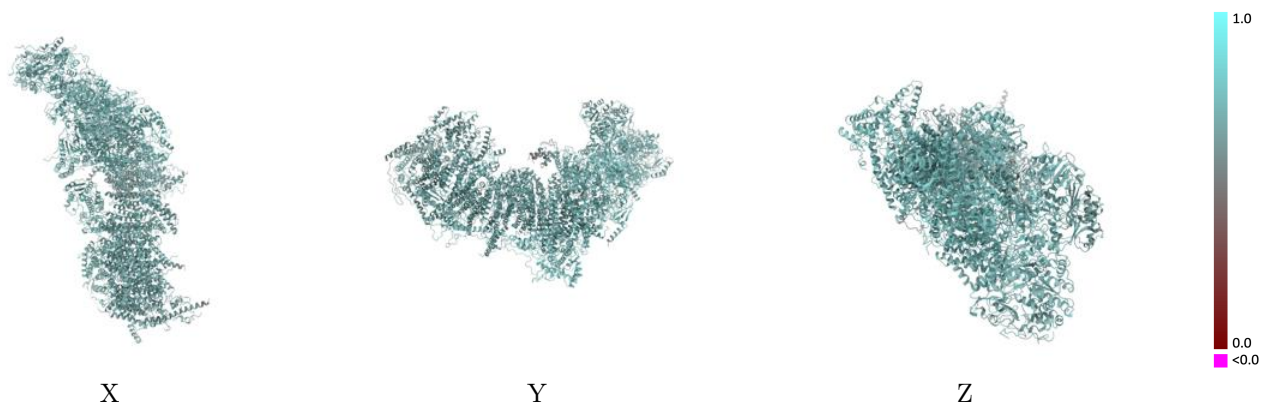
This section contains information regarding the fit between EMDB map EMD-16965 and PDB model 8OM1. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



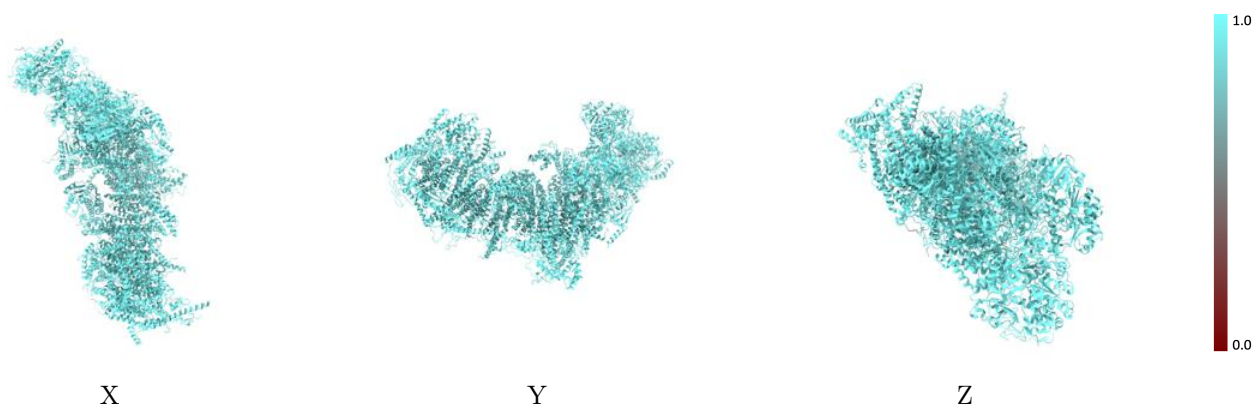
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



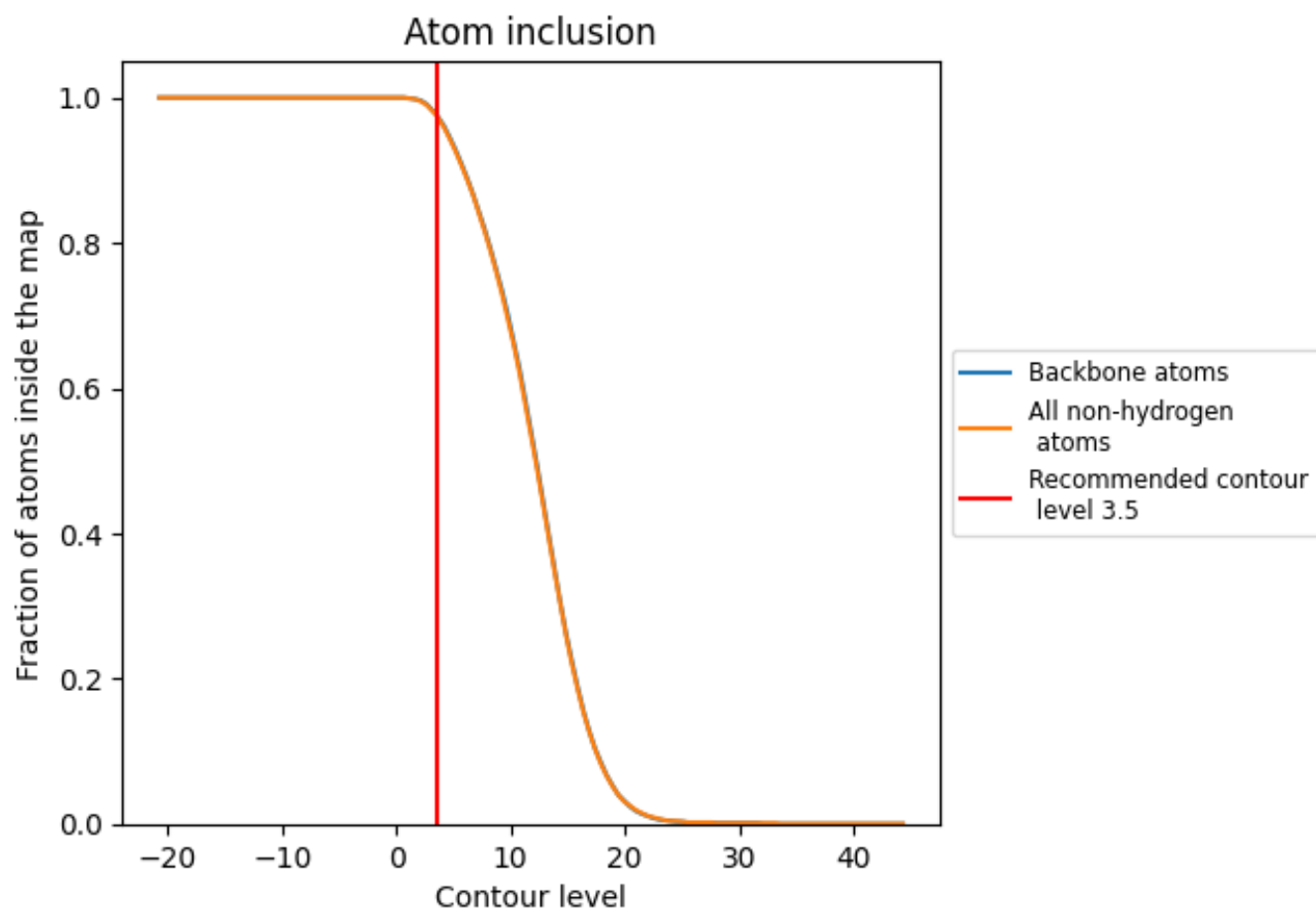
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9760	 0.6960
A	 0.9820	 0.7130
B	 0.9890	 0.7390
C	 0.9870	 0.7410
D	 0.9870	 0.7410
E	 0.9710	 0.6690
F	 0.9860	 0.6800
G	 0.9820	 0.7010
H	 0.9920	 0.7310
I	 0.9750	 0.7350
J	 0.9670	 0.6970
K	 0.9860	 0.7290
L	 0.9800	 0.6810
M	 0.9950	 0.7290
N	 0.9910	 0.7270
O	 0.9820	 0.7090
P	 0.9850	 0.7150
Q	 0.9750	 0.7180
R	 0.9840	 0.7070
S	 0.9700	 0.6370
T	 0.8920	 0.5780
U	 0.9610	 0.6330
V	 0.9710	 0.7130
W	 0.9790	 0.7120
X	 0.9740	 0.6960
Y	 0.9580	 0.6530
Z	 0.9850	 0.7070
a	 0.9960	 0.7230
b	 0.9770	 0.6820
c	 0.9370	 0.6540
d	 0.9720	 0.6940
e	 0.9720	 0.6980
f	 0.9350	 0.6500
g	 0.9770	 0.6930
h	 0.9640	 0.6890



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Chain	Atom inclusion	Q-score
i	 0.9520	 0.6290
j	 0.9420	 0.6120
k	 0.9580	 0.6190
l	 0.9620	 0.6640
m	 0.9640	 0.6750
n	 0.9600	 0.6550
o	 0.9410	 0.6080
p	 0.9700	 0.6640
q	 0.9790	 0.7060
r	 0.9600	 0.6970
s	 0.9440	 0.6380