



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 11:42 pm GMT

PDB ID : 7ZM7
EMDB ID : EMD-14791
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (inhibited by DDM)
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.77 Å (reported)
Based on initial models : 6RFR, 6RFQ

This is a Full wwPDB EM Validation 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:

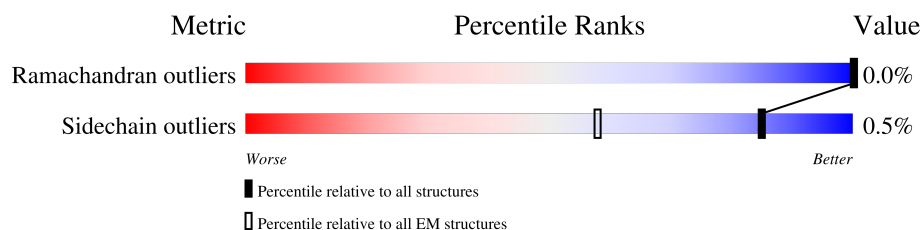
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 2.77 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.





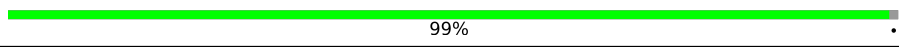
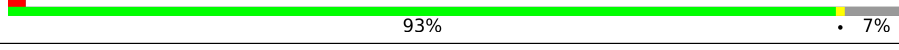
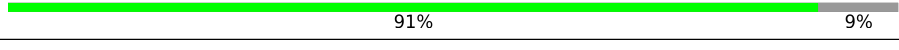

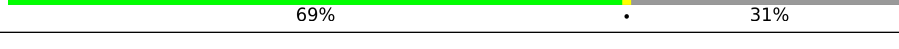
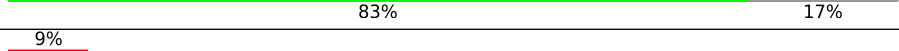
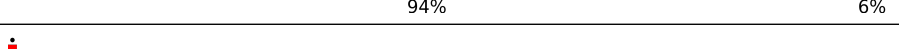
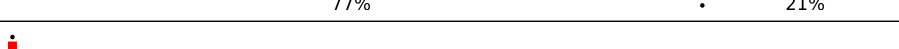
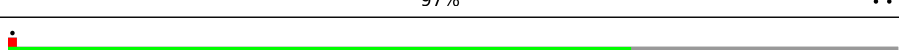

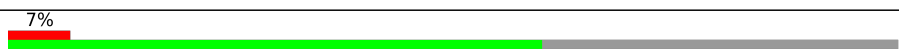
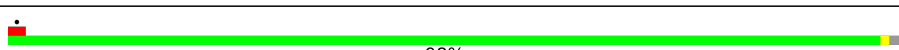
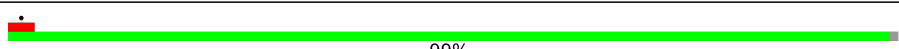


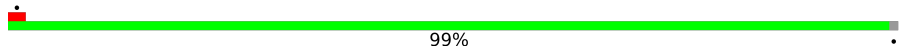
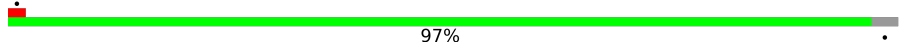

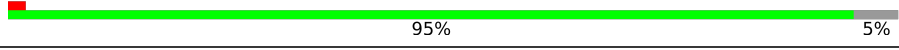
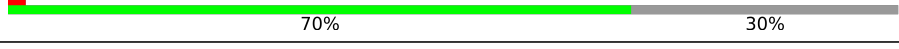



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	 11% 99%
2	2	571	 96%
3	3	146	 79% 21%
4	4	542	 90% 9%
5	5	679	 98%
6	6	224	 84% 16%
7	8	86	 10% 90% 10%
8	9	785	 13% 87%
9	A	749	 95% 5%

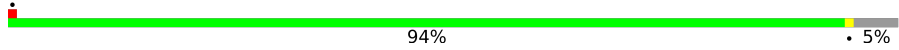

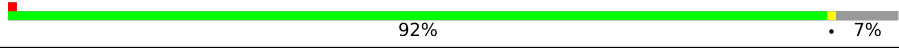
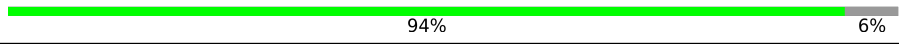
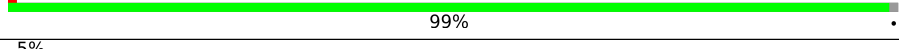

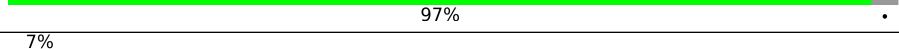
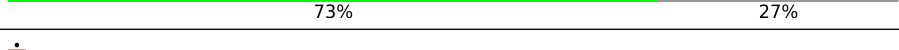
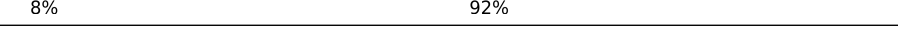
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	d	105	 94% 5%
35	e	46	 83% 17% 9%
36	f	95	 92% 7%
37	g	82	 94% 6%
38	h	134	 99%
39	i	93	 87% 13% 5%
40	j	75	 97%
41	n	184	 73% 27% 7%
42	o	380	 8% 92%

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 69157 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	378	Total	C	N	O	S	0	0
			2852	1916	430	496	10		

- 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	116	Total	C	N	O	S	0	0
			897	608	134	153	2		

- 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
			5276	3552	793	906	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

Continued on next page...

Continued from previous page...

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	189	Total	C	N	O	S	0	0
			1460	985	219	250	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
			654	405	125	118	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	102	Total	C	N	O	S	0	0
			802	497	146	153	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	427	Total	C	N	O	S	0	0
			3376	2152	585	620	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	353	Total	C	N	O	S	0	0
			2866	1816	510	530	10		

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	237	Total	C	N	O	S	0	0
			1877	1185	328	363	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	220	Total	C	N	O	S	0	0
			1695	1069	288	324	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	188	Total	C	N	O	S	0	0
			1408	892	263	251	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
			1439	916	253	255	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	87	Total	C	N	O	S	0	0
			673	453	102	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	118	Total	C	N	O	S	0	0
			937	585	178	169	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

Continued on next page...

Continued from previous page...

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	80	Total	C	N	O	S	0	0
			617	389	100	127	1		
22	Q	85	Total	C	N	O	S	0	0
			670	421	109	139	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	122	Total	C	N	O	S	0	0
			1035	658	197	177	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	72	Total	C	N	O	0	0
			598	393	96	109		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	167	Total	C	N	O	S	0	0
			1353	852	252	240	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	186	Total	C	N	O	S	0	0
			1467	934	266	259	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	80	Total	C	N	O	S	0	0
			675	440	124	109	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	64	Total	C	N	O	S	0	0
			510	332	90	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	100	Total	C	N	O	S	0	0
			827	526	146	151	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	38	Total	C	N	O	S	0	0
			320	217	58	44	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	77	Total	C	N	O	S	0	0
			604	395	104	104	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
			1124	726	197	200	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	81	Total	C	N	O	S	0	0
			686	453	119	112	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
			1068	683	189	195	1		

There are 52 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

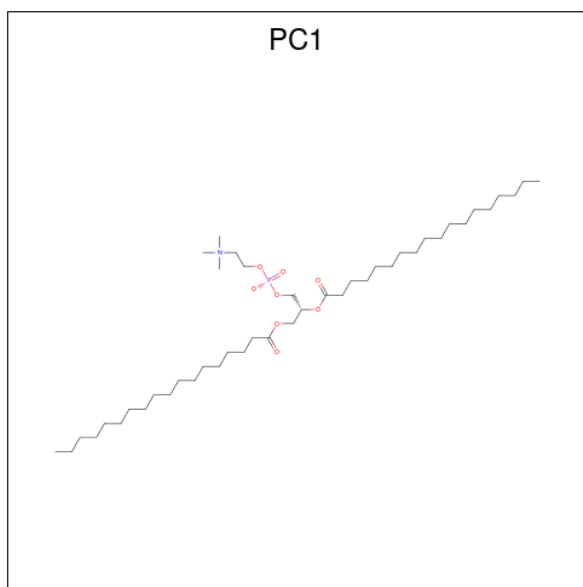
Continued from previous page...

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-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



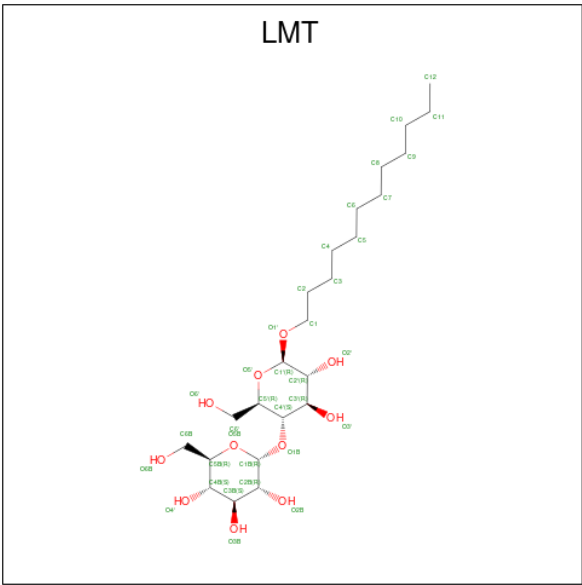
Mol	Chain	Residues	Atoms					AltConf
43	1	1	Total	C	N	O	P	0
			33	23	1	8	1	
43	2	1	Total	C	N	O	P	0
			45	35	1	8	1	
43	5	1	Total	C	N	O	P	0
			40	30	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
43	5	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 44 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



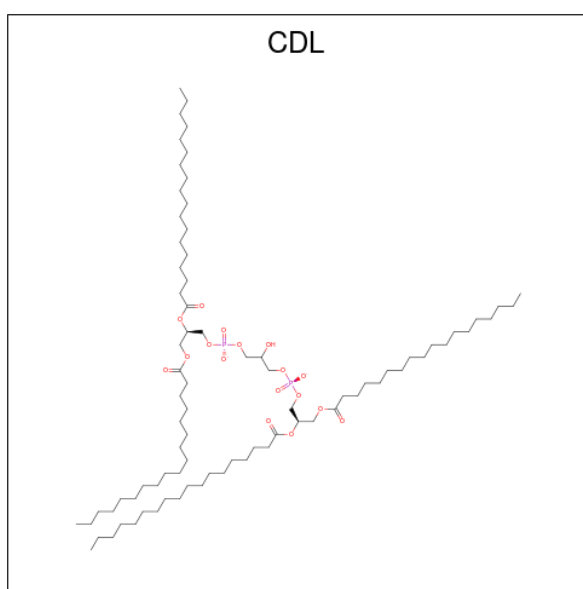
Mol	Chain	Residues	Atoms			AltConf
44	1	1	Total	C	O	0
			35	24	11	
44	1	1	Total	C	O	0
			35	24	11	
44	2	1	Total	C	O	0
			35	24	11	
44	2	1	Total	C	O	0
			33	22	11	
44	2	1	Total	C	O	0
			35	24	11	
44	3	1	Total	C	O	0
			35	24	11	
44	3	1	Total	C	O	0
			35	24	11	
44	4	1	Total	C	O	0
			35	24	11	
44	5	1	Total	C	O	0
			35	24	11	
44	J	1	Total	C	O	0
			31	20	11	

Continued on next page...

Continued from previous page...

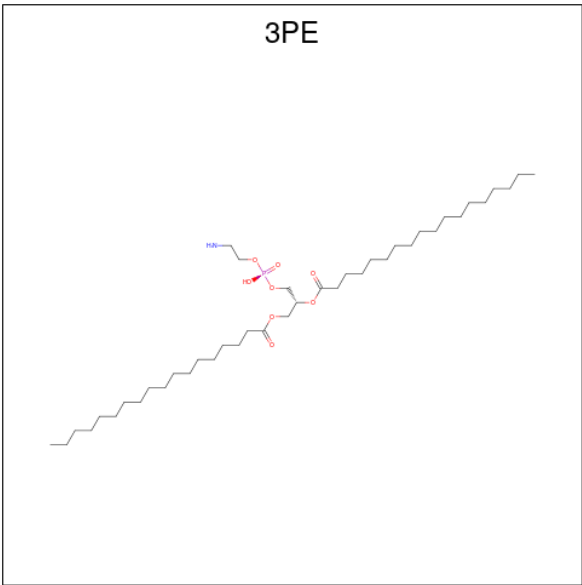
Mol	Chain	Residues	Atoms			AltConf
44	X	1	Total	C	O	0
			35	24	11	
44	a	1	Total	C	O	0
			35	24	11	
44	g	1	Total	C	O	0
			34	23	11	
44	j	1	Total	C	O	0
			35	24	11	

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



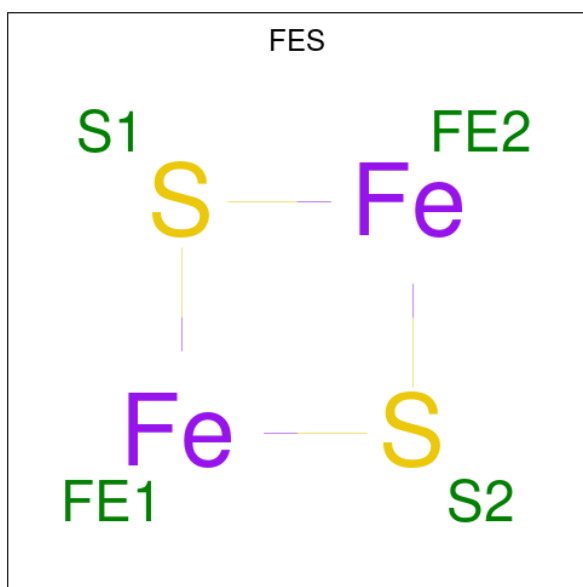
Mol	Chain	Residues	Atoms				AltConf
45	2	1	Total	C	O	P	0
			68	49	17	2	
45	D	1	Total	C	O	P	0
			59	40	17	2	
45	S	1	Total	C	O	P	0
			61	42	17	2	
45	X	1	Total	C	O	P	0
			52	33	17	2	
45	X	1	Total	C	O	P	0
			76	57	17	2	

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



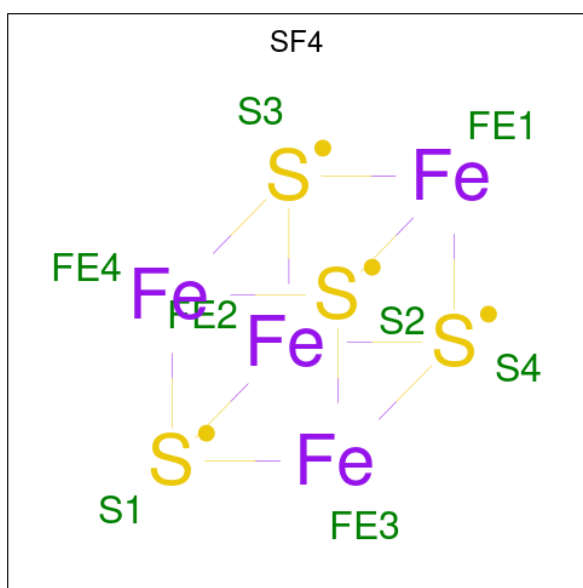
Mol	Chain	Residues	Atoms					AltConf
46	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	E	1	Total	C	N	O	P	0
			29	19	1	8	1	
46	I	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	W	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	W	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	i	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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).



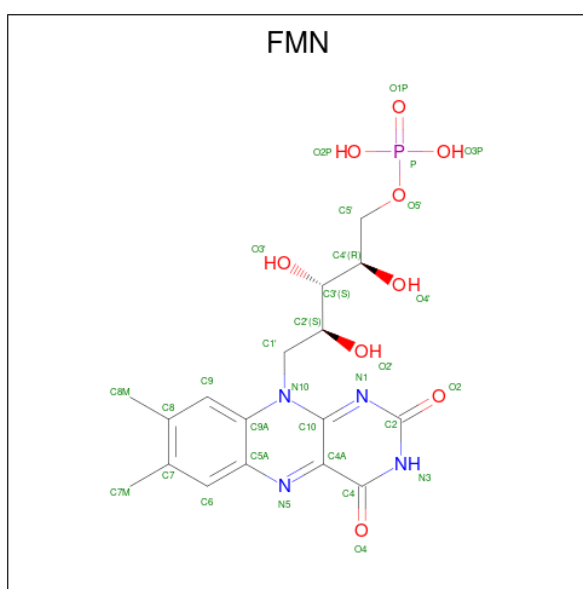
Mol	Chain	Residues	Atoms			AltConf
48	A	1	Total	Fe	S	0
			8	4	4	
48	A	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

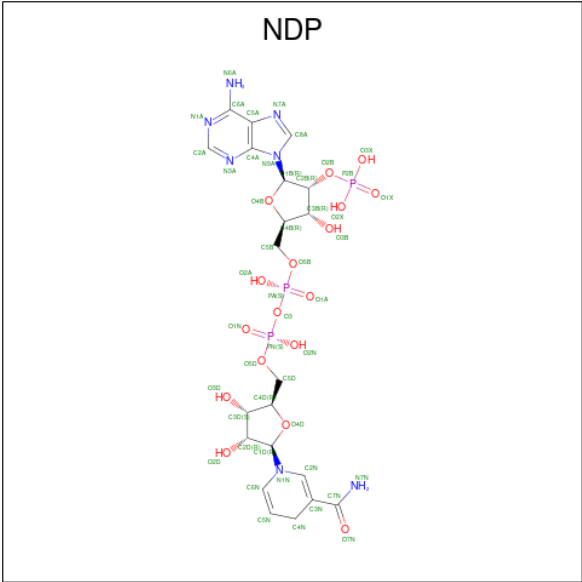
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	K	1	Total	Fe	S	0
			8	4	4	

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



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: $C_{21}H_{30}N_7O_{17}P_3$).

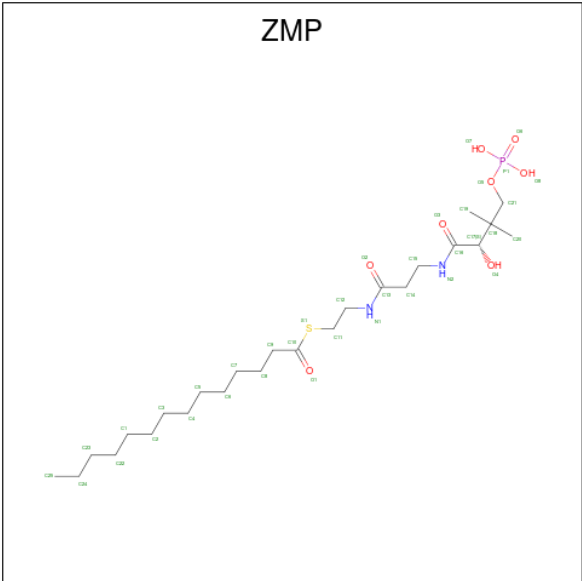


Mol	Chain	Residues	Atoms					AltConf
50	E	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).



Mol	Chain	Residues	Atoms						AltConf
52	O	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
52	Q	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	1	45	Total	O	0
			45	45	
53	2	115	Total	O	0
			115	115	
53	3	9	Total	O	0
			9	9	
53	4	79	Total	O	0
			79	79	
53	5	34	Total	O	0
			34	34	
53	6	21	Total	O	0
			21	21	
53	9	24	Total	O	0
			24	24	
53	A	123	Total	O	0
			123	123	
53	B	25	Total	O	0
			25	25	
53	C	114	Total	O	0
			114	114	
53	D	24	Total	O	0
			24	24	
53	E	31	Total	O	0
			31	31	
53	F	37	Total	O	0
			37	37	
53	G	76	Total	O	0
			76	76	
53	H	11	Total	O	0
			11	11	
53	I	68	Total	O	0
			68	68	
53	J	2	Total	O	0
			2	2	
53	K	38	Total	O	0
			38	38	

Continued on next page...

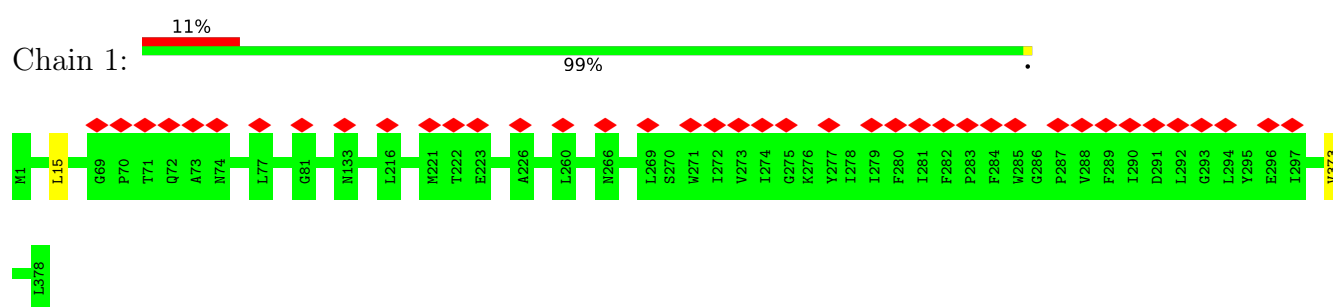
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
53	L	5	Total 5	O 5	0
53	M	26	Total 26	O 26	0
53	P	20	Total 20	O 20	0
53	R	2	Total 2	O 2	0
53	U	23	Total 23	O 23	0
53	W	41	Total 41	O 41	0
53	X	41	Total 41	O 41	0
53	Y	60	Total 60	O 60	0
53	Z	35	Total 35	O 35	0
53	a	5	Total 5	O 5	0
53	b	6	Total 6	O 6	0
53	d	14	Total 14	O 14	0
53	f	2	Total 2	O 2	0
53	g	2	Total 2	O 2	0
53	h	26	Total 26	O 26	0
53	i	1	Total 1	O 1	0
53	j	7	Total 7	O 7	0
53	n	27	Total 27	O 27	0

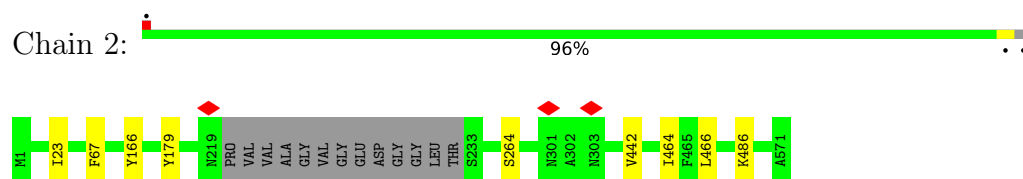
3 Residue-property plots [i](#)

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.

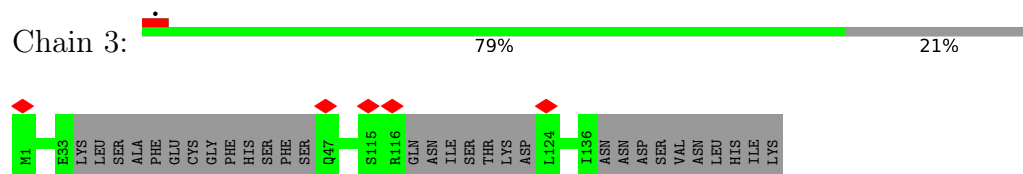
- Molecule 1: NADH-ubiquinone oxidoreductase chain 1



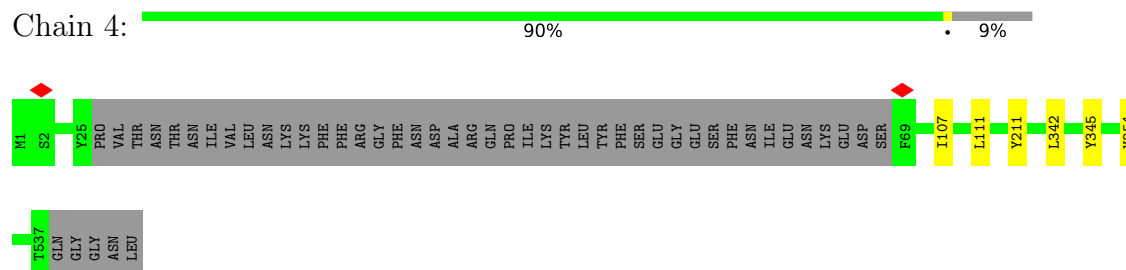
- Molecule 2: NADH dehydrogenase subunit 2



- Molecule 3: NADH-ubiquinone oxidoreductase chain 3



- Molecule 4: NADH-ubiquinone oxidoreductase chain 4

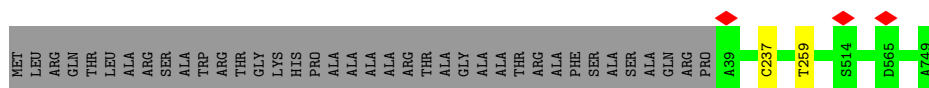


- Molecule 5: NADH-ubiquinone oxidoreductase chain 5



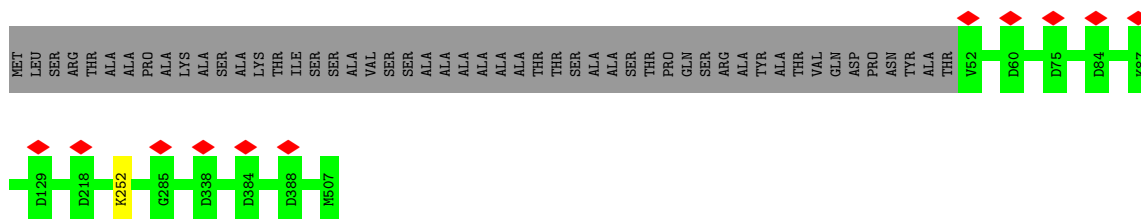
- Molecule 9: NADH-ubiquinone oxidoreductase-like protein

Chain A: 95% 5%



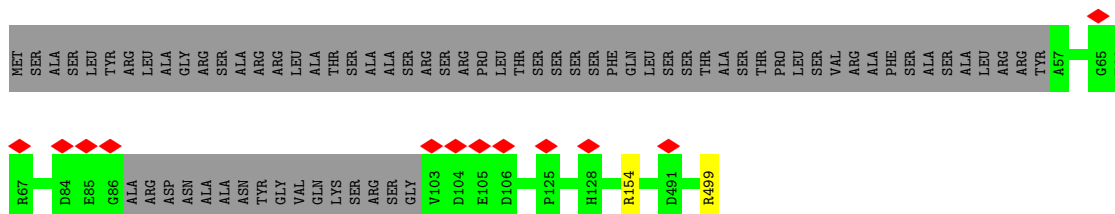
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B: 90% 10%



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

Chain C: 85% 14%



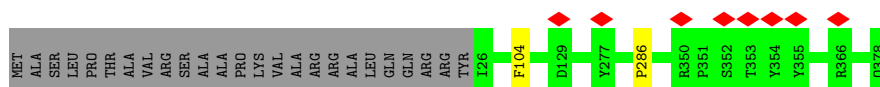
- Molecule 12: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

Chain D: 99%



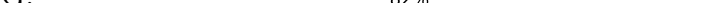
- Molecule 13: NADH dehydrogenase (Ubiquinone)-like protein

Chain E: 93% 7%



- Molecule 14: NADH-ubiquinone oxidoreductase-like protein

MET	ARG	ALA	THR	THR	ARG	LEU	LEU	ALA	VAL	VAL	ARG	PRO	ALA	THR	THR	GLN	ALA	ALA	ALA	SER	SER	ALA	SER	K24	K260	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----


- Chain G:  82% 17%

NET	ALA	SER	LYS	LEU	CYS	LYS	THR	ARG	ALA	ALA	LEU	SER	ALA	LEU	ARG	PRO	THR	ILE	SER	ARG	SER	SER	ARG	THR	GLU	ALA	ILE	ALA	ASN	VAL	VAL	VAL	VAL	ARG	SER	SER	PHE	ALA	ALA	THR	THR	THR	PRO	PRO	ARG	LEU	GLY	V45	560	T229	E266	GLU	GLN	SER	GLN	GLY	GLU	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----

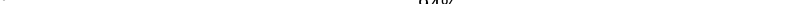
- Chain H:  69% 31%

[illegible]

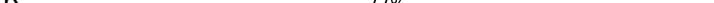
SER	LYS	LEU	THR	PRO	LEU	LEU	MET	ARG	THR	VAL	ALA	ARG	MET	GLY	SER	ARG	ALA	ALA	MET	TRP	ALA	MET	VAL	PRO	ALA	ALA	PRO	ALA	ARG	THR	SER	LEU	SER	THR	THR	ALA	MET	ARG	HIS	SER	SER	D99	H194	M250	F296	D317	I219
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------

- Chain I:  83% 17%

MET	LEU	PRO	THR	PRO	ALA	ALA	LEU	LEU	VAL	THR	ARG	ARG	GLN	LEU	PRO	LEU	ALA	ALA	ARG	VAL	PRO	SER	THR	LEU	VAL	ARG	THR	LEU	PRO	ILE	GLN	ALA	LEU	ILE	ALA	ARG	ARG	THR	TYR	A39	C173	B223
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------

- Chain J:  9% 94% 6%

[illegible]

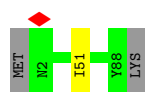
- Chain K:  77% 21%

MET	ILE	SER	SER	SER	ARG	THR	GLY	ALA	SER	SER	LEU	LEU	LEU	ARG	ALA	ARG	PRO	PRO	THR	THR	GLN	LEU	ILE	LEU	PRO	PRO	LEU	ARG	ALA	ALA	ALA	ALA	ALA	ALA	HIS	HIS	LEU	SER	SER	SER	SER	SER	SER	THR	THR	THR	ALA	V49	E50	G54	R58	F101	G102	C105
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------

Y176 K230

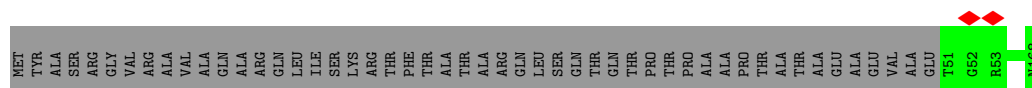
- 

Chain L:  97%



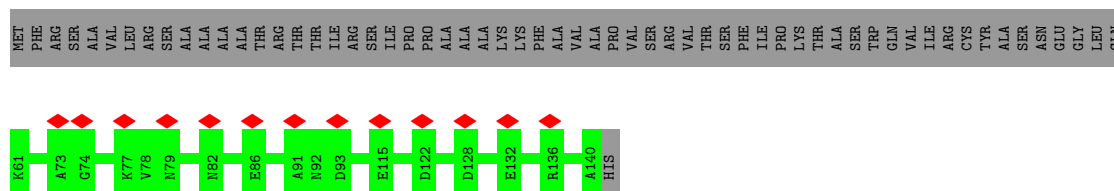
- Molecule 21: NADH-ubiquinone oxidoreductase-like protein

Chain M:  70%



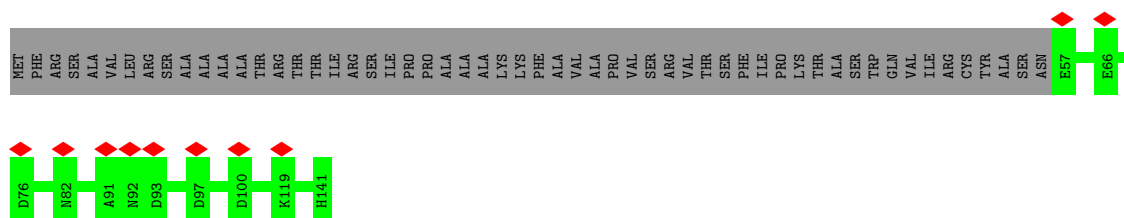
- Molecule 22: Acyl carrier protein

Chain O:  9%



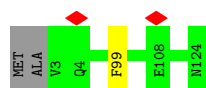
- Molecule 22: Acyl carrier protein

Chain Q:  7%



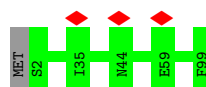
- Molecule 23: NADH-ubiquinone oxidoreductase B14 subunit-like protein

Chain P:  98%

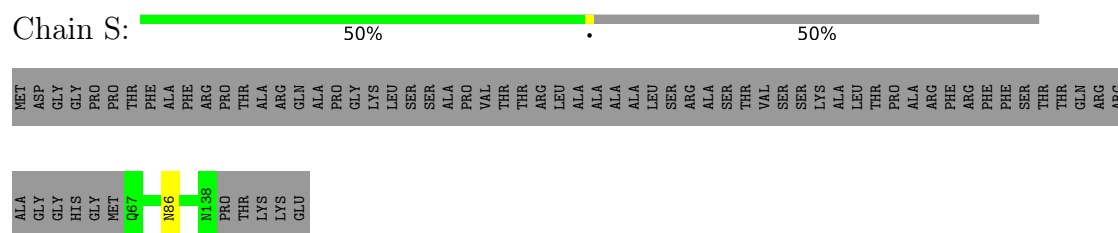


- Molecule 24: Complex I-B22

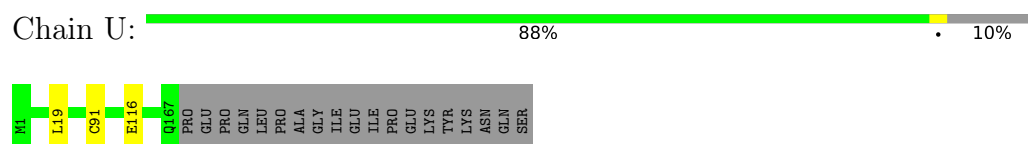
Chain R:  99%



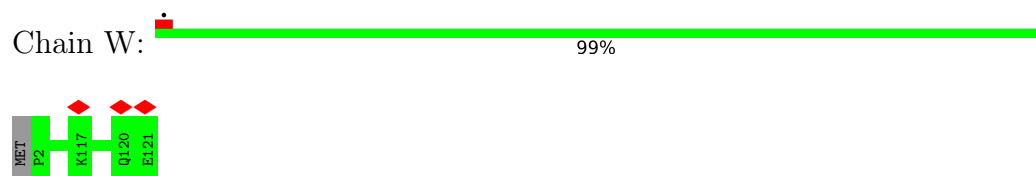
- Molecule 25: Complex I-ESSS



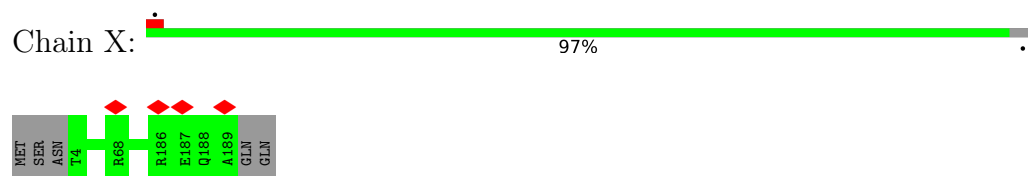
- Molecule 26: NADH-ubiquinone oxidoreductase



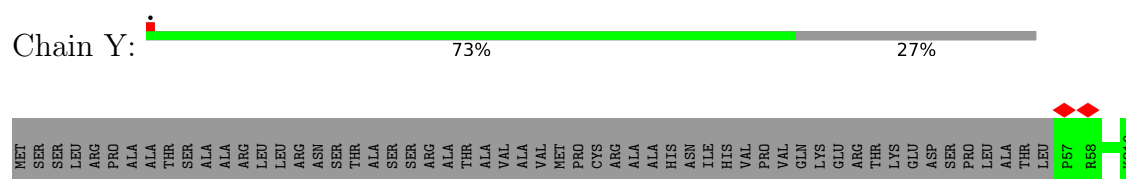
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



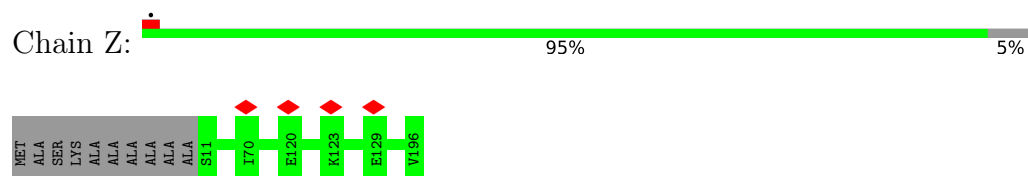
- Molecule 28: NADH-ubiquinone oxidoreductase-like protein



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

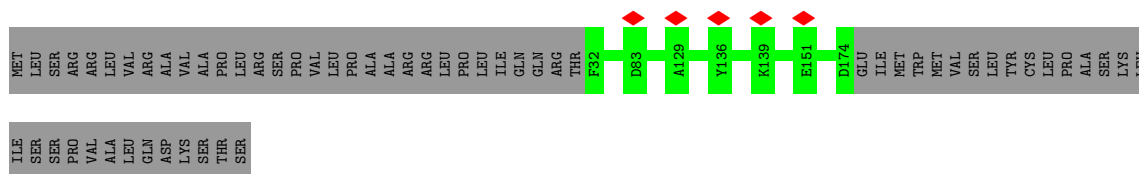


- Molecule 30: NADH-ubiquinone oxidoreductase-like protein



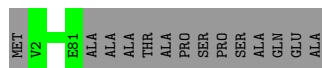
- Molecule 31: NADH dehydrogenase (Ubiquinone)-like protein





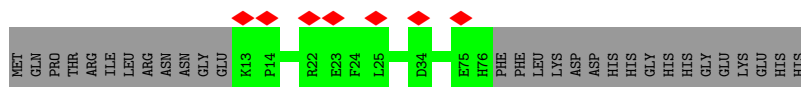
- Molecule 32: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)

Chain b: 85% 15%



- Molecule 33: Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I)

Chain c: 8% 69% 31%



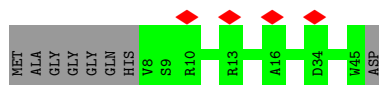
- Molecule 34: Subunit NDUF10 of NADH-ubiquinone oxidoreductase (Complex I)

Chain d: 94% 5%



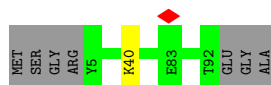
- Molecule 35: Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I)

Chain e: 9% 83% 17%



- Molecule 36: NADH dehydrogenase-like protein

Chain f: 92% 7%



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

Chain g: 94% 6%



-

- [illegible]

- MET
ALA
G3
R75

-

- MET ARG ARG THR ILE LEU GLN ALA ARG PRO SER ARG VAL LEU SER ARG ALA HIS GLY SER ALA R26 P27 R33 E37 N55 P56 V57 PRO LYS PRO GLN PRO ILE GLU PRO PRO PRO ALA VAL GLU GLU THR PRO ALA GLU

GLU	PRO	VAL	PRO	GLU	VAL	PRO	THR	THR	PRO	ALA	ALA	PRO	VAL	GLU	GLU	LYS	SER	ALA	ALA	PRO	PRO	VAL	GLU	GLU	ALA	ALA	PRO	PRO	VAL	GLU	GLU	LYS	ALA	ALA	VAL	PRO	PRO	GLU	GLU	ALA	ALA	PRO	PRO	GLU	GLU	ASP	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	PRO	GLU	GLU	LYS	LYS	SER	SER	ARG	ARG	LYS	ARG	GLN	GLN	GLN	GLU	GLU	GLU	SER	SER	SER	ALA	ALA	LYS	PRO	PRO	ILE	ARG	SER	SER	GLY	ARG	LEU	ASP	GLY	ALA	ALA	ALA	PRO	SER	PRO	PRO	GLU	GLN	GLN	PRO	PRO	LYS	GLU	SER	SER	ILE	THR	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LEU	SER	GLY	LEU	SER	GLY	PRO	THR	SER	SER	SER	SER	TYR	GLN	SER	ARG	GLU	SER	ILE	ARG	SER	SER	ARG	ARG	ARG	LEU	ILE	ALA	GLY	VAL	LEU	VAL	PRO	PRO	GLN	PRO	THR	GLU	ASP	ASN	CYS	CYS	MET	SER	GLY	CYS	VAL	ASN	CYS	VAL	TRP	ASP	ALA	TYR	ARG	GLU	GLU	LEU	MET	NIH
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	TRP	ALA	ALA	ALA	LYS	ALA	ALA	GLU	GLU	ARG	ARG	LEU	ALA	ALA	GLN	GLU	VAL	SER	SER	VAL	VAL	VAL	THR	THR	GLY	GLY	HIS	ALA	VAL	GLU	ASP	GLY	LYS	ARG	VAL	GLU	ARG	THR	LEU	GLY	VAL	HIS	GLY	GLU	VAL	ALA	ASP	ARG	THR	GLY	ASP	MET	ALA	ALA	ARG	GLU	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LYS
GLY
SER
THR
SER
MET
GLU
GLU
ASP
GLY
ALA
GLY
PHE
GLY
GLU
ARG
MET
GLU
TRP
ASP
GLU
GLY
LEU
TYR
LYS
ASP
VAL
PRO
VAL
GLY
TLE
ARG
GLU
PHE
MET
LYS
GLN
GLU
LYS
ARG
LEU
ARG
GLU
GLU
ARG
LEU
LYS
ARG
ASN
ARG
LYS
GLU
THR
GLU
HIS
GLN
GLN
GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37767	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)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.497	Depositor
Minimum map value	-1.728	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	154.48529, 228.63824, 305.8809	wwPDB
Map dimensions	297, 222, 150	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.029902, 1.029902, 1.029902	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CDL, 3PE, NDP, PC1, ZN, LMT, FMN, 2MR, ZMP, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.55	0/2921	0.65	0/3996
2	2	0.57	0/4562	0.69	2/6205 (0.0%)
3	3	0.54	0/918	0.58	0/1249
4	4	0.57	0/4002	0.63	1/5454 (0.0%)
5	5	0.52	0/5418	0.61	0/7376
6	6	0.53	0/1487	0.59	0/2026
7	8	0.39	0/667	0.47	0/892
8	9	0.51	0/819	0.67	0/1105
9	A	0.52	0/5589	0.61	0/7579
10	B	0.47	0/3621	0.57	0/4878
11	C	0.58	0/3447	0.62	0/4675
12	D	0.52	0/674	0.71	0/911
13	E	0.50	0/2932	0.59	0/3973
14	F	0.46	0/1916	0.56	0/2596
15	G	0.60	0/2026	0.61	0/2759
16	H	0.46	0/1734	0.56	0/2358
17	I	0.63	0/1527	0.67	0/2070
18	J	0.38	0/1435	0.55	0/1940
19	K	0.55	0/1478	0.66	0/2009
20	L	0.58	0/680	0.72	0/921
21	M	0.54	0/968	0.60	0/1319
22	O	0.31	0/626	0.45	0/852
22	Q	0.32	0/680	0.43	0/922
23	P	0.54	0/1062	0.60	0/1432
24	R	0.41	0/832	0.54	0/1133
25	S	0.56	0/622	0.65	0/850
26	U	0.56	0/1390	0.75	0/1885
27	W	0.55	0/1001	0.74	0/1354
28	X	0.54	0/1506	0.71	0/2036
29	Y	0.57	0/1277	0.63	0/1731
30	Z	0.54	0/1466	0.58	0/1997
31	a	0.47	0/1204	0.53	0/1632

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.47	0/693	0.66	0/929
33	c	0.36	0/529	0.48	0/720
34	d	0.53	0/845	0.61	0/1137
35	e	0.45	0/335	0.53	0/454
36	f	0.46	0/731	0.59	0/981
37	g	0.54	0/624	0.62	0/857
38	h	0.56	0/1164	0.60	0/1584
39	i	0.51	0/715	0.54	0/971
40	j	0.58	0/617	0.58	0/830
41	n	0.48	0/1100	0.65	0/1491
42	o	0.41	0/262	0.45	0/360
All	All	0.52	0/68102	0.62	3/92429 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	67	PHE	CB-CA-C	5.89	122.18	110.40
2	2	166	TYR	CB-CA-C	5.44	121.28	110.40
4	4	111	LEU	CA-CB-CG	5.11	127.04	115.30

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	376/378 (100%)	357 (95%)	19 (5%)	0	100	100
2	2	554/571 (97%)	541 (98%)	13 (2%)	0	100	100
3	3	110/146 (75%)	107 (97%)	3 (3%)	0	100	100
4	4	490/542 (90%)	472 (96%)	18 (4%)	0	100	100
5	5	668/679 (98%)	632 (95%)	36 (5%)	0	100	100
6	6	185/224 (83%)	175 (95%)	10 (5%)	0	100	100
7	8	75/86 (87%)	72 (96%)	3 (4%)	0	100	100
8	9	100/785 (13%)	98 (98%)	2 (2%)	0	100	100
9	A	709/749 (95%)	680 (96%)	29 (4%)	0	100	100
10	B	454/507 (90%)	434 (96%)	20 (4%)	0	100	100
11	C	422/499 (85%)	404 (96%)	18 (4%)	0	100	100
12	D	79/86 (92%)	76 (96%)	3 (4%)	0	100	100
13	E	351/378 (93%)	337 (96%)	13 (4%)	1 (0%)	37	64
14	F	235/261 (90%)	232 (99%)	3 (1%)	0	100	100
15	G	240/293 (82%)	233 (97%)	7 (3%)	0	100	100
16	H	218/318 (69%)	205 (94%)	13 (6%)	0	100	100
17	I	183/223 (82%)	179 (98%)	4 (2%)	0	100	100
18	J	186/199 (94%)	182 (98%)	4 (2%)	0	100	100
19	K	180/230 (78%)	172 (96%)	7 (4%)	1 (1%)	22	48
20	L	85/89 (96%)	85 (100%)	0	0	100	100
21	M	116/168 (69%)	114 (98%)	2 (2%)	0	100	100
22	O	78/141 (55%)	76 (97%)	2 (3%)	0	100	100
22	Q	83/141 (59%)	81 (98%)	2 (2%)	0	100	100
23	P	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
24	R	96/99 (97%)	91 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	S	70/143 (49%)	66 (94%)	4 (6%)	0	100	100
26	U	165/186 (89%)	161 (98%)	4 (2%)	0	100	100
27	W	118/121 (98%)	117 (99%)	1 (1%)	0	100	100
28	X	184/191 (96%)	179 (97%)	5 (3%)	0	100	100
29	Y	152/210 (72%)	144 (95%)	8 (5%)	0	100	100
30	Z	184/196 (94%)	174 (95%)	10 (5%)	0	100	100
31	a	141/203 (70%)	133 (94%)	8 (6%)	0	100	100
32	b	78/94 (83%)	77 (99%)	1 (1%)	0	100	100
33	c	62/93 (67%)	59 (95%)	3 (5%)	0	100	100
34	d	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
35	e	36/46 (78%)	34 (94%)	2 (6%)	0	100	100
36	f	86/95 (90%)	83 (96%)	3 (4%)	0	100	100
37	g	75/82 (92%)	71 (95%)	4 (5%)	0	100	100
38	h	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
39	i	79/93 (85%)	75 (95%)	4 (5%)	0	100	100
40	j	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
41	n	133/184 (72%)	127 (96%)	6 (4%)	0	100	100
42	o	30/380 (8%)	29 (97%)	1 (3%)	0	100	100
All	All	8286/10547 (79%)	7971 (96%)	313 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	E	286	PRO
19	K	102	GLY

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	298/326 (91%)	296 (99%)	2 (1%)	81	93
2	2	509/518 (98%)	502 (99%)	7 (1%)	62	85
3	3	95/128 (74%)	95 (100%)	0	100	100
4	4	431/477 (90%)	426 (99%)	5 (1%)	67	87
5	5	581/596 (98%)	578 (100%)	3 (0%)	86	95
6	6	167/203 (82%)	167 (100%)	0	100	100
7	8	68/75 (91%)	68 (100%)	0	100	100
8	9	84/687 (12%)	84 (100%)	0	100	100
9	A	577/602 (96%)	575 (100%)	2 (0%)	91	97
10	B	366/401 (91%)	366 (100%)	0	100	100
11	C	354/416 (85%)	353 (100%)	1 (0%)	91	97
12	D	68/69 (99%)	68 (100%)	0	100	100
13	E	311/335 (93%)	310 (100%)	1 (0%)	91	97
14	F	198/219 (90%)	198 (100%)	0	100	100
15	G	215/257 (84%)	214 (100%)	1 (0%)	86	95
16	H	190/272 (70%)	188 (99%)	2 (1%)	70	88
17	I	158/191 (83%)	157 (99%)	1 (1%)	84	94
18	J	131/146 (90%)	131 (100%)	0	100	100
19	K	154/191 (81%)	151 (98%)	3 (2%)	52	79
20	L	74/76 (97%)	73 (99%)	1 (1%)	62	85
21	M	98/135 (73%)	98 (100%)	0	100	100
22	O	67/119 (56%)	67 (100%)	0	100	100
22	Q	74/119 (62%)	74 (100%)	0	100	100
23	P	109/110 (99%)	108 (99%)	1 (1%)	75	91
24	R	87/89 (98%)	87 (100%)	0	100	100
25	S	58/111 (52%)	57 (98%)	1 (2%)	56	81
26	U	148/167 (89%)	145 (98%)	3 (2%)	50	78
27	W	100/102 (98%)	100 (100%)	0	100	100
28	X	143/152 (94%)	143 (100%)	0	100	100
29	Y	131/176 (74%)	131 (100%)	0	100	100
30	Z	152/155 (98%)	152 (100%)	0	100	100
31	a	123/177 (70%)	123 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	b	66/74 (89%)	66 (100%)	0	100	100
33	c	47/80 (59%)	47 (100%)	0	100	100
34	d	87/94 (93%)	86 (99%)	1 (1%)	70	88
35	e	30/35 (86%)	30 (100%)	0	100	100
36	f	76/80 (95%)	75 (99%)	1 (1%)	65	86
37	g	65/69 (94%)	65 (100%)	0	100	100
38	h	118/119 (99%)	118 (100%)	0	100	100
39	i	69/78 (88%)	69 (100%)	0	100	100
40	j	63/64 (98%)	63 (100%)	0	100	100
41	n	108/150 (72%)	108 (100%)	0	100	100
42	o	26/318 (8%)	26 (100%)	0	100	100
All	All	7074/8958 (79%)	7038 (100%)	36 (0%)	85	95

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	15	LEU
1	1	373	VAL
2	2	23	ILE
2	2	179	TYR
2	2	264	SER
2	2	442	VAL
2	2	464	ILE
2	2	466	LEU
2	2	486	LYS
4	4	107	ILE
4	4	211	TYR
4	4	342	LEU
4	4	345	TYR
4	4	354	TYR
5	5	372	VAL
5	5	378	LEU
5	5	503	ASN
9	A	237	CYS
9	A	259	THR
11	C	499	ARG
13	E	104	PHE
15	G	229	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	H	194	HIS
16	H	250	MET
17	I	173	CYS
19	K	101	PHE
19	K	105	CYS
19	K	176	TYR
20	L	51	ILE
23	P	99	PHE
25	S	86	ASN
26	U	19	LEU
26	U	91	CYS
26	U	116	GLU
34	d	31	LEU
36	f	40	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	54	GLN
1	1	147	GLN
2	2	68	HIS
2	2	80	GLN
2	2	155	GLN
2	2	364	GLN
3	3	47	GLN
3	3	83	ASN
4	4	86	ASN
4	4	519	HIS
5	5	131	ASN
5	5	161	ASN
9	A	142	GLN
9	A	289	ASN
9	A	680	GLN
11	C	123	GLN
11	C	218	ASN
11	C	270	GLN
11	C	410	ASN
11	C	473	HIS
12	D	48	GLN
13	E	42	GLN
13	E	134	ASN
13	E	162	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	E	167	ASN
13	E	298	ASN
14	F	54	HIS
15	G	266	GLN
16	H	104	HIS
16	H	122	ASN
16	H	128	GLN
16	H	186	ASN
16	H	194	HIS
19	K	120	GLN
21	M	105	GLN
23	P	63	HIS
23	P	114	ASN
25	S	86	ASN
26	U	107	GLN
27	W	19	ASN
28	X	65	GLN
29	Y	103	GLN
29	Y	181	GLN
29	Y	184	ASN
29	Y	195	ASN
31	a	88	GLN
31	a	101	HIS
32	b	29	ASN
41	n	84	HIS
41	n	113	HIS
41	n	153	HIS
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	0.42	0	5,13,15	1.04	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	2MR	C	154	11	-	0/10/13/15	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	154	2MR	NE-CZ-NH2	-2.20	117.46	119.48

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 44 ligands modelled in this entry, 1 is monoatomic - leaving 43 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CDL	X	201	-	51,51,99	0.38	0	57,63,111	0.51	0
43	PC1	1	401	-	32,32,53	0.33	0	38,40,61	0.35	0
44	LMT	4	601	-	36,36,36	1.09	2 (5%)	47,47,47	1.09	3 (6%)
47	FES	A	801	9	0,4,4	-	-	-	-	-
52	ZMP	O	201	22	29,35,36	0.23	0	34,42,45	0.45	0
46	3PE	E	401	-	28,28,50	0.37	0	31,33,55	0.48	0
44	LMT	g	101	-	35,35,36	1.10	2 (5%)	46,46,47	1.06	1 (2%)
44	LMT	2	603	-	34,34,36	0.37	0	45,45,47	0.84	1 (2%)
44	LMT	a	301	-	36,36,36	0.39	0	47,47,47	0.77	1 (2%)
45	CDL	S	201	-	60,60,99	0.33	0	66,72,111	0.43	0
46	3PE	5	704	-	41,41,50	0.30	0	44,46,55	0.37	0
46	3PE	I	303	-	36,36,50	0.34	0	39,41,55	0.55	0
46	3PE	5	701	-	40,40,50	0.29	0	43,45,55	0.32	0
44	LMT	1	403	-	36,36,36	0.35	0	47,47,47	0.61	0
49	FMN	B	602	-	33,33,33	0.66	0	48,50,50	0.72	1 (2%)
44	LMT	3	201	-	36,36,36	0.33	0	47,47,47	0.84	0
44	LMT	2	602	-	36,36,36	0.48	0	47,47,47	0.97	3 (6%)
44	LMT	j	101	-	36,36,36	0.38	0	47,47,47	0.94	3 (6%)
43	PC1	5	702	-	39,39,53	0.35	0	45,47,61	0.51	0
46	3PE	W	202	-	31,31,50	0.36	0	34,36,55	0.39	0
48	SF4	I	301	17	0,12,12	-	-	-	-	-
52	ZMP	Q	201	22	29,35,36	0.18	0	34,42,45	0.41	0
47	FES	H	401	16	0,4,4	-	-	-	-	-
48	SF4	I	302	17	0,12,12	-	-	-	-	-
46	3PE	W	201	-	39,39,50	0.30	0	42,44,55	0.35	0
48	SF4	B	601	10	0,12,12	-	-	-	-	-
48	SF4	A	802	9	0,12,12	-	-	-	-	-
44	LMT	3	202	-	36,36,36	0.40	0	47,47,47	0.93	4 (8%)
44	LMT	1	402	-	36,36,36	0.35	0	47,47,47	0.82	2 (4%)
45	CDL	D	101	-	58,58,99	0.35	0	64,70,111	0.42	0
46	3PE	5	706	-	41,41,50	0.94	4 (9%)	44,46,55	1.10	2 (4%)
48	SF4	A	803	9	0,12,12	-	-	-	-	-
46	3PE	i	101	-	37,37,50	0.32	0	40,42,55	0.36	0
45	CDL	2	601	-	67,67,99	0.33	0	73,79,111	0.42	0
44	LMT	2	604	-	36,36,36	0.41	0	47,47,47	0.70	0
48	SF4	K	301	19	0,12,12	-	-	-	-	-
45	CDL	X	202	-	75,75,99	0.33	0	81,87,111	0.38	0
50	NDP	E	402	-	45,52,52	0.61	0	53,80,80	0.67	1 (1%)
44	LMT	J	201	-	32,32,36	0.39	0	43,43,47	0.70	1 (2%)
44	LMT	5	705	-	36,36,36	0.33	0	47,47,47	1.15	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	PC1	2	605	-	44,44,53	0.28	0	50,52,61	0.52	0
43	PC1	5	703	-	44,44,53	0.30	0	50,52,61	0.33	0
44	LMT	X	203	-	36,36,36	0.38	0	47,47,47	0.70	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
45	CDL	X	201	-	-	25/62/62/110	-
43	PC1	1	401	-	-	10/36/36/57	-
44	LMT	4	601	-	-	8/21/61/61	0/2/2/2
47	FES	A	801	9	-	-	0/1/1/1
52	ZMP	O	201	22	-	10/40/42/43	-
46	3PE	E	401	-	-	8/32/32/54	-
44	LMT	g	101	-	-	10/20/60/61	0/2/2/2
44	LMT	2	603	-	-	7/19/59/61	0/2/2/2
44	LMT	a	301	-	-	6/21/61/61	0/2/2/2
45	CDL	S	201	-	-	20/70/70/110	-
46	3PE	5	704	-	-	17/45/45/54	-
46	3PE	I	303	-	-	15/40/40/54	-
46	3PE	5	701	-	-	8/44/44/54	-
44	LMT	1	403	-	-	3/21/61/61	0/2/2/2
49	FMN	B	602	-	-	3/18/18/18	0/3/3/3
44	LMT	3	201	-	-	3/21/61/61	0/2/2/2
44	LMT	2	602	-	-	7/21/61/61	0/2/2/2
44	LMT	j	101	-	-	5/21/61/61	0/2/2/2
43	PC1	5	702	-	-	18/43/43/57	-
46	3PE	W	202	-	-	7/35/35/54	-
48	SF4	I	301	17	-	-	0/6/5/5
52	ZMP	Q	201	22	-	17/40/42/43	-
47	FES	H	401	16	-	-	0/1/1/1
48	SF4	I	302	17	-	-	0/6/5/5
46	3PE	W	201	-	-	14/43/43/54	-
48	SF4	B	601	10	-	-	0/6/5/5
48	SF4	A	802	9	-	-	0/6/5/5
44	LMT	3	202	-	-	10/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	LMT	1	402	-	-	3/21/61/61	0/2/2/2
45	CDL	D	101	-	-	25/69/69/110	-
46	3PE	5	706	-	-	14/45/45/54	-
48	SF4	A	803	9	-	-	0/6/5/5
46	3PE	i	101	-	-	11/41/41/54	-
45	CDL	2	601	-	-	19/78/78/110	-
44	LMT	2	604	-	-	9/21/61/61	0/2/2/2
48	SF4	K	301	19	-	-	0/6/5/5
45	CDL	X	202	-	-	36/86/86/110	-
50	NDP	E	402	-	-	7/30/77/77	0/5/5/5
44	LMT	J	201	-	-	6/17/57/61	0/2/2/2
44	LMT	5	705	-	-	6/21/61/61	0/2/2/2
43	PC1	2	605	-	-	7/48/48/57	-
43	PC1	5	703	-	-	8/48/48/57	-
44	LMT	X	203	-	-	4/21/61/61	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	4	601	LMT	O5B-C1B	3.28	1.50	1.41
44	g	101	LMT	O5B-C1B	3.18	1.49	1.41
44	g	101	LMT	O5'-C1'	3.13	1.49	1.41
44	4	601	LMT	O5'-C1'	2.79	1.48	1.41
46	5	706	3PE	O21-C2	-2.46	1.40	1.46
46	5	706	3PE	O31-C31	2.35	1.40	1.33
46	5	706	3PE	O31-C3	-2.18	1.40	1.45
46	5	706	3PE	O21-C21	2.12	1.40	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	5	706	3PE	O21-C21-C22	3.86	119.82	111.50
44	4	601	LMT	C1B-O1B-C4'	-3.46	109.40	117.96
44	5	705	LMT	C1-O1'-C1'	-3.39	108.22	113.84
44	5	705	LMT	O1'-C1'-C2'	3.35	113.53	108.30
44	j	101	LMT	C1-O1'-C1'	-2.94	108.97	113.84
44	2	603	LMT	C1-O1'-C1'	-2.76	109.27	113.84
44	2	602	LMT	C1B-O1B-C4'	-2.75	111.17	117.96
44	g	101	LMT	C1B-O1B-C4'	-2.70	111.28	117.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	402	LMT	C4B-C3B-C2B	-2.63	106.24	110.82
44	a	301	LMT	C1B-O1B-C4'	-2.60	111.53	117.96
44	3	202	LMT	O1B-C4'-C3'	2.58	114.13	107.28
44	j	101	LMT	O1'-C1'-C2'	2.50	112.20	108.30
44	2	602	LMT	C3B-C4B-C5B	-2.42	105.92	110.24
46	5	706	3PE	O31-C31-C32	2.33	119.22	111.91
44	5	705	LMT	C1'-O5'-C5'	-2.30	109.17	113.69
44	2	602	LMT	O5B-C5B-C6B	2.29	112.12	106.44
44	4	601	LMT	C1'-C2'-C3'	2.19	114.56	110.00
50	E	402	NDP	C5A-C6A-N6A	2.18	123.67	120.35
44	5	705	LMT	O5'-C1'-C2'	-2.13	105.85	110.35
44	j	101	LMT	C1'-O5'-C5'	-2.11	109.54	113.69
44	3	202	LMT	C1'-C2'-C3'	2.06	114.29	110.00
44	3	202	LMT	O1B-C4'-C5'	-2.04	103.85	109.45
44	4	601	LMT	C2'-C3'-C4'	2.03	114.31	109.68
44	J	201	LMT	C1B-O1B-C4'	-2.02	112.96	117.96
44	3	202	LMT	O3'-C3'-C2'	-2.01	105.70	110.35
49	B	602	FMN	C4-N3-C2	-2.00	121.94	125.64
44	1	402	LMT	C6B-C5B-C4B	-2.00	108.31	113.00

There are no chirality outliers.

All (386) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1	401	PC1	C11-O13-P-O14
43	1	401	PC1	C11-O13-P-O11
43	1	401	PC1	C1-O11-P-O12
43	1	401	PC1	C1-O11-P-O14
43	1	401	PC1	C22-C21-O21-C2
43	2	605	PC1	C22-C21-O21-C2
43	2	605	PC1	O32-C31-O31-C3
43	2	605	PC1	C32-C31-O31-C3
43	5	702	PC1	C11-O13-P-O12
43	5	702	PC1	C11-O13-P-O14
43	5	702	PC1	C1-O11-P-O14
44	1	402	LMT	C2-C1-O1'-C1'
44	2	602	LMT	C2'-C1'-O1'-C1
44	2	602	LMT	O5'-C1'-O1'-C1
44	3	202	LMT	C2'-C1'-O1'-C1
44	4	601	LMT	O5'-C1'-O1'-C1
44	J	201	LMT	O5'-C1'-O1'-C1
44	J	201	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
44	a	301	LMT	C2'-C1'-O1'-C1
44	a	301	LMT	O5'-C1'-O1'-C1
44	g	101	LMT	O5B-C1B-O1B-C4'
44	j	101	LMT	C2-C1-O1'-C1'
45	2	601	CDL	CA2-OA2-PA1-OA5
45	2	601	CDL	CA3-OA5-PA1-OA3
45	2	601	CDL	OB7-CB5-OB6-CB4
45	D	101	CDL	CA3-OA5-PA1-OA2
45	D	101	CDL	CA3-OA5-PA1-OA3
45	D	101	CDL	CA3-OA5-PA1-OA4
45	D	101	CDL	CB2-OB2-PB2-OB4
45	D	101	CDL	CB3-OB5-PB2-OB3
45	S	201	CDL	C1-CA2-OA2-PA1
45	S	201	CDL	CA2-OA2-PA1-OA4
45	S	201	CDL	CB2-OB2-PB2-OB3
45	S	201	CDL	CB2-OB2-PB2-OB4
45	S	201	CDL	CB3-OB5-PB2-OB3
45	S	201	CDL	OB6-CB4-CB6-OB8
45	X	201	CDL	C11-CA5-OA6-CA4
45	X	201	CDL	OB7-CB5-OB6-CB4
45	X	202	CDL	CA2-C1-CB2-OB2
45	X	202	CDL	CB2-OB2-PB2-OB3
46	5	701	3PE	C11-O13-P-O14
46	5	704	3PE	C1-O11-P-O14
46	5	704	3PE	C11-O13-P-O11
46	5	706	3PE	C1-O11-P-O12
46	5	706	3PE	C1-O11-P-O13
46	5	706	3PE	C1-O11-P-O14
46	5	706	3PE	C11-O13-P-O14
46	5	706	3PE	O13-C11-C12-N
46	5	706	3PE	O21-C2-C3-O31
46	I	303	3PE	C11-O13-P-O12
46	I	303	3PE	C11-O13-P-O14
46	W	201	3PE	C2-C1-O11-P
46	i	101	3PE	C11-O13-P-O11
46	i	101	3PE	C11-O13-P-O14
52	O	201	ZMP	O4-C17-C18-C21
52	O	201	ZMP	O4-C17-C18-C19
52	Q	201	ZMP	O3-C16-C17-C18
52	Q	201	ZMP	N2-C16-C17-C18
52	Q	201	ZMP	O3-C16-C17-O4
52	Q	201	ZMP	N2-C16-C17-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	Q	201	ZMP	O1-C10-S1-C11
52	Q	201	ZMP	C9-C10-S1-C11
44	2	603	LMT	O5B-C1B-O1B-C4'
44	5	705	LMT	O5B-C1B-O1B-C4'
46	I	303	3PE	O32-C31-O31-C3
44	J	201	LMT	O5B-C1B-O1B-C4'
44	2	603	LMT	C2B-C1B-O1B-C4'
46	I	303	3PE	C32-C31-O31-C3
43	1	401	PC1	O22-C21-O21-C2
43	2	605	PC1	O22-C21-O21-C2
45	X	201	CDL	OA7-CA5-OA6-CA4
46	5	704	3PE	O22-C21-O21-C2
45	2	601	CDL	C51-CB5-OB6-CB4
45	X	201	CDL	C51-CB5-OB6-CB4
46	5	704	3PE	C22-C21-O21-C2
52	Q	201	ZMP	C14-C13-N1-C12
44	3	202	LMT	C3'-C4'-O1B-C1B
46	I	303	3PE	O22-C21-O21-C2
45	X	201	CDL	O1-C1-CA2-OA2
45	X	202	CDL	O1-C1-CA2-OA2
45	X	202	CDL	O1-C1-CB2-OB2
46	I	303	3PE	C22-C21-O21-C2
44	2	604	LMT	O5'-C5'-C6'-O6'
44	3	202	LMT	O5'-C1'-O1'-C1
52	Q	201	ZMP	O2-C13-N1-C12
45	X	201	CDL	CB2-C1-CA2-OA2
45	X	202	CDL	CB2-C1-CA2-OA2
44	4	601	LMT	C7-C8-C9-C10
45	X	201	CDL	OB5-CB3-CB4-OB6
44	2	602	LMT	C4B-C5B-C6B-O6B
44	J	201	LMT	C2'-C1'-O1'-C1
44	g	101	LMT	C2'-C1'-O1'-C1
44	2	603	LMT	C3-C4-C5-C6
45	S	201	CDL	C11-CA5-OA6-CA4
46	5	704	3PE	C21-C22-C23-C24
44	g	101	LMT	O5'-C5'-C6'-O6'
44	2	603	LMT	O5'-C5'-C6'-O6'
45	D	101	CDL	CB5-C51-C52-C53
45	X	202	CDL	CB7-C71-C72-C73
44	2	603	LMT	C4'-C5'-C6'-O6'
44	1	402	LMT	O5'-C1'-O1'-C1
46	I	303	3PE	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	S	201	CDL	OA7-CA5-OA6-CA4
45	D	101	CDL	C51-CB5-OB6-CB4
43	1	401	PC1	C1-O11-P-O13
43	5	702	PC1	C11-O13-P-O11
43	5	702	PC1	C1-O11-P-O13
45	2	601	CDL	CA3-OA5-PA1-OA2
45	D	101	CDL	CB2-OB2-PB2-OB5
45	S	201	CDL	CA2-OA2-PA1-OA5
45	S	201	CDL	CB2-OB2-PB2-OB5
45	X	202	CDL	CA3-OA5-PA1-OA2
45	X	202	CDL	CB2-OB2-PB2-OB5
46	5	701	3PE	C11-O13-P-O11
46	5	706	3PE	C11-O13-P-O11
46	E	401	3PE	C1-O11-P-O13
46	I	303	3PE	C11-O13-P-O11
46	W	201	3PE	C1-O11-P-O13
44	2	602	LMT	O5B-C5B-C6B-O6B
45	D	101	CDL	OB7-CB5-OB6-CB4
43	5	702	PC1	C11-C12-N-C13
43	5	702	PC1	C11-C12-N-C14
43	5	703	PC1	C32-C33-C34-C35
46	E	401	3PE	C22-C21-O21-C2
46	5	704	3PE	C33-C34-C35-C36
45	D	101	CDL	CA4-CA3-OA5-PA1
46	i	101	3PE	C2-C1-O11-P
44	2	604	LMT	C2'-C1'-O1'-C1
46	W	201	3PE	C31-C32-C33-C34
46	i	101	3PE	C31-C32-C33-C34
44	3	202	LMT	C4-C5-C6-C7
44	2	604	LMT	O5B-C1B-O1B-C4'
44	J	201	LMT	C4-C5-C6-C7
46	E	401	3PE	O22-C21-O21-C2
46	W	202	3PE	C22-C21-O21-C2
44	4	601	LMT	C3-C4-C5-C6
44	5	705	LMT	C3-C4-C5-C6
44	2	604	LMT	O5'-C1'-O1'-C1
44	g	101	LMT	C7-C8-C9-C10
46	5	704	3PE	C23-C24-C25-C26
44	4	601	LMT	C2-C1-O1'-C1'
44	1	403	LMT	C1-C2-C3-C4
45	2	601	CDL	O1-C1-CA2-OA2
45	X	201	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	W	202	3PE	O22-C21-O21-C2
46	I	303	3PE	C2-C1-O11-P
43	5	702	PC1	C11-C12-N-C15
44	3	201	LMT	O5B-C5B-C6B-O6B
44	2	604	LMT	C11-C10-C9-C8
44	4	601	LMT	C11-C10-C9-C8
45	X	202	CDL	C75-C76-C77-C78
44	2	603	LMT	O5B-C5B-C6B-O6B
45	X	201	CDL	CA7-C31-C32-C33
45	X	202	CDL	CA7-C31-C32-C33
44	5	705	LMT	C2-C3-C4-C5
43	5	702	PC1	C22-C21-O21-C2
45	2	601	CDL	C11-CA5-OA6-CA4
45	D	101	CDL	C11-CA5-OA6-CA4
44	g	101	LMT	C1-C2-C3-C4
43	5	702	PC1	O22-C21-O21-C2
44	2	604	LMT	O5B-C5B-C6B-O6B
44	4	601	LMT	C4-C5-C6-C7
45	X	201	CDL	OA9-CA7-OA8-CA6
52	O	201	ZMP	C22-C1-C2-C3
45	X	202	CDL	C31-C32-C33-C34
46	I	303	3PE	C22-C23-C24-C25
45	X	201	CDL	OB5-CB3-CB4-CB6
46	E	401	3PE	O11-C1-C2-C3
45	S	201	CDL	C73-C74-C75-C76
46	i	101	3PE	C26-C27-C28-C29
44	a	301	LMT	O5'-C5'-C6'-O6'
44	X	203	LMT	O5'-C5'-C6'-O6'
44	3	202	LMT	C5'-C4'-O1B-C1B
45	S	201	CDL	CB3-CB4-CB6-OB8
44	1	403	LMT	O5B-C5B-C6B-O6B
44	4	601	LMT	O5B-C5B-C6B-O6B
44	j	101	LMT	O5'-C5'-C6'-O6'
43	1	401	PC1	C32-C31-O31-C3
43	2	605	PC1	C1-C2-O21-C21
45	X	201	CDL	CB6-CB4-OB6-CB5
44	2	604	LMT	C4'-C5'-C6'-O6'
46	I	303	3PE	C23-C24-C25-C26
45	X	202	CDL	CA5-C11-C12-C13
45	D	101	CDL	C52-C51-CB5-OB6
45	X	202	CDL	C72-C71-CB7-OB8
52	O	201	ZMP	O4-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	Q	201	ZMP	C17-C16-N2-C15
45	X	202	CDL	C51-CB5-OB6-CB4
45	2	601	CDL	C31-CA7-OA8-CA6
52	O	201	ZMP	O3-C16-C17-C18
45	D	101	CDL	C13-C14-C15-C16
45	S	201	CDL	CA4-CA3-OA5-PA1
45	X	201	CDL	C1-CB2-OB2-PB2
45	X	202	CDL	C1-CB2-OB2-PB2
46	E	401	3PE	C2-C1-O11-P
43	1	401	PC1	O32-C31-O31-C3
44	2	602	LMT	C2-C1-O1'-C1'
44	2	603	LMT	C2-C1-O1'-C1'
44	3	201	LMT	C2-C1-O1'-C1'
46	W	201	3PE	C2B-C2C-C2D-C2E
52	Q	201	ZMP	O3-C16-N2-C15
43	5	702	PC1	C1-C2-C3-O31
46	5	706	3PE	C1-C2-C3-O31
45	2	601	CDL	OA7-CA5-OA6-CA4
45	2	601	CDL	CB5-C51-C52-C53
44	g	101	LMT	C4-C5-C6-C7
45	S	201	CDL	CB3-OB5-PB2-OB2
45	X	201	CDL	CB2-OB2-PB2-OB5
45	X	202	CDL	OB5-CB3-CB4-OB6
44	5	705	LMT	C4-C5-C6-C7
52	Q	201	ZMP	C3-C4-C5-C6
46	5	704	3PE	O21-C2-C3-O31
45	X	201	CDL	C32-C31-CA7-OA8
44	g	101	LMT	O5'-C1'-O1'-C1
45	D	101	CDL	OA7-CA5-OA6-CA4
45	X	202	CDL	OB7-CB5-OB6-CB4
43	5	702	PC1	C24-C25-C26-C27
45	X	202	CDL	C76-C77-C78-C79
45	D	101	CDL	C32-C31-CA7-OA8
45	S	201	CDL	C51-C52-C53-C54
43	5	703	PC1	C25-C26-C27-C28
45	X	201	CDL	OA5-CA3-CA4-CA6
50	E	402	NDP	O4B-C4B-C5B-O5B
52	Q	201	ZMP	C2-C3-C4-C5
45	X	202	CDL	CA4-CA3-OA5-PA1
45	X	202	CDL	CA3-CA4-CA6-OA8
45	D	101	CDL	OA5-CA3-CA4-OA6
44	2	602	LMT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	Q	201	ZMP	C16-C17-C18-C20
45	2	601	CDL	OA9-CA7-OA8-CA6
50	E	402	NDP	PN-O3-PA-O2A
46	W	202	3PE	C25-C26-C27-C28
45	D	101	CDL	C71-C72-C73-C74
46	5	706	3PE	C32-C31-O31-C3
43	5	703	PC1	C11-O13-P-O11
45	D	101	CDL	CB3-OB5-PB2-OB2
46	5	704	3PE	C1-O11-P-O13
43	5	702	PC1	C2A-C2B-C2C-C2D
50	E	402	NDP	C2D-C1D-N1N-C6N
43	5	702	PC1	C1-O11-P-O12
45	2	601	CDL	CA2-OA2-PA1-OA4
45	2	601	CDL	CA3-OA5-PA1-OA4
45	D	101	CDL	CB3-OB5-PB2-OB4
45	X	201	CDL	CB2-OB2-PB2-OB4
45	X	202	CDL	CA3-OA5-PA1-OA3
45	X	202	CDL	CB2-OB2-PB2-OB4
46	5	701	3PE	C11-O13-P-O12
46	5	704	3PE	C1-O11-P-O12
46	5	704	3PE	C11-O13-P-O14
46	E	401	3PE	C1-O11-P-O14
46	W	201	3PE	C1-O11-P-O12
46	W	201	3PE	C1-O11-P-O14
44	3	202	LMT	C7-C8-C9-C10
45	D	101	CDL	OB5-CB3-CB4-CB6
45	X	202	CDL	OB5-CB3-CB4-CB6
46	W	201	3PE	O11-C1-C2-C3
43	2	605	PC1	C31-C32-C33-C34
44	2	602	LMT	C5-C6-C7-C8
44	a	301	LMT	C5-C6-C7-C8
46	5	701	3PE	C12-C11-O13-P
46	i	101	3PE	C12-C11-O13-P
46	5	706	3PE	C33-C34-C35-C36
45	2	601	CDL	CB2-C1-CA2-OA2
45	X	201	CDL	OA5-CA3-CA4-OA6
52	Q	201	ZMP	C16-C17-C18-C21
45	X	202	CDL	C32-C31-CA7-OA8
52	O	201	ZMP	C1-C2-C3-C4
43	1	401	PC1	O13-C11-C12-N
45	X	202	CDL	C51-C52-C53-C54
46	I	303	3PE	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
43	5	702	PC1	O21-C2-C3-O31
45	X	201	CDL	OA6-CA4-CA6-OA8
46	I	303	3PE	O21-C2-C3-O31
45	X	201	CDL	C72-C73-C74-C75
44	3	202	LMT	C3-C4-C5-C6
46	5	706	3PE	O32-C31-O31-C3
44	4	601	LMT	C1-C2-C3-C4
46	W	201	3PE	C2C-C2D-C2E-C2F
45	S	201	CDL	CA6-CA4-OA6-CA5
44	5	705	LMT	C5-C6-C7-C8
46	W	202	3PE	C2-C1-O11-P
46	E	401	3PE	O11-C1-C2-O21
44	g	101	LMT	C5-C6-C7-C8
45	X	202	CDL	C11-CA5-OA6-CA4
44	3	202	LMT	O5B-C1B-O1B-C4'
52	O	201	ZMP	C2-C3-C4-C5
43	2	605	PC1	C11-O13-P-O11
43	5	703	PC1	C1-O11-P-O13
45	X	202	CDL	CA2-OA2-PA1-OA5
46	5	701	3PE	C1-O11-P-O13
46	W	201	3PE	C11-O13-P-O11
45	2	601	CDL	CB3-CB4-CB6-OB8
46	5	704	3PE	C1-C2-C3-O31
50	E	402	NDP	O4D-C1D-N1N-C6N
43	5	702	PC1	C25-C26-C27-C28
45	X	202	CDL	C72-C73-C74-C75
44	3	202	LMT	C2B-C1B-O1B-C4'
45	X	202	CDL	C31-CA7-OA8-CA6
46	5	701	3PE	C24-C25-C26-C27
52	O	201	ZMP	C5-C6-C7-C8
46	5	704	3PE	C24-C25-C26-C27
46	5	701	3PE	O11-C1-C2-O21
44	3	201	LMT	C3-C4-C5-C6
45	X	202	CDL	OA9-CA7-OA8-CA6
44	2	604	LMT	C7-C8-C9-C10
49	B	602	FMN	C4'-C5'-O5'-P
45	X	202	CDL	OA7-CA5-OA6-CA4
44	g	101	LMT	C4'-C5'-C6'-O6'
43	5	703	PC1	C21-C22-C23-C24
43	5	702	PC1	C28-C29-C2A-C2B
45	2	601	CDL	CA3-CA4-CA6-OA8
45	X	201	CDL	CA3-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
44	2	604	LMT	C1-C2-C3-C4
52	Q	201	ZMP	C20-C18-C21-O5
46	i	101	3PE	C27-C28-C29-C2A
44	X	203	LMT	O5'-C1'-O1'-C1
50	E	402	NDP	C2D-C1D-N1N-C2N
45	X	202	CDL	C71-CB7-OB8-CB6
45	D	101	CDL	OA5-CA3-CA4-CA6
46	5	704	3PE	C36-C37-C38-C39
52	Q	201	ZMP	C12-C11-S1-C10
43	5	703	PC1	C3D-C3E-C3F-C3G
45	S	201	CDL	OA6-CA4-CA6-OA8
45	X	202	CDL	C35-C36-C37-C38
50	E	402	NDP	PN-O3-PA-O1A
44	X	203	LMT	C2-C3-C4-C5
45	D	101	CDL	C72-C73-C74-C75
46	W	201	3PE	C33-C34-C35-C36
45	D	101	CDL	C52-C51-CB5-OB7
44	1	402	LMT	C1-C2-C3-C4
46	W	201	3PE	O11-C1-C2-O21
45	2	601	CDL	C54-C55-C56-C57
49	B	602	FMN	C2'-C3'-C4'-O4'
46	I	303	3PE	C38-C39-C3A-C3B
44	X	203	LMT	C2'-C1'-O1'-C1
45	X	202	CDL	C72-C71-CB7-OB9
52	O	201	ZMP	N2-C16-C17-O4
46	5	701	3PE	C34-C35-C36-C37
45	2	601	CDL	C56-C57-C58-C59
43	5	703	PC1	O22-C21-O21-C2
45	S	201	CDL	OB7-CB5-OB6-CB4
44	J	201	LMT	C2-C3-C4-C5
44	j	101	LMT	O5B-C1B-O1B-C4'
45	X	202	CDL	OB9-CB7-OB8-CB6
46	W	202	3PE	O11-C1-C2-O21
46	W	201	3PE	C24-C25-C26-C27
52	Q	201	ZMP	C16-C17-C18-C19
50	E	402	NDP	O4D-C1D-N1N-C2N
46	W	202	3PE	O11-C1-C2-C3
46	5	706	3PE	C34-C35-C36-C37
44	5	705	LMT	O1'-C1-C2-C3
44	a	301	LMT	C7-C8-C9-C10
45	S	201	CDL	C51-CB5-OB6-CB4
43	5	703	PC1	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

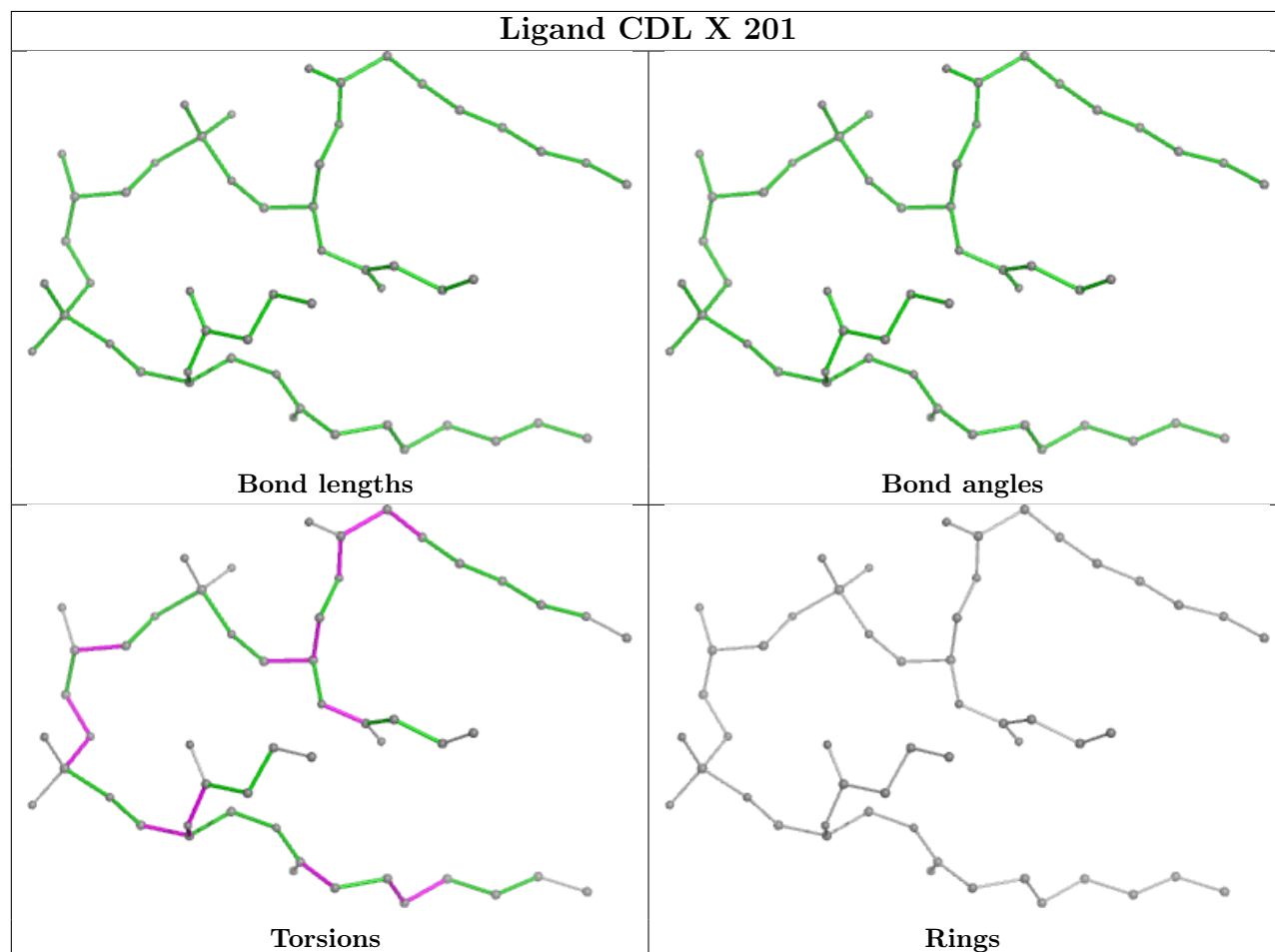
Mol	Chain	Res	Type	Atoms
46	5	704	3PE	C35-C36-C37-C38
45	S	201	CDL	C54-C55-C56-C57
45	X	201	CDL	C71-C72-C73-C74
44	j	101	LMT	C2B-C1B-O1B-C4'
45	D	101	CDL	CA2-OA2-PA1-OA3
45	X	202	CDL	CA2-OA2-PA1-OA3
46	W	201	3PE	C11-O13-P-O14
46	i	101	3PE	C1-O11-P-O12
46	i	101	3PE	C1-O11-P-O14
45	X	201	CDL	C32-C31-CA7-OA9
44	g	101	LMT	C11-C10-C9-C8
52	O	201	ZMP	O3-C16-N2-C15
46	W	201	3PE	C32-C33-C34-C35
46	5	706	3PE	C12-C11-O13-P
46	E	401	3PE	C12-C11-O13-P
43	5	702	PC1	C26-C27-C28-C29
45	D	101	CDL	C32-C31-CA7-OA9
46	W	202	3PE	C32-C33-C34-C35
45	X	201	CDL	C72-C71-CB7-OB8
44	a	301	LMT	C9-C10-C11-C12
46	5	704	3PE	C26-C27-C28-C29
49	B	602	FMN	N10-C1'-C2'-O2'
46	5	706	3PE	O31-C31-C32-C33
46	i	101	3PE	O31-C31-C32-C33
44	3	202	LMT	C2-C1-O1'-C1'
46	5	704	3PE	C32-C33-C34-C35
44	j	101	LMT	C6-C7-C8-C9
46	i	101	3PE	O32-C31-C32-C33
45	X	201	CDL	C72-C71-CB7-OB9
44	1	403	LMT	C11-C10-C9-C8
45	2	601	CDL	C52-C51-CB5-OB6
46	I	303	3PE	O21-C21-C22-C23

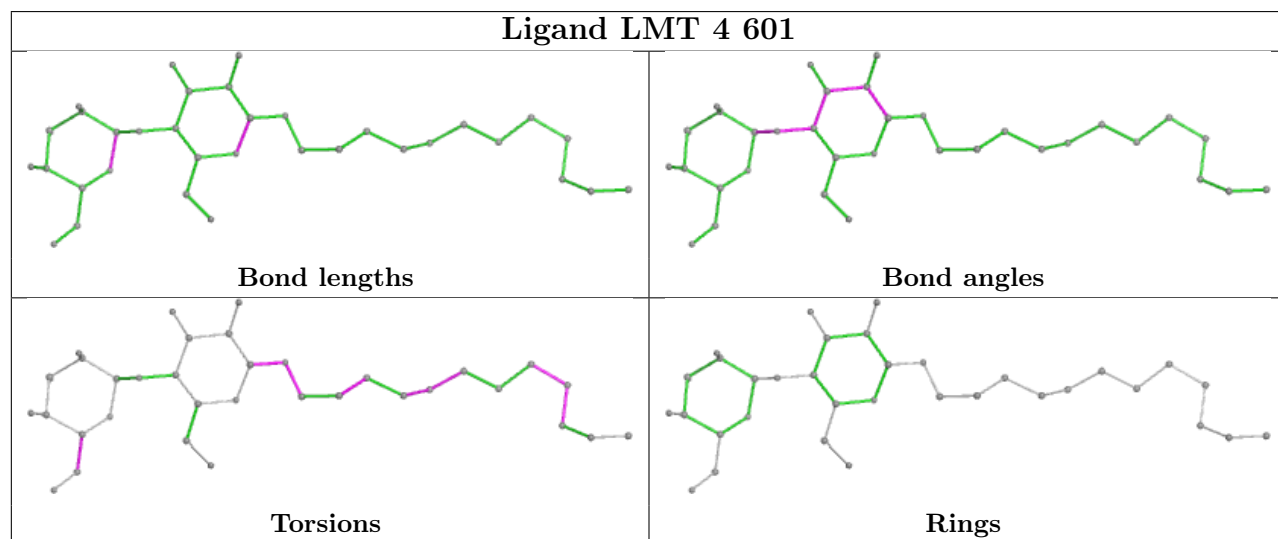
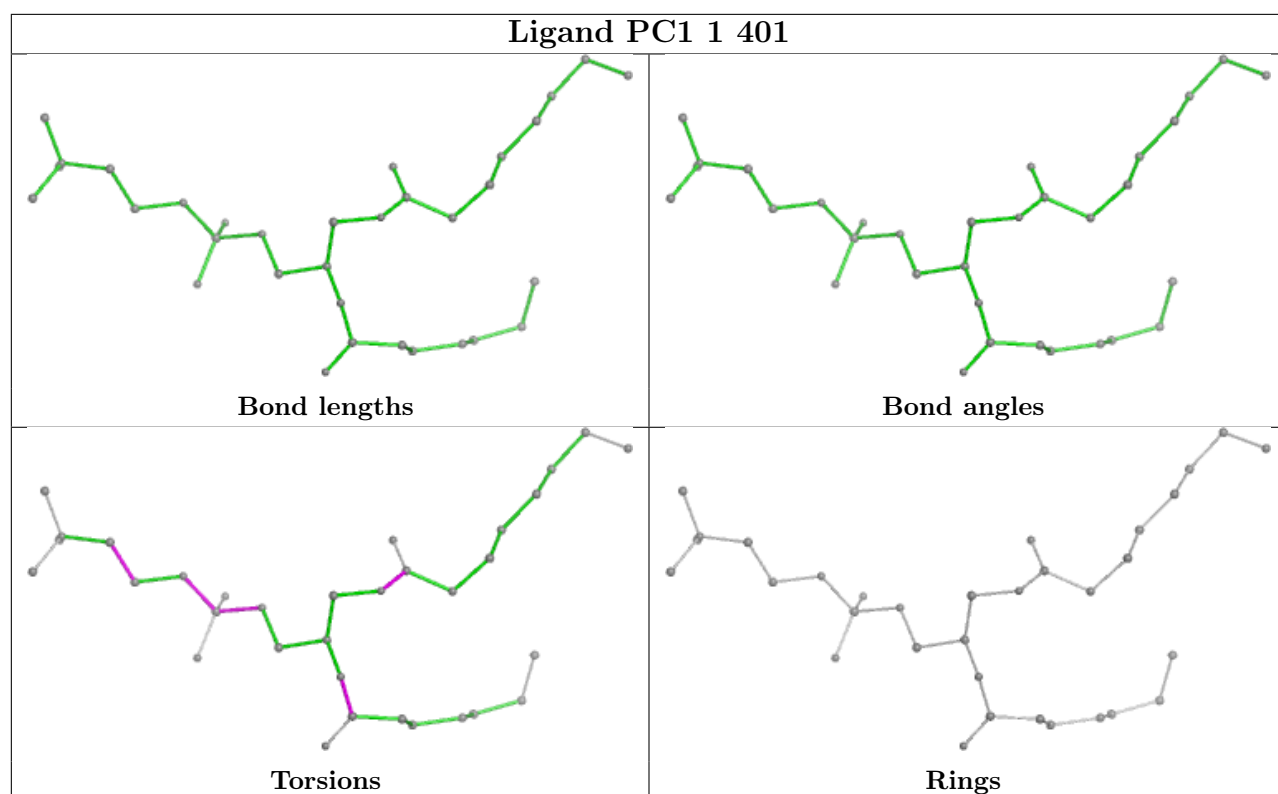
There are no ring outliers.

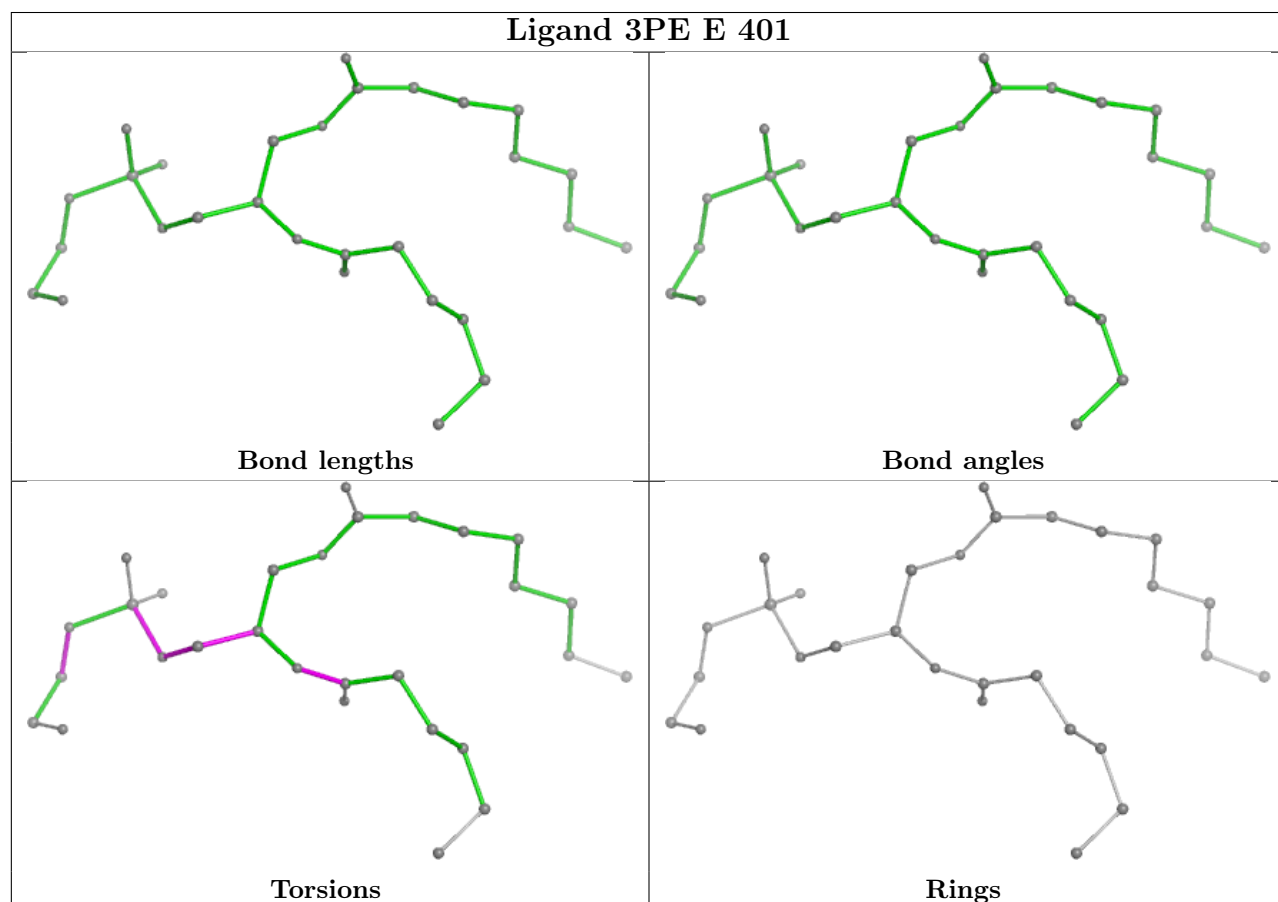
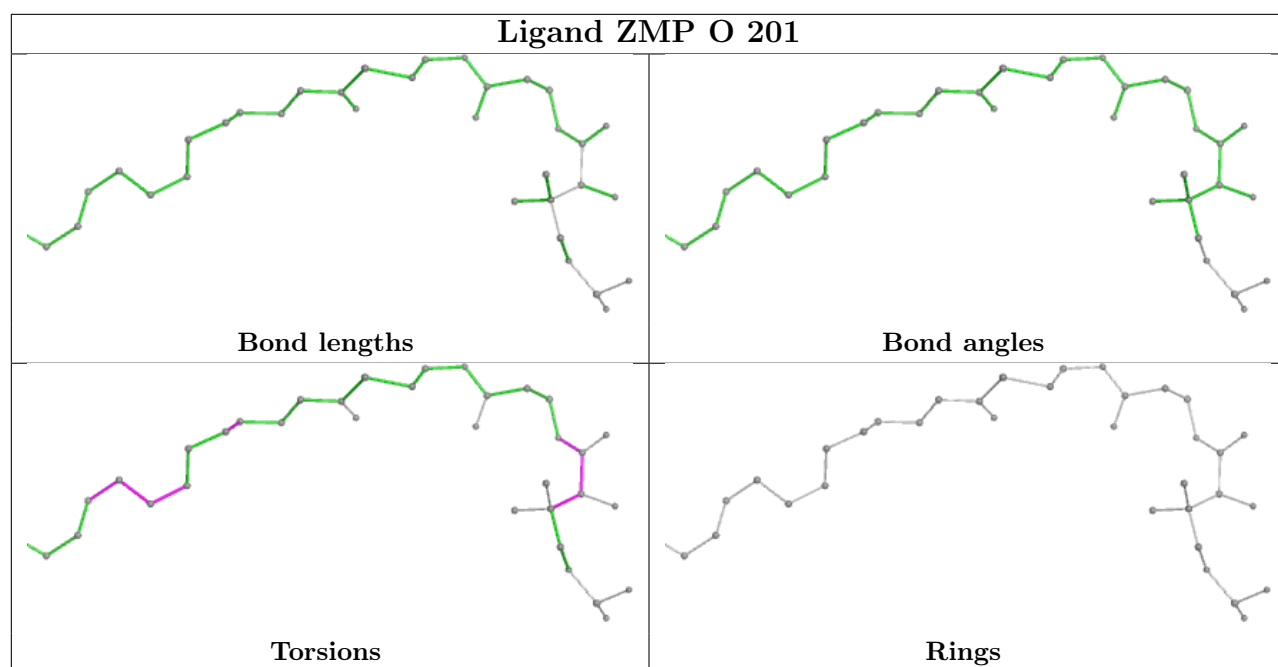
No monomer is involved in short contacts.

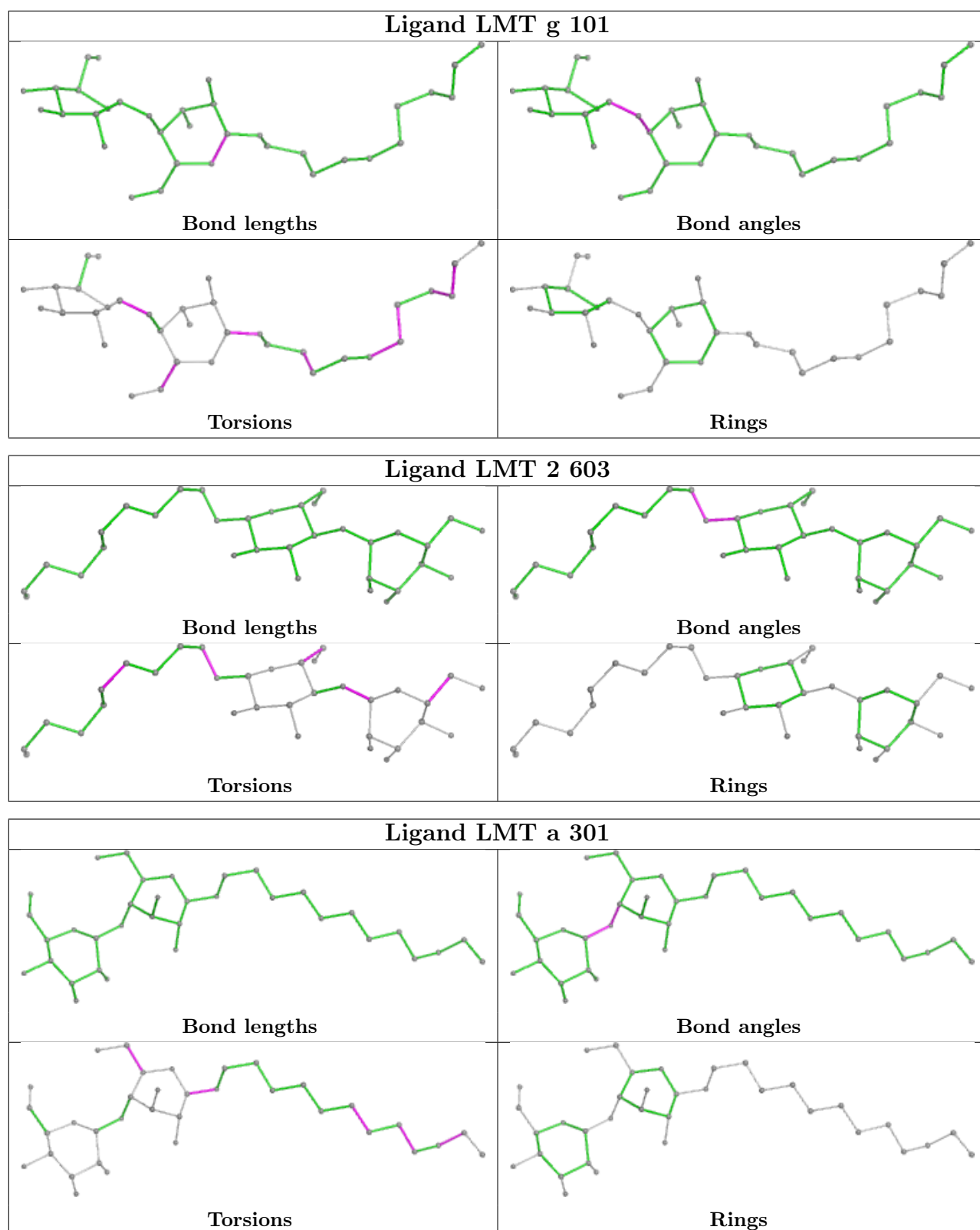
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

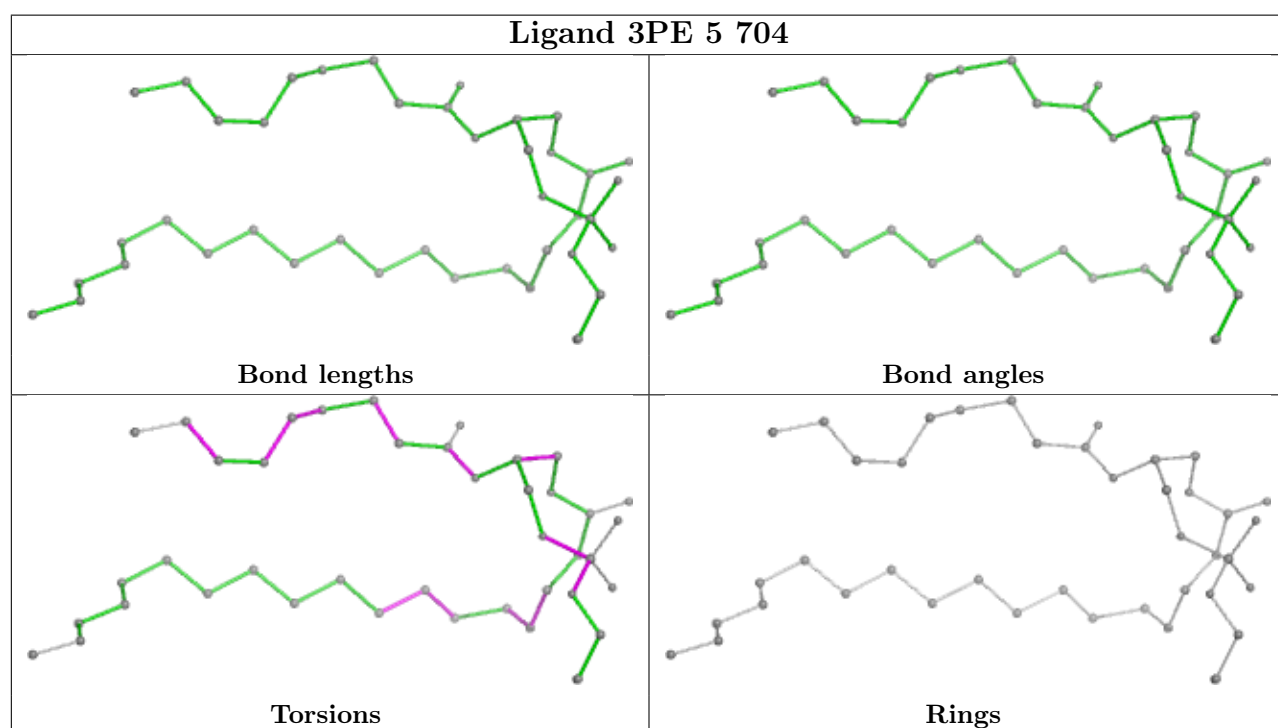
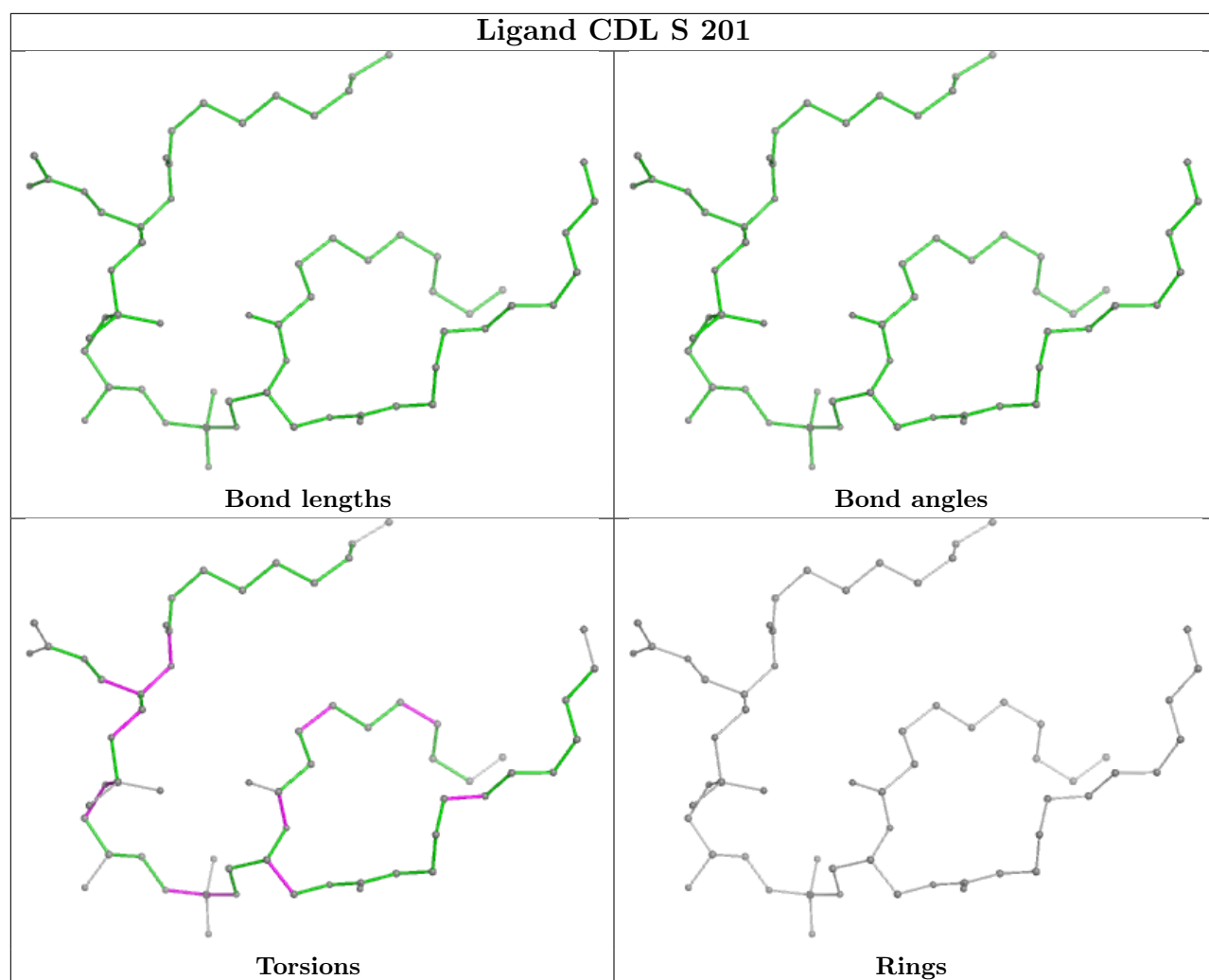
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

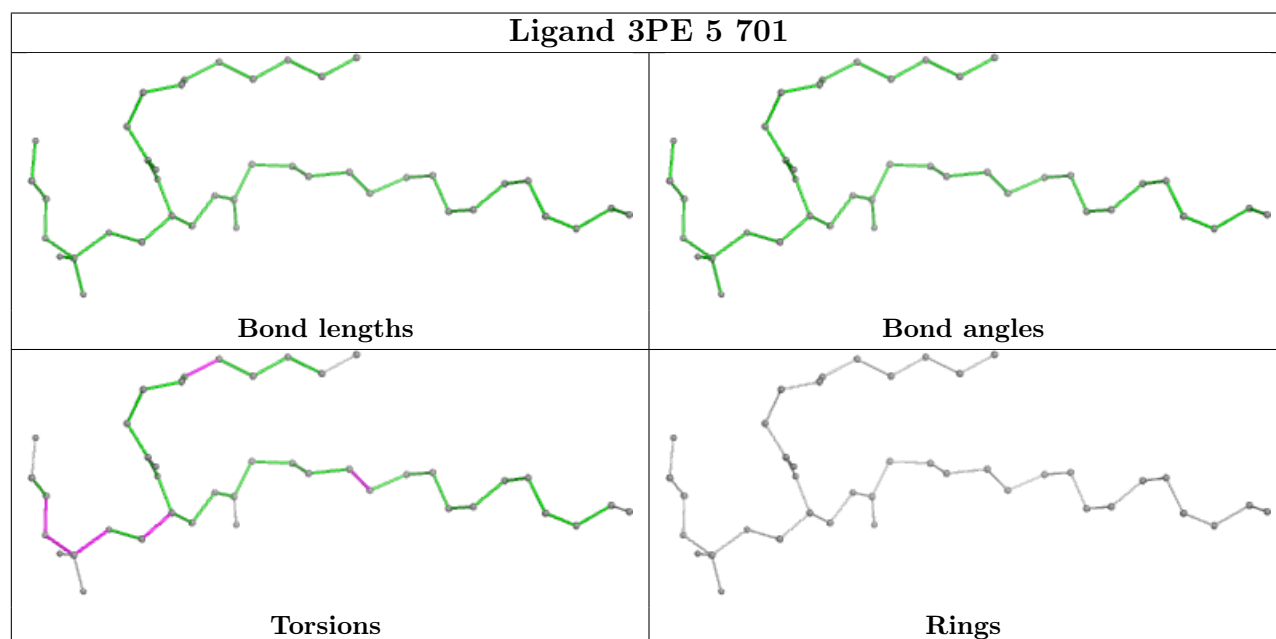
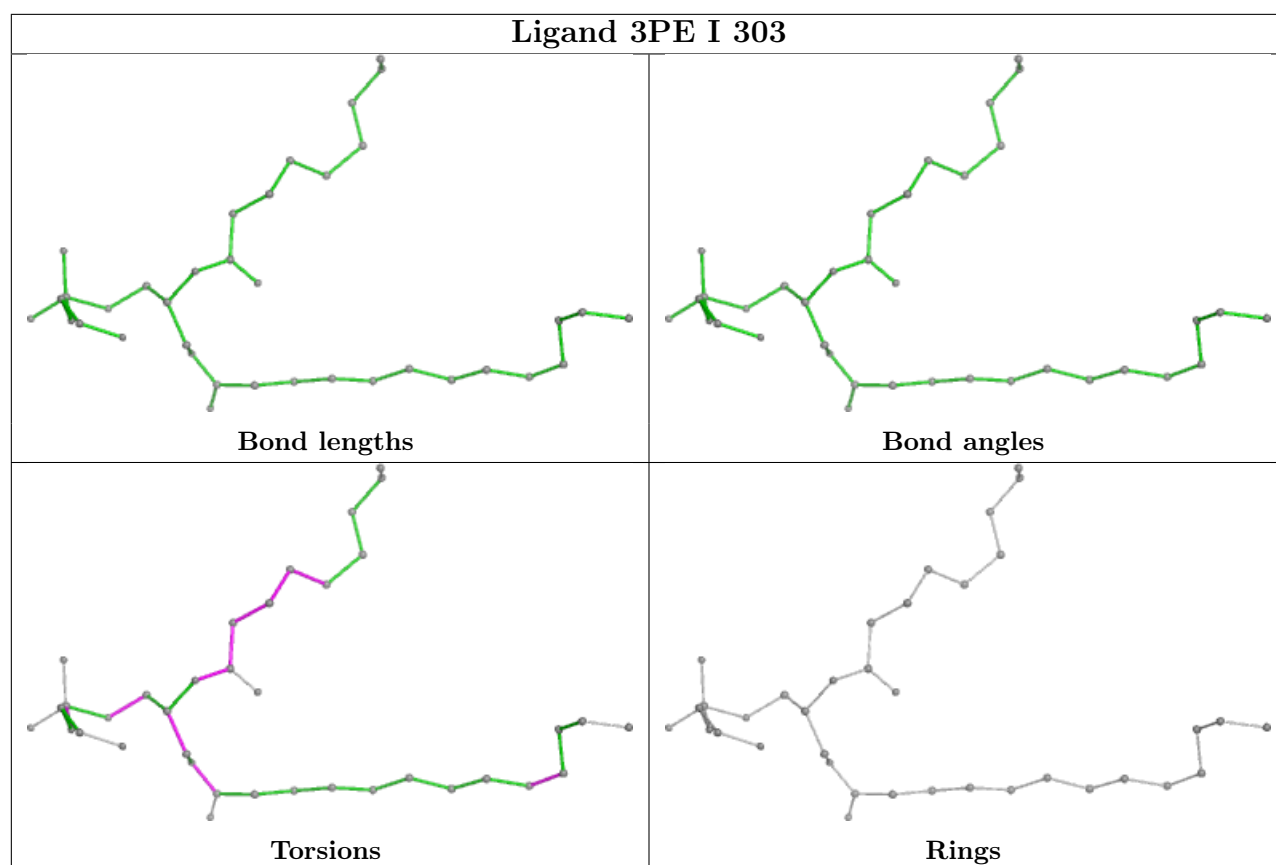




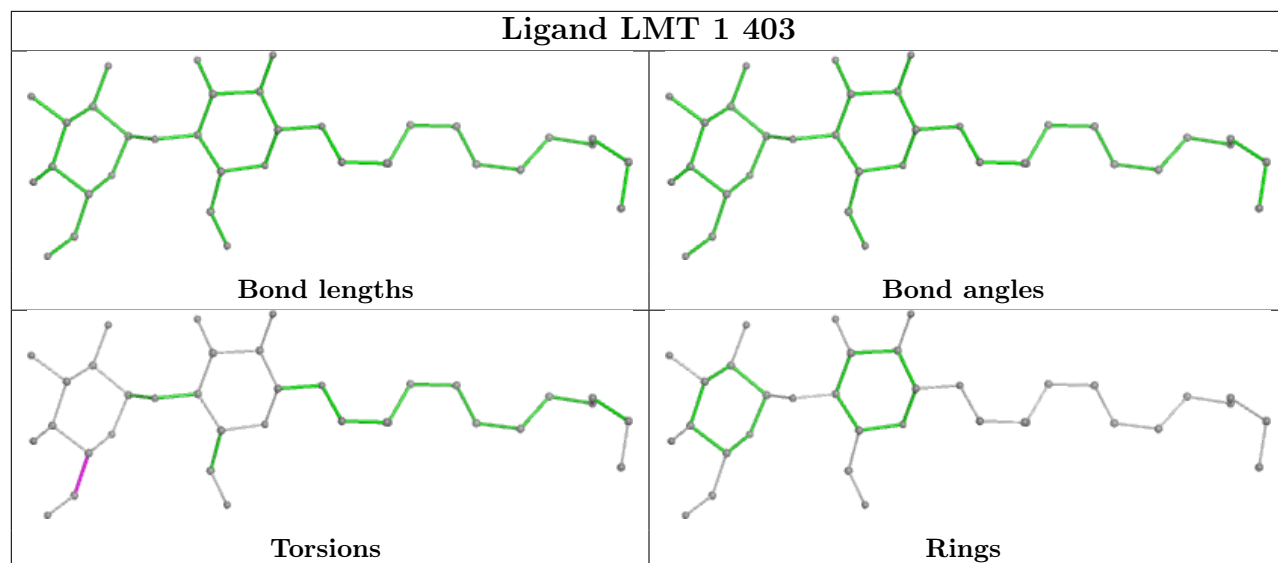




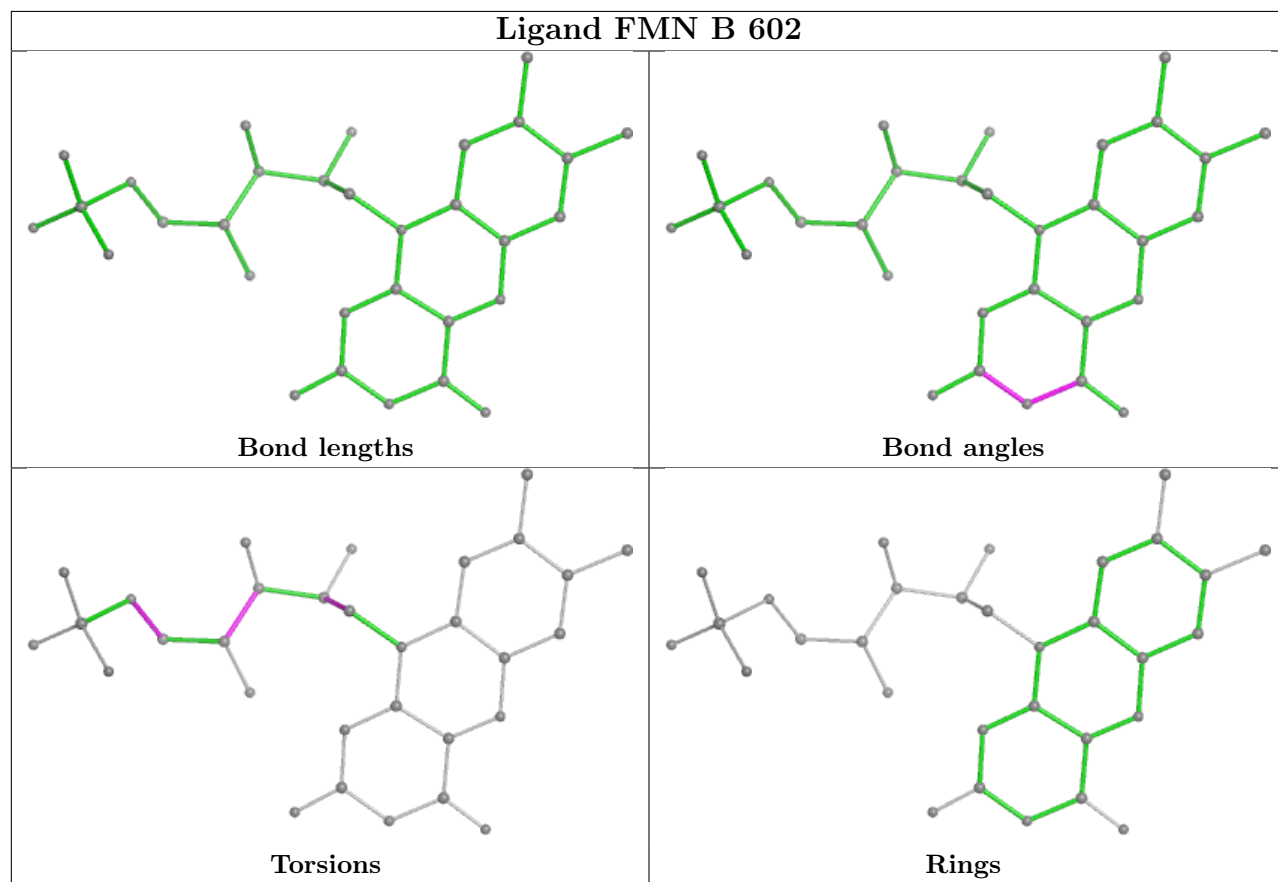


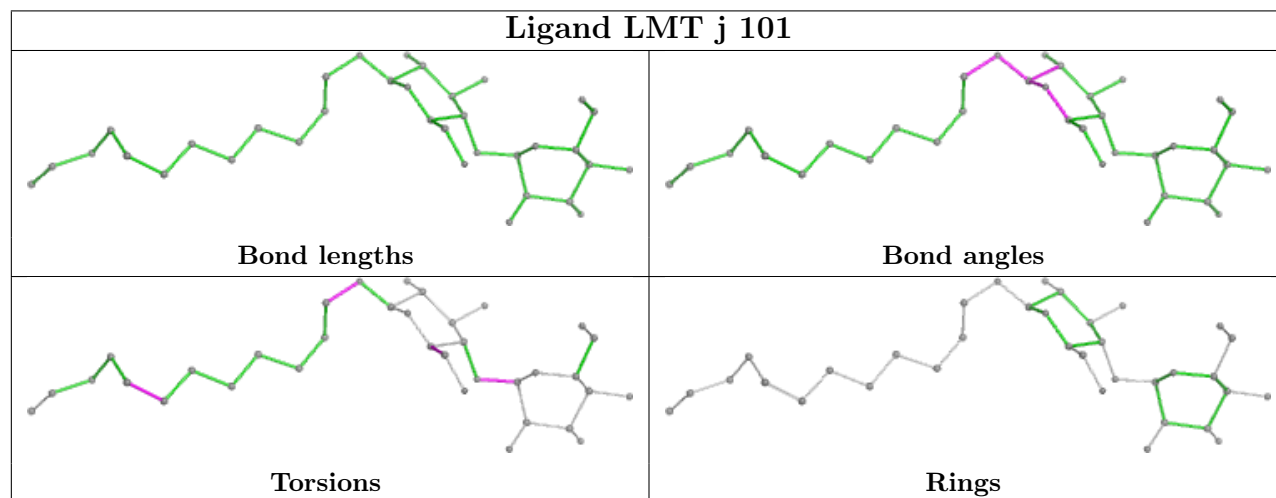
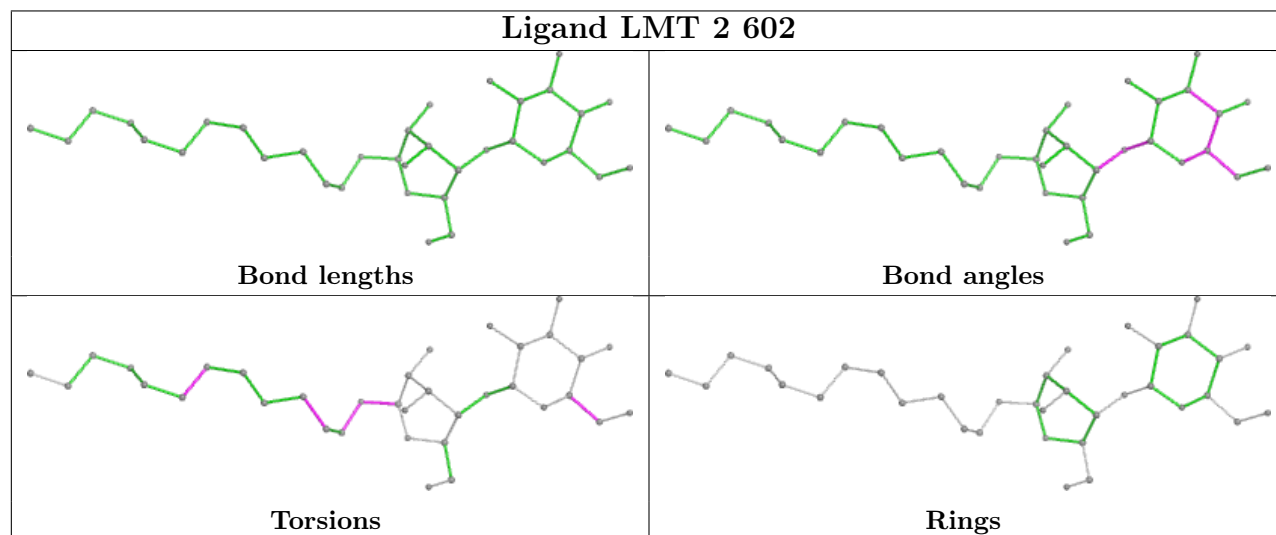
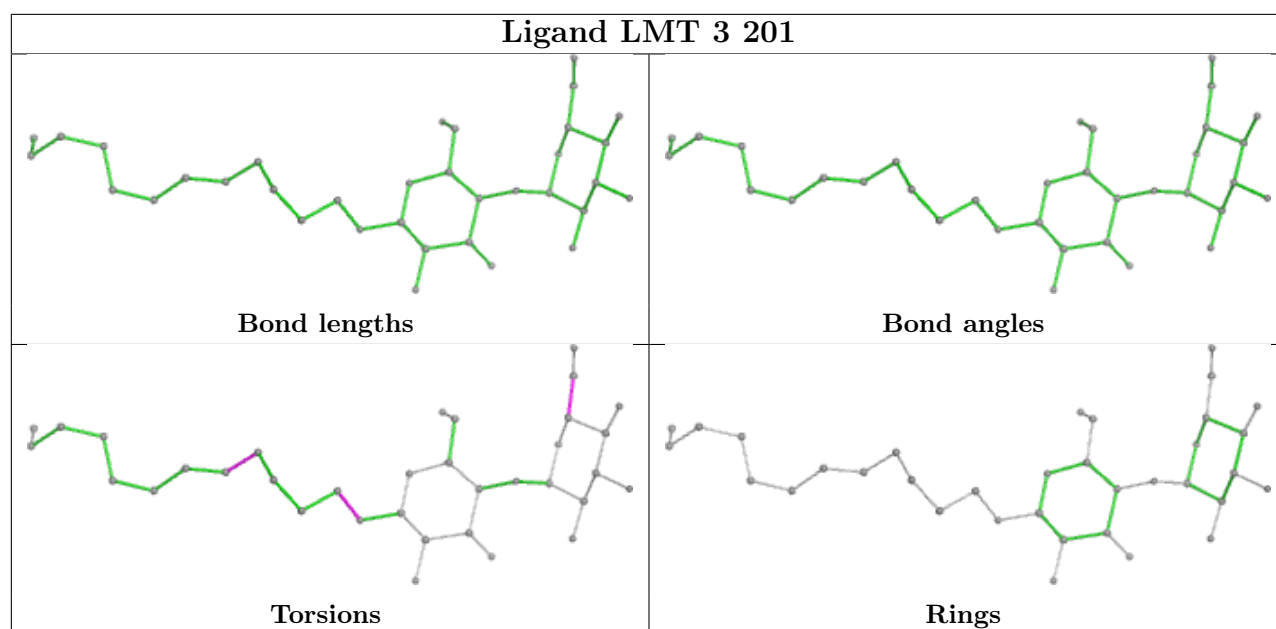


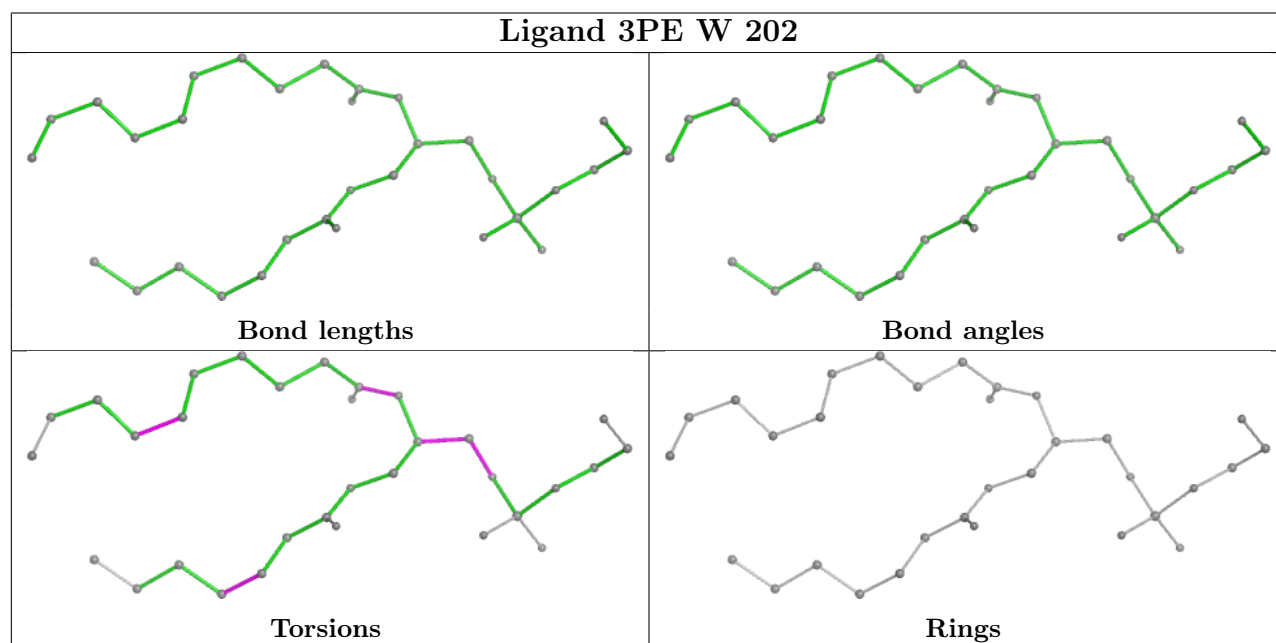
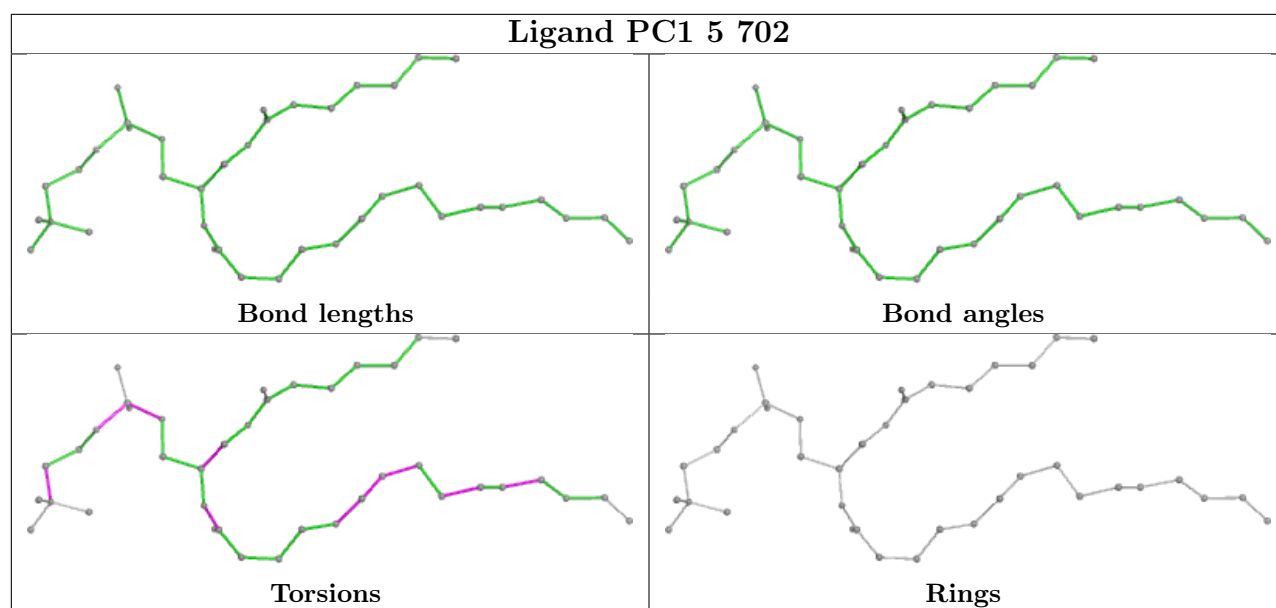
Ligand LMT 1 403

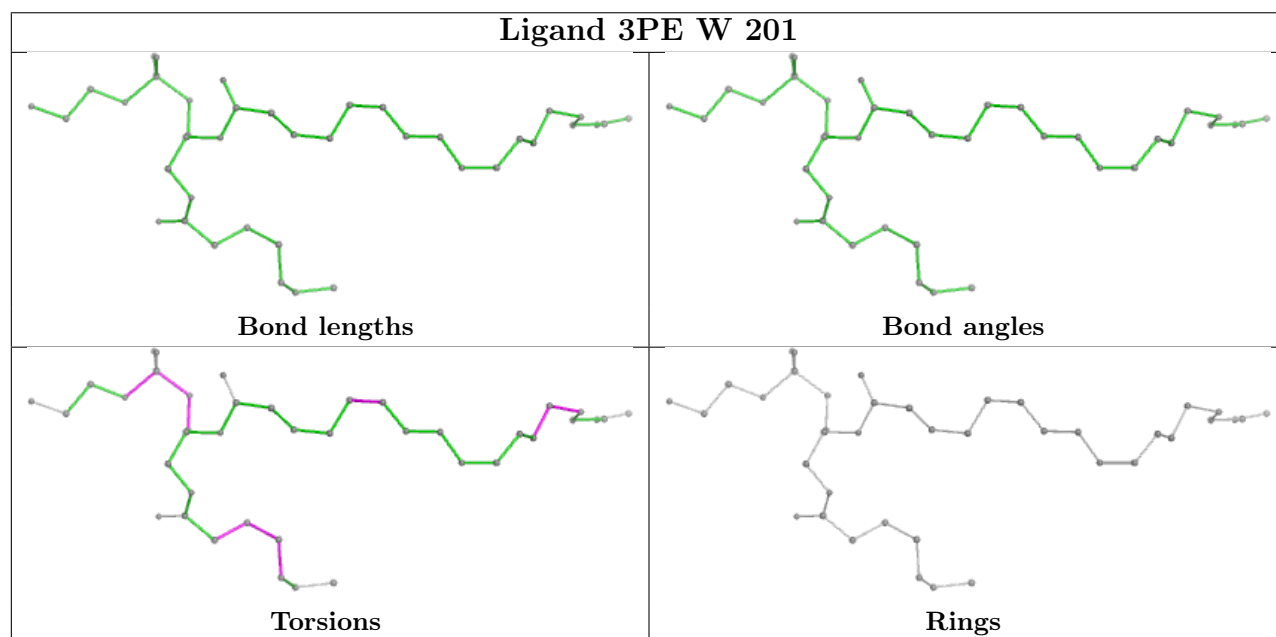
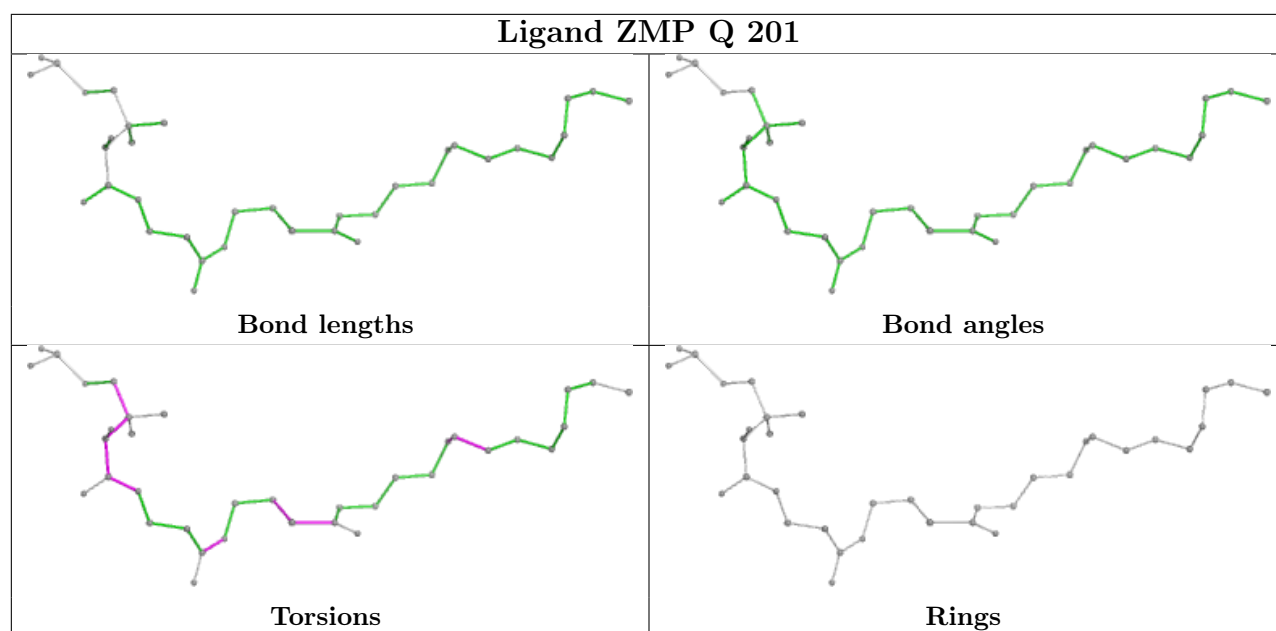


Ligand FMN B 602

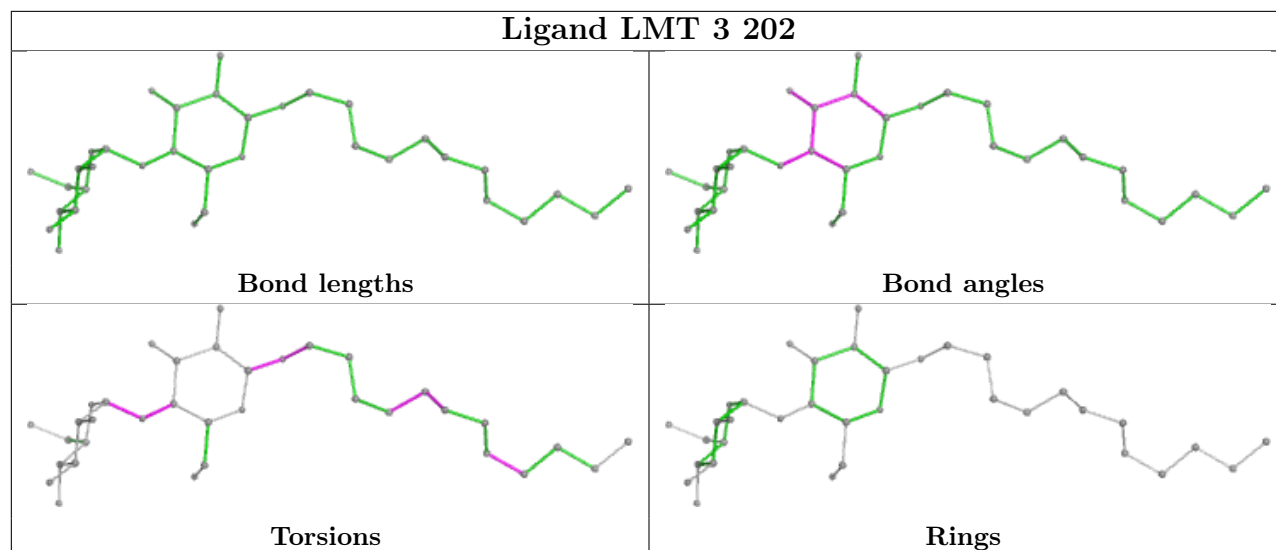




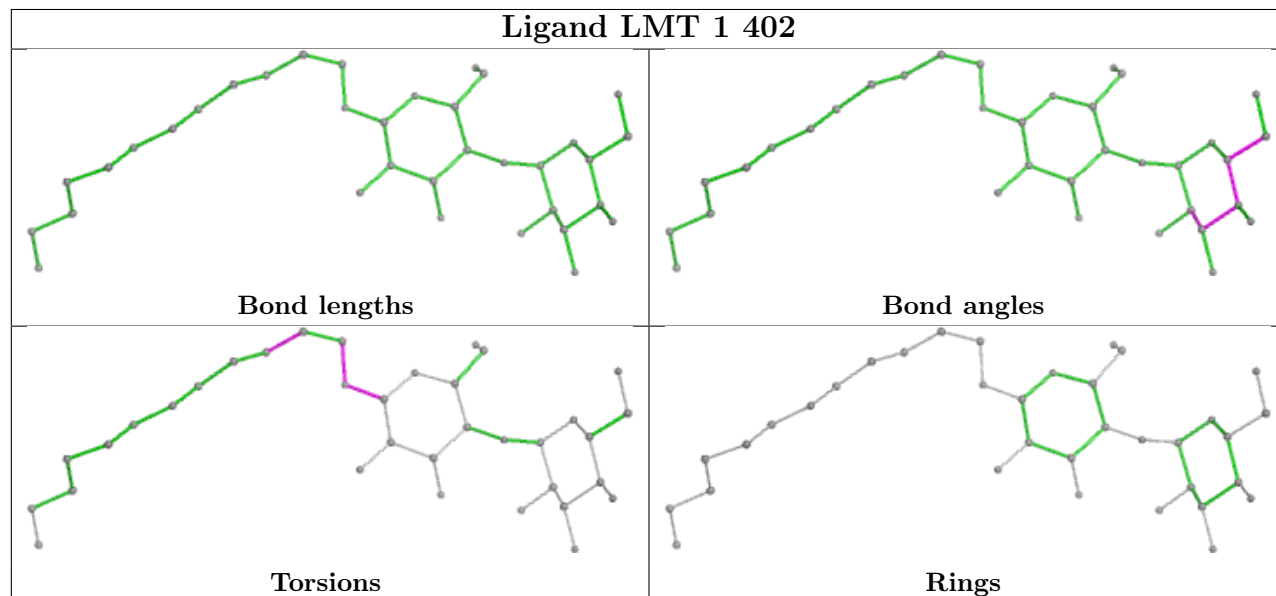


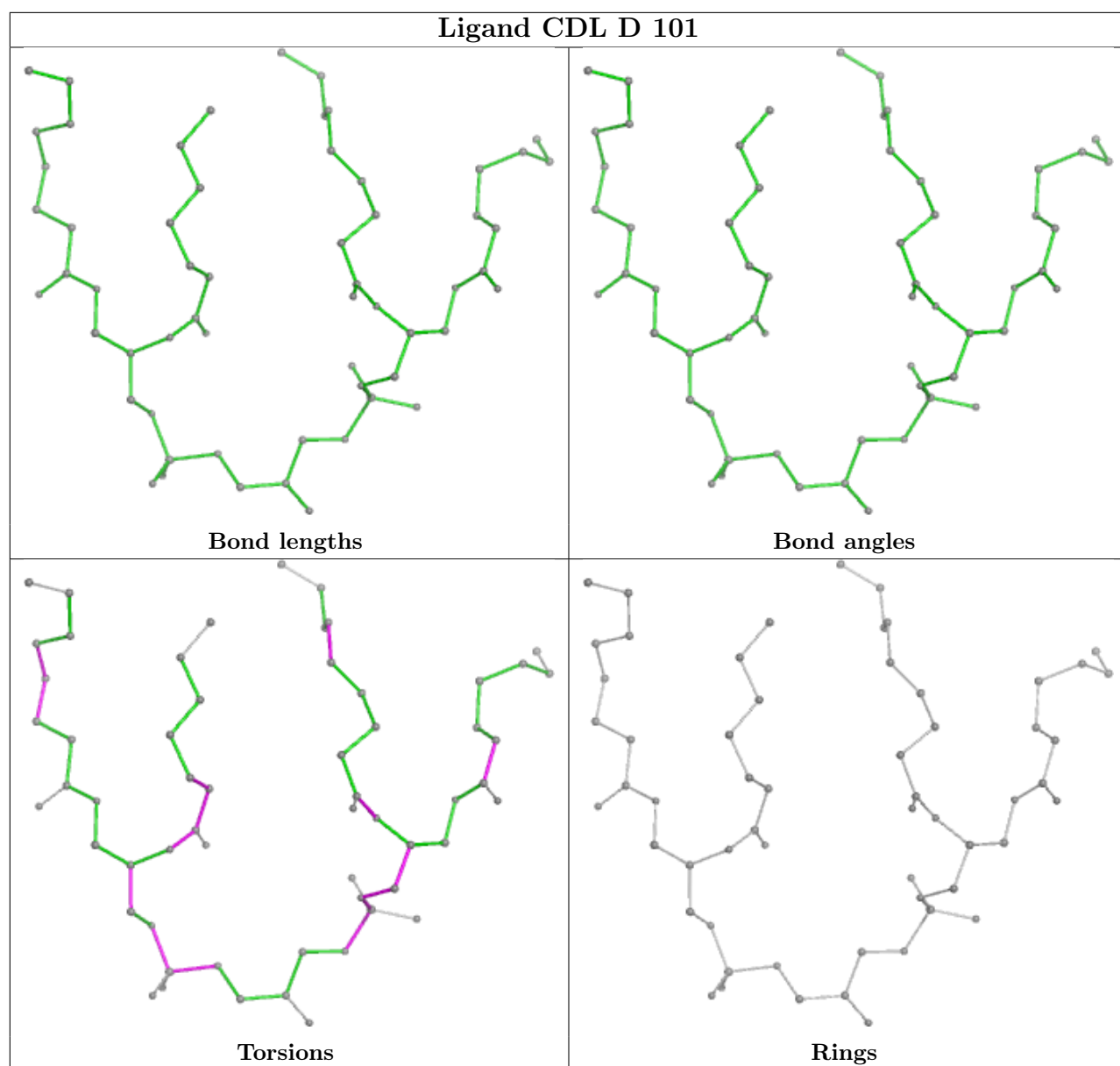


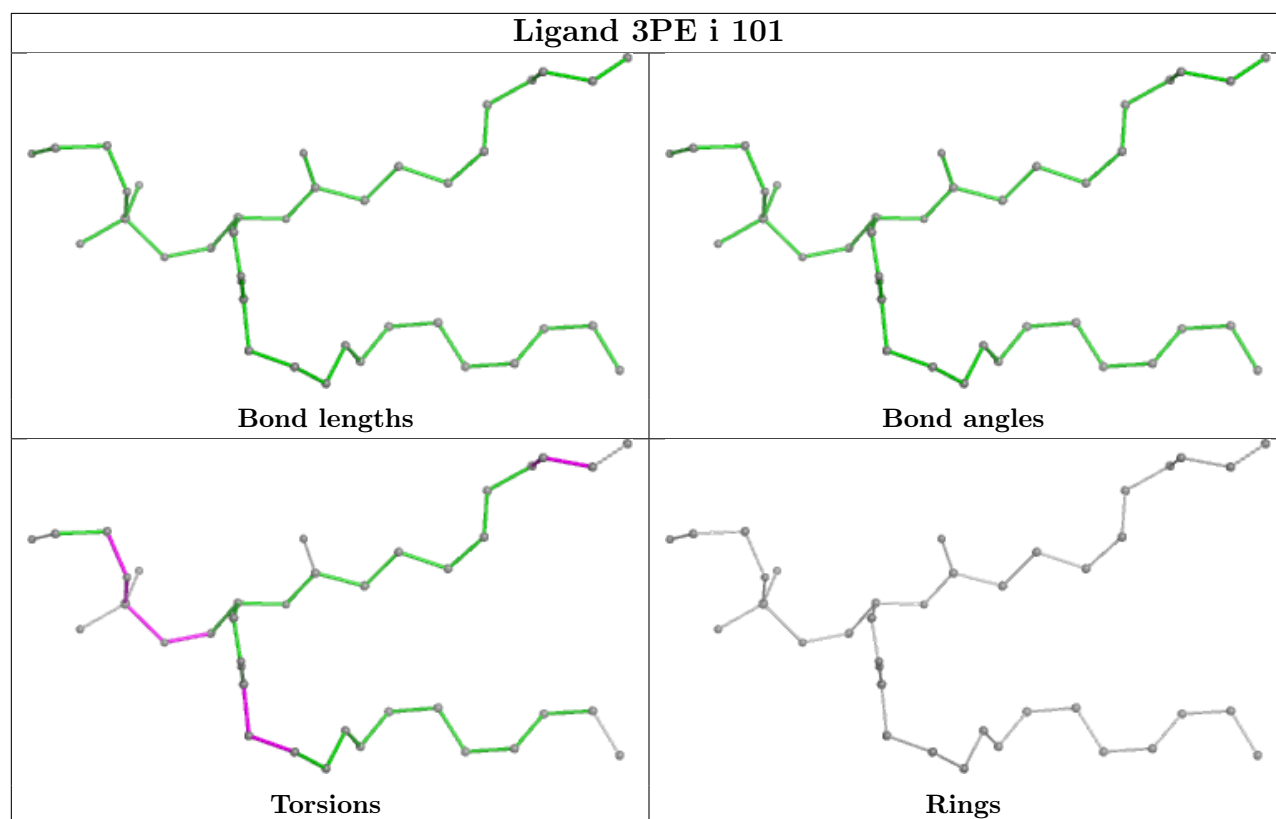
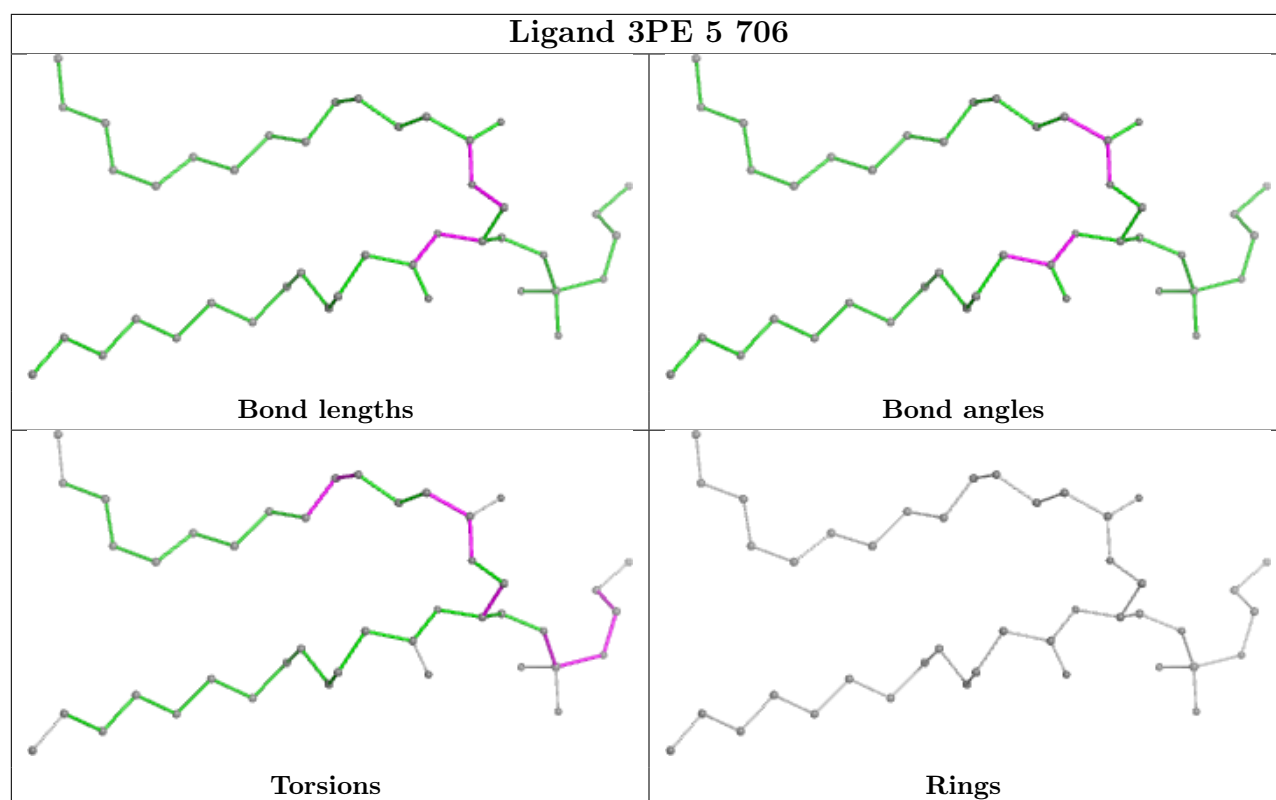
Ligand LMT 3 202

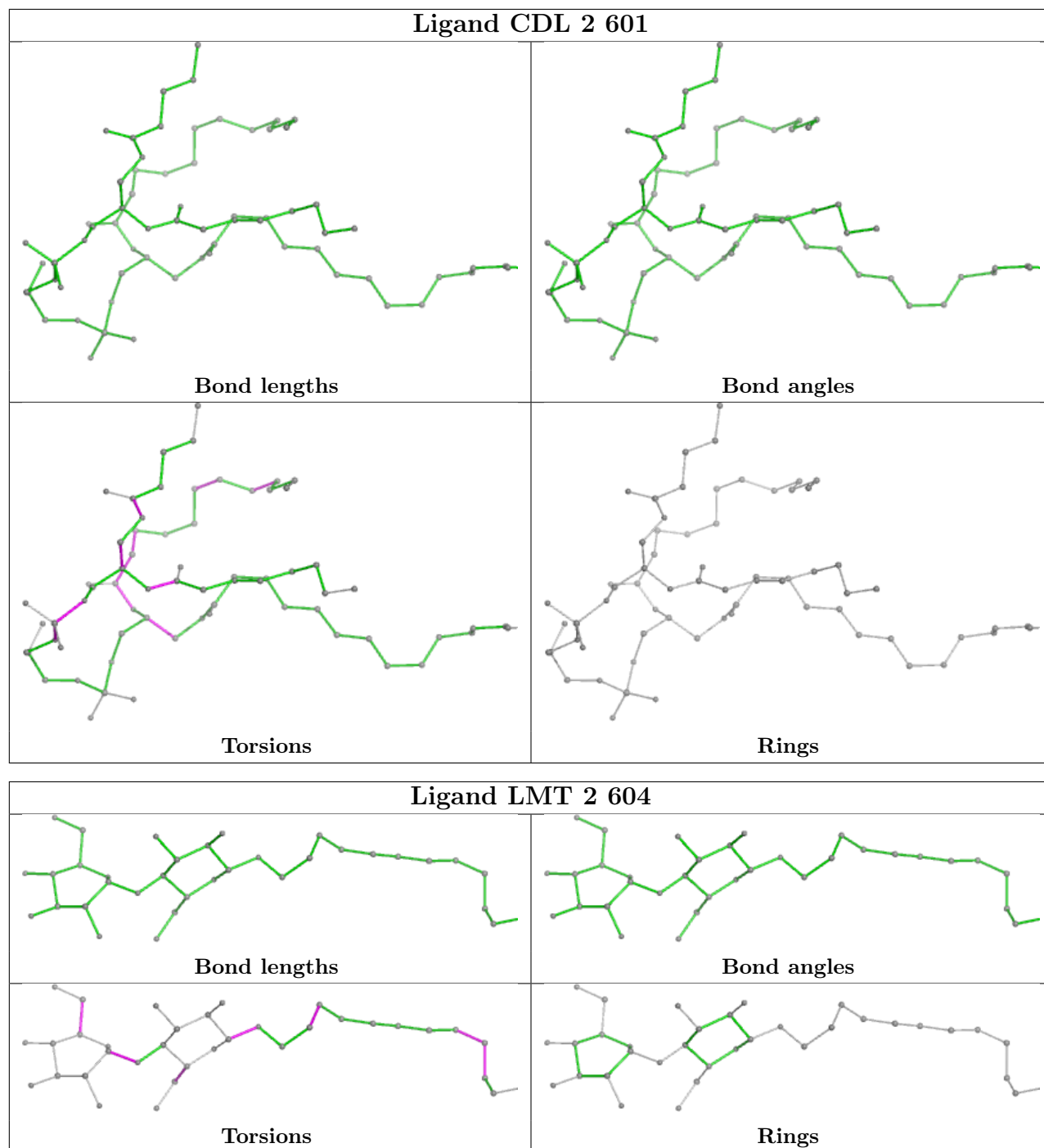


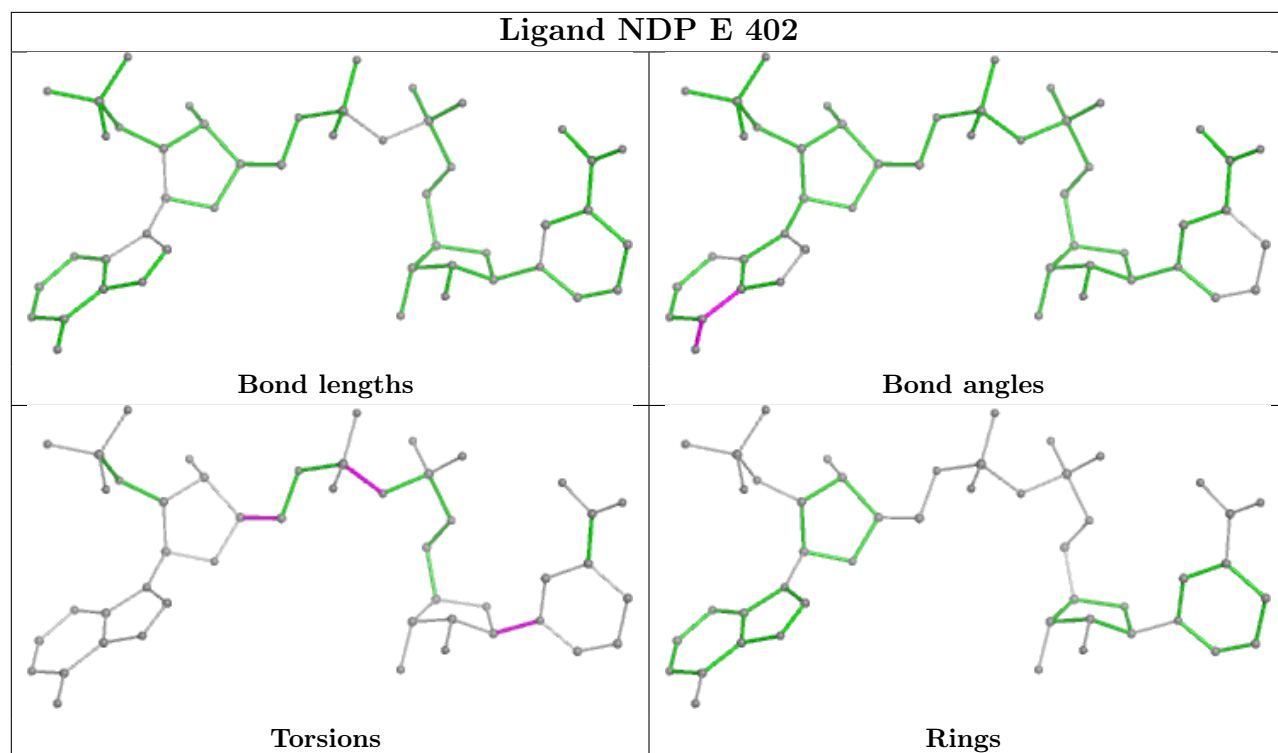
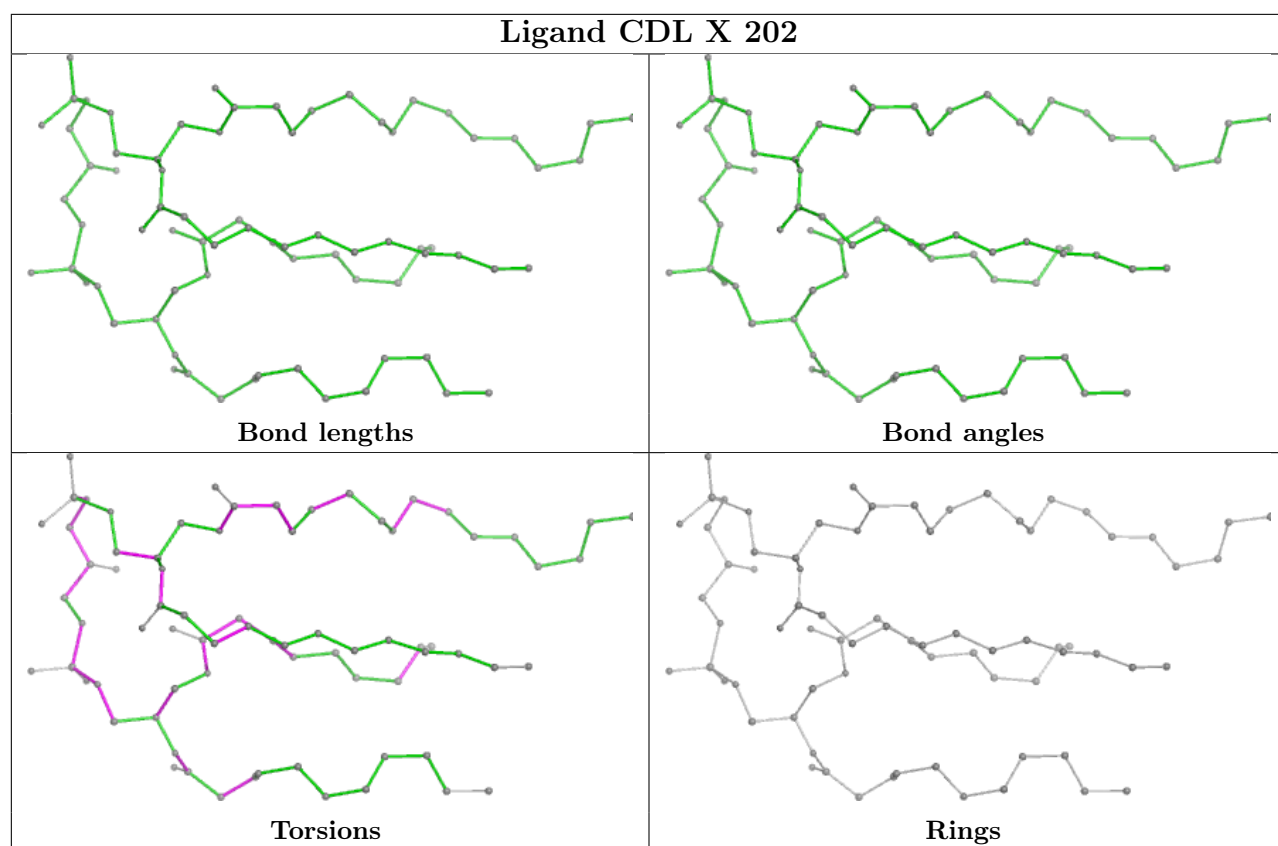
Ligand LMT 1 402

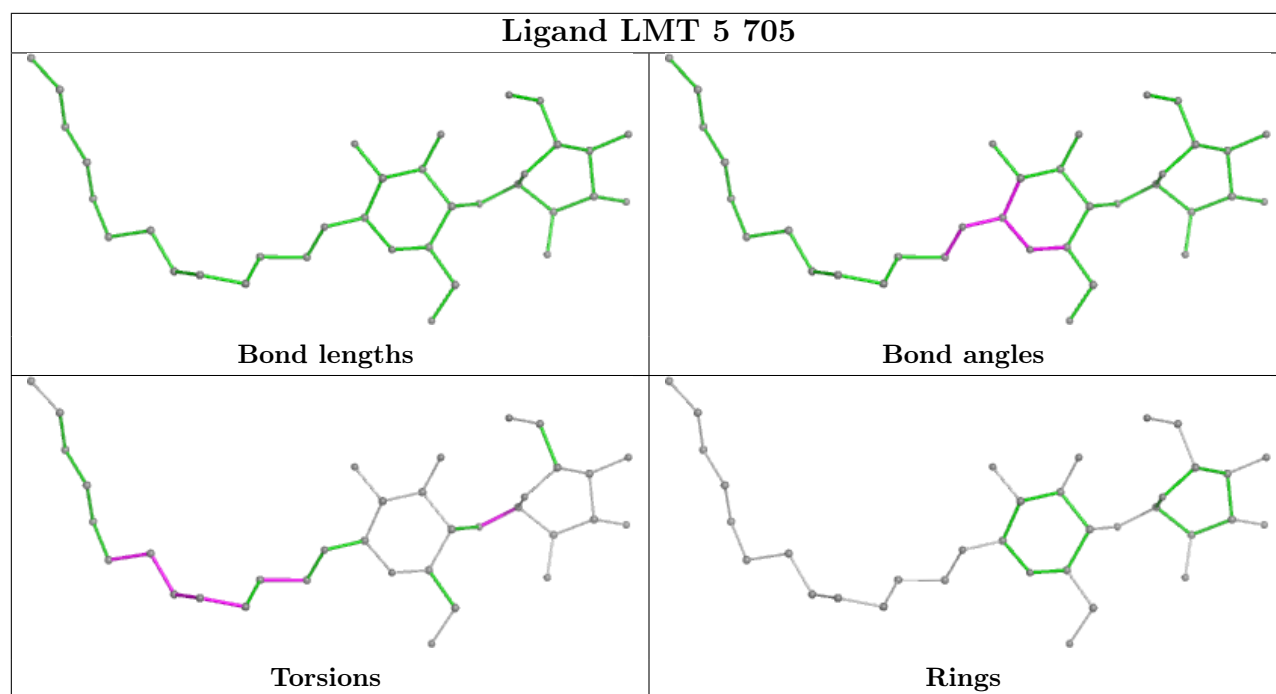
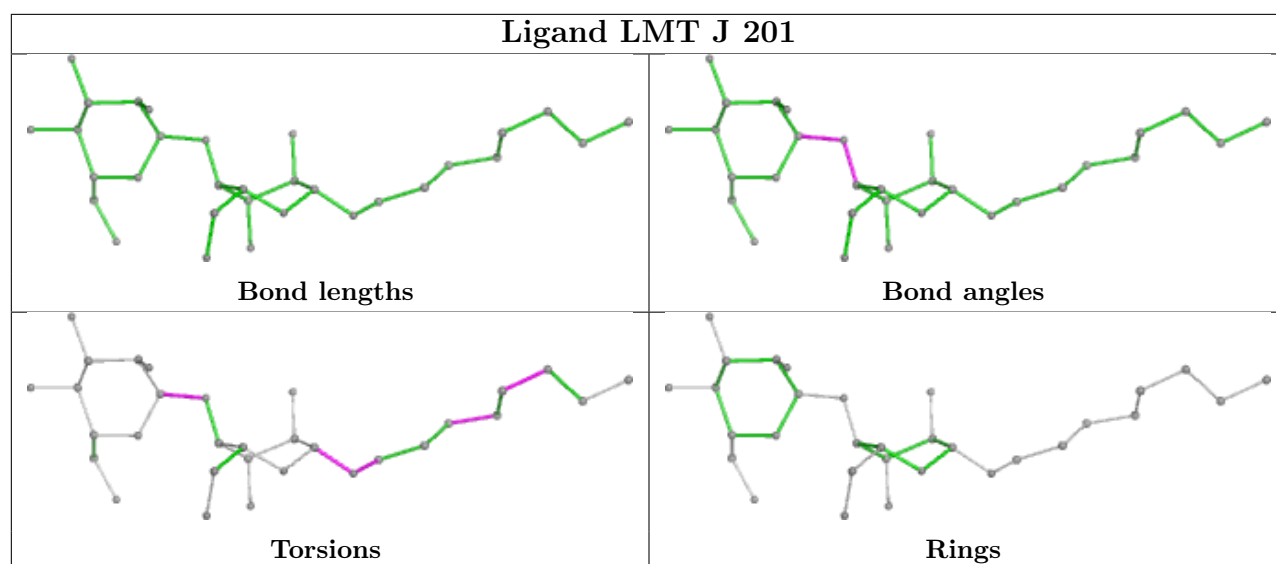


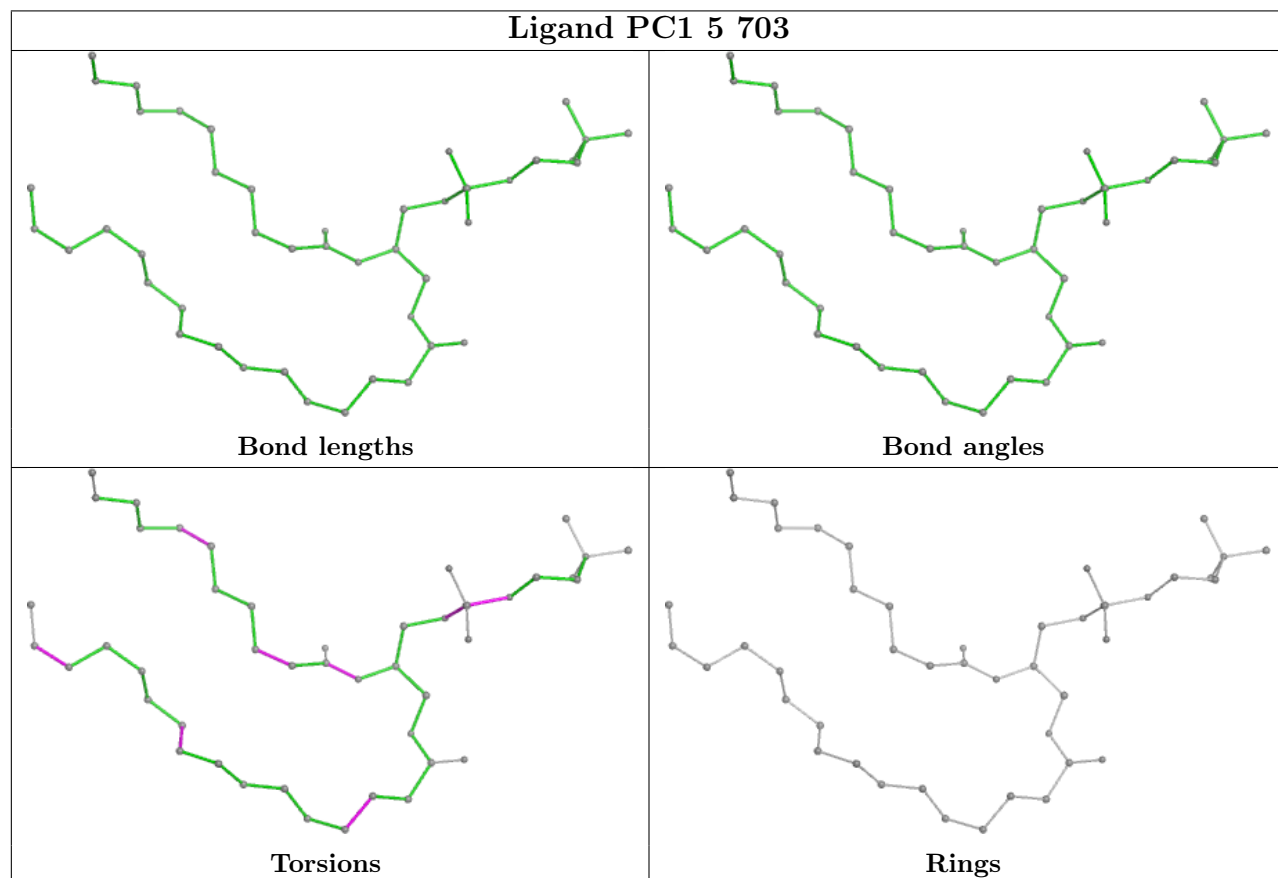
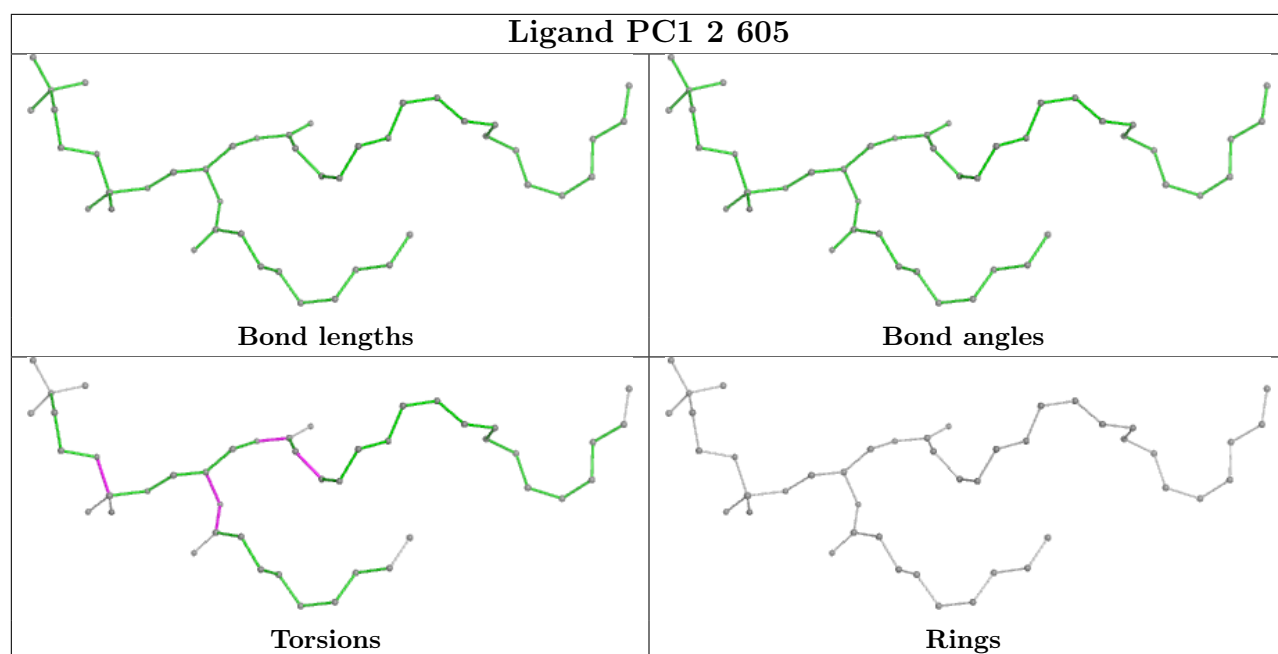


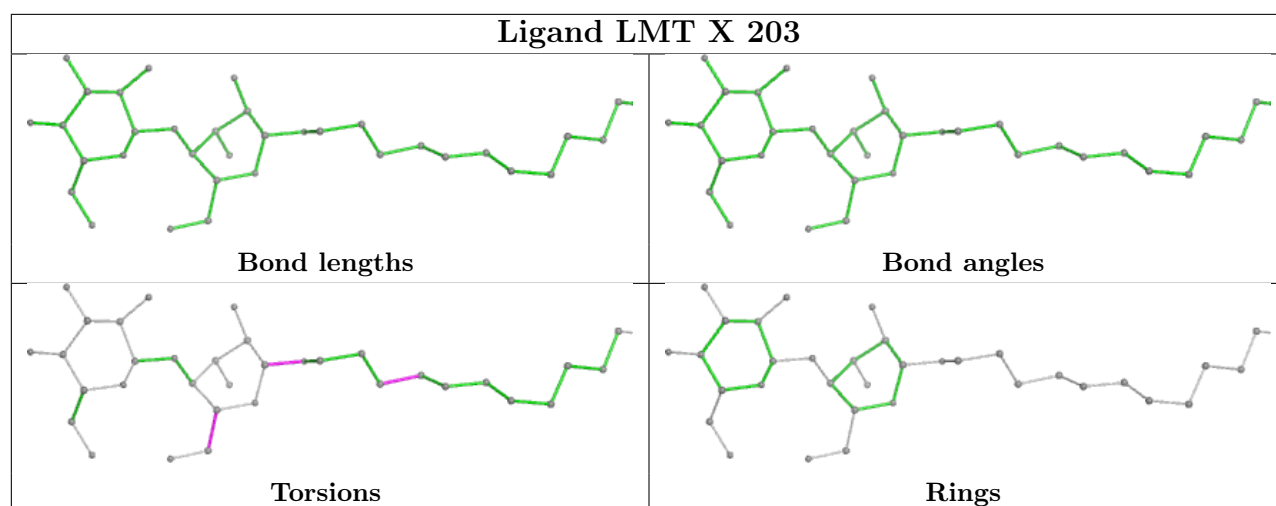












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

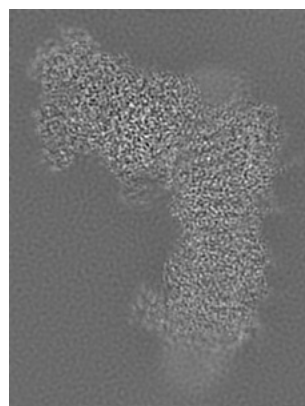
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14791. These allow visual inspection of the internal detail of the map and identification of artifacts.

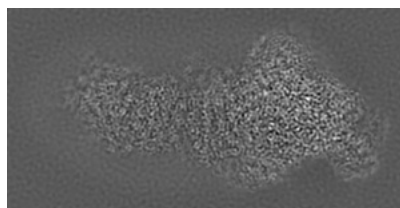
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

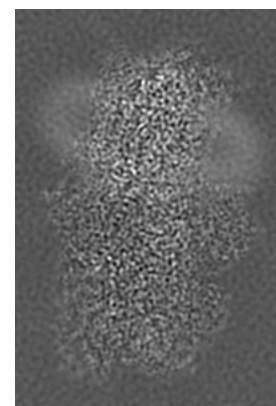
6.1.1 Primary map



X

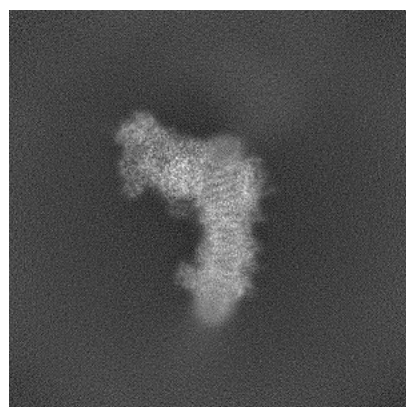


Y

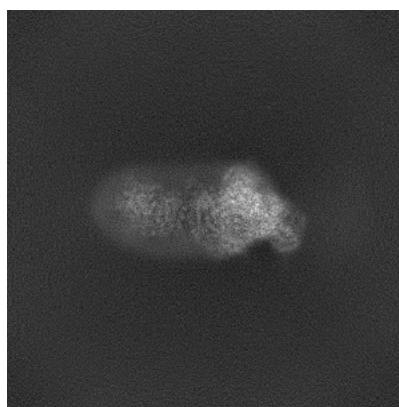


Z

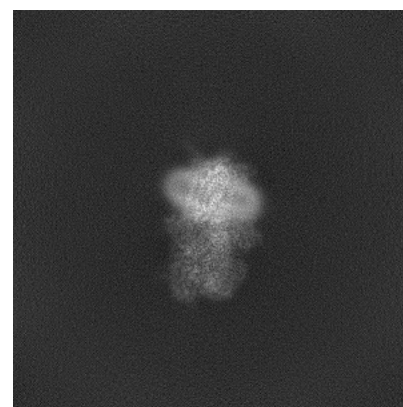
6.1.2 Raw map



X



Y

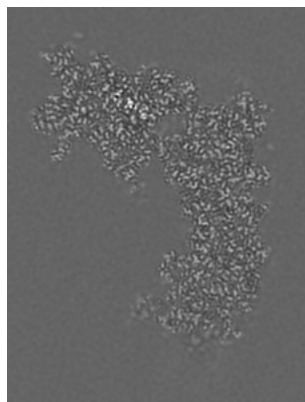


Z

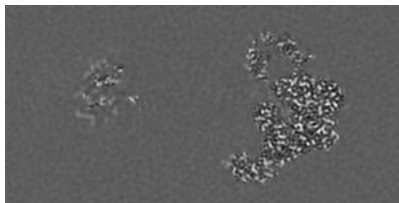
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

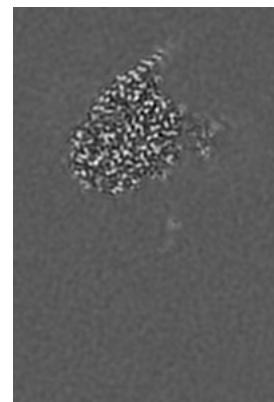
6.2.1 Primary map



X Index: 75

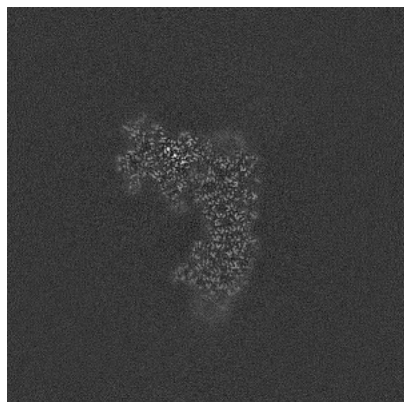


Y Index: 111

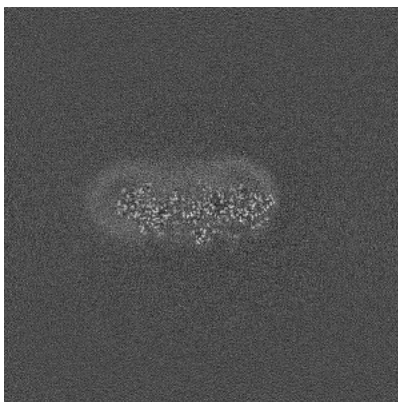


Z Index: 148

6.2.2 Raw map



X Index: 256



Y Index: 256

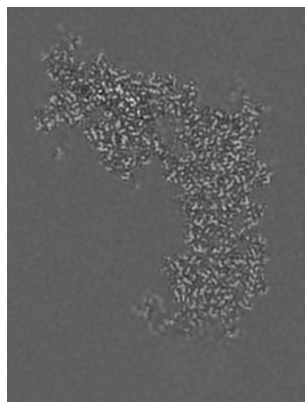


Z Index: 256

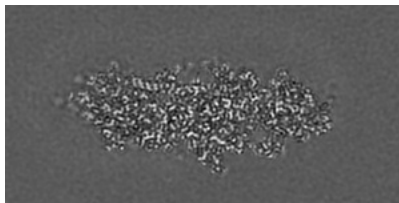
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

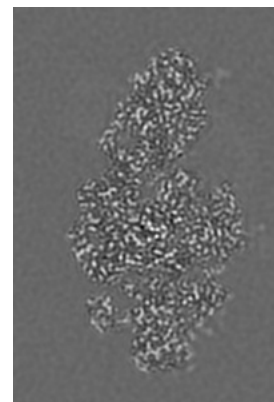
6.3.1 Primary map



X Index: 71

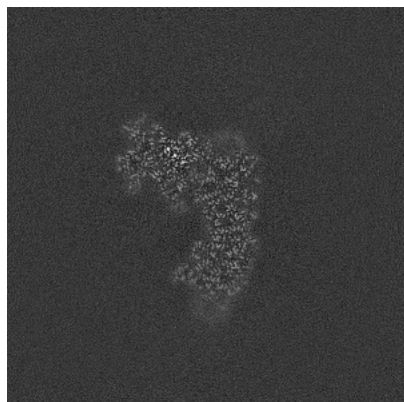


Y Index: 139

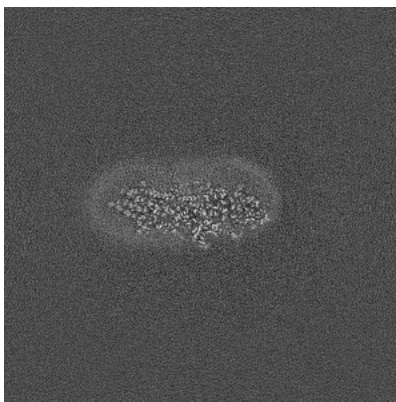


Z Index: 214

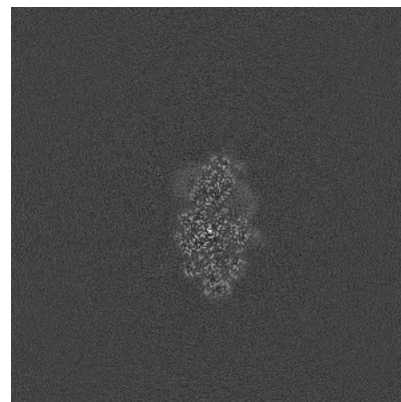
6.3.2 Raw map



X Index: 256



Y Index: 262

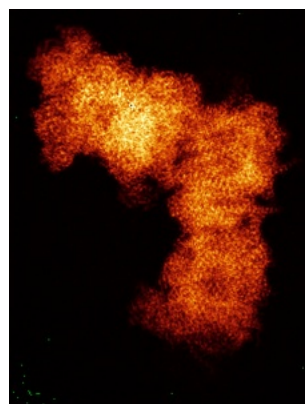


Z Index: 312

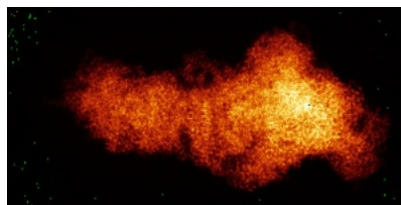
The images above show the largest variance slices of the map in three orthogonal directions.

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

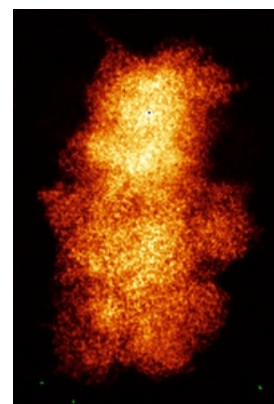
6.4.1 Primary map



X

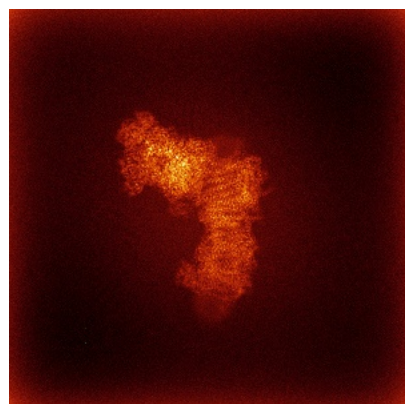


Y

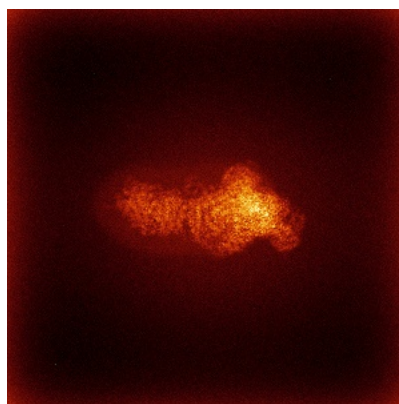


Z

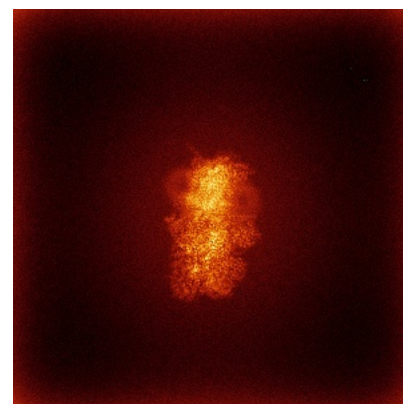
6.4.2 Raw map



X



Y

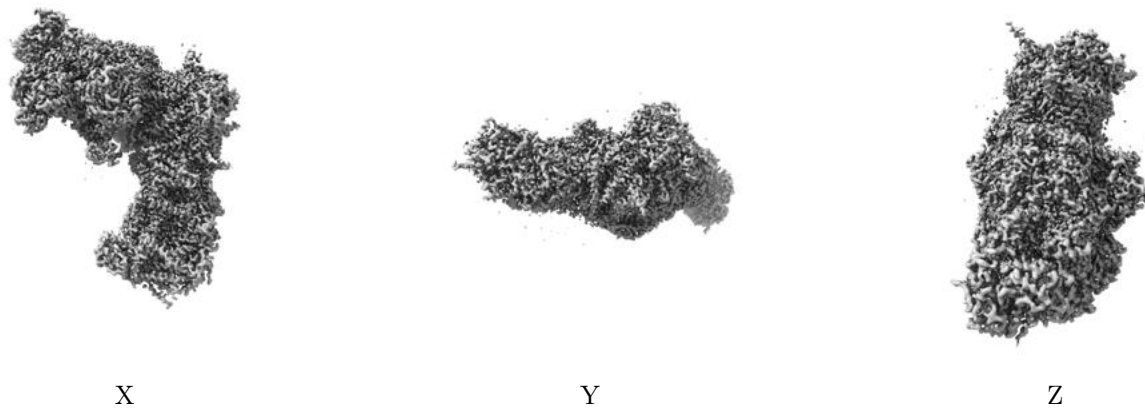


Z

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.

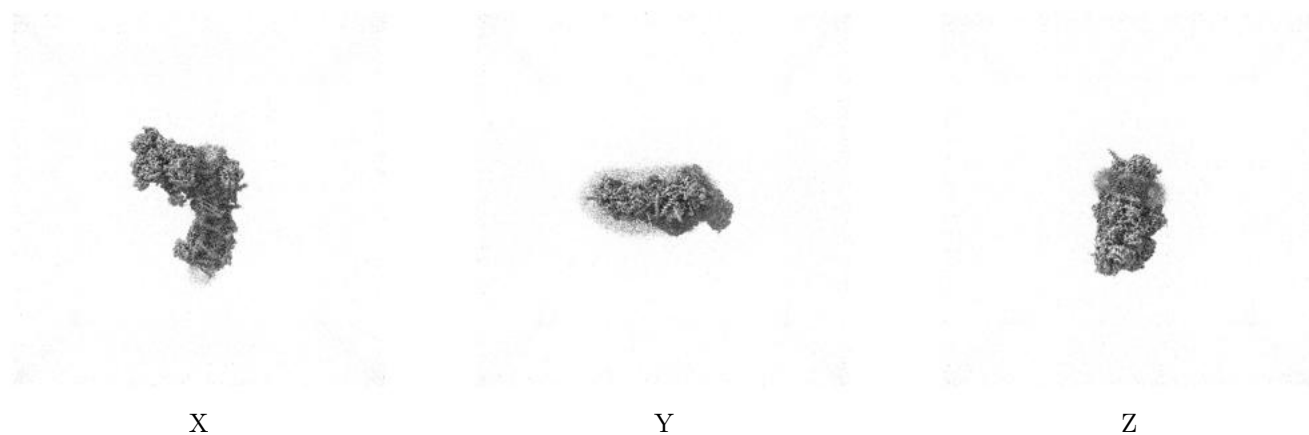
6.5 Orthogonal surface views [i](#)

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.

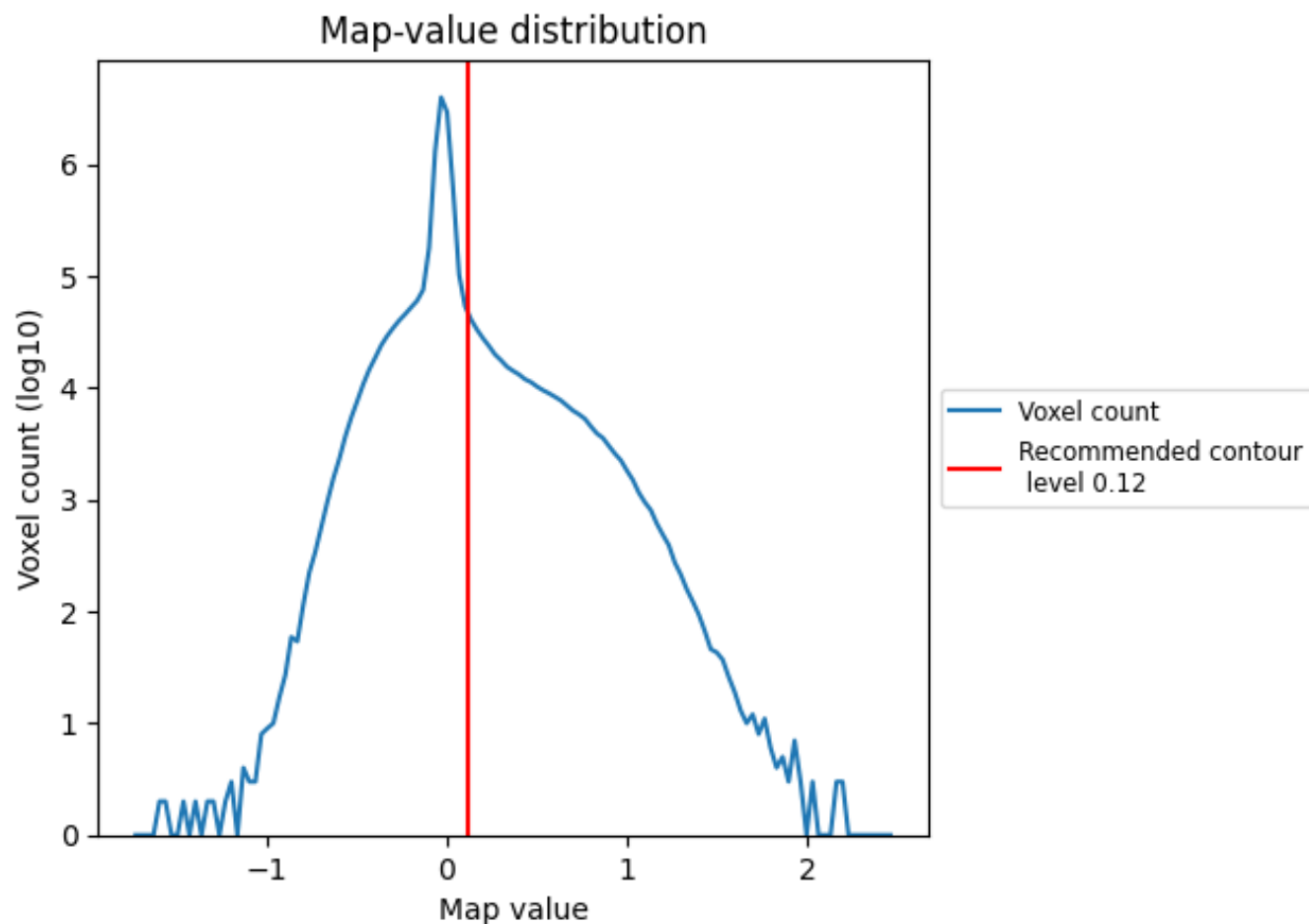
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

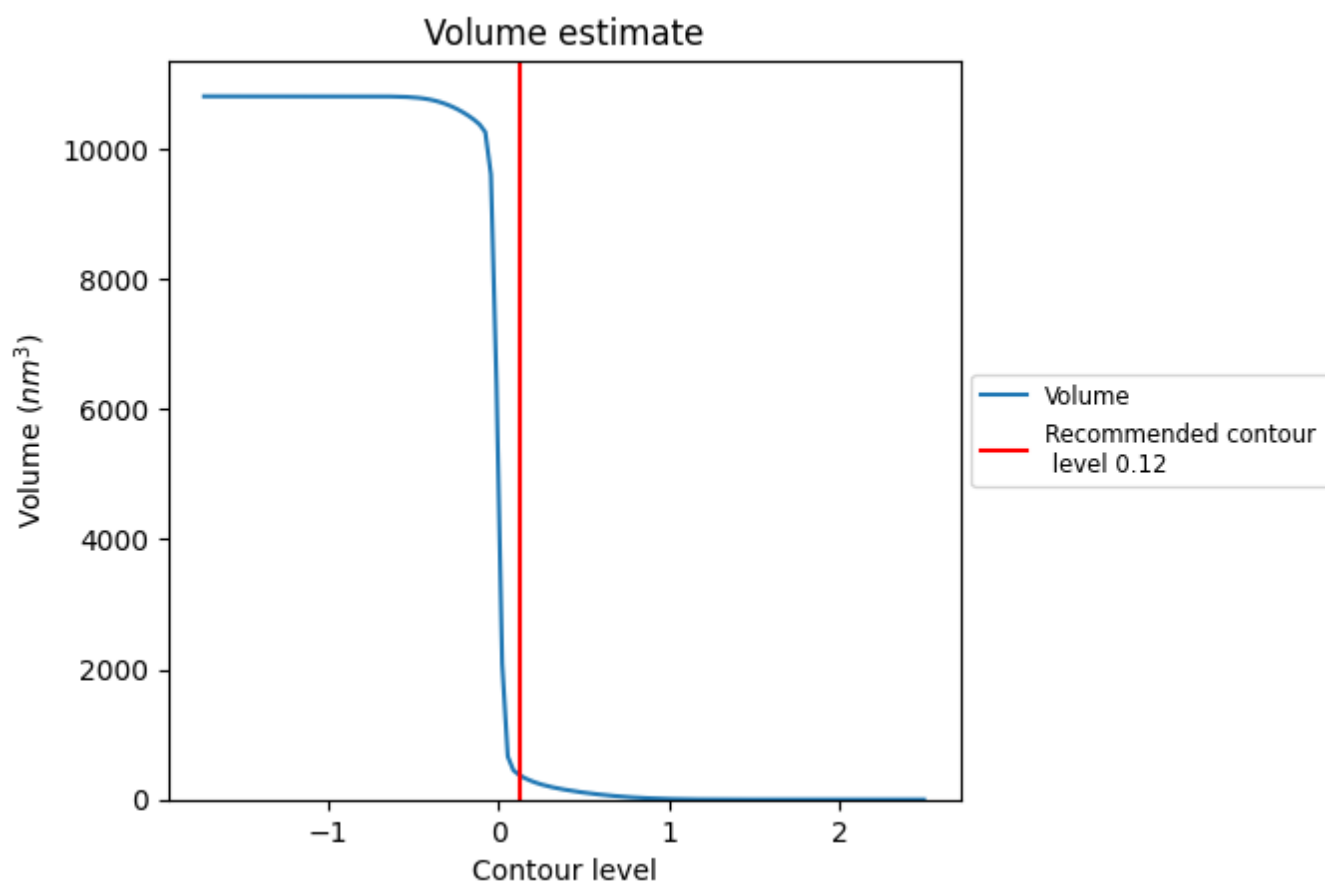
This section contains the results of statistical analysis of the map.

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 382 nm³; this corresponds to an approximate mass of 345 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.

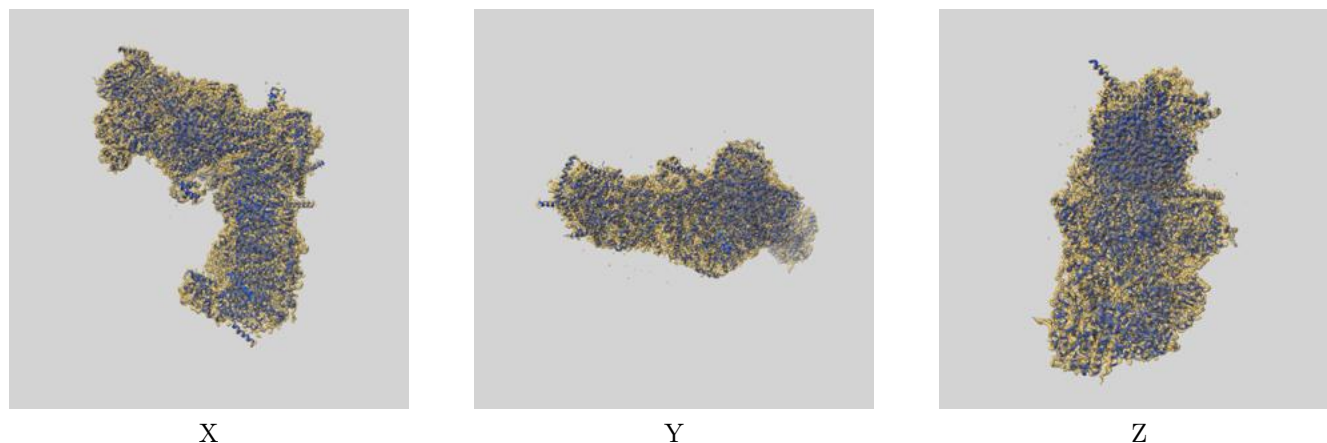
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

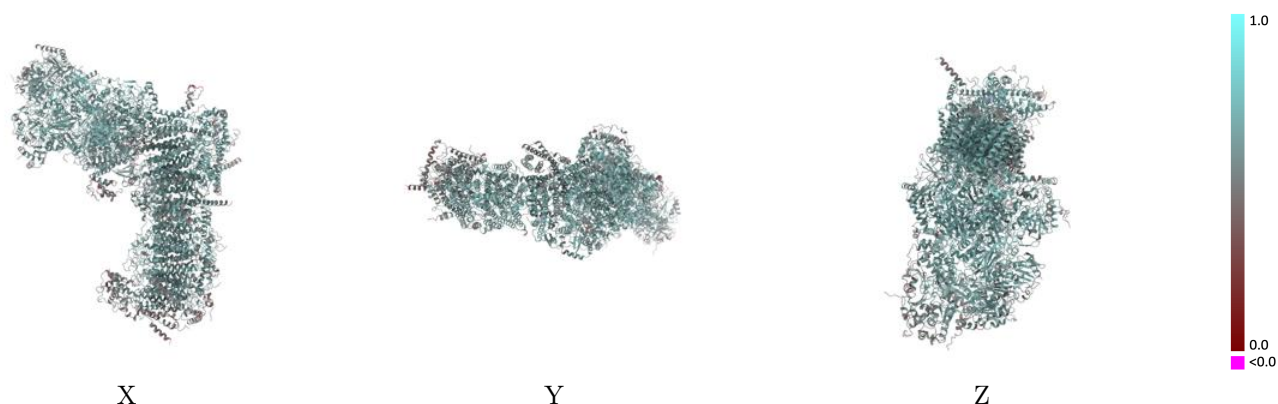
This section contains information regarding the fit between EMDB map EMD-14791 and PDB model 7ZM7. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



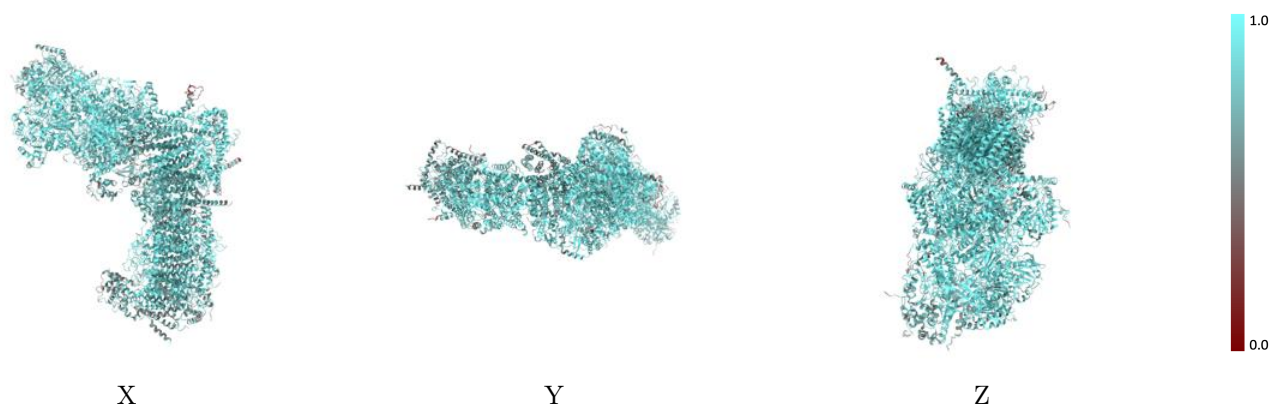
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



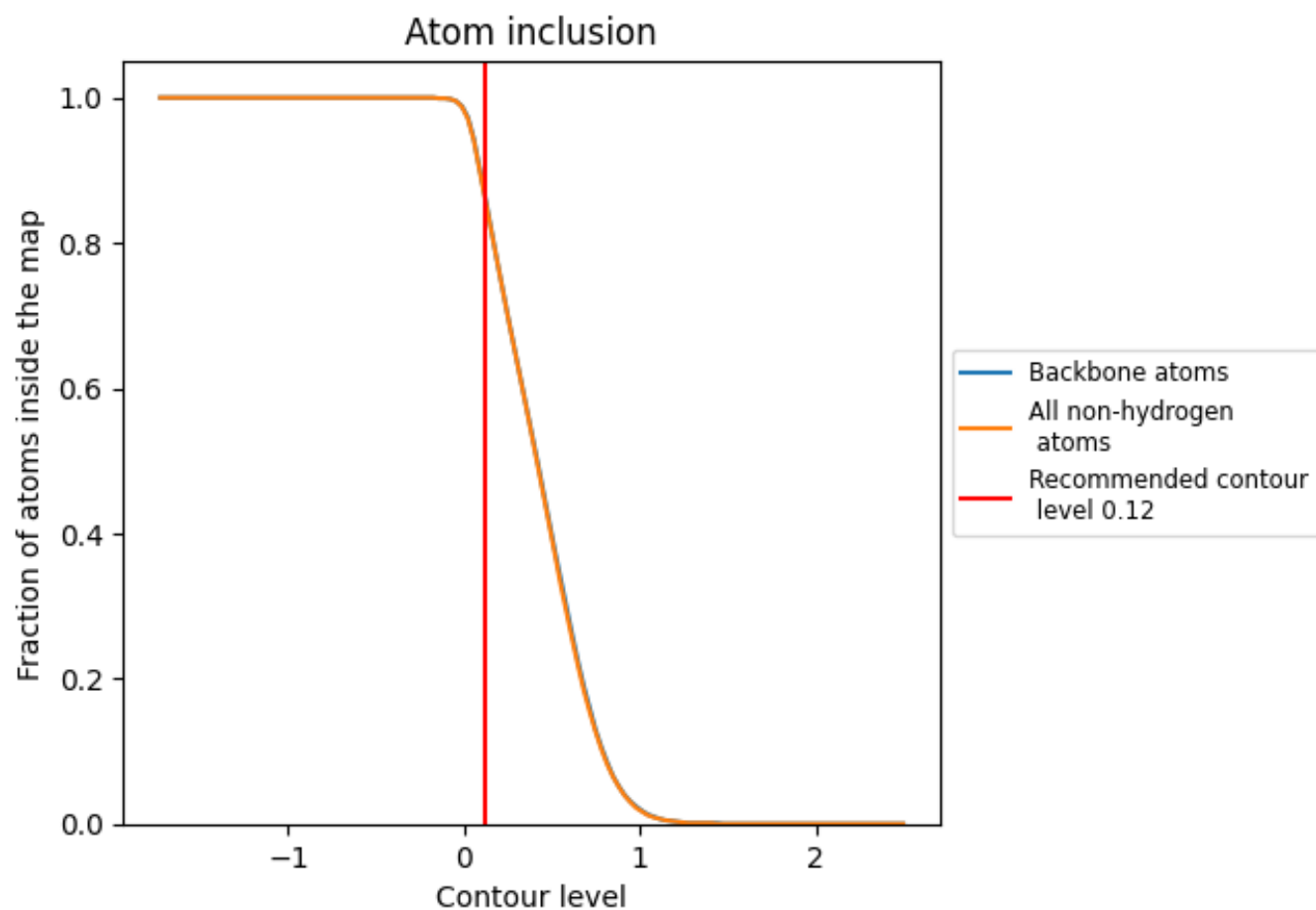
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



















The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.5980
1	 0.8390	 0.5950
2	 0.9270	 0.6390
3	 0.8270	 0.5880
4	 0.9500	 0.6400
5	 0.8450	 0.5820
6	 0.8710	 0.6040
8	 0.6820	 0.4830
9	 0.8110	 0.5780
A	 0.9100	 0.6200
B	 0.8300	 0.5650
C	 0.9330	 0.6490
D	 0.9230	 0.6350
E	 0.8580	 0.5840
F	 0.8550	 0.5930
G	 0.9410	 0.6580
H	 0.8300	 0.5630
I	 0.9450	 0.6540
J	 0.7010	 0.5290
K	 0.9260	 0.6300
L	 0.9200	 0.6260
M	 0.9120	 0.6240
O	 0.6440	 0.4590
P	 0.8830	 0.5880
Q	 0.6160	 0.4750
R	 0.7400	 0.5230
S	 0.8520	 0.5770
U	 0.9030	 0.6110
W	 0.8530	 0.6070
X	 0.8960	 0.6180
Y	 0.9230	 0.6330
Z	 0.8610	 0.5970
a	 0.7730	 0.5380
b	 0.8510	 0.5980
c	 0.6430	 0.4690



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.8680	 0.5980
e	 0.6410	 0.4690
f	 0.8140	 0.5510
g	 0.8450	 0.5910
h	 0.9100	 0.6340
i	 0.7690	 0.5560
j	 0.8400	 0.5850
n	 0.7880	 0.5660
o	 0.5890	 0.5030