



## wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 12:06 pm GMT

PDB ID : 7O6Y  
EMDB ID : EMD-12741  
Title : Cryo-EM structure of respiratory complex I under turnover  
Authors : Parey, K.; Vonck, J.  
Deposited on : 2021-04-12  
Resolution : 3.40 Å (reported)  
Based on initial model : 6RFR

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

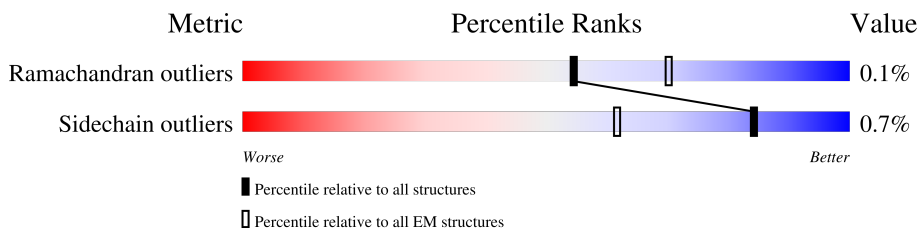
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	728	6% 94% 5%
2	B	488	25% 93% 6%
3	C	466	6% 87% 12%
4	G	281	85% 15%
5	H	243	28% 88% 11%
6	I	229	7% 83% 17%
7	K	210	82% 16%
8	L	89	7% 92%
9	S	249	46% 72% 27%

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Mol	Chain	Length	Quality of chain
10	j	93	33% 97%
11	1	341	99%
12	2	469	99%
13	3	128	11% 90% 9%
14	4	486	5% 99%
15	5	655	49% 98%
16	6	185	8% 69% 27%
17	g	78	21% 96%
18	D	87	99%
19	E	375	6% 87% 11%
20	F	144	7% 83% 17%
21	J	198	46% 87% 13%
22	M	136	6% 86% 14%
23	O	109	50% 65% 35%
24	P	124	18% 99%
25	Q	132	58% 64% 36%
26	R	109	67% 94%
27	U	172	16% 98%
28	W	123	12% 98%
29	X	169	11% 97%
30	Y	161	76% 22%
31	Z	182	5% 99%
32	a	149	56% 83% 17%
33	b	74	8% 86% 14%
34	c	60	67% 73% 27%

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Mol	Chain	Length	Quality of chain
35	d	92	
36	e	67	
37	f	87	
38	h	138	
39	i	90	
40	n	139	
41	8	99	
42	9	89	

## 2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 64866 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 Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	693	5269	3272	927	1041	29	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	457	3528	2230	619	655	24	0	0

- Molecule 3 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	410	3247	2070	553	602	22	0	0

- Molecule 4 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	239	1978	1272	336	366	4	0	0

- Molecule 5 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	216	1688	1060	284	326	18	0	0

- Molecule 6 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	190	1519	966	254	289	10	0	0

- Molecule 7 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	177	1395	885	246	249	15	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	86	669	448	106	112	3	0	0

- Molecule 9 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	182	1492	961	255	274	2	0	0

- Molecule 10 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	j	90	724	465	132	127	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	1	340	2716	1850	393	466	7	0	0

- Molecule 12 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	2	469	3776	2558	550	656	12	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	3	117	930	642	129	156	3	0	0

- Molecule 14 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	4	481	3815	2573	581	647	14	0	0

- Molecule 15 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	5	648	5151	3453	775	895	28	0	0

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	6	135	1078	740	150	180	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	1	FME	-	insertion	UNP S5U3X7

- Molecule 17 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	g	76	622	408	113	101	0	0

- Molecule 18 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 19 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	334	Total	C	N	O	S	0	0
			2673	1697	468	498	10		

- Molecule 20 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	120	Total	C	N	O	S	0	0
			981	624	164	191	2		

- Molecule 21 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	172	Total	C	N	O	S	0	0
			1274	811	228	230	5		

- Molecule 22 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	117	Total	C	N	O	S	0	0
			912	568	163	176	5		

- Molecule 23 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
23	O	71	Total	C	N	O	0	0
			543	344	83	116		

- Molecule 24 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	123	1036	667	182	185	2	0	0

- Molecule 25 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	85	648	405	103	138	2	0	0

- Molecule 26 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	106	884	562	168	151	3	0	0

- Molecule 27 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	171	1345	847	236	252	10	0	0

- Molecule 28 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	W	121	974	623	178	168	5	0	0

- Molecule 29 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	X	164	1275	828	217	226	4	0	0

- Molecule 30 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Y	125	1037	659	190	186	2	0	0

- Molecule 31 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Z	181	1389	893	240	255	1	0	0

- Molecule 32 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	a	124	1030	669	165	194	2	0	0

- Molecule 33 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	b	64	490	326	83	81	0	0

- Molecule 34 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	c	44	353	229	67	57	0	0

- Molecule 35 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	d	89	751	467	136	145	3	0	0

- Molecule 36 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 37 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	82	Total	C	N	O	S	0	0
			642	403	121	117	1		

- Molecule 38 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	136	Total	C	N	O	S	0	0
			1130	727	193	208	2		

- Molecule 39 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	83	Total	C	N	O	S	0	0
			646	413	117	115	1		

- Molecule 40 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	114	Total	C	N	O	S	0	0
			913	587	154	171	1		

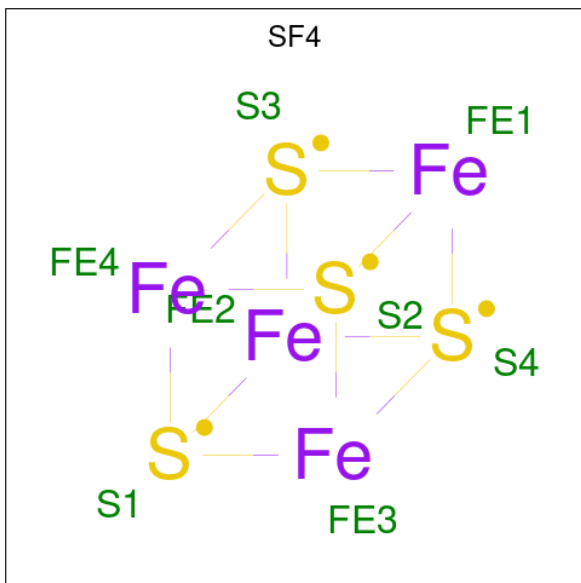
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	71	Total	C	N	O	S	0	0
			594	375	109	102	8		

- Molecule 42 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

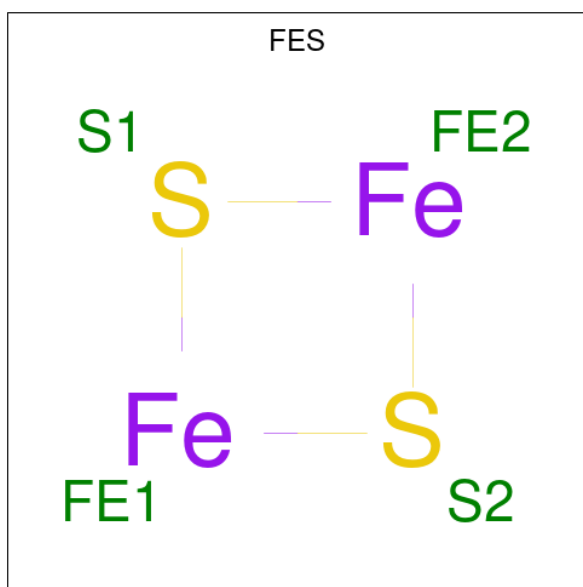
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	9	86	672	422	122	122	6	0	0

- Molecule 43 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



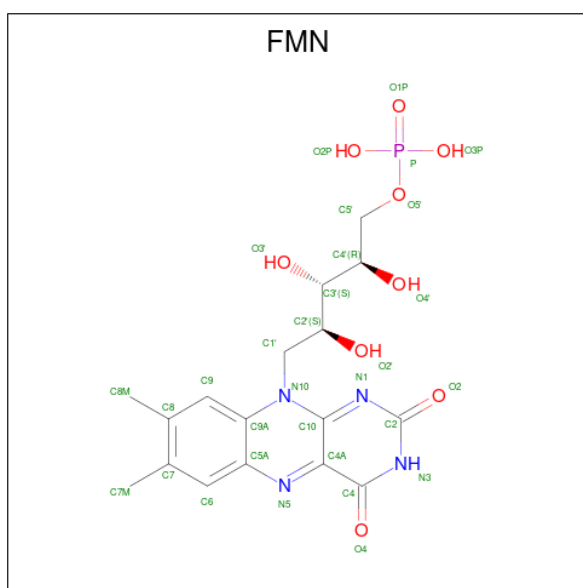
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
43	A	1	16	8	8	0
43	A	1	16	8	8	0
43	B	1	8	4	4	0
43	I	1	16	8	8	0
43	I	1	16	8	8	0
43	K	1	8	4	4	0

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	Fe	S	0
			4	2	2	
44	H	1	Total	Fe	S	0
			4	2	2	

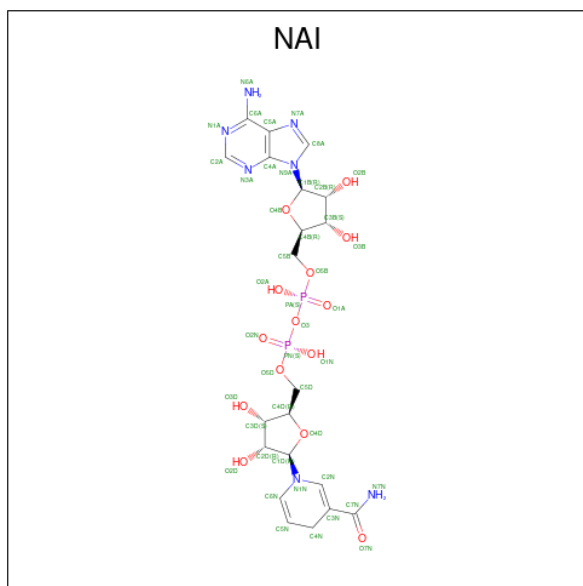
- Molecule 45 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

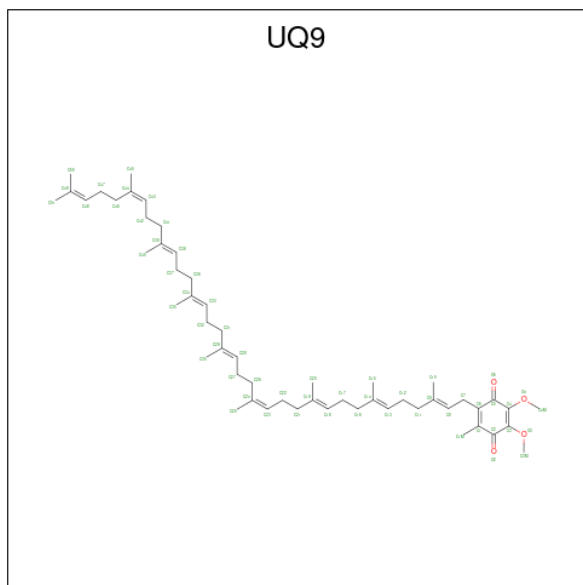
- Molecule 46 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter

code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
46	B	1	44	21	7	14	2	0

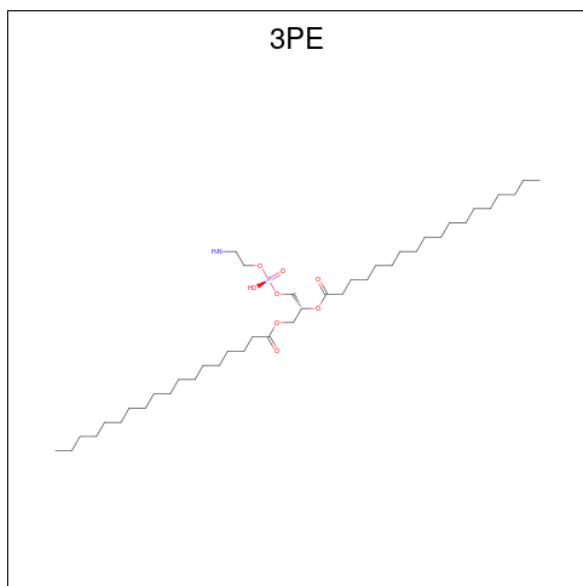
- Molecule 47 is Ubiquinone-9 (three-letter code: UQ9) (formula:  $C_{54}H_{82}O_4$ ).



Mol	Chain	Residues	Atoms		AltConf
			Total	C O	
47	C	1	14	10 4	0

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE)

(formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



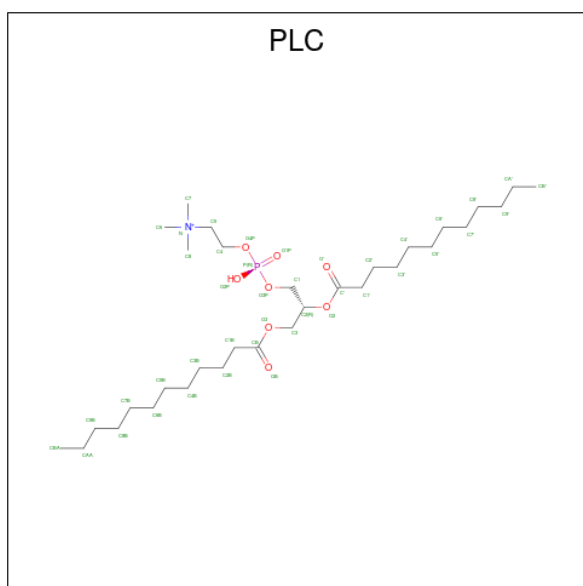
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	1	1	Total	C	N	O	P	0
			77	57	2	16	2	
48	1	1	Total	C	N	O	P	0
			77	57	2	16	2	
48	2	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	4	1	Total	C	N	O	P	0
			136	106	3	24	3	
48	4	1	Total	C	N	O	P	0
			136	106	3	24	3	
48	4	1	Total	C	N	O	P	0
			136	106	3	24	3	
48	5	1	Total	C	N	O	P	0
			127	97	3	24	3	
48	5	1	Total	C	N	O	P	0
			127	97	3	24	3	
48	5	1	Total	C	N	O	P	0
			127	97	3	24	3	
48	6	1	Total	C	N	O	P	0
			84	64	2	16	2	
48	6	1	Total	C	N	O	P	0
			84	64	2	16	2	
48	g	1	Total	C	N	O	P	0
			43	33	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	E	1	Total 36	C 26	N 1	O 8	P 1	0
48	J	1	Total 41	C 31	N 1	O 8	P 1	0
48	b	1	Total 42	C 32	N 1	O 8	P 1	0

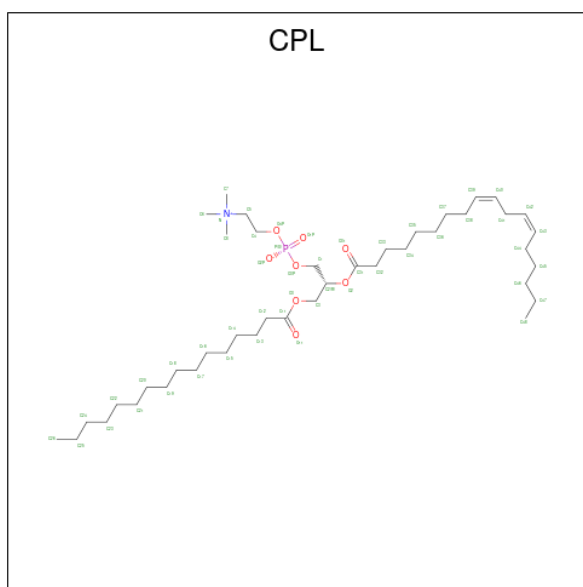
- Molecule 49 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula:  $C_{32}H_{65}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	K	1	Total 36	C 26	N 1	O 8	P 1	0
49	1	1	Total 77	C 57	N 2	O 16	P 2	0
49	1	1	Total 77	C 57	N 2	O 16	P 2	0
49	4	1	Total 35	C 25	N 1	O 8	P 1	0
49	W	1	Total 41	C 31	N 1	O 8	P 1	0
49	i	1	Total 42	C 32	N 1	O 8	P 1	0

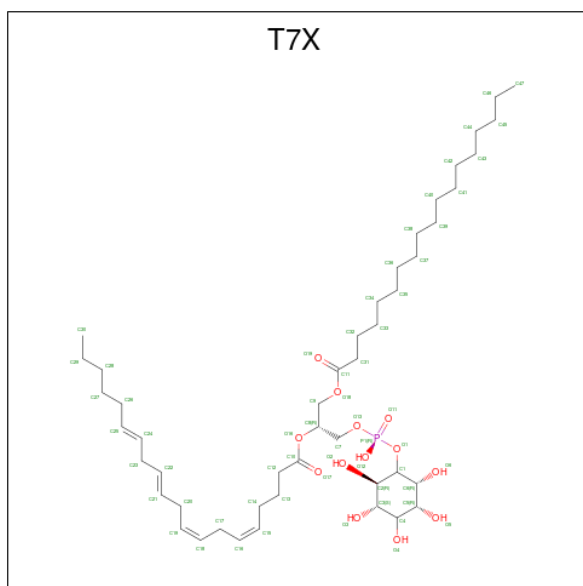
- Molecule 50 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula:  $C_{42}H_{80}NO_8P$ ).





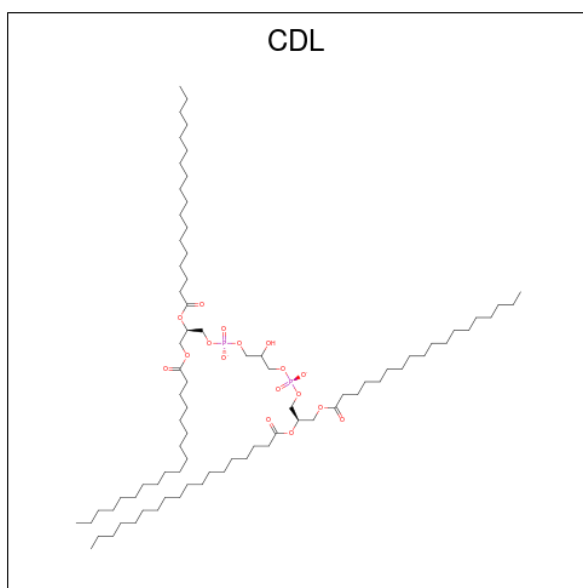
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	2	1	52	42	1	8	1	0

- Molecule 51 is Phosphatidylinositol (three-letter code: T7X) (formula:  $C_{47}H_{83}O_{13}P$ ).



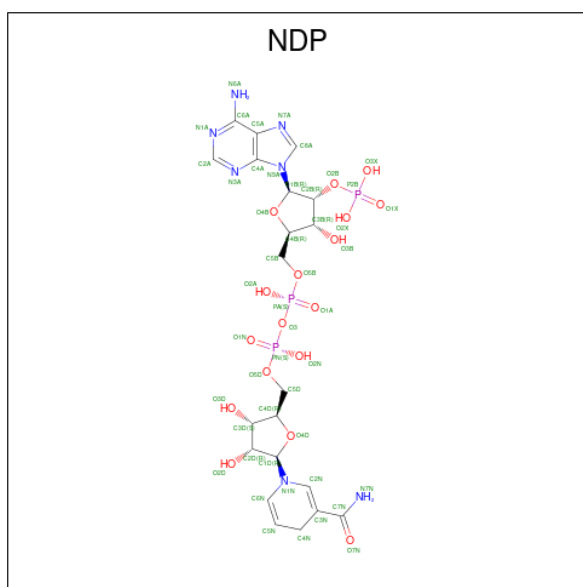
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	2	1	52	38	13	1	0
51	3	1	44	30	13	1	0
51	b	1	48	34	13	1	0

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



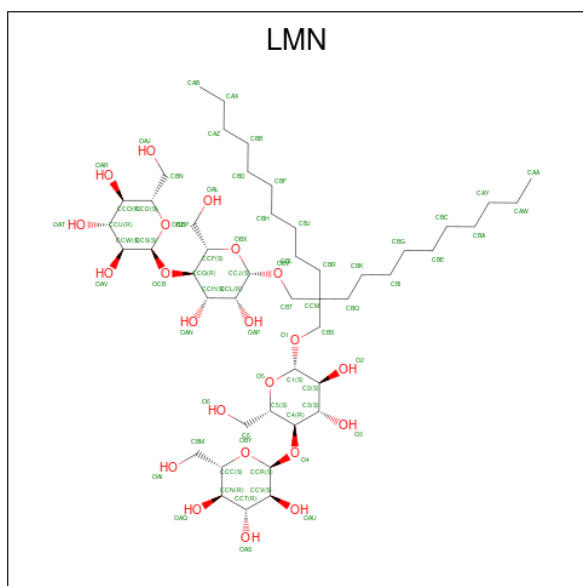
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	g	1	80	61	17	2	0
52	E	1	72	53	17	2	0
52	W	1	54	35	17	2	0
52	X	1	86	67	17	2	0
52	Z	1	76	57	17	2	0
52	n	1	92	73	17	2	0

- Molecule 53 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	
53	E	1	48	21	7	17	3	0

- Molecule 54 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula:  $C_{47}H_{88}O_{22}$ ).

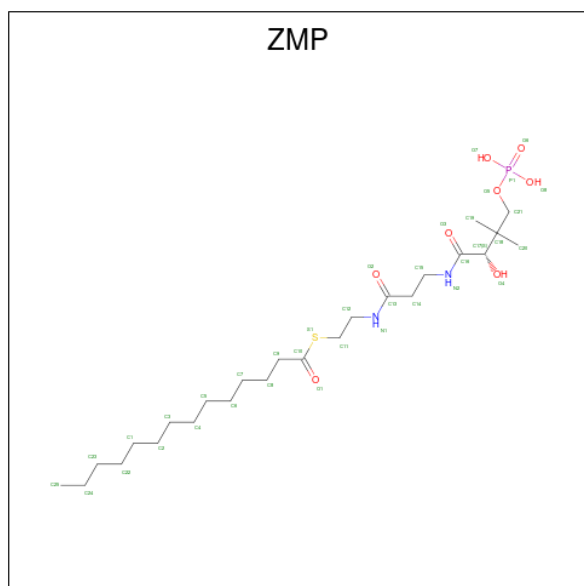


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
54	J	1	69	47	22	0
54	a	1	65	43	22	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	M	1	Total	Zn	0
			1	1	

- Molecule 56 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).

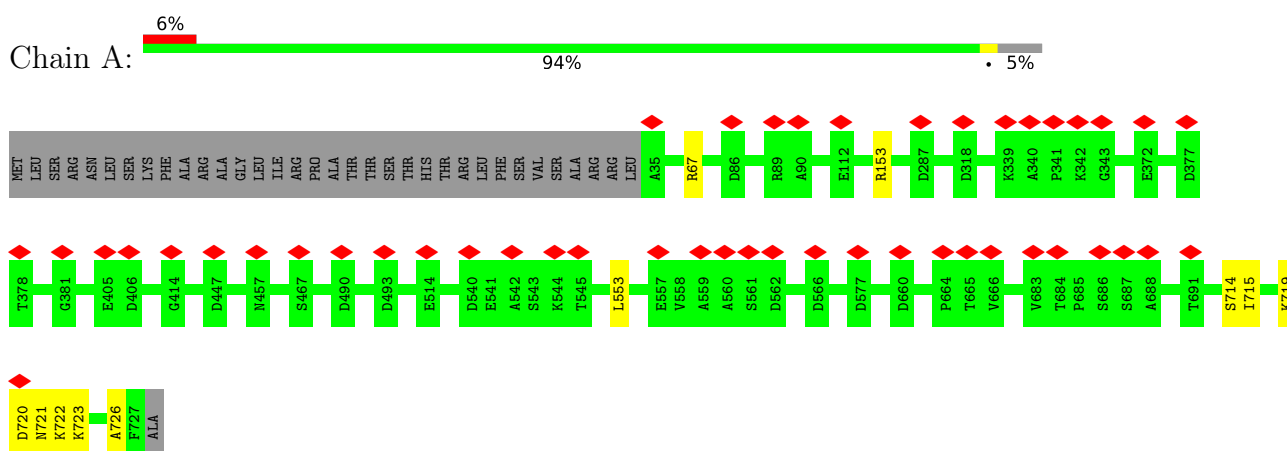


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
56	O	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	
56	R	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

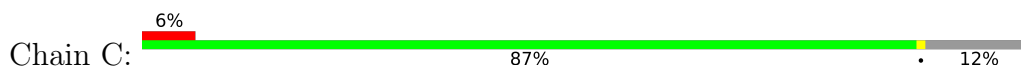
- Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)

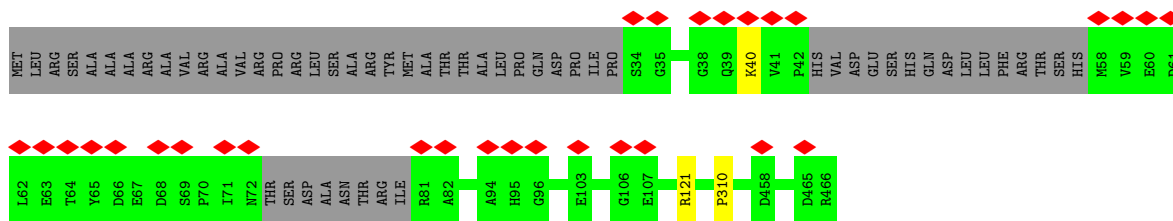


- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

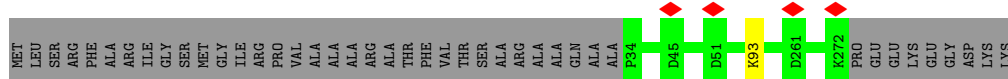
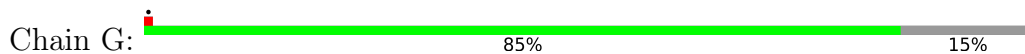


- Molecule 3: NUCM protein

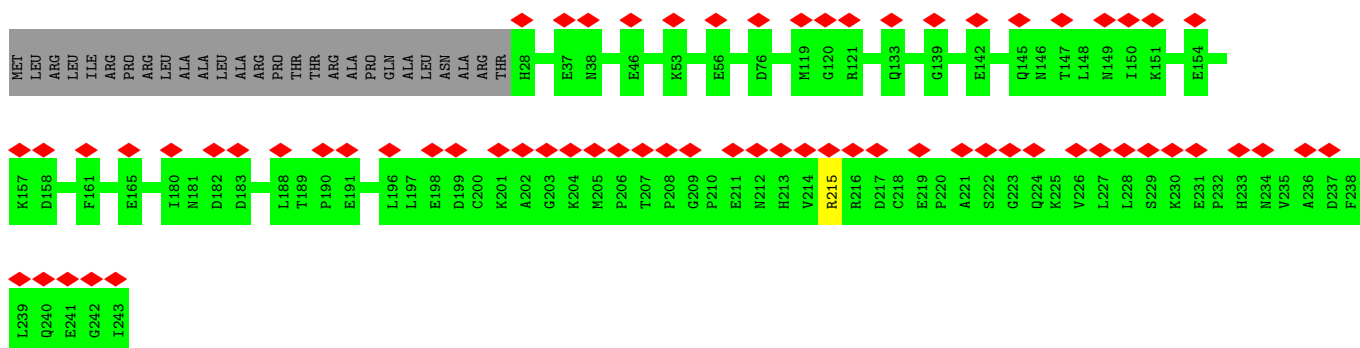
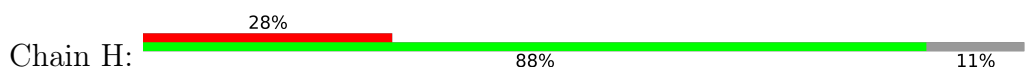




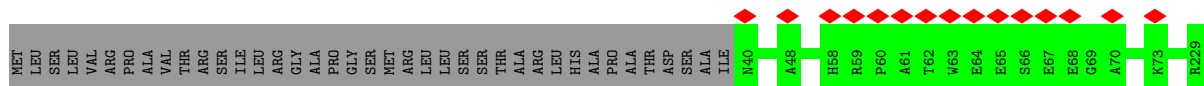
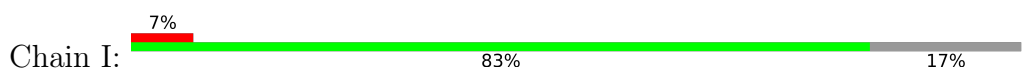
• Molecule 4: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)



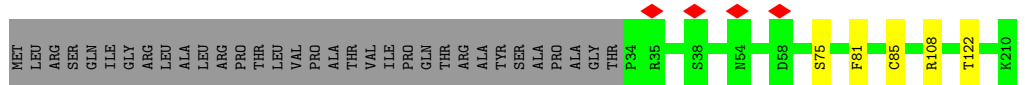
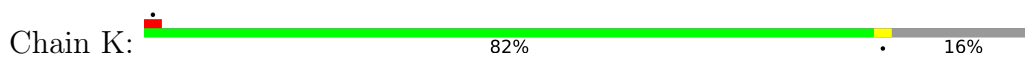
• Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)



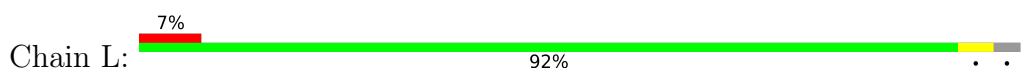
• Molecule 6: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

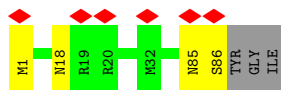


• Molecule 7: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

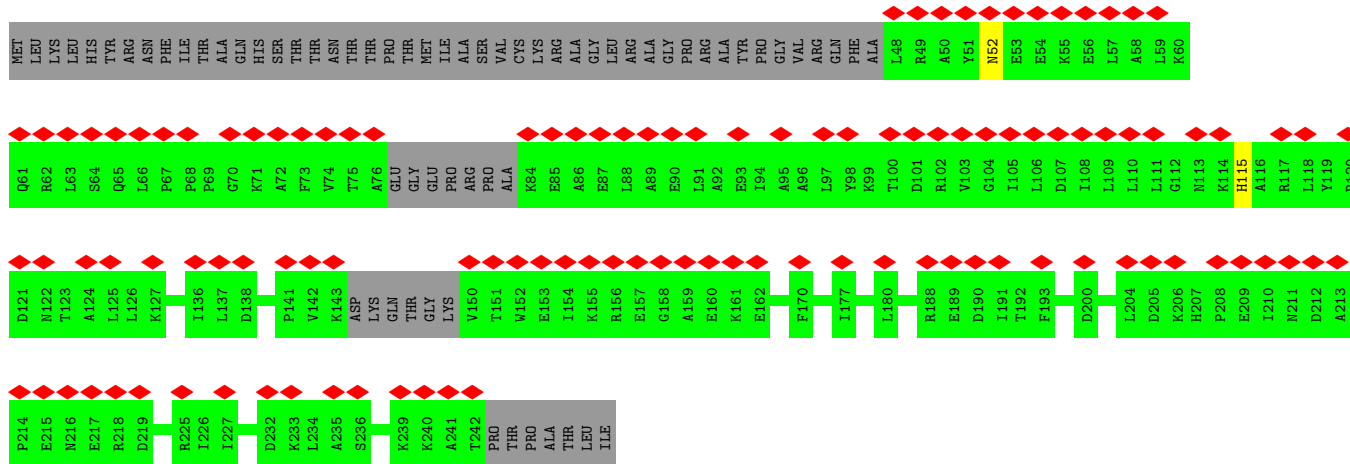


• Molecule 8: NADH-ubiquinone oxidoreductase chain 4L

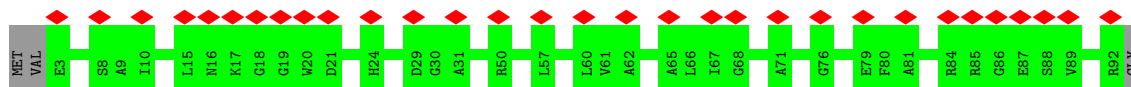




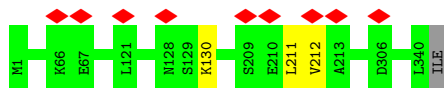
- Molecule 9: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)



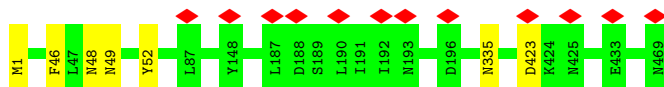
- Molecule 10: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)



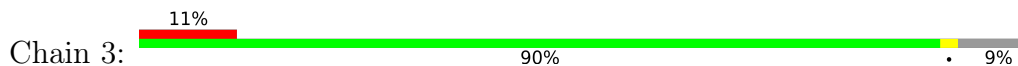
- Molecule 11: NADH-ubiquinone oxidoreductase chain 1



- Molecule 12: NADH dehydrogenase subunit 2

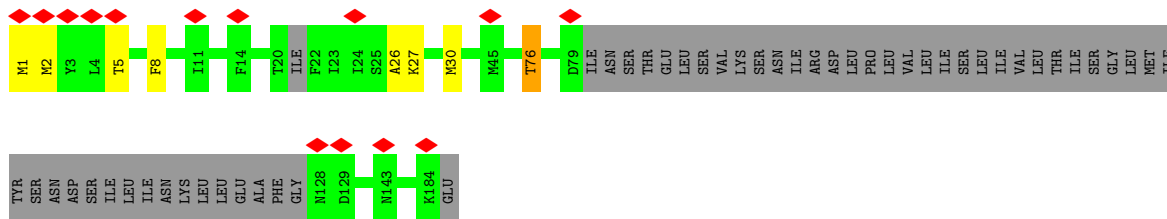


- Molecule 13: NADH-ubiquinone oxidoreductase chain 3

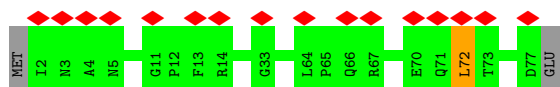




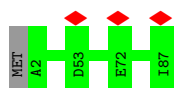




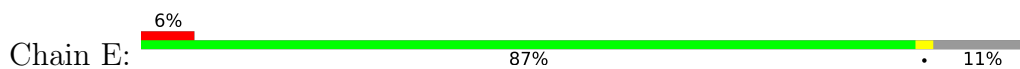
- Molecule 17: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



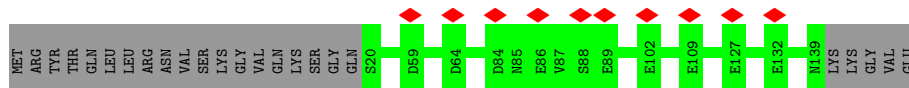
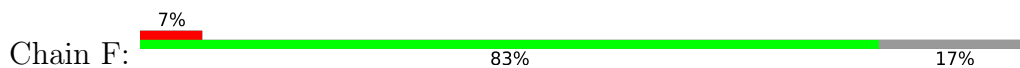
- Molecule 18: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)



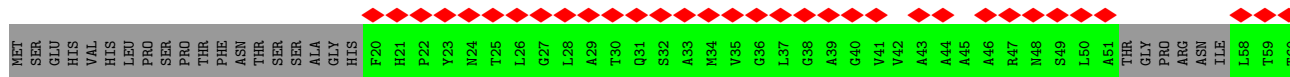
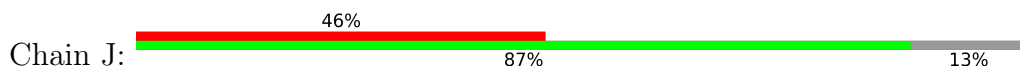
- Molecule 19: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

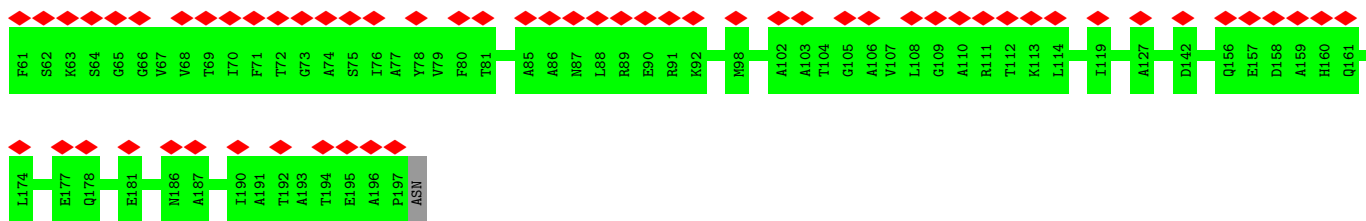


- Molecule 20: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)

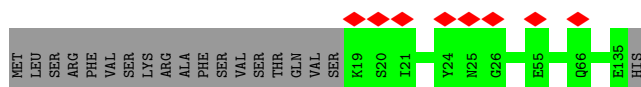
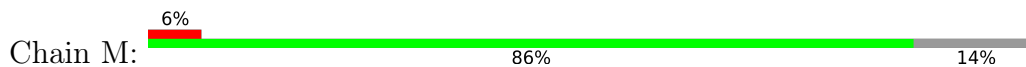


- Molecule 21: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)

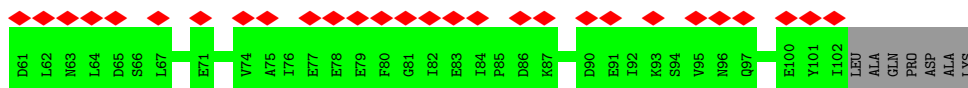




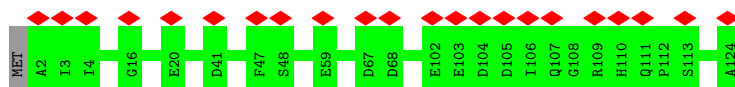
- Molecule 22: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



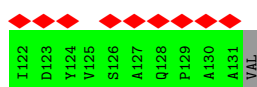
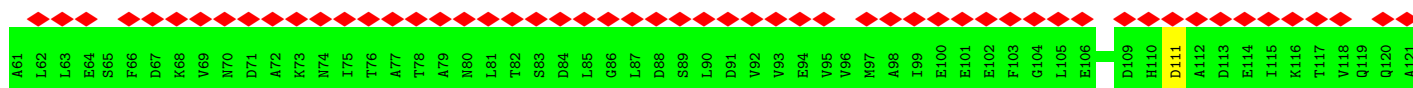
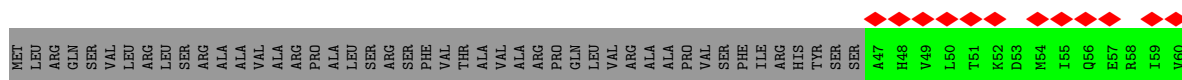
- Molecule 23: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)



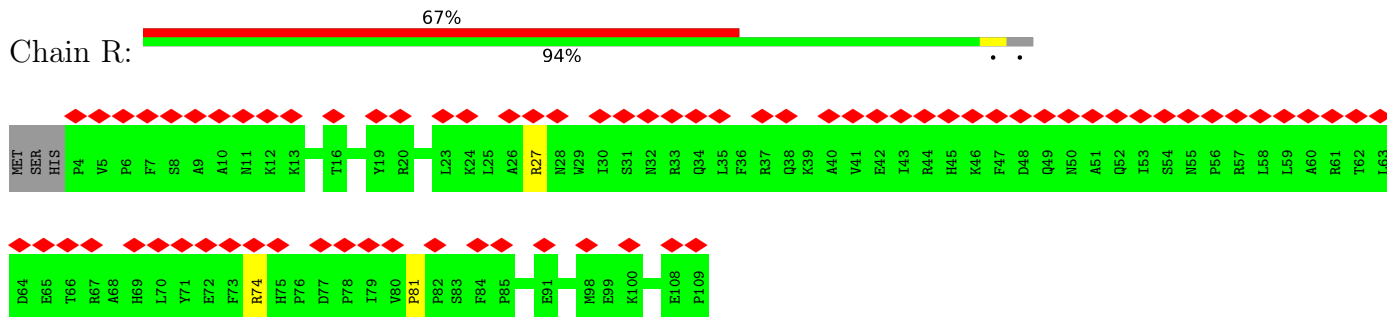
- Molecule 24: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



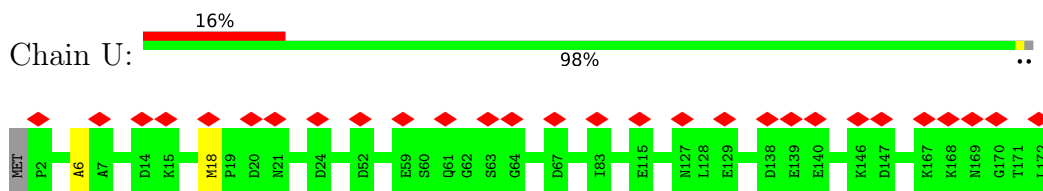
- Molecule 25: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)



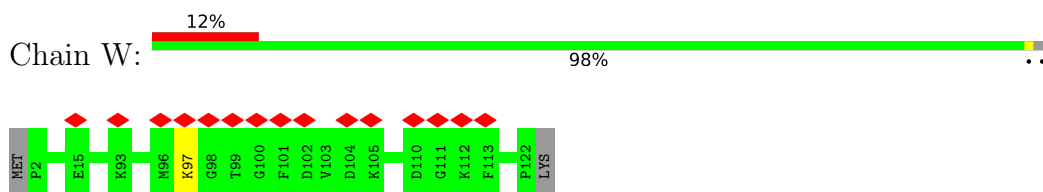
- Molecule 26: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)



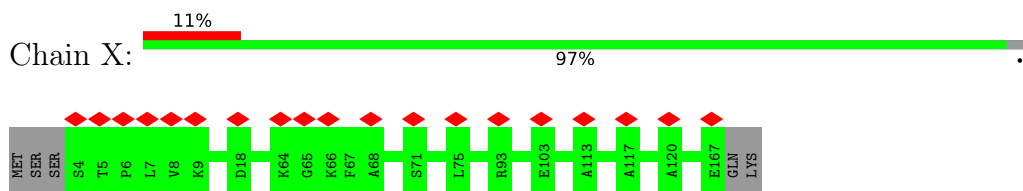
- Molecule 27: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



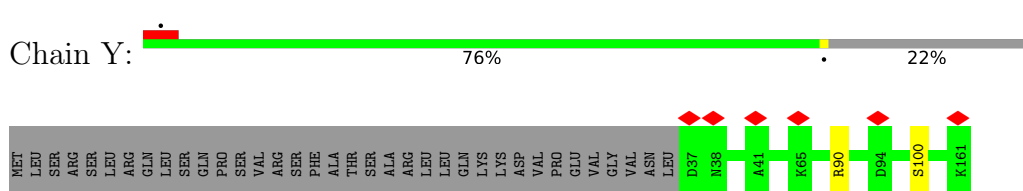
- Molecule 28: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)



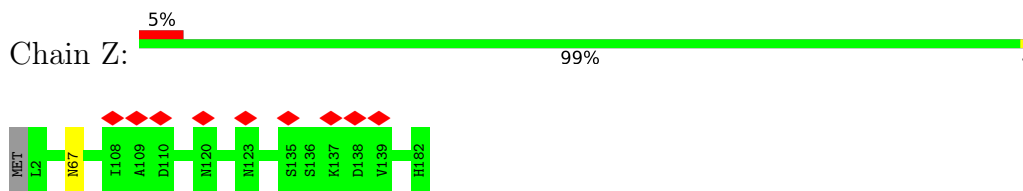
- Molecule 29: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)



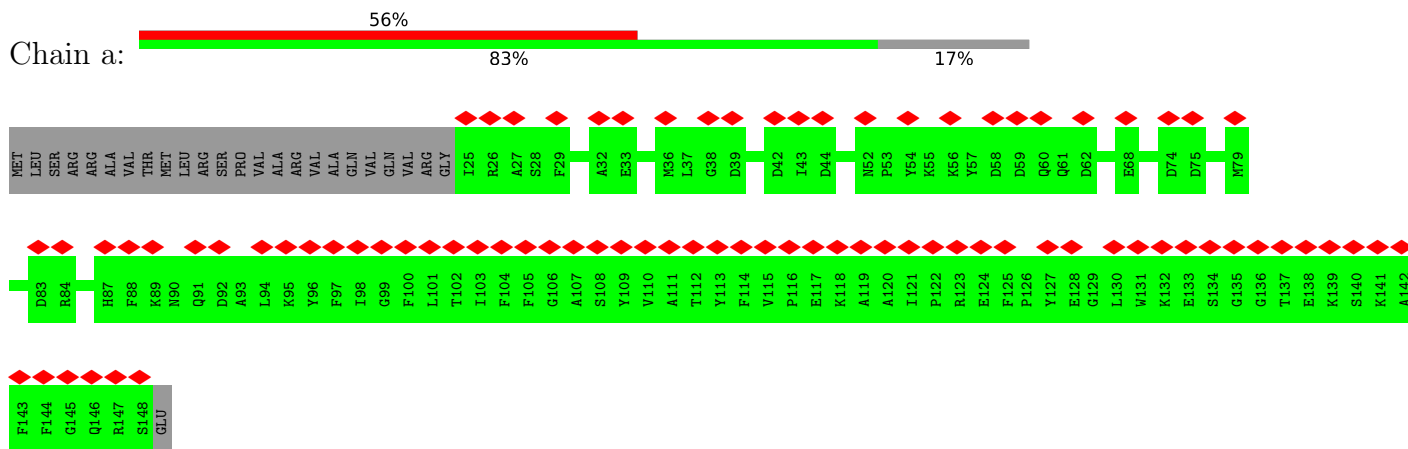
- Molecule 30: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 31: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)



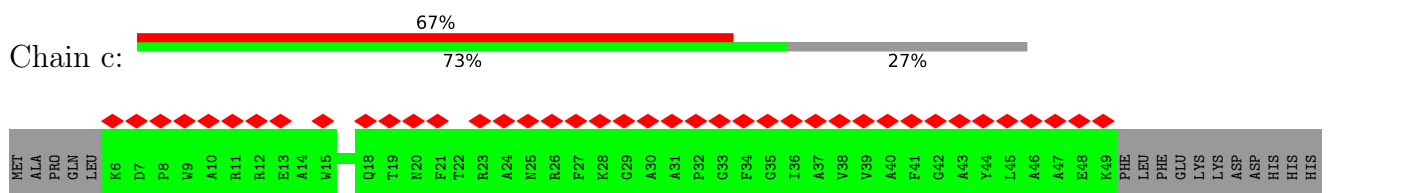
- Molecule 32: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



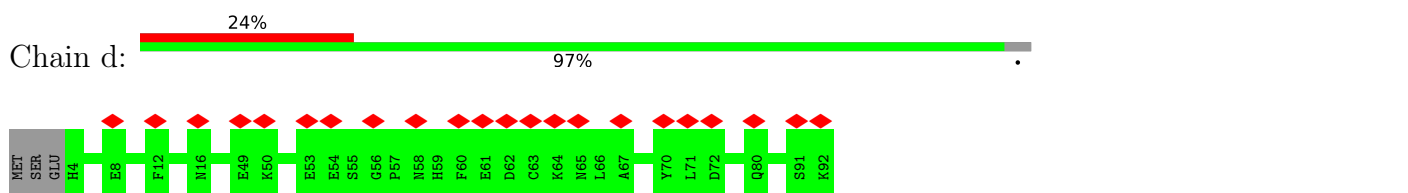
- Molecule 33: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



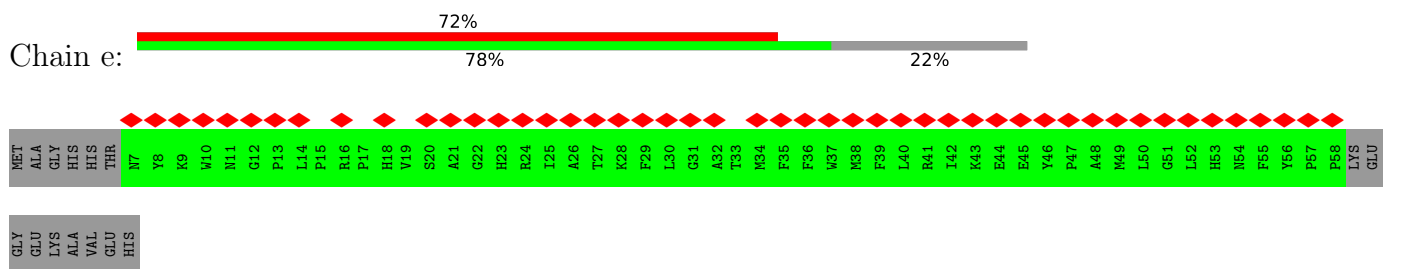
- Molecule 34: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 35: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)

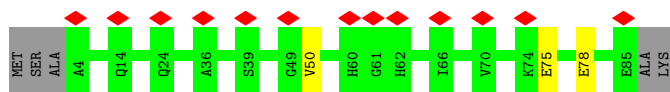


- Molecule 36: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)



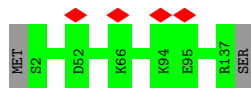
- Molecule 37: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)





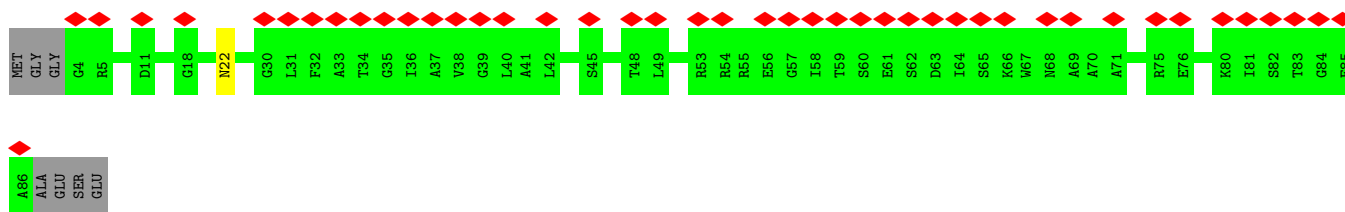
- Molecule 38: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain h: 99%



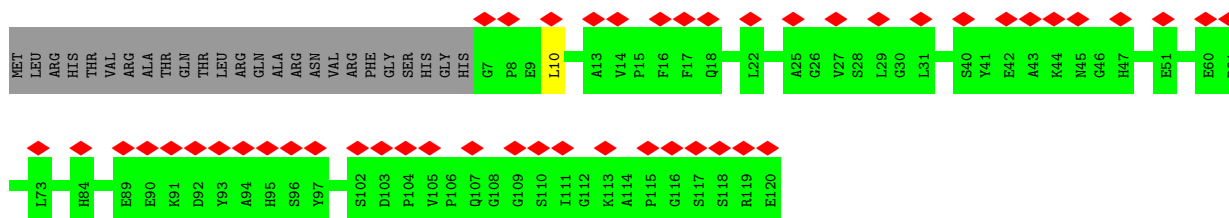
- Molecule 39: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain i: 49% 91% 8%



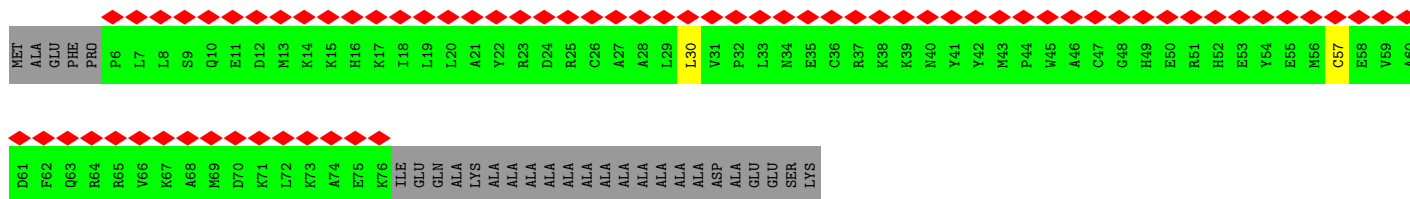
- Molecule 40: Subunit NUMM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain n: 35% 81% 18%



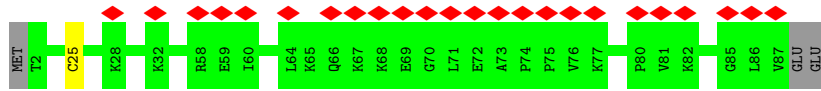
- Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 8: 72% 70% 28%



- Molecule 42: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 9: 27% 96% 2%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54863	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-3200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0115	Depositor
Map size ( $\text{\AA}$ )	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.828, 0.828, 0.828	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: FES, ZN, ZMP, FME, 2MR, SF4, FMN, LMN, NDP, T7X, 3PE, CDL, CPL, NAI, PLC, UQ9

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	0/5363	0.55	1/7278 (0.0%)
2	B	0.37	0/3605	0.53	2/4866 (0.0%)
3	C	0.49	0/3307	0.56	0/4475
4	G	0.49	0/2040	0.54	0/2781
5	H	0.44	1/1725 (0.1%)	0.63	3/2343 (0.1%)
6	I	0.55	0/1557	0.54	0/2110
7	K	0.57	1/1434 (0.1%)	0.61	0/1950
8	L	0.43	0/667	0.68	3/903 (0.3%)
9	S	0.39	0/1517	0.56	0/2046
10	j	0.36	0/745	0.50	0/1006
11	1	0.46	0/2781	0.56	0/3798
12	2	0.49	2/3846 (0.1%)	0.59	3/5242 (0.1%)
13	3	0.42	0/939	0.57	0/1280
14	4	0.39	0/3908	0.53	0/5337
15	5	0.38	0/5280	0.53	2/7208 (0.0%)
16	6	0.52	2/1088 (0.2%)	0.67	2/1483 (0.1%)
17	g	0.37	0/648	0.51	0/887
18	D	0.36	0/697	0.50	0/940
19	E	0.40	0/2732	0.53	0/3702
20	F	0.40	0/1002	0.52	0/1359
21	J	0.34	0/1304	0.53	0/1774
22	M	0.39	0/935	0.47	0/1268
23	O	0.31	0/549	0.53	0/746
24	P	0.43	0/1061	0.50	0/1427
25	Q	0.36	0/654	0.61	2/890 (0.2%)
26	R	0.46	0/909	0.66	2/1229 (0.2%)
27	U	0.35	0/1374	0.51	1/1856 (0.1%)
28	W	0.40	0/998	0.52	0/1346
29	X	0.39	0/1314	0.47	0/1783
30	Y	0.46	0/1067	0.53	0/1442
31	Z	0.42	0/1430	0.54	0/1955
32	a	0.36	0/1064	0.51	0/1439



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	b	0.34	0/503	0.40	0/679
34	c	0.33	0/364	0.46	0/491
35	d	0.35	0/767	0.47	0/1031
36	e	0.31	0/456	0.50	0/619
37	f	0.51	2/652 (0.3%)	0.67	2/874 (0.2%)
38	h	0.47	0/1168	0.52	0/1589
39	i	0.31	0/666	0.45	0/907
40	n	0.37	0/940	0.52	1/1273 (0.1%)
41	8	0.46	1/606 (0.2%)	0.66	2/808 (0.2%)
42	9	0.57	1/684 (0.1%)	0.63	1/918 (0.1%)
All	All	0.43	10/64346 (0.0%)	0.55	27/87338 (0.0%)

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
8	L	0	1
16	6	0	1
27	U	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	9	25	CYS	CB-SG	-9.75	1.65	1.82
5	H	215	ARG	C-N	8.46	1.53	1.34
7	K	75	SER	CA-CB	-7.93	1.41	1.52
12	2	49	ASN	C-O	-6.17	1.11	1.23
41	8	57	CYS	CB-SG	-5.75	1.72	1.81

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	9	25	CYS	CA-CB-SG	8.47	129.25	114.00
5	H	215	ARG	O-C-N	8.22	135.85	122.70
41	8	57	CYS	CA-CB-SG	8.12	128.62	114.00
8	L	18	ASN	O-C-N	7.97	135.45	122.70
25	Q	111	ASP	CB-CG-OD1	7.76	125.29	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	6	76	THR	Mainchain
8	L	1	FME	Mainchain
27	U	6	ALA	Peptide

## 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	691/728 (95%)	667 (96%)	23 (3%)	1 (0%)	51	82
2	B	455/488 (93%)	441 (97%)	14 (3%)	0	100	100
3	C	403/466 (86%)	386 (96%)	16 (4%)	1 (0%)	47	78
4	G	237/281 (84%)	231 (98%)	5 (2%)	1 (0%)	34	67
5	H	214/243 (88%)	192 (90%)	22 (10%)	0	100	100
6	I	188/229 (82%)	182 (97%)	6 (3%)	0	100	100
7	K	175/210 (83%)	168 (96%)	6 (3%)	1 (1%)	25	57
8	L	84/89 (94%)	84 (100%)	0	0	100	100
9	S	176/249 (71%)	166 (94%)	10 (6%)	0	100	100
10	j	88/93 (95%)	83 (94%)	5 (6%)	0	100	100
11	1	338/341 (99%)	323 (96%)	15 (4%)	0	100	100
12	2	467/469 (100%)	463 (99%)	4 (1%)	0	100	100
13	3	111/128 (87%)	108 (97%)	3 (3%)	0	100	100
14	4	479/486 (99%)	464 (97%)	15 (3%)	0	100	100
15	5	644/655 (98%)	622 (97%)	21 (3%)	1 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	6	129/185 (70%)	125 (97%)	4 (3%)	0	100	100
17	g	74/78 (95%)	63 (85%)	10 (14%)	1 (1%)	11	37
18	D	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
19	E	332/375 (88%)	317 (96%)	14 (4%)	1 (0%)	41	72
20	F	118/144 (82%)	111 (94%)	7 (6%)	0	100	100
21	J	168/198 (85%)	164 (98%)	4 (2%)	0	100	100
22	M	115/136 (85%)	114 (99%)	1 (1%)	0	100	100
23	O	69/109 (63%)	65 (94%)	4 (6%)	0	100	100
24	P	121/124 (98%)	121 (100%)	0	0	100	100
25	Q	83/132 (63%)	80 (96%)	3 (4%)	0	100	100
26	R	104/109 (95%)	103 (99%)	1 (1%)	0	100	100
27	U	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
28	W	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
29	X	162/169 (96%)	158 (98%)	4 (2%)	0	100	100
30	Y	123/161 (76%)	119 (97%)	4 (3%)	0	100	100
31	Z	179/182 (98%)	171 (96%)	8 (4%)	0	100	100
32	a	122/149 (82%)	116 (95%)	6 (5%)	0	100	100
33	b	62/74 (84%)	62 (100%)	0	0	100	100
34	c	42/60 (70%)	40 (95%)	2 (5%)	0	100	100
35	d	87/92 (95%)	84 (97%)	3 (3%)	0	100	100
36	e	50/67 (75%)	47 (94%)	3 (6%)	0	100	100
37	f	80/87 (92%)	77 (96%)	3 (4%)	0	100	100
38	h	134/138 (97%)	130 (97%)	4 (3%)	0	100	100
39	i	81/90 (90%)	79 (98%)	2 (2%)	0	100	100
40	n	111/139 (80%)	107 (96%)	4 (4%)	0	100	100
41	8	69/99 (70%)	66 (96%)	3 (4%)	0	100	100
42	9	84/89 (94%)	80 (95%)	4 (5%)	0	100	100
All	All	7821/8723 (90%)	7542 (96%)	272 (4%)	7 (0%)	54	82

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	81	PHE

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Mol	Chain	Res	Type
1	A	726	ALA
17	g	72	LEU
4	G	93	LYS
19	E	344	MET

### 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	566/595 (95%)	557 (98%)	9 (2%)	62	81
2	B	364/389 (94%)	362 (100%)	2 (0%)	88	94
3	C	346/393 (88%)	345 (100%)	1 (0%)	92	97
4	G	216/245 (88%)	216 (100%)	0	100	100
5	H	191/212 (90%)	191 (100%)	0	100	100
6	I	156/187 (83%)	156 (100%)	0	100	100
7	K	154/180 (86%)	151 (98%)	3 (2%)	57	78
8	L	74/76 (97%)	72 (97%)	2 (3%)	44	70
9	S	157/211 (74%)	155 (99%)	2 (1%)	69	84
10	j	71/73 (97%)	71 (100%)	0	100	100
11	1	300/301 (100%)	297 (99%)	3 (1%)	76	88
12	2	432/432 (100%)	430 (100%)	2 (0%)	88	94
13	3	102/113 (90%)	101 (99%)	1 (1%)	76	88
14	4	429/434 (99%)	428 (100%)	1 (0%)	93	98
15	5	573/580 (99%)	568 (99%)	5 (1%)	78	90
16	6	119/166 (72%)	115 (97%)	4 (3%)	37	65
17	g	63/65 (97%)	62 (98%)	1 (2%)	62	81
18	D	68/69 (99%)	68 (100%)	0	100	100
19	E	290/329 (88%)	285 (98%)	5 (2%)	60	80
20	F	108/129 (84%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	J	124/147 (84%)	124 (100%)	0	100	100
22	M	97/115 (84%)	97 (100%)	0	100	100
23	O	60/91 (66%)	60 (100%)	0	100	100
24	P	109/110 (99%)	109 (100%)	0	100	100
25	Q	72/111 (65%)	72 (100%)	0	100	100
26	R	97/100 (97%)	96 (99%)	1 (1%)	76	88
27	U	147/148 (99%)	147 (100%)	0	100	100
28	W	100/102 (98%)	99 (99%)	1 (1%)	76	88
29	X	128/133 (96%)	128 (100%)	0	100	100
30	Y	107/140 (76%)	105 (98%)	2 (2%)	57	78
31	Z	147/148 (99%)	146 (99%)	1 (1%)	84	92
32	a	108/129 (84%)	108 (100%)	0	100	100
33	b	50/59 (85%)	50 (100%)	0	100	100
34	c	30/45 (67%)	30 (100%)	0	100	100
35	d	82/85 (96%)	82 (100%)	0	100	100
36	e	44/55 (80%)	44 (100%)	0	100	100
37	f	70/73 (96%)	70 (100%)	0	100	100
38	h	121/123 (98%)	121 (100%)	0	100	100
39	i	64/68 (94%)	63 (98%)	1 (2%)	62	81
40	n	98/119 (82%)	98 (100%)	0	100	100
41	8	63/76 (83%)	63 (100%)	0	100	100
42	9	73/76 (96%)	73 (100%)	0	100	100
All	All	6770/7432 (91%)	6723 (99%)	47 (1%)	84	92

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	5	556	SER
17	g	72	LEU
15	5	612	SER
16	6	5	THR
19	E	127	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
25	Q	119	GLN
37	f	11	HIS
30	Y	93	ASN
32	a	146	GLN
41	8	16	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](#)

6 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
8	FME	L	1	8	8,9,10	0.98	0	7,9,11	0.84	0
16	FME	6	1	16	8,9,10	0.49	0	7,9,11	0.97	1 (14%)
13	FME	3	1	13	8,9,10	0.87	0	7,9,11	1.49	1 (14%)
11	FME	1	1	11	8,9,10	0.94	0	7,9,11	0.70	0
12	FME	2	1	12	8,9,10	0.97	1 (12%)	7,9,11	1.04	0
3	2MR	C	121	3	10,12,13	1.90	1 (10%)	5,13,15	2.61	2 (40%)

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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	L	1	8	-	3/7/9/11	-
16	FME	6	1	16	-	6/7/9/11	-
13	FME	3	1	13	-	2/7/9/11	-
11	FME	1	1	11	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	2	1	12	-	5/7/9/11	-
3	2MR	C	121	3	-	2/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	121	2MR	CZ-NE	5.19	1.45	1.34
12	2	1	FME	CA-N	-2.02	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	121	2MR	CD-NE-CZ	4.13	131.15	123.41
3	C	121	2MR	NE-CZ-NH2	3.95	123.10	119.48
13	3	1	FME	C-CA-N	2.96	115.07	109.73
16	6	1	FME	O-C-CA	-2.43	118.41	124.78

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	121	2MR	C-CA-CB-CG
8	L	1	FME	O1-CN-N-CA
12	2	1	FME	C-CA-CB-CG
12	2	1	FME	O-C-CA-CB
16	6	1	FME	O1-CN-N-CA

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 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	CDL	n	201	-	91,91,99	0.94	7 (7%)	97,103,111	0.97	4 (4%)
45	FMN	B	502	-	33,33,33	1.14	2 (6%)	48,50,50	1.29	6 (12%)
52	CDL	X	201	-	85,85,99	0.96	6 (7%)	91,97,111	1.00	4 (4%)
43	SF4	I	503	6	0,12,12	-	-	-	-	-
43	SF4	A	801	1	0,12,12	-	-	-	-	-
49	PLC	K	302	-	35,35,41	0.32	0	41,43,49	0.34	0
48	3PE	6	202	-	46,46,50	0.88	4 (8%)	49,51,55	0.90	2 (4%)
48	3PE	I	501	-	50,50,50	0.85	3 (6%)	53,55,55	0.98	3 (5%)
48	3PE	5	703	-	43,43,50	0.29	0	46,48,55	0.33	0
48	3PE	5	701	-	41,41,50	0.94	4 (9%)	44,46,55	0.99	2 (4%)
56	ZMP	O	201	23	26,32,36	1.85	5 (19%)	31,39,45	2.00	8 (25%)
48	3PE	1	403	11	40,40,50	0.92	3 (7%)	43,45,55	0.81	1 (2%)
46	NAI	B	503	-	42,48,48	0.60	0	47,73,73	0.85	2 (4%)
48	3PE	b	502	-	41,41,50	0.94	4 (9%)	44,46,55	0.86	2 (4%)
48	3PE	2	503	-	41,41,50	0.94	4 (9%)	44,46,55	0.90	2 (4%)
52	CDL	W	402	-	53,53,99	1.24	6 (11%)	59,65,111	1.17	4 (6%)
54	LMN	a	201	-	68,68,72	1.65	14 (20%)	92,94,98	0.95	3 (3%)
49	PLC	4	504	-	34,34,41	1.32	5 (14%)	40,42,49	1.22	3 (7%)
48	3PE	4	502	-	42,42,50	0.94	4 (9%)	45,47,55	1.02	3 (6%)
43	SF4	I	502	6	0,12,12	-	-	-	-	-
44	FES	H	301	5	0,4,4	-	-	-	-	-
48	3PE	6	201	-	35,35,50	1.01	4 (11%)	38,40,55	1.13	2 (5%)
51	T7X	3	201	-	44,44,61	1.01	3 (6%)	54,56,73	1.07	5 (9%)
48	3PE	5	702	-	40,40,50	0.95	4 (10%)	43,45,55	1.08	3 (6%)
48	3PE	J	201	-	40,40,50	0.95	3 (7%)	43,45,55	0.98	3 (6%)
54	LMN	J	202	-	72,72,72	1.54	13 (18%)	96,98,98	1.27	13 (13%)
48	3PE	1	402	-	35,35,50	1.00	4 (11%)	38,40,55	1.00	2 (5%)
53	NDP	E	401	-	45,52,52	2.25	8 (17%)	53,80,80	1.83	11 (20%)
47	UQ9	C	601	-	14,14,58	2.63	6 (42%)	18,20,73	0.99	0
56	ZMP	R	201	26,25	26,32,36	1.74	4 (15%)	31,39,45	1.47	3 (9%)
43	SF4	B	501	2	0,12,12	-	-	-	-	-
49	PLC	1	401	-	34,34,41	1.31	4 (11%)	40,42,49	1.29	4 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	CDL	E	403	-	71,71,99	1.04	7 (9%)	77,83,111	1.06	6 (7%)
52	CDL	g	201	-	79,79,99	1.01	7 (8%)	85,91,111	1.08	6 (7%)
48	3PE	g	202	-	42,42,50	0.94	4 (9%)	45,47,55	0.88	2 (4%)
51	T7X	2	502	-	52,52,61	0.91	5 (9%)	62,64,73	1.41	8 (12%)
49	PLC	1	404	-	41,41,41	1.23	5 (12%)	47,49,49	1.20	5 (10%)
50	CPL	2	501	-	51,51,51	1.13	3 (5%)	57,59,59	1.23	5 (8%)
44	FES	A	803	1	0,4,4	-	-	-		
48	3PE	4	501	-	41,41,50	0.93	4 (9%)	44,46,55	0.96	2 (4%)
52	CDL	Z	201	-	75,75,99	1.04	7 (9%)	81,87,111	1.00	4 (4%)
48	3PE	4	503	-	50,50,50	0.85	3 (6%)	53,55,55	0.93	3 (5%)
48	3PE	E	402	-	35,35,50	1.00	3 (8%)	38,40,55	1.14	3 (7%)
51	T7X	b	501	-	48,48,61	0.94	4 (8%)	57,60,73	1.17	4 (7%)
43	SF4	A	802	1	0,12,12	-	-	-		
43	SF4	K	301	7	0,12,12	-	-	-		
49	PLC	W	401	-	40,40,41	1.21	3 (7%)	46,48,49	1.17	4 (8%)
49	PLC	i	1101	-	41,41,41	1.22	5 (12%)	47,49,49	1.13	3 (6%)

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
52	CDL	n	201	-	-	59/102/102/110	-
45	FMN	B	502	-	-	7/18/18/18	0/3/3/3
52	CDL	X	201	-	-	40/96/96/110	-
43	SF4	A	801	1	-	-	0/6/5/5
43	SF4	I	503	6	-	-	0/6/5/5
49	PLC	K	302	-	-	7/39/39/45	-
48	3PE	6	202	-	-	22/50/50/54	-
48	3PE	I	501	-	-	29/54/54/54	-
48	3PE	5	703	-	-	26/47/47/54	-
48	3PE	5	701	-	-	18/45/45/54	-
56	ZMP	O	201	23	-	18/37/39/43	-
48	3PE	1	403	11	-	16/44/44/54	-
48	3PE	b	502	-	-	26/45/45/54	-
46	NAI	B	503	-	-	7/25/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	3PE	2	503	-	-	21/45/45/54	-
52	CDL	W	402	-	-	34/64/64/110	-
54	LMN	a	201	-	-	22/46/126/130	0/4/4/4
49	PLC	4	504	-	-	23/38/38/45	-
48	3PE	4	502	-	-	24/46/46/54	-
43	SF4	I	502	6	-	-	0/6/5/5
44	FES	H	301	5	-	-	0/1/1/1
48	3PE	6	201	-	-	21/39/39/54	-
51	T7X	3	201	-	-	13/39/63/80	0/1/1/1
48	3PE	5	702	-	-	22/44/44/54	-
48	3PE	J	201	-	-	18/44/44/54	-
54	LMN	J	202	-	-	40/50/130/130	0/4/4/4
48	3PE	1	402	-	-	20/39/39/54	-
53	NDP	E	401	-	-	6/30/77/77	0/5/5/5
47	UQ9	C	601	-	-	1/4/28/81	0/1/1/1
56	ZMP	R	201	26,25	-	10/37/39/43	-
43	SF4	B	501	2	-	-	0/6/5/5
49	PLC	1	401	-	-	15/38/38/45	-
52	CDL	E	403	-	-	36/82/82/110	-
52	CDL	g	201	-	-	36/90/90/110	-
48	3PE	g	202	-	-	22/46/46/54	-
51	T7X	2	502	-	-	23/47/71/80	0/1/1/1
49	PLC	1	404	-	-	22/45/45/45	-
50	CPL	2	501	-	-	22/55/55/55	-
44	FES	A	803	1	-	-	0/1/1/1
48	3PE	4	501	-	-	22/45/45/54	-
52	CDL	Z	201	-	-	38/86/86/110	-
48	3PE	4	503	-	-	26/54/54/54	-
48	3PE	E	402	-	-	16/39/39/54	-
51	T7X	b	501	-	-	18/43/67/80	0/1/1/1
43	SF4	A	802	1	-	-	0/6/5/5
43	SF4	K	301	7	-	-	0/6/5/5
49	PLC	W	401	-	-	19/44/44/45	-
49	PLC	i	1101	-	-	25/45/45/45	-

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	E	401	NDP	P2B-O2B	12.05	1.82	1.59
56	O	201	ZMP	C16-N2	5.69	1.46	1.33
47	C	601	UQ9	O4-C4	-5.55	1.23	1.36
56	R	201	ZMP	C16-N2	5.54	1.45	1.33
47	C	601	UQ9	O3-C3	-5.33	1.23	1.36

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	E	401	NDP	PN-O3-PA	-7.25	107.96	132.83
56	O	201	ZMP	C9-C10-S1	6.98	121.58	113.46
51	2	502	T7X	C6-C1-C2	5.47	118.75	110.85
56	R	201	ZMP	C9-C10-S1	5.25	119.57	113.46
50	2	501	CPL	C37-C38-C39	-4.71	85.46	112.43

There are no chirality outliers.

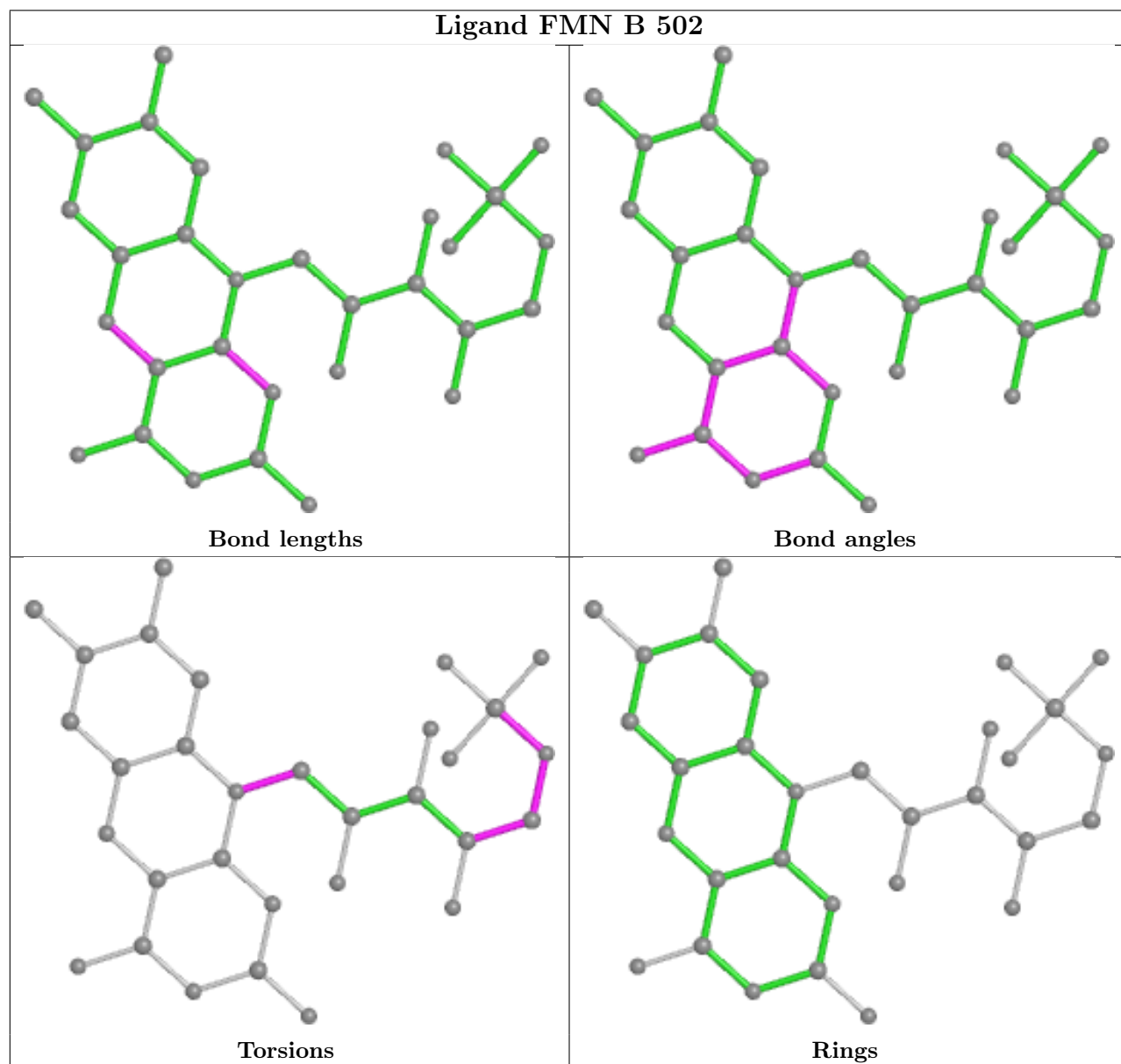
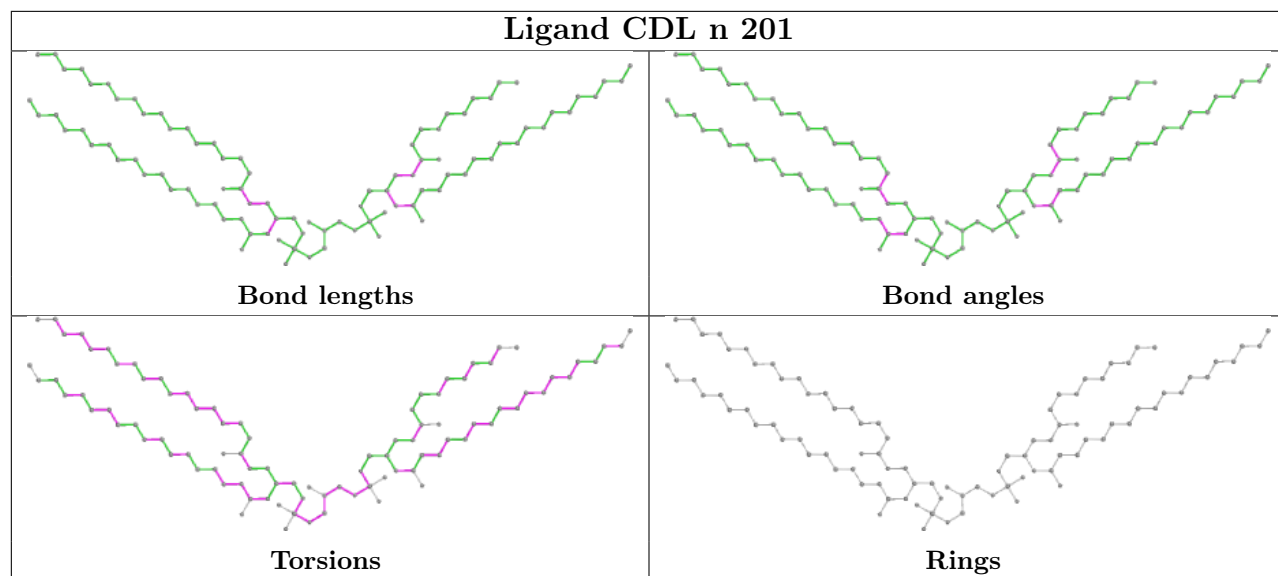
5 of 890 torsion outliers are listed below:

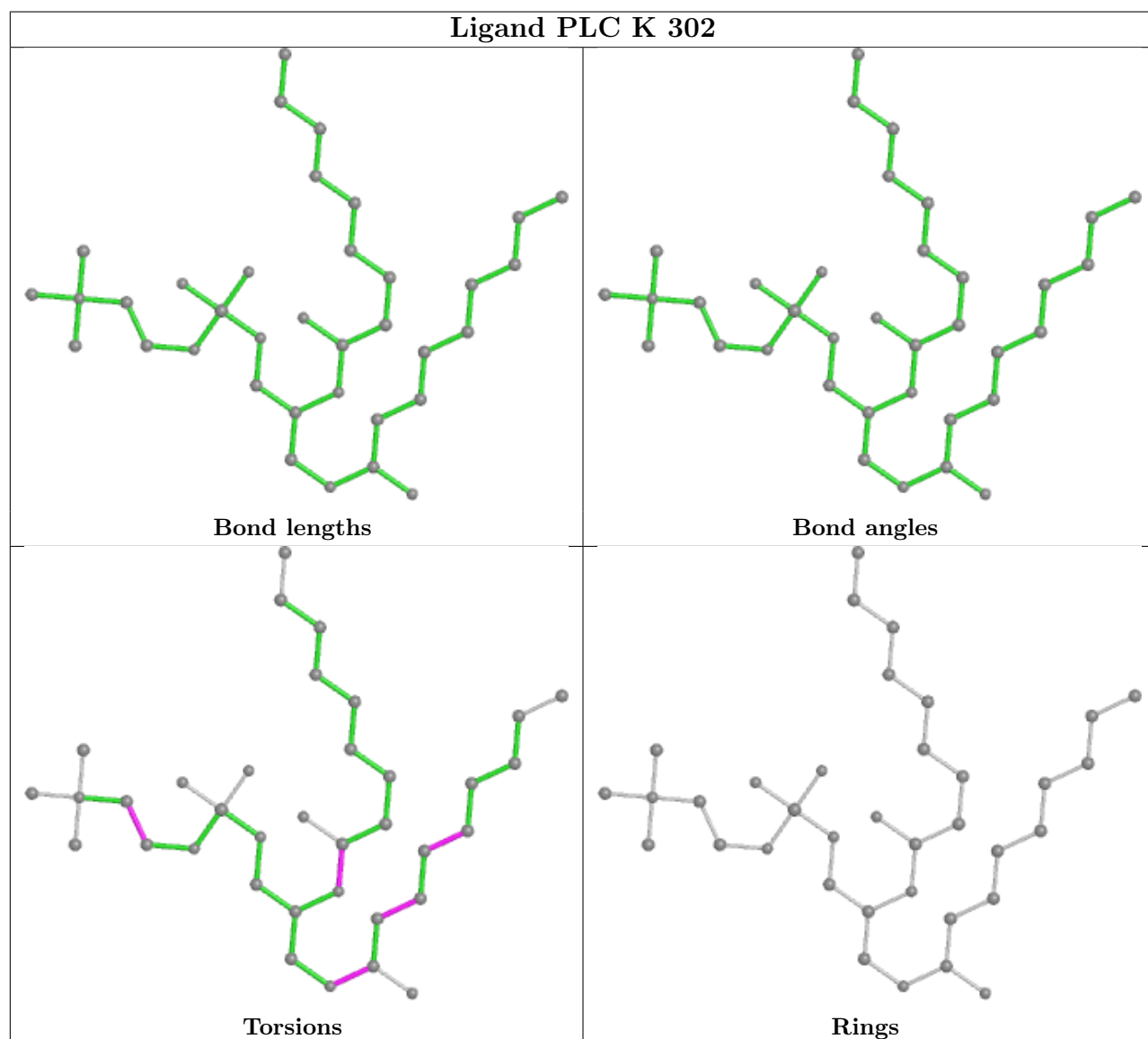
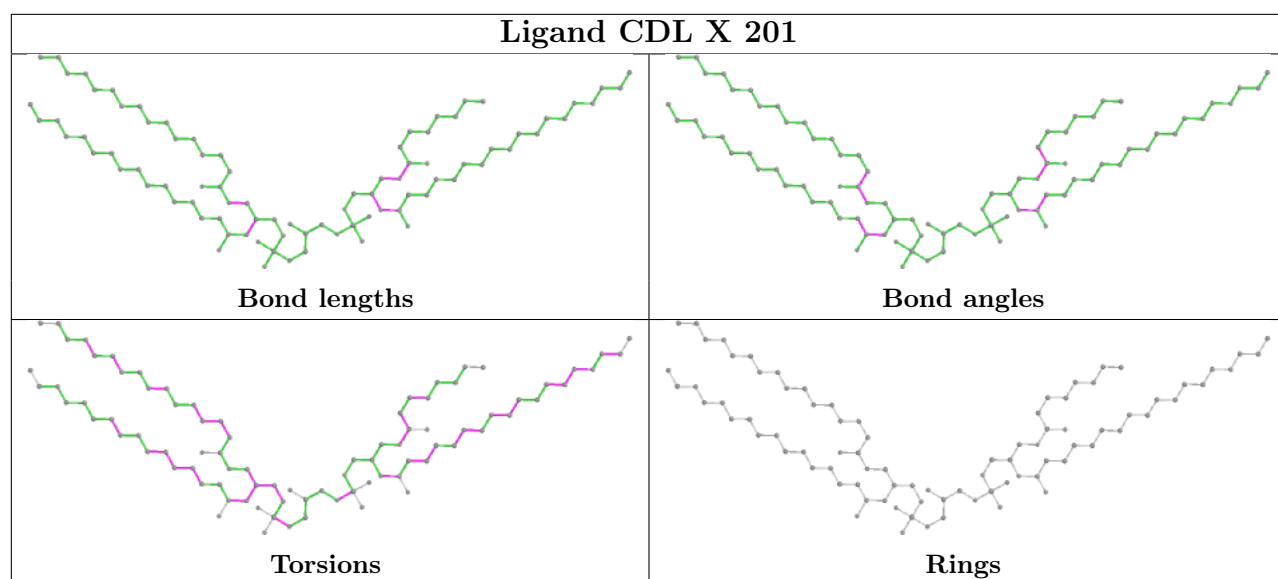
Mol	Chain	Res	Type	Atoms
45	B	502	FMN	C3'-C4'-C5'-O5'
45	B	502	FMN	O4'-C4'-C5'-O5'
45	B	502	FMN	C5'-O5'-P-O1P
45	B	502	FMN	C5'-O5'-P-O2P
45	B	502	FMN	C5'-O5'-P-O3P

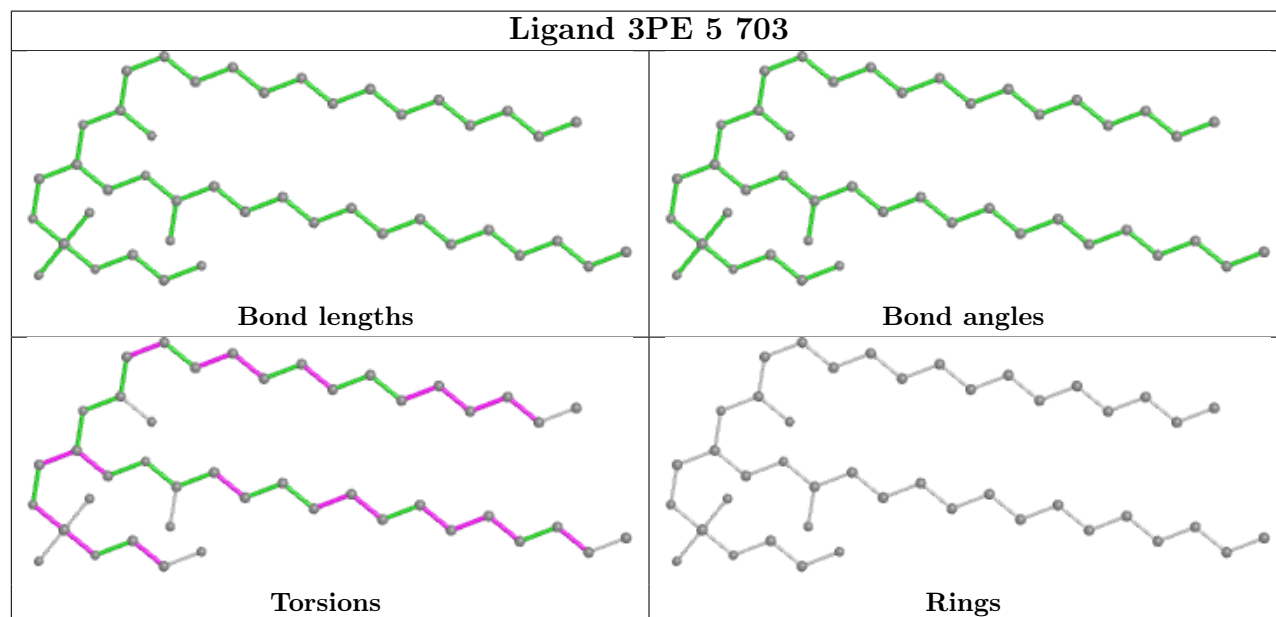
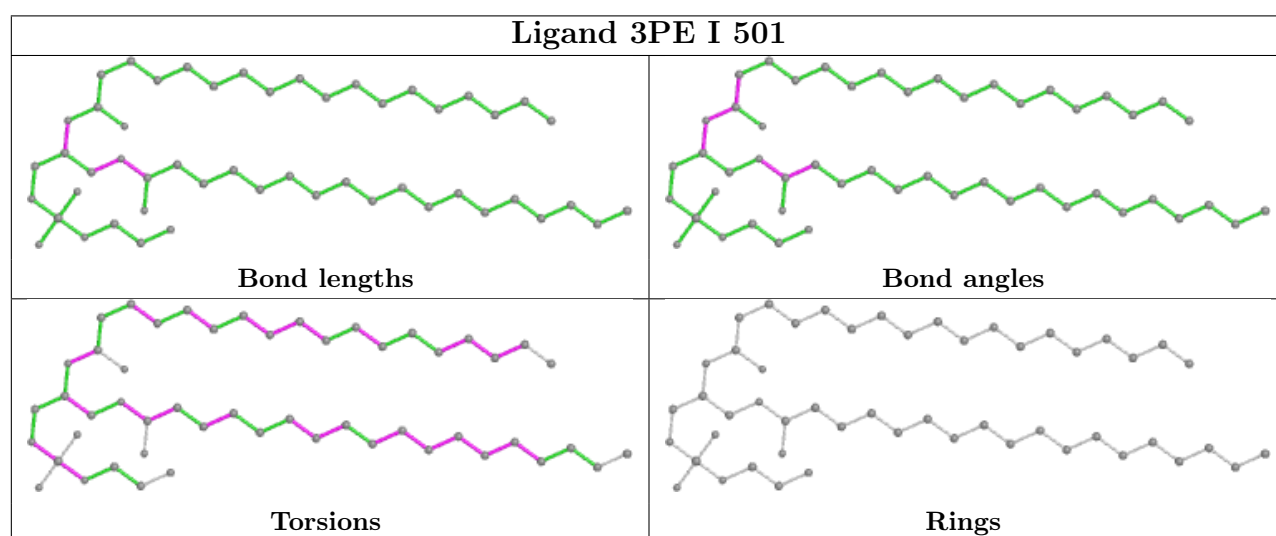
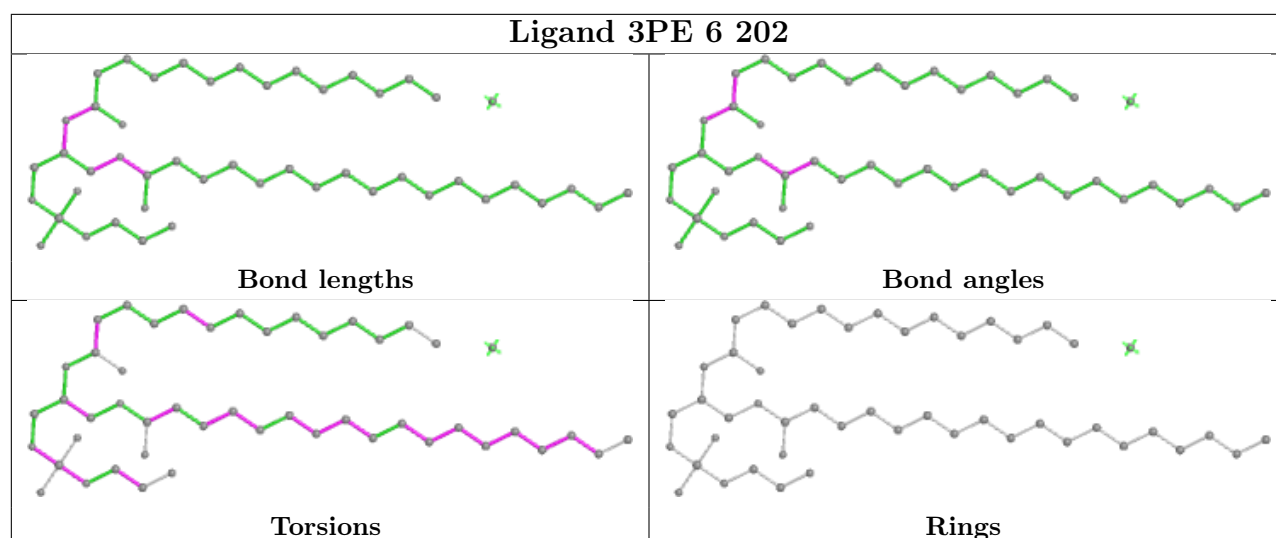
There are no ring outliers.

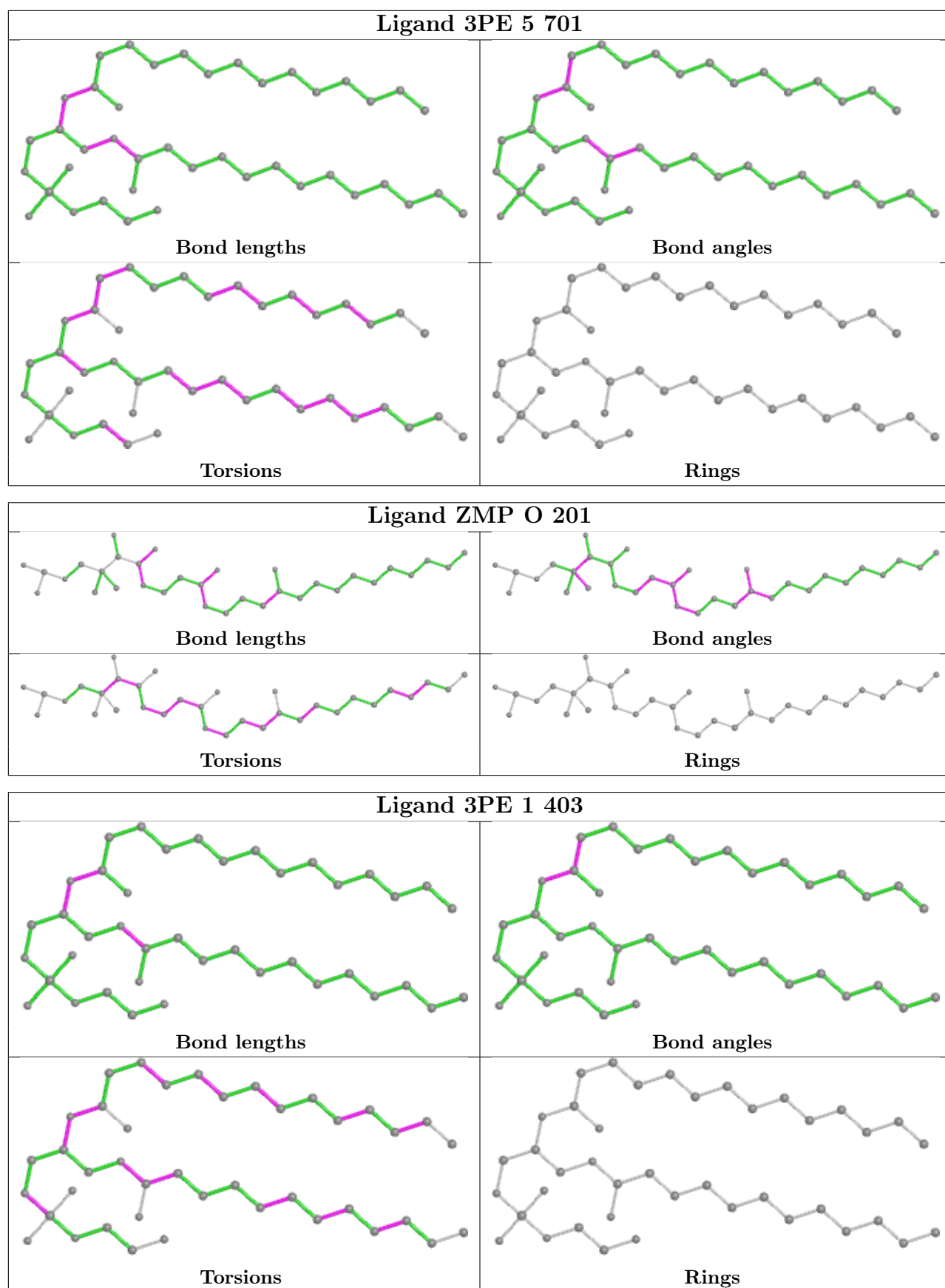
No monomer is involved in short contacts.

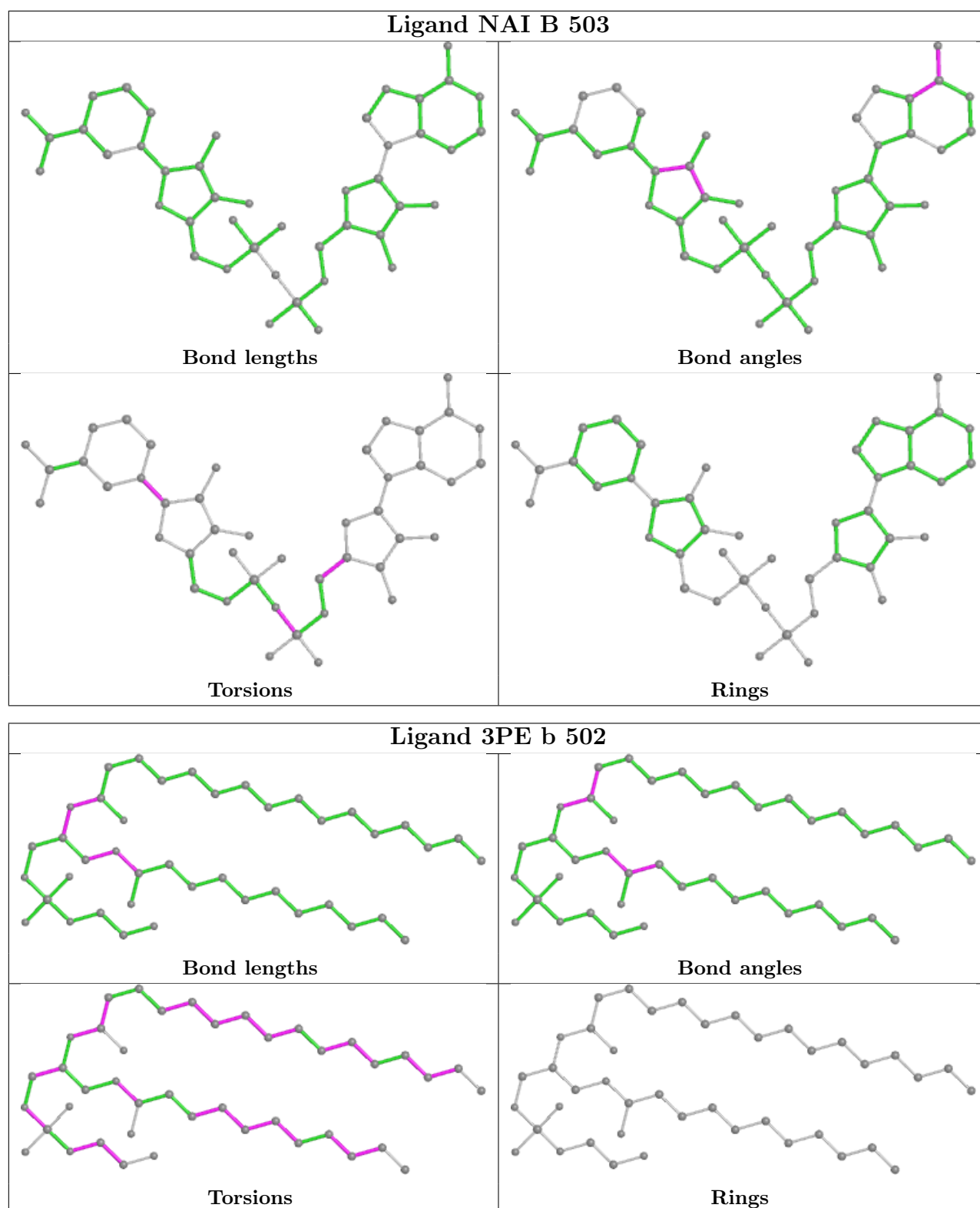
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



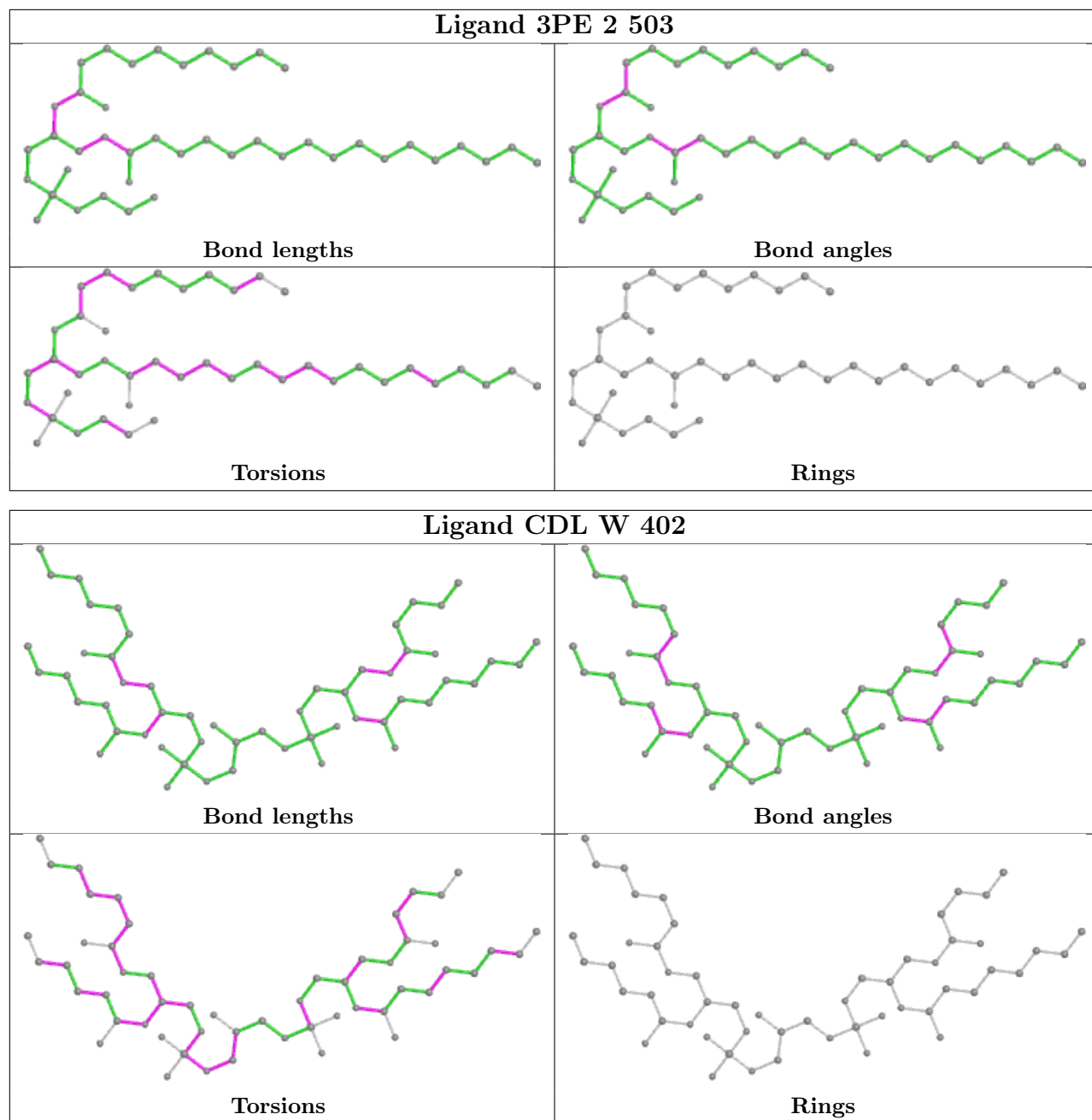


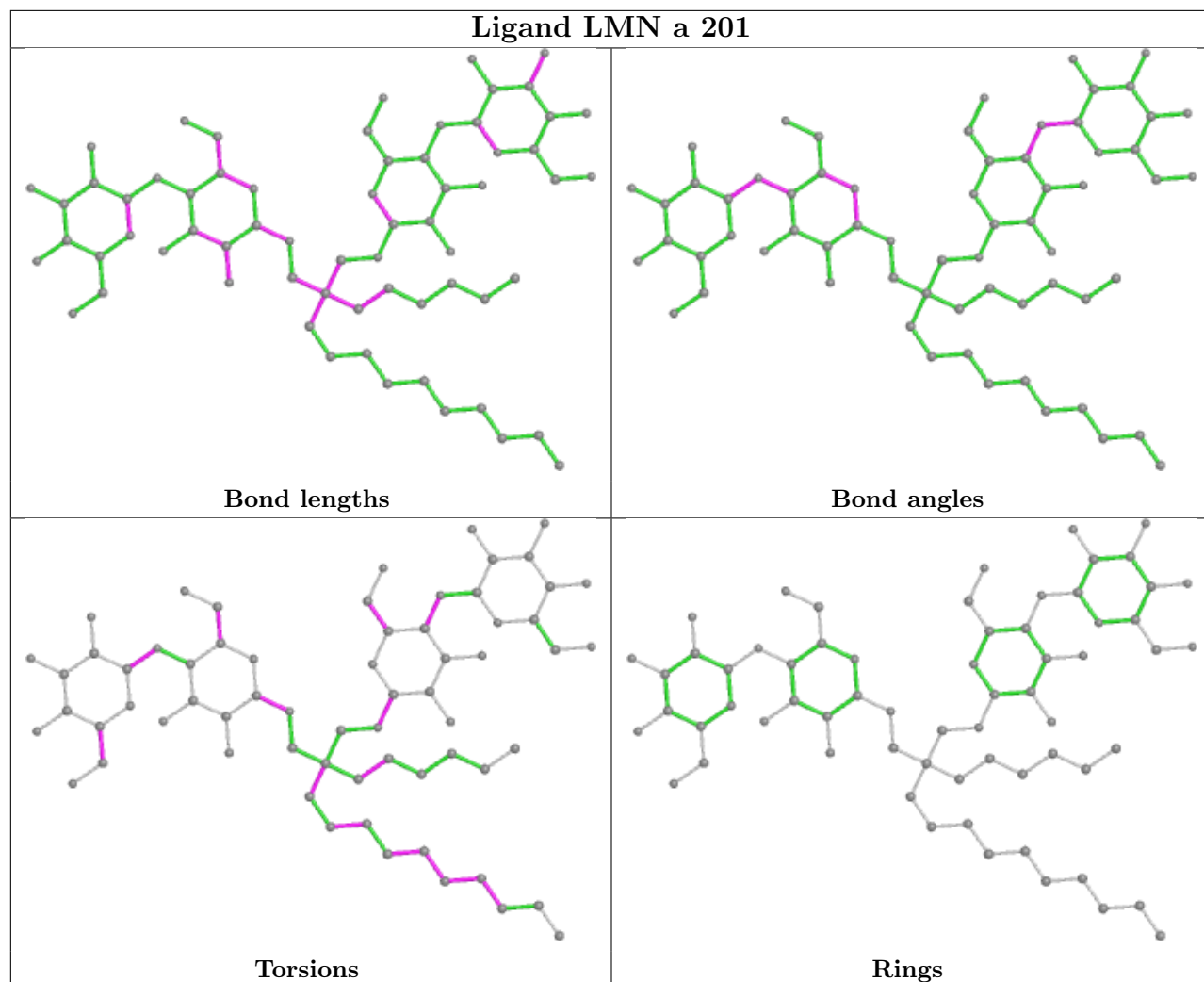


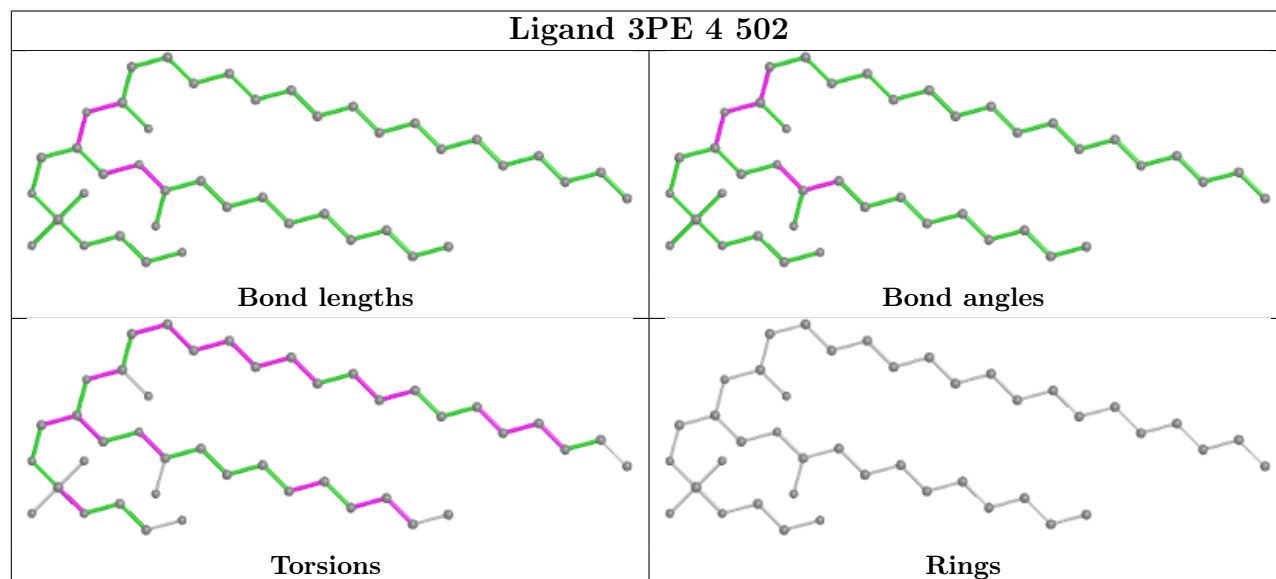
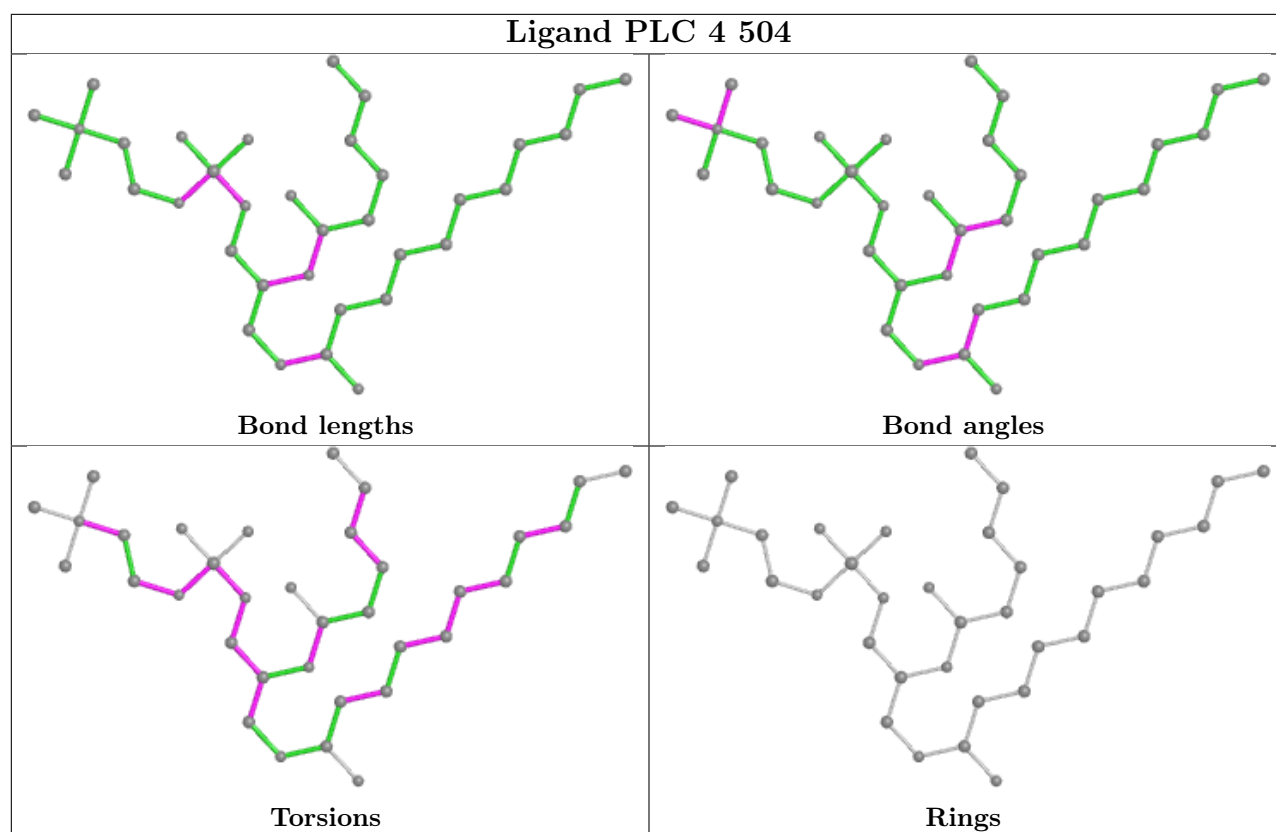


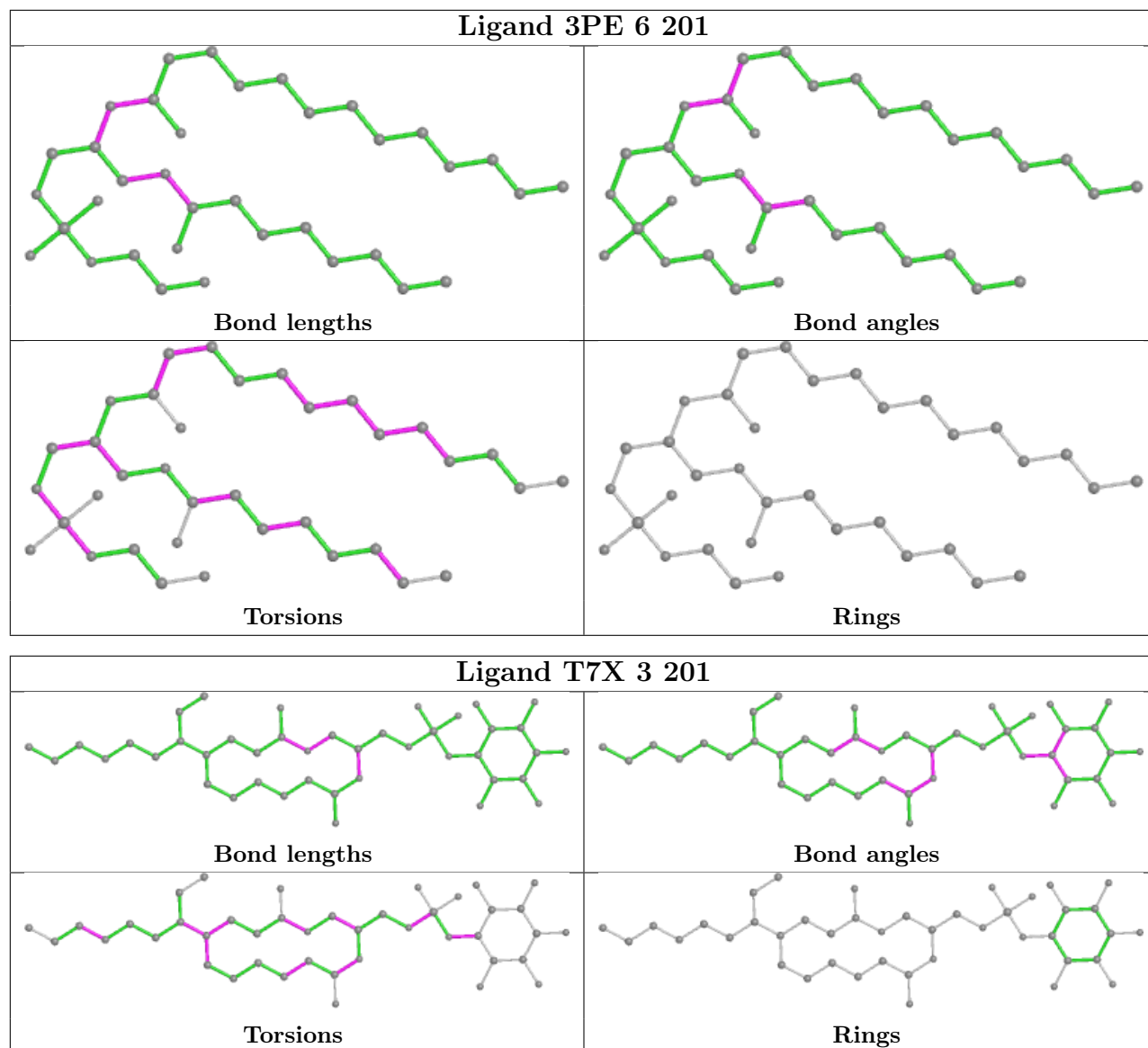


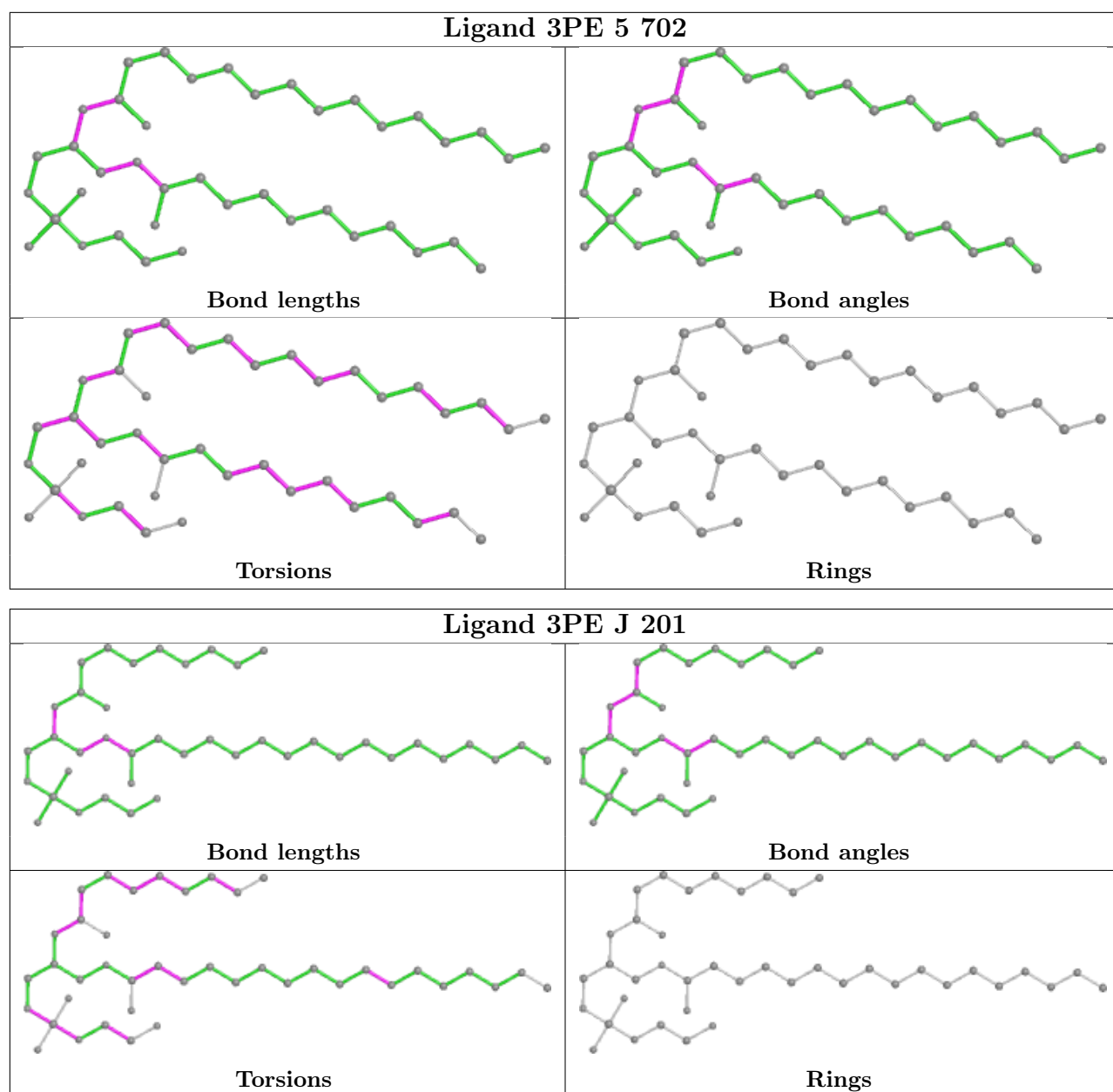


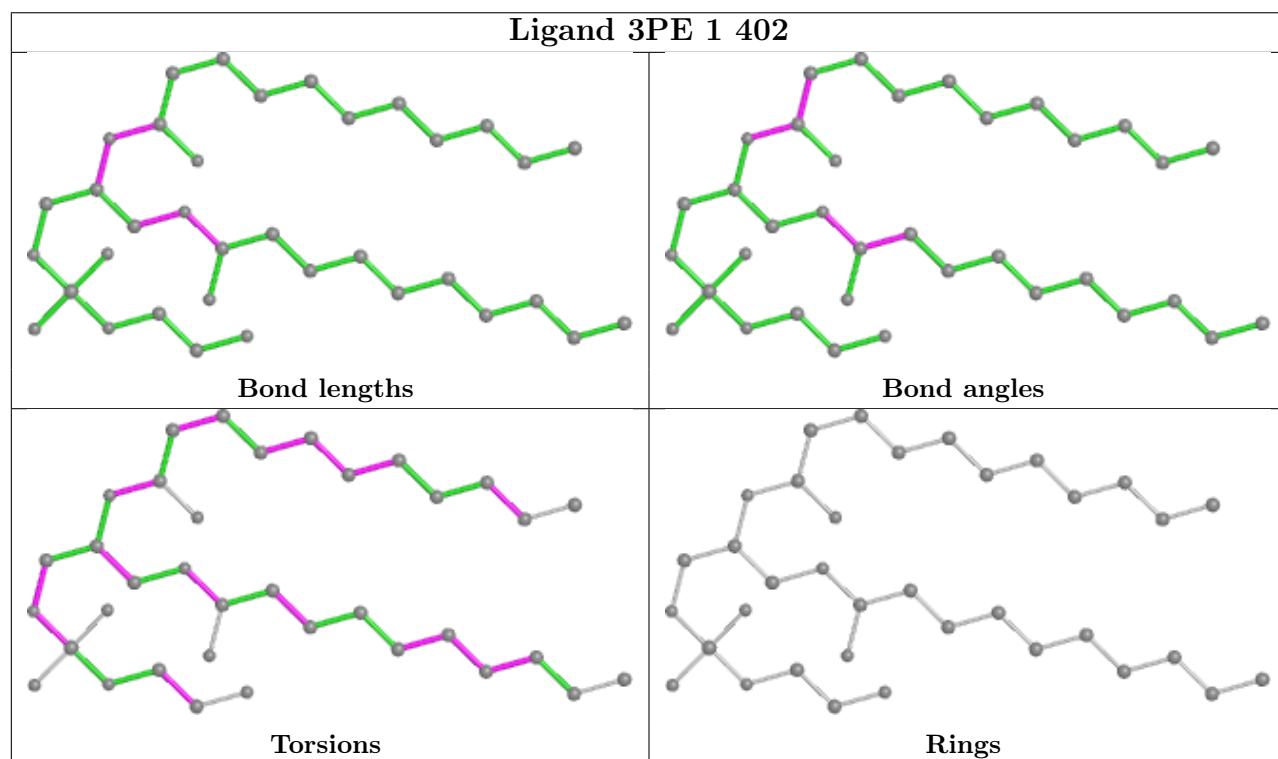
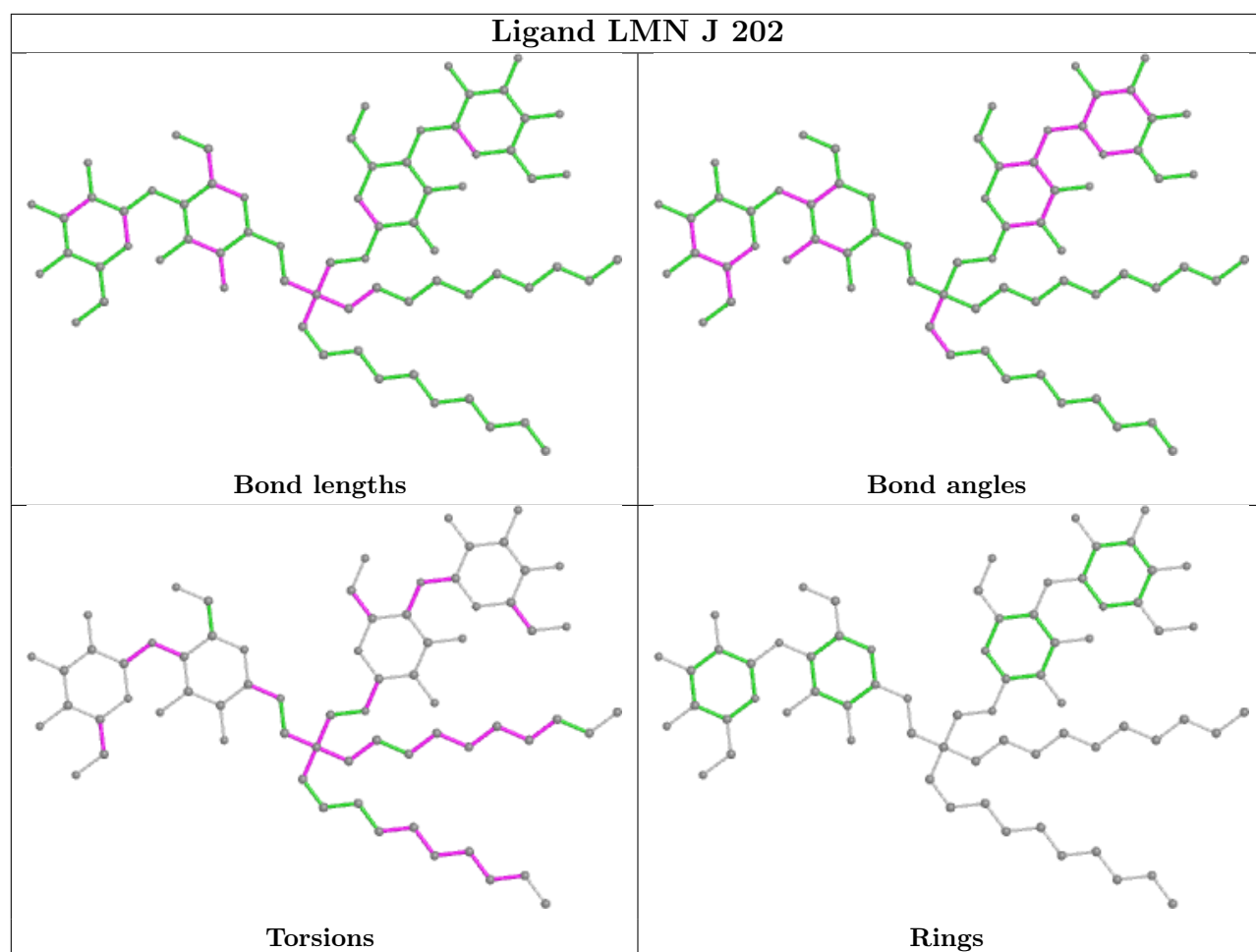


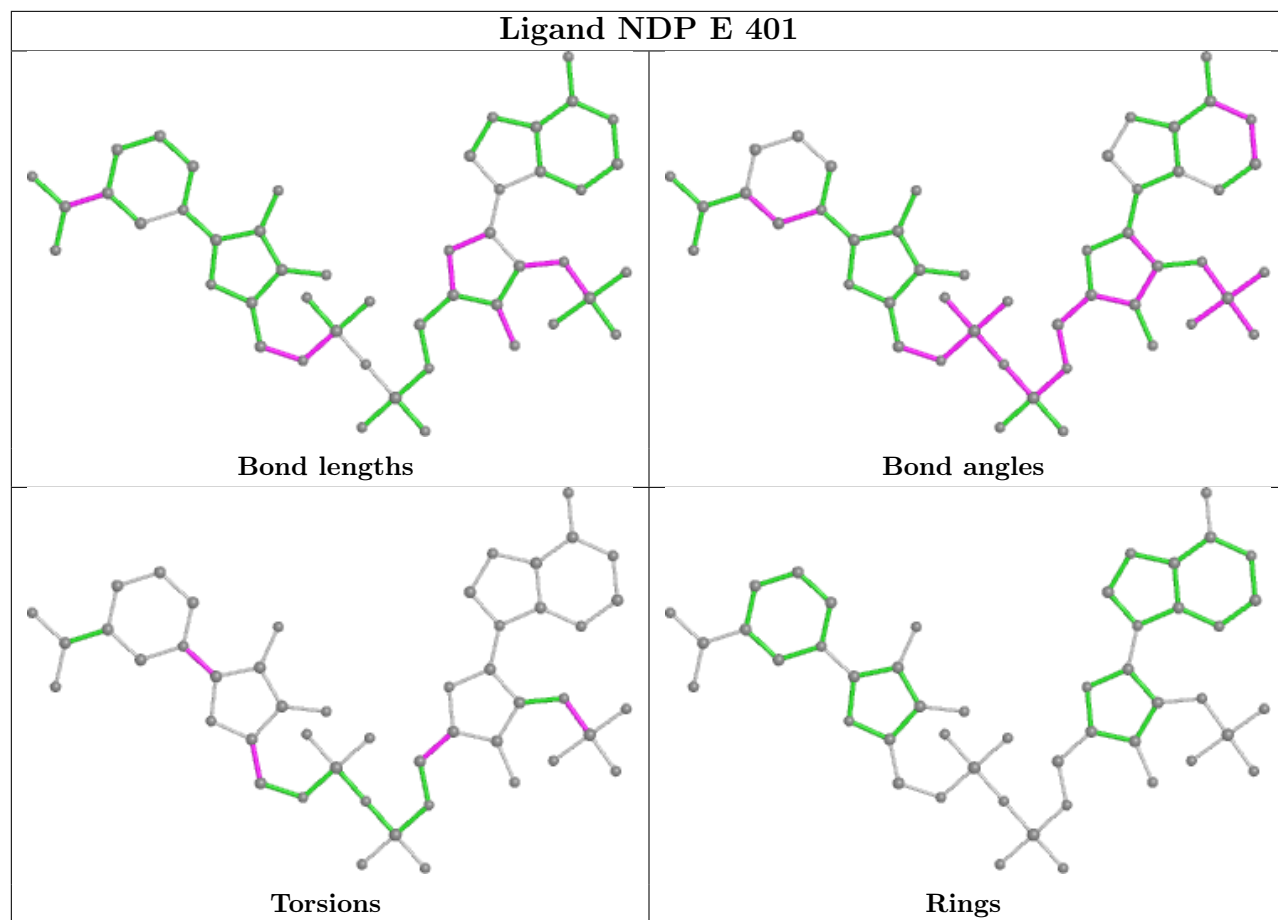


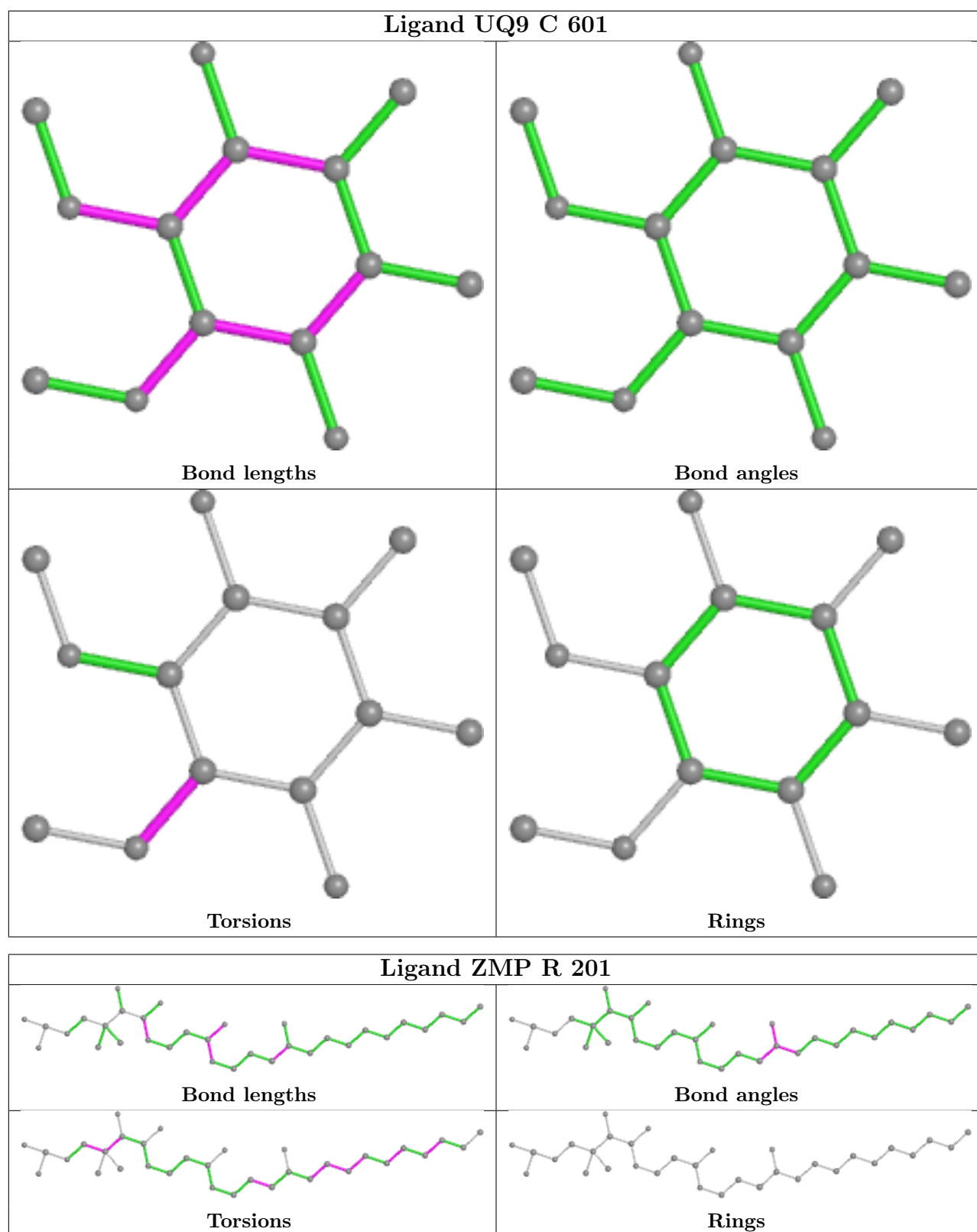




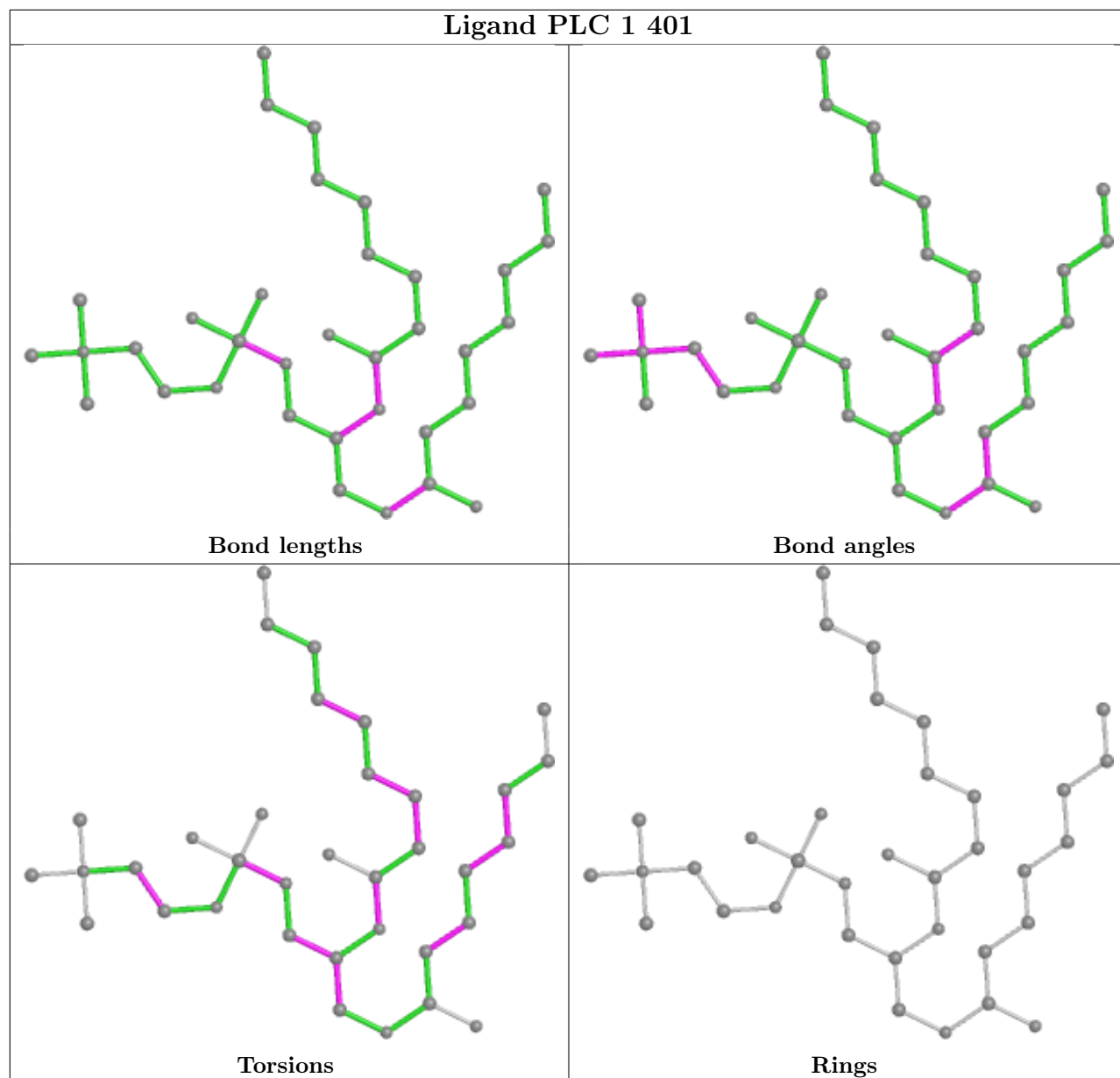


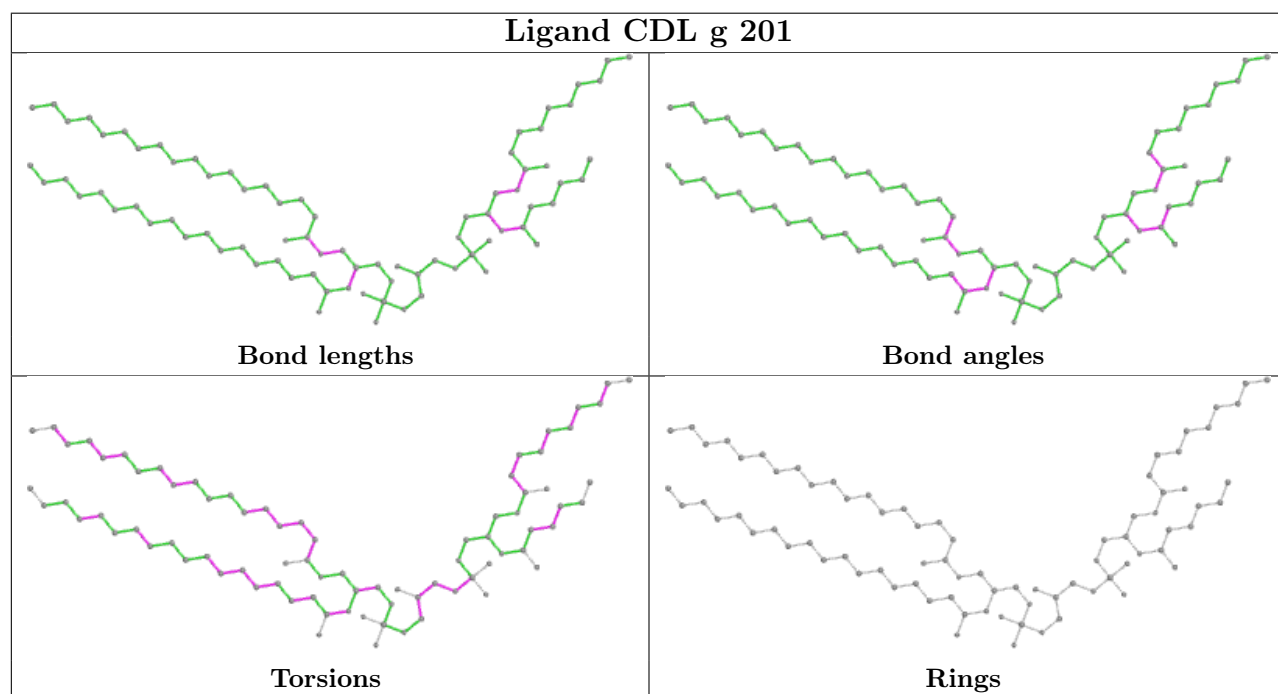
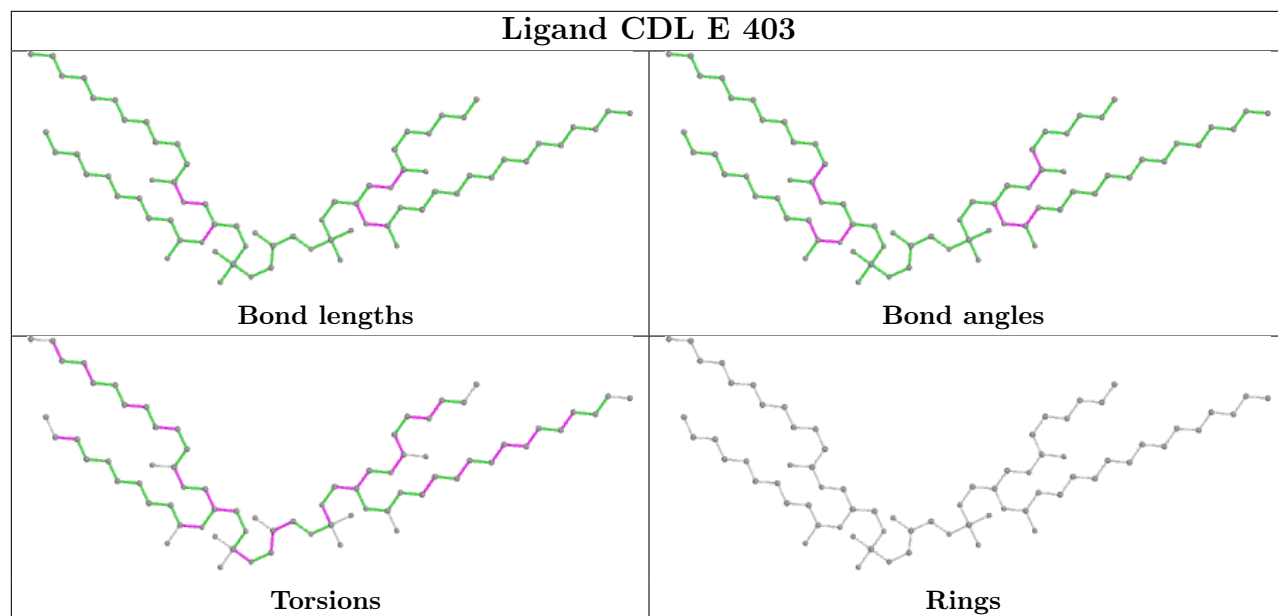


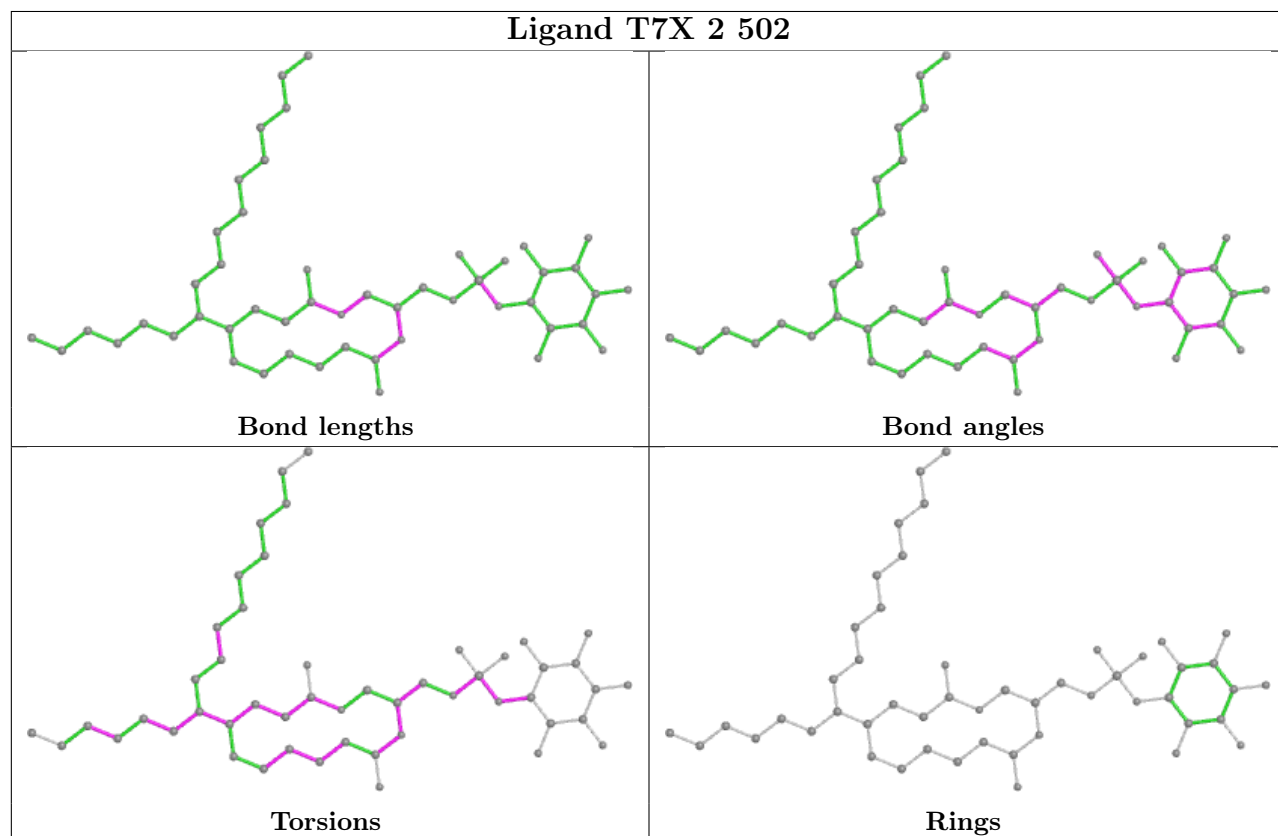
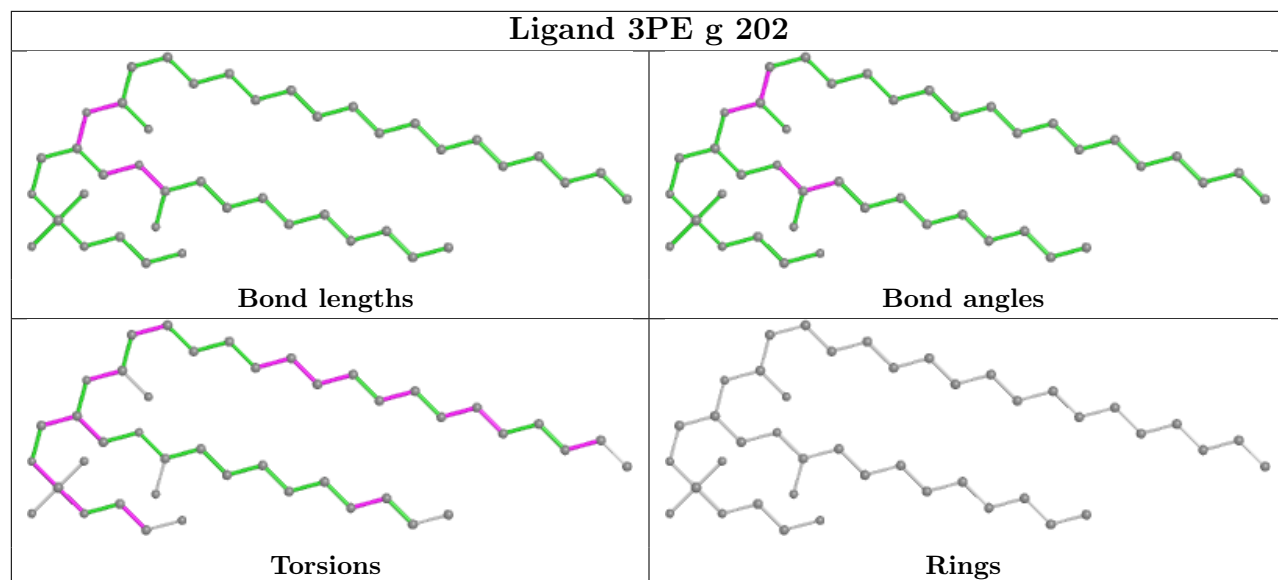


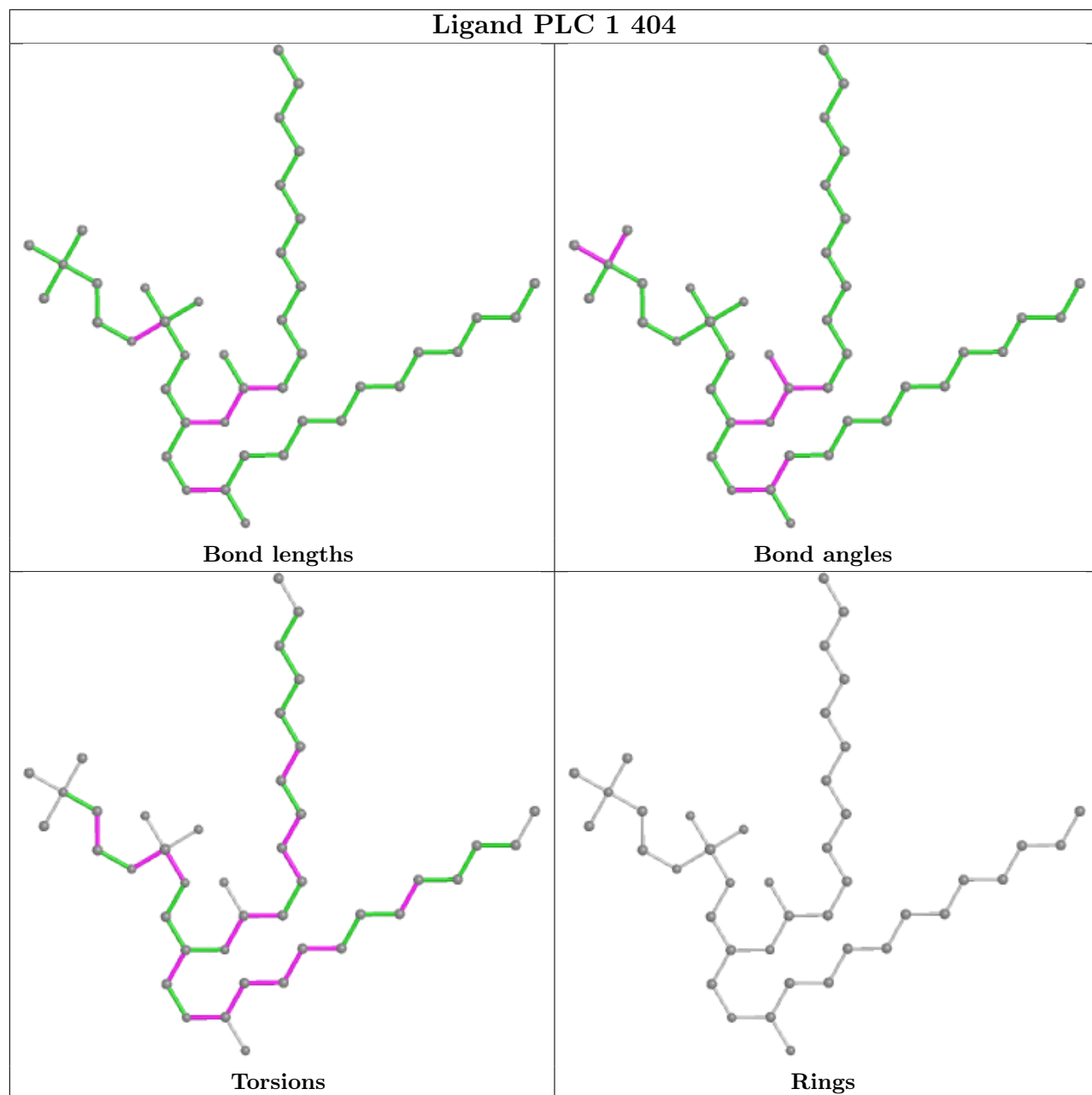


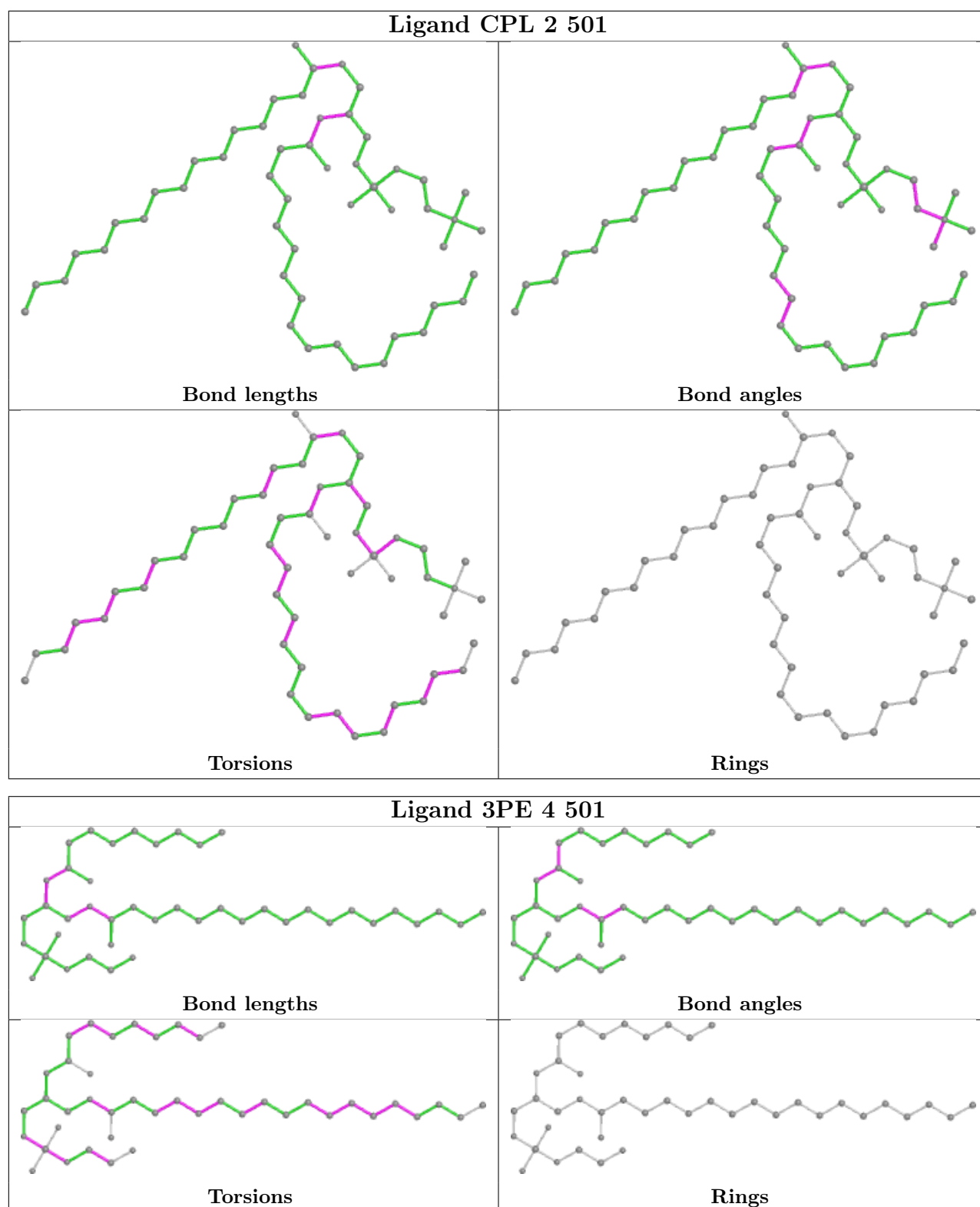


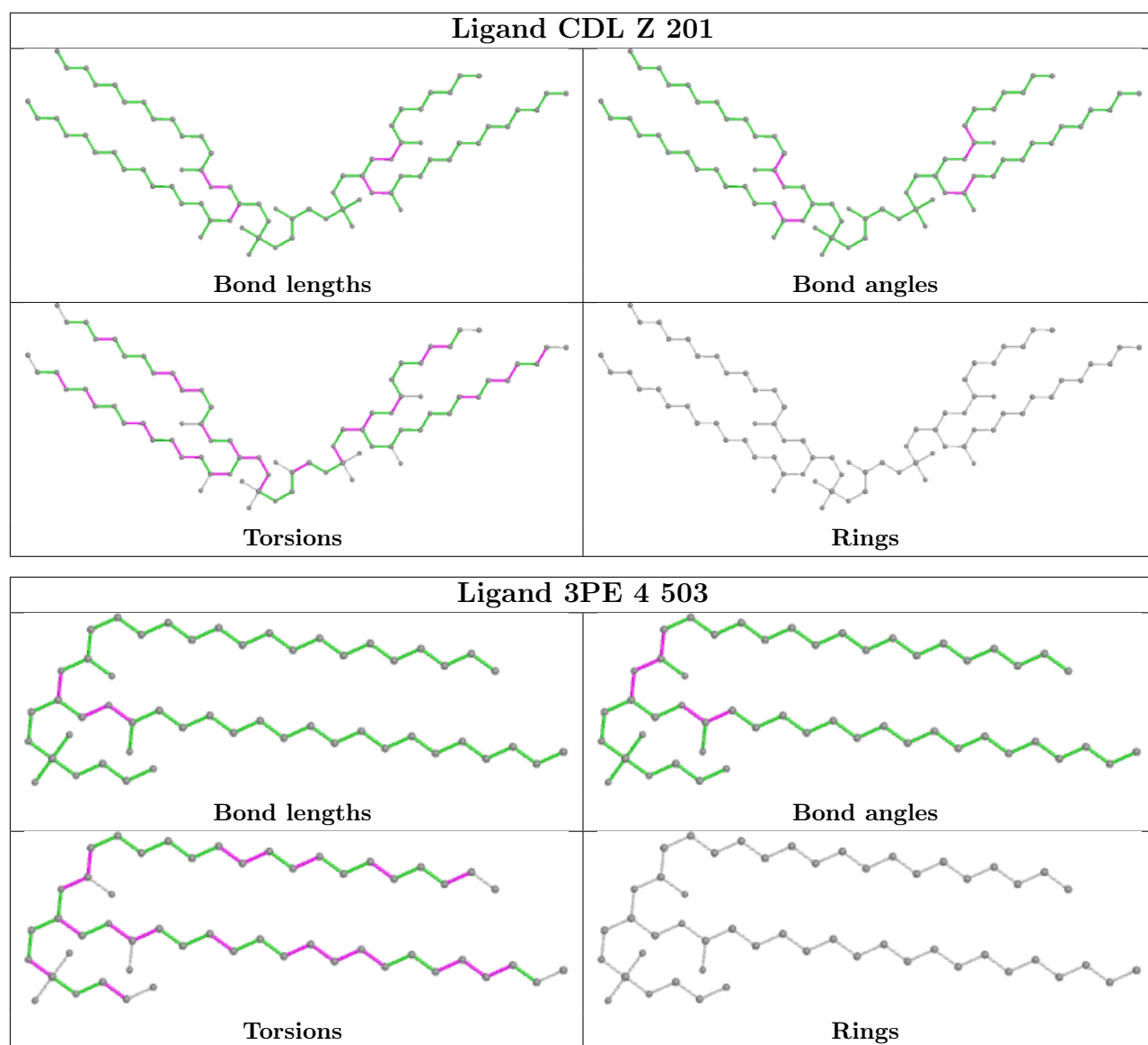


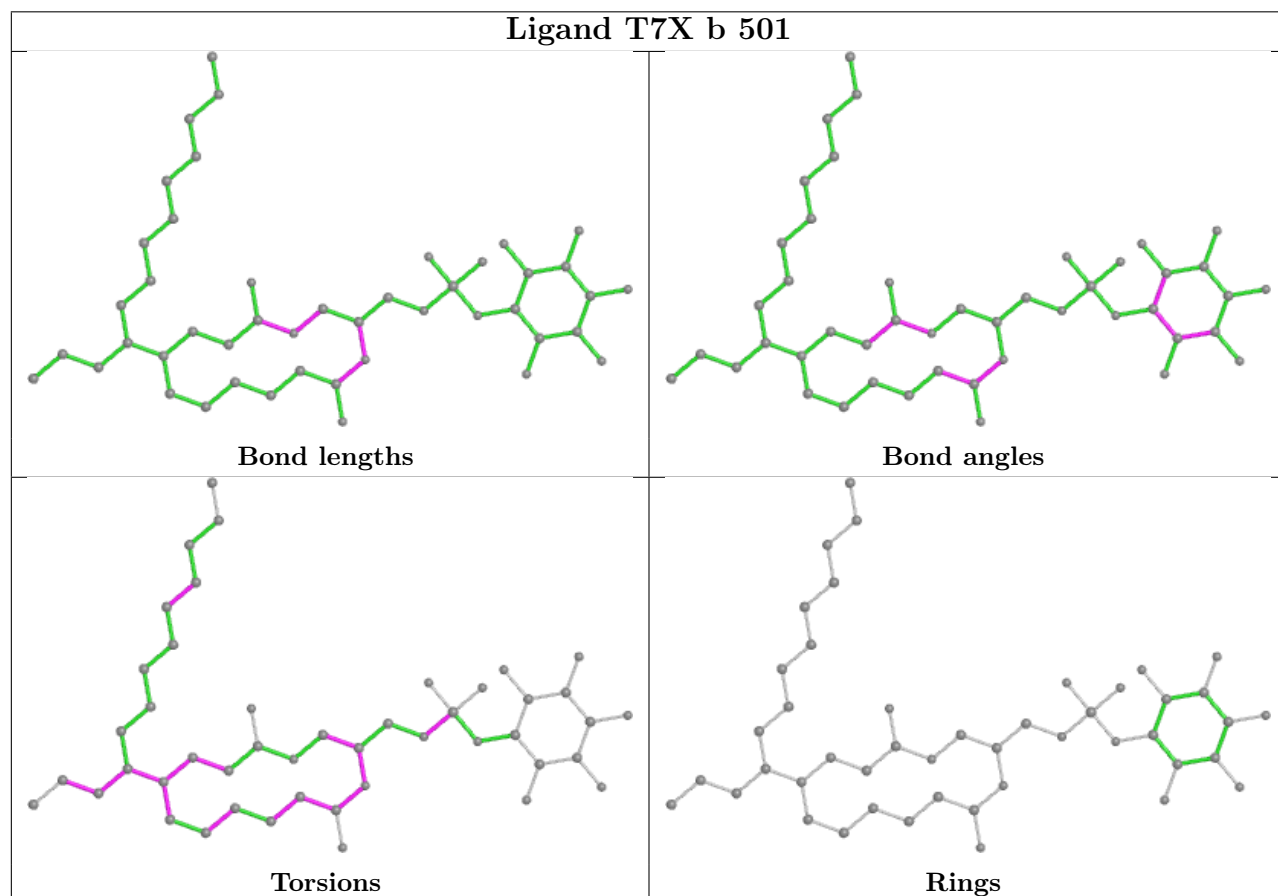
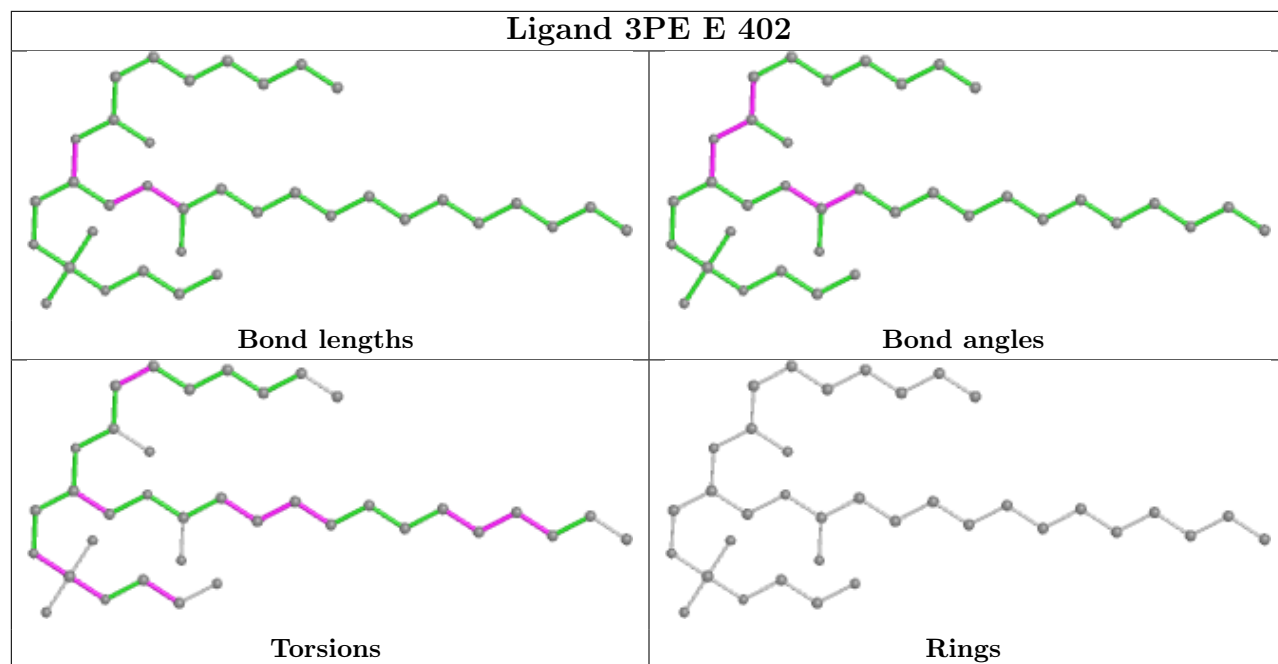


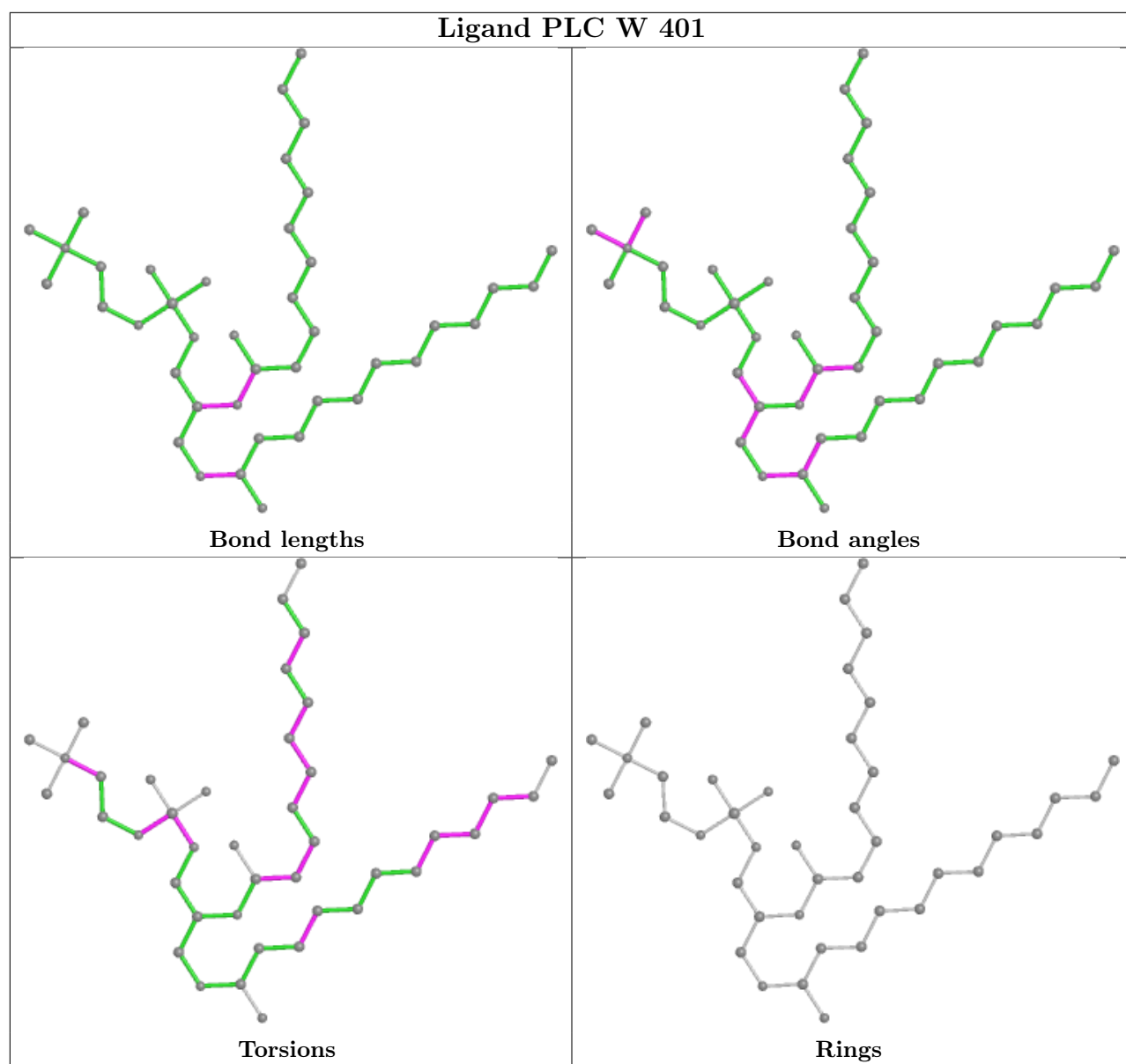




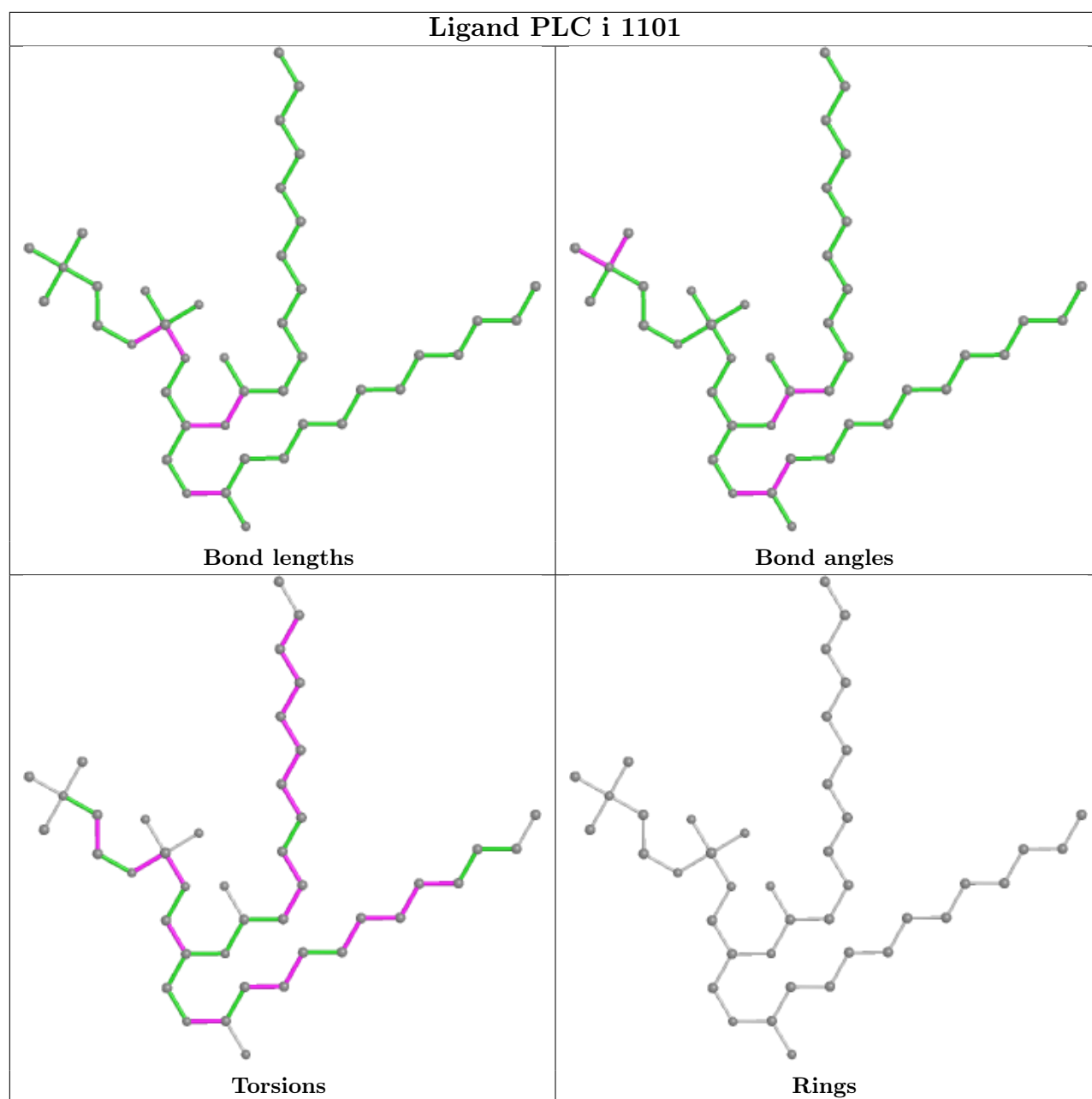












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	n	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	n	119:ARG	C	120:GLU	N	3.11

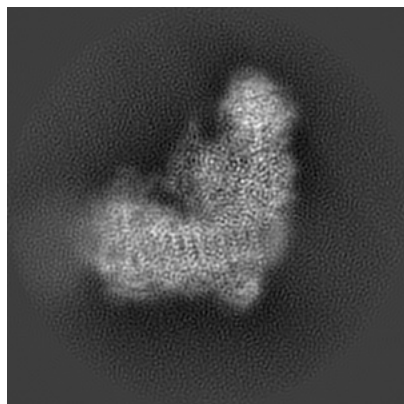
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12741. These allow visual inspection of the internal detail of the map and identification of artifacts.

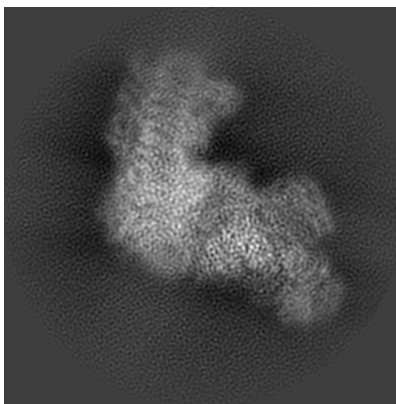
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

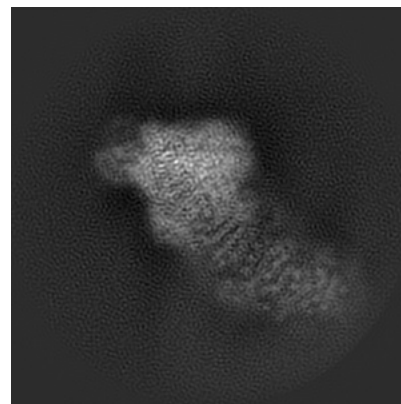
#### 6.1.1 Primary map



X

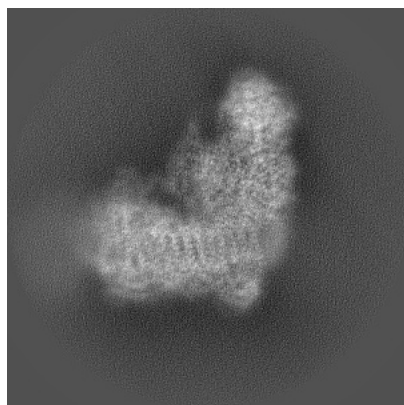


Y

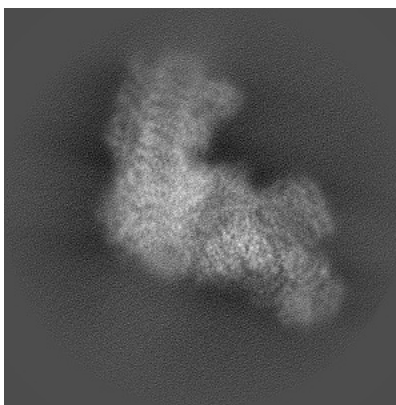


Z

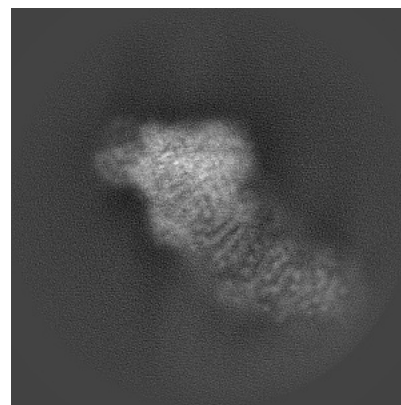
#### 6.1.2 Raw map



X



Y

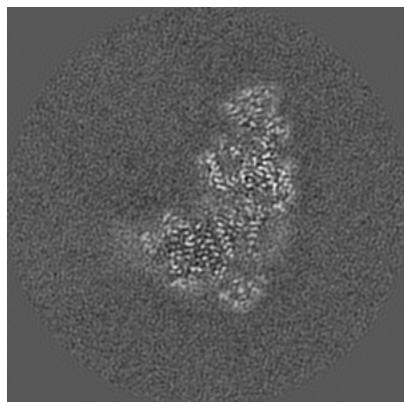


Z

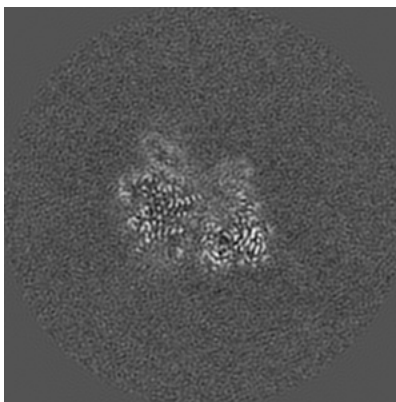
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

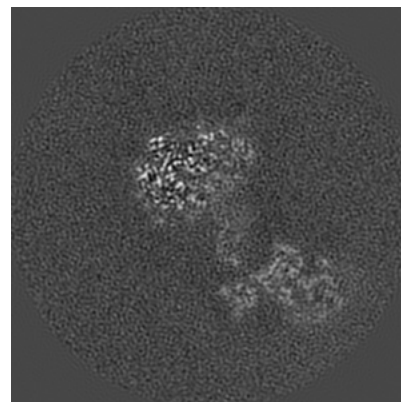
### 6.2.1 Primary map



X Index: 200

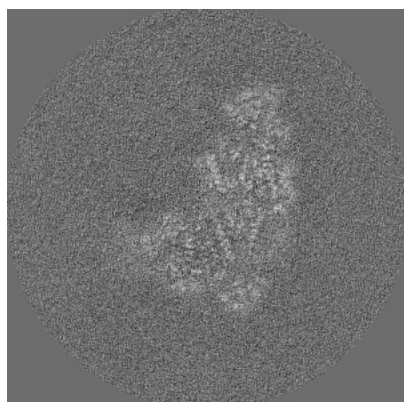


Y Index: 200

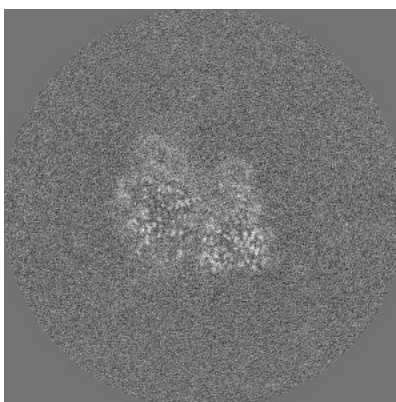


Z Index: 200

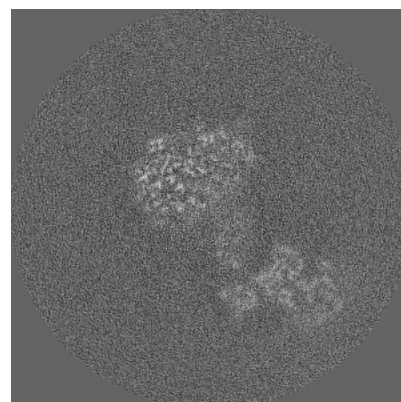
### 6.2.2 Raw map



X Index: 200



Y Index: 200

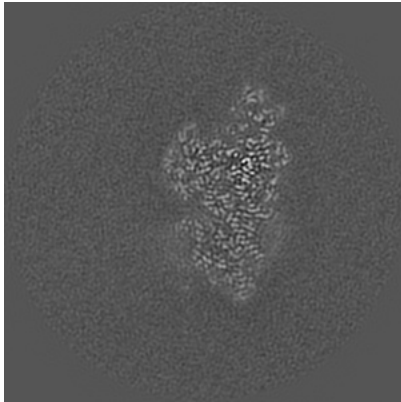


Z Index: 200

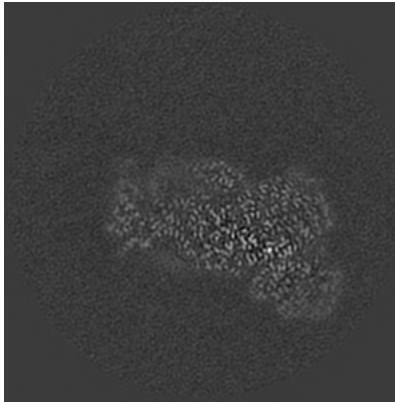
The images above show central slices of the map in three orthogonal directions.

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

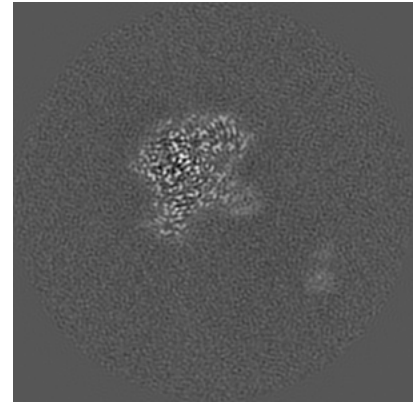
### 6.3.1 Primary map



X Index: 166

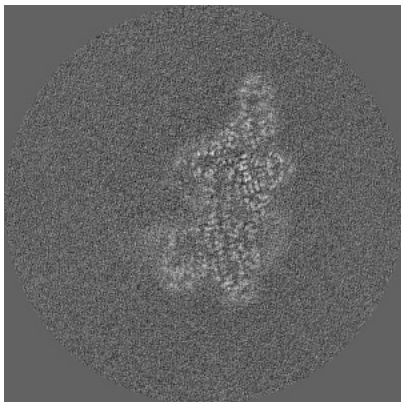


Y Index: 248

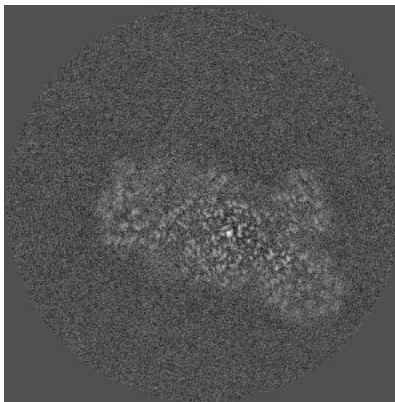


Z Index: 233

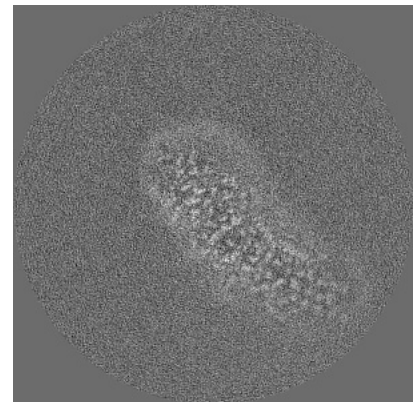
### 6.3.2 Raw map



X Index: 179



Y Index: 236

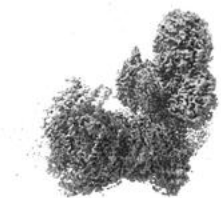


Z Index: 175

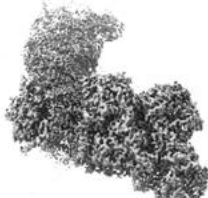
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



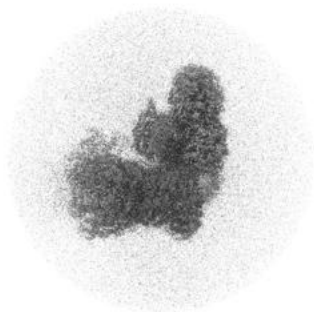
Y



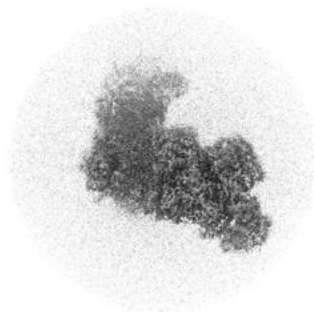
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

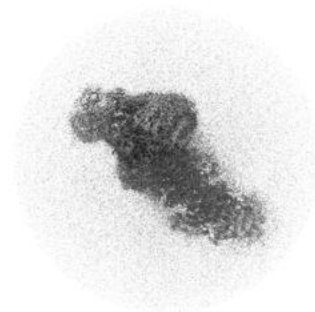
### 6.4.2 Raw map



X



Y



Z

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.

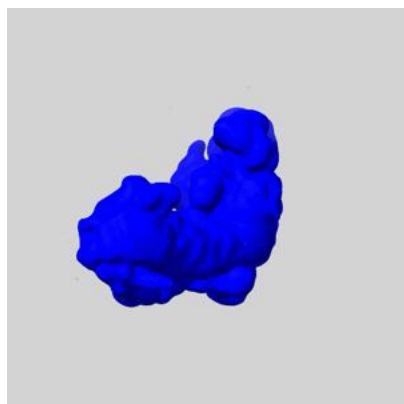
## 6.5 Mask visualisation [i](#)

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

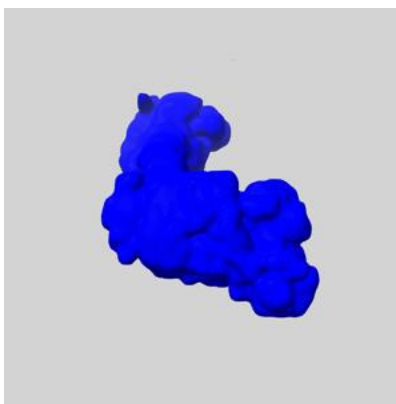
A mask typically either:

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

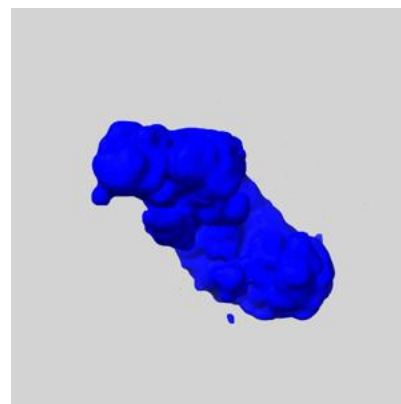
### 6.5.1 emd\_12741\_msk\_1.map [i](#)



X



Y

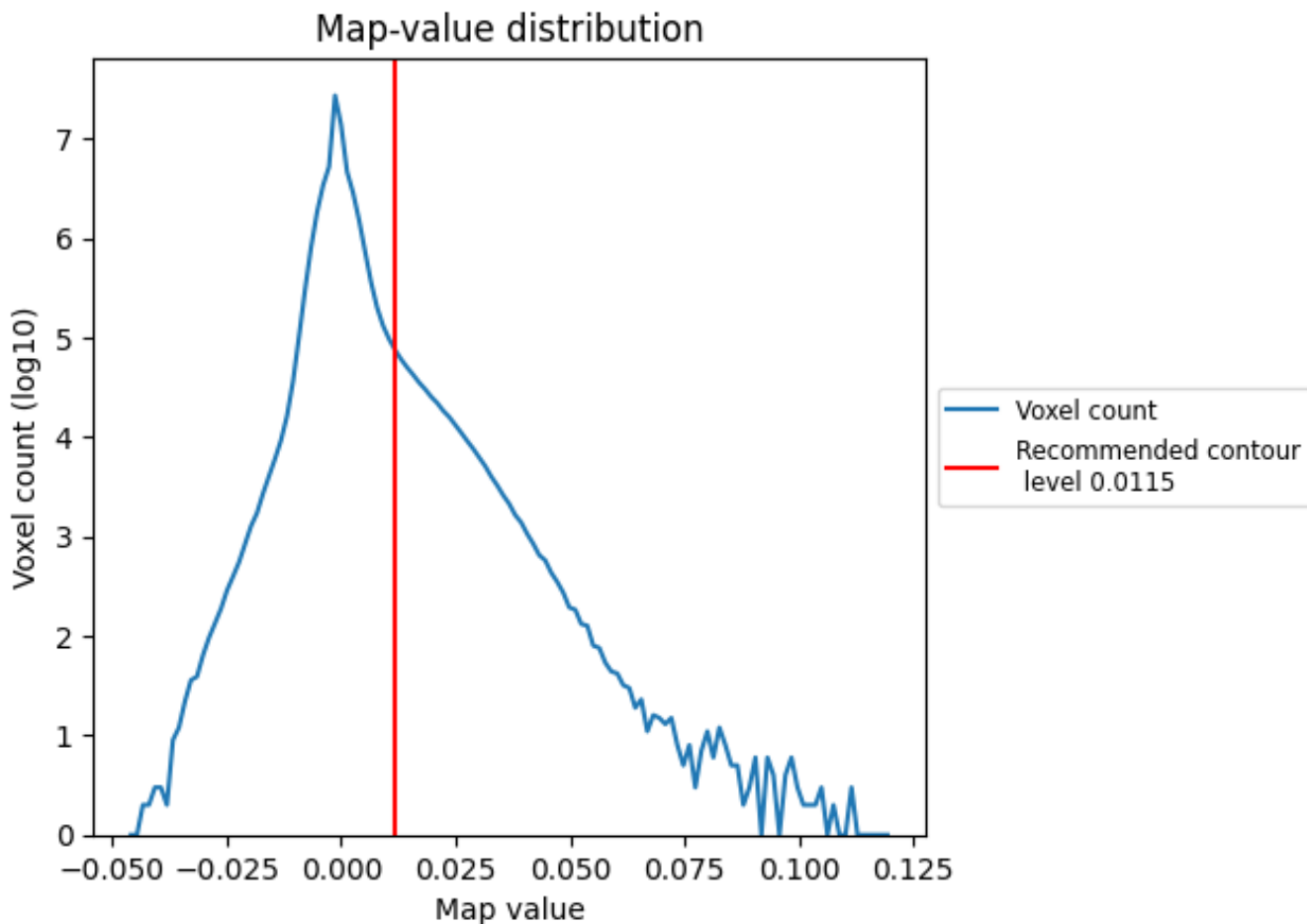


Z

## 7 Map analysis [i](#)

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

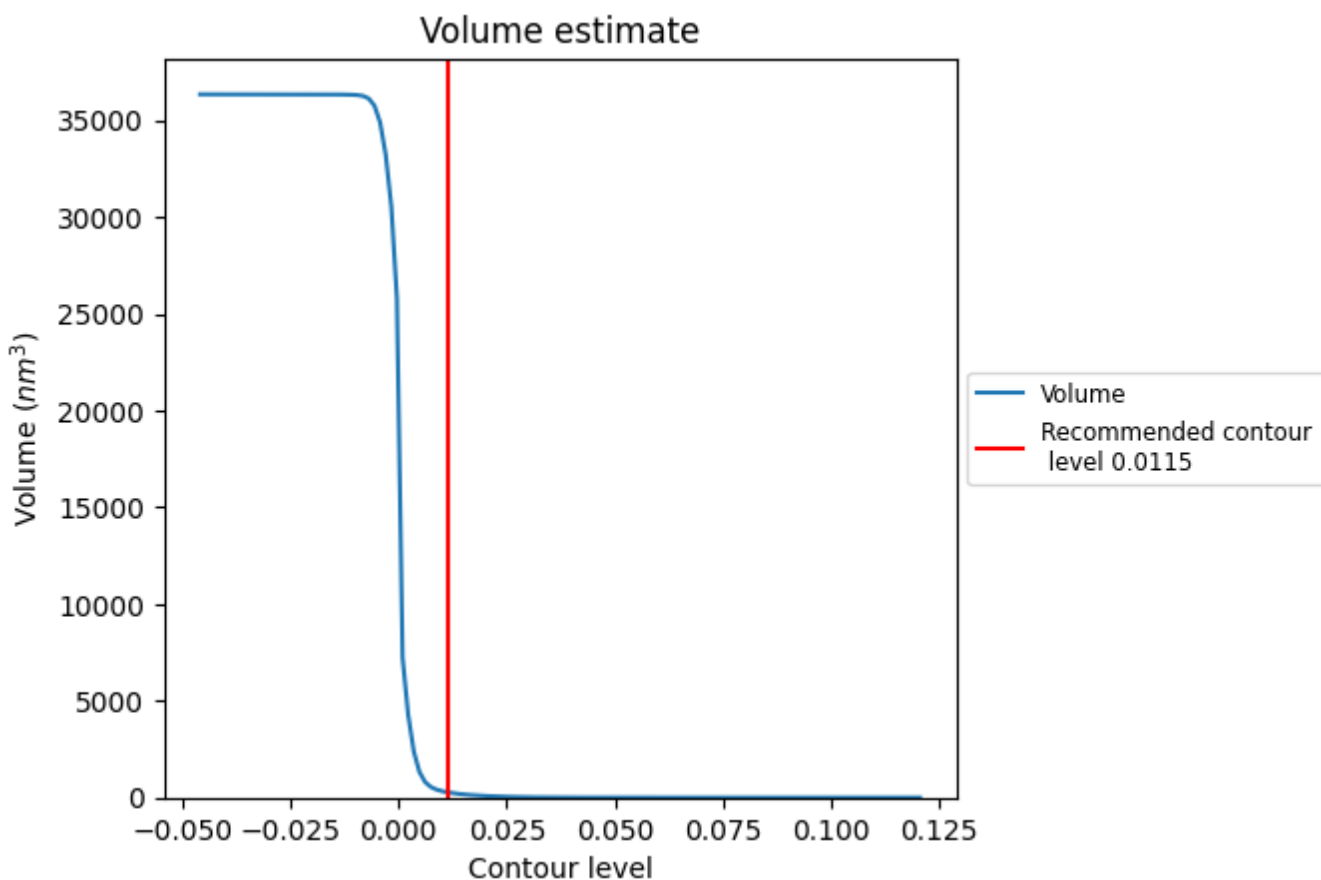
### 7.1 Map-value distribution [i](#)



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.



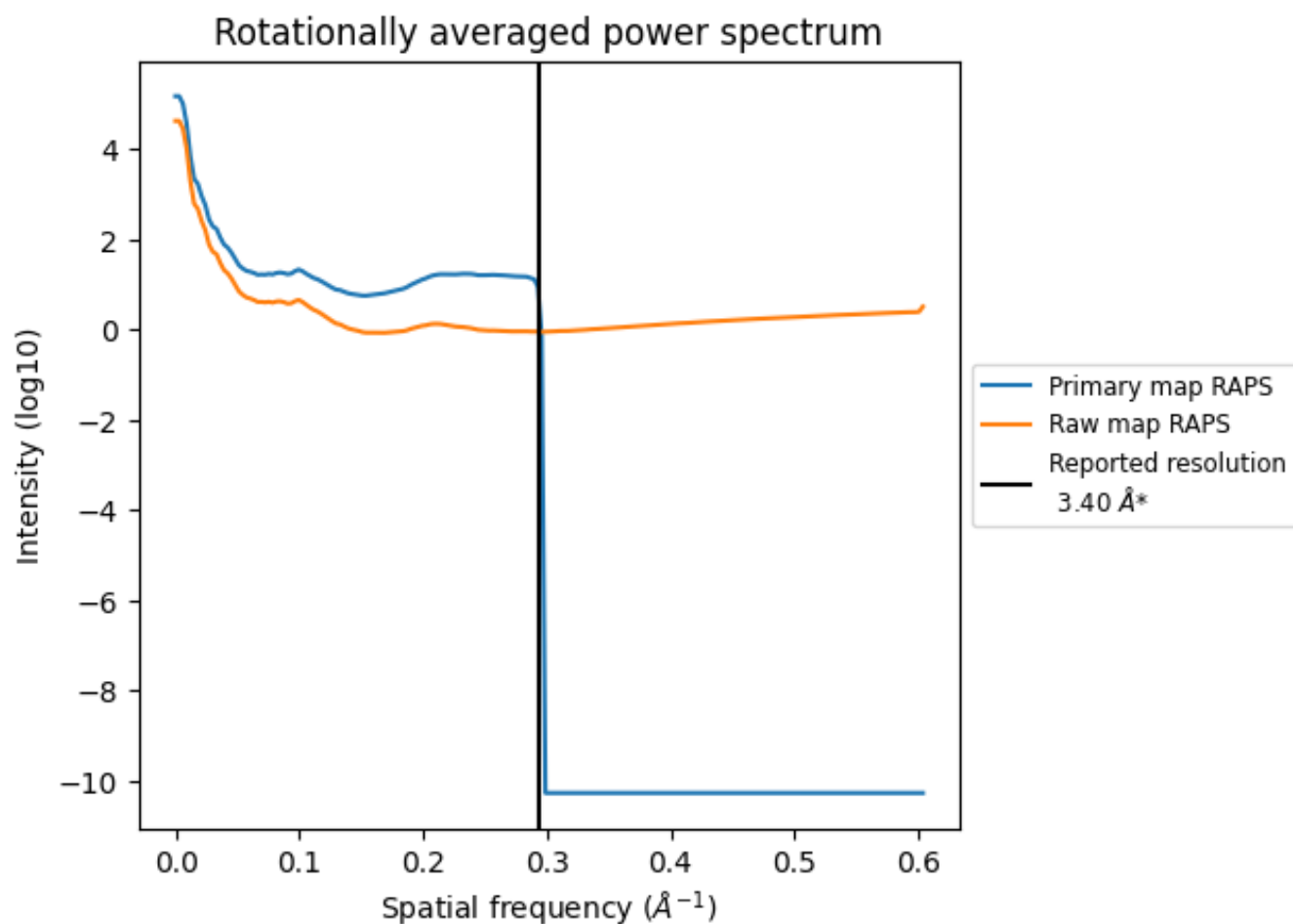
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 266  $\text{nm}^3$ ; this corresponds to an approximate mass of 240 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 [\(i\)](#)

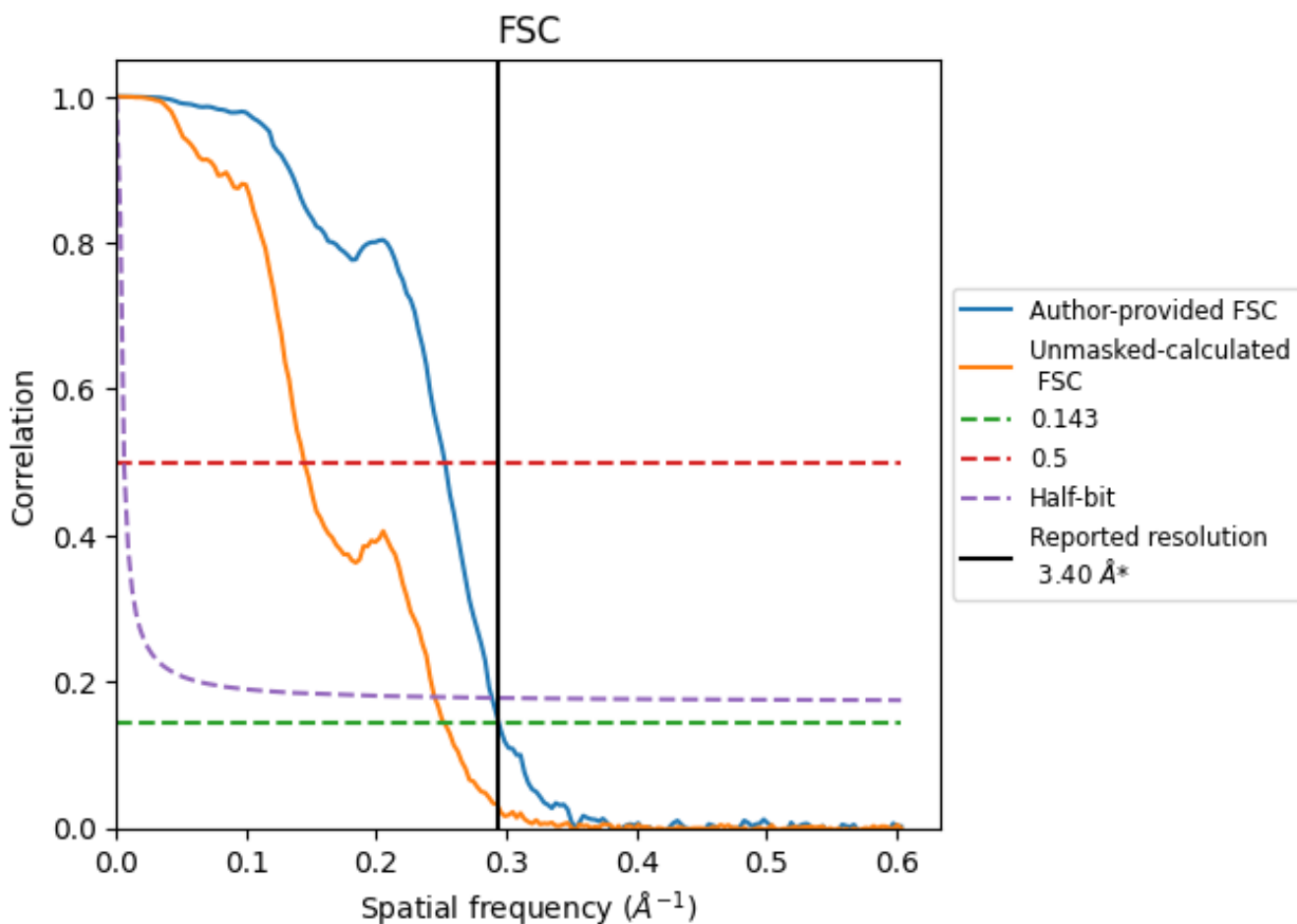


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

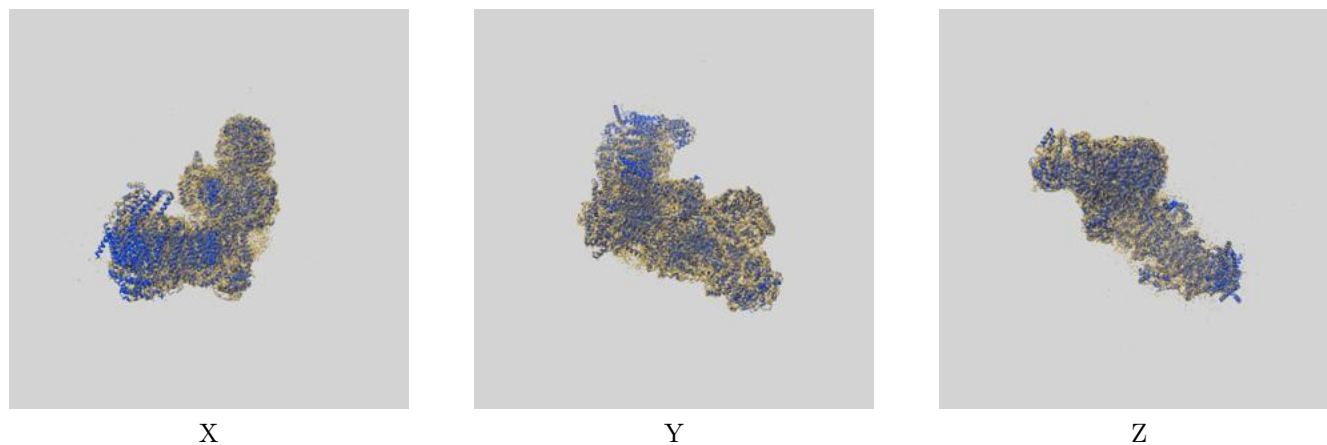
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.96	3.46
Unmasked-calculated*	3.96	6.92	4.08

\*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 3.96 differs from the reported value 3.4 by more than 10 %

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

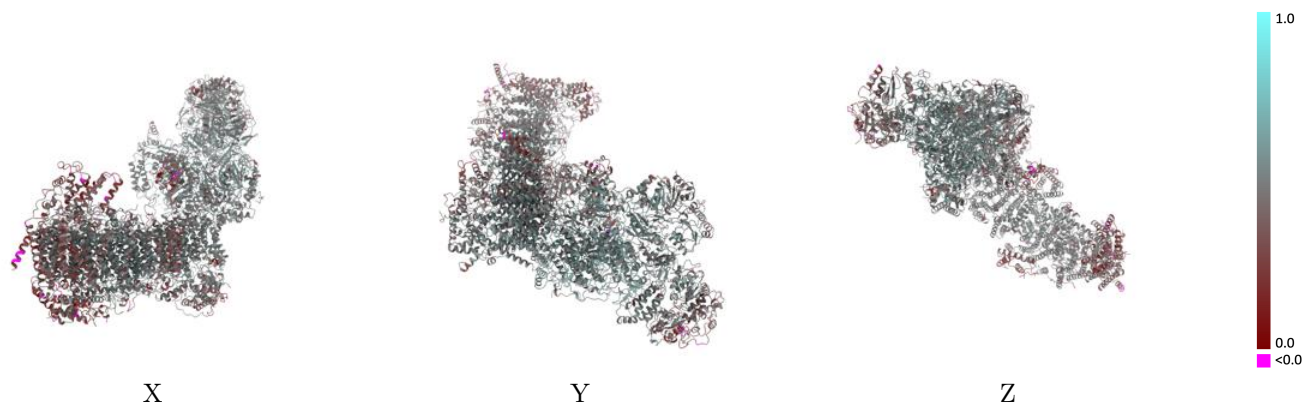
This section contains information regarding the fit between EMDB map EMD-12741 and PDB model 7O6Y. Per-residue inclusion information can be found in section 3 on page 21.

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



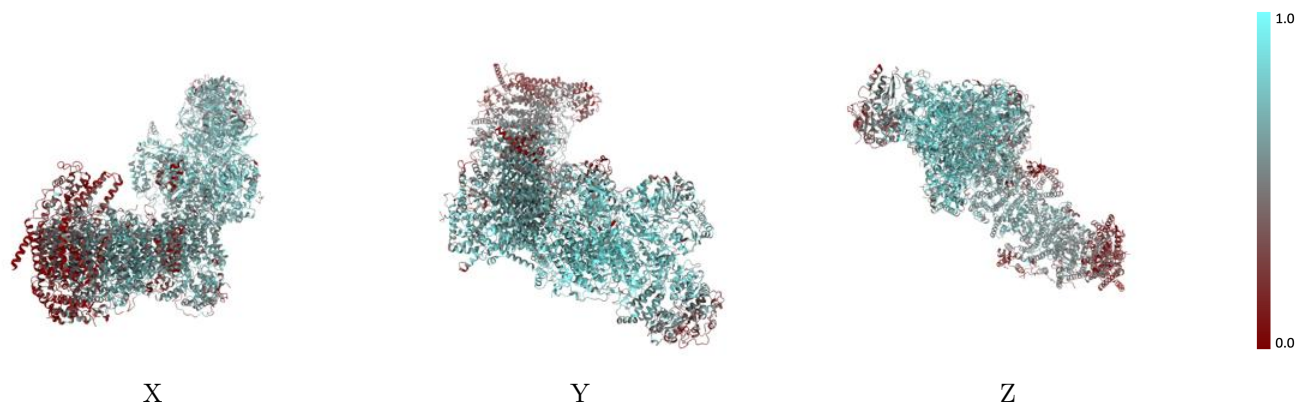
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



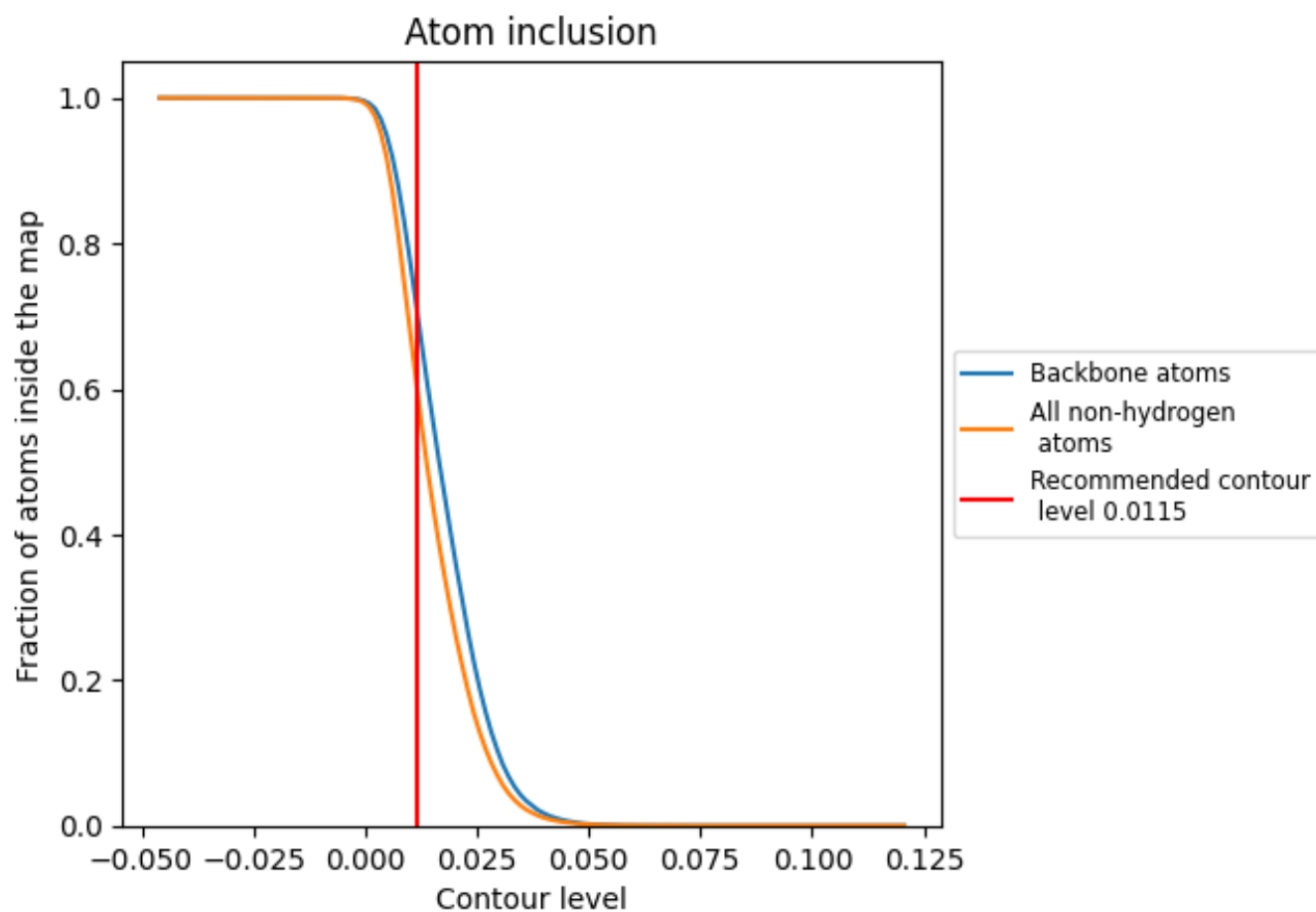
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0115).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 61% 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 (0.0115) and Q-score for the entire model and for each chain.

















Chain	Atom inclusion	Q-score
All	 0.6050	 0.4680
1	 0.7027	 0.5090
2	 0.7168	 0.5060
3	 0.6412	 0.4750
4	 0.6329	 0.5010
5	 0.4041	 0.4330
6	 0.6082	 0.4630
8	 0.1109	 0.2870
9	 0.5167	 0.4090
A	 0.7222	 0.5040
B	 0.5712	 0.4530
C	 0.7647	 0.5240
D	 0.7134	 0.5050
E	 0.6864	 0.4930
F	 0.7081	 0.5010
G	 0.8106	 0.5390
H	 0.5192	 0.3980
I	 0.8097	 0.5410
J	 0.3756	 0.3910
K	 0.8033	 0.5410
L	 0.6408	 0.4780
M	 0.7561	 0.5150
O	 0.2705	 0.2780
P	 0.6502	 0.4550
Q	 0.1628	 0.2710
R	 0.3157	 0.3550
S	 0.3505	 0.3580
U	 0.6177	 0.4590
W	 0.6667	 0.4770
X	 0.6667	 0.4760
Y	 0.7653	 0.5240
Z	 0.7324	 0.5110
a	 0.3007	 0.3720
b	 0.5436	 0.4440
c	 0.1711	 0.3080



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
d	 0.5239	 0.4490
e	 0.1082	 0.3150
f	 0.5984	 0.4370
g	 0.5345	 0.4480
h	 0.8058	 0.5400
i	 0.3787	 0.4050
j	 0.5150	 0.4520
n	 0.4283	 0.4110