



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 05:28 am GMT

PDB ID : 7ZMB
EMDB ID : EMD-14794
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (state 2)
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.75 Å (reported)
Based on initial models : 6RFR, 6RFQ

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:

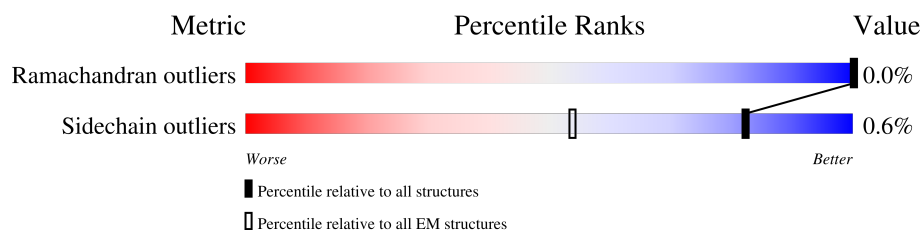
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.75 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1	378	
2	2	571	
3	3	146	
4	4	542	
5	5	679	
6	6	224	
7	8	86	
8	9	785	
9	A	749	

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Mol	Chain	Length	Quality of chain
10	B	507	
11	C	499	
12	D	86	
13	E	378	
14	F	261	
15	G	293	
16	H	318	
17	I	223	
18	J	199	
19	K	230	
20	L	89	
21	M	168	
22	O	141	
22	Q	141	
23	P	124	
24	R	99	
25	S	143	
26	U	186	
27	W	121	
28	X	191	
29	Y	210	
30	Z	196	
31	a	203	
32	b	94	
33	c	93	

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Mol	Chain	Length	Quality of chain
34	d	105	 5% 94% 6%
35	e	46	 30% 80% 20%
36	f	95	 1% 93% 7%
37	g	82	 1% 95% 5%
38	h	134	 1% 99% 0%
39	i	93	 19% 86% 14%
40	j	75	 1% 96% 3% 2%
41	n	184	 17% 73% 27%
42	o	380	 8% 92% 0%

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 69495 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	334	Total	C	N	O	S	0	0
			2573	1728	388	446	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	558	Total	C	N	O	S	0	0
			4456	2993	672	780	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	130	Total	C	N	O	S	0	0
			1026	695	153	175	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	494	Total	C	N	O	S	0	0
			3904	2650	572	670	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	670	Total	C	N	O	S	0	0
			5272	3551	792	904	25		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	445	ARG	-	insertion	UNP G1DJA3
5	446	LEU	-	insertion	UNP G1DJA3
5	447	ALA	-	insertion	UNP G1DJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
5	448	ILE	-	insertion	UNP G1DJA3
5	449	ASP	-	insertion	UNP G1DJA3
5	450	ASN	-	insertion	UNP G1DJA3
5	451	PHE	-	insertion	UNP G1DJA3
5	452	PHE	-	insertion	UNP G1DJA3
5	453	SER	-	insertion	UNP G1DJA3
5	454	ALA	-	insertion	UNP G1DJA3
5	455	GLN	-	insertion	UNP G1DJA3
5	456	ALA	-	insertion	UNP G1DJA3
5	457	ILE	-	insertion	UNP G1DJA3
5	458	LYS	-	insertion	UNP G1DJA3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	190	Total	C	N	O	S	0	0
			1452	982	217	247	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	77	Total	C	N	O	S	0	0
			658	408	126	118	6		

- Molecule 8 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	103	Total	C	N	O	S	0	0
			807	500	147	154	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	100	VAL	-	insertion	UNP G0SG48

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	711	Total	C	N	O	S	0	0
			5476	3444	966	1035	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP G0RYA1
A	72	TYR	VAL	conflict	UNP G0RYA1
A	73	CYS	SER	conflict	UNP G0RYA1
A	74	TYR	MET	conflict	UNP G0RYA1
A	75	HIS	ARG	conflict	UNP G0RYA1
A	76	GLU	ARG	conflict	UNP G0RYA1

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	456	Total	C	N	O	S	0	0
			3538	2225	638	648	27		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	441	Total	C	N	O	S	0	0
			3468	2205	604	640	19		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LYS	deletion	UNP G0SCG0
C	?	-	LEU	deletion	UNP G0SCG0
C	?	-	THR	deletion	UNP G0SCG0
C	?	-	ILE	deletion	UNP G0SCG0
C	?	-	ALA	deletion	UNP G0SCG0
C	?	-	PRO	deletion	UNP G0SCG0
C	?	-	LYS	deletion	UNP G0SCG0

- Molecule 12 is a protein called Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	85	Total	C	N	O	S	0	0
			678	432	127	115	4		

- Molecule 13 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	337	Total	C	N	O	S	0	0
			2741	1743	484	505	9		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	103	GLU	-	insertion	UNP G0SB35
E	104	PHE	-	insertion	UNP G0SB35
E	105	ASP	-	insertion	UNP G0SB35
E	106	LEU	-	insertion	UNP G0SB35
E	107	ARG	-	insertion	UNP G0SB35
E	108	ASN	-	insertion	UNP G0SB35
E	109	THR	-	insertion	UNP G0SB35
E	110	GLN	-	insertion	UNP G0SB35
E	233	HIS	-	insertion	UNP G0SB35
E	234	VAL	-	insertion	UNP G0SB35

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	238	Total	C	N	O	S	0	0
			1884	1189	328	366	1		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase 30.4 kDa subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	242	Total	C	N	O	S	0	0
			1968	1271	329	361	7		

- Molecule 16 is a protein called Subunit NDUFV2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	221	Total	C	N	O	S	0	0
			1698	1069	288	327	14		

- Molecule 17 is a protein called Oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	185	Total	C	N	O	S	0	0
			1487	941	252	282	12		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	186	Total	C	N	O	S	0	0
			1375	872	259	242	2		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	182	Total	C	N	O	S	0	0
			1454	927	255	257	15		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	88	Total	C	N	O	S	0	0
			671	450	103	115	3		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	117	Total	C	N	O	S	0	0
			930	581	177	167	5		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	149	ALA	SER	conflict	UNP G0S6J1
M	150	ASN	-	insertion	UNP G0S6J1
M	151	GLU	-	insertion	UNP G0S6J1
M	152	HIS	-	insertion	UNP G0S6J1
M	153	HIS	-	insertion	UNP G0S6J1
M	154	ARG	-	insertion	UNP G0S6J1
M	155	LYS	-	insertion	UNP G0S6J1
M	156	TYR	-	insertion	UNP G0S6J1
M	157	LEU	-	insertion	UNP G0S6J1
M	158	GLU	-	insertion	UNP G0S6J1
M	159	SER	-	insertion	UNP G0S6J1
M	160	LEU	-	insertion	UNP G0S6J1
M	161	PRO	-	insertion	UNP G0S6J1
M	162	GLN	-	insertion	UNP G0S6J1
M	163	THR	-	insertion	UNP G0S6J1
M	164	SER	-	insertion	UNP G0S6J1
M	165	TYR	-	insertion	UNP G0S6J1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	166	PRO	-	insertion	UNP G0S6J1
M	167	LEU	-	insertion	UNP G0S6J1
M	168	ASN	-	insertion	UNP G0S6J1

- Molecule 22 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	82	Total	C	N	O	S	0	0
			631	397	102	131	1		
22	Q	85	Total	C	N	O	S	0	0
			666	419	109	137	1		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase B14 subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	115	Total	C	N	O	S	0	0
			962	613	180	166	3		

- Molecule 24 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	98	Total	C	N	O	S	0	0
			807	520	149	137	1		

- Molecule 25 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	S	74	Total	C	N	O	0	0
			610	401	98	111		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	169	Total	C	N	O	S	0	0
			1365	860	254	242	9		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	120	Total	C	N	O	S	0	0
			976	623	182	168	3		

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	187	Total	C	N	O	S	0	0
			1472	937	267	260	8		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	154	Total	C	N	O	S	0	0
			1240	788	219	229	4		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	186	Total	C	N	O	S	0	0
			1432	898	254	278	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	189	SER	-	insertion	UNP G0SEF0
Z	190	TYR	-	insertion	UNP G0SEF0
Z	191	PRO	-	insertion	UNP G0SEF0
Z	192	CYS	-	insertion	UNP G0SEF0
Z	193	ARG	-	insertion	UNP G0SEF0
Z	194	SER	-	insertion	UNP G0SEF0
Z	195	PHE	-	insertion	UNP G0SEF0
Z	196	VAL	-	insertion	UNP G0SEF0

- Molecule 31 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	143	Total	C	N	O	S	0	0
			1167	750	195	217	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	166	VAL	ALA	conflict	UNP G0RXU4
a	168	ALA	MET	conflict	UNP G0RXU4
a	?	-	GLU	deletion	UNP G0RXU4
a	?	-	GLY	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4

- Molecule 32 is a protein called Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	81	Total	C	N	O	S	0	0
			683	445	125	110	3		

- Molecule 33 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	60	Total	C	N	O	S	0	0
			490	320	86	82	2		

- Molecule 34 is a protein called Subunit NDUF10 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	99	Total	C	N	O	S	0	0
			822	523	145	150	4		

- Molecule 35 is a protein called Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	37	Total	C	N	O	S	0	0
			309	211	54	43	1		

- Molecule 36 is a protein called NADH dehydrogenase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	88	Total	C	N	O	S	0	0
			717	459	127	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	?	-	ALA	deletion	UNP G0S1P3

- Molecule 37 is a protein called Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	78	Total	C	N	O	S	0	0
			610	399	105	105	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	133	Total	C	N	O	S	0	0
			1118	723	194	200	1		

- Molecule 39 is a protein called Subunit NDUF6 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	80	Total	C	N	O	S	0	0
			677	447	117	111	2		

- Molecule 40 is a protein called Subunit NDUF4 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	73	Total	C	N	O	S	0	0
			603	391	108	101	3		

- Molecule 41 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	135	Total	C	N	O	S	0	0
			1061	680	186	194	1		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086

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Chain	Residue	Modelled	Actual	Comment	Reference
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP G0S086
n	9	ALA	-	insertion	UNP G0S086
n	10	LEU	-	insertion	UNP G0S086
n	11	LEU	-	insertion	UNP G0S086
n	12	ALA	-	insertion	UNP G0S086
n	13	ARG	-	insertion	UNP G0S086
n	14	ARG	-	insertion	UNP G0S086
n	15	VAL	-	insertion	UNP G0S086
n	16	ARG	-	insertion	UNP G0S086
n	17	PRO	-	insertion	UNP G0S086
n	18	THR	-	insertion	UNP G0S086
n	19	VAL	-	insertion	UNP G0S086
n	20	VAL	-	insertion	UNP G0S086
n	21	VAL	-	insertion	UNP G0S086
n	22	PRO	-	insertion	UNP G0S086
n	23	ARG	-	insertion	UNP G0S086
n	24	ASN	-	insertion	UNP G0S086
n	25	ALA	-	insertion	UNP G0S086
n	26	ARG	-	insertion	UNP G0S086
n	27	THR	-	insertion	UNP G0S086
n	28	TYR	-	insertion	UNP G0S086
n	29	ALA	-	insertion	UNP G0S086
n	30	SER	-	insertion	UNP G0S086
n	31	SER	-	insertion	UNP G0S086
n	32	HIS	-	insertion	UNP G0S086
n	33	ASP	-	insertion	UNP G0S086
n	34	HIS	-	insertion	UNP G0S086
n	35	ASP	-	insertion	UNP G0S086
n	36	HIS	-	insertion	UNP G0S086
n	37	HIS	-	insertion	UNP G0S086
n	38	ASP	-	insertion	UNP G0S086
n	39	HIS	-	insertion	UNP G0S086
n	40	HIS	-	insertion	UNP G0S086
n	41	HIS	-	insertion	UNP G0S086
n	42	ASP	-	insertion	UNP G0S086
n	43	HIS	-	insertion	UNP G0S086

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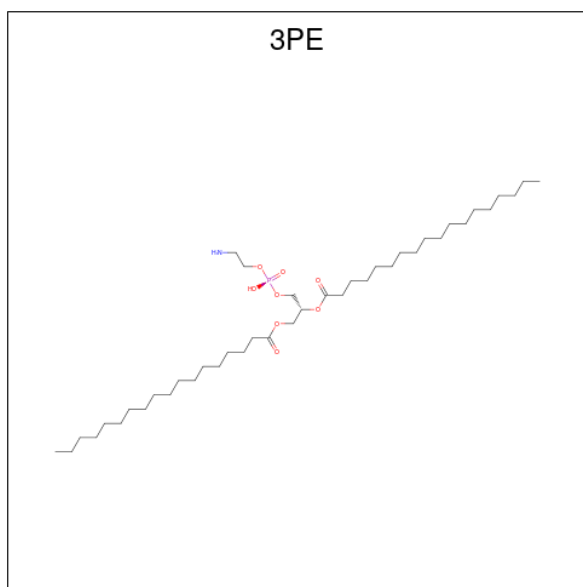
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Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	insertion	UNP G0S086
n	51	LEU	-	insertion	UNP G0S086
n	52	GLY	-	insertion	UNP G0S086

- Molecule 42 is a protein called Oxidoreductase-like domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	o	32	Total	C	N	O	0	0
			252	165	43	44		

- Molecule 43 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



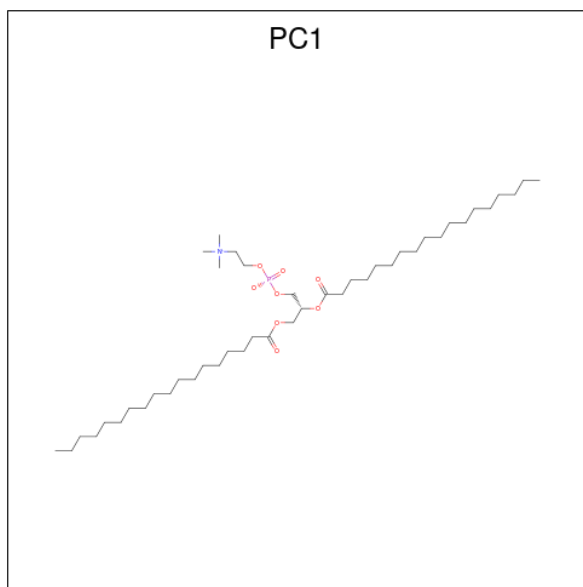
Mol	Chain	Residues	Atoms					AltConf
43	1	1	Total	C	N	O	P	0
			50	40	1	8	1	
43	1	1	Total	C	N	O	P	0
			27	18	1	7	1	
43	4	1	Total	C	N	O	P	0
			33	23	1	8	1	

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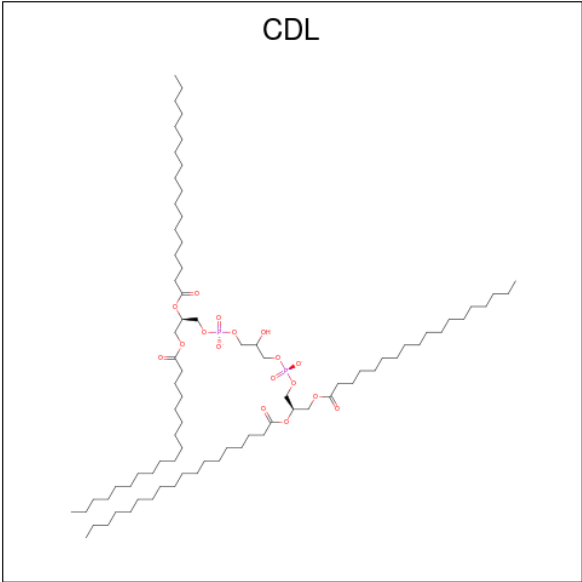
Mol	Chain	Residues	Atoms					AltConf
43	4	1	Total	C	N	O	P	0
			31	21	1	8	1	
43	5	1	Total	C	N	O	P	0
			40	30	1	8	1	
43	5	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	5	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
43	8	1	Total	C	N	O	P	0
			36	26	1	8	1	
43	E	1	Total	C	N	O	P	0
			27	17	1	8	1	
43	J	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
43	W	1	Total	C	N	O	P	0
			40	30	1	8	1	
43	g	1	Total	C	N	O	P	0
			35	25	1	8	1	
43	i	1	Total	C	N	O	P	0
			39	29	1	8	1	
43	n	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 44 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



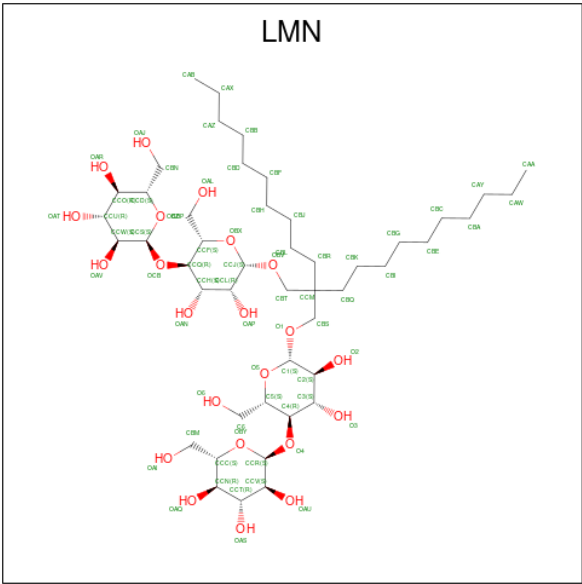
Mol	Chain	Residues	Atoms					AltConf
44	1	1	Total	C	N	O	P	0
			43	33	1	8	1	
44	2	1	Total	C	N	O	P	0
			30	20	1	8	1	
44	3	1	Total	C	N	O	P	0
			49	39	1	8	1	
44	4	1	Total	C	N	O	P	0
			50	40	1	8	1	
44	5	1	Total	C	N	O	P	0
			46	36	1	8	1	
44	5	1	Total	C	N	O	P	0
			43	33	1	8	1	
44	K	1	Total	C	N	O	P	0
			34	24	1	8	1	
44	S	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 45 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



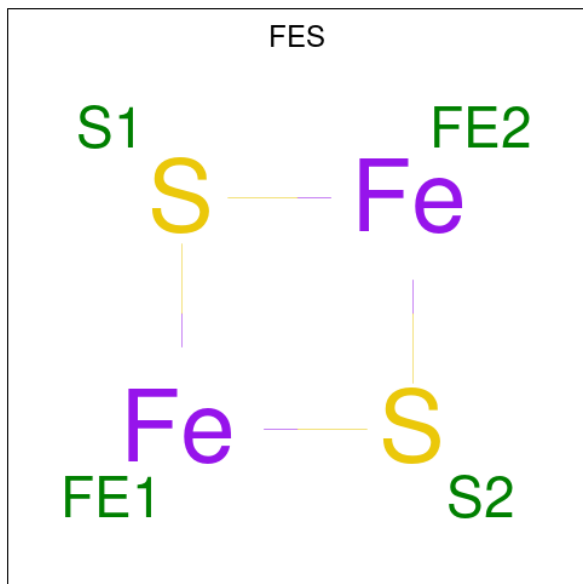
Mol	Chain	Residues	Atoms				AltConf
45	2	1	Total	C	O	P	0
			85	66	17	2	
45	4	1	Total	C	O	P	0
			83	64	17	2	
45	X	1	Total	C	O	P	0
			78	59	17	2	
45	g	1	Total	C	O	P	0
			57	38	17	2	
45	h	1	Total	C	O	P	0
			65	46	17	2	

- Molecule 46 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms			AltConf
46	2	1	Total	C	O	0
			58	41	17	
46	J	1	Total	C	O	0
			58	41	17	
46	j	1	Total	C	O	0
			68	46	22	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



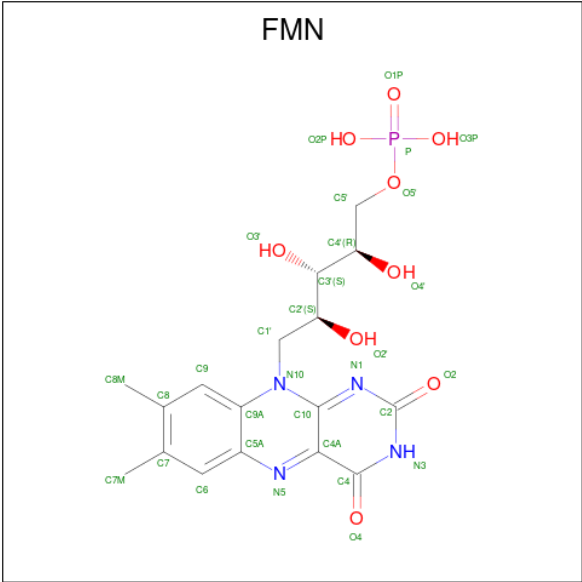
Mol	Chain	Residues	Atoms			AltConf
47	A	1	Total	Fe	S	0
			4	2	2	
47	H	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



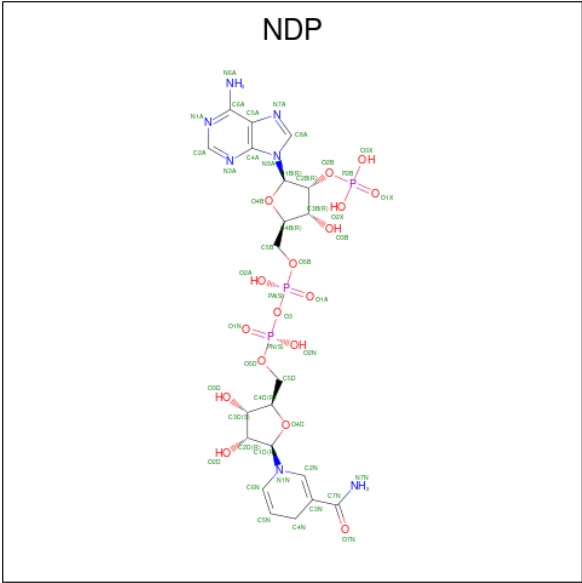
Mol	Chain	Residues	Atoms			AltConf
48	A	1	Total	Fe	S	0
			8	4	4	
48	A	1	Total	Fe	S	0
			8	4	4	
48	B	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



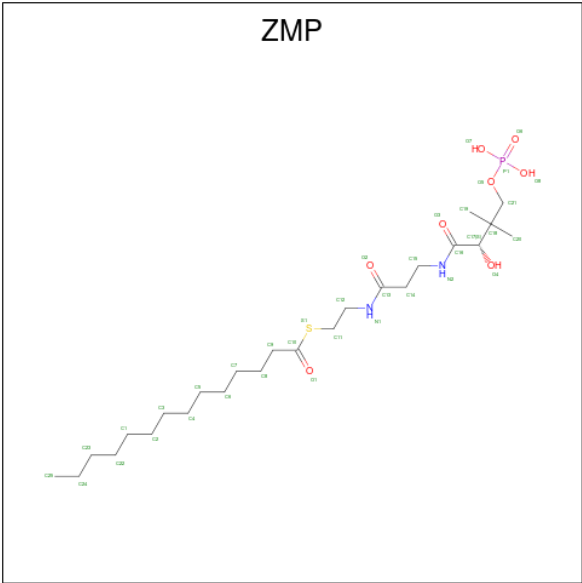
Mol	Chain	Residues	Atoms					AltConf
49	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 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
51	M	1	Total	Zn	0
			1	1	

- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



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Mol	Chain	Residues	Atoms		AltConf
53	9	14	Total 14	O 14	0
53	A	197	Total 197	O 197	0
53	B	30	Total 30	O 30	0
53	C	166	Total 166	O 166	0
53	D	22	Total 22	O 22	0
53	E	62	Total 62	O 62	0
53	F	29	Total 29	O 29	0
53	G	99	Total 99	O 99	0
53	H	5	Total 5	O 5	0
53	I	84	Total 84	O 84	0
53	K	83	Total 83	O 83	0
53	L	11	Total 11	O 11	0
53	M	34	Total 34	O 34	0
53	P	24	Total 24	O 24	0
53	S	1	Total 1	O 1	0
53	U	38	Total 38	O 38	0
53	W	39	Total 39	O 39	0
53	X	50	Total 50	O 50	0
53	Y	91	Total 91	O 91	0
53	Z	40	Total 40	O 40	0
53	a	4	Total 4	O 4	0

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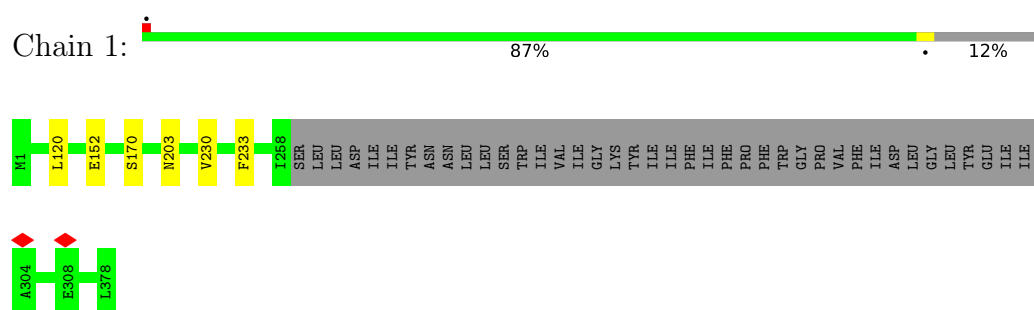
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Mol	Chain	Residues	Atoms		AltConf
53	b	2	Total 2	O 2	0
53	d	4	Total 4	O 4	0
53	f	1	Total 1	O 1	0
53	g	9	Total 9	O 9	0
53	h	46	Total 46	O 46	0
53	j	3	Total 3	O 3	0
53	n	24	Total 24	O 24	0

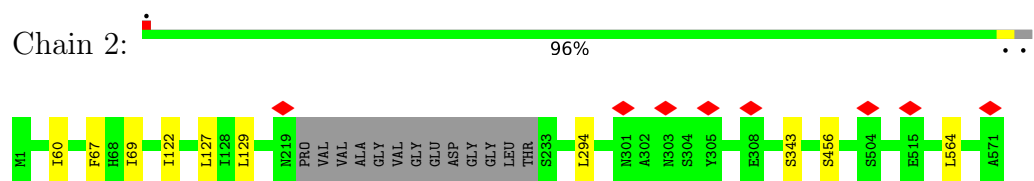
3 Residue-property plots [i](#)

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.

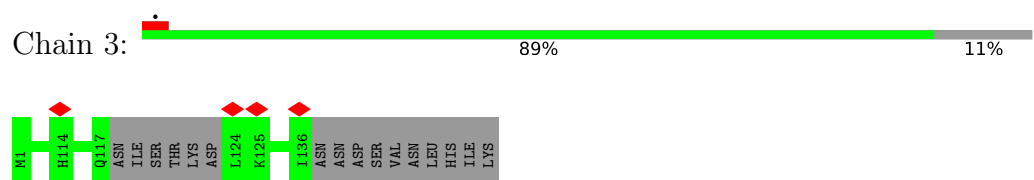
- Molecule 1: NADH-ubiquinone oxidoreductase chain 1



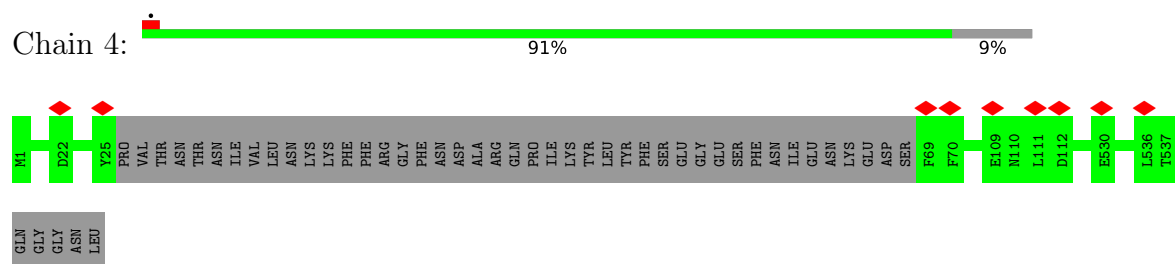
- Molecule 2: NADH dehydrogenase subunit 2



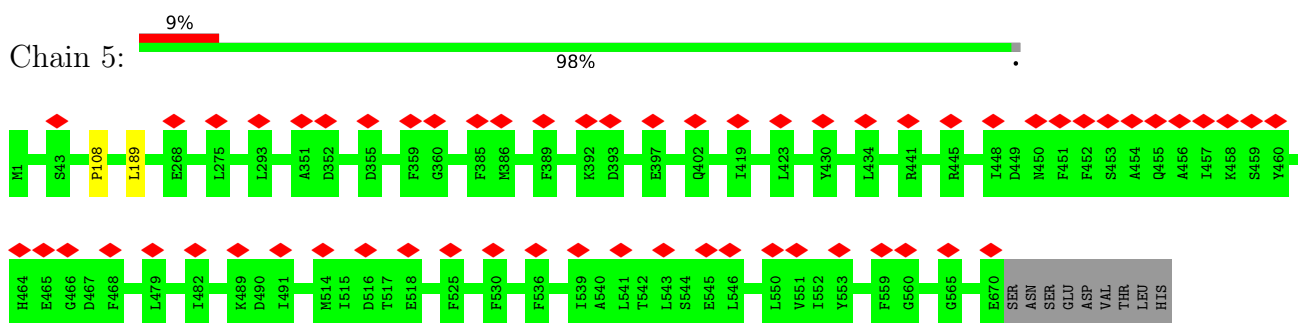
- Molecule 3: NADH-ubiquinone oxidoreductase chain 3



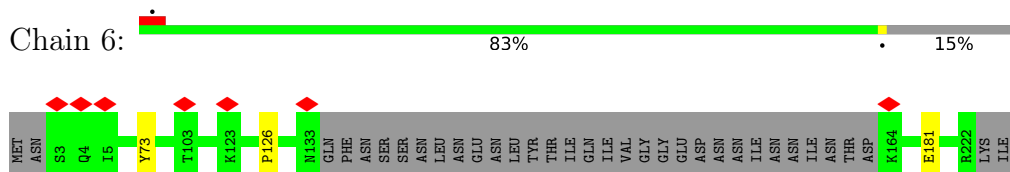
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4



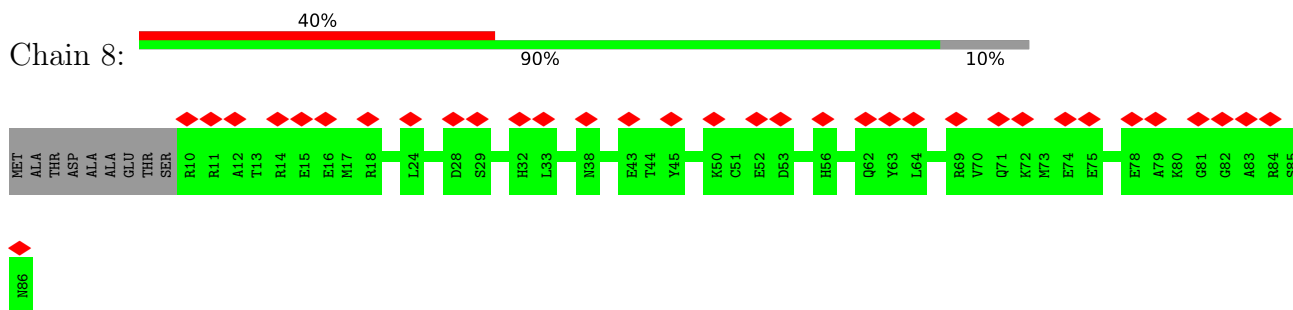
- Molecule 5: NADH-ubiquinone oxidoreductase chain 5



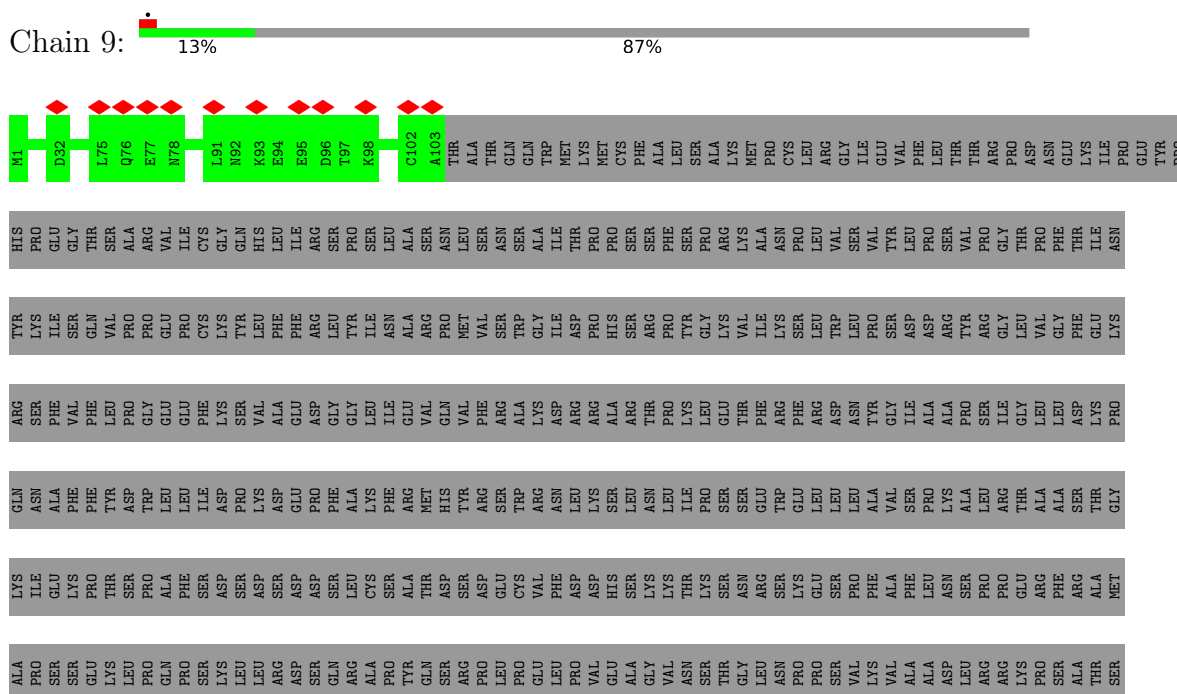
- Molecule 6: NADH-ubiquinone oxidoreductase chain 6

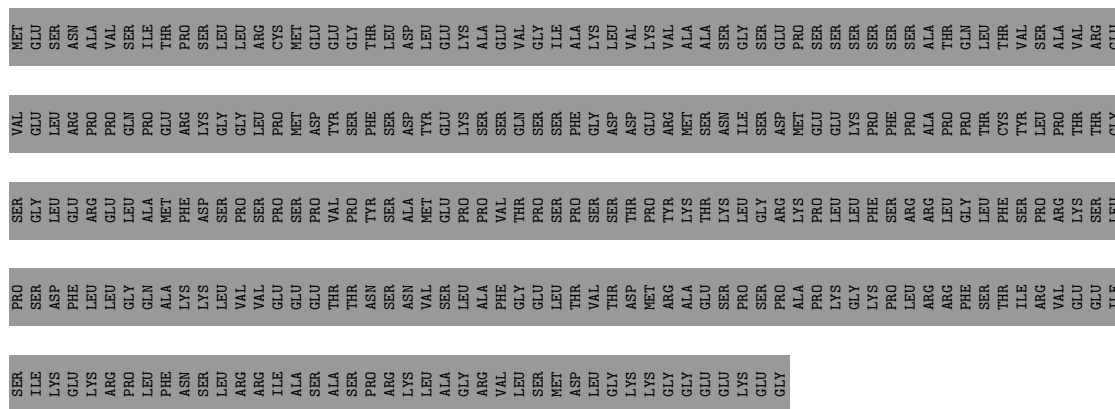


- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

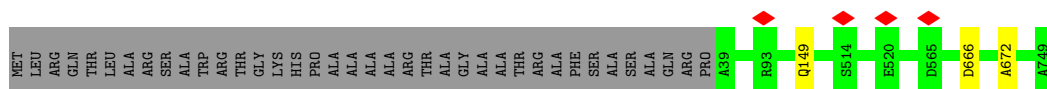


- Molecule 8: Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I)

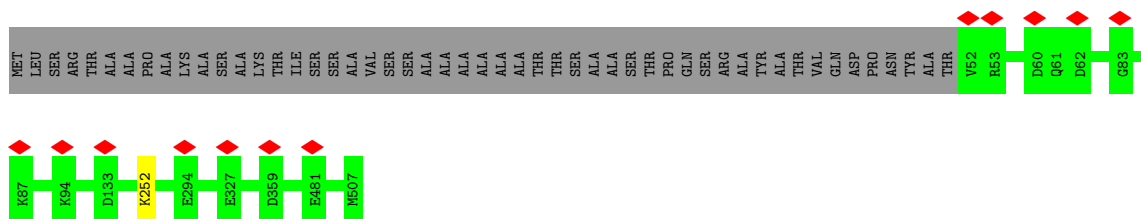
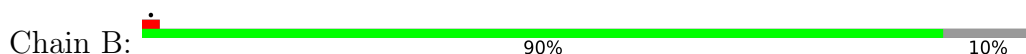




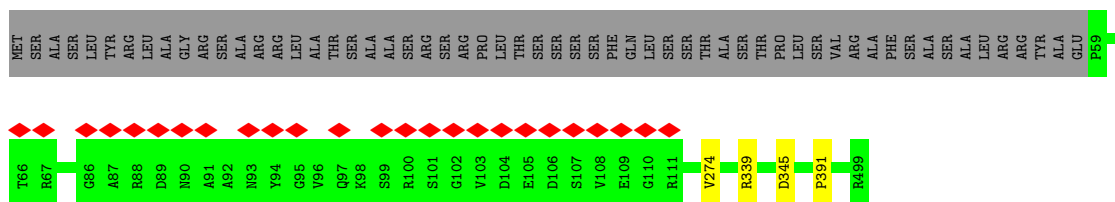
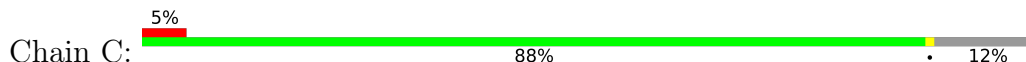
- Molecule 9: NADH-ubiquinone oxidoreductase-like protein



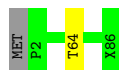
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 11: NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein



- Molecule 12: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

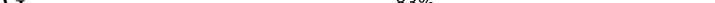


- Molecule 13: NADH dehydrogenase (Ubiquinone)-like protein

MET	ALA	SER	LEU	PRO	THR	VAL	ARG	SER	ALA	ALA	PRO	LYS	VAL	ALA	ARG	ARG	ALA	LEU	GLN	GLN	ARG	ARG	TYR	I26	M218	E227	R281	R299	T361	E362	LYS	GLU	MET	ARG	GLU	GLU	ARG	LYS	TYR	LEU	HIS	VAL	LEU	ASP	ASP	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain F:  91% 9%


MET
 ARG
 ALA
 THR
 THR
 ARG
 LEU
 LEU
 ALA
 VAL
 VAL
 ARG
 PRO
 ALA
 THR
 THR
 GLN
 ALA
 ALA
 ALA
 SER
 SER
 ALA
 SER
 SER
 K24
 E104
 E118
 E175
 E179
 E195
 P261

- Chain G:  83% 17%

MET ALA SER SER LYS LEU CYS LYS THR ARG ALA LEU ALA SER SER LEU LEU ARG ARG PRO ARG ILE SER ARG SER SER SER ARG SER THR GLU ALA ILE ALA ALA ASN VAL VAL VAL VAL ARG SER SER PHE ALA ALA THR THR THR PRO ARG ARG ARG LEU LEU GLY V45 P285 F286

- Chain H: 69% 31%

Met	Arg	Arg	Arg	Gln	Leu	Ser	Gln	Ala	Gly	Pro	Phe	Pro	Ala	Glu	Pro	Lys	Ala	Asn	Gln	Arg	Lys	Ser	Ser	Gly	Glu	Arg	Ser	Thr	Thr	Ser	Asp	His	Asp	Pro	Val	Arg	Pro	Gly	Ala	Ala	Leu	Met				
Ser	Lys	Leu	Thr	Pro	Leu	Leu	Met	Arg	Thr	Val	Ala	Arg	Met	Gly	Ser	Arg	Ala	Ala	Trp	Met	Val	Pro	Ala	Pro	Arg	Thr	Leu	Ser	Thr	Ser	Ala	Met	Arg	His	S98	D99	M102	T200	D256	N278	D279	K282	E312	P316	D317	L318

- Chain I:  83% 17%

MET
 LEU
 PRO
 THR
 PRO
 THR
 ALA
 ALA
 LEU
 LEU
 LEU
 VAL
 VAL
 THR
 ARG
 ARG
 GLN
 LEU
 PRO
 PRO
 LEU
 ALA
 ALA
 ARG
 VAL
 VAL
 PRO
 SER
 THR
 LEU
 LEU
 VAL
 VAL
 ARG
 THR
 THR
 LEU
 PRO
 ILE
 ILE
 GLN
 ALA
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 ARG
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 THR
 TYR
 A39
 N56
 C173
 F223

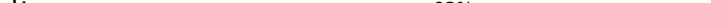
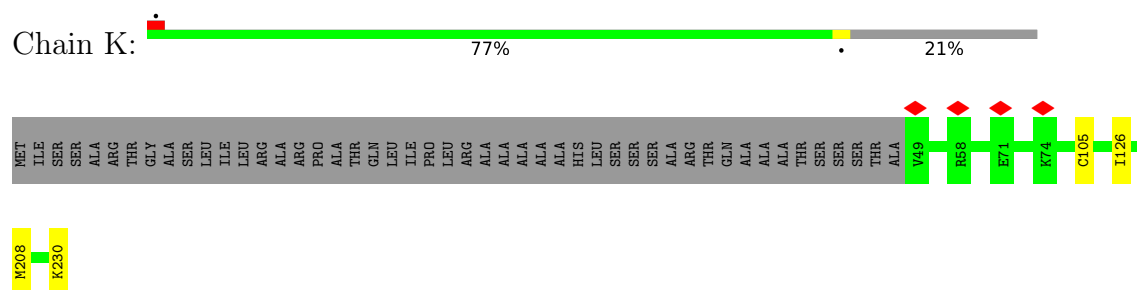
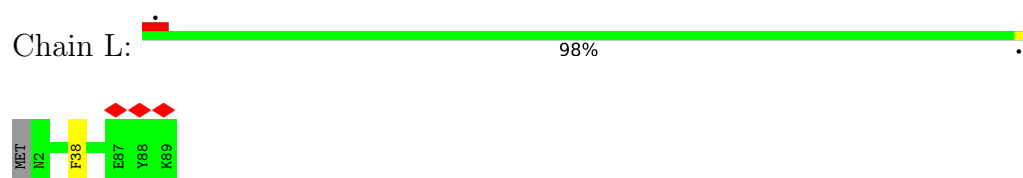
- Chain J:  20% 93% 7%

Diagram illustrating the distribution of 100 SNPs across the human genome. The genome is represented as a horizontal bar with a color gradient from blue to red. SNPs are marked with colored diamonds: red for SNPs with a frequency of 100% (e.g., MET, ALA, PRO, ILE, GLU, GLU, GLU, HIS, HIS, HIS, TYR, P13, R43, R44, R45, R46, R47, R48, R49, A50, A51, F52, T53, R54, R55, G56, A77, E81, A97, L101, R108, R131, G132, R135, R136, D137, V138, L181, R182, F183) and green for SNPs with a frequency of 50% (e.g., G186, N190, C193, A194, G198, ALA). The SNPs are distributed across the genome, with a higher density in the red region.

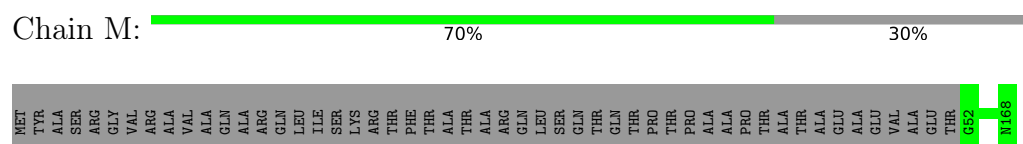
- Molecule 19: NADH-ubiquinone oxidoreductase-like protein



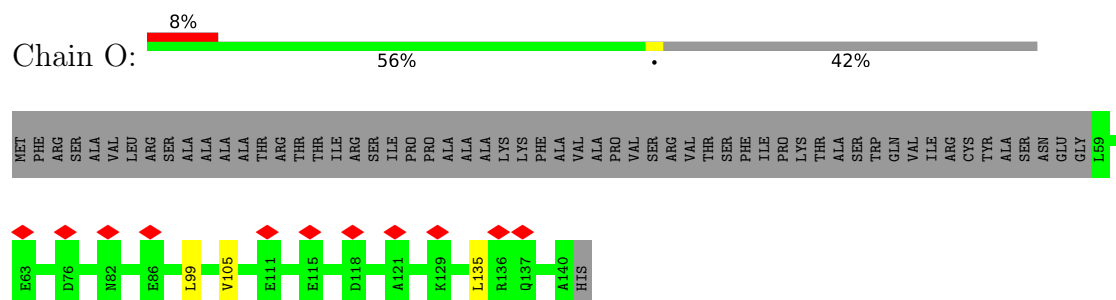
- Molecule 20: NADH-ubiquinone oxidoreductase chain 4L



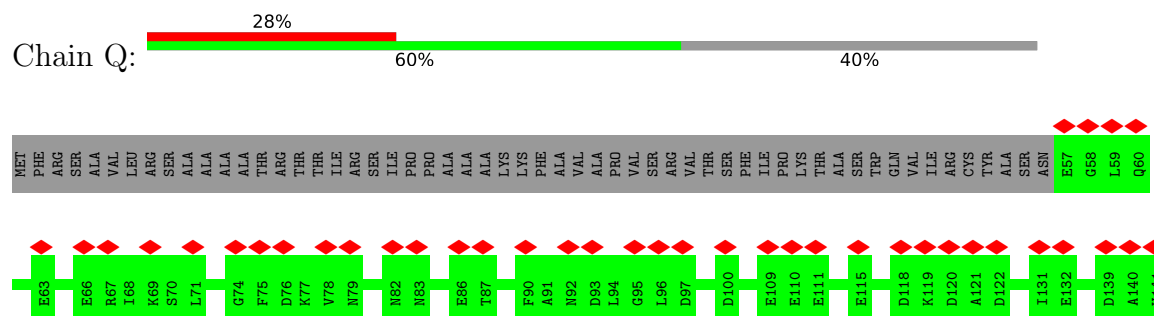
- Molecule 21: NADH-ubiquinone oxidoreductase-like protein



- Molecule 22: Acyl carrier protein

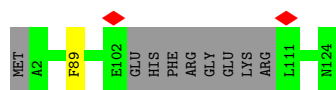


- Molecule 22: Acyl carrier protein

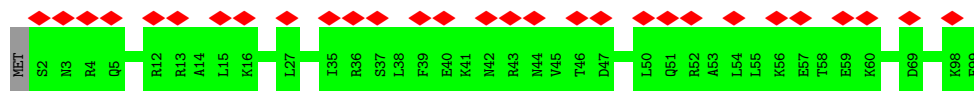


- Molecule 23: NADH-ubiquinone oxidoreductase B14 subunit-like protein

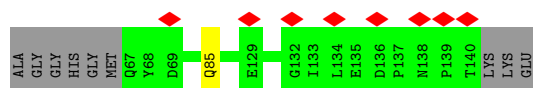




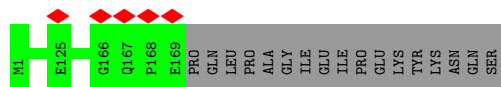
- Molecule 24: Complex I-B22



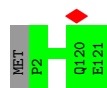
- Molecule 25: Complex I-ESSS



- Molecule 26: NADH-ubiquinone oxidoreductase



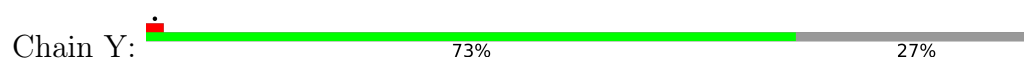
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

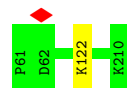
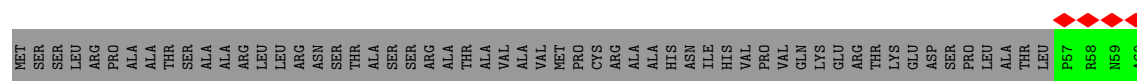


- Molecule 28: NADH-ubiquinone oxidoreductase-like protein

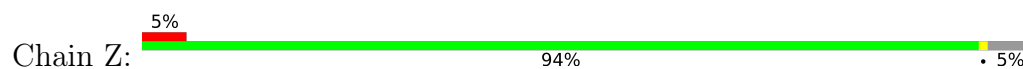


- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

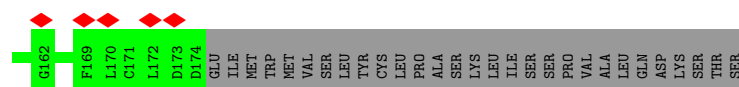
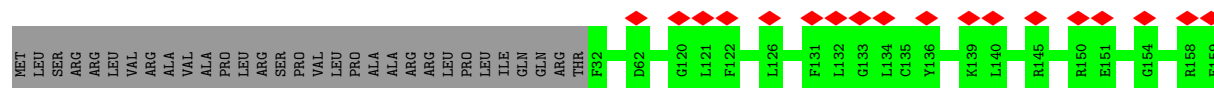




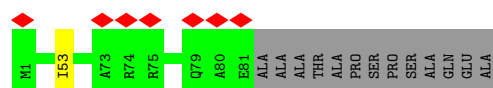
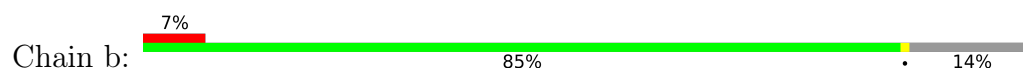
- Molecule 30: NADH-ubiquinone oxidoreductase-like protein



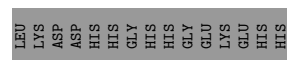
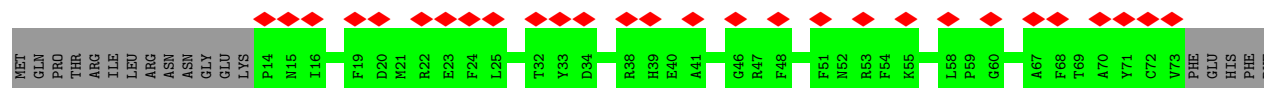
- Molecule 31: NADH dehydrogenase (Ubiquinone)-like protein



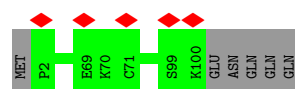
- Molecule 32: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)



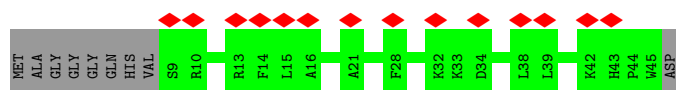
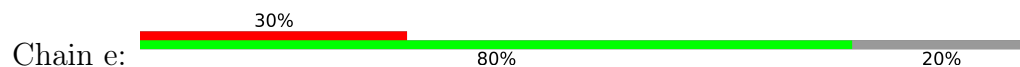
- Molecule 33: Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I)



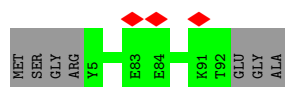
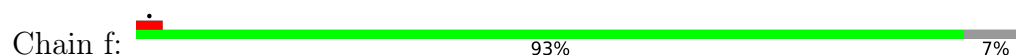
- Molecule 34: Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I)



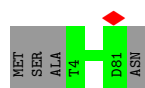
- Molecule 35: Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I)



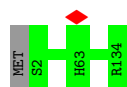
- Molecule 36: NADH dehydrogenase-like protein



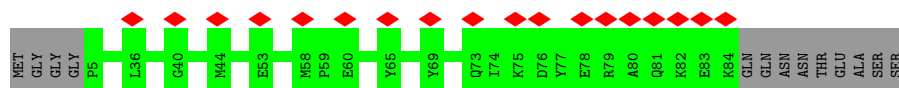
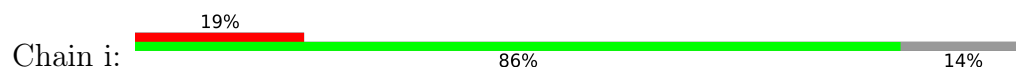
- Molecule 37: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)



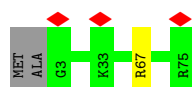
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit



- Molecule 39: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)

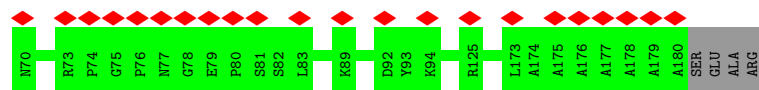


- Molecule 40: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 41: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)





- Molecule 42: Oxidoreductase-like domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.675	Depositor
Minimum map value	-1.374	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	159.03, 221.80501, 319.734	wwPDB
Map dimensions	382, 265, 190	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.837, 0.837, 0.837	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: LMN, NDP, ZN, 3PE, FES, PC1, CDL, ZMP, FMN, SF4, 2MR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.50	0/2633	0.65	0/3593
2	2	0.50	1/4562 (0.0%)	0.64	2/6205 (0.0%)
3	3	0.51	0/1053	0.64	0/1428
4	4	0.41	0/4002	0.54	0/5454
5	5	0.36	0/5414	0.51	0/7371
6	6	0.49	0/1479	0.68	0/2017
7	8	0.25	0/671	0.42	0/896
8	9	0.46	0/824	0.62	0/1112
9	A	0.42	0/5589	0.59	1/7579 (0.0%)
10	B	0.39	0/3621	0.54	0/4878
11	C	0.46	0/3542	0.60	2/4806 (0.0%)
12	D	0.47	0/674	0.70	0/911
13	E	0.40	0/2807	0.54	0/3807
14	F	0.38	0/1924	0.51	0/2609
15	G	0.43	0/2026	0.55	0/2759
16	H	0.40	0/1737	0.58	1/2362 (0.0%)
17	I	0.50	0/1527	0.67	0/2070
18	J	0.32	0/1400	0.46	0/1892
19	K	0.47	0/1493	0.66	1/2026 (0.0%)
20	L	0.50	0/677	0.67	0/917
21	M	0.47	0/961	0.60	0/1309
22	O	0.49	0/640	0.56	0/871
22	Q	0.28	0/676	0.47	0/917
23	P	0.39	0/986	0.48	0/1333
24	R	0.27	0/832	0.45	0/1133
25	S	0.36	0/635	0.49	0/869
26	U	0.51	0/1403	0.71	0/1904
27	W	0.48	0/1001	0.66	0/1354
28	X	0.48	0/1511	0.65	0/2043
29	Y	0.38	0/1277	0.54	0/1731
30	Z	0.42	0/1466	0.55	0/1997
31	a	0.31	0/1204	0.46	0/1632

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.35	0/701	0.50	0/939
33	c	0.27	0/509	0.41	0/691
34	d	0.41	0/840	0.56	0/1130
35	e	0.29	0/324	0.41	0/440
36	f	0.42	0/731	0.59	0/981
37	g	0.44	0/631	0.58	0/868
38	h	0.40	0/1158	0.53	0/1577
39	i	0.37	0/706	0.45	0/960
40	j	0.37	0/617	0.51	0/830
41	n	0.45	0/1092	0.58	0/1481
42	o	0.32	0/262	0.41	0/360
All	All	0.42	1/67818 (0.0%)	0.57	7/92042 (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
10	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	122	ILE	C-N	5.69	1.47	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	339	ARG	CB-CA-C	5.79	121.99	110.40
16	H	102	MET	CB-CG-SD	5.60	129.21	112.40
11	C	345	ASP	CB-CA-C	5.51	121.42	110.40
2	2	122	ILE	O-C-N	5.45	131.42	122.70
9	A	149	GLN	CB-CA-C	-5.42	99.55	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	B	252	LYS	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	330/378 (87%)	318 (96%)	12 (4%)	0	100	100
2	2	554/571 (97%)	543 (98%)	11 (2%)	0	100	100
3	3	126/146 (86%)	117 (93%)	9 (7%)	0	100	100
4	4	490/542 (90%)	476 (97%)	14 (3%)	0	100	100
5	5	668/679 (98%)	614 (92%)	53 (8%)	1 (0%)	48	70
6	6	186/224 (83%)	173 (93%)	13 (7%)	0	100	100
7	8	75/86 (87%)	68 (91%)	7 (9%)	0	100	100
8	9	101/785 (13%)	100 (99%)	1 (1%)	0	100	100
9	A	709/749 (95%)	680 (96%)	28 (4%)	1 (0%)	48	70
10	B	454/507 (90%)	437 (96%)	17 (4%)	0	100	100
11	C	438/499 (88%)	417 (95%)	21 (5%)	0	100	100
12	D	79/86 (92%)	77 (98%)	2 (2%)	0	100	100
13	E	335/378 (89%)	319 (95%)	16 (5%)	0	100	100
14	F	236/261 (90%)	224 (95%)	12 (5%)	0	100	100
15	G	240/293 (82%)	231 (96%)	9 (4%)	0	100	100
16	H	219/318 (69%)	207 (94%)	12 (6%)	0	100	100
17	I	183/223 (82%)	178 (97%)	5 (3%)	0	100	100
18	J	184/199 (92%)	178 (97%)	6 (3%)	0	100	100
19	K	180/230 (78%)	171 (95%)	9 (5%)	0	100	100
20	L	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	M	115/168 (68%)	110 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	O	80/141 (57%)	78 (98%)	2 (2%)	0	100	100
22	Q	83/141 (59%)	79 (95%)	4 (5%)	0	100	100
23	P	111/124 (90%)	108 (97%)	3 (3%)	0	100	100
24	R	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
25	S	72/143 (50%)	69 (96%)	3 (4%)	0	100	100
26	U	167/186 (90%)	166 (99%)	1 (1%)	0	100	100
27	W	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
28	X	185/191 (97%)	181 (98%)	3 (2%)	1 (0%)	25	41
29	Y	152/210 (72%)	148 (97%)	4 (3%)	0	100	100
30	Z	184/196 (94%)	175 (95%)	9 (5%)	0	100	100
31	a	141/203 (70%)	141 (100%)	0	0	100	100
32	b	79/94 (84%)	77 (98%)	2 (2%)	0	100	100
33	c	58/93 (62%)	54 (93%)	4 (7%)	0	100	100
34	d	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
35	e	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
36	f	86/95 (90%)	82 (95%)	4 (5%)	0	100	100
37	g	76/82 (93%)	73 (96%)	3 (4%)	0	100	100
38	h	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
39	i	78/93 (84%)	74 (95%)	4 (5%)	0	100	100
40	j	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
41	n	133/184 (72%)	128 (96%)	5 (4%)	0	100	100
42	o	30/380 (8%)	29 (97%)	1 (3%)	0	100	100
All	All	8251/10547 (78%)	7915 (96%)	333 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	A	672	ALA
28	X	67	GLY
5	5	108	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	284/326 (87%)	278 (98%)	6 (2%)	48	69
2	2	509/518 (98%)	501 (98%)	8 (2%)	58	75
3	3	111/128 (87%)	111 (100%)	0	100	100
4	4	431/477 (90%)	431 (100%)	0	100	100
5	5	579/596 (97%)	578 (100%)	1 (0%)	92	96
6	6	162/203 (80%)	159 (98%)	3 (2%)	52	71
7	8	69/75 (92%)	69 (100%)	0	100	100
8	9	84/687 (12%)	84 (100%)	0	100	100
9	A	577/602 (96%)	576 (100%)	1 (0%)	92	96
10	B	366/401 (91%)	366 (100%)	0	100	100
11	C	362/416 (87%)	360 (99%)	2 (1%)	84	90
12	D	68/69 (99%)	67 (98%)	1 (2%)	60	76
13	E	299/335 (89%)	298 (100%)	1 (0%)	91	95
14	F	199/219 (91%)	199 (100%)	0	100	100
15	G	215/257 (84%)	215 (100%)	0	100	100
16	H	190/272 (70%)	189 (100%)	1 (0%)	86	92
17	I	158/191 (83%)	157 (99%)	1 (1%)	84	90
18	J	126/146 (86%)	126 (100%)	0	100	100
19	K	158/191 (83%)	155 (98%)	3 (2%)	52	71
20	L	73/76 (96%)	72 (99%)	1 (1%)	62	78
21	M	97/135 (72%)	97 (100%)	0	100	100
22	O	68/119 (57%)	65 (96%)	3 (4%)	24	43
22	Q	73/119 (61%)	73 (100%)	0	100	100
23	P	101/110 (92%)	100 (99%)	1 (1%)	73	84
24	R	87/89 (98%)	87 (100%)	0	100	100
25	S	59/111 (53%)	58 (98%)	1 (2%)	56	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	U	149/167 (89%)	149 (100%)	0	100	100
27	W	100/102 (98%)	100 (100%)	0	100	100
28	X	143/152 (94%)	139 (97%)	4 (3%)	38	60
29	Y	131/176 (74%)	130 (99%)	1 (1%)	79	88
30	Z	152/155 (98%)	150 (99%)	2 (1%)	65	80
31	a	123/177 (70%)	123 (100%)	0	100	100
32	b	67/74 (90%)	66 (98%)	1 (2%)	60	76
33	c	47/80 (59%)	47 (100%)	0	100	100
34	d	87/94 (93%)	87 (100%)	0	100	100
35	e	29/35 (83%)	29 (100%)	0	100	100
36	f	76/80 (95%)	76 (100%)	0	100	100
37	g	65/69 (94%)	65 (100%)	0	100	100
38	h	117/119 (98%)	117 (100%)	0	100	100
39	i	68/78 (87%)	68 (100%)	0	100	100
40	j	63/64 (98%)	62 (98%)	1 (2%)	58	75
41	n	106/150 (71%)	106 (100%)	0	100	100
42	o	26/318 (8%)	26 (100%)	0	100	100
All	All	7054/8958 (79%)	7011 (99%)	43 (1%)	82	90

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

Mol	Chain	Res	Type
20	L	38	PHE
28	X	130	ARG
22	O	99	LEU
23	P	89	PHE
28	X	167	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
28	X	10	GLN
39	i	52	HIS
28	X	136	GLN
30	Z	99	GLN

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Mol	Chain	Res	Type
41	n	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
11	2MR	C	154	11	10,12,13	0.28	0	5,13,15	0.92	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
11	2MR	C	154	11	-	0/10/13/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 1 is monoatomic - leaving 45 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	3PE	E	401	-	26,26,50	1.16	4 (15%)	29,31,55	1.32	2 (6%)
44	PC1	K	302	-	33,33,53	1.18	4 (12%)	39,41,61	1.13	2 (5%)
45	CDL	2	601	-	84,84,99	0.30	0	90,96,111	0.34	0
50	NDP	E	402	-	45,52,52	0.66	0	53,80,80	0.65	1 (1%)
52	ZMP	Q	201	22	29,35,36	0.19	0	34,42,45	0.46	0
44	PC1	5	701	-	45,45,53	1.05	5 (11%)	51,53,61	1.11	2 (3%)
48	SF4	B	601	10	0,12,12	-	-	-		
48	SF4	K	301	19	0,12,12	-	-	-		
45	CDL	h	201	-	64,64,99	0.34	0	70,76,111	0.44	0
43	3PE	n	201	-	38,38,50	0.98	4 (10%)	41,43,55	1.12	2 (4%)
48	SF4	A	802	9	0,12,12	-	-	-		
46	LMN	2	602	-	60,60,72	0.20	0	78,80,98	0.39	0
43	3PE	5	707	-	40,40,50	0.95	4 (10%)	43,45,55	1.11	2 (4%)
45	CDL	g	101	-	56,56,99	1.13	7 (12%)	62,68,111	1.29	5 (8%)
44	PC1	3	201	-	48,48,53	0.31	0	54,56,61	0.30	0
47	FES	A	801	9	0,4,4	-	-	-		
49	FMN	B	602	-	33,33,33	0.64	0	48,50,50	0.71	1 (2%)
43	3PE	5	705	-	41,41,50	0.94	4 (9%)	44,46,55	1.10	2 (4%)
43	3PE	8	101	-	35,35,50	1.01	4 (11%)	38,40,55	1.15	2 (5%)
43	3PE	J	201	-	31,31,50	1.09	4 (12%)	34,36,55	1.16	2 (5%)
44	PC1	4	603	-	49,49,53	0.98	4 (8%)	55,57,61	1.05	2 (3%)
43	3PE	i	101	-	38,38,50	0.98	4 (10%)	41,43,55	1.13	2 (4%)
46	LMN	j	101	-	71,71,72	1.63	14 (19%)	95,97,98	1.08	5 (5%)
43	3PE	5	703	-	31,31,50	1.06	4 (12%)	34,36,55	1.16	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	3PE	W	201	-	33,33,50	0.93	2 (6%)	34,37,55	1.04	1 (2%)
43	3PE	1	401	-	49,49,50	0.86	3 (6%)	52,54,55	1.13	2 (3%)
43	3PE	5	704	-	31,31,50	1.06	4 (12%)	34,36,55	1.23	2 (5%)
43	3PE	g	102	-	34,34,50	1.05	4 (11%)	37,39,55	1.24	2 (5%)
48	SF4	A	803	9	0,12,12	-	-	-	-	-
43	3PE	4	604	-	30,30,50	1.10	4 (13%)	33,35,55	1.14	2 (6%)
52	ZMP	O	201	22	29,35,36	0.25	0	34,42,45	0.51	0
43	3PE	W	202	-	39,39,50	0.96	4 (10%)	42,44,55	1.13	2 (4%)
43	3PE	4	602	-	32,32,50	0.37	0	35,37,55	0.55	1 (2%)
45	CDL	4	601	-	82,82,99	0.29	0	88,94,111	0.32	0
47	FES	H	401	16	0,4,4	-	-	-	-	-
46	LMN	J	202	-	60,60,72	1.73	14 (23%)	78,80,98	0.95	1 (1%)
44	PC1	5	706	-	42,42,53	1.06	4 (9%)	48,50,61	1.04	2 (4%)
43	3PE	1	402	-	26,26,50	0.33	0	28,30,55	0.55	0
44	PC1	2	603	-	29,29,53	1.25	4 (13%)	35,37,61	1.12	2 (5%)
44	PC1	1	403	-	42,42,53	1.07	4 (9%)	48,50,61	1.17	2 (4%)
45	CDL	X	201	-	77,77,99	0.98	7 (9%)	83,89,111	1.11	4 (4%)
43	3PE	5	702	-	39,39,50	0.32	0	42,44,55	0.38	0
48	SF4	I	302	17	0,12,12	-	-	-	-	-
44	PC1	S	201	-	50,50,53	0.96	4 (8%)	56,58,61	1.06	2 (3%)
48	SF4	I	301	17	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	3PE	E	401	-	-	15/30/30/54	-
44	PC1	K	302	-	-	22/37/37/57	-
45	CDL	2	601	-	-	25/95/95/110	-
50	NDP	E	402	-	-	2/30/77/77	0/5/5/5
52	ZMP	Q	201	22	-	8/40/42/43	-
44	PC1	5	701	-	-	25/49/49/57	-
48	SF4	B	601	10	-	-	0/6/5/5
48	SF4	K	301	19	-	-	0/6/5/5
45	CDL	h	201	-	-	26/75/75/110	-
43	3PE	n	201	-	-	13/42/42/54	-

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SF4	A	802	9	-	-	0/6/5/5
46	LMN	2	602	-	-	17/44/104/130	0/3/3/4
43	3PE	5	707	-	-	15/44/44/54	-
45	CDL	g	101	-	-	21/67/67/110	-
44	PC1	3	201	-	-	16/52/52/57	-
47	FES	A	801	9	-	-	0/1/1/1
49	FMN	B	602	-	-	7/18/18/18	0/3/3/3
43	3PE	5	705	-	-	18/45/45/54	-
43	3PE	8	101	-	-	18/39/39/54	-
43	3PE	J	201	-	-	21/35/35/54	-
44	PC1	4	603	-	-	32/53/53/57	-
43	3PE	i	101	-	-	13/42/42/54	-
46	LMN	j	101	-	-	22/49/129/130	0/4/4/4
43	3PE	5	703	-	-	16/35/35/54	-
43	3PE	W	201	-	-	14/36/36/54	-
43	3PE	1	401	-	-	28/53/53/54	-
43	3PE	5	704	-	-	13/35/35/54	-
43	3PE	g	102	-	-	21/38/38/54	-
48	SF4	A	803	9	-	-	0/6/5/5
43	3PE	4	604	-	-	13/34/34/54	-
52	ZMP	O	201	22	-	18/40/42/43	-
43	3PE	W	202	-	-	17/43/43/54	-
43	3PE	4	602	-	-	12/36/36/54	-
45	CDL	4	601	-	-	29/93/93/110	-
47	FES	H	401	16	-	-	0/1/1/1
46	LMN	J	202	-	-	27/44/104/130	0/3/3/4
44	PC1	5	706	-	-	18/46/46/57	-
43	3PE	1	402	-	-	9/29/29/54	-
44	PC1	2	603	-	-	18/33/33/57	-
44	PC1	1	403	-	-	22/46/46/57	-
45	CDL	X	201	-	-	35/88/88/110	-
43	3PE	5	702	-	-	18/43/43/54	-
48	SF4	I	302	17	-	-	0/6/5/5
44	PC1	S	201	-	-	20/54/54/57	-
48	SF4	I	301	17	-	-	0/6/5/5

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	J	202	LMN	O5-C1	4.75	1.53	1.41
46	j	101	LMN	O5-C1	4.60	1.53	1.41
46	J	202	LMN	CBS-CCM	4.18	1.63	1.53
46	j	101	LMN	CBS-CCM	4.06	1.62	1.53
46	j	101	LMN	CBT-CCM	3.81	1.62	1.53

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	g	101	CDL	OB6-CB5-C51	4.61	121.43	111.50
43	E	401	3PE	O21-C21-C22	4.52	121.25	111.50
43	5	704	3PE	O21-C21-C22	4.32	120.82	111.50
43	1	401	3PE	O21-C21-C22	4.27	120.71	111.50
44	4	603	PC1	O21-C21-C22	4.24	120.64	111.50

There are no chirality outliers.

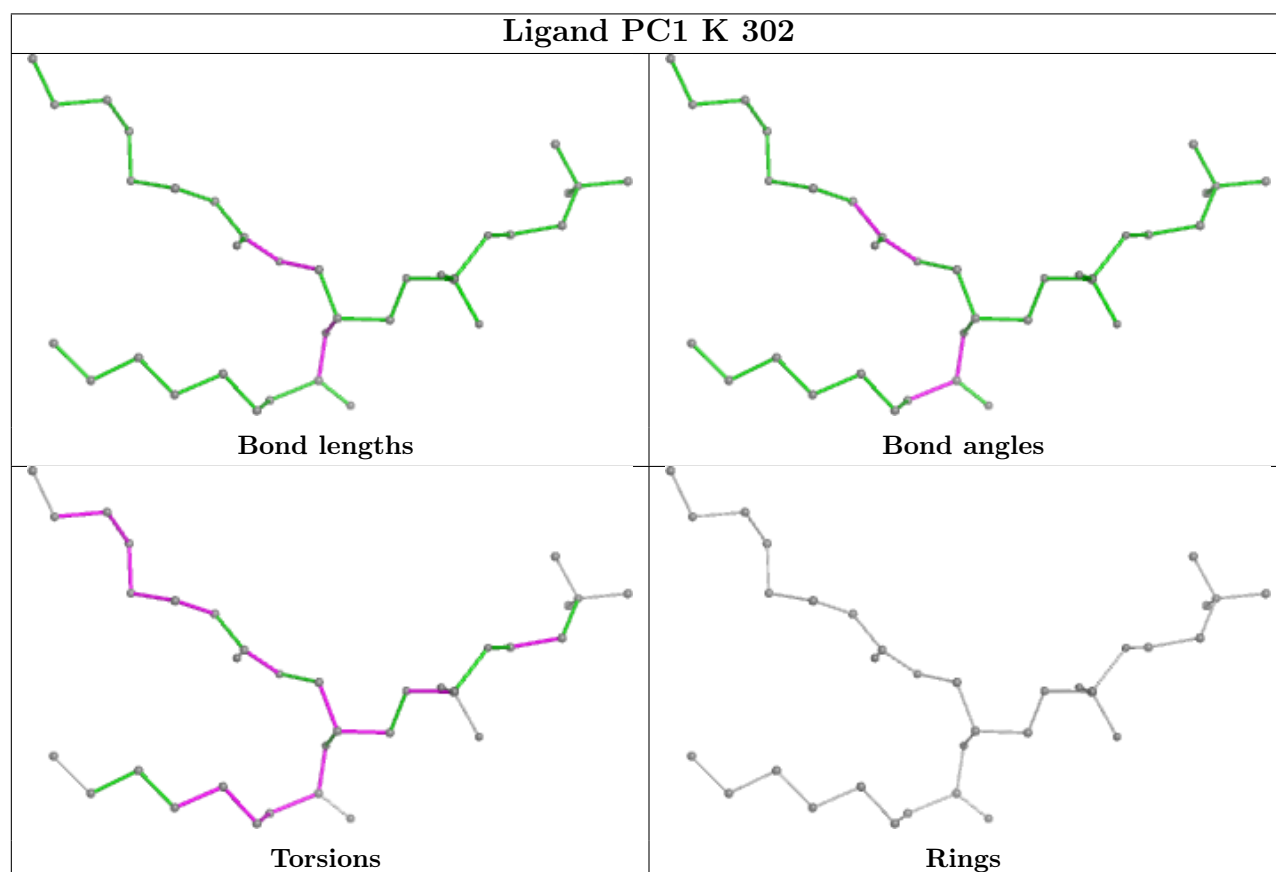
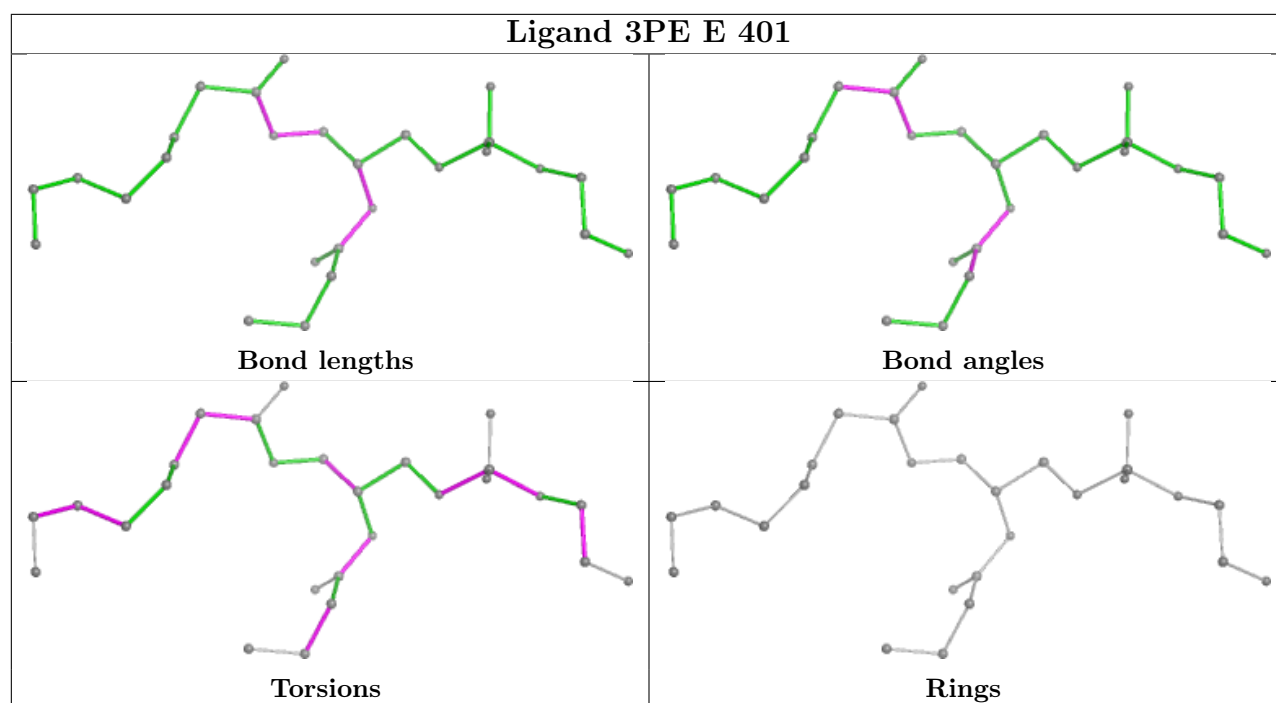
5 of 684 torsion outliers are listed below:

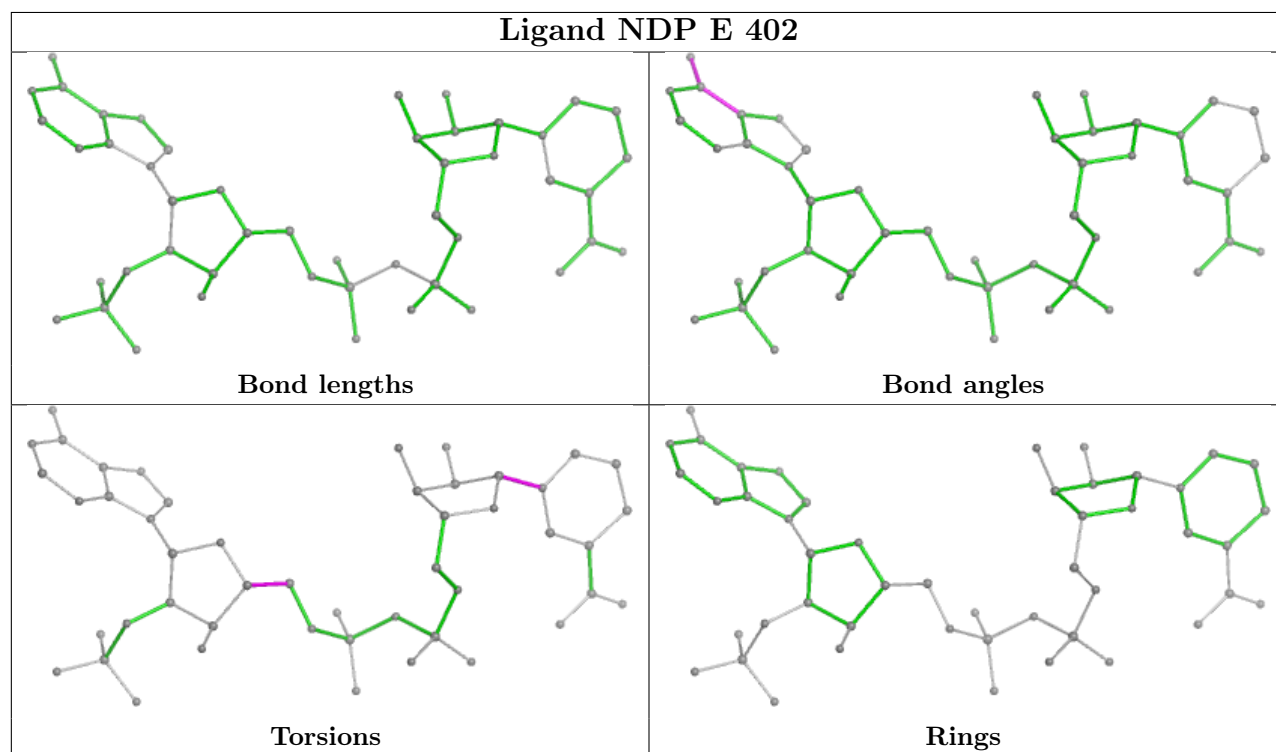
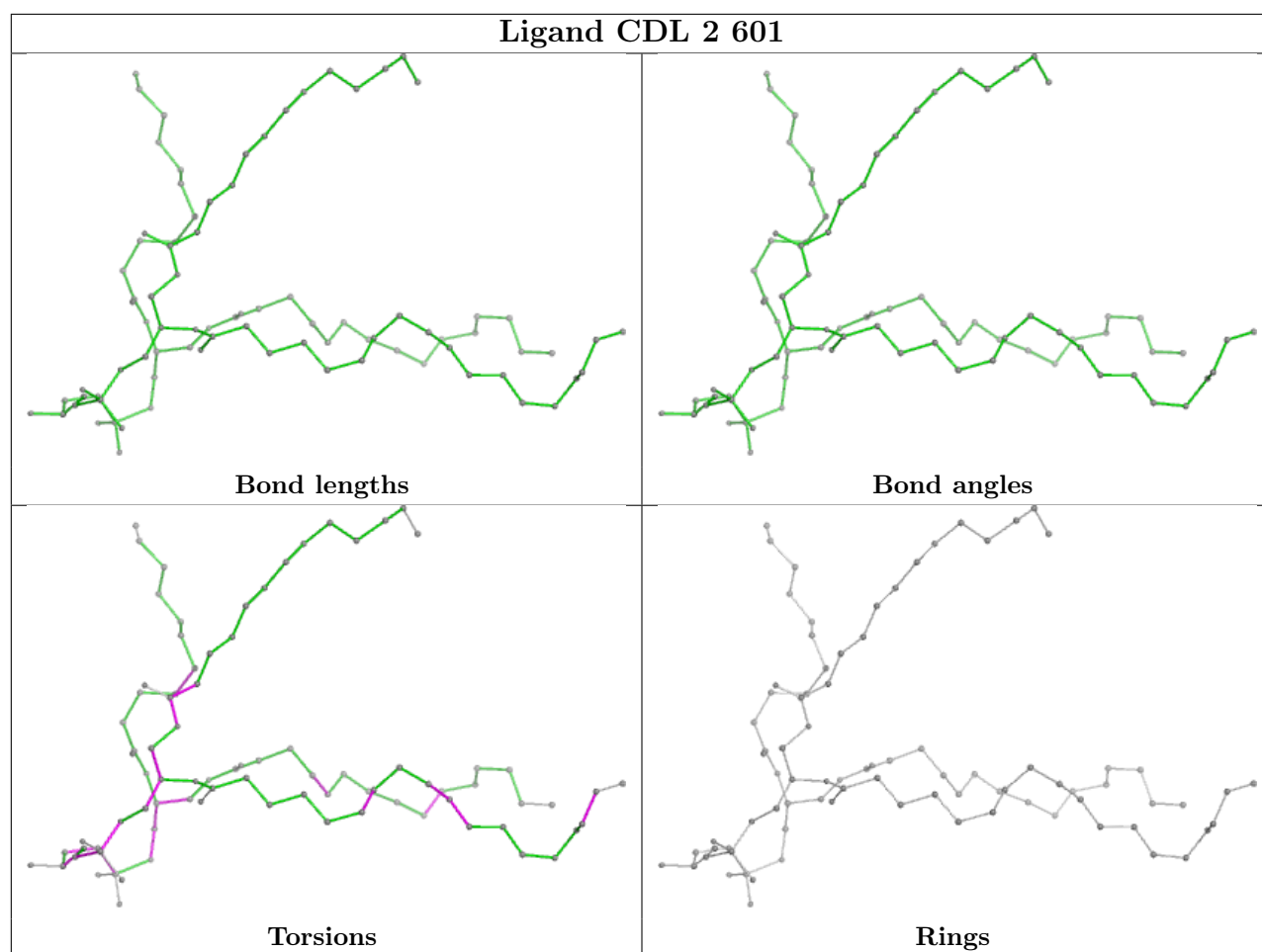
Mol	Chain	Res	Type	Atoms
43	1	401	3PE	C1-O11-P-O12
43	1	401	3PE	C1-O11-P-O14
43	1	401	3PE	C12-C11-O13-P
43	1	402	3PE	C11-O13-P-O11
43	1	402	3PE	C11-O13-P-O12

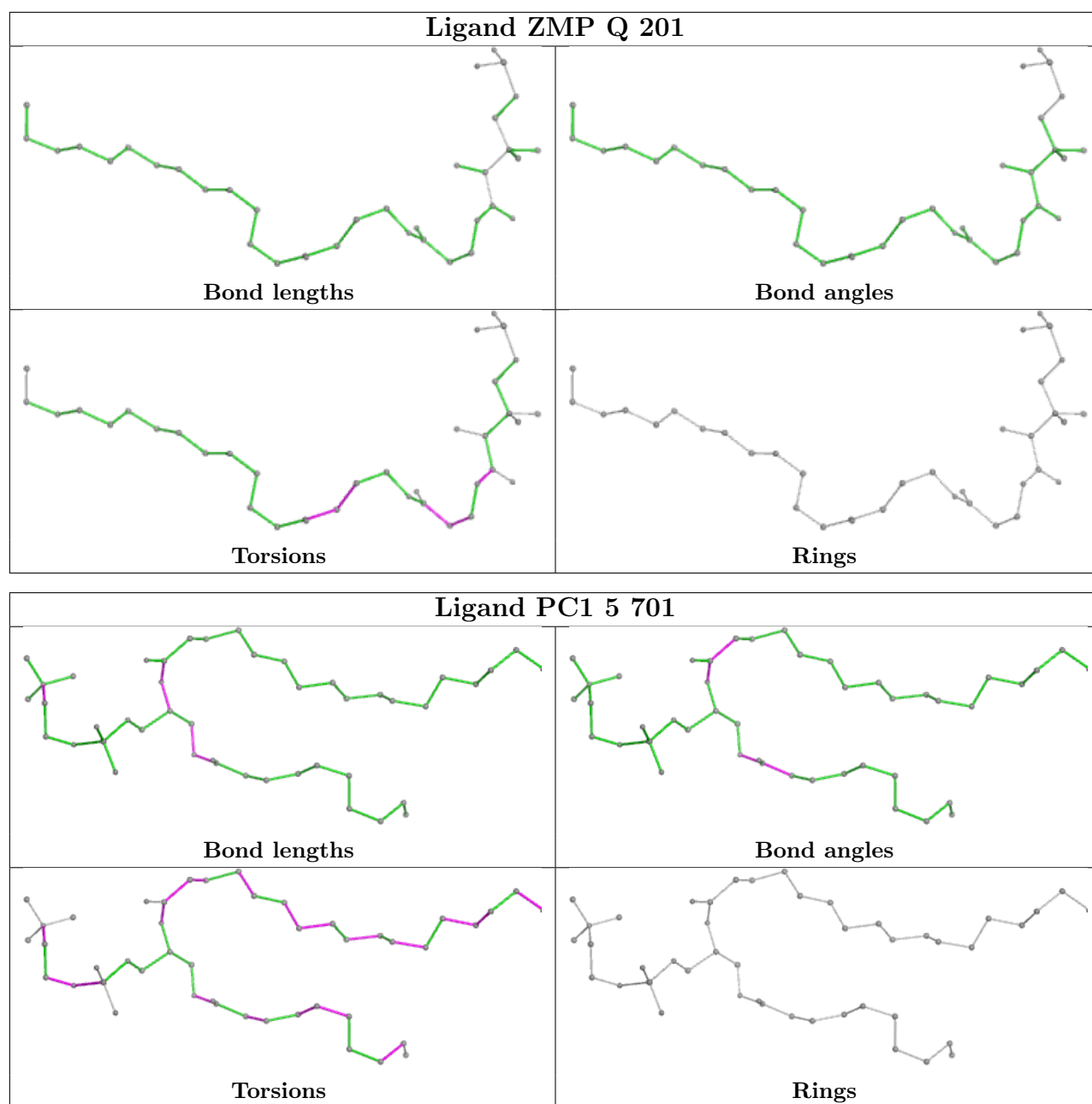
There are no ring outliers.

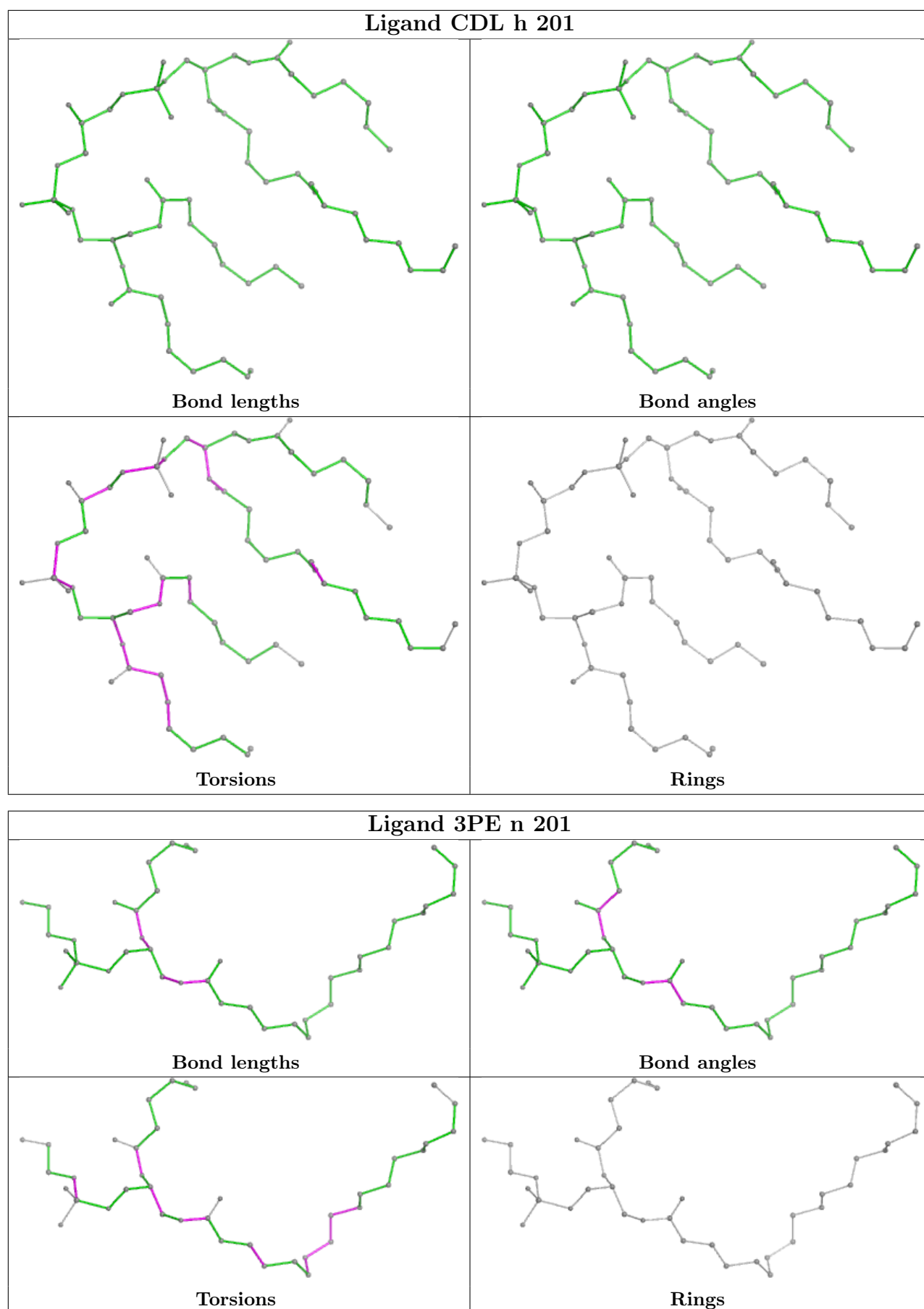
No monomer is involved in short contacts.

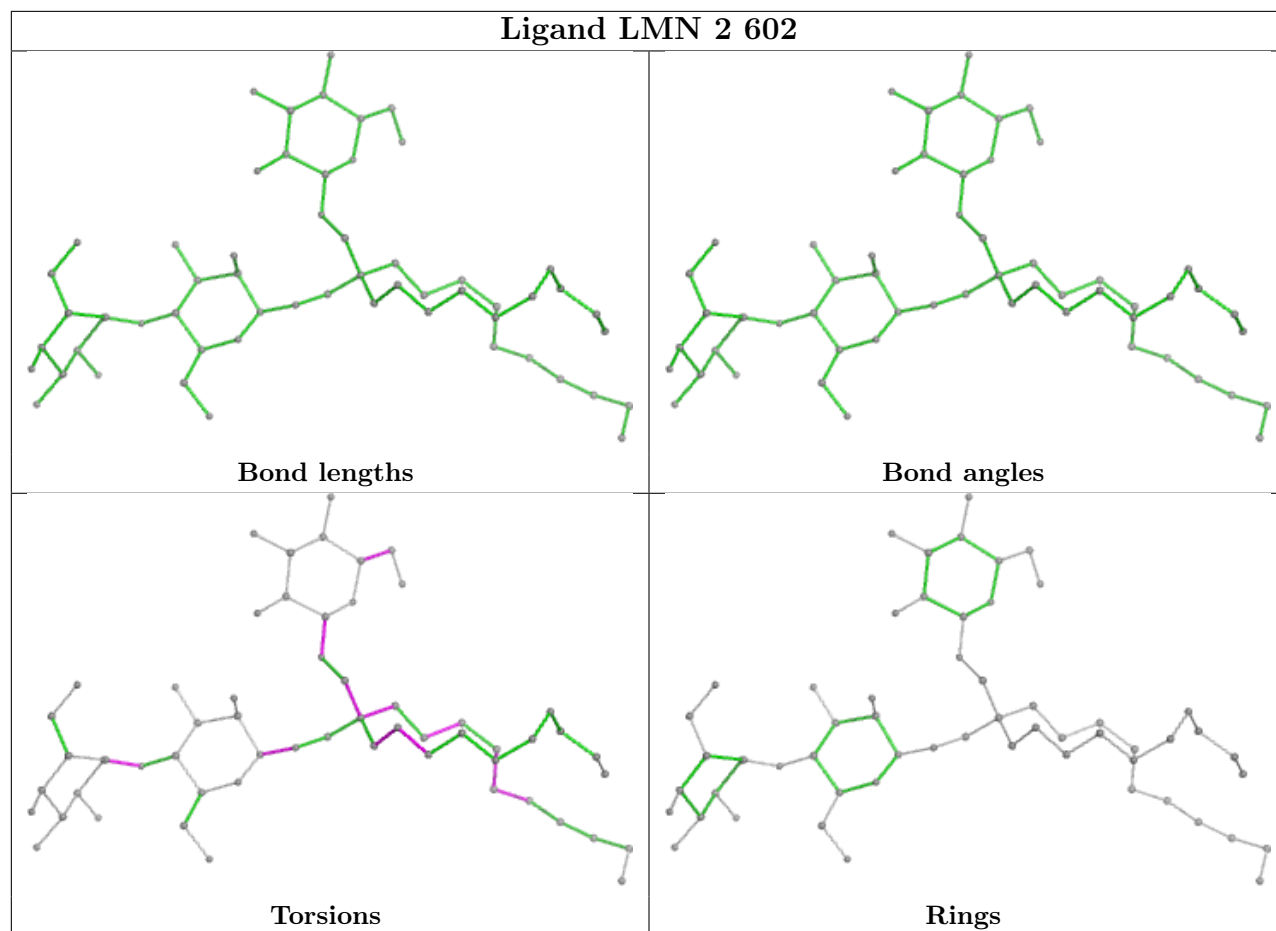
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



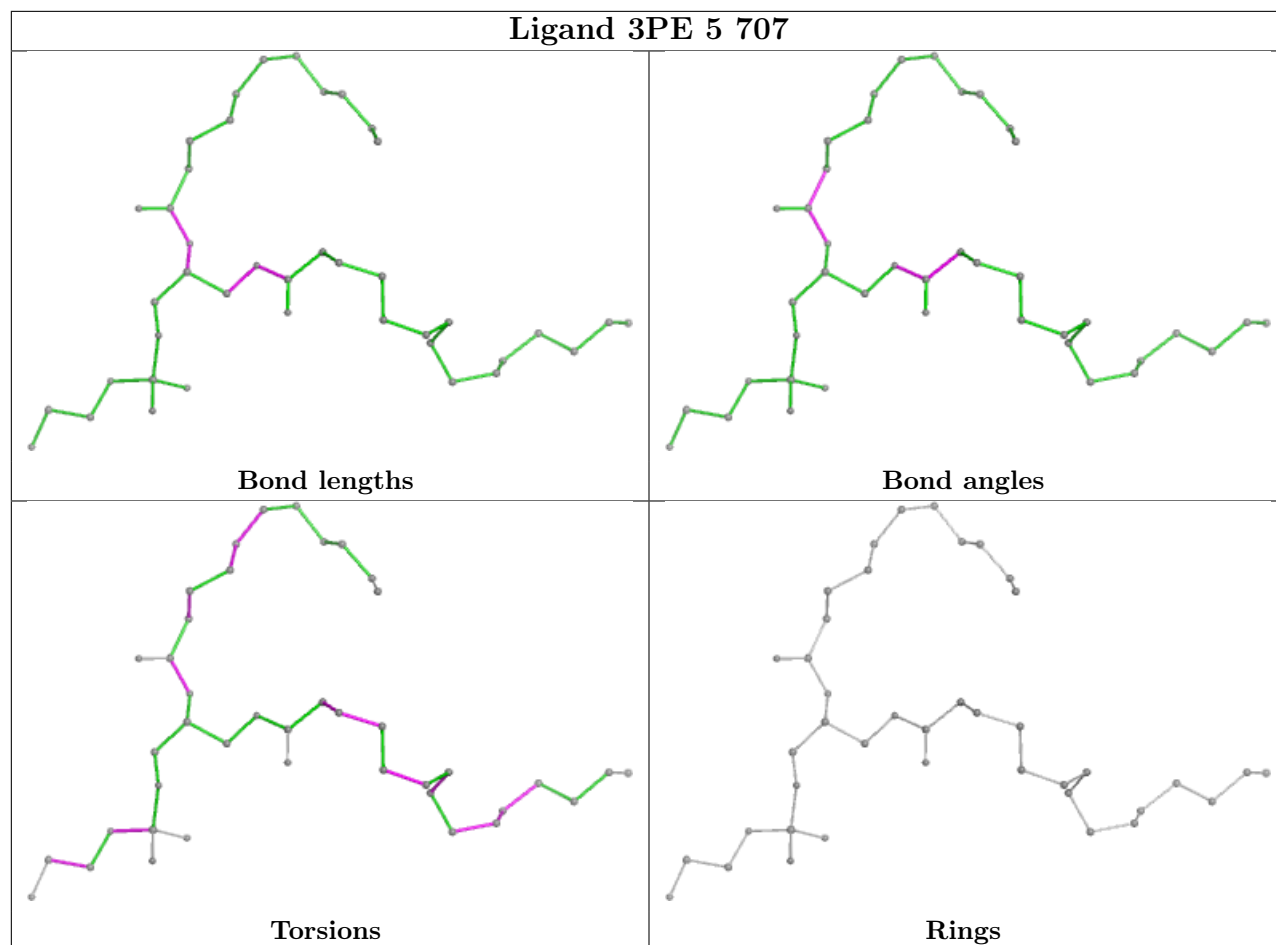




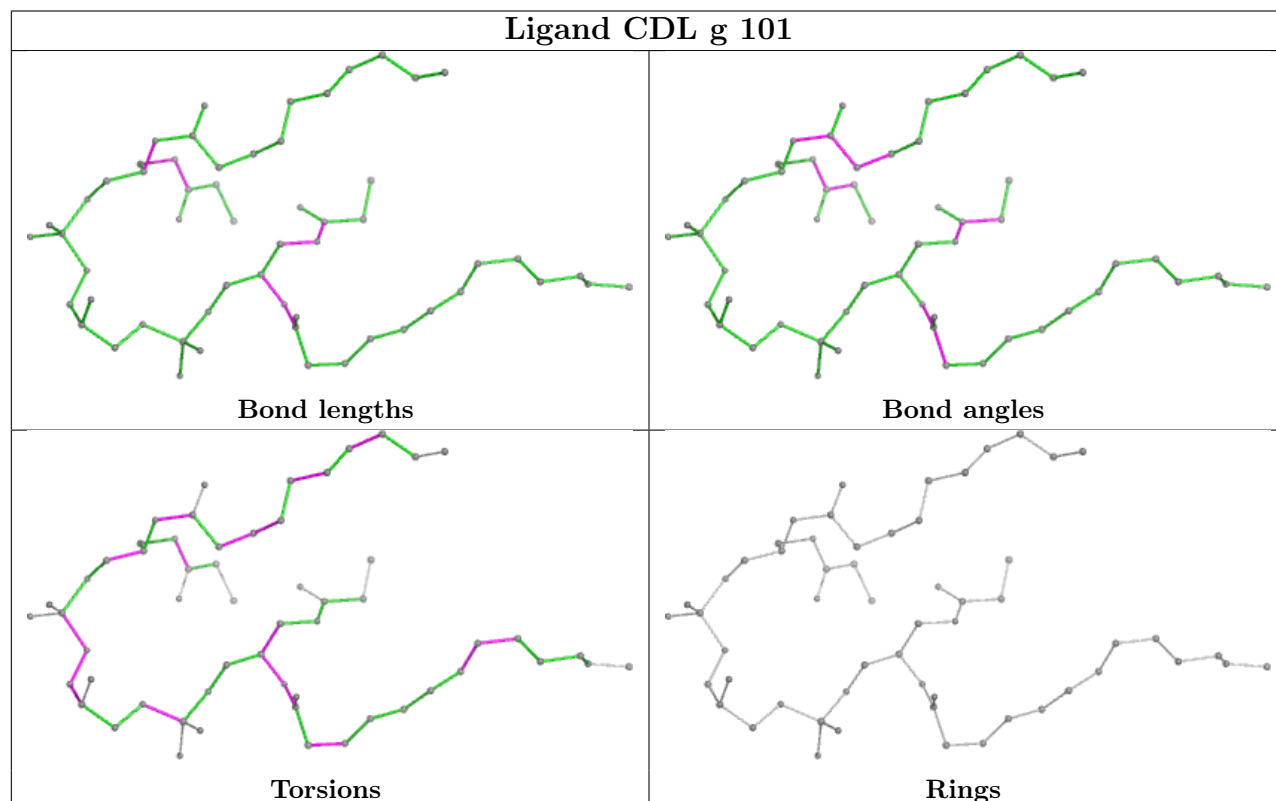


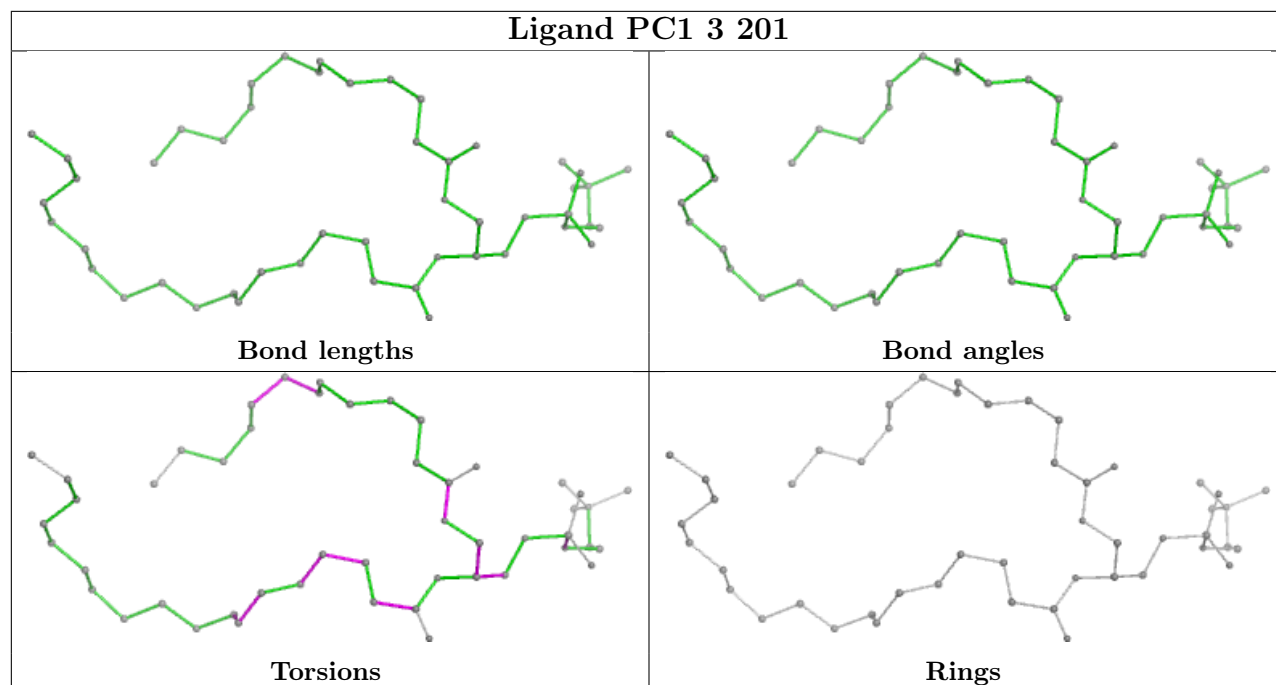
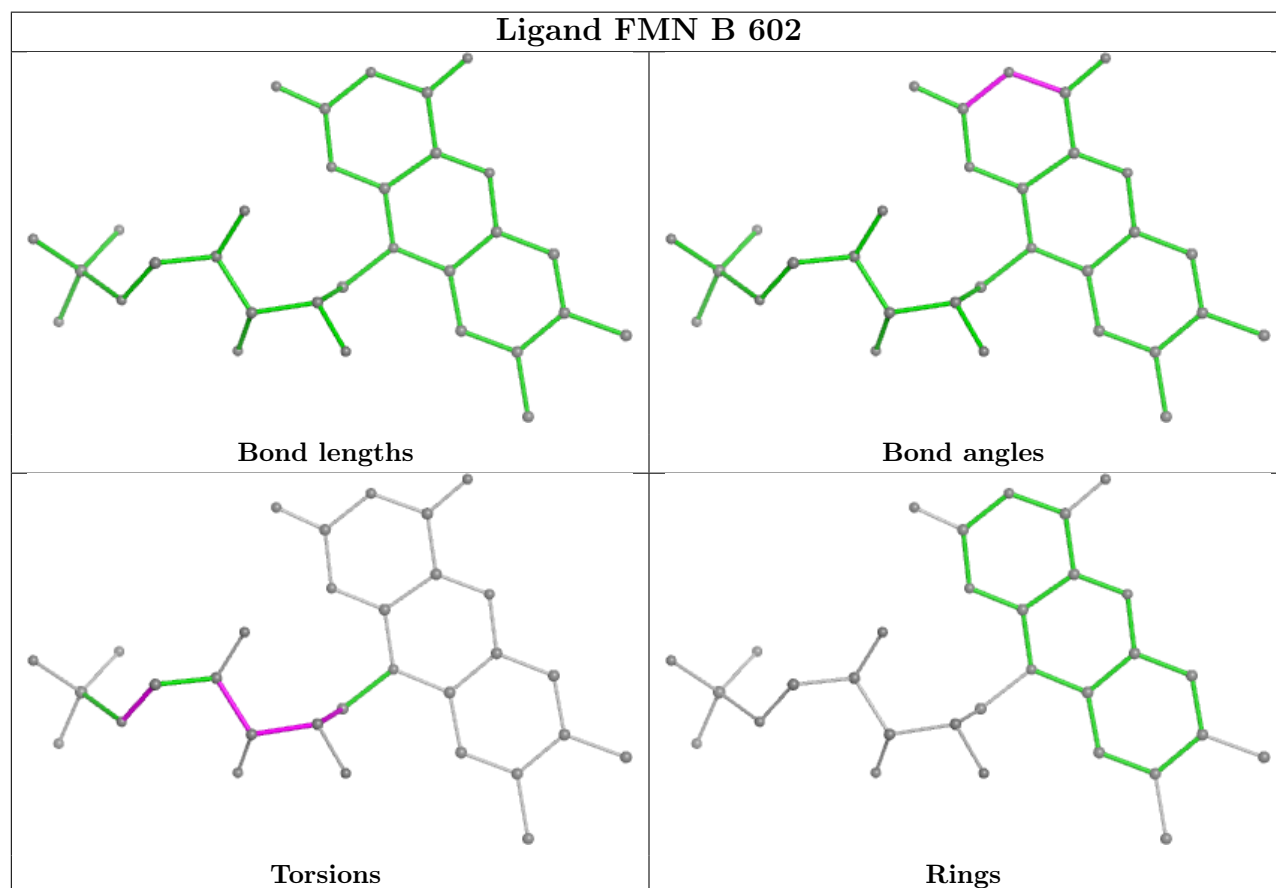


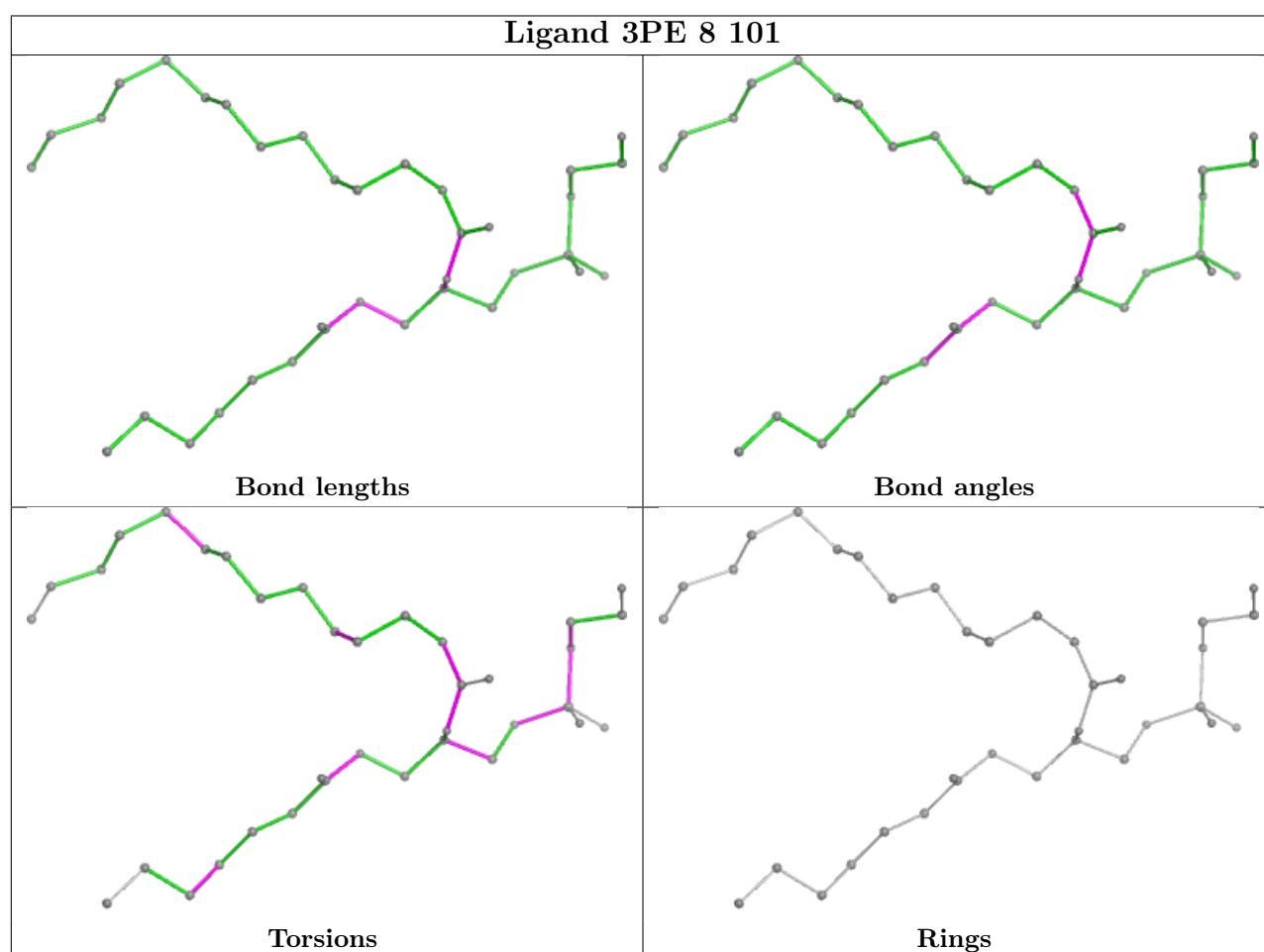
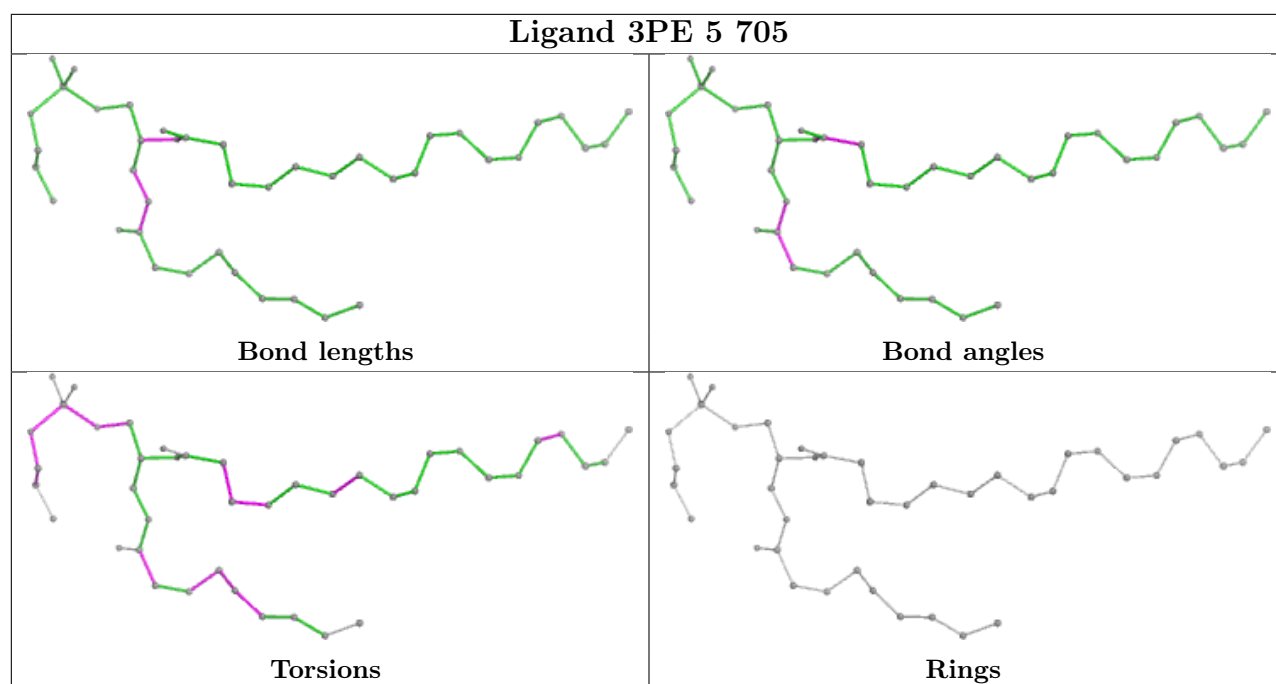
Ligand 3PE 5 707

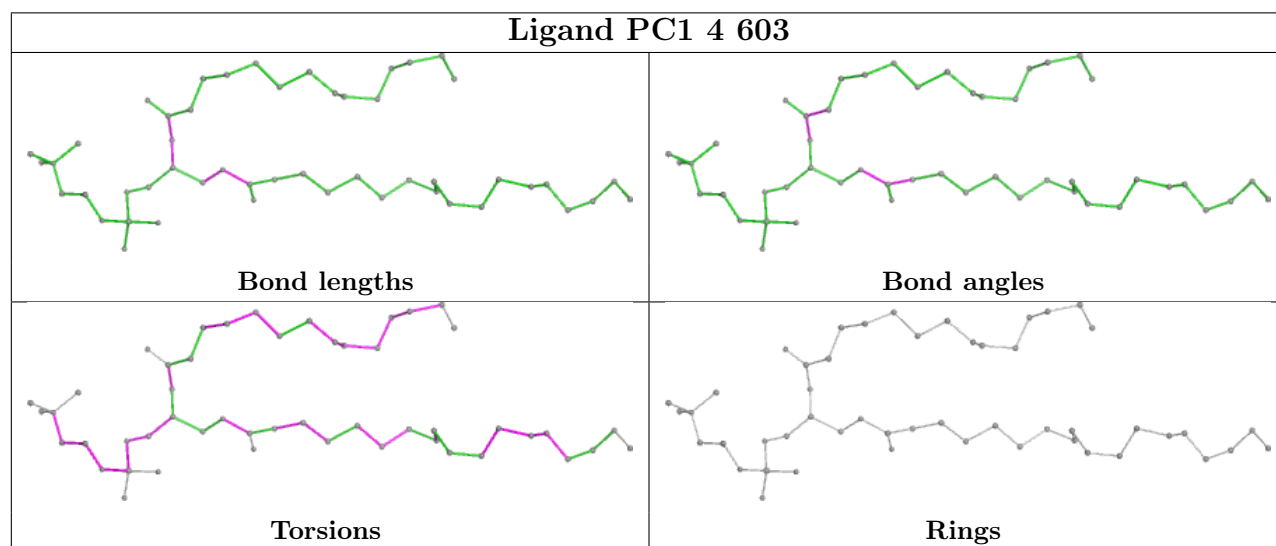
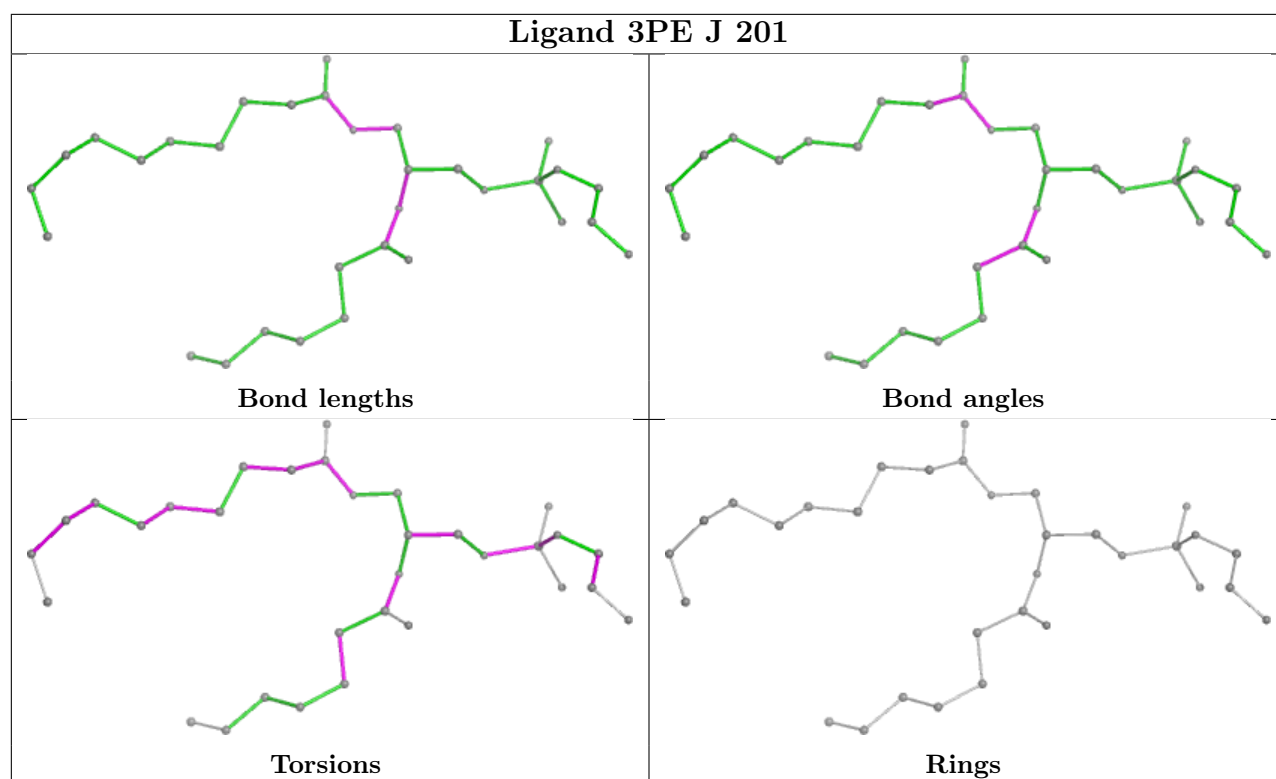


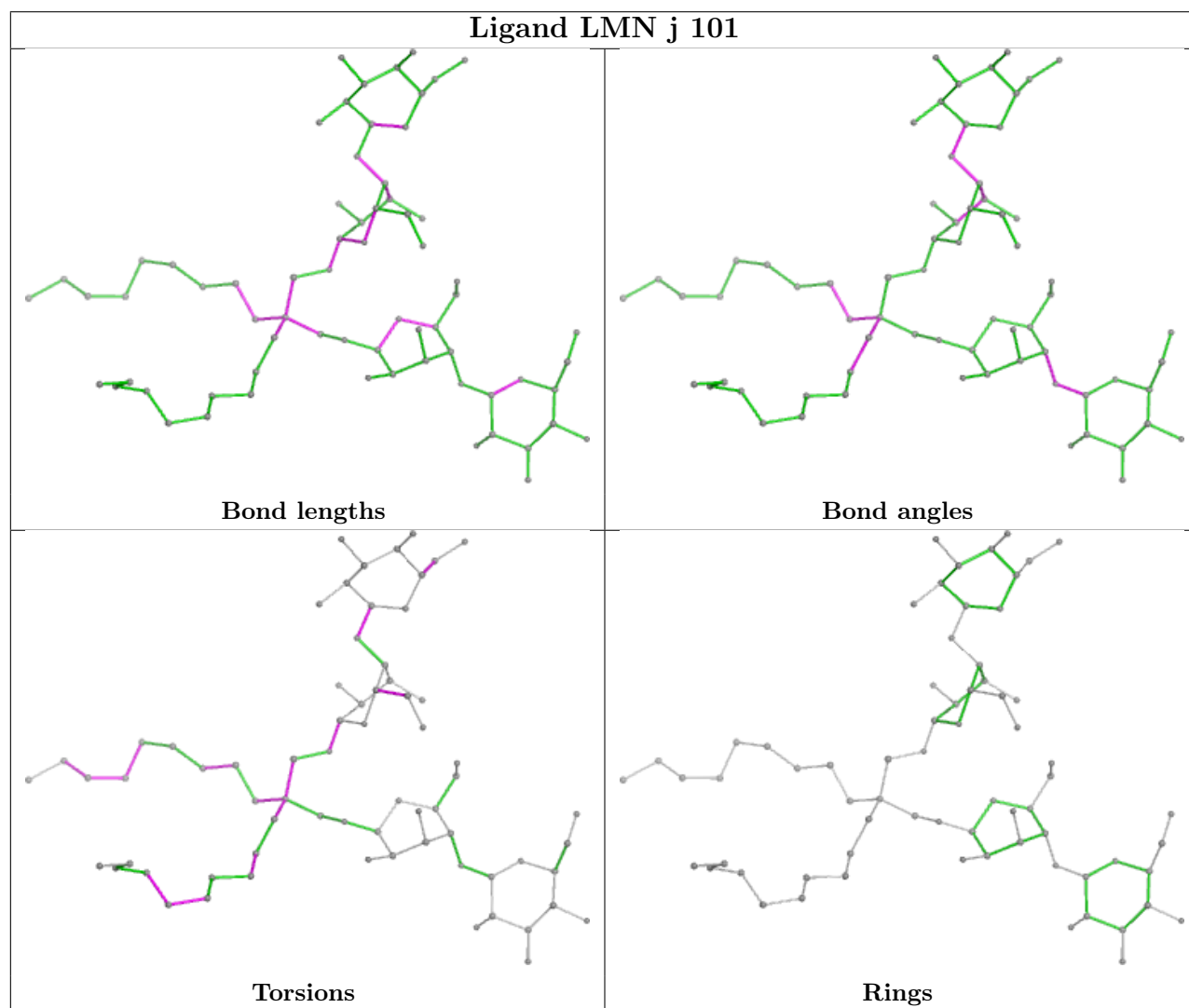
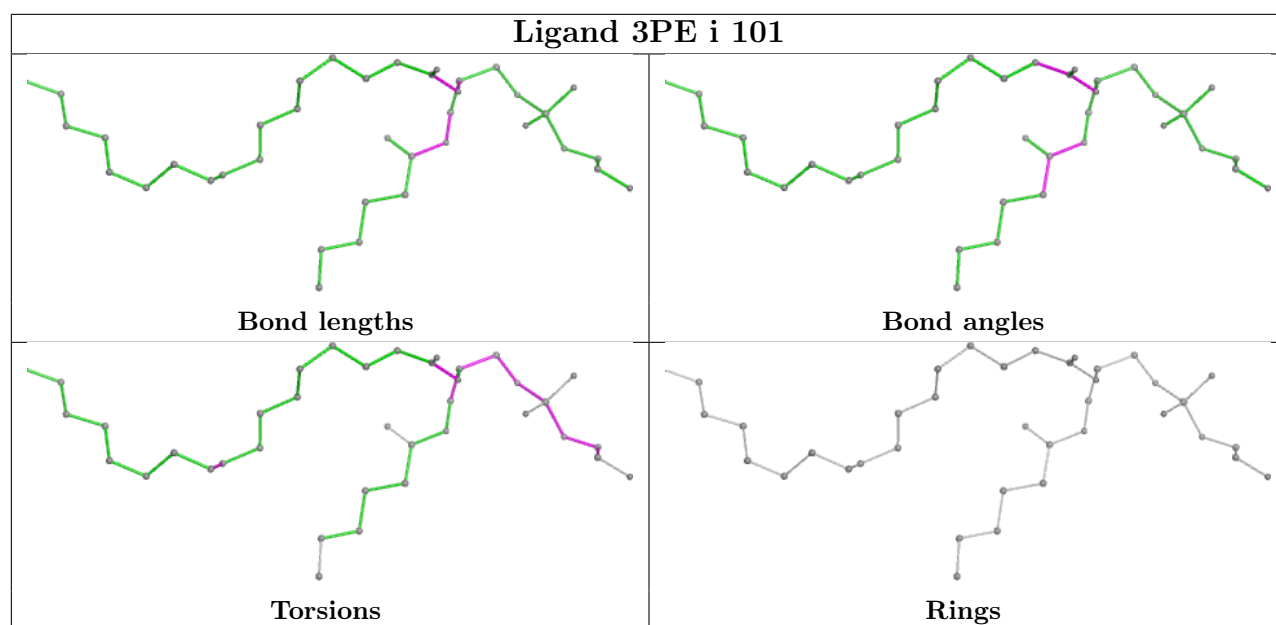
Ligand CDL g 101

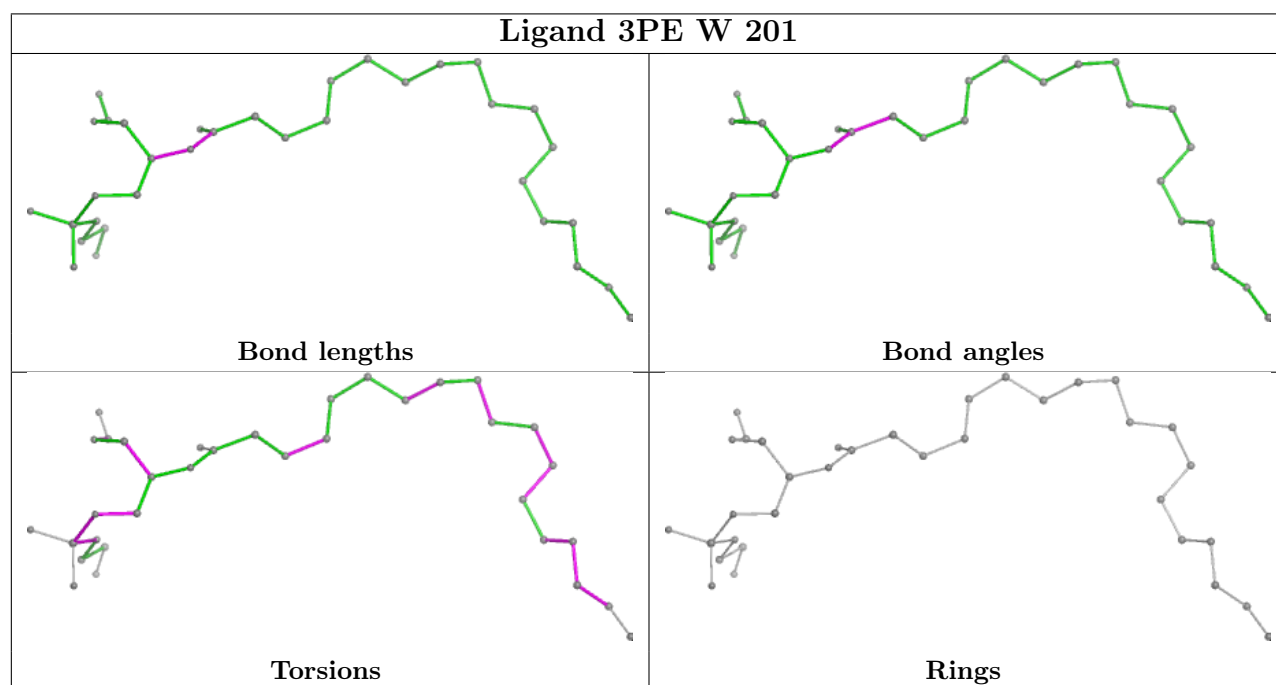
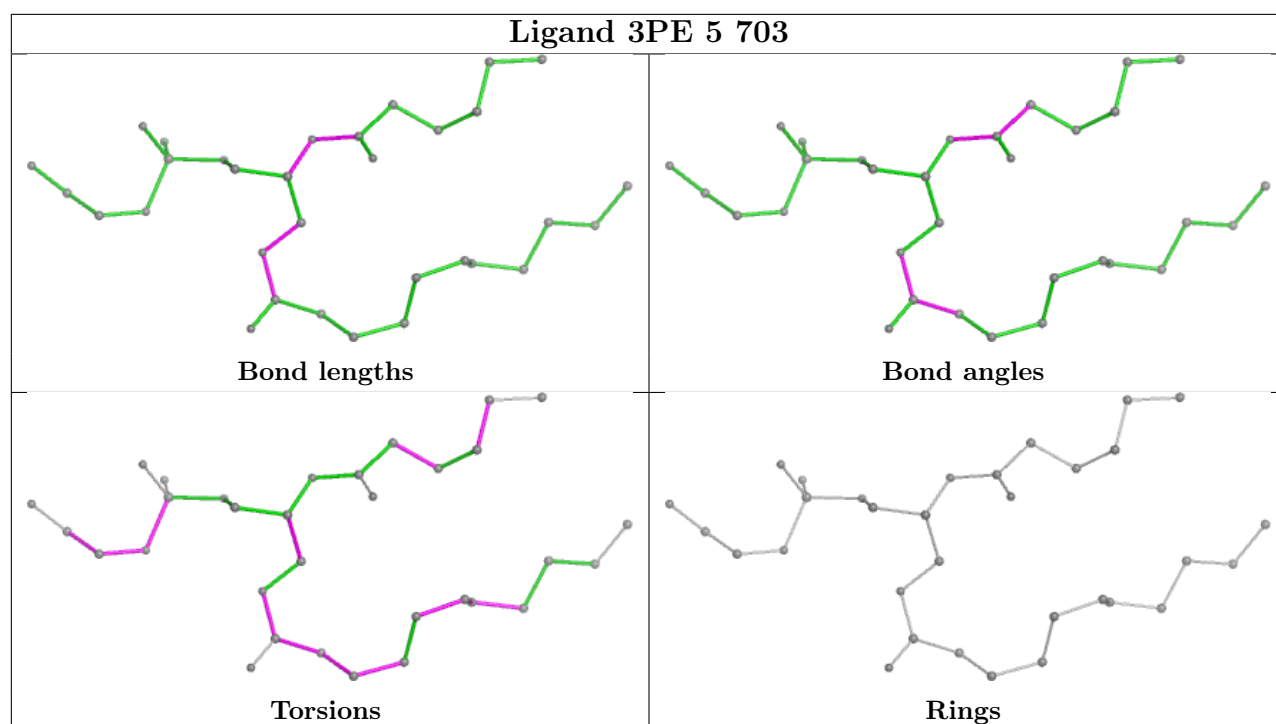


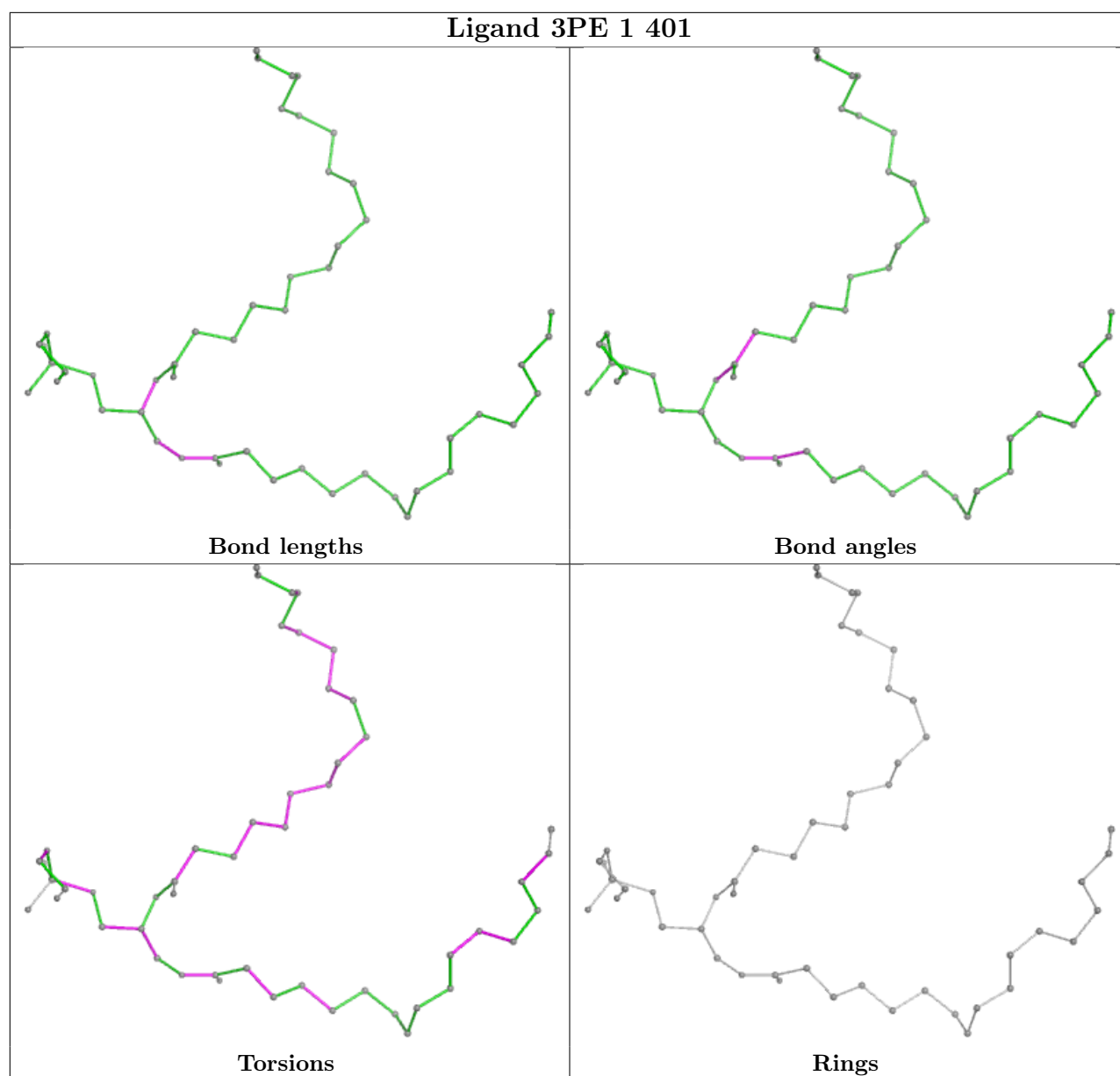
Ligand PC1 3 201**Ligand FMN B 602**

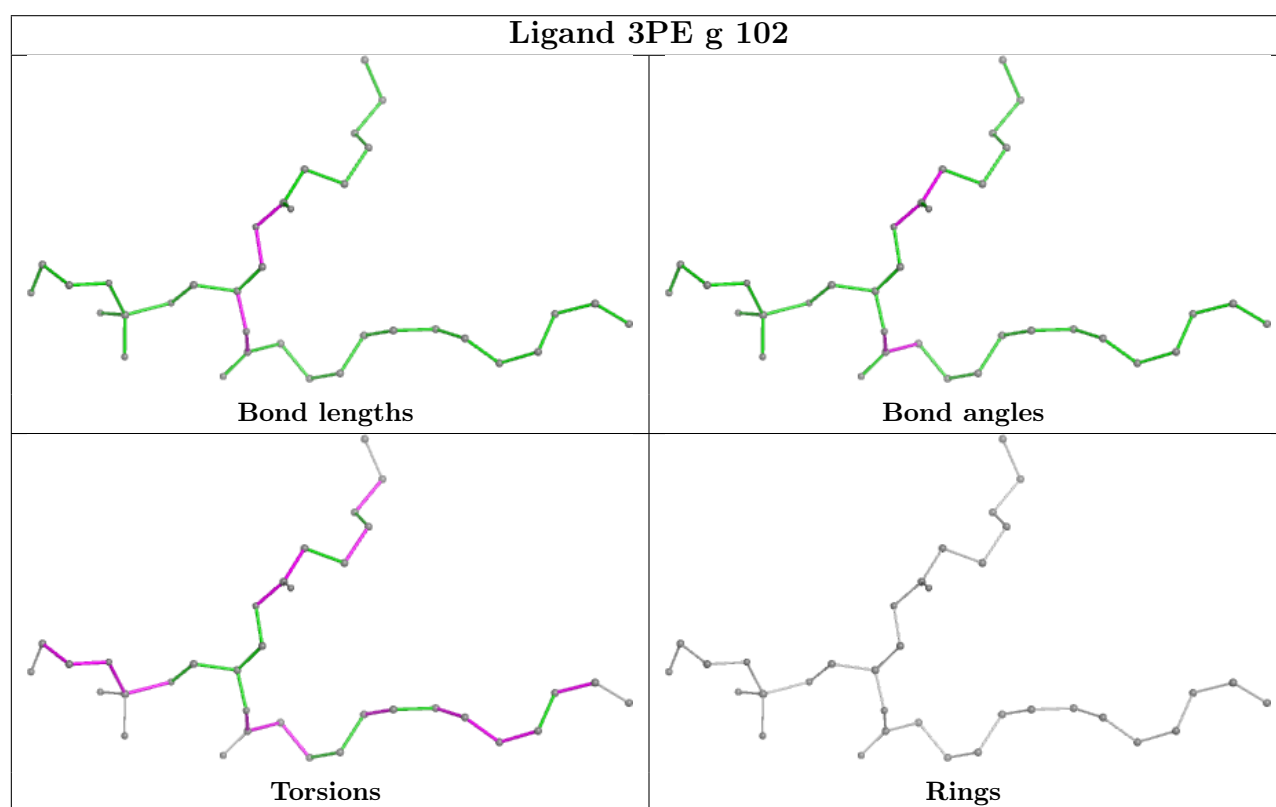
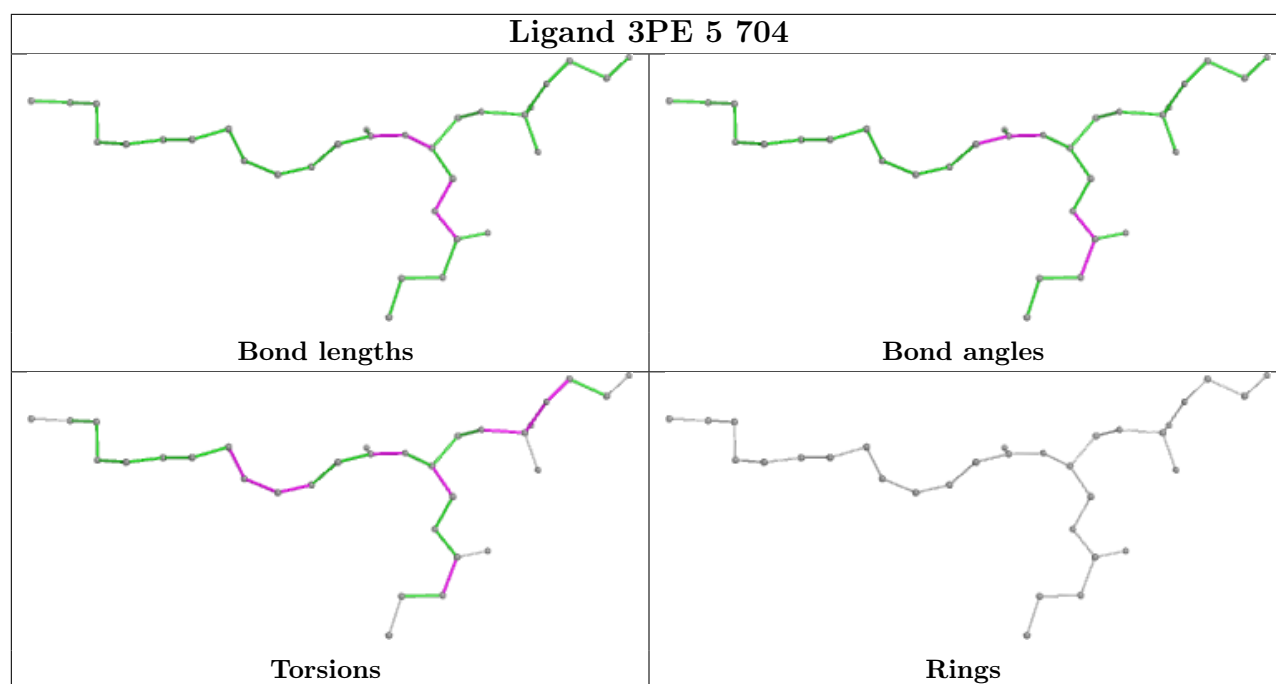


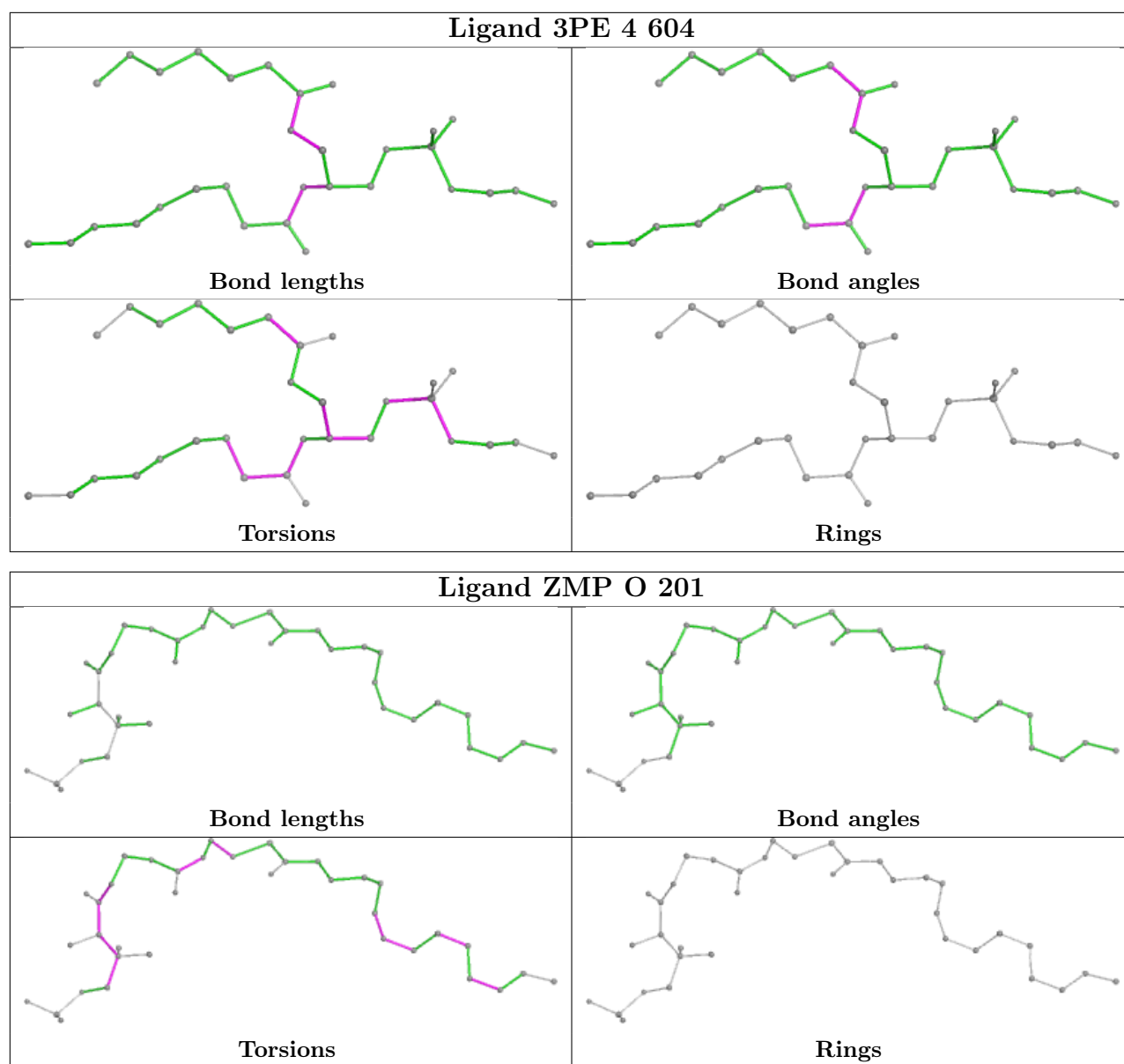


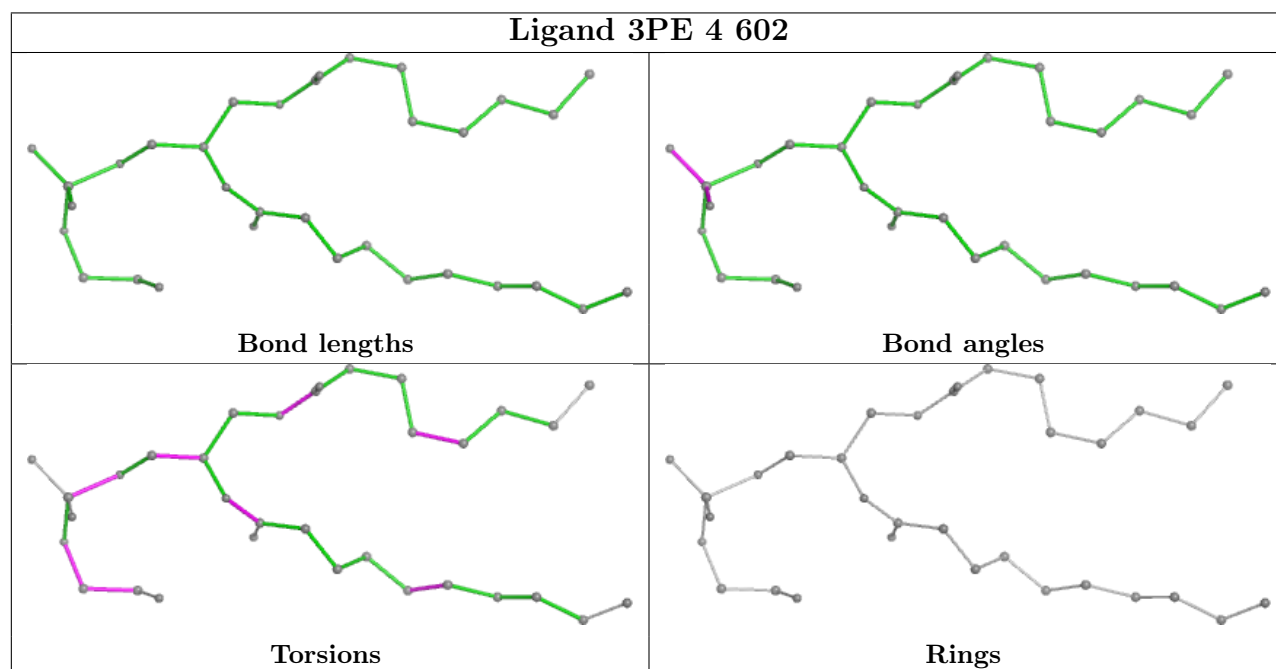
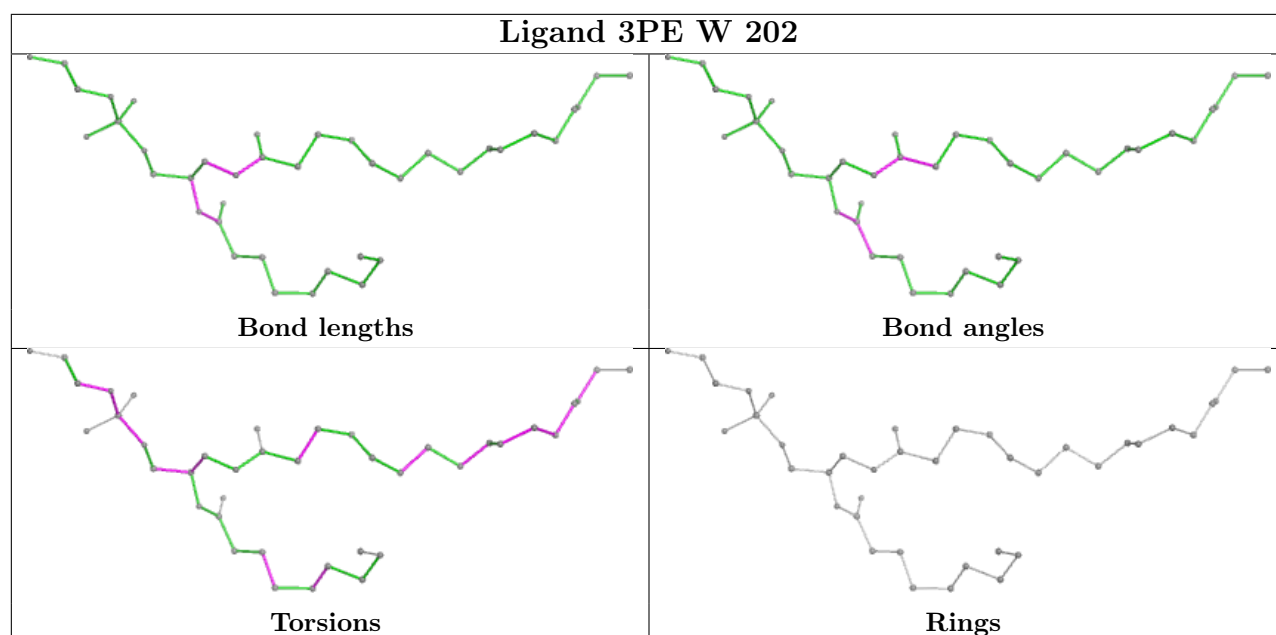


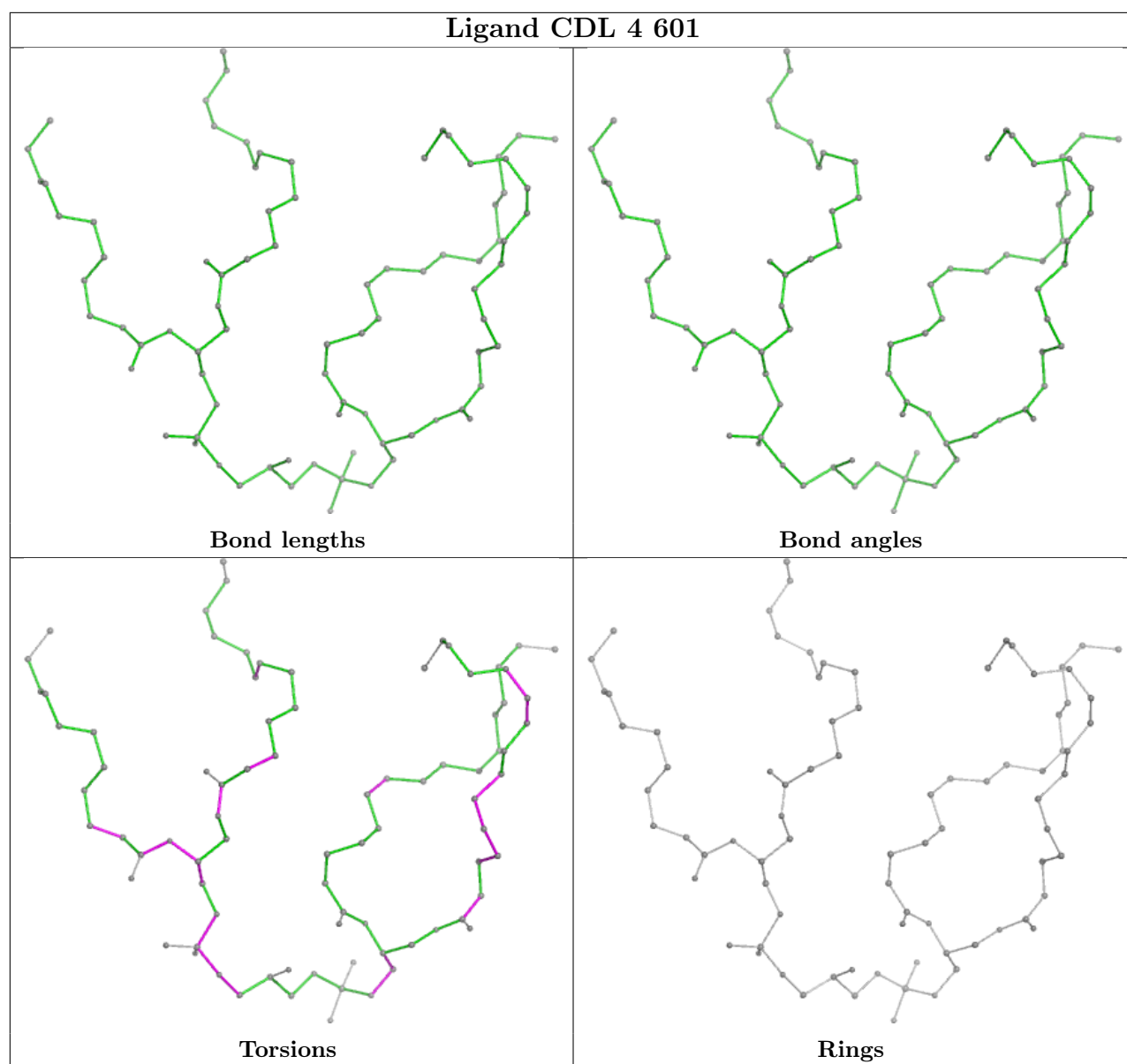




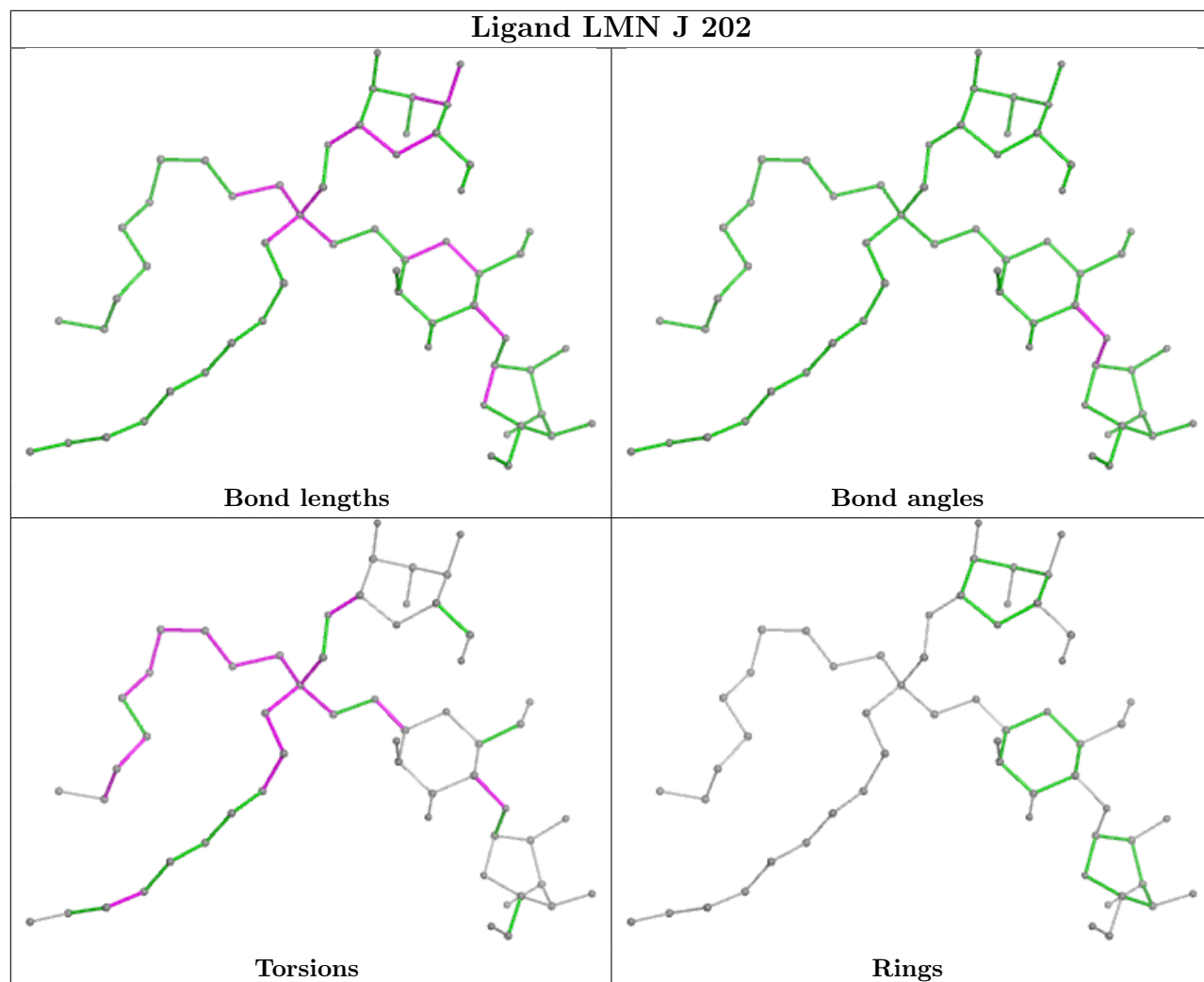


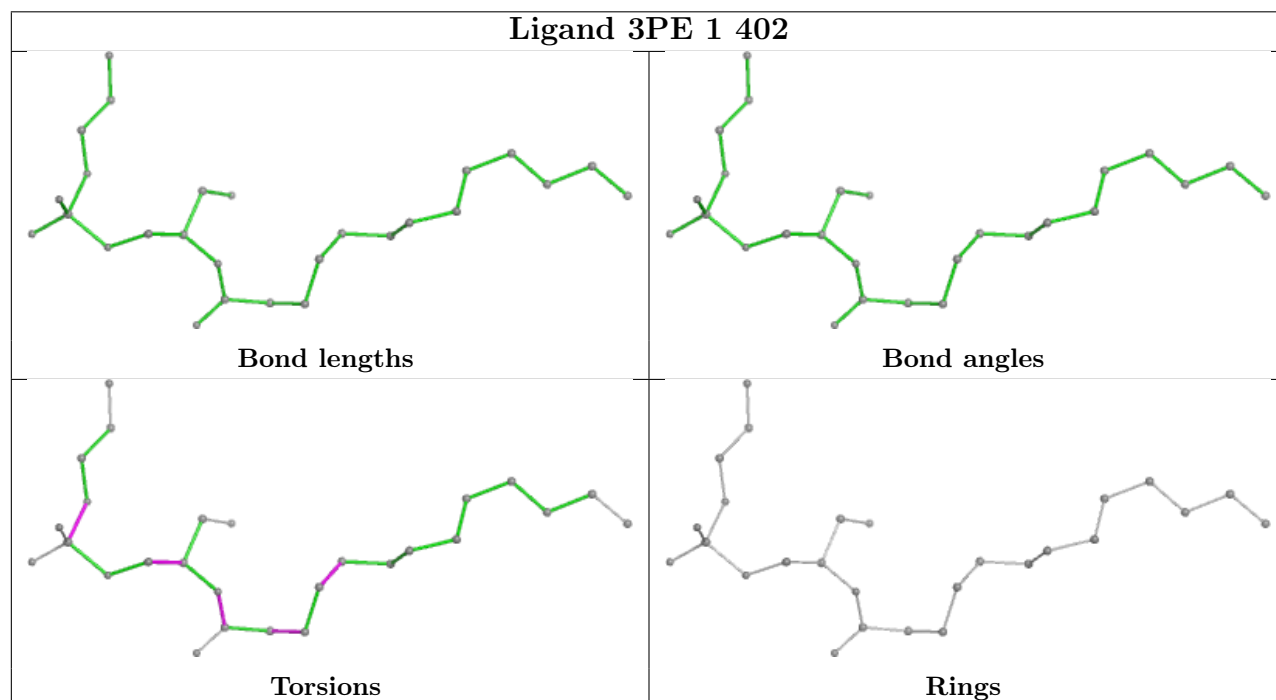
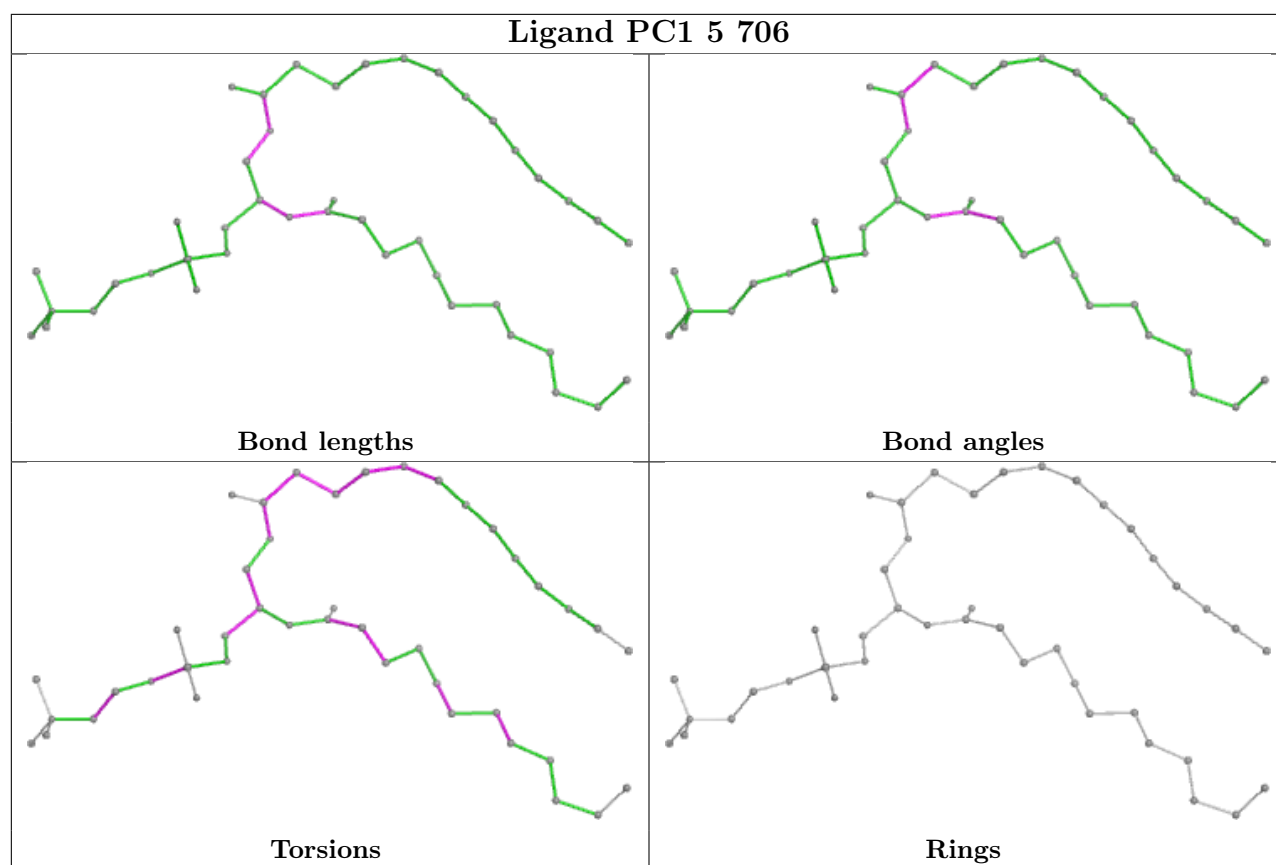


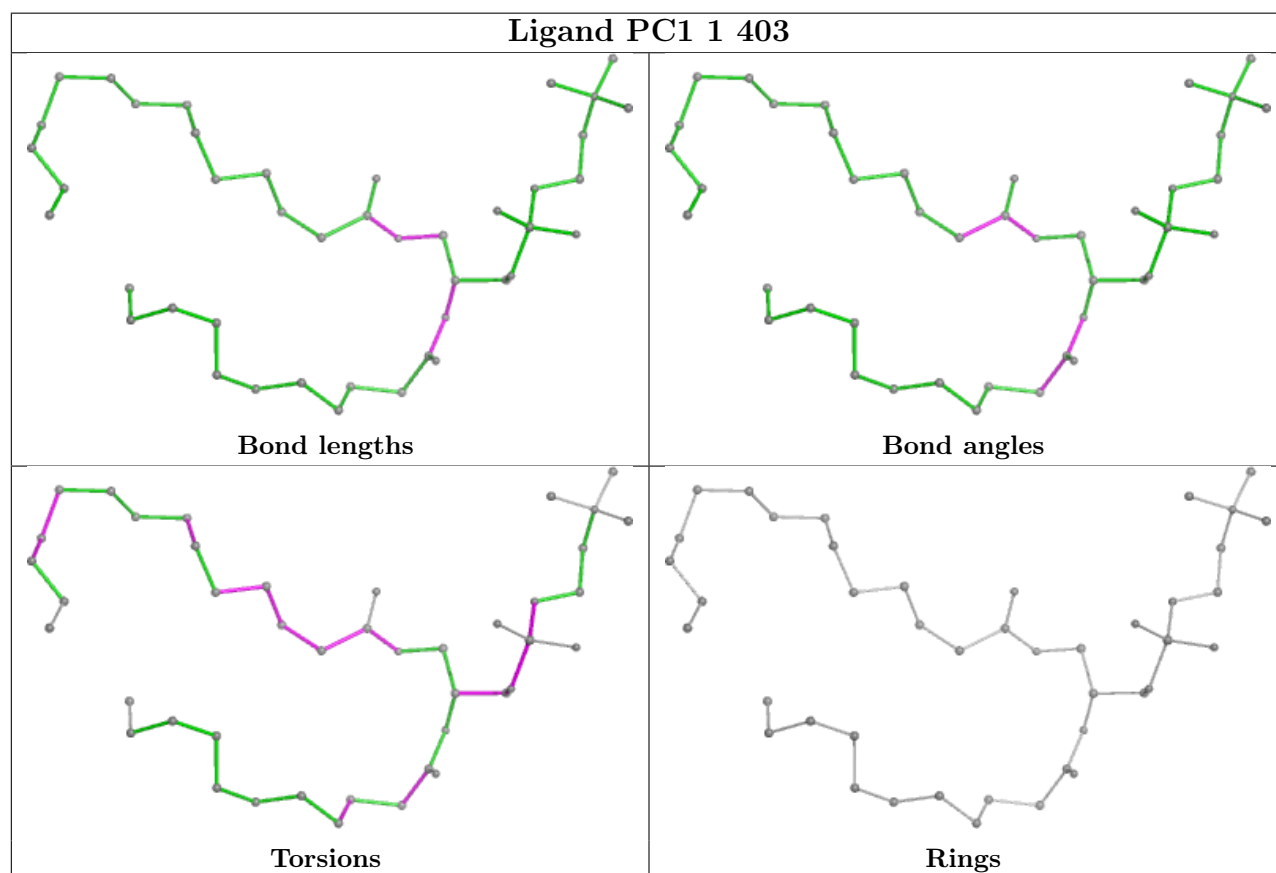
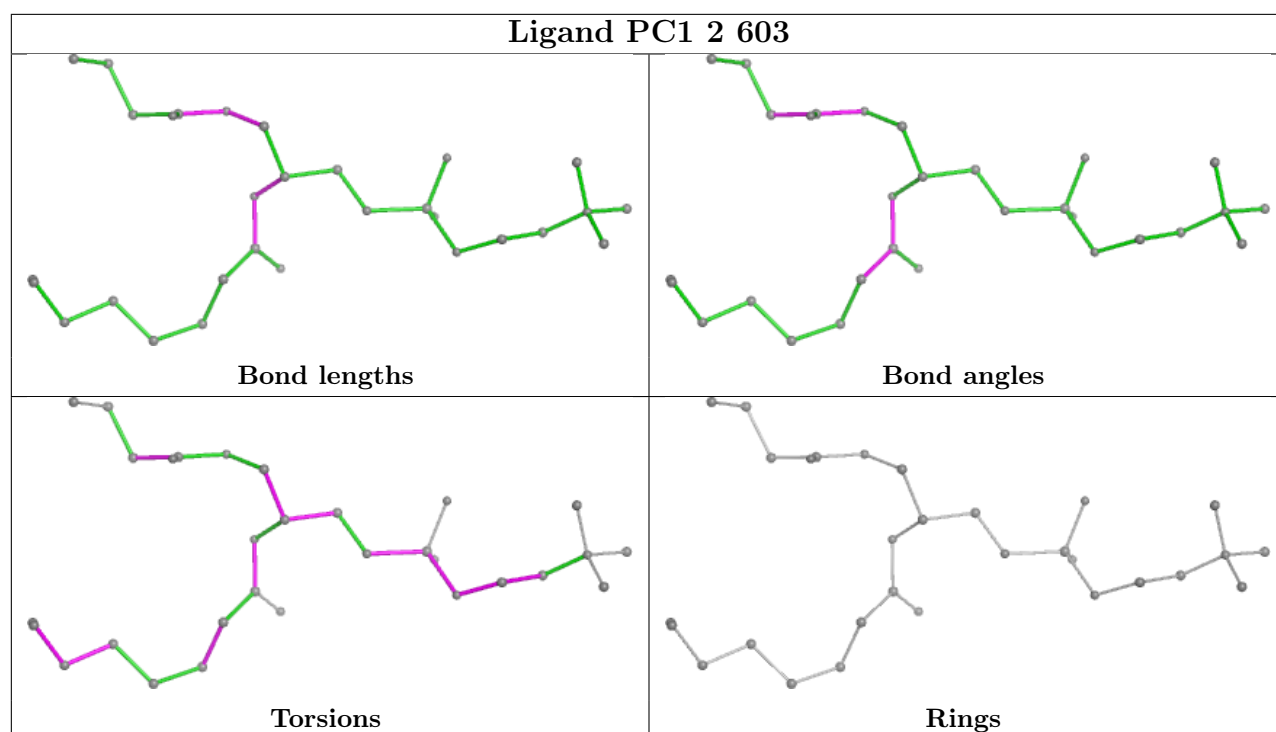


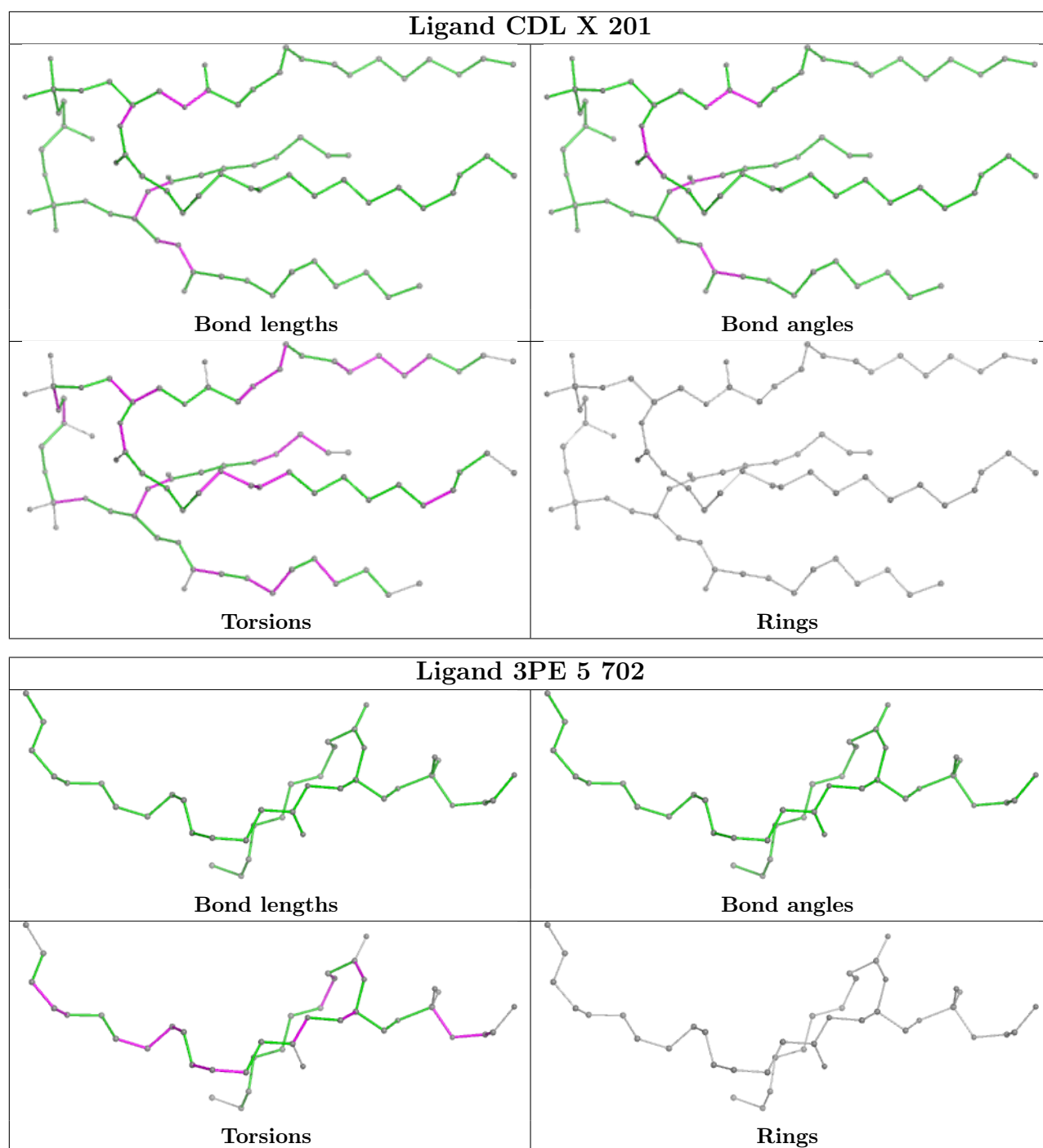


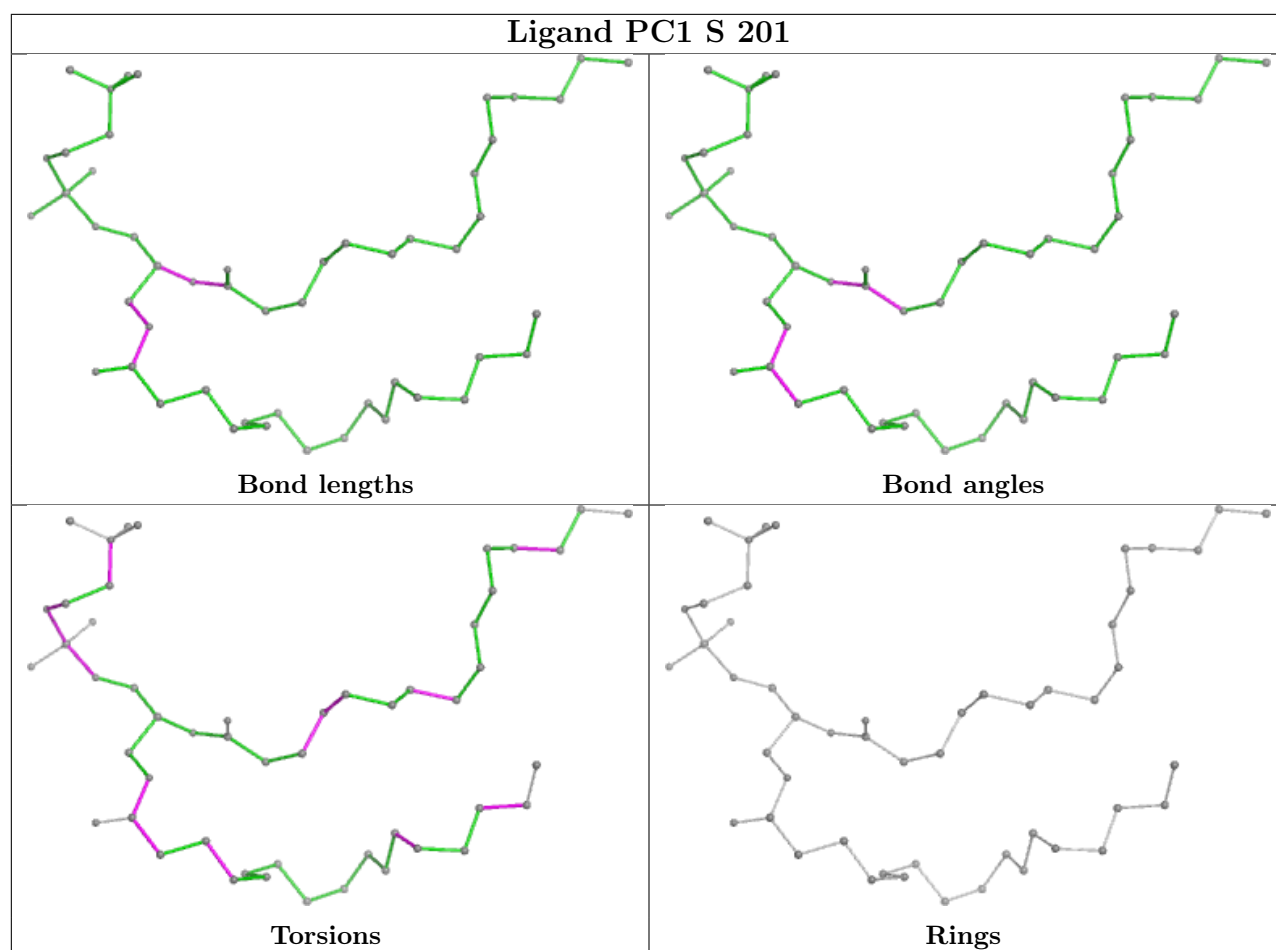
Ligand LMN J 202











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.

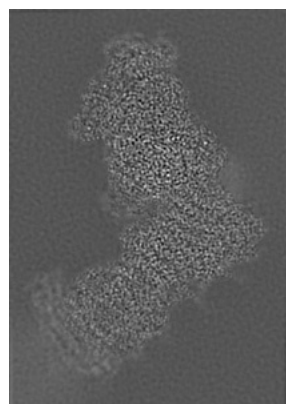
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14794. These allow visual inspection of the internal detail of the map and identification of artifacts.

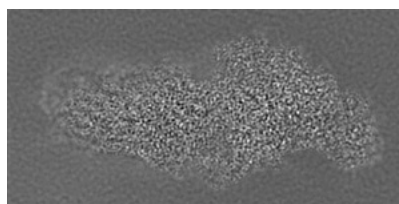
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

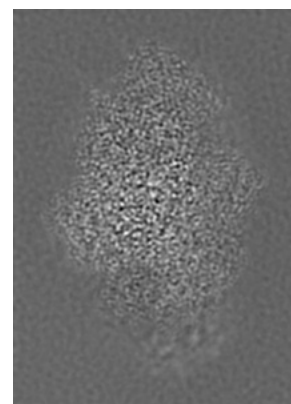
6.1.1 Primary map



X

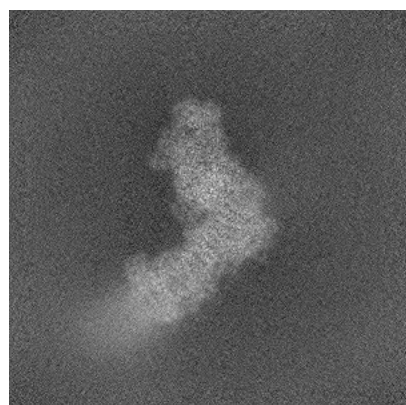


Y

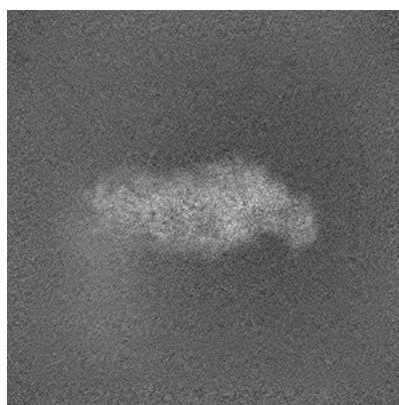


Z

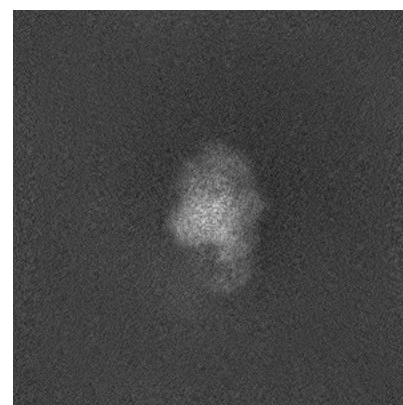
6.1.2 Raw map



X



Y

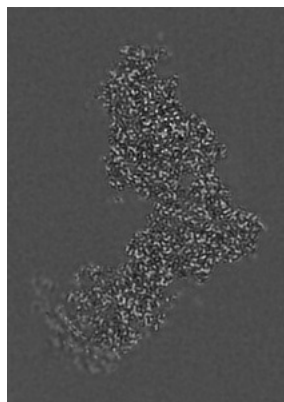


Z

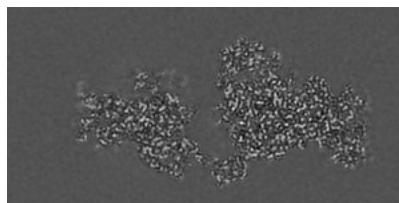
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

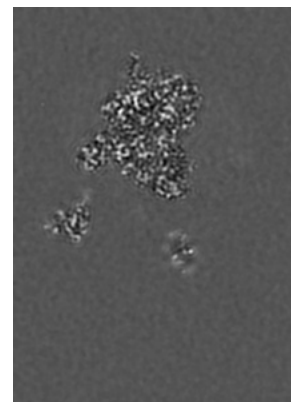
6.2.1 Primary map



X Index: 95

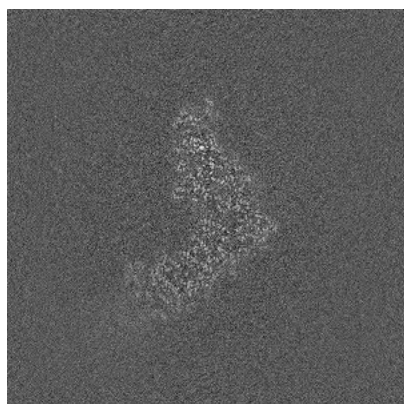


Y Index: 132

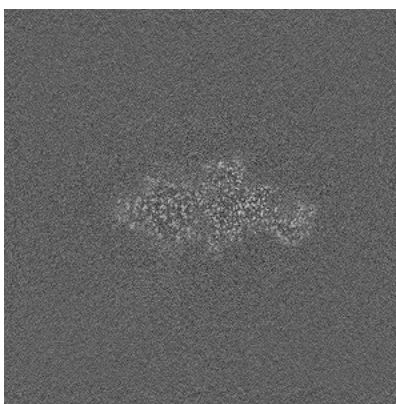


Z Index: 191

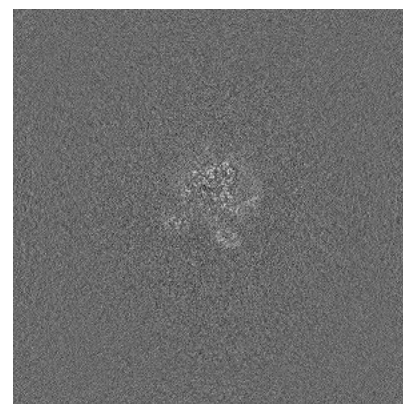
6.2.2 Raw map



X Index: 294



Y Index: 294

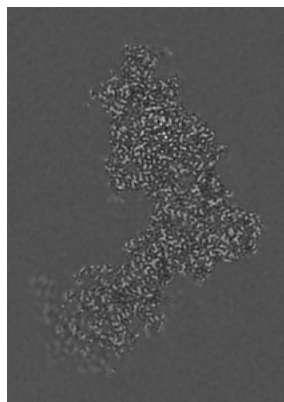


Z Index: 294

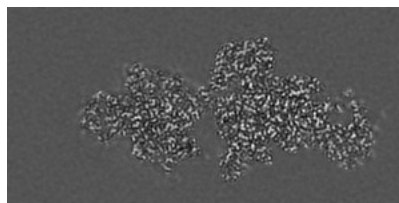
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

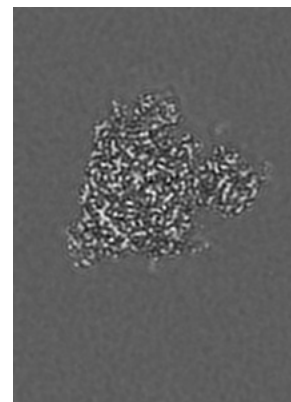
6.3.1 Primary map



X Index: 97

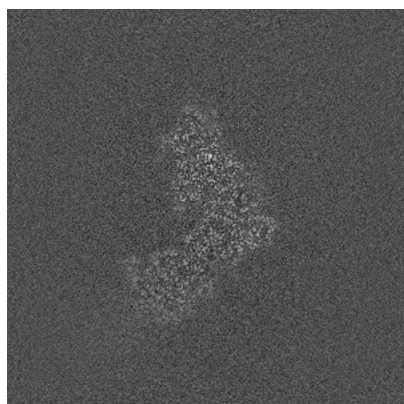


Y Index: 140

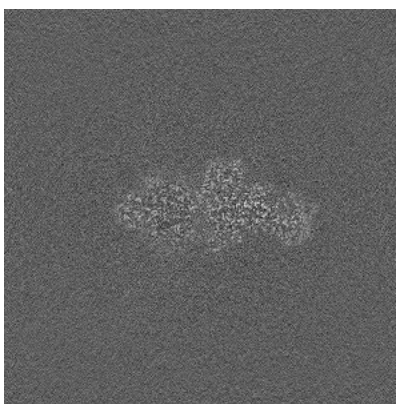


Z Index: 240

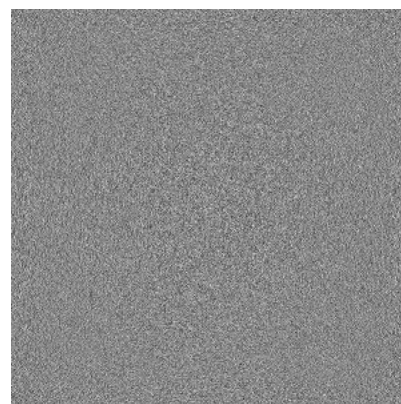
6.3.2 Raw map



X Index: 302



Y Index: 292

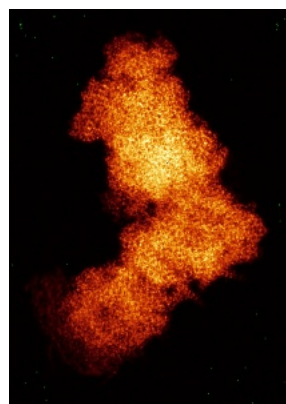


Z Index: 0

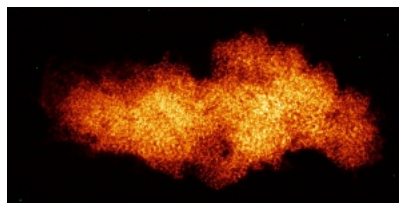
The images above show the largest variance slices of the map in three orthogonal directions.

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

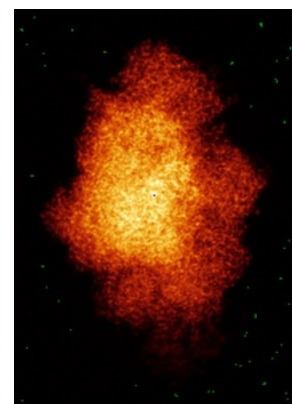
6.4.1 Primary map



X

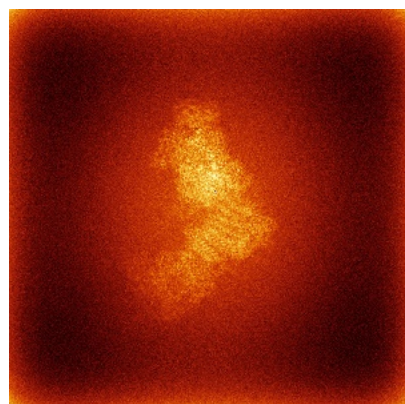


Y

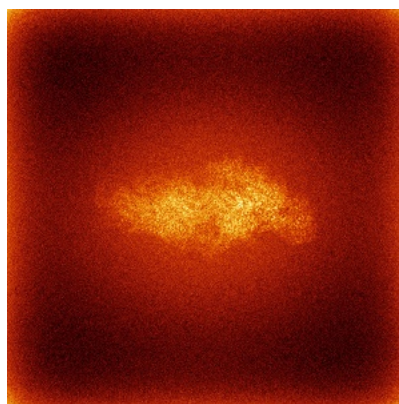


Z

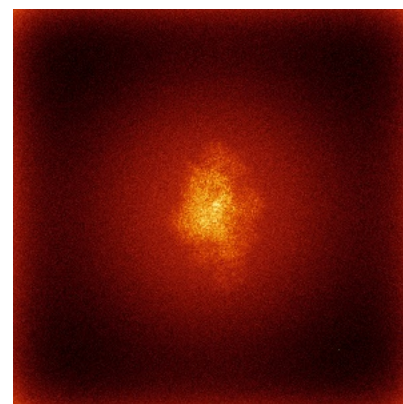
6.4.2 Raw map



X



Y

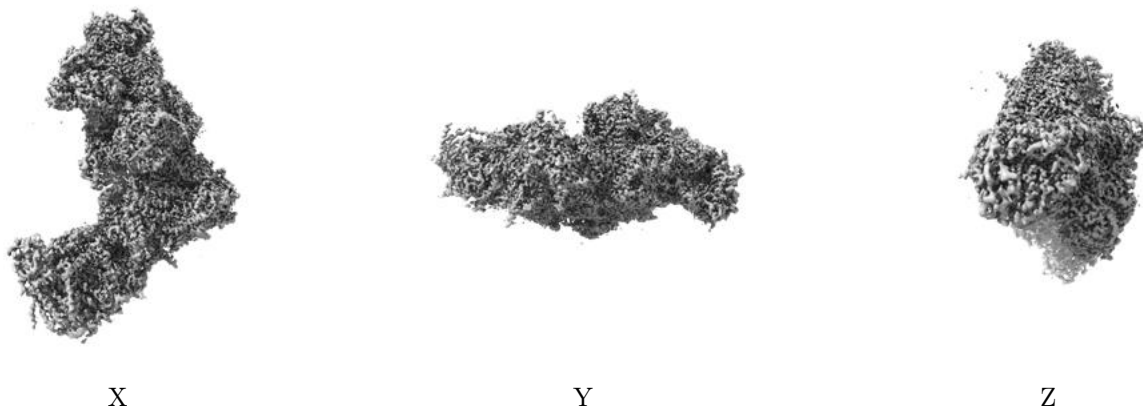


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

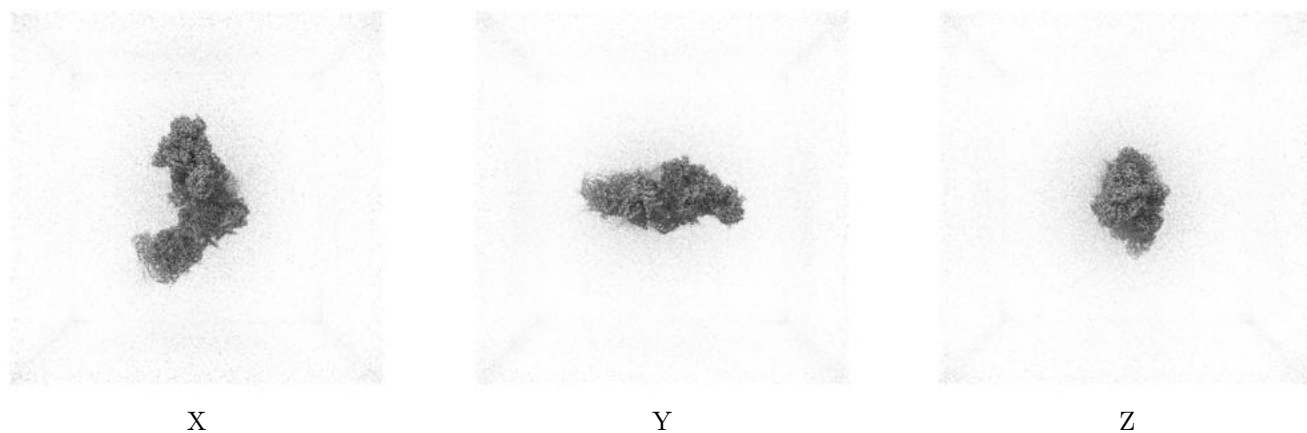
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

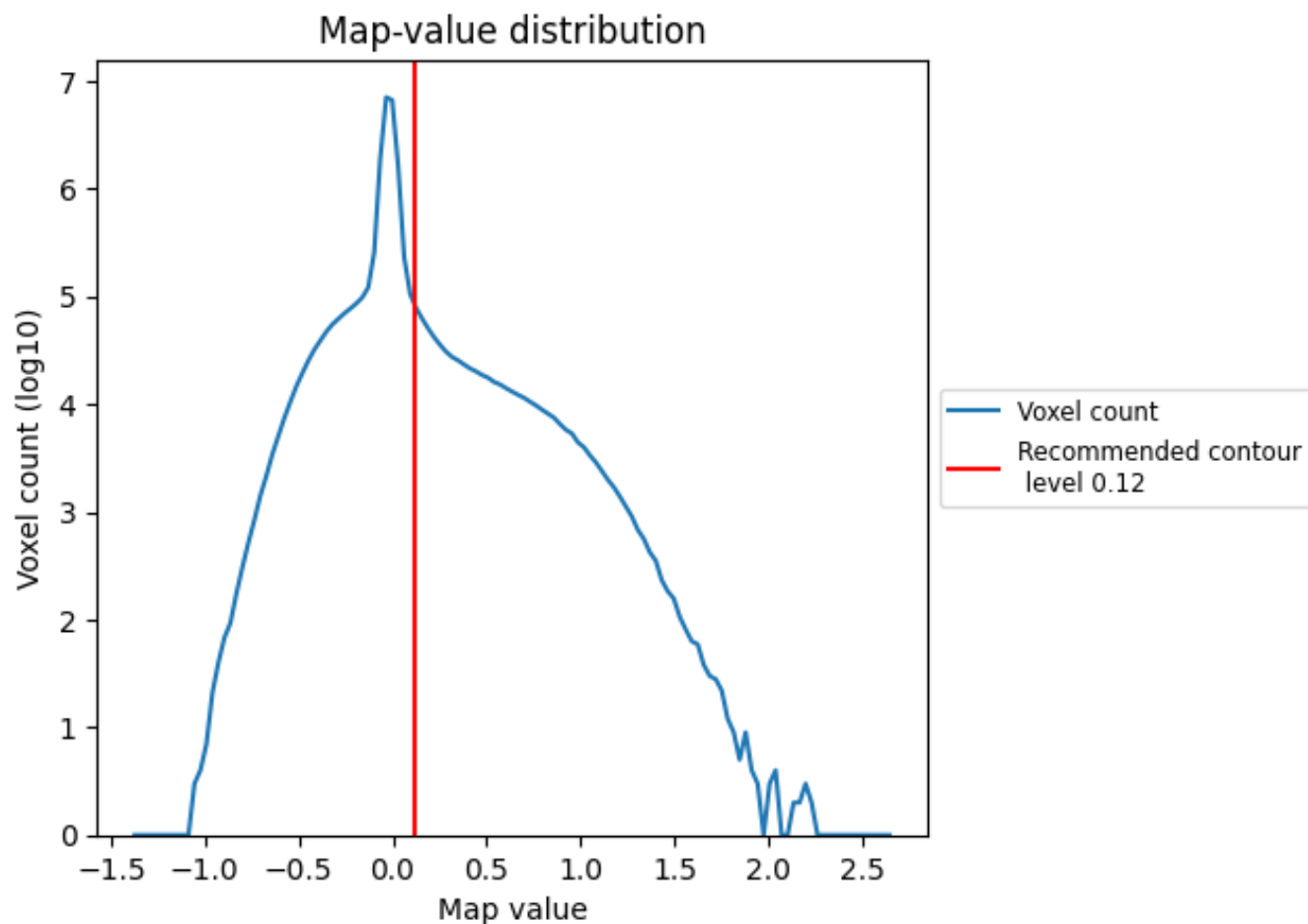
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

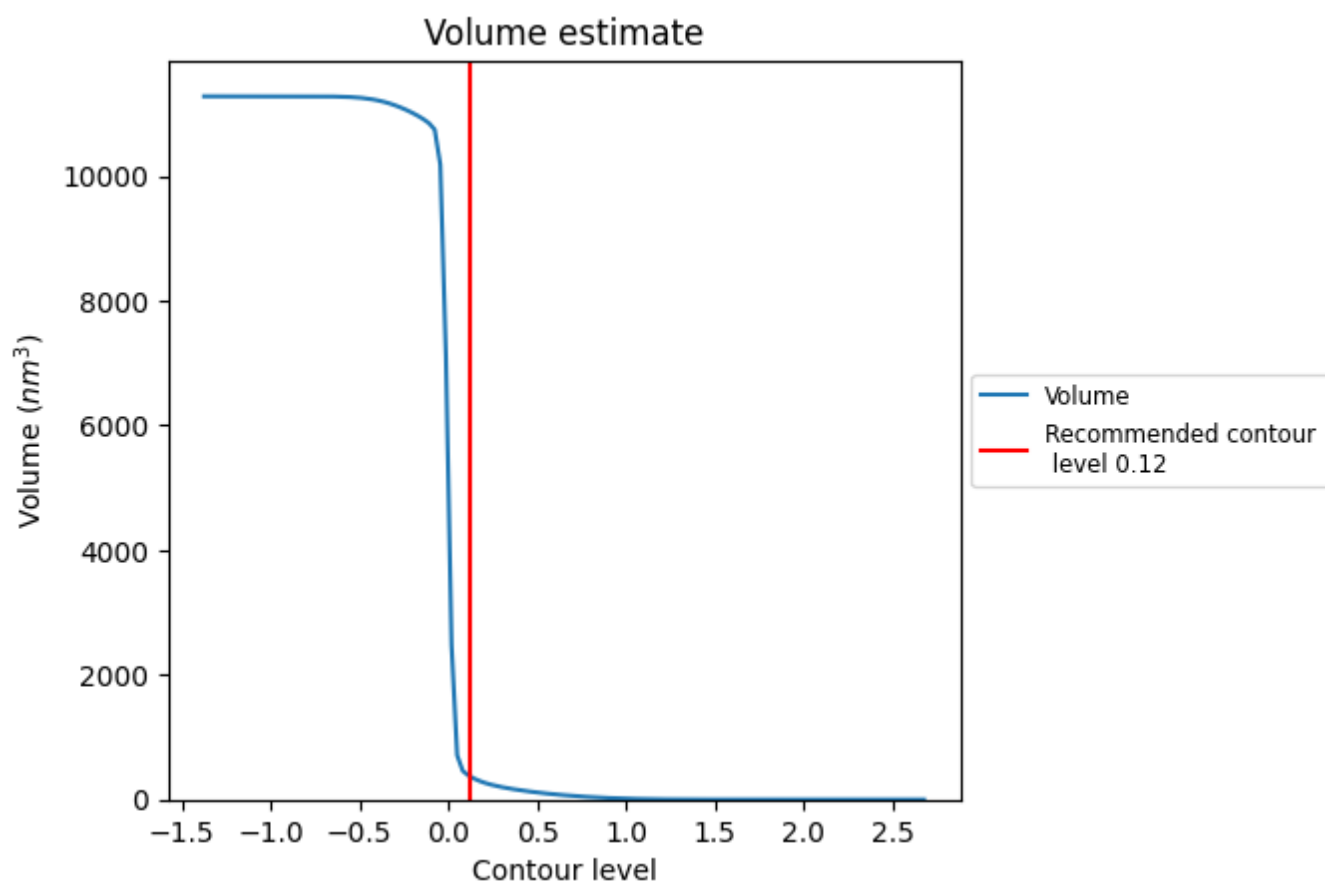
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 375 nm³; this corresponds to an approximate mass of 339 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

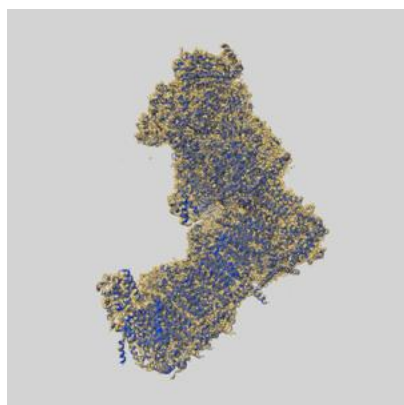
8 Fourier-Shell correlation

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

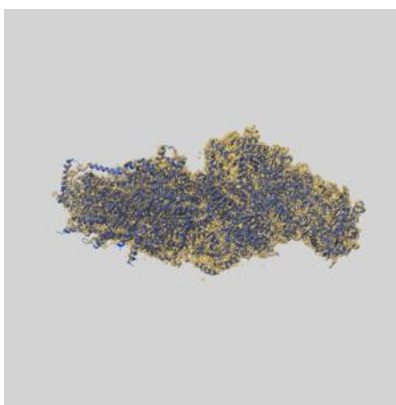
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14794 and PDB model 7ZMB. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

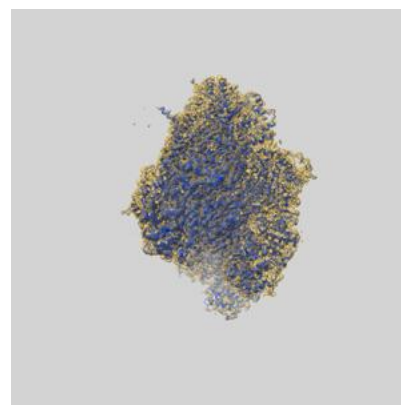
9.1 Map-model overlay [i](#)



X



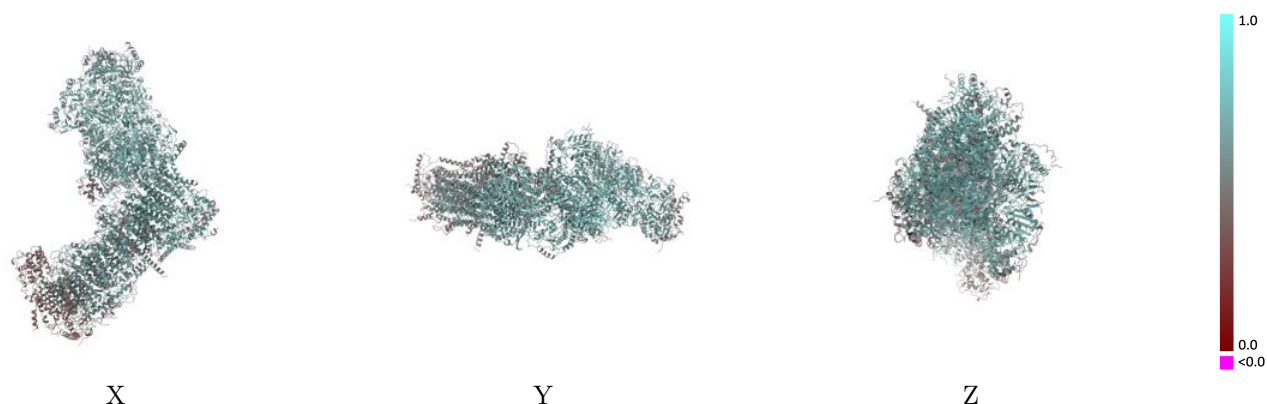
Y



Z

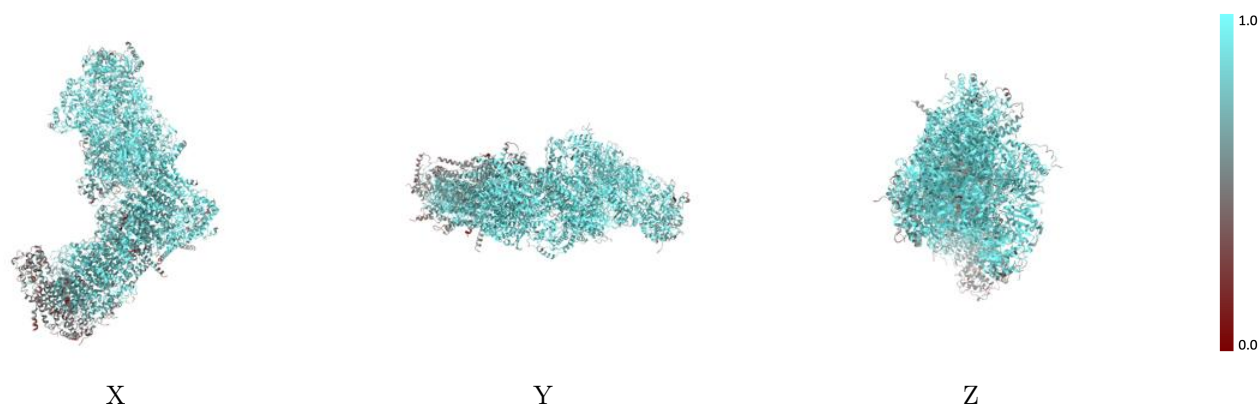
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



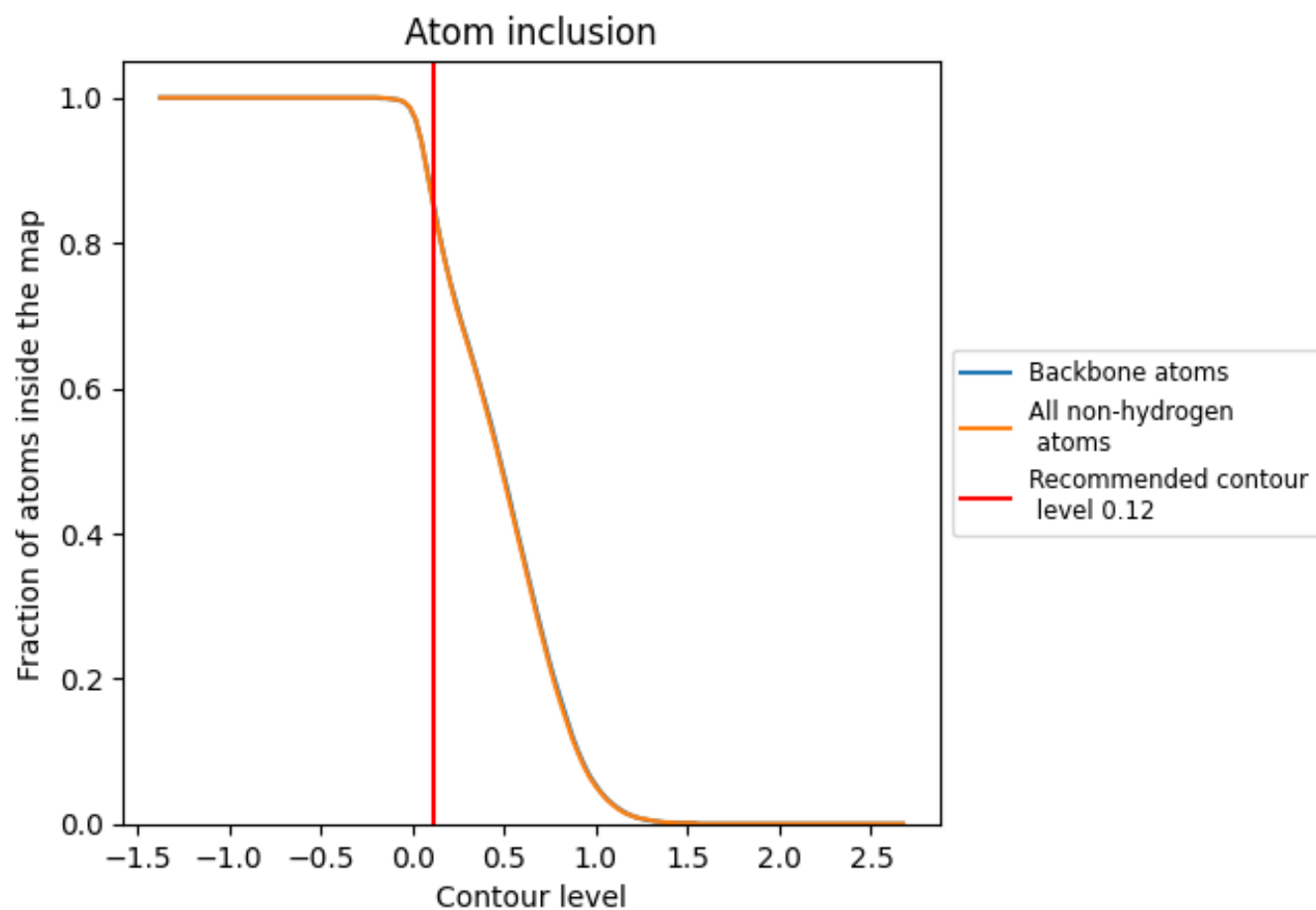
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.5980
1	 0.9530	 0.6590
2	 0.9330	 0.6510
3	 0.9090	 0.6350
4	 0.9070	 0.6290
5	 0.7220	 0.5290
6	 0.8960	 0.6190
8	 0.4190	 0.4030
9	 0.7950	 0.5650
A	 0.9250	 0.6390
B	 0.8610	 0.5790
C	 0.9320	 0.6630
D	 0.9490	 0.6510
E	 0.9010	 0.6200
F	 0.8740	 0.6030
G	 0.9510	 0.6670
H	 0.8200	 0.5640
I	 0.9530	 0.6640
J	 0.6490	 0.5030
K	 0.9210	 0.6430
L	 0.9330	 0.6540
M	 0.9440	 0.6440
O	 0.6260	 0.4410
P	 0.9150	 0.6320
Q	 0.4070	 0.3900
R	 0.5590	 0.4520
S	 0.7450	 0.5330
U	 0.9000	 0.6100
W	 0.8880	 0.6250
X	 0.8980	 0.6280
Y	 0.9130	 0.6460
Z	 0.8500	 0.5860
a	 0.6750	 0.5040
b	 0.8230	 0.5810
c	 0.4270	 0.3900



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Chain	Atom inclusion	Q-score
d	 0.7790	 0.5440
e	 0.4670	 0.4090
f	 0.8200	 0.5560
g	 0.9030	 0.6210
h	 0.9080	 0.6290
i	 0.6180	 0.4950
j	 0.7800	 0.5600
n	 0.6830	 0.5300
o	 0.5770	 0.4630