



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 06:16 pm BST

PDB ID : 6YJ4 / pdb_00006yj4
EMDB ID : EMD-10815
Title : Structure of Yarrowia lipolytica complex I at 2.7 Å
Authors : Hirst, J.; Grba, D.
Deposited on : 2020-04-02
Resolution : 2.70 Å (reported)
Based on initial model : 6G2J

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
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) : 2.42

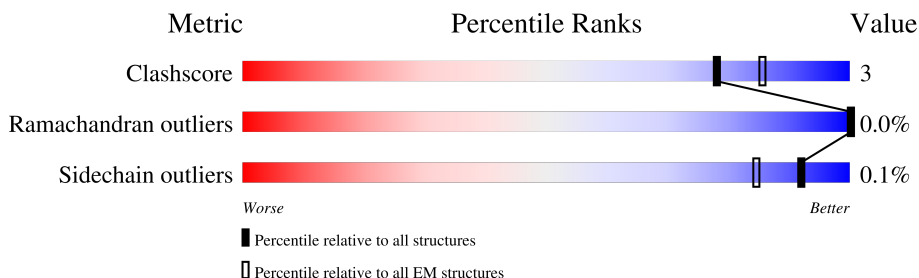
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.




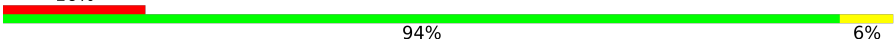
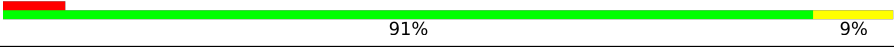
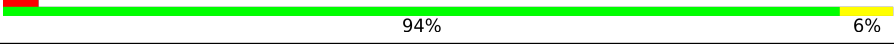
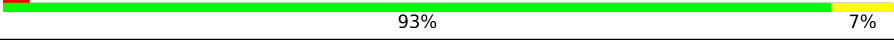
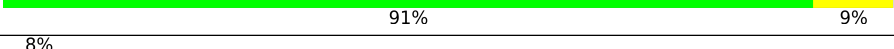
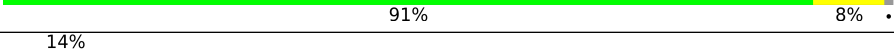
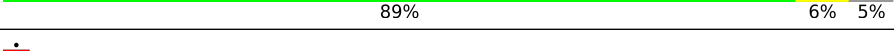
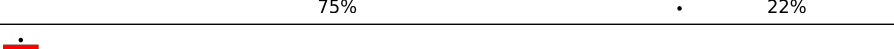
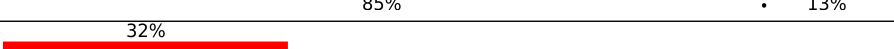


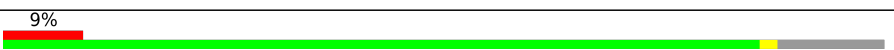

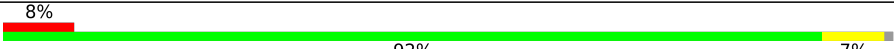


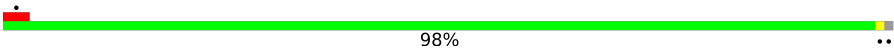
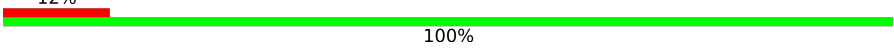
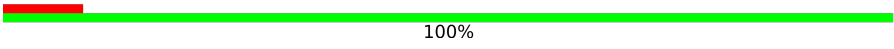
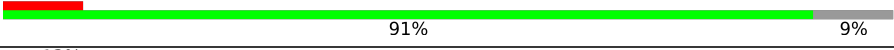
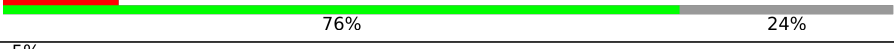
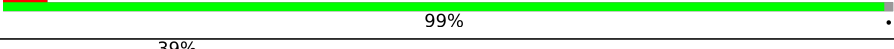


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	128	<div> <div>40%</div> <div> <div>92%</div> <div>8%</div> </div> </div>
2	B	210	<div> <div>79%</div> <div>5%</div> <div>16%</div> </div>
3	C	293	<div> <div>78%</div> <div>5%</div> <div>17%</div> </div>
4	D	466	<div> <div>6%</div> <div>82%</div> <div>11%</div> <div>6%</div> </div>
5	E	243	<div> <div>22%</div> <div>81%</div> <div>7%</div> <div>11%</div> </div>
6	F	488	<div> <div>14%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
7	G	728	<div> <div>7%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
8	H	341	<div> <div>13%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	229	
10	J	185	
11	K	89	
12	L	655	
13	M	486	
14	N	469	
15	O	169	
16	P	375	
17	Q	161	
18	R	136	
19	S	87	
20	T	109	
21	U	132	
22	V	144	
23	W	124	
24	X	172	
25	Y	198	
26	Z	123	
27	a	87	
28	b	78	
29	c	182	
30	d	74	
31	e	89	
32	f	138	
33	g	249	

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Mol	Chain	Length	Quality of chain
34	h	139	
35	i	90	
36	j	91	
37	k	60	
38	l	149	
39	m	93	
40	n	109	
41	o	99	
42	p	92	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	3PE	A	501	X	-	-	-
43	3PE	H	602	X	-	-	-
43	3PE	M	502	X	-	-	-
43	3PE	Y	4203	X	-	-	-
43	3PE	Z	202	X	-	-	-
43	3PE	d	4603	X	-	-	-
45	LMT	B	302	X	-	-	-
45	LMT	M	503	X	-	-	-
45	LMT	Y	4201	X	-	-	-
45	LMT	Y	4202	X	-	-	-
45	LMT	Y	4204	X	-	-	-
48	FMN	F	501	X	-	-	-
52	EHZ	T	201	X	-	-	-
52	EHZ	U	201	X	-	-	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 66311 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	128	Total	C	N	O	S	0	0
			1006	684	150	169	3		

- Molecule 2 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

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

- Molecule 3 is a protein called NUGM protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	242	Total	C	N	O	S	0	0
			1999	1285	339	371	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	282	ALA	-	expression tag	UNP Q9UUU0
C	283	ALA	-	expression tag	UNP Q9UUU0
C	284	ALA	-	expression tag	UNP Q9UUU0
C	285	ALA	-	expression tag	UNP Q9UUU0
C	286	ALA	-	expression tag	UNP Q9UUU0
C	287	ALA	-	expression tag	UNP Q9UUU0
C	288	HIS	-	expression tag	UNP Q9UUU0
C	289	HIS	-	expression tag	UNP Q9UUU0
C	290	HIS	-	expression tag	UNP Q9UUU0
C	291	HIS	-	expression tag	UNP Q9UUU0
C	292	HIS	-	expression tag	UNP Q9UUU0
C	293	HIS	-	expression tag	UNP Q9UUU0

- Molecule 4 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	437	Total	C	N	O	S	0	0
			3465	2202	594	647	22		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	460	Total	C	N	O	S	0	0
			3559	2248	629	658	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	694	Total	C	N	O	S	0	0
			5274	3275	928	1042	29		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	341	Total	C	N	O	S	0	0
			2709	1843	394	465	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	191	Total	C	N	O	S	0	0
			1526	972	255	289	10		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	185	Total	C	N	O	S	0	0
			1462	990	209	254	9		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	89	Total	C	N	O	S	0	0
			693	465	109	116	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	655	Total	C	N	O	S	0	0
			5207	3485	786	907	29		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	486	Total	C	N	O	S	0	0
			3857	2601	586	655	15		

- Molecule 14 is a protein called NADH dehydrogenase subunit 2.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	168	Total	C	N	O	S	0	0
			1305	845	223	233	4		

- Molecule 16 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	355	Total	C	N	O	S	0	0
			2812	1785	493	524	10		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	118	Total	C	N	O	S	0	0
			922	574	166	177	5		

- Molecule 19 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	86	Total	C	N	O	S	0	0
			667	418	126	122	1		

- Molecule 20 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	81	Total	C	N	O	S	0	0
			620	391	98	131			

- Molecule 21 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	88	Total	C	N	O	S	0	0
			667	416	106	143	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	126	Total	C	N	O	S	0	0
			1028	653	173	200	2		

- Molecule 23 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

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

- Molecule 25 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	179	Total	C	N	O	S	0	0
			1327	842	240	240	5		

- Molecule 26 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	122	Total	C	N	O	S	0	0
			983	629	180	169	5		

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

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

- Molecule 28 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	78	Total	C	N	O	S	0	0
			639	418	115	105	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	182	Total	C	N	O	S	0	0
			1397	898	241	256	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	67	Total	C	N	O	S	0	0
			510	339	86	85			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	68	Total	C	N	O	S	0	0
			546	336	102	102	6		

- Molecule 32 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	137	Total	C	N	O	S	0	0
			1136	730	194	210	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	198	Total	C	N	O	S	0	0
			1585	1019	273	291	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	113	Total	C	N	O	S	0	0
			909	585	153	170	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	86	Total	C	N	O	S	0	0
			659	420	120	118	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	53	Total	C	N	O	S	0	0
			445	299	77	66	3		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-23	MET	-	initiating methionine	UNP A0A1D8NFX6
j	-22	HIS	-	expression tag	UNP A0A1D8NFX6
j	-21	ASN	-	expression tag	UNP A0A1D8NFX6
j	-20	SER	-	expression tag	UNP A0A1D8NFX6
j	-19	SER	-	expression tag	UNP A0A1D8NFX6
j	-18	SER	-	expression tag	UNP A0A1D8NFX6
j	-17	VAL	-	expression tag	UNP A0A1D8NFX6
j	-16	HIS	-	expression tag	UNP A0A1D8NFX6
j	-15	HIS	-	expression tag	UNP A0A1D8NFX6
j	-14	HIS	-	expression tag	UNP A0A1D8NFX6
j	-13	TYR	-	expression tag	UNP A0A1D8NFX6
j	-12	ILE	-	expression tag	UNP A0A1D8NFX6
j	-11	SER	-	expression tag	UNP A0A1D8NFX6
j	-10	LYS	-	expression tag	UNP A0A1D8NFX6
j	-9	THR	-	expression tag	UNP A0A1D8NFX6
j	-8	THR	-	expression tag	UNP A0A1D8NFX6
j	-7	GLY	-	expression tag	UNP A0A1D8NFX6
j	-6	PHE	-	expression tag	UNP A0A1D8NFX6
j	-5	PHE	-	expression tag	UNP A0A1D8NFX6
j	-4	ARG	-	expression tag	UNP A0A1D8NFX6
j	-3	PHE	-	expression tag	UNP A0A1D8NFX6
j	-2	ARG	-	expression tag	UNP A0A1D8NFX6
j	-1	TYR	-	expression tag	UNP A0A1D8NFX6
j	0	LYS	-	expression tag	UNP A0A1D8NFX6

- Molecule 37 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	47	Total	C	N	O	0	0
			373	242	70	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	125	Total	C	N	O	S	0	0
			1039	674	166	197	2		

- Molecule 39 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
39	m	92	Total	C	N	O	0	0
			735	472	134	129		

- Molecule 40 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	108	Total	C	N	O	S	0	0
			900	571	172	154	3		

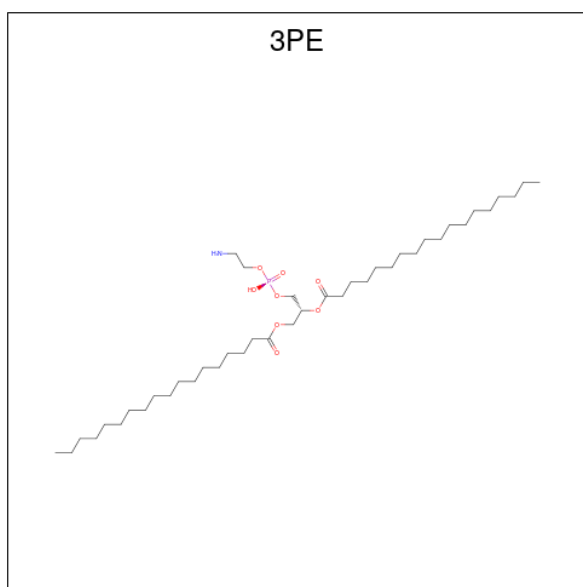
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	83	Total	C	N	O	S	0	0
			681	431	123	119	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	91	Total	C	N	O	S	0	0
			766	475	138	150	3		

- Molecule 43 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



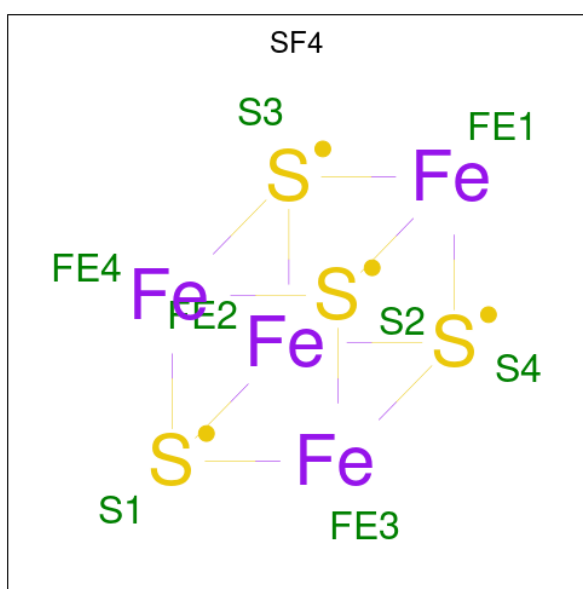
Mol	Chain	Residues	Atoms					AltConf
43	A	1	Total	C	N	O	P	0
			27	17	1	8	1	
43	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	H	1	Total	C	N	O	P	0
			22	12	1	8	1	
43	I	1	Total	C	N	O	P	0
			46	36	1	8	1	
43	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	L	1	Total	C	N	O	P	0
			33	23	1	8	1	
43	M	1	Total	C	N	O	P	0
			30	20	1	8	1	
43	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
43	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	Y	1	Total	C	N	O	P	0
			24	14	1	8	1	
43	Z	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	Z	1	Total	C	N	O	P	0
			43	33	1	8	1	

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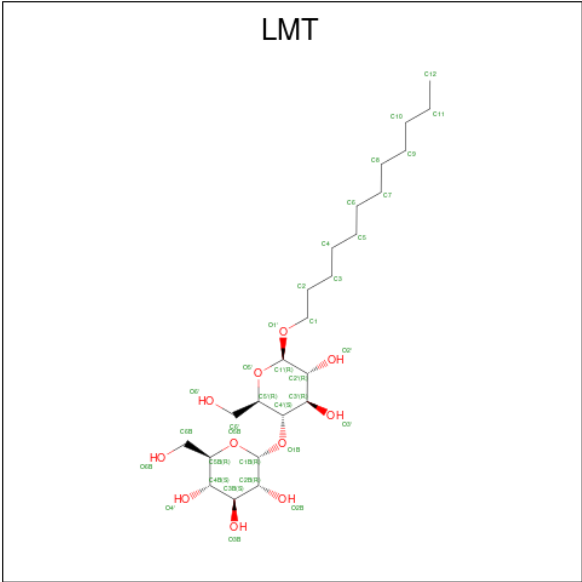
Mol	Chain	Residues	Atoms					AltConf
43	b	1	Total	C	N	O	P	0
			43	33	1	8	1	
43	b	1	Total	C	N	O	P	0
			26	16	1	8	1	
43	d	1	Total	C	N	O	P	0
			24	14	1	8	1	
43	d	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 44 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



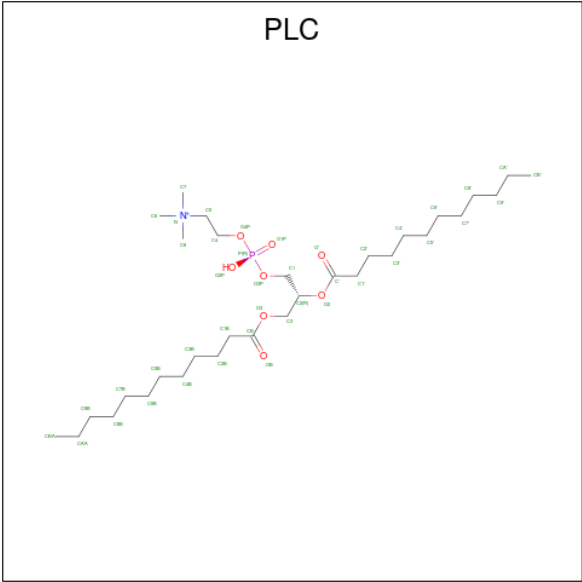
Mol	Chain	Residues	Atoms			AltConf
44	B	1	Total	Fe	S	0
			8	4	4	
44	F	1	Total	Fe	S	0
			8	4	4	
44	G	1	Total	Fe	S	0
			8	4	4	
44	G	1	Total	Fe	S	0
			8	4	4	
44	I	1	Total	Fe	S	0
			8	4	4	
44	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



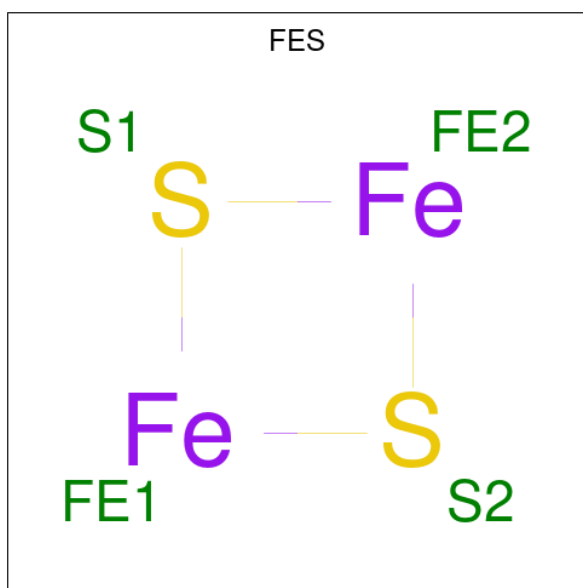
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	

- Molecule 46 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



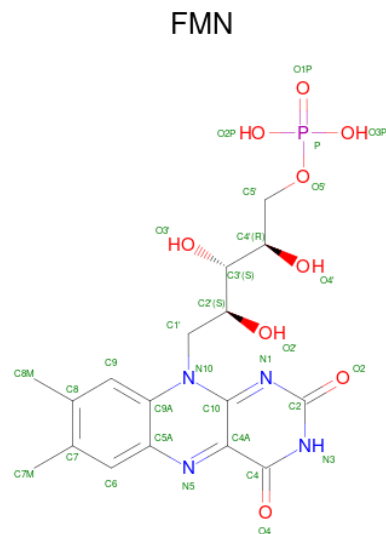
Mol	Chain	Residues	Atoms					AltConf
46	D	1	Total	C	N	O	P	0
			27	17	1	8	1	
46	H	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	L	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	L	1	Total	C	N	O	P	0
			29	19	1	8	1	
46	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	P	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	d	1	Total	C	N	O	P	0
			27	17	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



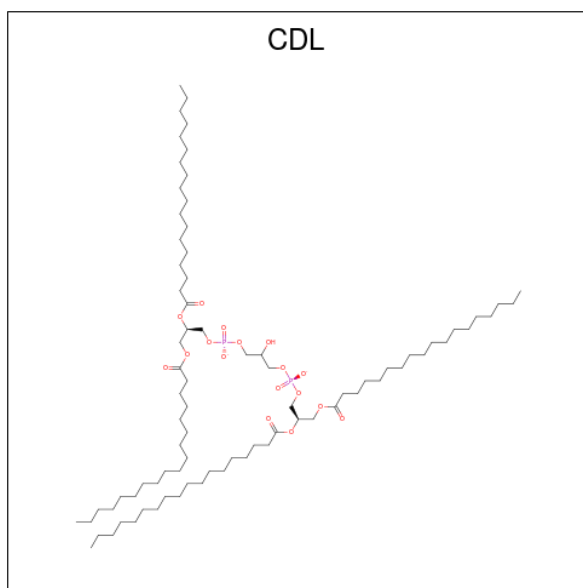
Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



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

- Molecule 49 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



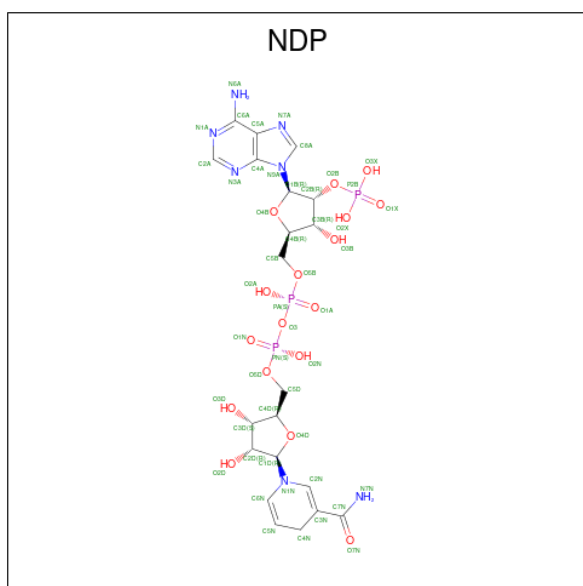
Mol	Chain	Residues	Atoms				AltConf
49	M	1	Total 83	C 64	O 17	P 2	0
49	O	1	Total 63	C 44	O 17	P 2	0
49	P	1	Total 48	C 29	O 17	P 2	0

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Mol	Chain	Residues	Atoms				AltConf
49	Z	1	Total	C	O	P	0
			57	38	17	2	
49	a	1	Total	C	O	P	0
			52	33	17	2	
49	b	1	Total	C	O	P	0
			48	29	17	2	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

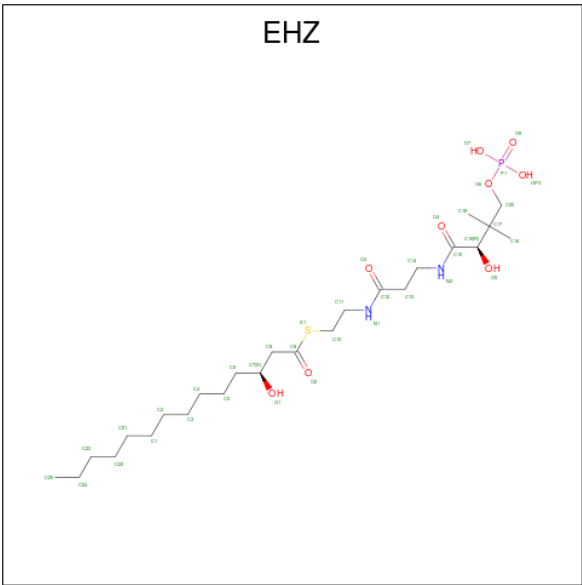


Mol	Chain	Residues	Atoms					AltConf
50	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 52 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms						AltConf
52	T	1	Total	C	N	O	P	S	0
			34	22	2	8	1	1	
52	U	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 53 is water.

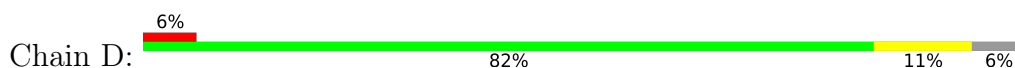
Mol	Chain	Residues	Atoms		AltConf
53	A	2	Total	O	0
			2	2	
53	B	15	Total	O	0
			15	15	
53	C	15	Total	O	0
			15	15	
53	D	20	Total	O	0
			20	20	
53	E	2	Total	O	0
			2	2	
53	F	7	Total	O	0
			7	7	
53	G	25	Total	O	0
			25	25	
53	H	10	Total	O	0
			10	10	
53	I	18	Total	O	0
			18	18	
53	J	4	Total	O	0
			4	4	

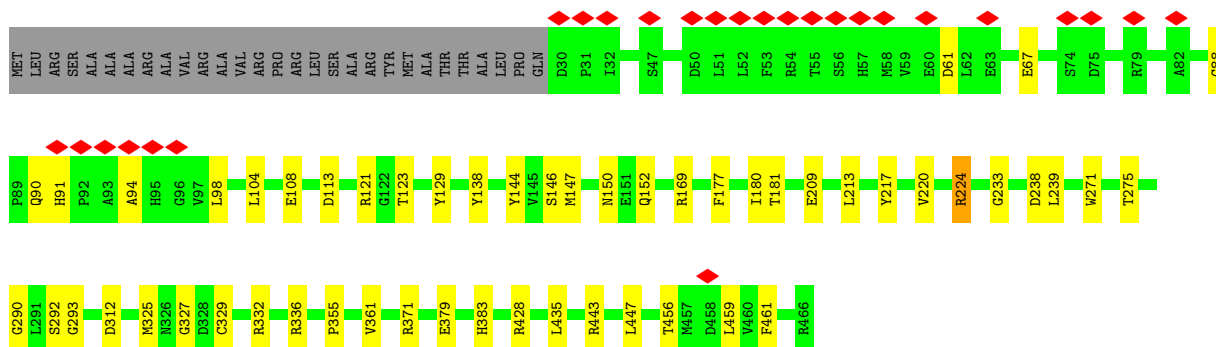
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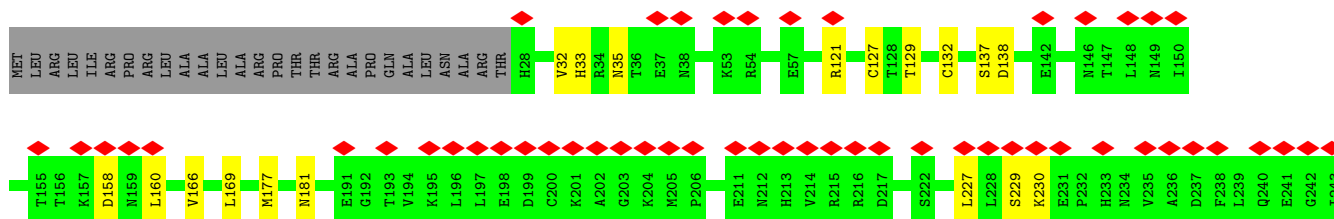
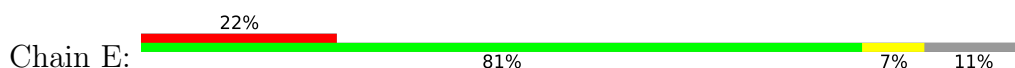
Mol	Chain	Residues	Atoms		AltConf
53	K	3	Total 3	O 3	0
53	L	27	Total 27	O 27	0
53	M	25	Total 25	O 25	0
53	N	37	Total 37	O 37	0
53	O	4	Total 4	O 4	0
53	P	14	Total 14	O 14	0
53	Q	7	Total 7	O 7	0
53	R	3	Total 3	O 3	0
53	W	4	Total 4	O 4	0
53	X	1	Total 1	O 1	0
53	Z	3	Total 3	O 3	0
53	a	3	Total 3	O 3	0
53	c	3	Total 3	O 3	0
53	f	4	Total 4	O 4	0
53	h	1	Total 1	O 1	0
53	i	2	Total 2	O 2	0
53	l	4	Total 4	O 4	0
53	m	4	Total 4	O 4	0
53	n	2	Total 2	O 2	0
53	o	1	Total 1	O 1	0
53	p	5	Total 5	O 5	0

- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

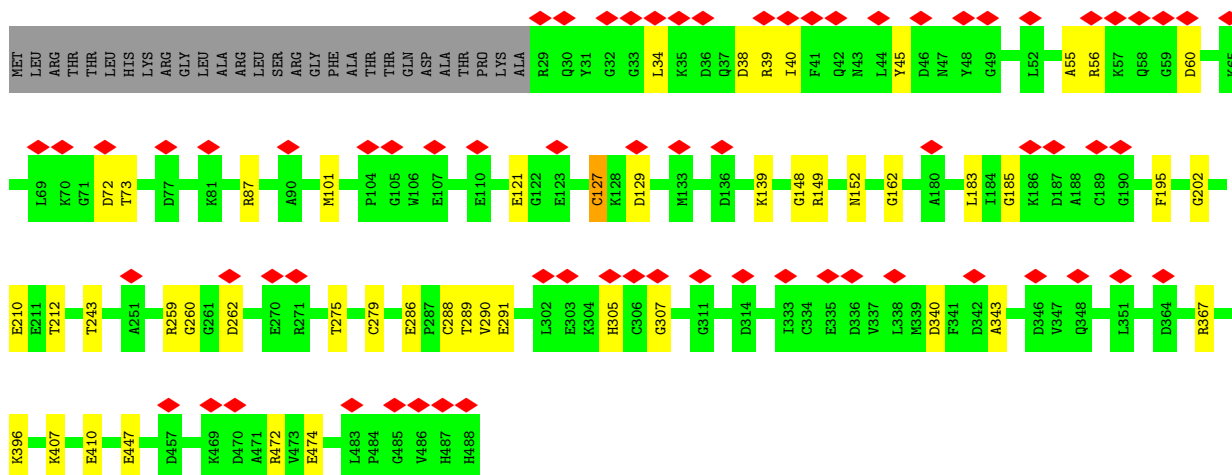
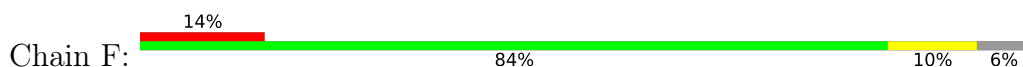




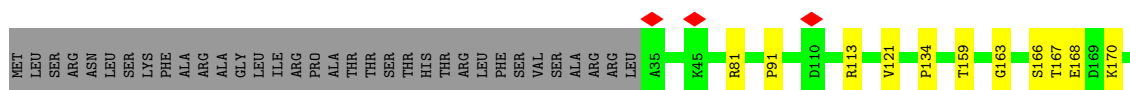
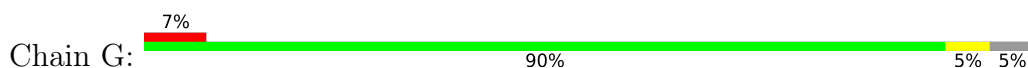
• Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

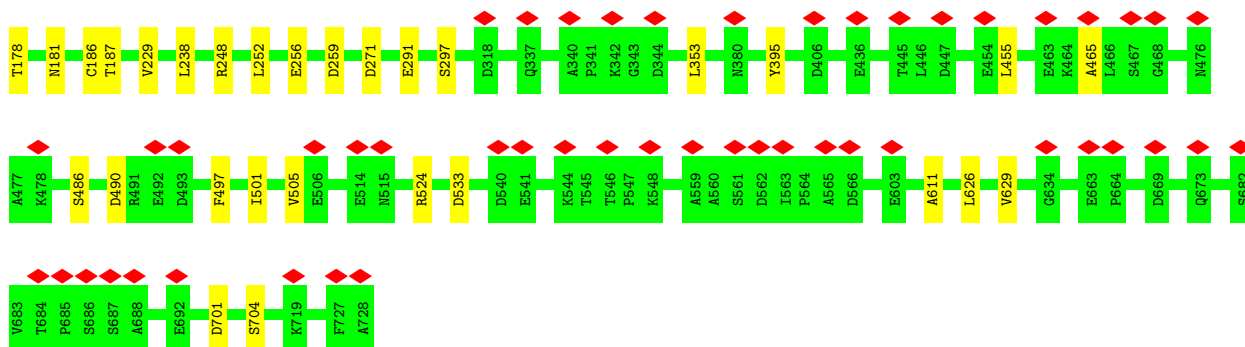


• Molecule 6: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)

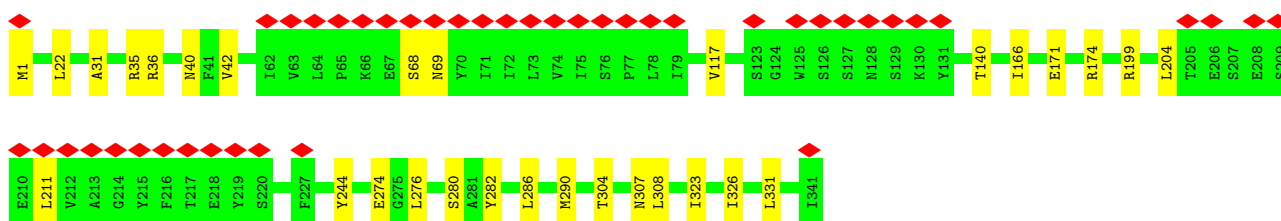


• Molecule 7: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)

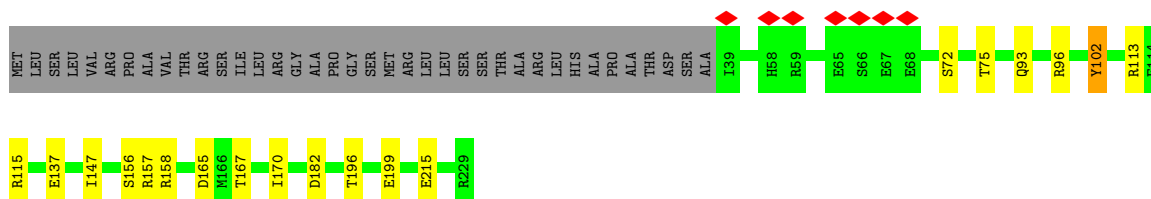




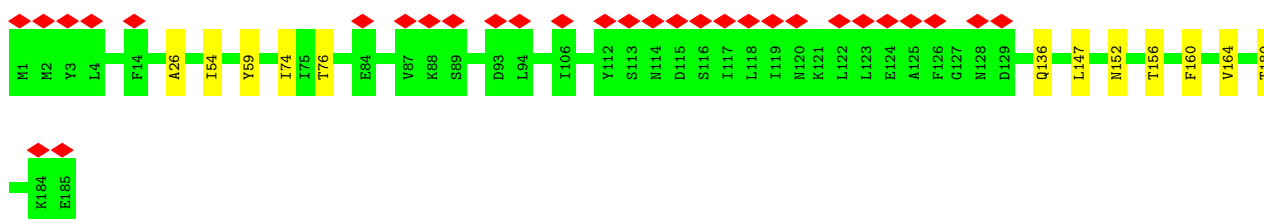
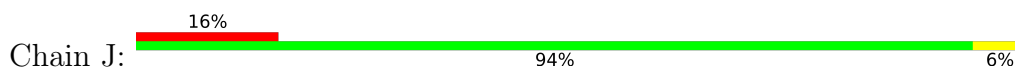
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



• Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

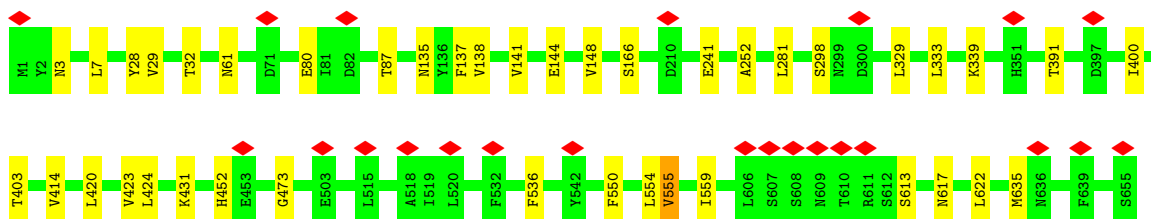


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

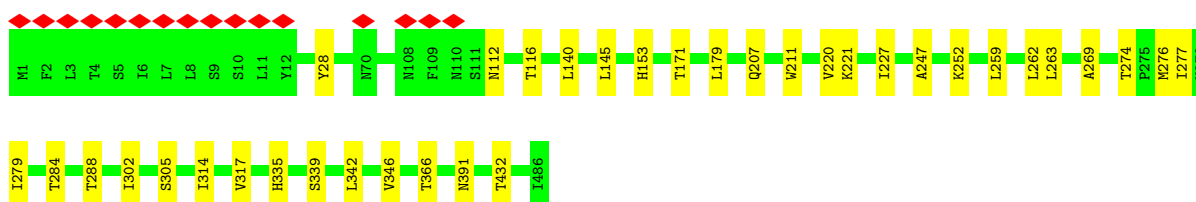




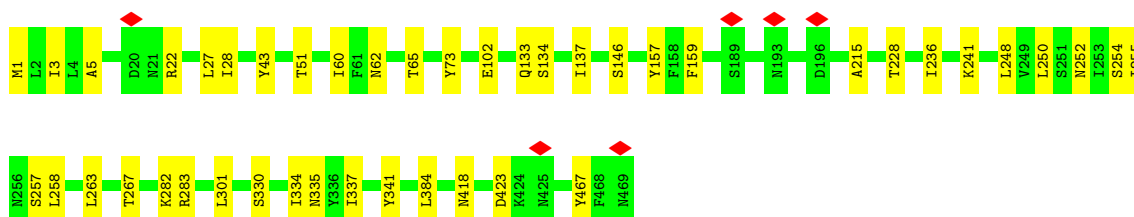
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



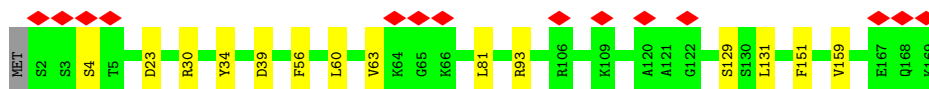
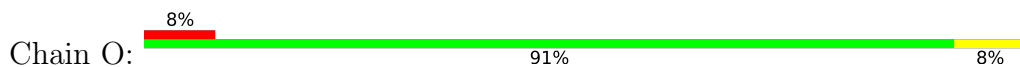
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



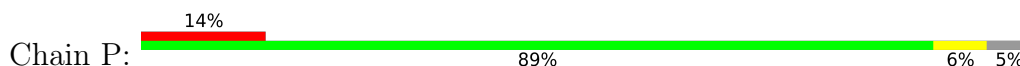
- Molecule 14: NADH dehydrogenase subunit 2

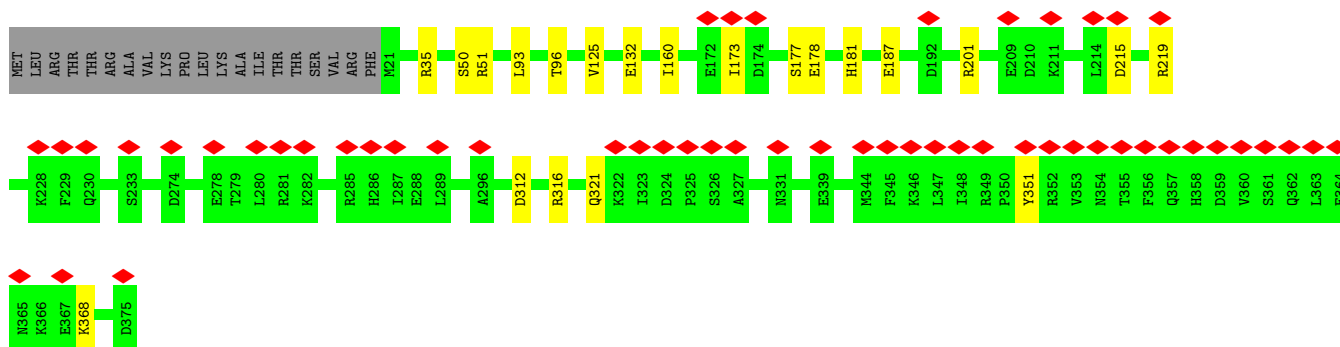


- Molecule 15: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

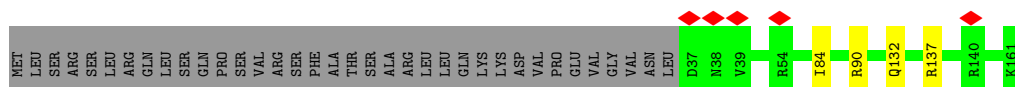
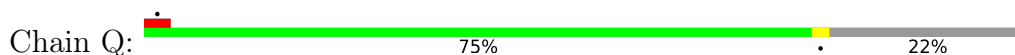


- Molecule 16: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

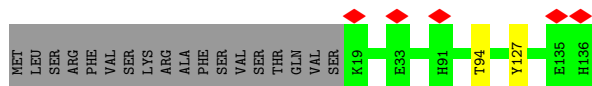
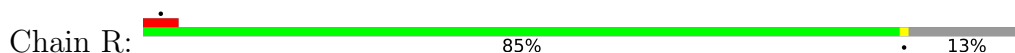




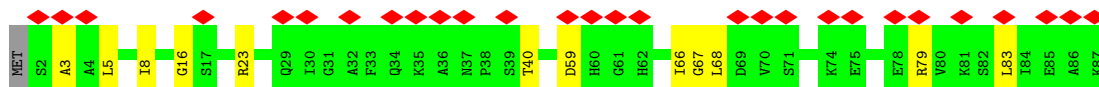
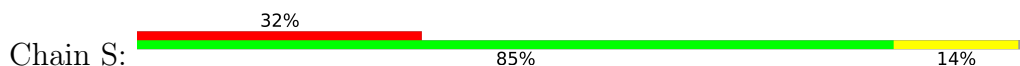
- Molecule 17: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)



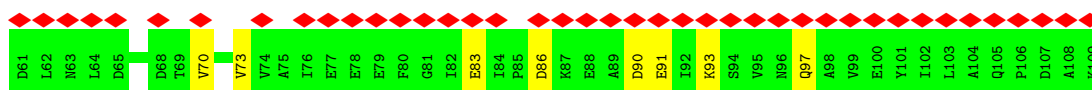
- Molecule 18: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



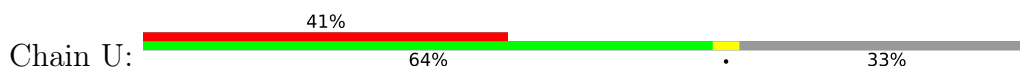
- Molecule 19: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)

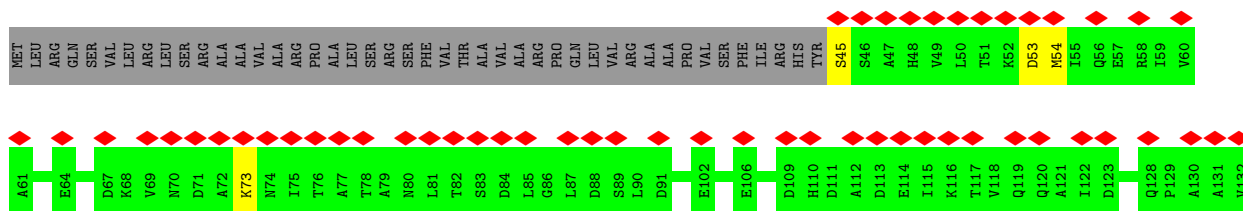


- Molecule 20: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)

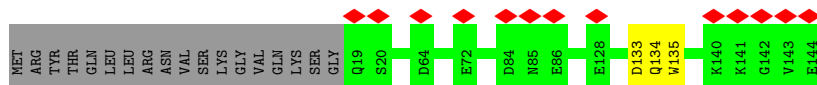
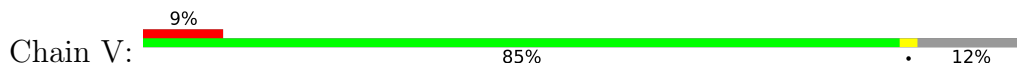


- Molecule 21: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)

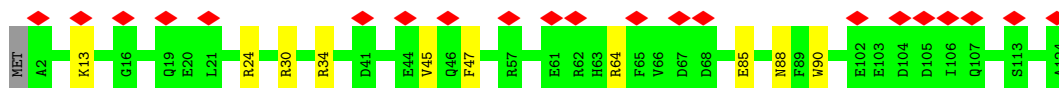




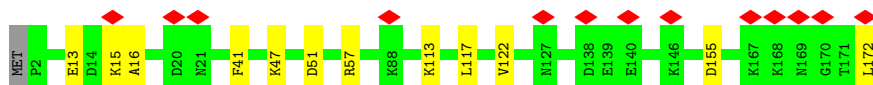
- Molecule 22: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



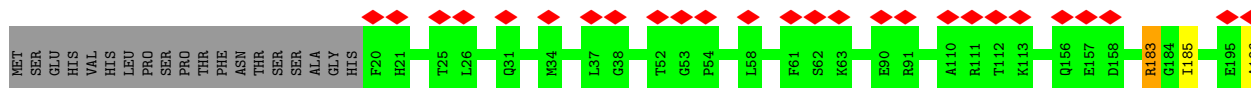
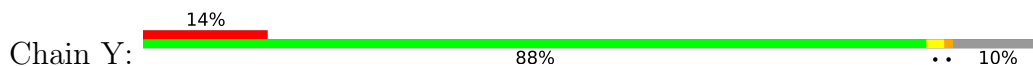
- Molecule 23: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



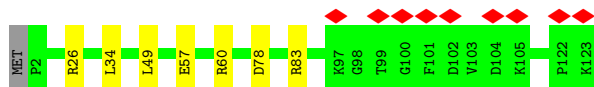
- Molecule 24: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 25: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)

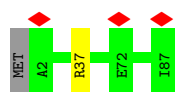


- Molecule 26: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)



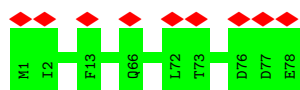
- Molecule 27: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain a:  98%



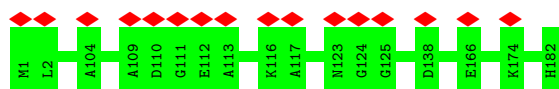
- Molecule 28: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain b:  12% 100%



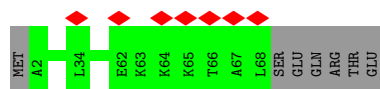
- Molecule 29: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain c:  9% 100%




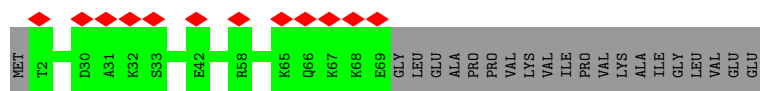
- Molecule 30: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain d:  9% 91% 9%



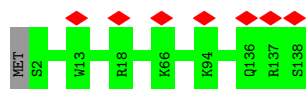
- Molecule 31: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain e:  13% 76% 24%




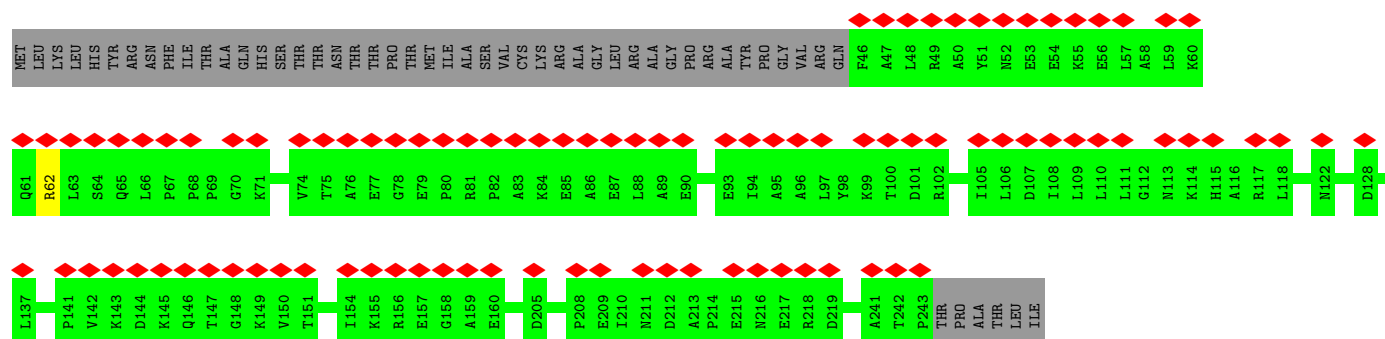
- Molecule 32: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain f:  5% 99%

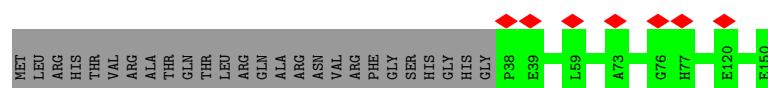
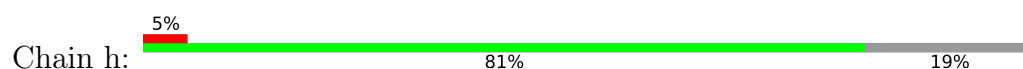


- Molecule 33: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

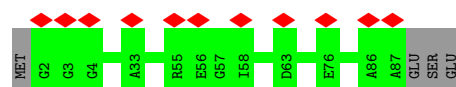
Chain g:  39% 79% 20%



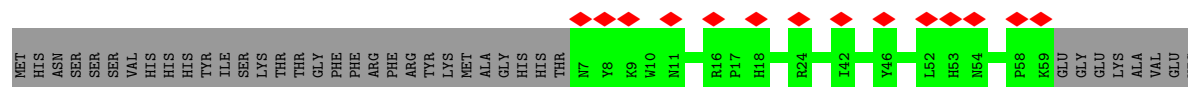
- Molecule 34: subunit NUNM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



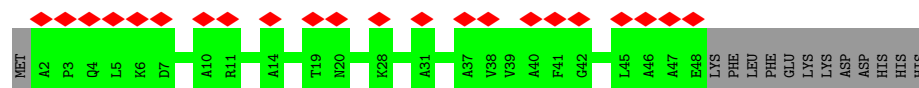
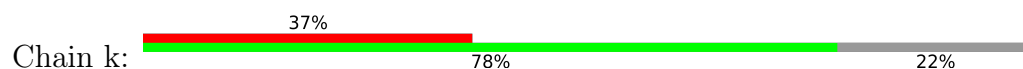
- Molecule 35: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)



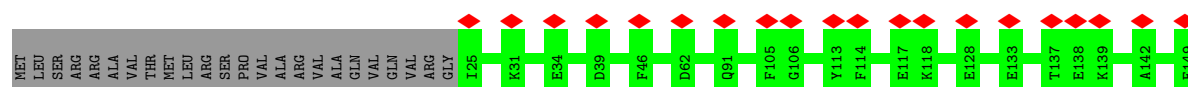
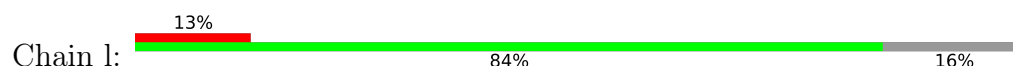
- Molecule 36: subunit NIGM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 37: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)

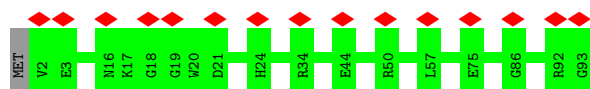


- Molecule 38: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



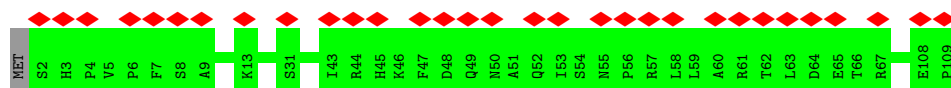
- Molecule 39: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain m:  16% 99%




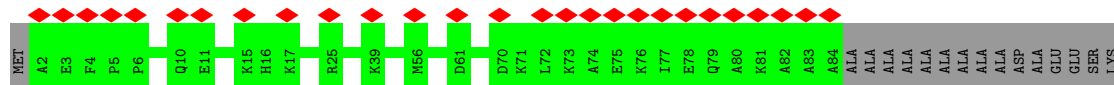
- Molecule 40: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain n:  28% 99%



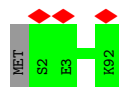
- Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain o:  27% 84% 16%



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

Chain p:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49669	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	474.74997, 474.74997, 474.74997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/1018	0.56	0/1390
2	B	0.65	3/1434 (0.2%)	0.68	1/1950 (0.1%)
3	C	0.55	0/2062	0.62	2/2813 (0.1%)
4	D	0.54	0/3533	0.61	2/4788 (0.0%)
5	E	0.44	0/1725	0.62	0/2343
6	F	0.45	1/3638 (0.0%)	0.62	0/4910
7	G	0.47	0/5368	0.59	0/7285
8	H	0.51	0/2772	0.64	3/3786 (0.1%)
9	I	0.66	1/1564 (0.1%)	0.67	2/2121 (0.1%)
10	J	0.41	0/1477	0.53	0/2015
11	K	0.45	0/692	0.61	0/937
12	L	0.46	0/5327	0.56	0/7273
13	M	0.50	0/3941	0.58	0/5382
14	N	0.55	0/3846	0.56	0/5242
15	O	0.46	0/1344	0.56	0/1822
16	P	0.41	0/2873	0.60	0/3894
17	Q	0.49	0/1067	0.58	1/1442 (0.1%)
18	R	0.48	0/946	0.56	0/1283
19	S	0.36	0/677	0.63	0/907
20	T	0.48	1/628 (0.2%)	0.72	1/854 (0.1%)
21	U	0.32	0/673	0.54	0/916
22	V	0.44	0/1049	0.57	0/1420
23	W	0.45	0/1061	0.57	0/1427
24	X	0.43	0/1374	0.59	0/1856
25	Y	0.40	0/1359	0.58	0/1851
26	Z	0.48	0/1007	0.69	0/1357
27	a	0.44	0/697	0.60	1/940 (0.1%)
28	b	0.47	0/665	0.57	0/909
29	c	0.48	0/1438	0.58	0/1965
30	d	0.44	0/523	0.50	0/707
31	e	0.40	0/555	0.53	0/740
32	f	0.53	0/1174	0.56	0/1597

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.39	0/1614	0.58	0/2182
34	h	0.44	0/937	0.52	0/1270
35	i	0.37	0/679	0.59	0/924
36	j	0.36	0/465	0.53	0/630
37	k	0.37	0/385	0.62	0/522
38	l	0.41	0/1073	0.54	0/1451
39	m	0.44	0/756	0.59	0/1021
40	n	0.38	0/926	0.57	0/1253
41	o	0.38	0/695	0.54	0/930
42	p	0.47	0/782	0.61	0/1051
All	All	0.48	6/65819 (0.0%)	0.59	13/89356 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	102	TYR	CD1-CE1	-8.28	1.26	1.39
2	B	156	TYR	CD2-CE2	-7.00	1.28	1.39
6	F	279	CYS	CB-SG	6.17	1.92	1.82
2	B	156	TYR	CD1-CE1	-5.16	1.31	1.39
20	T	33	GLU	CG-CD	-5.09	1.44	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	94	ASP	CB-CG-OD1	7.05	124.65	118.30
8	H	211	LEU	CB-CG-CD1	6.04	121.27	111.00
20	T	31	ASP	CB-CG-OD2	5.75	123.47	118.30
8	H	199	ARG	NE-CZ-NH2	5.54	123.07	120.30
9	I	115	ARG	NE-CZ-NH1	5.48	123.04	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1006	0	1056	10	0
2	B	1395	0	1375	11	0
3	C	1999	0	1925	10	0
4	D	3465	0	3397	37	0
5	E	1688	0	1660	13	0
6	F	3559	0	3513	30	0
7	G	5274	0	5173	25	0
8	H	2709	0	2805	17	0
9	I	1526	0	1471	12	0
10	J	1462	0	1582	11	0
11	K	693	0	753	9	0
12	L	5207	0	5364	27	0
13	M	3857	0	4053	26	0
14	N	3776	0	4004	34	0
15	O	1305	0	1281	10	0
16	P	2812	0	2763	13	0
17	Q	1037	0	994	3	0
18	R	922	0	876	2	0
19	S	667	0	684	8	0
20	T	620	0	614	6	0
21	U	667	0	655	2	0
22	V	1028	0	1021	2	0
23	W	1036	0	1018	7	0
24	X	1345	0	1333	7	0
25	Y	1327	0	1310	2	0
26	Z	983	0	1000	6	0
27	a	681	0	671	0	0
28	b	639	0	620	0	0
29	c	1397	0	1407	0	0
30	d	510	0	532	0	0
31	e	546	0	536	0	0
32	f	1136	0	1089	0	0
33	g	1585	0	1603	0	0
34	h	909	0	877	0	0
35	i	659	0	641	0	0
36	j	445	0	439	0	0
37	k	373	0	361	0	0
38	l	1039	0	973	0	0
39	m	735	0	718	0	0
40	n	900	0	904	0	0
41	o	681	0	685	0	0
42	p	766	0	726	0	0
43	A	78	0	110	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	H	22	0	18	0	0
43	I	46	0	69	1	0
43	L	186	0	286	1	0
43	M	70	0	91	1	0
43	N	51	0	82	1	0
43	Y	24	0	22	0	0
43	Z	75	0	98	0	0
43	b	69	0	89	0	0
43	d	54	0	56	0	0
44	B	8	0	0	0	0
44	F	8	0	0	0	0
44	G	16	0	0	0	0
44	I	16	0	0	0	0
45	B	35	0	46	0	0
45	M	35	0	46	0	0
45	Y	105	0	138	0	0
46	D	27	0	28	0	0
46	H	28	0	30	0	0
46	L	105	0	138	3	0
46	N	42	0	64	0	0
46	P	35	0	47	0	0
46	d	27	0	28	0	0
47	E	4	0	0	1	0
47	G	4	0	0	0	0
48	F	31	0	19	0	0
49	M	83	0	113	1	0
49	O	63	0	73	2	0
49	P	48	0	40	0	0
49	Z	57	0	58	1	0
49	a	52	0	48	0	0
49	b	48	0	40	0	0
50	P	48	0	26	0	0
51	R	1	0	0	0	0
52	T	34	0	0	2	0
52	U	35	0	0	2	0
53	A	2	0	0	0	0
53	B	15	0	0	3	0
53	C	15	0	0	2	0
53	D	20	0	0	2	0
53	E	2	0	0	0	0
53	F	7	0	0	0	0
53	G	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	H	10	0	0	2	0
53	I	18	0	0	1	0
53	J	4	0	0	1	0
53	K	3	0	0	0	0
53	L	27	0	0	1	0
53	M	25	0	0	1	0
53	N	37	0	0	5	0
53	O	4	0	0	0	0
53	P	14	0	0	2	0
53	Q	7	0	0	0	0
53	R	3	0	0	0	0
53	W	4	0	0	1	0
53	X	1	0	0	0	0
53	Z	3	0	0	0	0
53	a	3	0	0	0	0
53	c	3	0	0	0	0
53	f	4	0	0	0	0
53	h	1	0	0	0	0
53	i	2	0	0	0	0
53	l	4	0	0	0	0
53	m	4	0	0	0	0
53	n	2	0	0	0	0
53	o	1	0	0	0	0
53	p	5	0	0	0	0
All	All	66311	0	66365	296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 296 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:T:201:EHZ:O9	23:W:64:ARG:NH2	1.66	1.25
14:N:137:ILE:HD11	14:N:236:ILE:HG22	1.46	0.93
2:B:102:ARG:NH2	53:B:403:HOH:O	2.18	0.77
5:E:129:THR:OG1	47:E:301:FES:S2	2.46	0.74
2:B:80:THR:O	4:D:90:GLN:NE2	2.20	0.74

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
2	B	175/210 (83%)	169 (97%)	6 (3%)	0	100	100
3	C	240/293 (82%)	234 (98%)	6 (2%)	0	100	100
4	D	434/466 (93%)	417 (96%)	17 (4%)	0	100	100
5	E	214/243 (88%)	204 (95%)	10 (5%)	0	100	100
6	F	458/488 (94%)	433 (94%)	25 (6%)	0	100	100
7	G	692/728 (95%)	657 (95%)	35 (5%)	0	100	100
8	H	339/341 (99%)	324 (96%)	15 (4%)	0	100	100
9	I	189/229 (82%)	179 (95%)	10 (5%)	0	100	100
10	J	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
11	K	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
12	L	653/655 (100%)	624 (96%)	28 (4%)	1 (0%)	44	68
13	M	484/486 (100%)	469 (97%)	15 (3%)	0	100	100
14	N	467/469 (100%)	460 (98%)	7 (2%)	0	100	100
15	O	166/169 (98%)	158 (95%)	8 (5%)	0	100	100
16	P	353/375 (94%)	340 (96%)	13 (4%)	0	100	100
17	Q	123/161 (76%)	119 (97%)	4 (3%)	0	100	100
18	R	116/136 (85%)	111 (96%)	5 (4%)	0	100	100
19	S	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
20	T	79/109 (72%)	71 (90%)	8 (10%)	0	100	100
21	U	86/132 (65%)	83 (96%)	3 (4%)	0	100	100
22	V	124/144 (86%)	116 (94%)	8 (6%)	0	100	100
23	W	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
24	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
25	Y	177/198 (89%)	171 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
27	a	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
28	b	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
29	c	180/182 (99%)	168 (93%)	12 (7%)	0	100	100
30	d	65/74 (88%)	65 (100%)	0	0	100	100
31	e	66/89 (74%)	64 (97%)	2 (3%)	0	100	100
32	f	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
33	g	196/249 (79%)	190 (97%)	6 (3%)	0	100	100
34	h	111/139 (80%)	107 (96%)	4 (4%)	0	100	100
35	i	84/90 (93%)	82 (98%)	2 (2%)	0	100	100
36	j	51/91 (56%)	50 (98%)	1 (2%)	0	100	100
37	k	45/60 (75%)	40 (89%)	5 (11%)	0	100	100
38	l	123/149 (83%)	113 (92%)	10 (8%)	0	100	100
39	m	90/93 (97%)	86 (96%)	4 (4%)	0	100	100
40	n	106/109 (97%)	101 (95%)	5 (5%)	0	100	100
41	o	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
42	p	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
All	All	8041/8759 (92%)	7707 (96%)	333 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	555	VAL

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	A	107/113 (95%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	154/180 (86%)	154 (100%)	0	100	100
3	C	218/251 (87%)	218 (100%)	0	100	100
4	D	372/393 (95%)	372 (100%)	0	100	100
5	E	191/212 (90%)	191 (100%)	0	100	100
6	F	367/389 (94%)	366 (100%)	1 (0%)	91	97
7	G	566/595 (95%)	566 (100%)	0	100	100
8	H	298/301 (99%)	298 (100%)	0	100	100
9	I	157/187 (84%)	157 (100%)	0	100	100
10	J	166/166 (100%)	166 (100%)	0	100	100
11	K	76/76 (100%)	76 (100%)	0	100	100
12	L	579/579 (100%)	579 (100%)	0	100	100
13	M	433/433 (100%)	433 (100%)	0	100	100
14	N	432/432 (100%)	432 (100%)	0	100	100
15	O	132/133 (99%)	132 (100%)	0	100	100
16	P	299/329 (91%)	299 (100%)	0	100	100
17	Q	107/140 (76%)	107 (100%)	0	100	100
18	R	98/115 (85%)	98 (100%)	0	100	100
19	S	72/73 (99%)	72 (100%)	0	100	100
20	T	68/91 (75%)	68 (100%)	0	100	100
21	U	75/111 (68%)	74 (99%)	1 (1%)	65	85
22	V	113/129 (88%)	113 (100%)	0	100	100
23	W	109/110 (99%)	109 (100%)	0	100	100
24	X	147/148 (99%)	147 (100%)	0	100	100
25	Y	130/147 (88%)	129 (99%)	1 (1%)	79	91
26	Z	101/102 (99%)	101 (100%)	0	100	100
27	a	68/69 (99%)	68 (100%)	0	100	100
28	b	65/65 (100%)	65 (100%)	0	100	100
29	c	148/148 (100%)	148 (100%)	0	100	100
30	d	52/59 (88%)	52 (100%)	0	100	100
31	e	59/76 (78%)	59 (100%)	0	100	100
32	f	122/123 (99%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	g	161/211 (76%)	160 (99%)	1 (1%)	84	94
34	h	98/119 (82%)	98 (100%)	0	100	100
35	i	64/68 (94%)	64 (100%)	0	100	100
36	j	45/78 (58%)	45 (100%)	0	100	100
37	k	32/45 (71%)	32 (100%)	0	100	100
38	l	109/129 (84%)	109 (100%)	0	100	100
39	m	72/73 (99%)	72 (100%)	0	100	100
40	n	99/100 (99%)	99 (100%)	0	100	100
41	o	70/76 (92%)	70 (100%)	0	100	100
42	p	84/85 (99%)	84 (100%)	0	100	100
All	All	6915/7459 (93%)	6911 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	127	CYS
21	U	73	LYS
25	Y	183	ARG
33	g	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	237	HIS
23	W	22	GLN
40	n	11	ASN
33	g	207	HIS
5	E	174	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	FME	J	1	10	8,9,10	0.91	0	7,9,11	1.10	0
1	FME	A	1	1	8,9,10	0.99	0	7,9,11	0.84	0
8	FME	H	1	8	8,9,10	0.98	0	7,9,11	1.35	1 (14%)
11	FME	K	1	11	8,9,10	0.96	0	7,9,11	1.00	0
12	FME	L	1	12	8,9,10	0.98	0	7,9,11	0.95	0
4	2MR	D	121	4	10,12,13	2.41	3 (30%)	5,13,15	2.15	1 (20%)
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	0.90	0
14	FME	N	1	14	8,9,10	1.10	1 (12%)	7,9,11	1.22	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FME	J	1	10	-	3/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
4	2MR	D	121	4	-	3/10/13/15	-
13	FME	M	1	13	-	0/7/9/11	-
14	FME	N	1	14	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	121	2MR	CZ-NE	5.01	1.45	1.34
4	D	121	2MR	CZ-NH2	4.72	1.43	1.33
4	D	121	2MR	CQ1-NH1	-2.54	1.41	1.46
14	N	1	FME	CA-N	-2.46	1.42	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	121	2MR	CD-NE-CZ	4.46	131.76	123.41
8	H	1	FME	C-CA-N	2.90	114.96	109.73
14	N	1	FME	C-CA-N	2.73	114.66	109.73

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	O-C-CA-CB
4	D	121	2MR	O-C-CA-CB
8	H	1	FME	O1-CN-N-CA
8	H	1	FME	CB-CA-N-CN

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	3PE	A	501	-	26,26,50	1.26	3 (11%)	29,31,55	1.31	3 (10%)
44	SF4	G	802	7	0,12,12	-	-	-	-	-
49	CDL	Z	201	-	56,56,99	1.22	8 (14%)	62,68,111	1.12	6 (9%)
49	CDL	b	401	-	47,47,99	1.33	9 (19%)	53,59,111	1.36	6 (11%)
52	EHZ	U	201	21	27,34,37	1.74	6 (22%)	33,42,47	1.37	7 (21%)
46	PLC	L	1007	-	41,41,41	1.28	6 (14%)	47,49,49	1.11	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	CDL	P	403	-	47,47,99	1.31	8 (17%)	53,59,111	1.23	6 (11%)
49	CDL	O	401	-	62,62,99	1.14	8 (12%)	68,74,111	1.16	6 (8%)
52	EHZ	T	201	20	26,33,37	1.71	5 (19%)	32,41,47	1.60	6 (18%)
44	SF4	I	6302	9	0,12,12	-	-	-	-	-
46	PLC	d	4602	-	26,26,41	1.38	2 (7%)	32,34,49	1.24	3 (9%)
43	3PE	M	504	-	39,39,50	1.03	4 (10%)	42,44,55	1.12	3 (7%)
43	3PE	L	1005	-	50,50,50	0.91	3 (6%)	53,55,55	1.29	3 (5%)
43	3PE	b	403	-	25,25,50	1.27	4 (16%)	28,30,55	1.25	3 (10%)
45	LMT	Y	4201	-	36,36,36	0.85	0	47,47,47	1.07	5 (10%)
43	3PE	H	602	-	21,21,50	1.31	2 (9%)	24,26,55	1.21	2 (8%)
49	CDL	M	501	-	82,82,99	1.32	7 (8%)	88,94,111	1.05	6 (6%)
43	3PE	Z	203	-	42,42,50	0.97	4 (9%)	45,47,55	1.08	3 (6%)
44	SF4	G	801	7	0,12,12	-	-	-	-	-
46	PLC	L	1001	-	33,33,41	1.38	3 (9%)	39,41,49	1.09	3 (7%)
46	PLC	H	601	-	27,27,41	1.44	3 (11%)	33,35,49	3.95	8 (24%)
46	PLC	P	401	-	34,34,41	1.34	4 (11%)	40,42,49	1.15	3 (7%)
45	LMT	Y	4204	-	36,36,36	0.88	2 (5%)	47,47,47	1.65	10 (21%)
50	NDP	P	402	-	45,52,52	2.22	5 (11%)	53,80,80	1.66	9 (16%)
46	PLC	N	2401	-	41,41,41	1.11	4 (9%)	47,49,49	1.10	3 (6%)
47	FES	E	301	5	0,4,4	-	-	-	-	-
43	3PE	d	4603	-	29,29,50	1.18	4 (13%)	32,34,55	1.15	3 (9%)
46	PLC	L	1002	-	28,28,41	1.30	4 (14%)	34,36,49	1.12	3 (8%)
44	SF4	I	6303	9	0,12,12	-	-	-	-	-
43	3PE	M	502	-	29,29,50	1.18	4 (13%)	32,34,55	1.22	3 (9%)
43	3PE	Y	4203	-	23,23,50	1.32	4 (17%)	26,28,55	1.53	4 (15%)
45	LMT	B	302	-	36,36,36	0.83	1 (2%)	47,47,47	0.80	1 (2%)
46	PLC	D	501	-	26,26,41	1.39	4 (15%)	32,34,49	1.15	3 (9%)
49	CDL	a	101	-	51,51,99	1.26	8 (15%)	57,63,111	1.25	6 (10%)
43	3PE	A	502	-	50,50,50	0.90	4 (8%)	53,55,55	1.12	5 (9%)
43	3PE	L	1003	-	50,50,50	0.88	4 (8%)	53,55,55	0.93	2 (3%)
47	FES	G	803	7	0,4,4	-	-	-	-	-
43	3PE	L	1004	-	50,50,50	0.88	3 (6%)	53,55,55	1.03	2 (3%)
43	3PE	d	4601	-	23,23,50	1.29	4 (17%)	26,28,55	1.31	3 (11%)
48	FMN	F	501	6	33,33,33	2.89	10 (30%)	48,50,50	1.99	16 (33%)
45	LMT	M	503	-	36,36,36	0.77	0	47,47,47	0.85	2 (4%)
43	3PE	N	2402	-	50,50,50	0.89	3 (6%)	53,55,55	0.97	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	LMT	Y	4202	-	36,36,36	0.79	0	47,47,47	1.25	7 (14%)
43	3PE	I	6301	-	45,45,50	1.21	3 (6%)	48,50,55	1.01	3 (6%)
43	3PE	Z	202	-	31,31,50	1.15	4 (12%)	34,36,55	1.31	3 (8%)
44	SF4	B	301	2	0,12,12	-	-	-	-	-
44	SF4	F	502	6	0,12,12	-	-	-	-	-
43	3PE	L	1006	-	32,32,50	1.13	4 (12%)	35,37,55	1.17	3 (8%)
43	3PE	b	402	-	42,42,50	1.21	4 (9%)	45,47,55	1.02	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	3PE	A	501	-	1/1/4/4	16/30/30/54	-
44	SF4	G	802	7	-	-	0/6/5/5
52	EHZ	U	201	21	1/1/7/9	11/40/42/45	-
49	CDL	Z	201	-	-	33/67/67/110	-
49	CDL	b	401	-	-	19/58/58/110	-
46	PLC	L	1007	-	-	21/45/45/45	-
49	CDL	P	403	-	-	26/58/58/110	-
49	CDL	O	401	-	-	26/73/73/110	-
52	EHZ	T	201	20	1/1/7/9	7/39/41/45	-
44	SF4	I	6302	9	-	-	0/6/5/5
46	PLC	d	4602	-	-	9/30/30/45	-
43	3PE	M	504	-	-	17/43/43/54	-
43	3PE	L	1005	-	-	25/54/54/54	-
43	3PE	b	403	-	-	9/29/29/54	-
45	LMT	Y	4201	-	4/4/10/10	4/21/61/61	0/2/2/2
43	3PE	H	602	-	1/1/4/4	11/24/24/54	-
49	CDL	M	501	-	-	41/93/93/110	-
43	3PE	Z	203	-	-	14/46/46/54	-
44	SF4	G	801	7	-	-	0/6/5/5
46	PLC	L	1001	-	-	18/37/37/45	-
46	PLC	H	601	-	-	12/31/31/45	-
46	PLC	P	401	-	-	9/38/38/45	-
45	LMT	Y	4204	-	4/4/10/10	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	NDP	P	402	-	-	9/30/77/77	0/5/5/5
46	PLC	N	2401	-	-	18/45/45/45	-
47	FES	E	301	5	-	-	0/1/1/1
43	3PE	d	4603	-	1/1/4/4	16/33/33/54	-
46	PLC	L	1002	-	-	10/32/32/45	-
44	SF4	I	6303	9	-	-	0/6/5/5
43	3PE	M	502	-	1/1/4/4	18/33/33/54	-
43	3PE	Y	4203	-	1/1/4/4	13/26/26/54	-
45	LMT	B	302	-	4/4/10/10	9/21/61/61	0/2/2/2
46	PLC	D	501	-	-	12/30/30/45	-
49	CDL	a	101	-	-	25/62/62/110	-
43	3PE	A	502	-	-	20/54/54/54	-
43	3PE	L	1003	-	-	20/54/54/54	-
47	FES	G	803	7	-	-	0/1/1/1
43	3PE	L	1004	-	-	27/54/54/54	-
48	FMN	F	501	6	2/2/4/4	8/18/18/18	0/3/3/3
43	3PE	d	4601	-	-	8/27/27/54	-
45	LMT	M	503	-	4/4/10/10	13/21/61/61	0/2/2/2
45	LMT	Y	4202	-	4/4/10/10	13/21/61/61	0/2/2/2
43	3PE	N	2402	-	-	27/54/54/54	-
43	3PE	I	6301	-	-	17/49/49/54	-
43	3PE	Z	202	-	1/1/4/4	18/35/35/54	-
44	SF4	B	301	2	-	-	0/6/5/5
44	SF4	F	502	6	-	-	0/6/5/5
43	3PE	L	1006	-	-	11/36/36/54	-
43	3PE	b	402	-	-	12/46/46/54	-

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	P	402	NDP	P2B-O2B	11.90	1.81	1.59
48	F	501	FMN	O2-C2	8.75	1.40	1.24
48	F	501	FMN	O4-C4	8.61	1.40	1.23
48	F	501	FMN	C2-N1	5.84	1.50	1.36
52	U	201	EHZ	C15-N2	5.19	1.44	1.33

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H	601	PLC	C8-N-C7	14.48	146.20	108.97
46	H	601	PLC	C6-N-C5	10.05	151.06	109.92
46	H	601	PLC	C7-N-C6	-8.86	86.19	108.97
46	H	601	PLC	C8-N-C6	-8.00	88.39	108.97
43	L	1005	3PE	O21-C21-C22	6.46	125.43	111.50

5 of 30 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	A	501	3PE	C2
43	H	602	3PE	C2
43	M	502	3PE	C2
43	Y	4203	3PE	C2
43	Z	202	3PE	C2

5 of 665 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	A	501	3PE	C11-O13-P-O12
43	A	501	3PE	C11-O13-P-O14
43	A	501	3PE	O13-C11-C12-N
43	A	501	3PE	C22-C21-O21-C2
43	A	502	3PE	C1-O11-P-O14

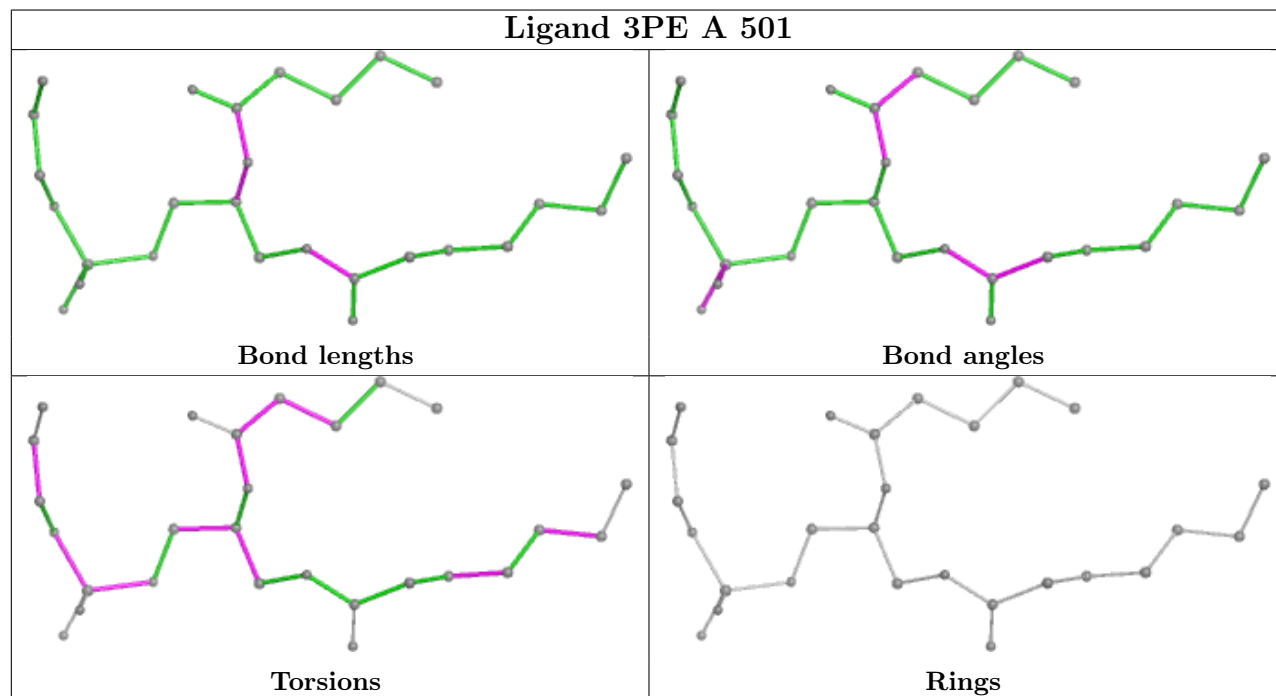
There are no ring outliers.

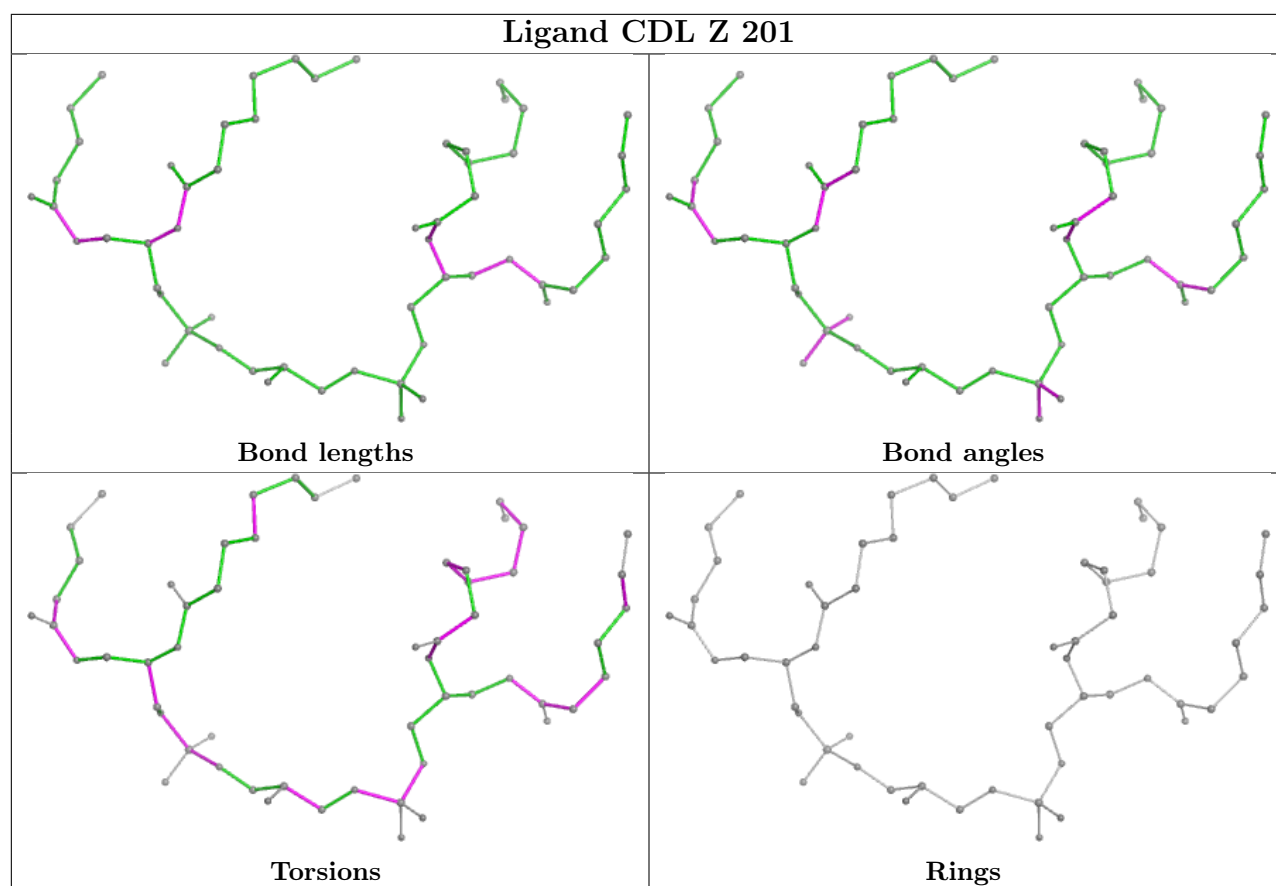
12 monomers are involved in 16 short contacts:

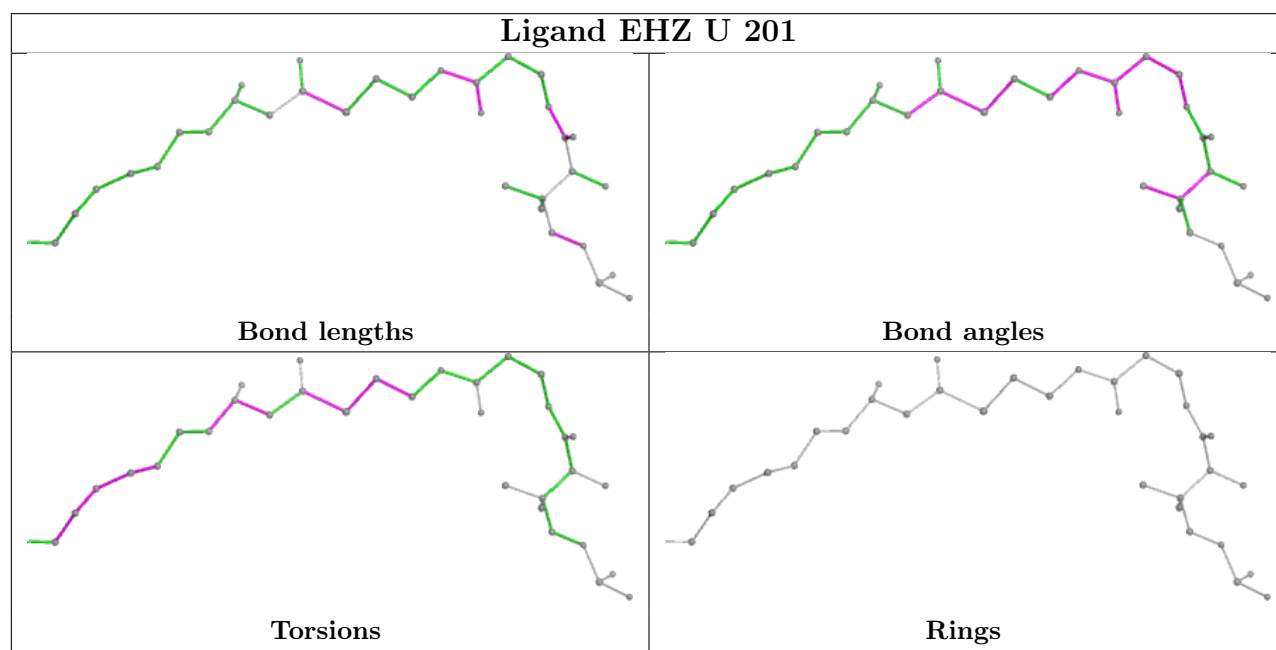
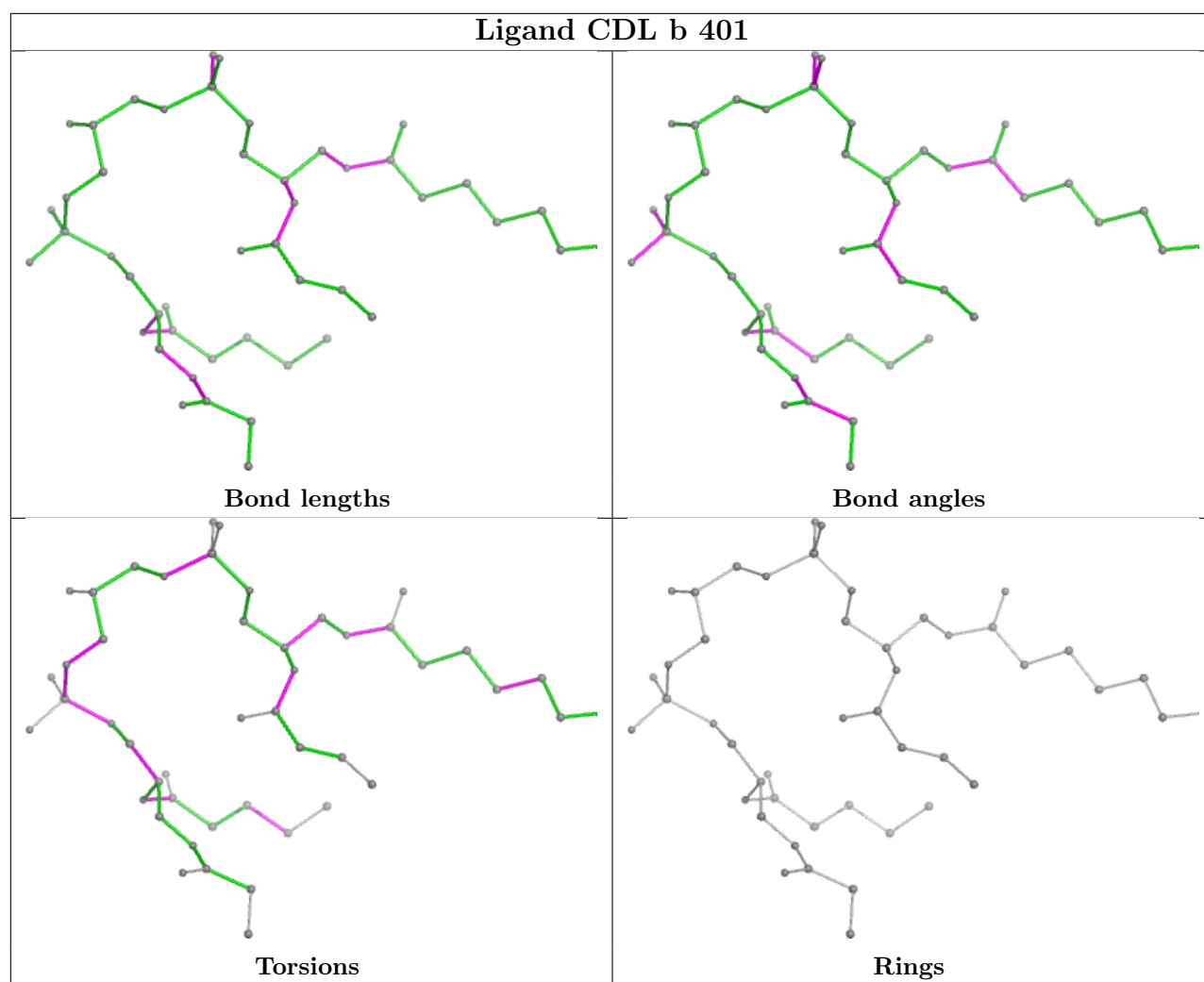
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	Z	201	CDL	1	0
52	U	201	EHZ	2	0
46	L	1007	PLC	2	0
49	O	401	CDL	2	0
52	T	201	EHZ	2	0
43	M	504	3PE	1	0
49	M	501	CDL	1	0
46	L	1001	PLC	1	0
47	E	301	FES	1	0
43	L	1003	3PE	1	0
43	N	2402	3PE	1	0
43	I	6301	3PE	1	0

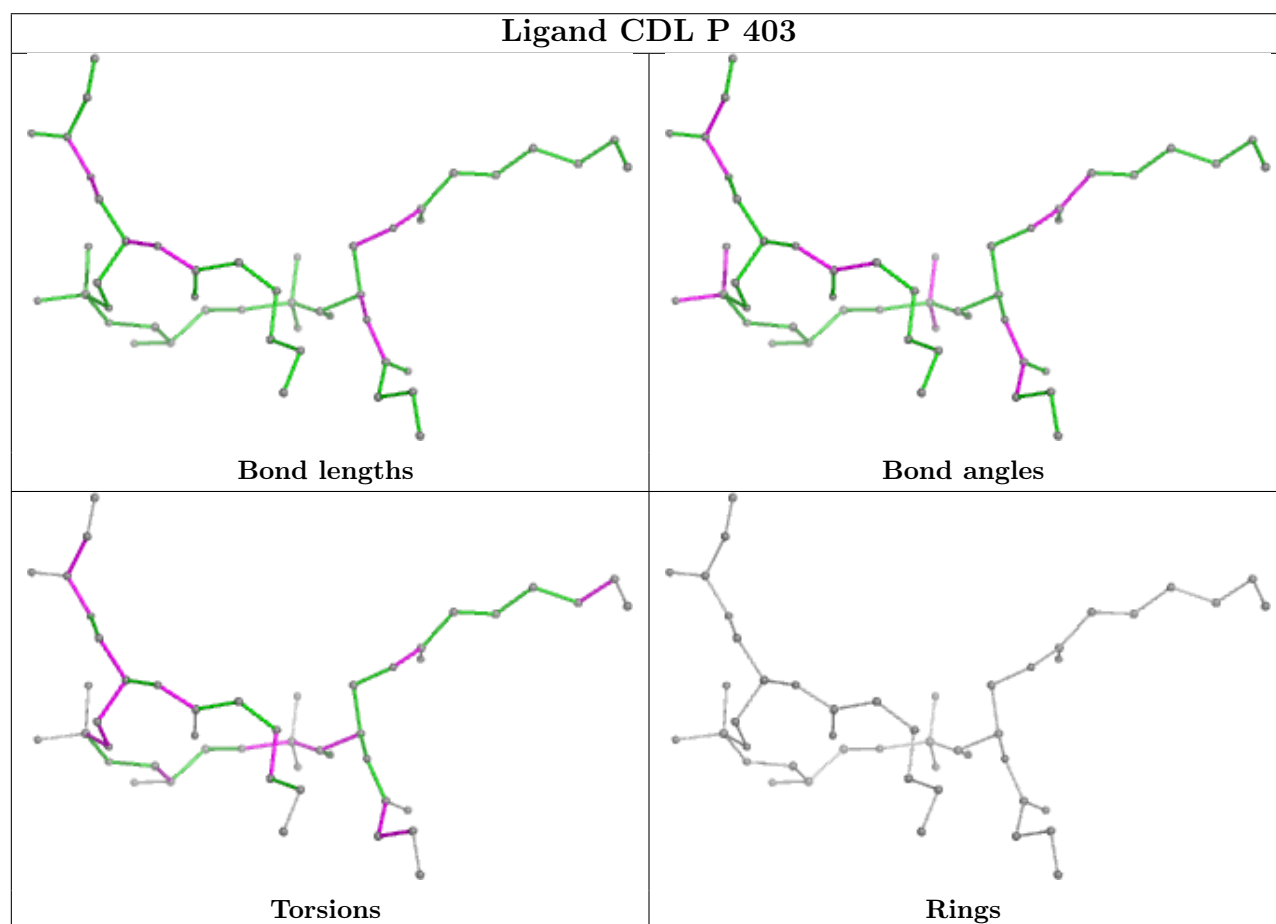
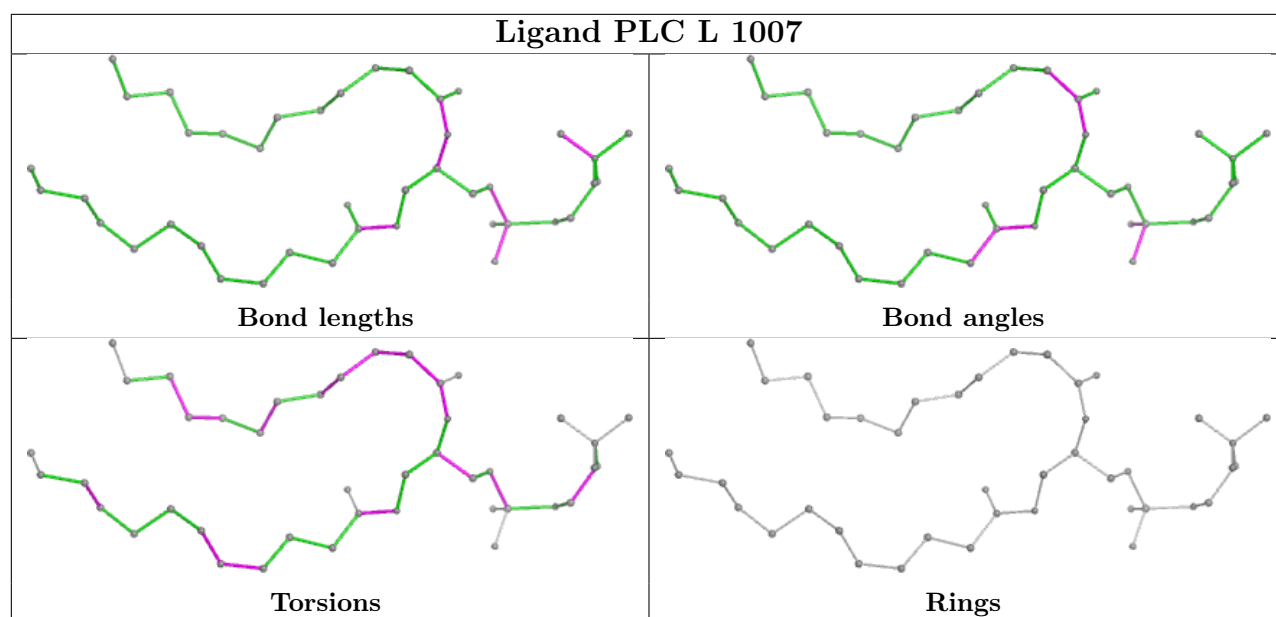
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

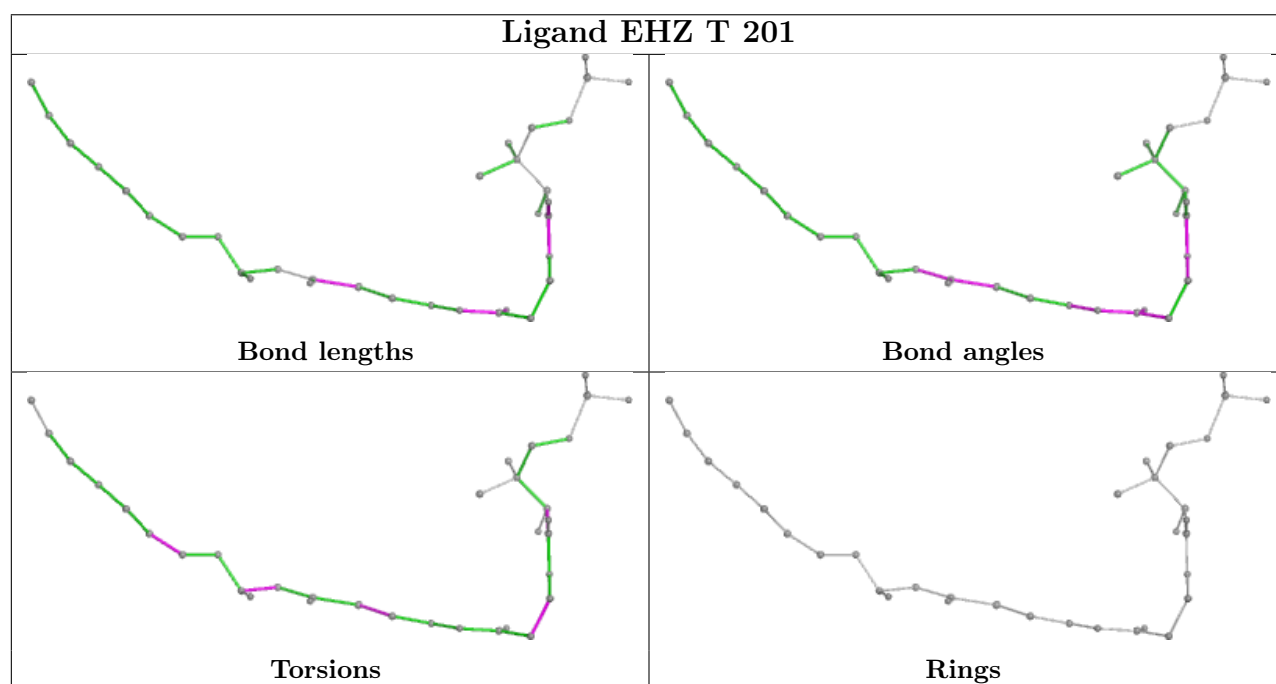
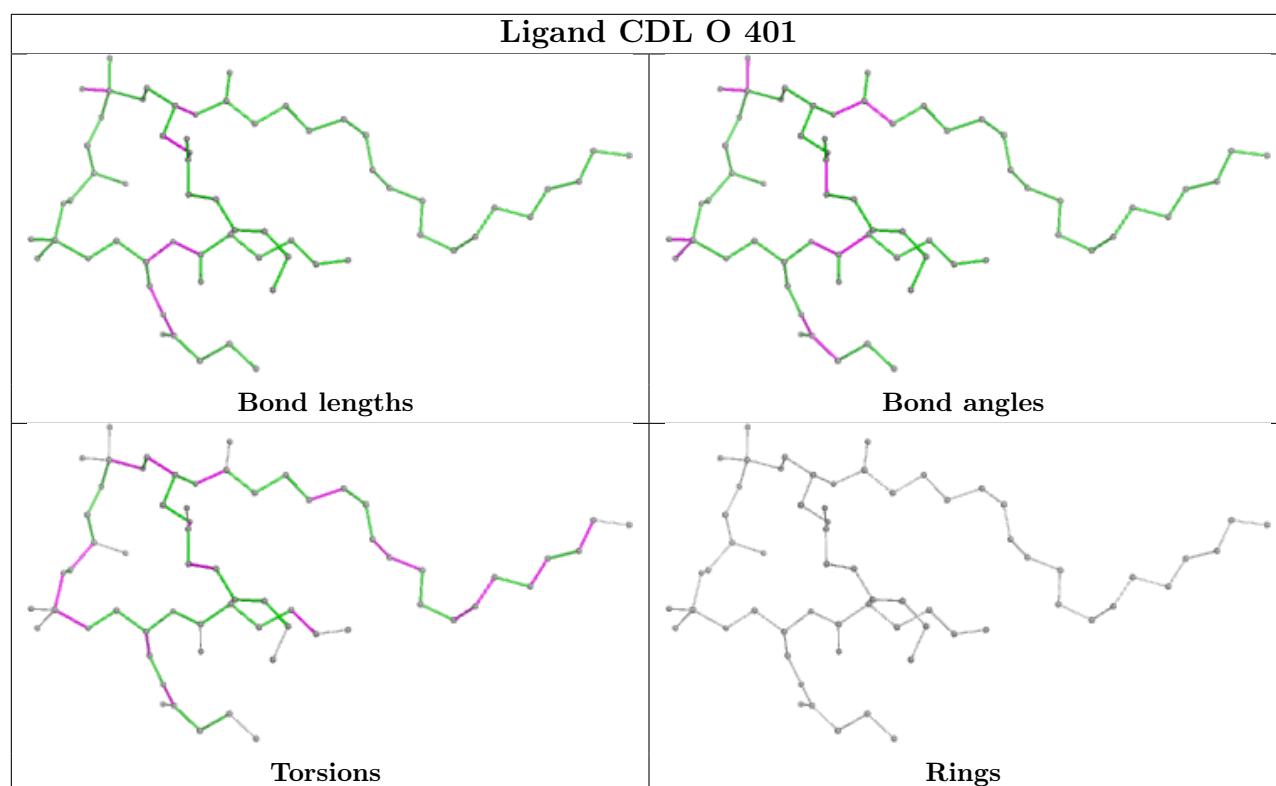
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

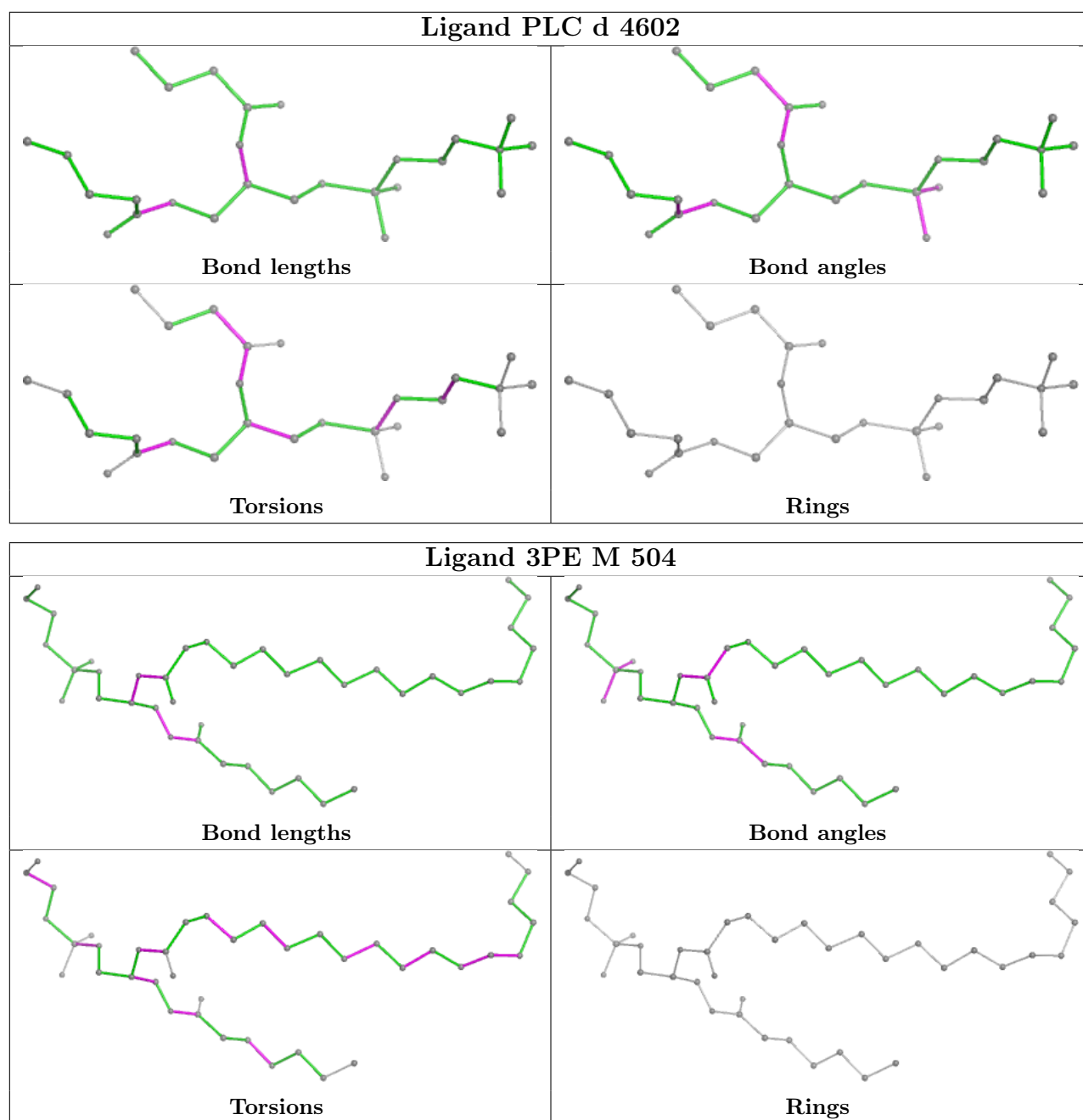


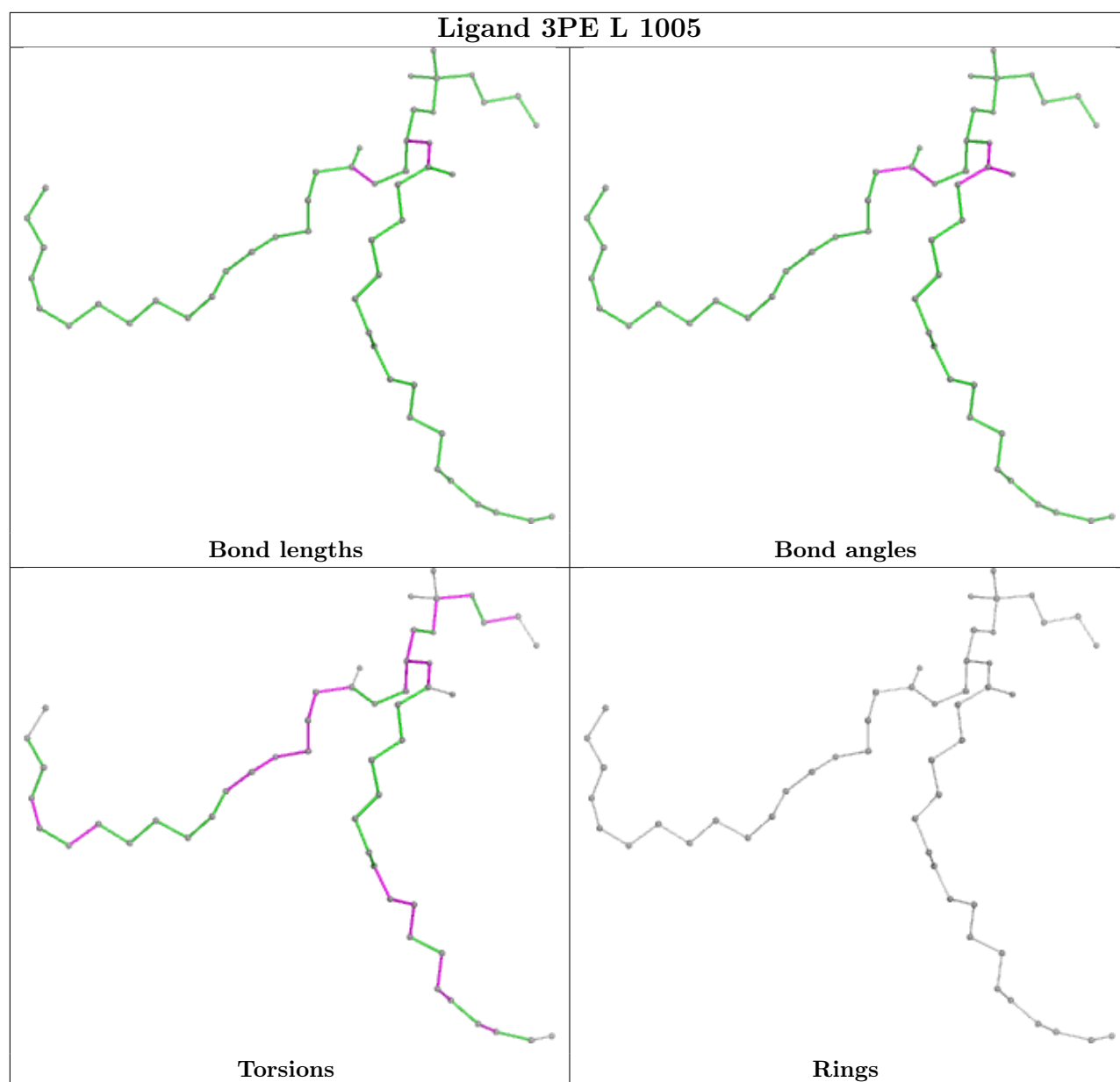


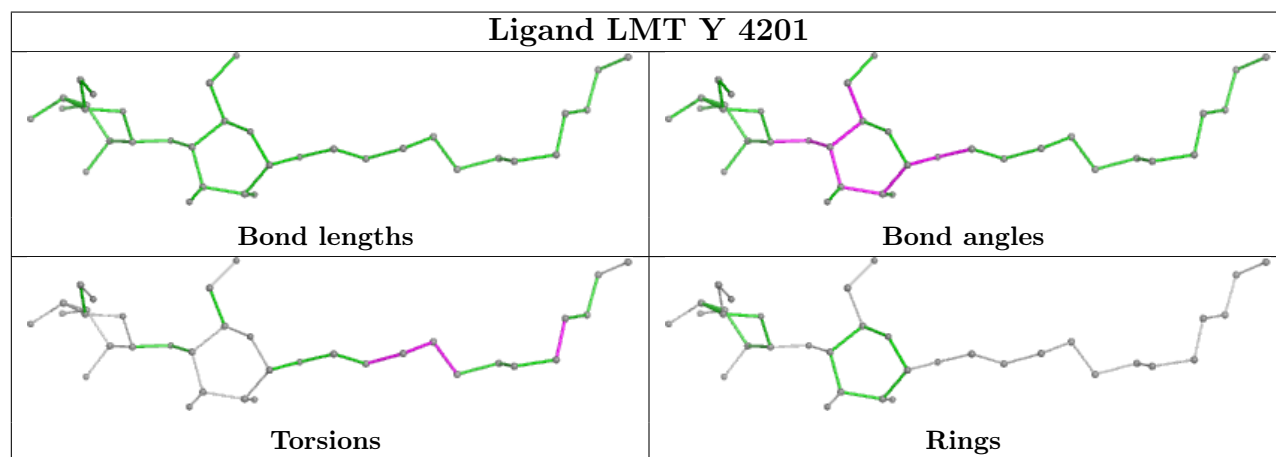
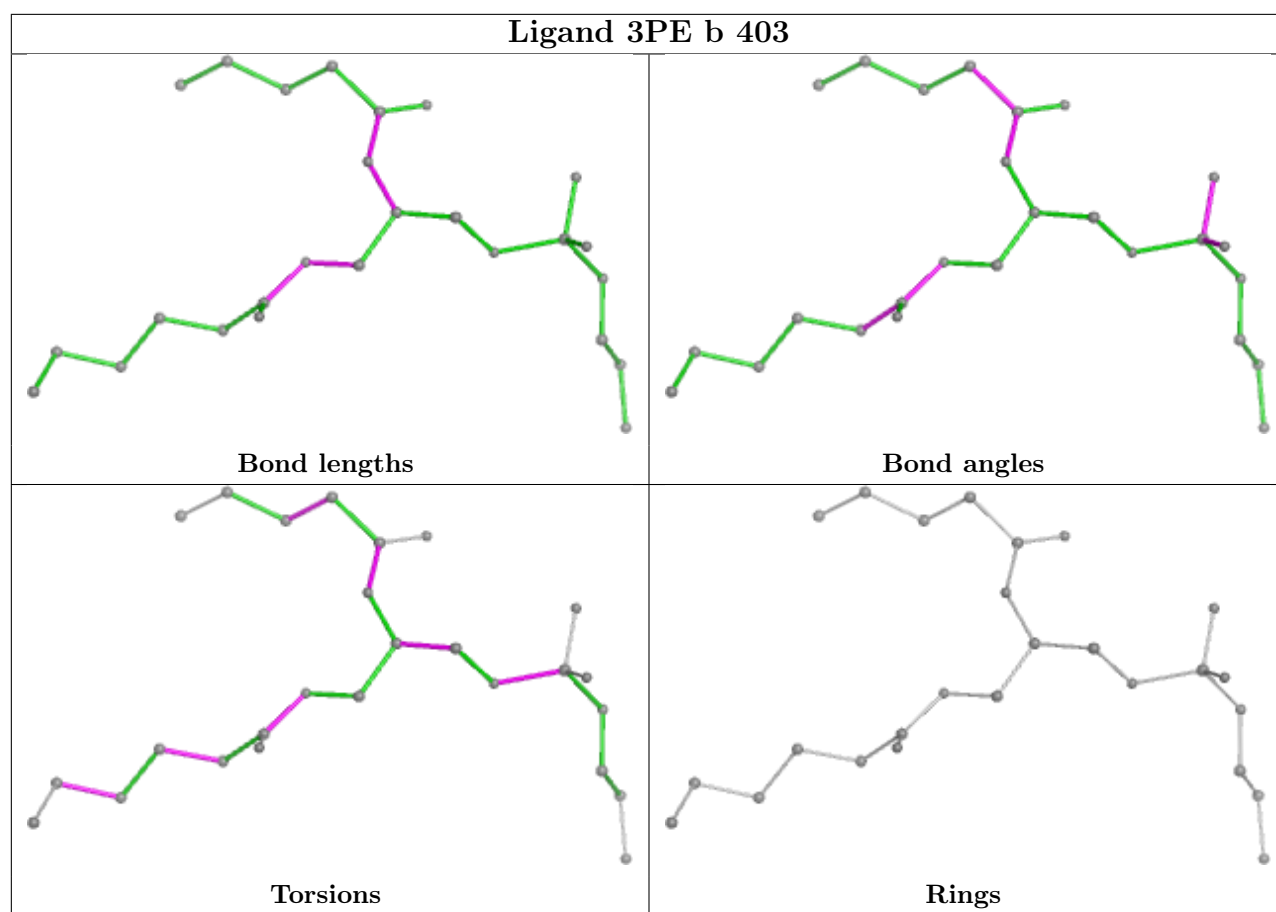


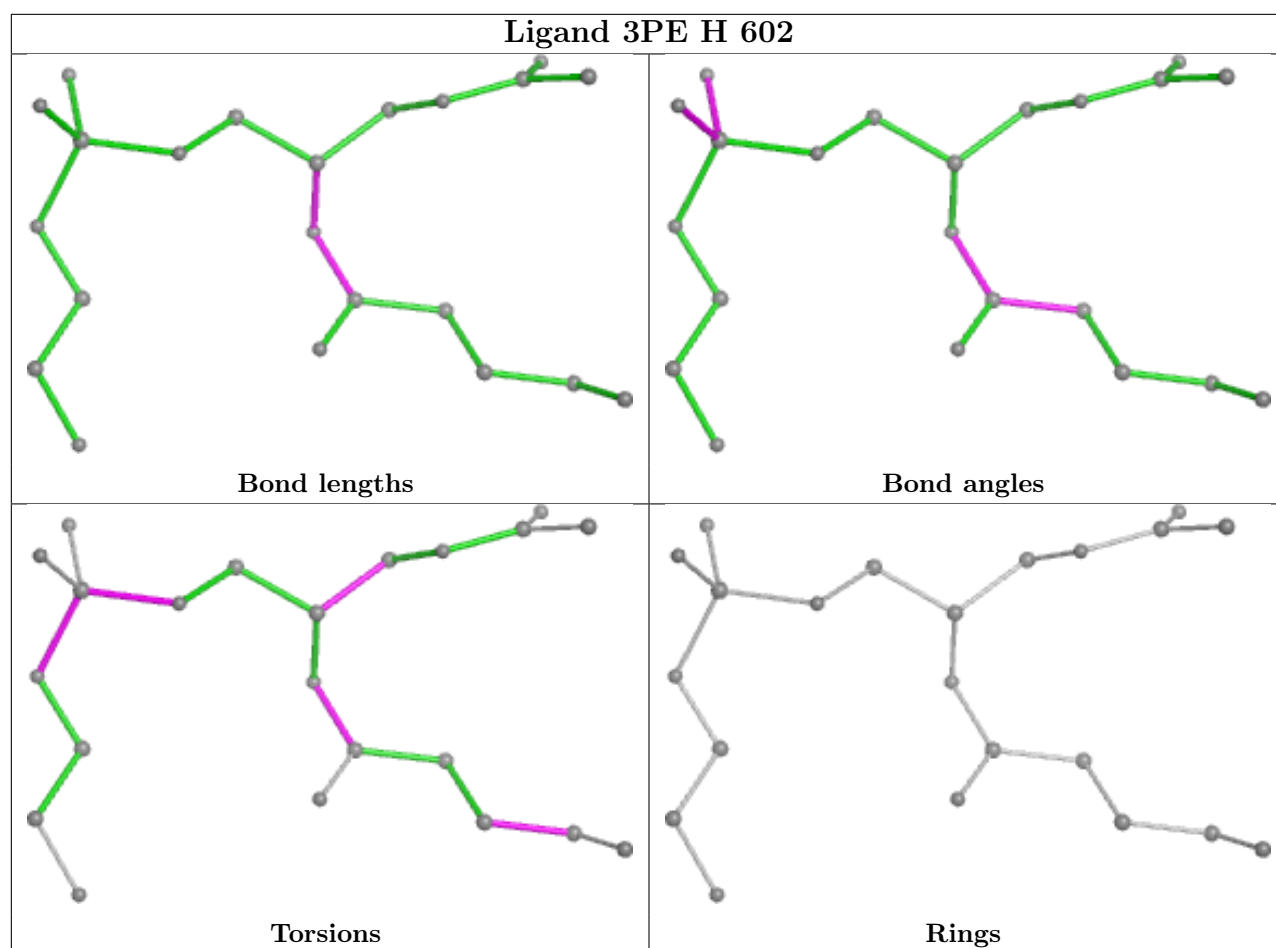


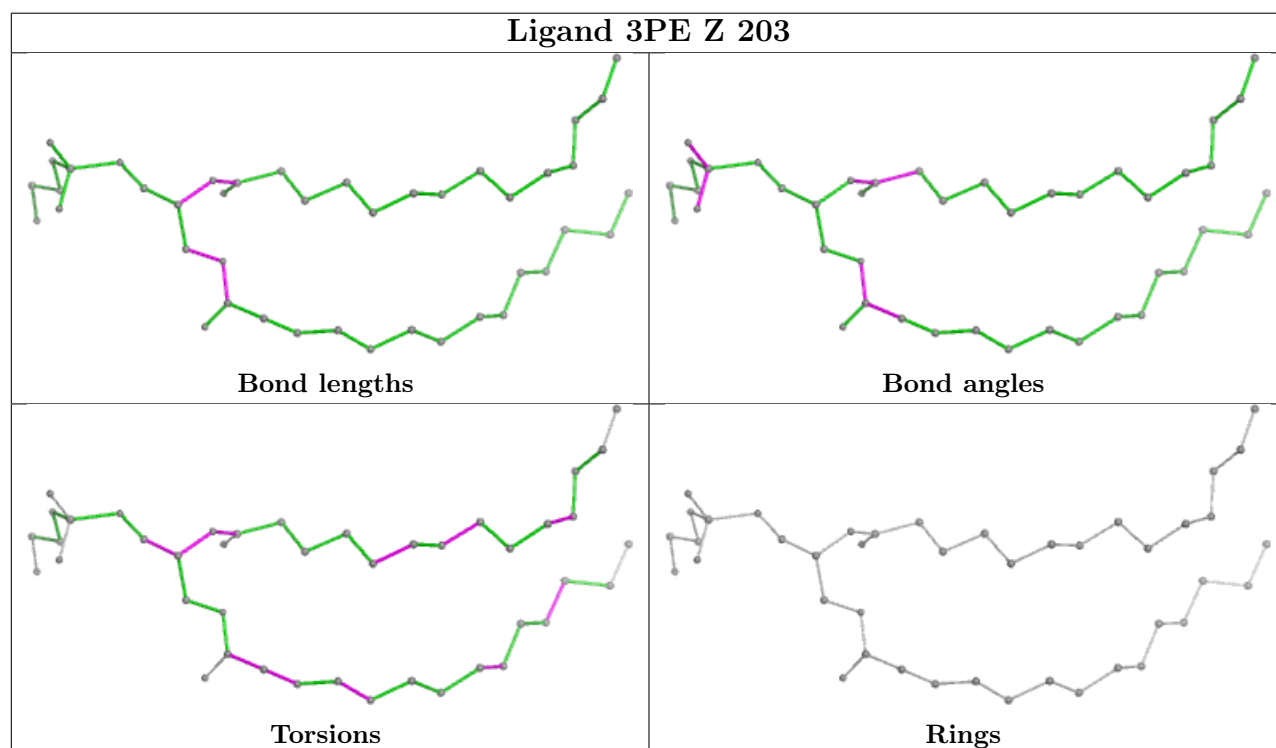
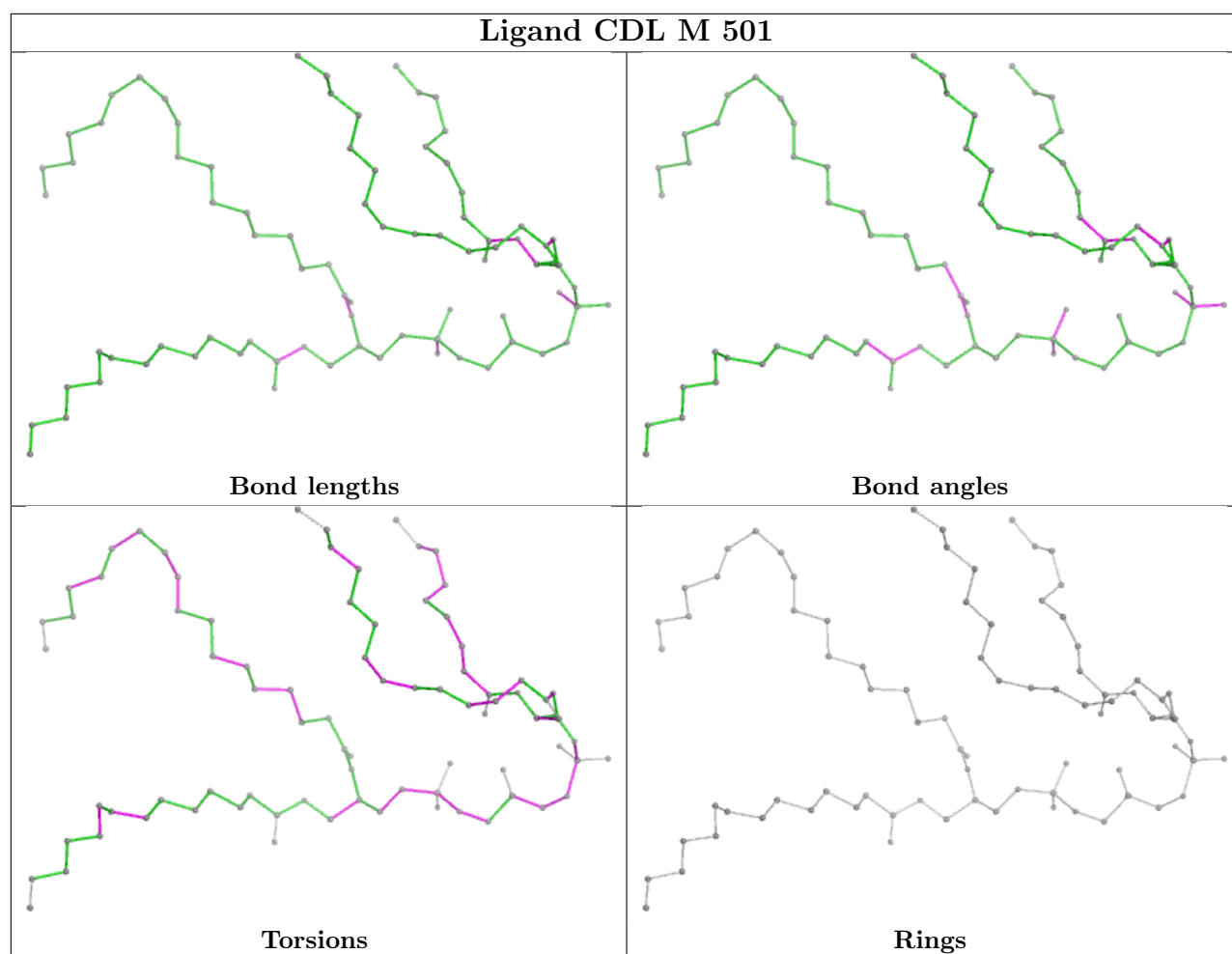


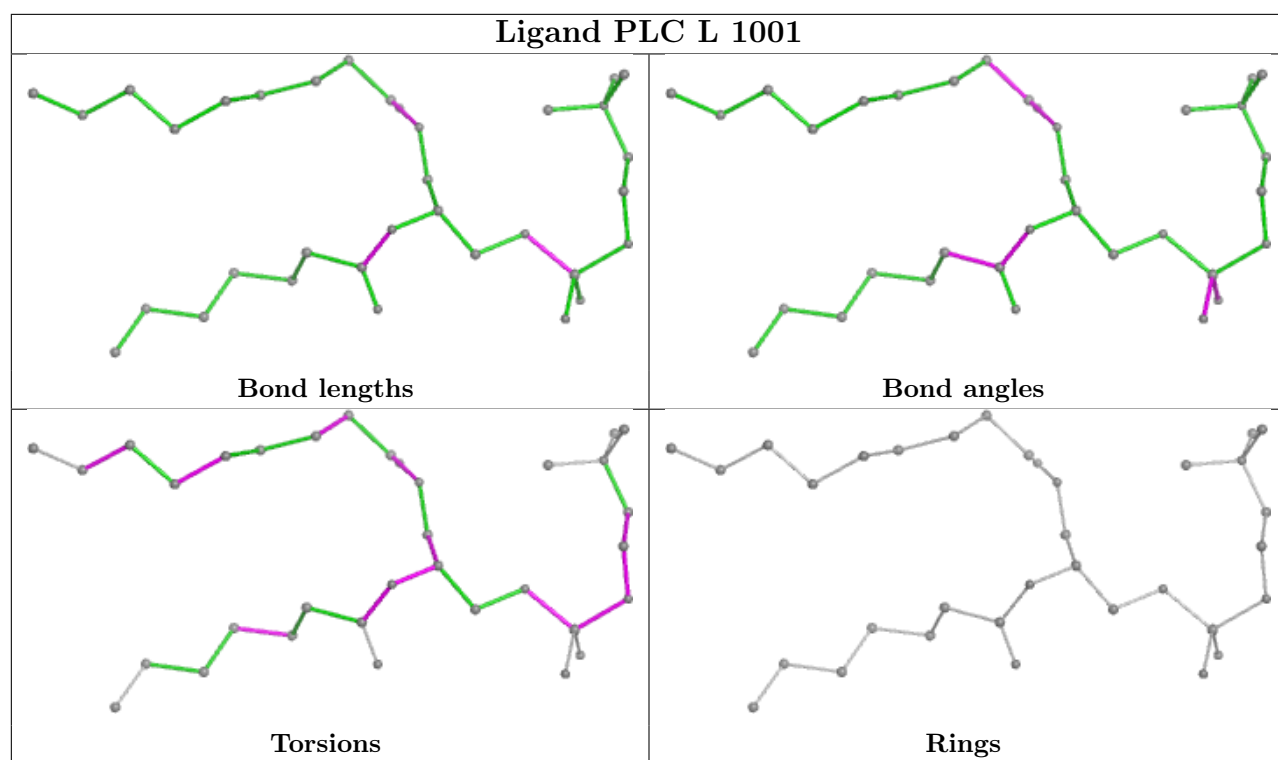


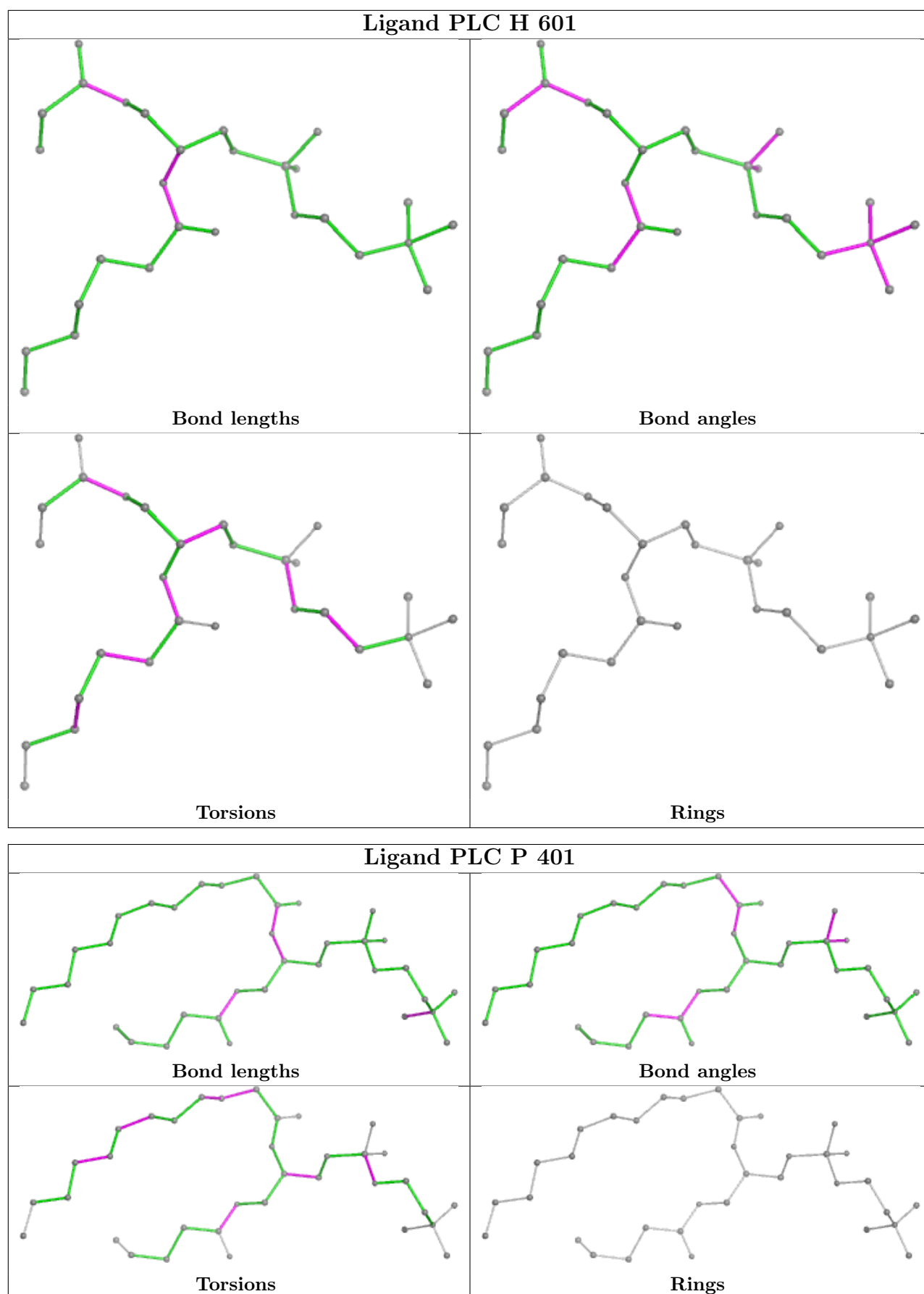


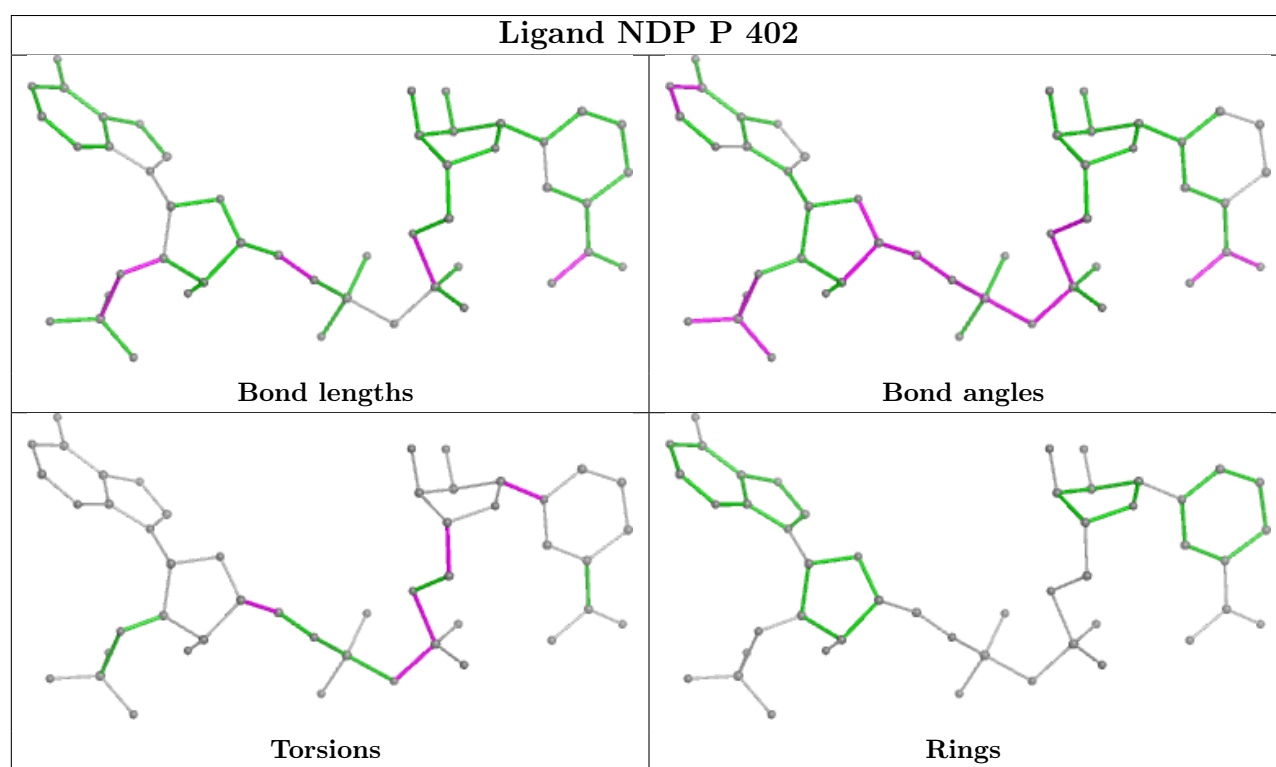
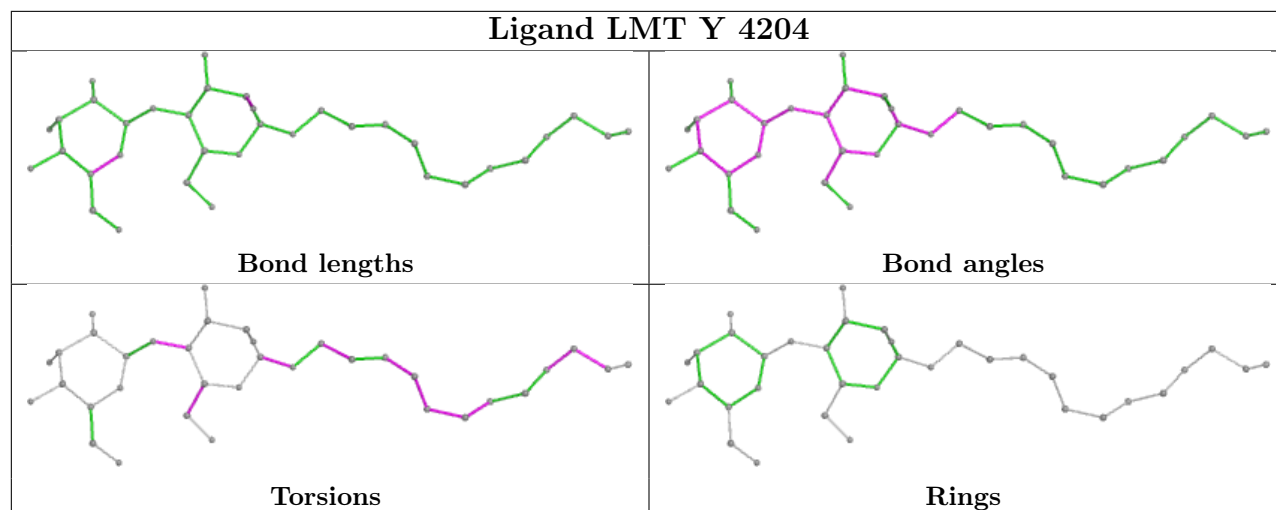


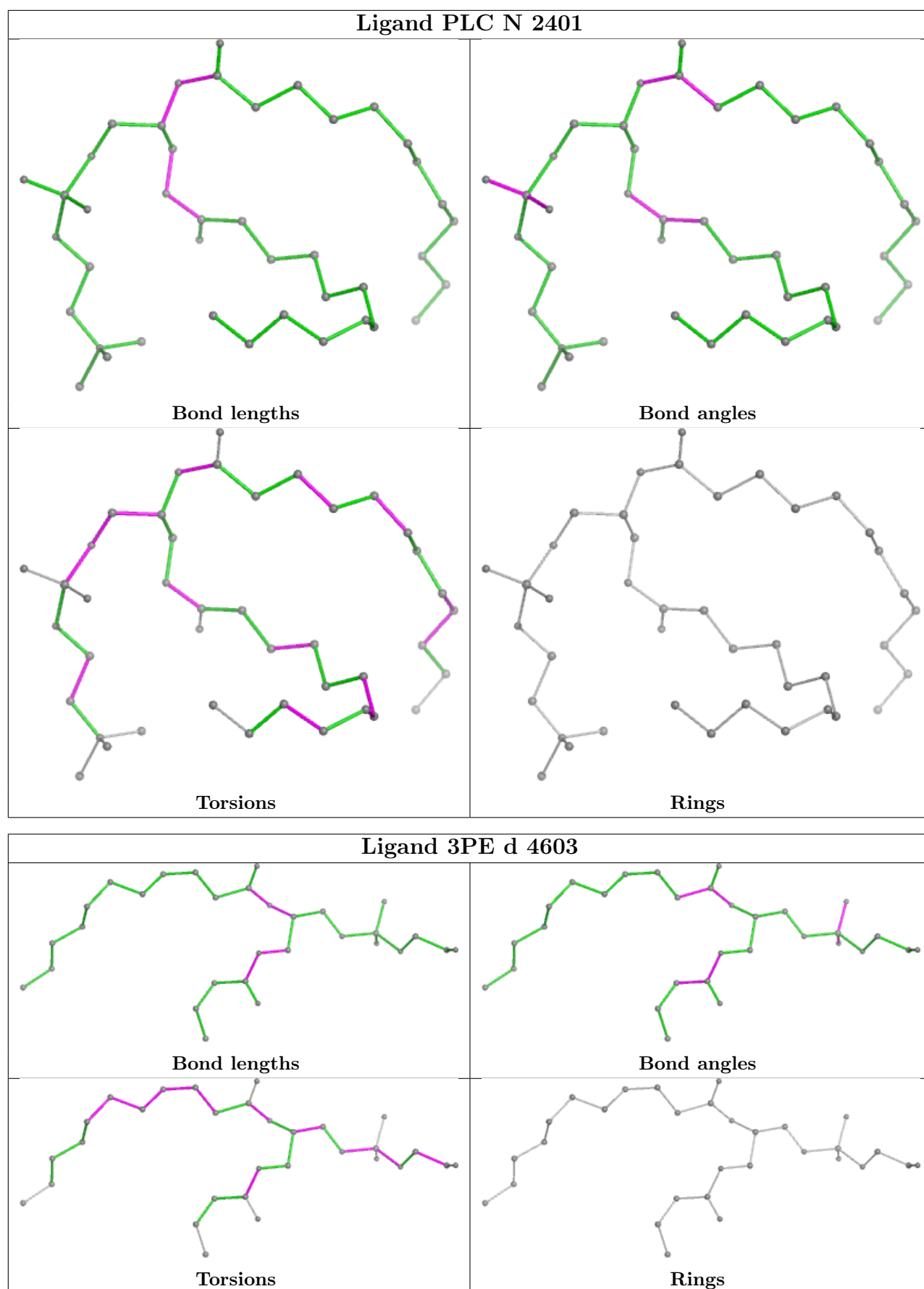


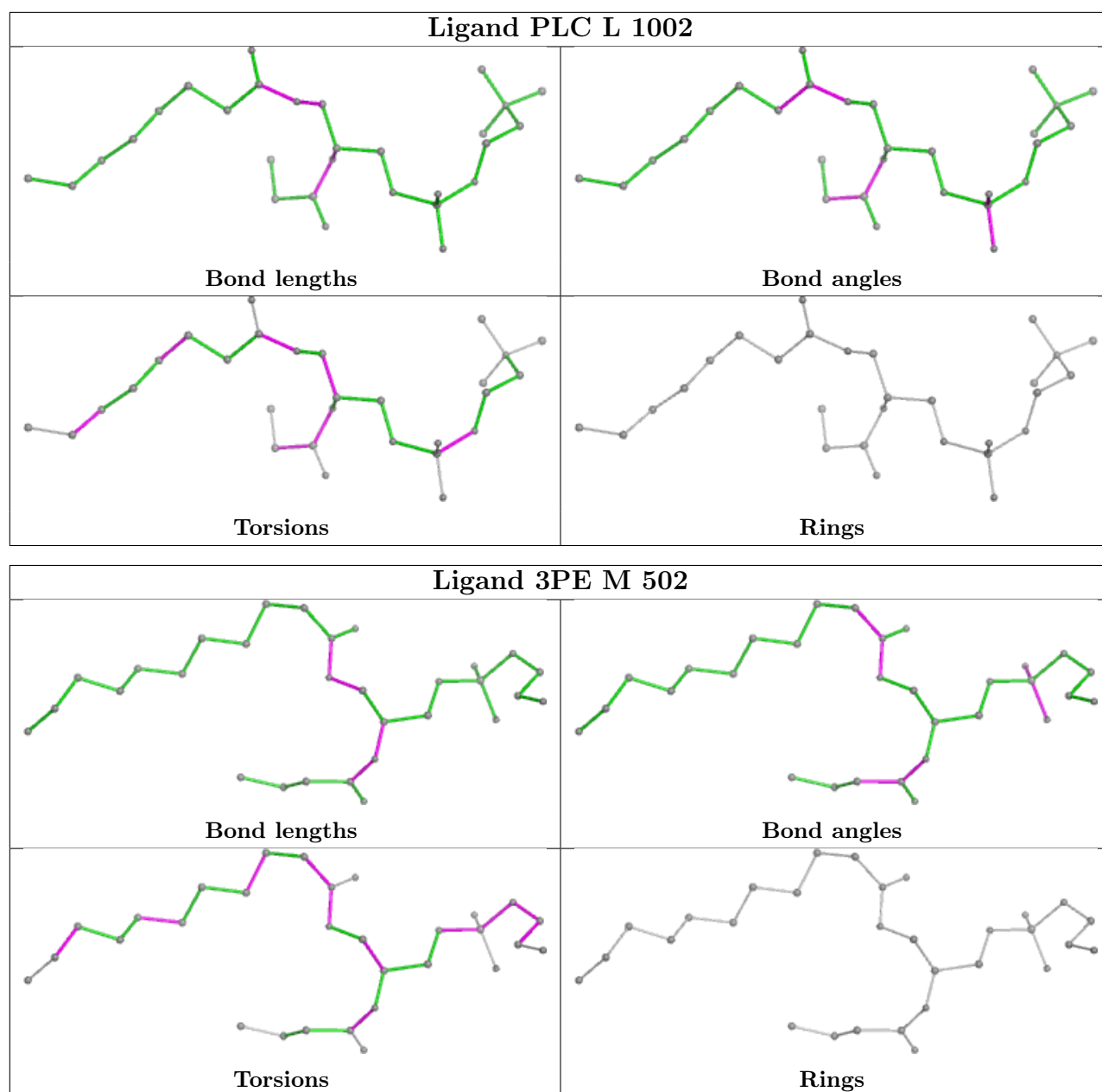


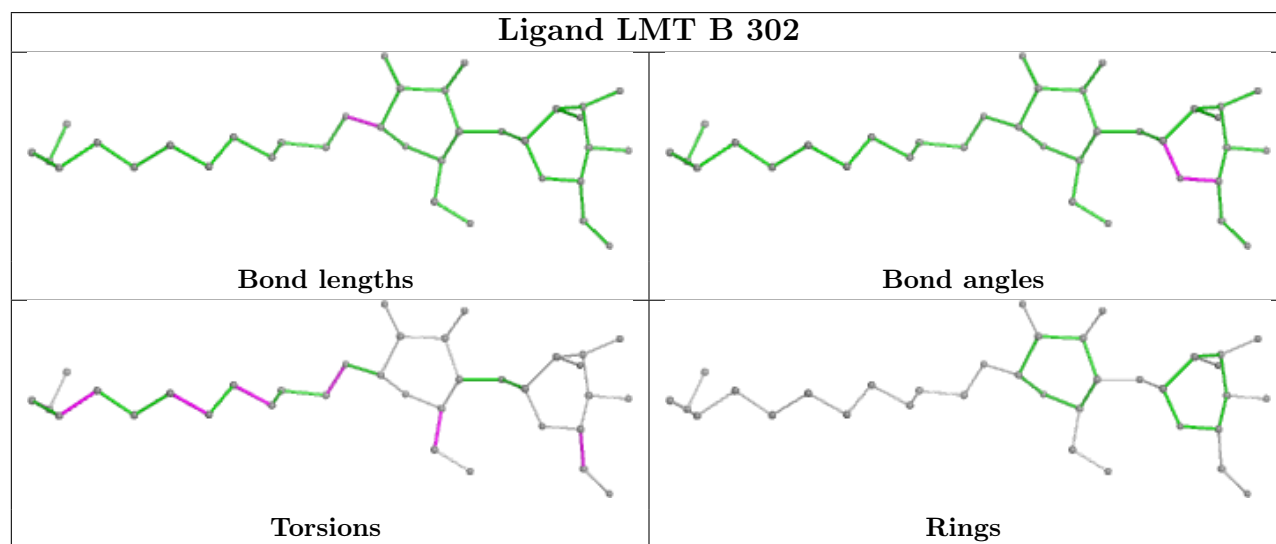
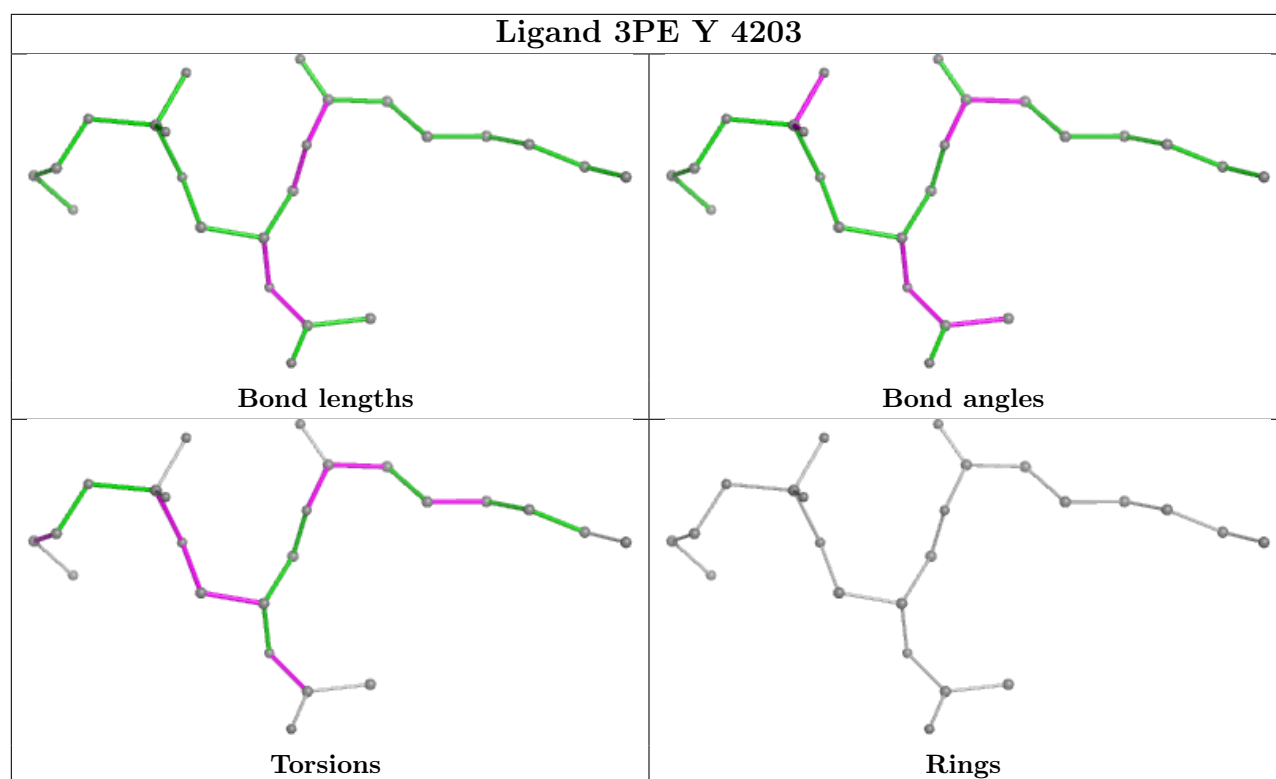


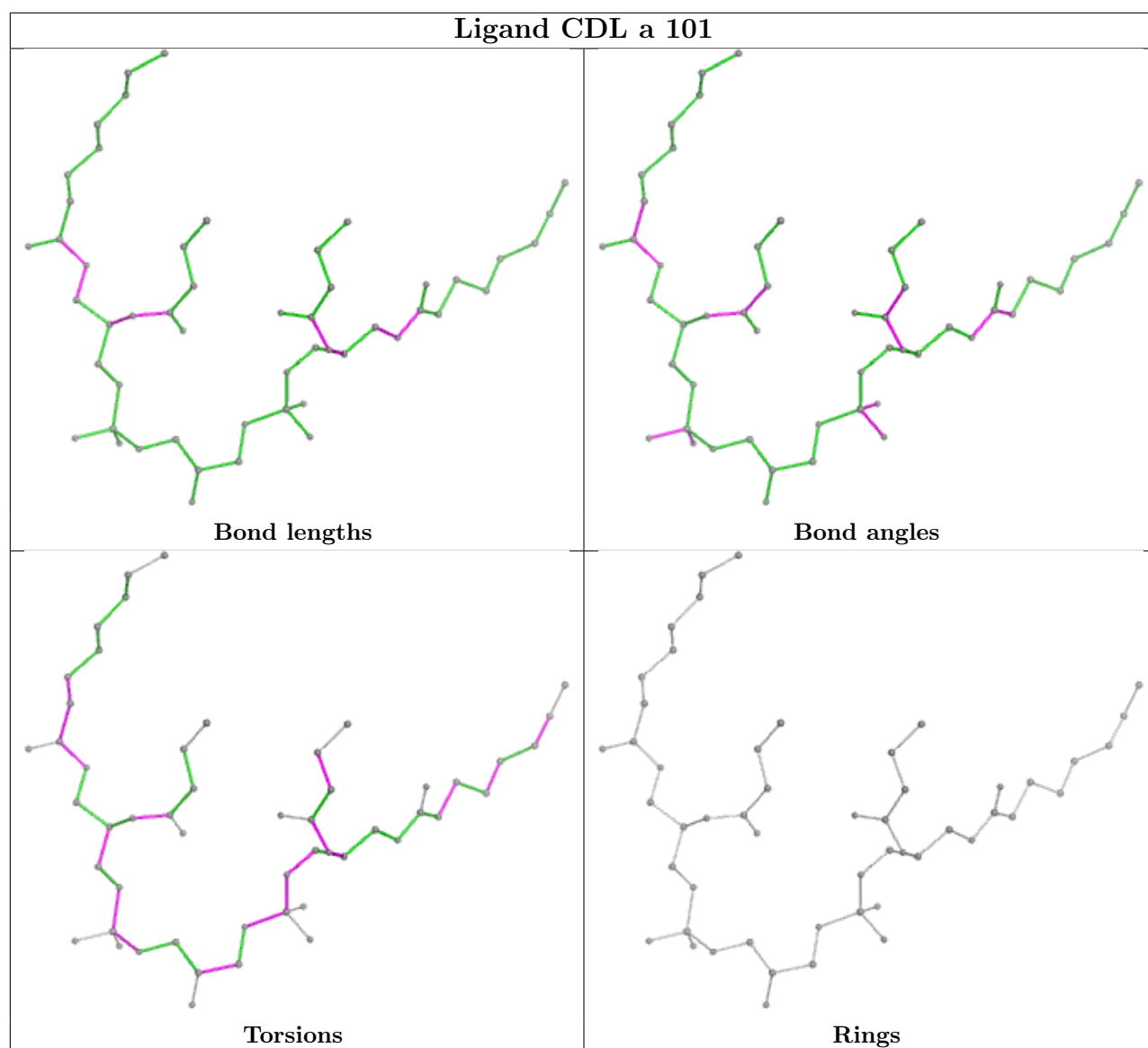
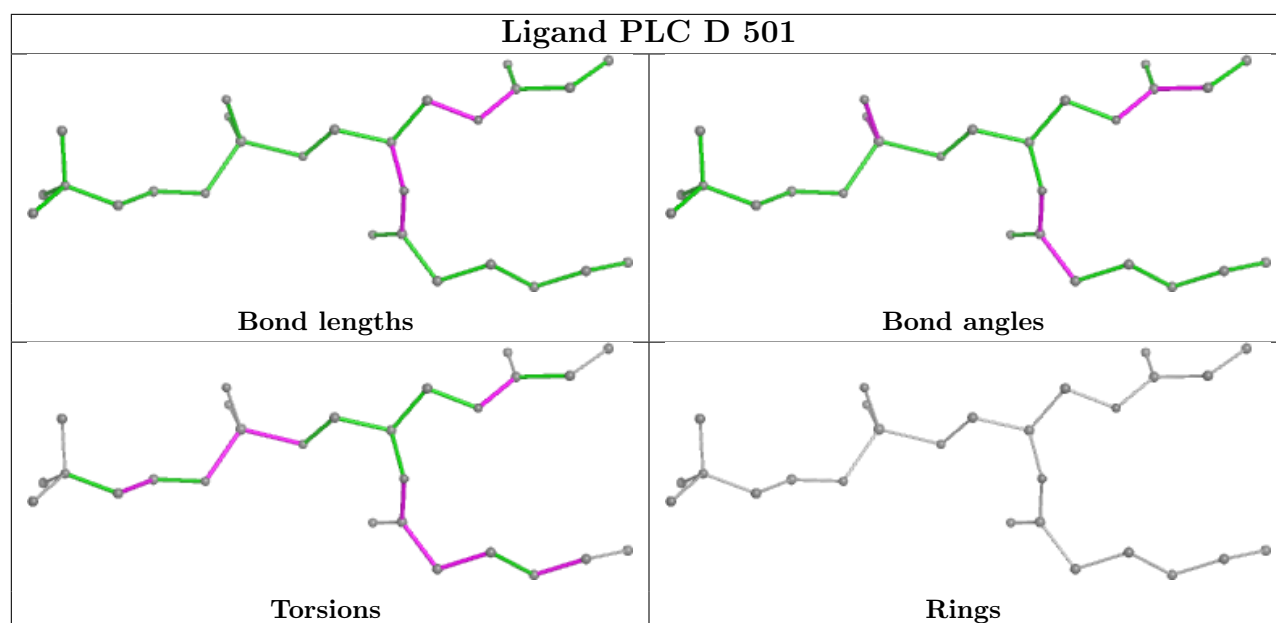


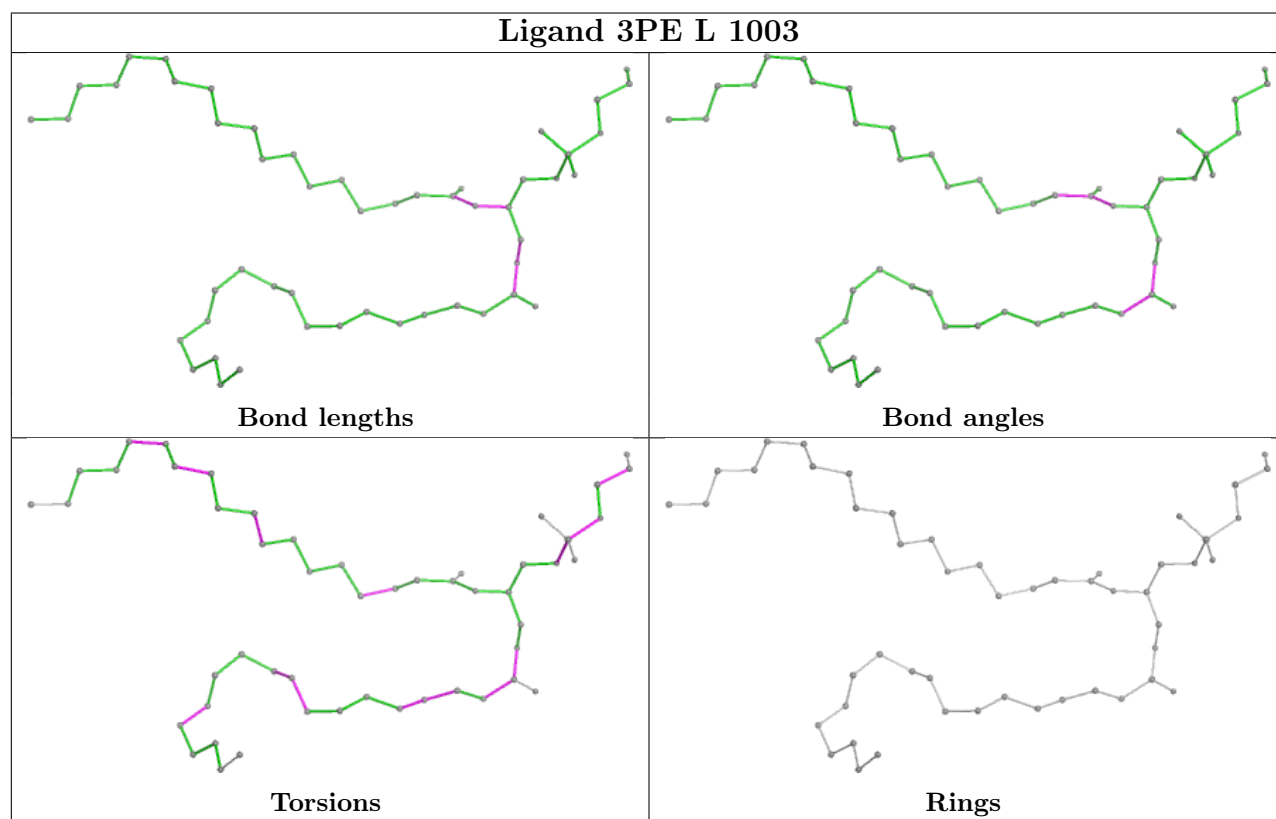
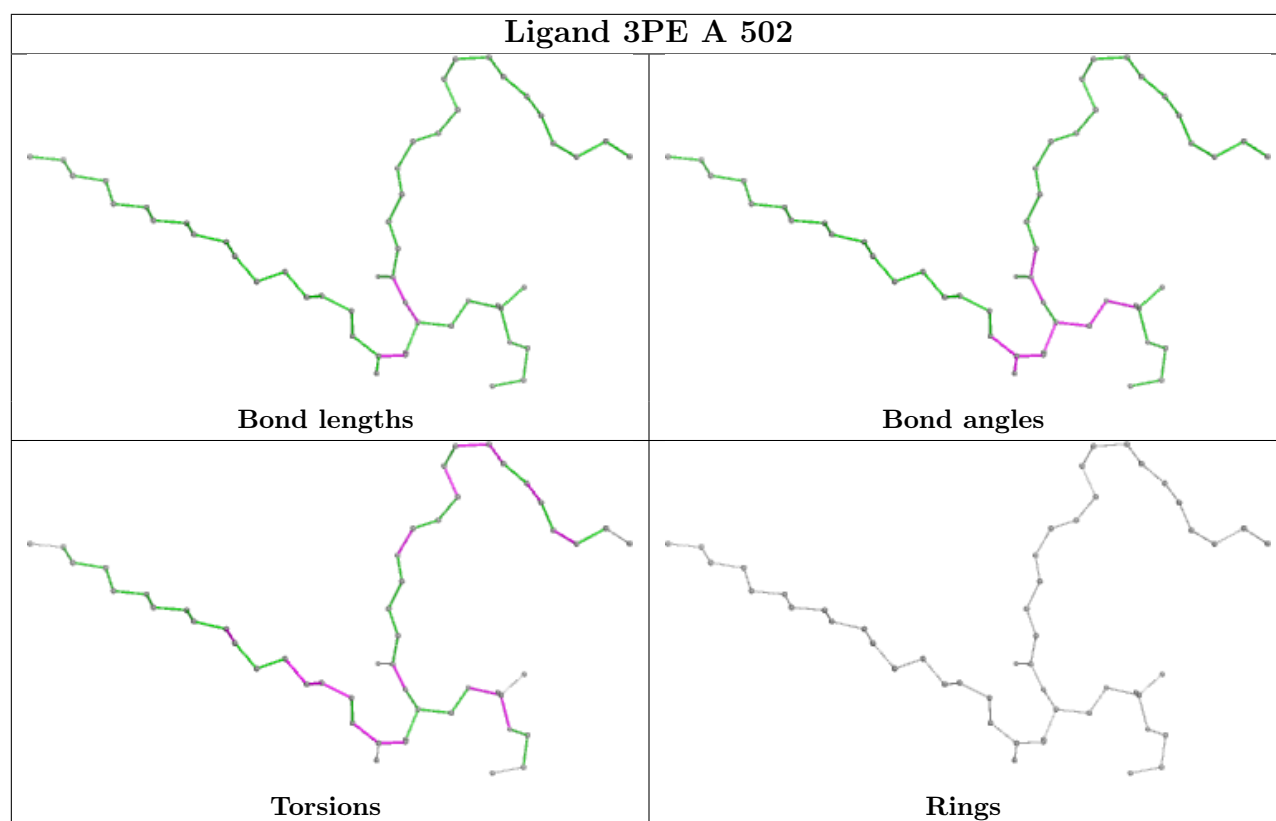


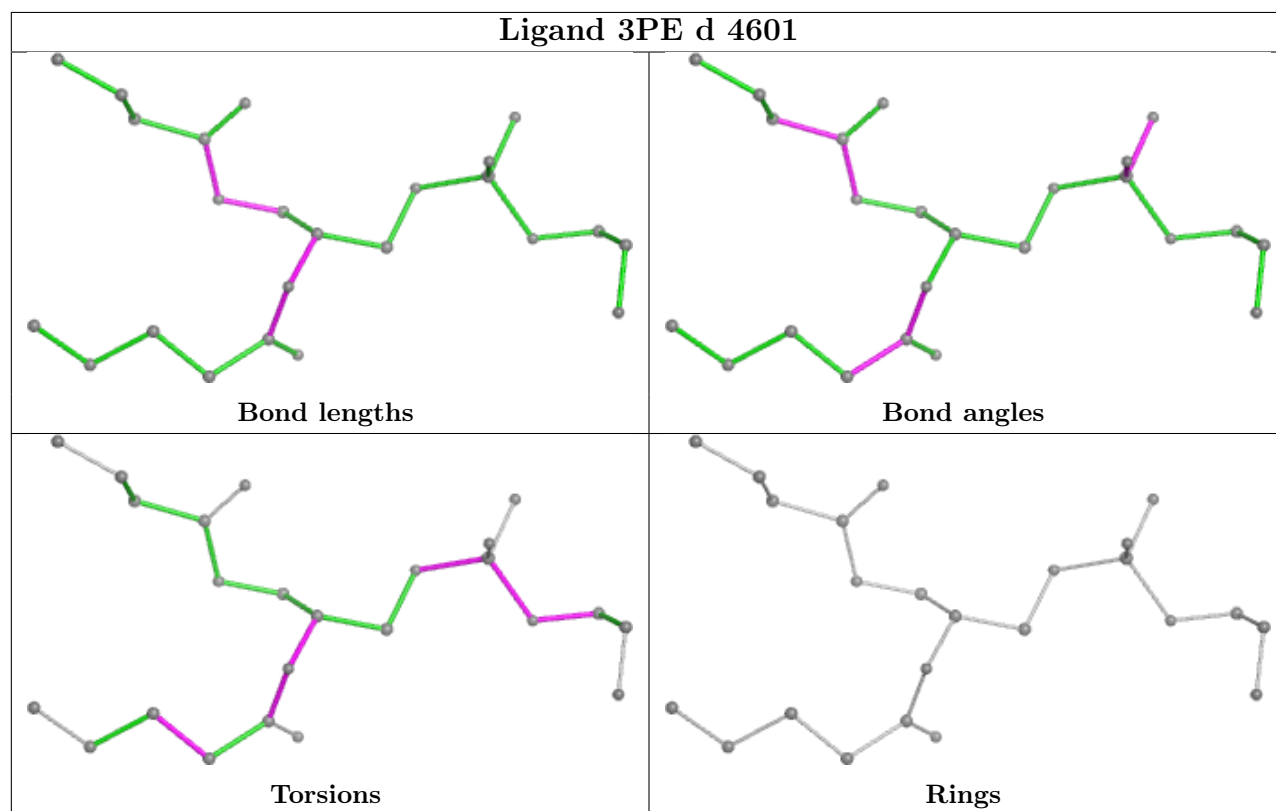
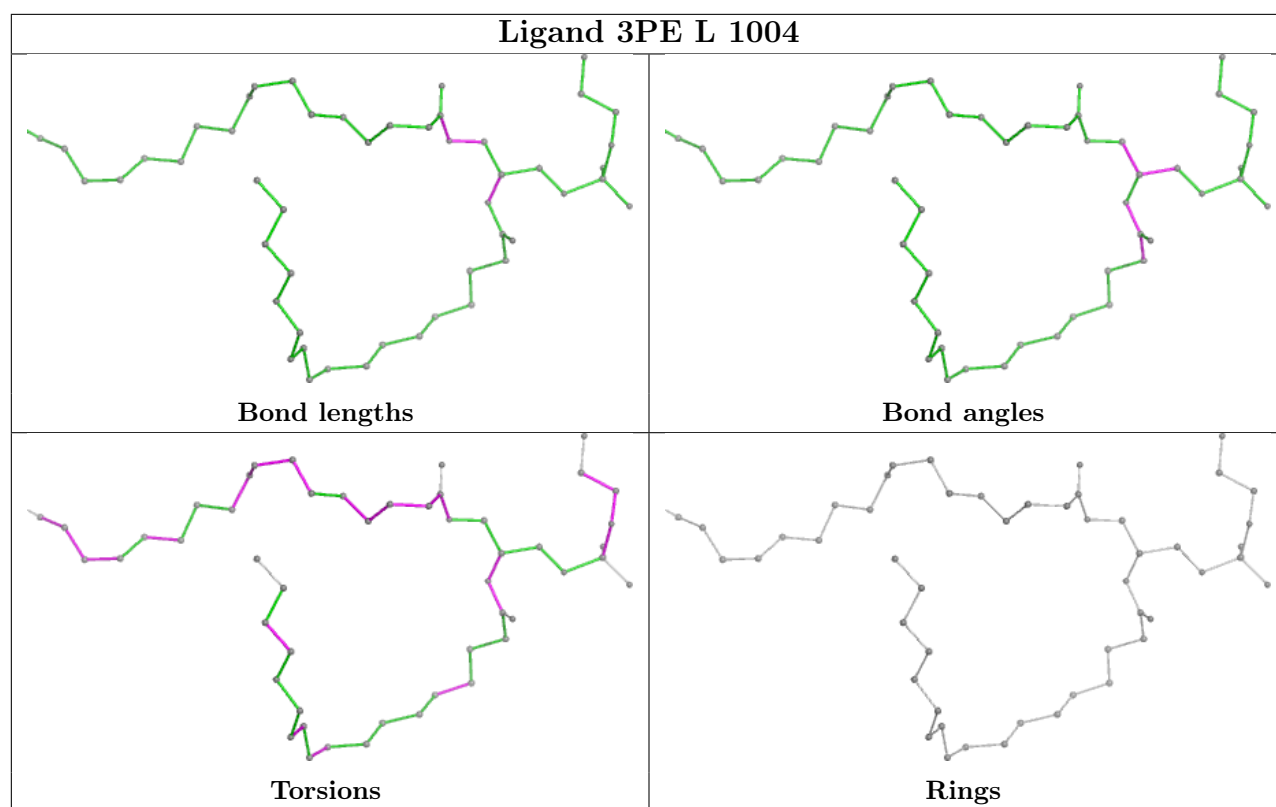


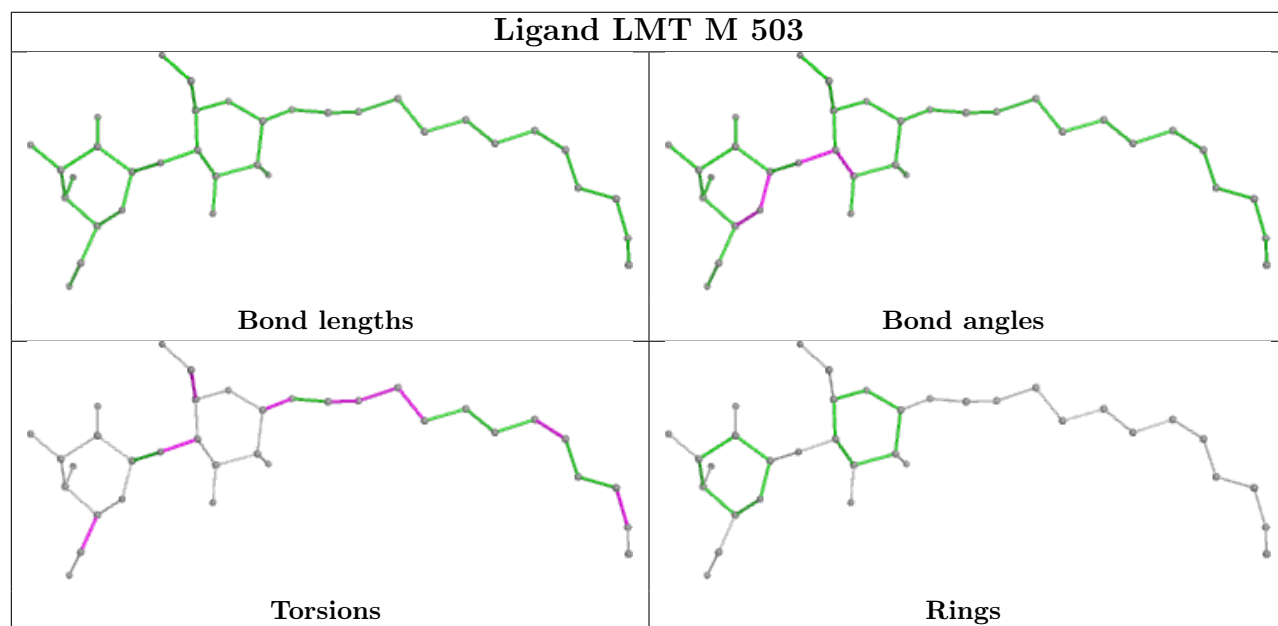
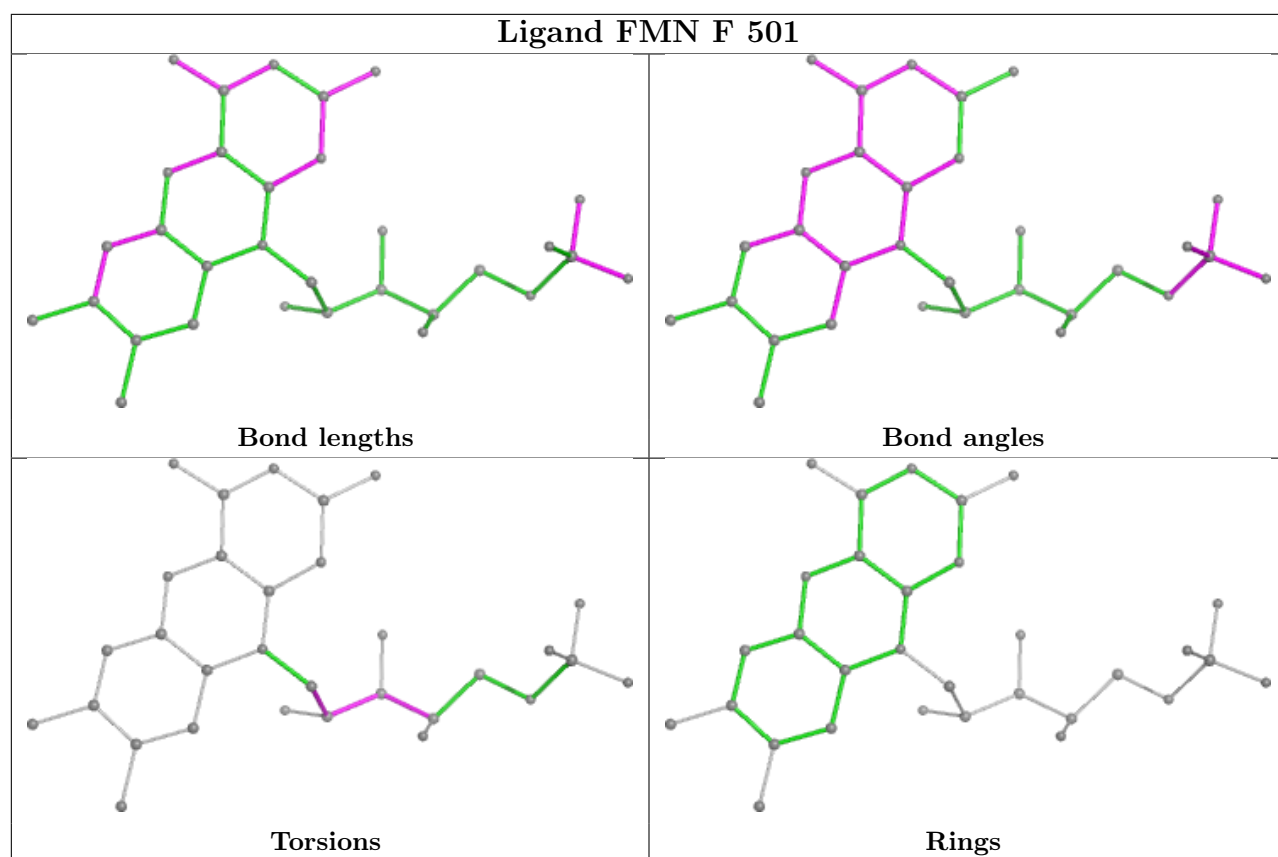


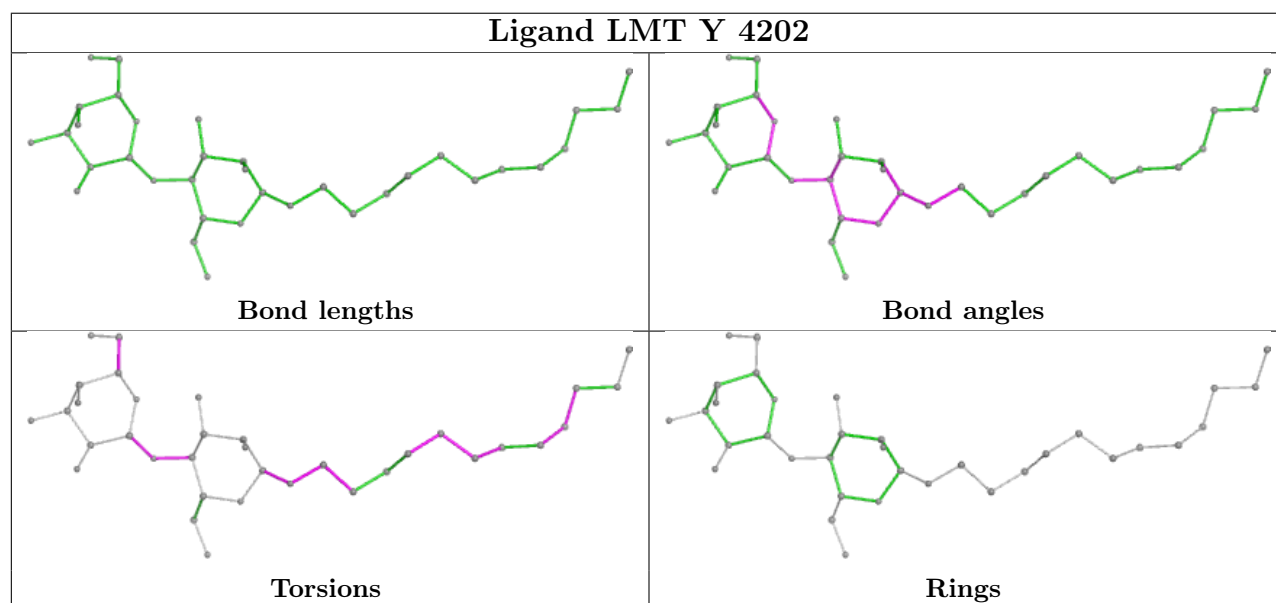
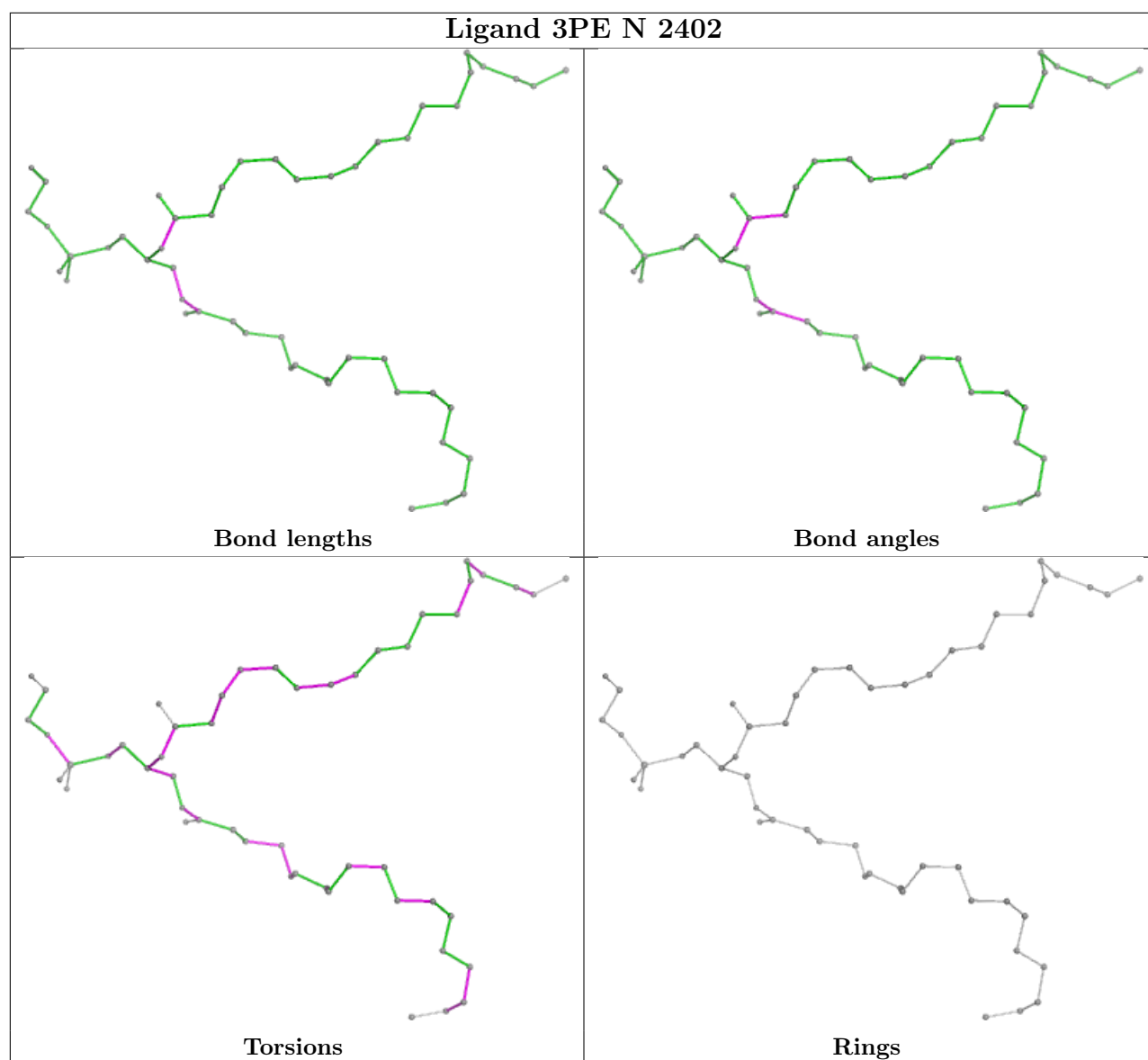


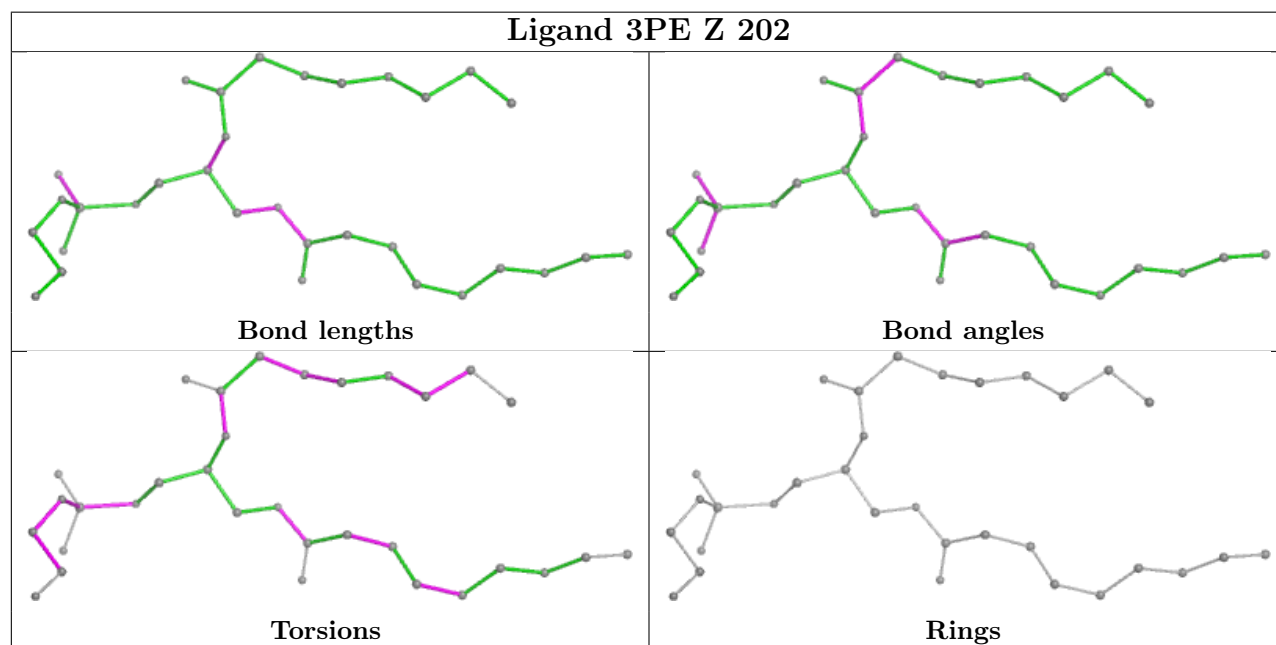
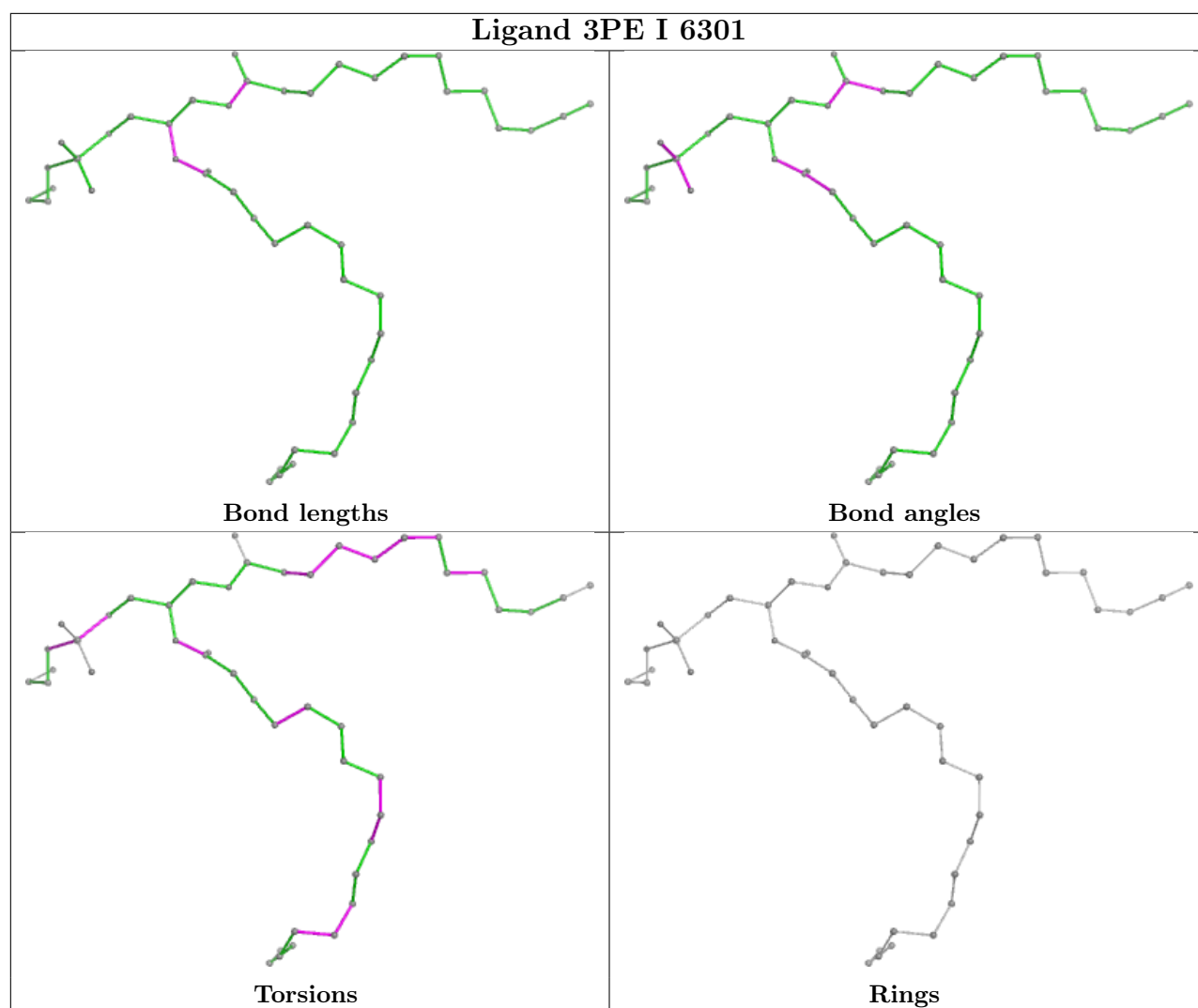


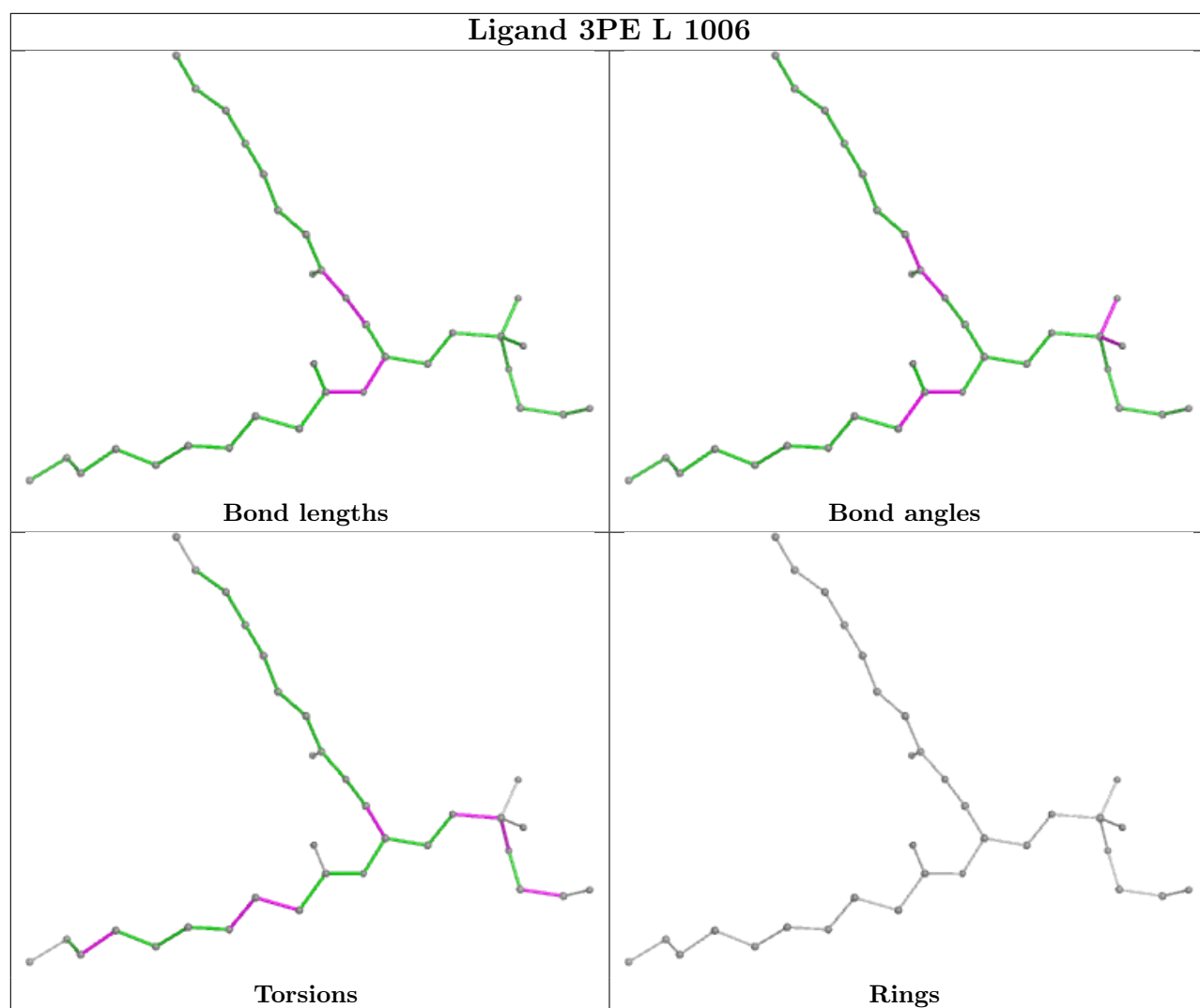


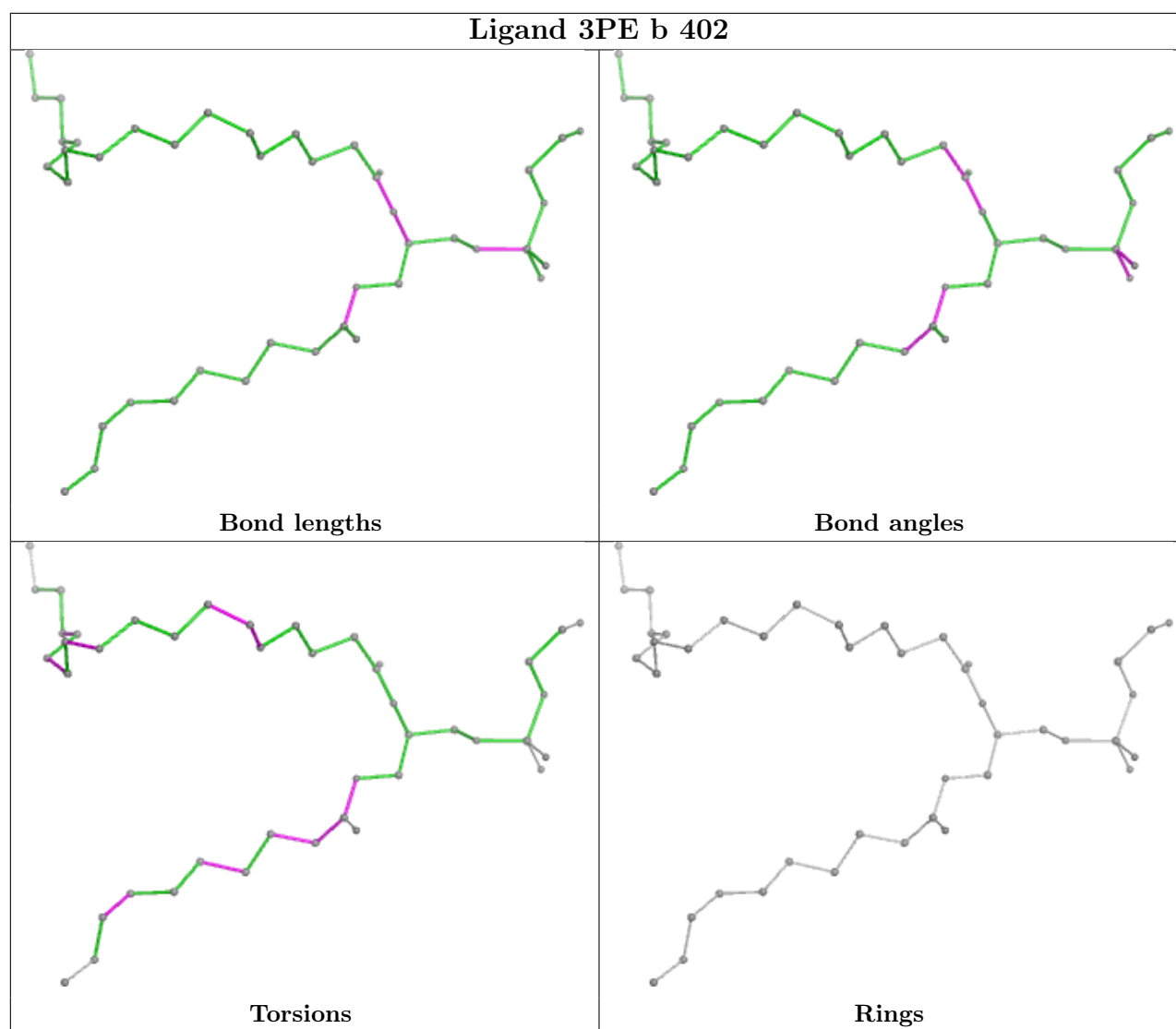












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

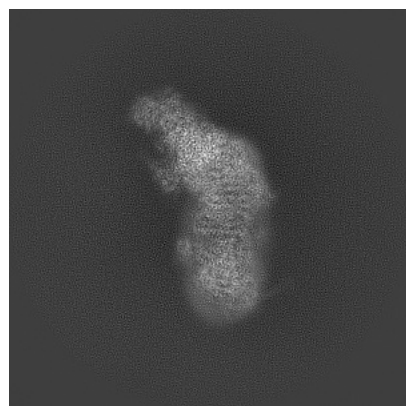
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10815. These allow visual inspection of the internal detail of the map and identification of artifacts.

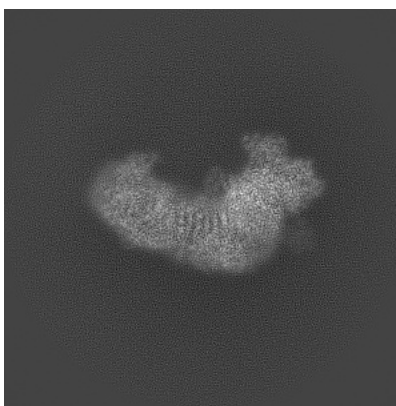
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

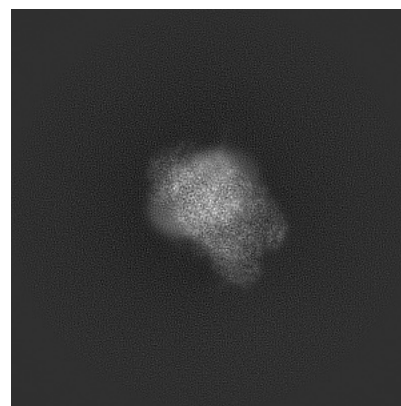
6.1.1 Primary map



X

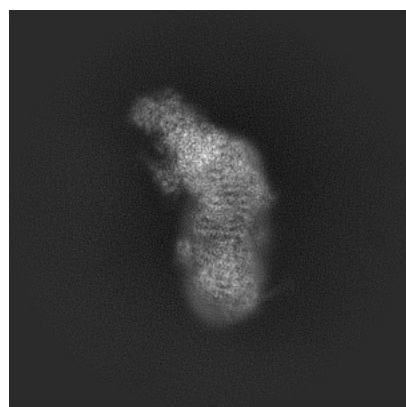


Y

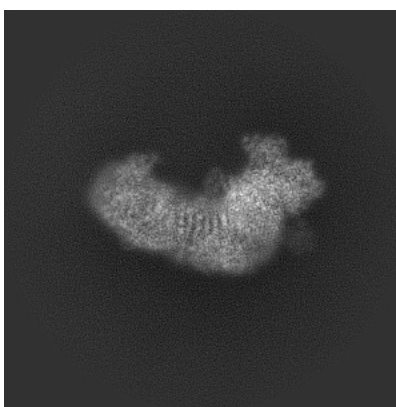


Z

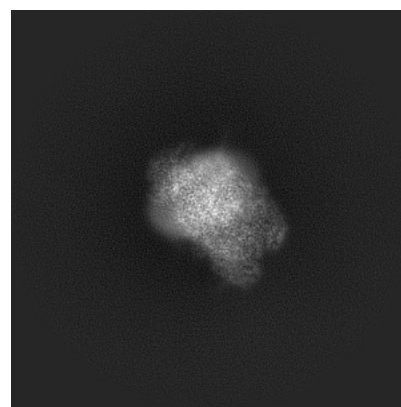
6.1.2 Raw map



X



Y

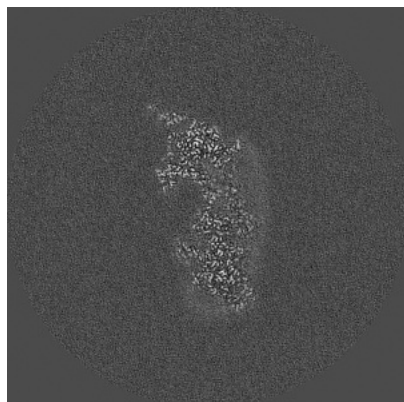


Z

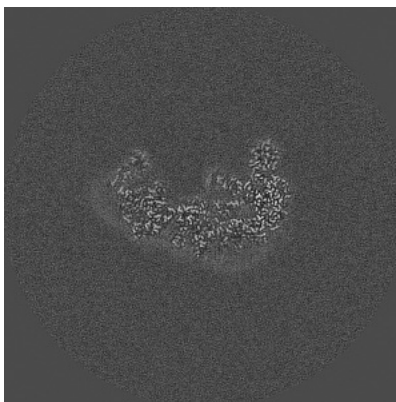
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

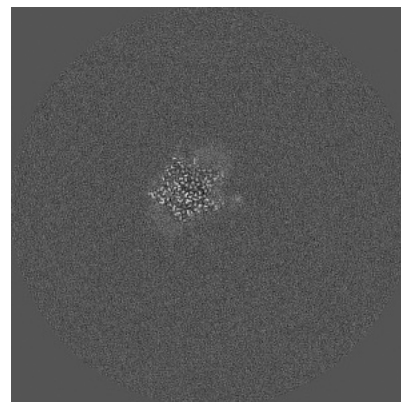
6.2.1 Primary map



X Index: 225

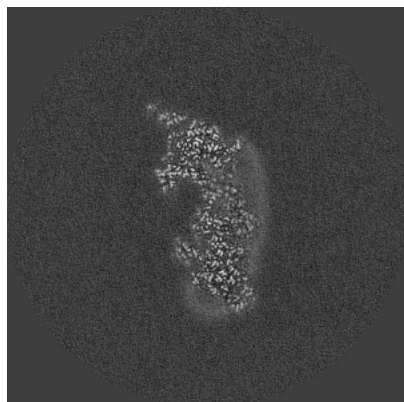


Y Index: 225



Z Index: 225

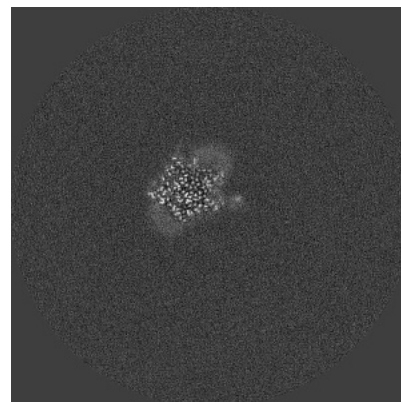
6.2.2 Raw map



X Index: 225



Y Index: 225

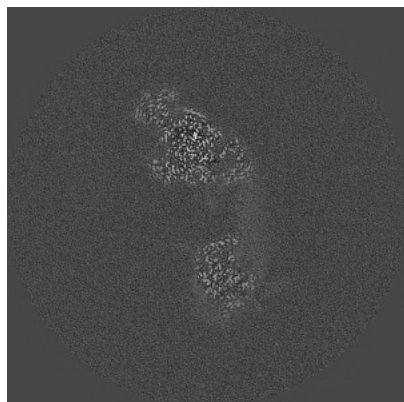


Z Index: 225

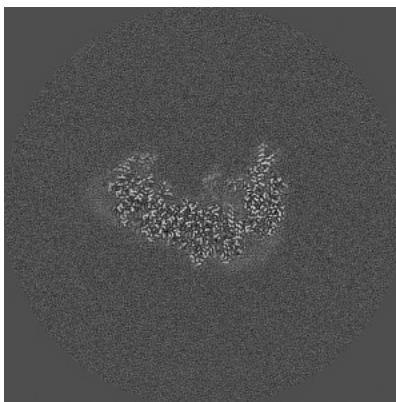
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

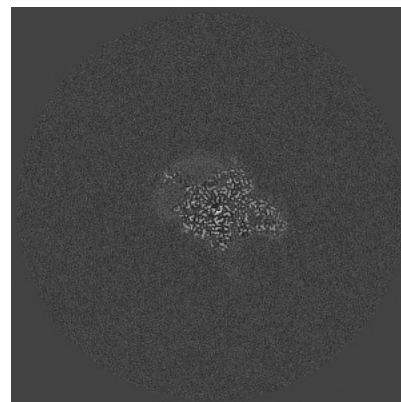
6.3.1 Primary map



X Index: 242

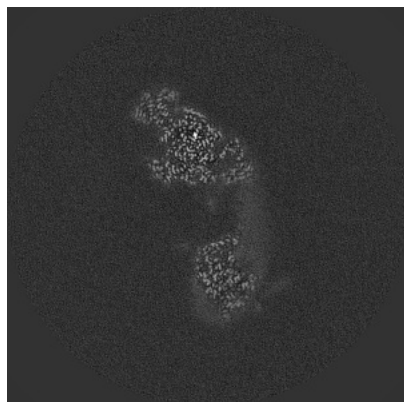


Y Index: 234

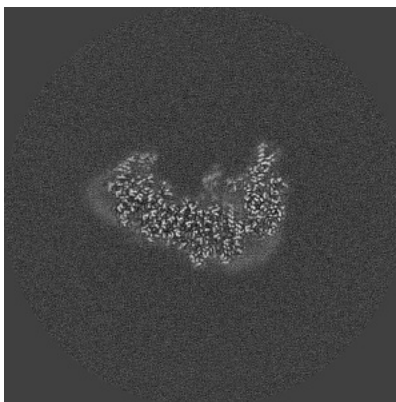


Z Index: 284

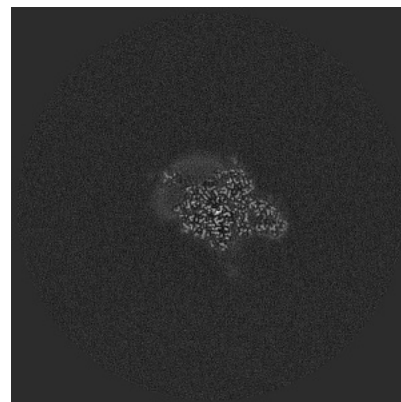
6.3.2 Raw map



X Index: 242



Y Index: 234

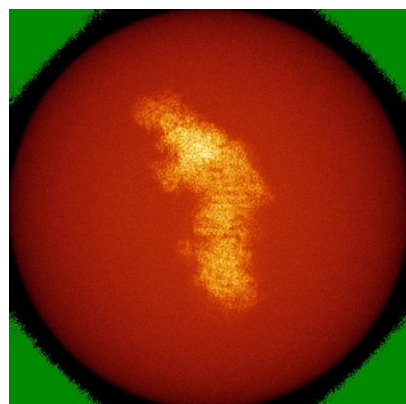


Z Index: 284

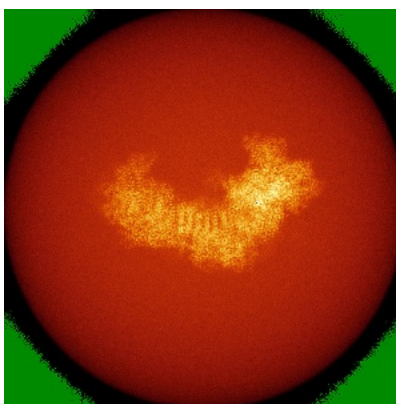
The images above show the largest variance slices of the map in three orthogonal directions.

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

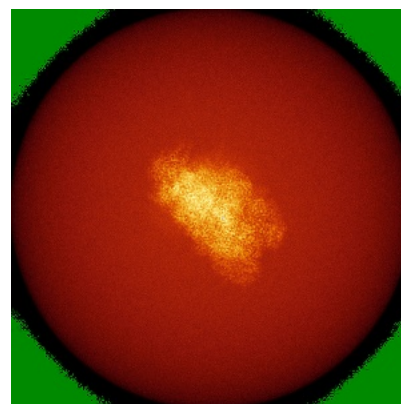
6.4.1 Primary map



X

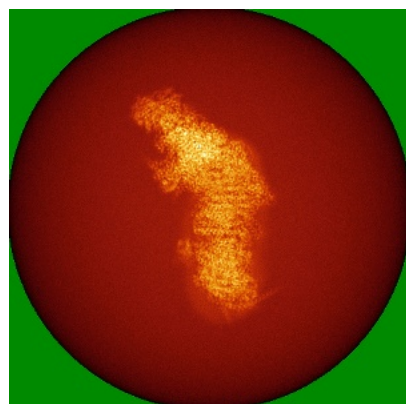


Y

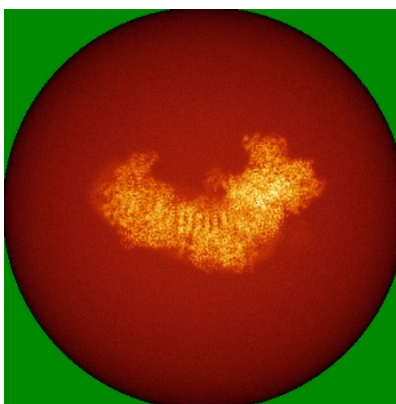


Z

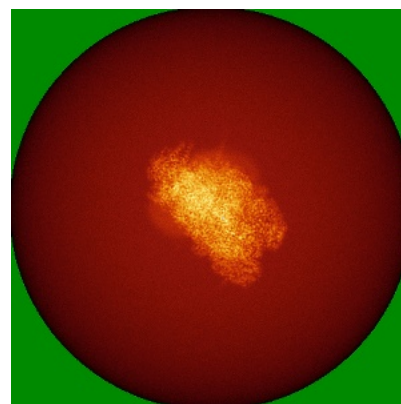
6.4.2 Raw map



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



X



Y



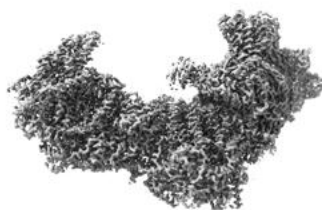
Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

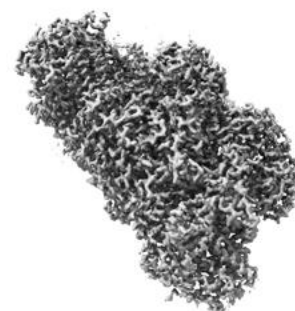
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

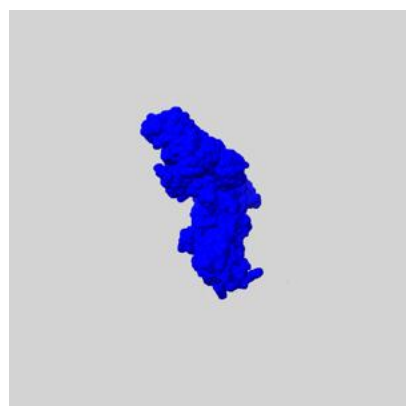
6.6 Mask visualisation [i](#)

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

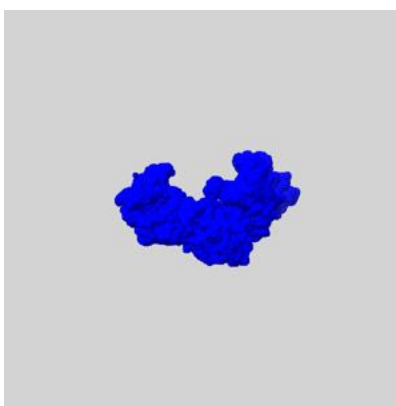
A mask typically either:

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

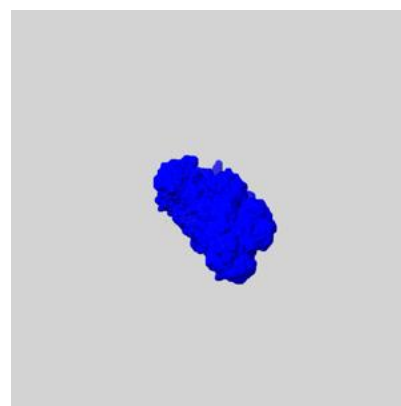
6.6.1 emd_10815_msk_1.map [i](#)



X



Y

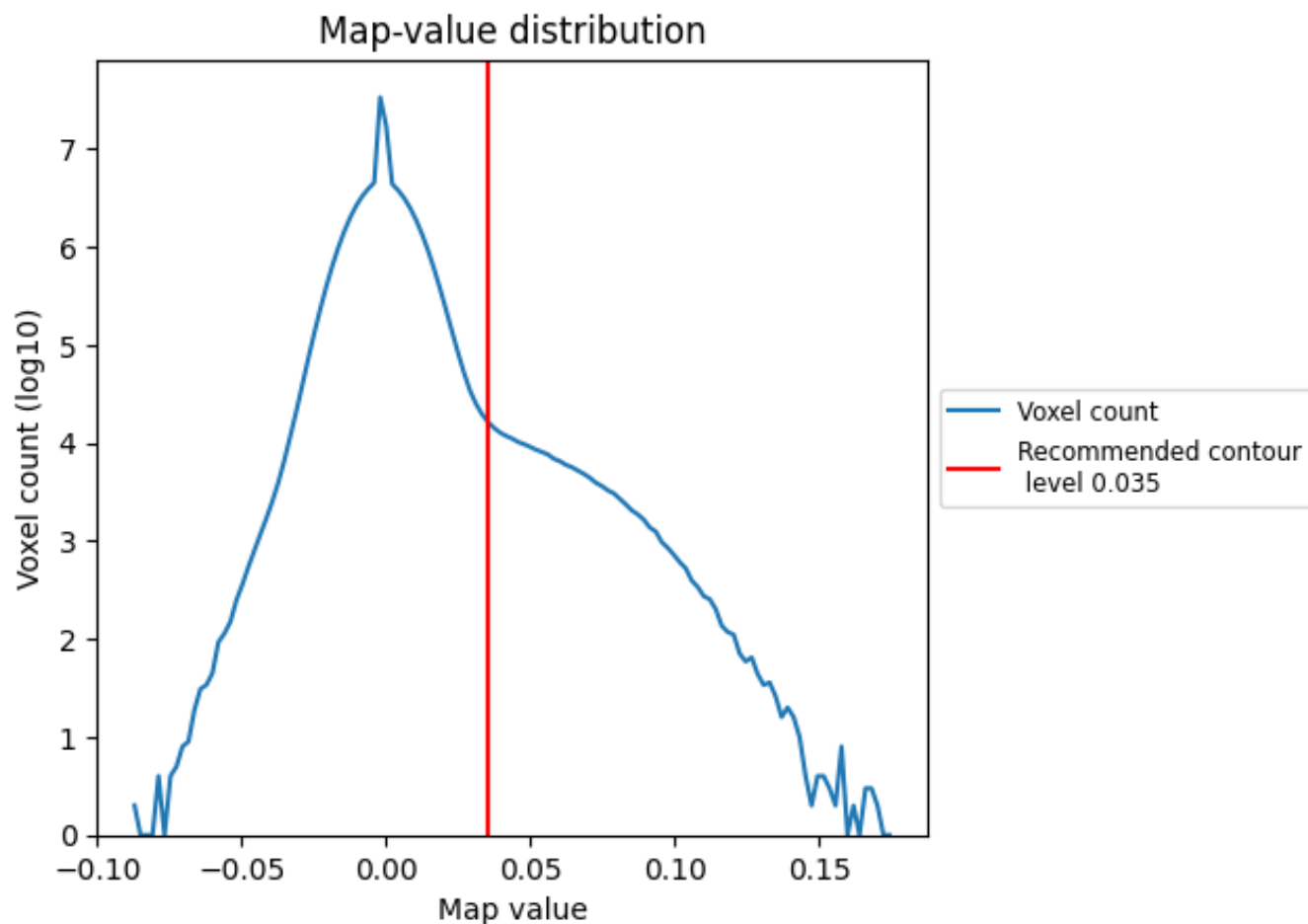


Z

7 Map analysis [i](#)

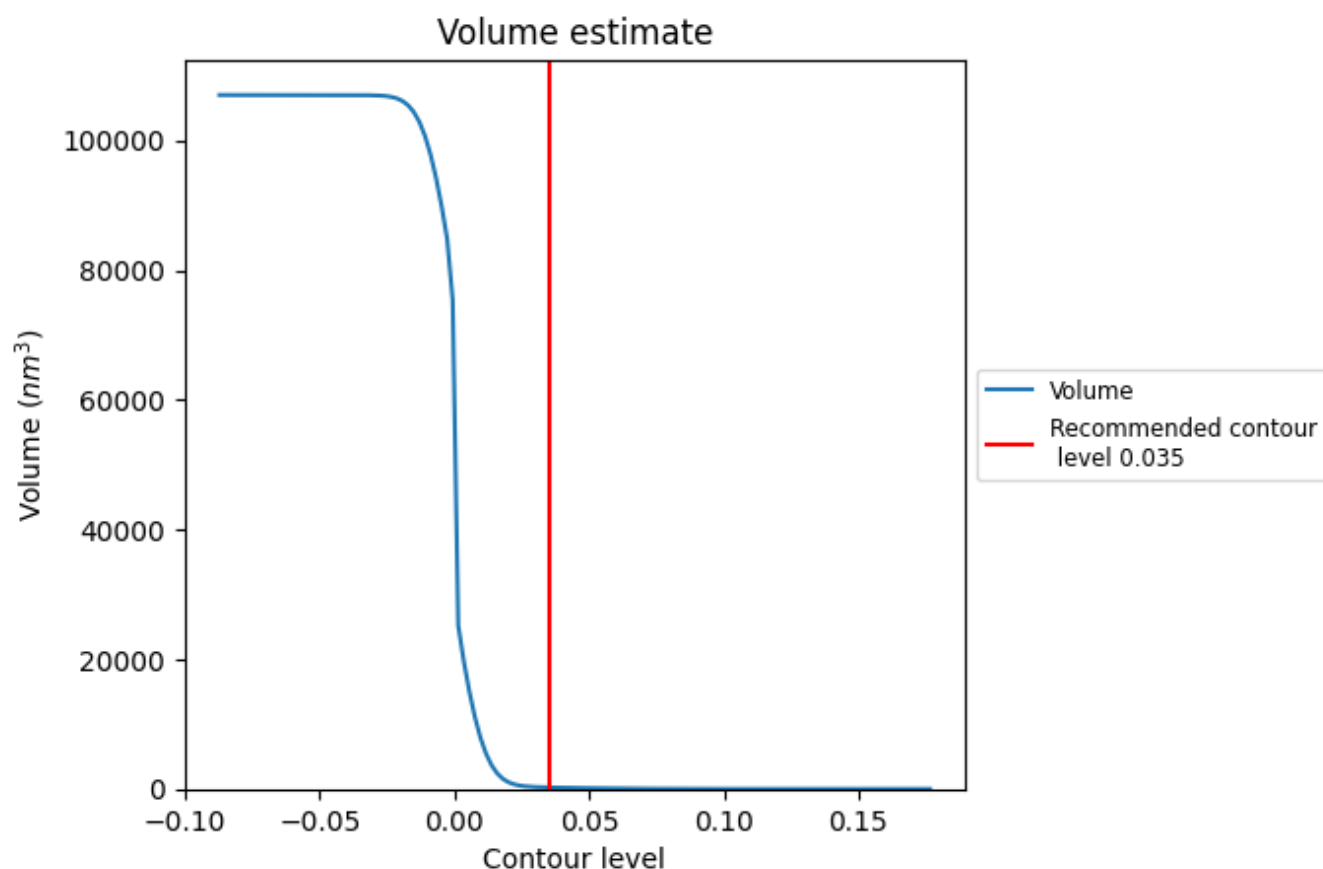
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

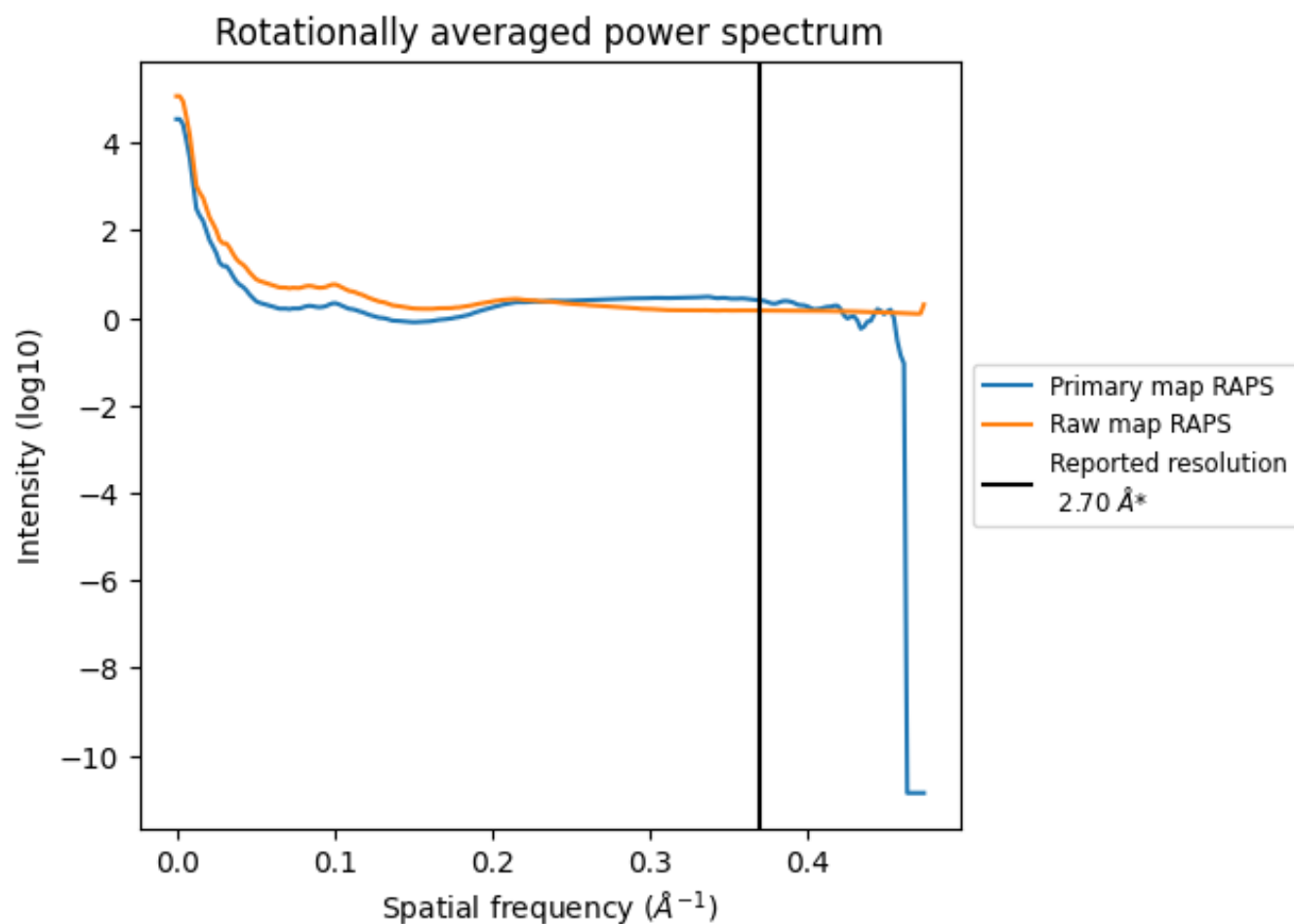
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm³; this corresponds to an approximate mass of 208 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 ⓘ

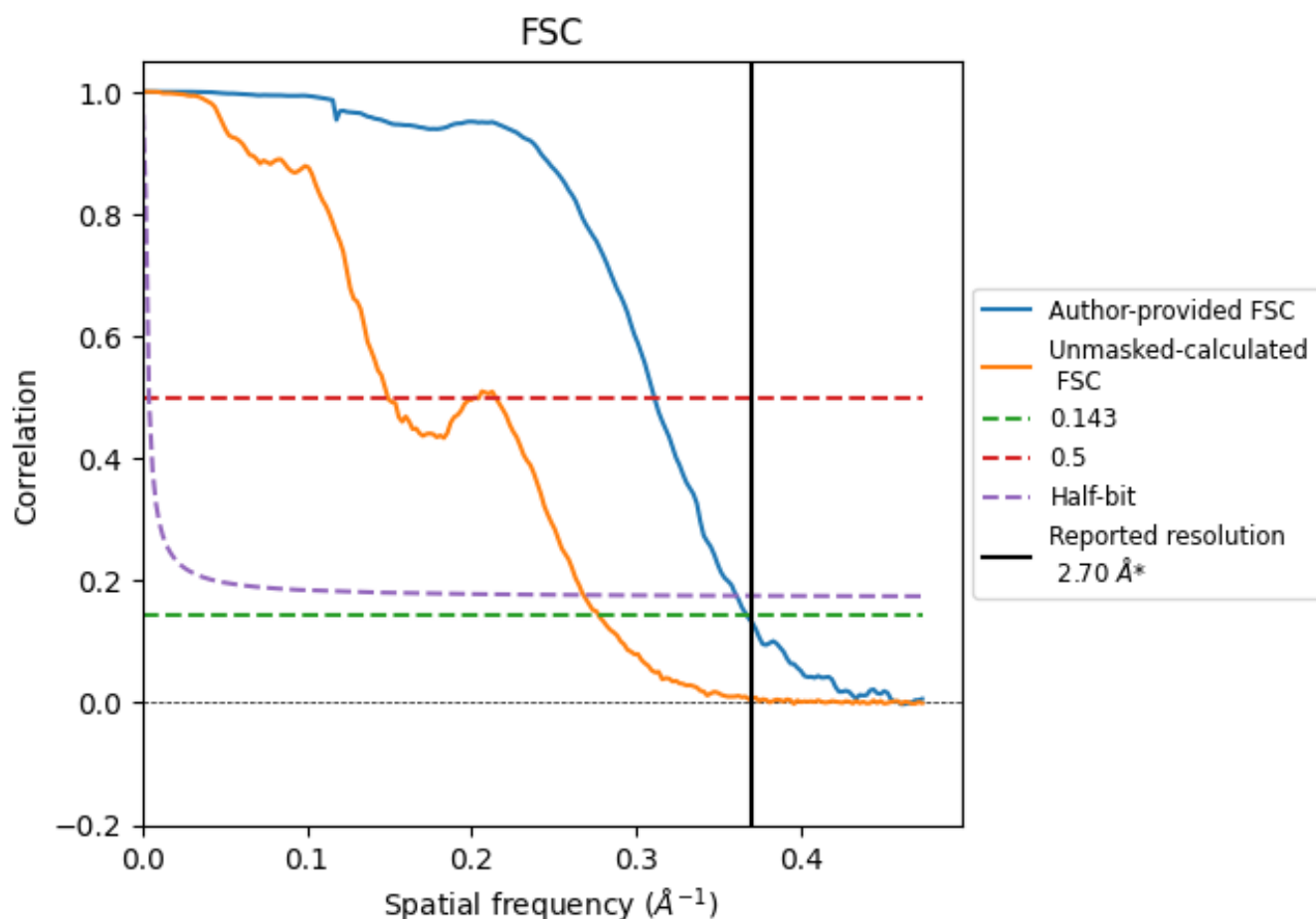


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

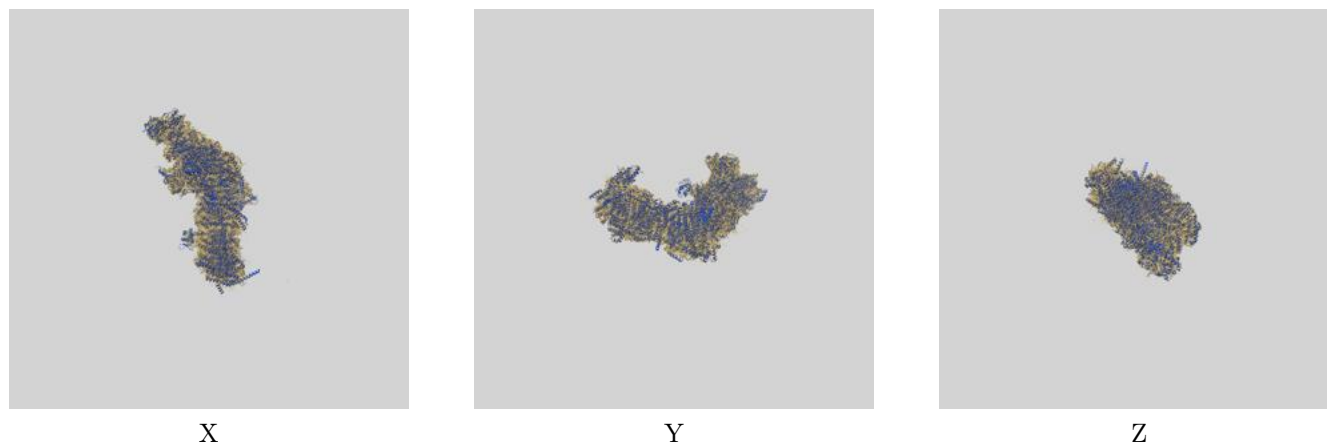
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.21	2.77
Unmasked-calculated*	3.60	6.70	3.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

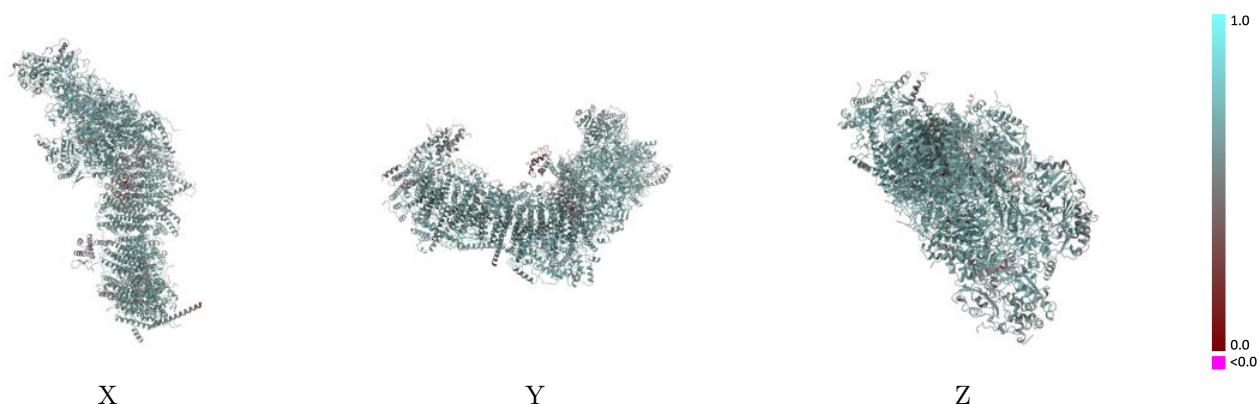
This section contains information regarding the fit between EMDB map EMD-10815 and PDB model 6YJ4. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



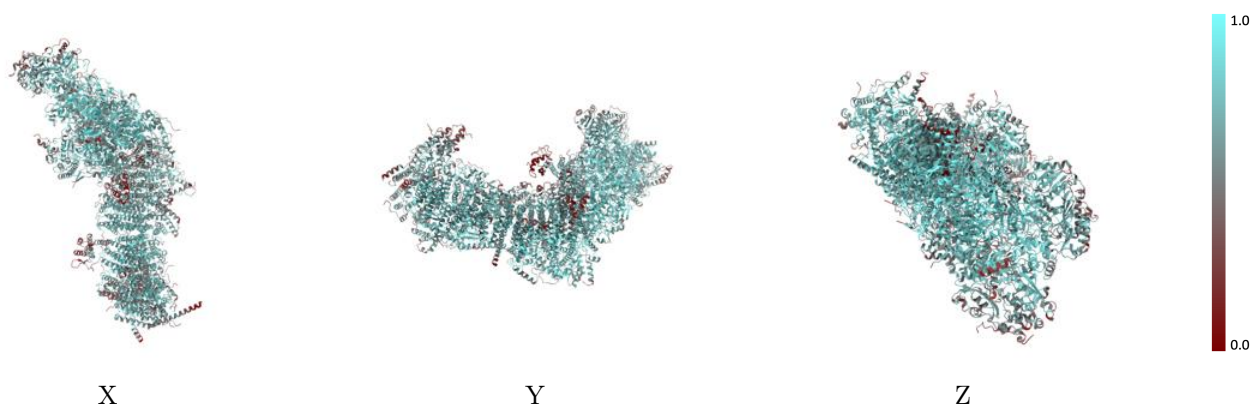
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



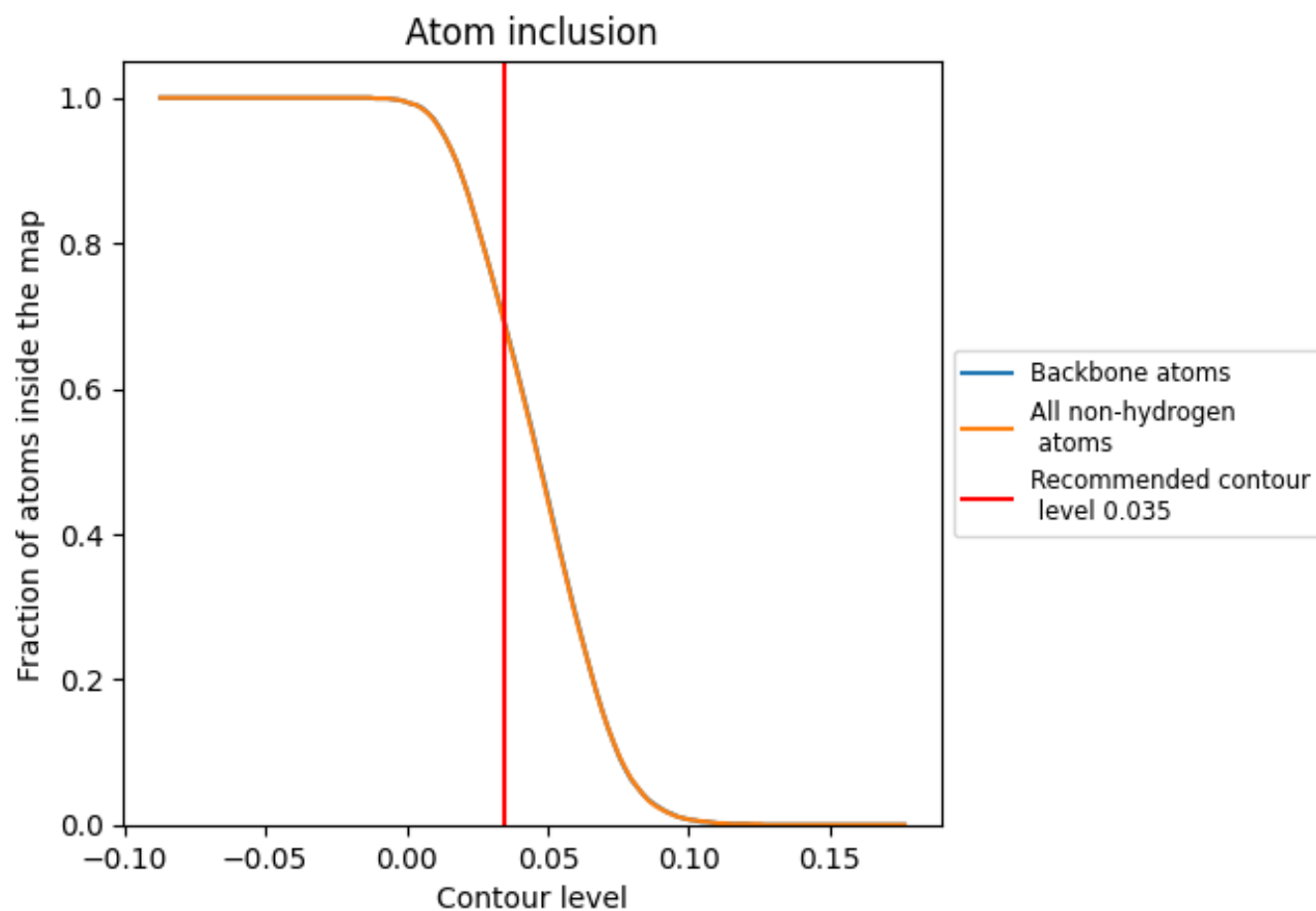
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.6020
A	 0.4610	 0.5350
B	 0.8240	 0.6470
C	 0.8190	 0.6420
D	 0.7970	 0.6390
E	 0.5920	 0.5690
F	 0.6420	 0.5810
G	 0.7410	 0.6130
H	 0.6950	 0.6100
I	 0.8330	 0.6520
J	 0.6420	 0.6030
K	 0.7370	 0.6340
L	 0.7050	 0.6110
M	 0.7730	 0.6360
N	 0.8170	 0.6520
O	 0.7280	 0.6170
P	 0.6590	 0.5860
Q	 0.7760	 0.6310
R	 0.7860	 0.6210
S	 0.5240	 0.5430
T	 0.1930	 0.3900
U	 0.3660	 0.4980
V	 0.6410	 0.5800
W	 0.6870	 0.5970
X	 0.6850	 0.6030
Y	 0.5840	 0.5790
Z	 0.6840	 0.6050
a	 0.7460	 0.6120
b	 0.6580	 0.5910
c	 0.7280	 0.6100
d	 0.6630	 0.5910
e	 0.6650	 0.5800
f	 0.7710	 0.6210
g	 0.4430	 0.4960
h	 0.6740	 0.6030



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Chain	Atom inclusion	Q-score
i	 0.6460	 0.5860
j	 0.5070	 0.5320
k	 0.4650	 0.5150
l	 0.6210	 0.5830
m	 0.6740	 0.5990
n	 0.5490	 0.5260
o	 0.5120	 0.5380
p	 0.7520	 0.6180