



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 04:04 am BST

PDB ID : 6Y79 / pdb_00006y79
EMDB ID : EMD-10711
Title : Cryo-EM structure of a respiratory complex I F89A mutant
Authors : Parey, K.
Deposited on : 2020-02-28
Resolution : 2.96 Å(reported)
Based on initial model : 6RFR

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

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

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

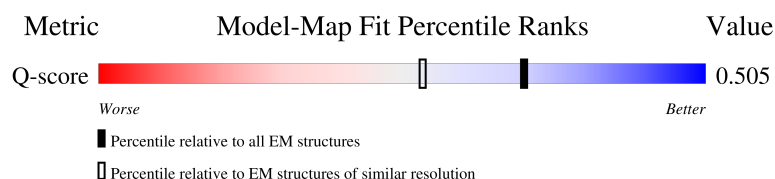
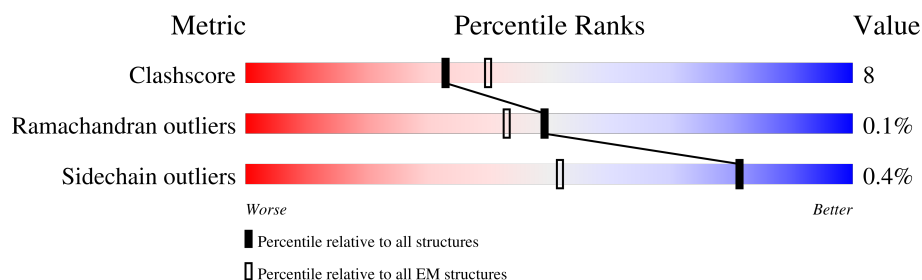
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	728	
2	B	488	
3	C	466	
4	D	87	

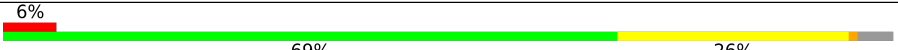
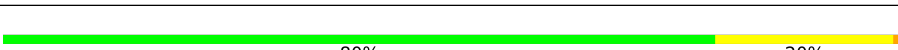
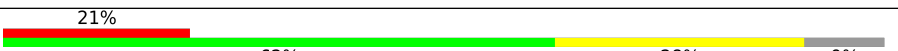
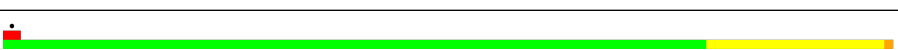
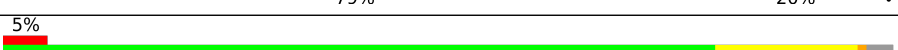
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	375	
6	F	144	
7	G	281	
8	H	243	
9	I	229	
10	J	198	
11	K	210	
12	L	89	
13	M	136	
14	O	109	
15	P	124	
16	Q	132	
17	R	109	
18	S	249	
19	U	172	
20	W	123	
21	X	169	
22	Y	161	
23	Z	182	
24	a	149	
25	b	74	
26	c	60	
27	d	92	
28	e	67	
29	f	87	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	g	78	
31	h	138	
32	i	90	
33	j	93	
34	n	120	
35	1	341	
36	2	469	
37	3	128	
38	4	486	
39	5	655	
40	6	185	
41	8	99	
42	9	89	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 65173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	692	Total	C	N	O	S	0	0
			5258	3263	926	1040	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	456	Total	C	N	O	S	0	0
			3528	2229	621	654	24		

- Molecule 3 is a protein called Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	433	Total	C	N	O	S	0	0
			3426	2177	586	641	22		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	317	Total	C	N	O	S	0	0
			2527	1606	435	478	8		

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

plex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	121	Total	C	N	O	S	0	0
			990	629	166	193	2		

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

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

- Molecule 8 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	179	Total	C	N	O	S	0	0
			1329	844	241	239	5		

- Molecule 11 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	175	Total	C	N	O	S	0	0
			1377	874	241	247	15		

- Molecule 12 is a protein called Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	89	Total	C	N	O	S	0	0
			691	464	109	115	3		

- Molecule 13 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

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

- Molecule 14 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	77	Total	C	N	O	0	0
			591	373	93	125		

- Molecule 15 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	123	Total	C	N	O	S	0	0
			1030	661	182	185	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	89	ALA	PHE	conflict	UNP A0A1D8N3C8

- Molecule 16 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

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

- Molecule 17 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	174	Total	C	N	O	S	0	0
			1430	920	245	263	2		

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

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

- Molecule 20 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	167	Total	C	N	O	S	0	0
			1296	839	221	232	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	123	Total	C	N	O	S	0	0
			1021	651	187	181	2		

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

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

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

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

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

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

- Molecule 26 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	90	Total	C	N	O	S	0	0
			760	472	137	148	3		

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

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

- Molecule 29 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	80	Total	C	N	O	S	0	0
			629	394	119	115	1		

- Molecule 30 is a protein called Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	76	Total	C	N	O	0	0
			617	405	112	100		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	71	GLY	GLN	conflict	UNP A0A1D8NJR0

- Molecule 31 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

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

- Molecule 33 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	114	Total	C	N	O	S	0	0
			914	588	156	169	1		

- Molecule 35 is a protein called Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	329	Total	C	N	O	S	0	0
			2627	1793	382	445	7		

- Molecule 36 is a protein called Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	469	Total	C	N	O	S	0	0
			3774	2557	550	655	12		

- Molecule 37 is a protein called Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	116	Total	C	N	O	S	0	0
			933	641	137	153	2		

- Molecule 38 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4	485	Total	C	N	O	S	0	0
			3847	2595	585	653	14		

- Molecule 39 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	654	Total	C	N	O	S	0	0
			5197	3479	785	905	28		

- Molecule 40 is a protein called Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6	180	Total	C	N	O	S	0	0
			1415	959	204	245	7		

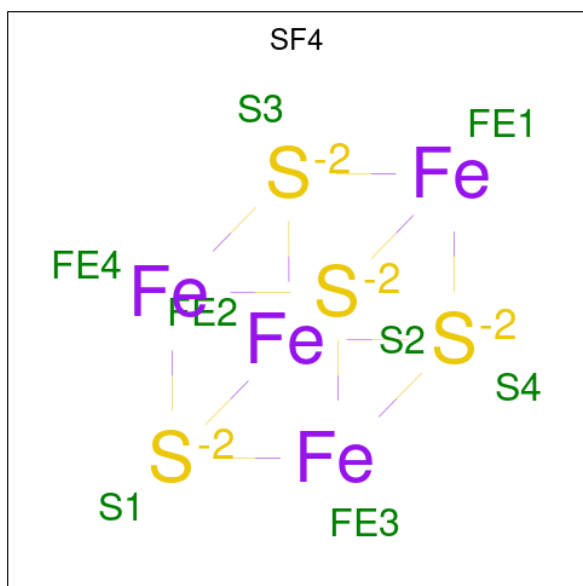
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	77	Total	C	N	O	S	0	0
			643	408	116	111	8		

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

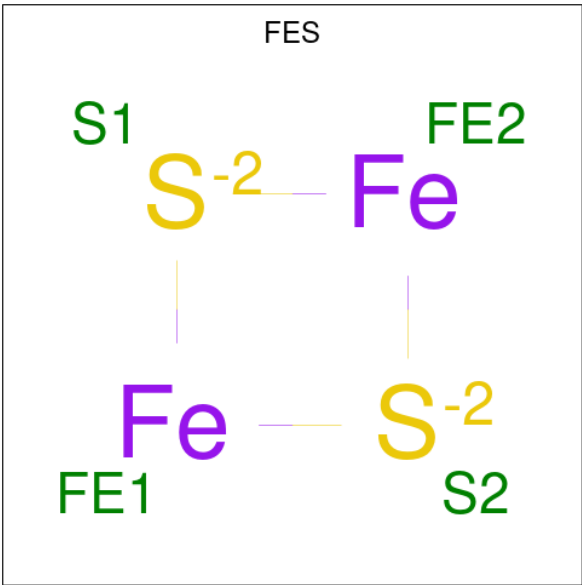
Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



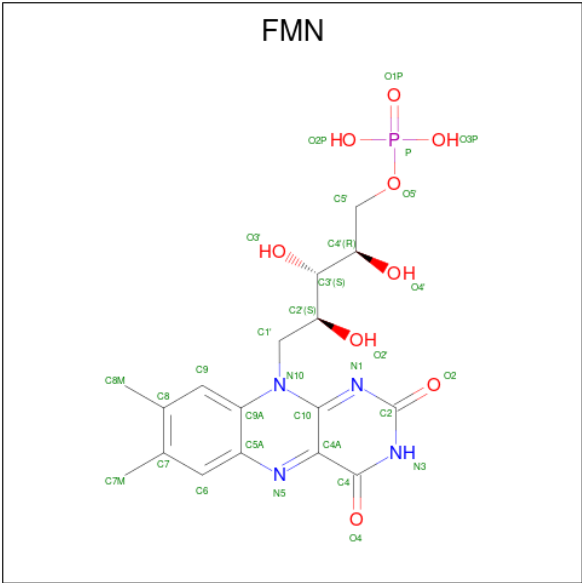
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			8	4	4	
43	A	1	Total	Fe	S	0
			8	4	4	
43	B	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

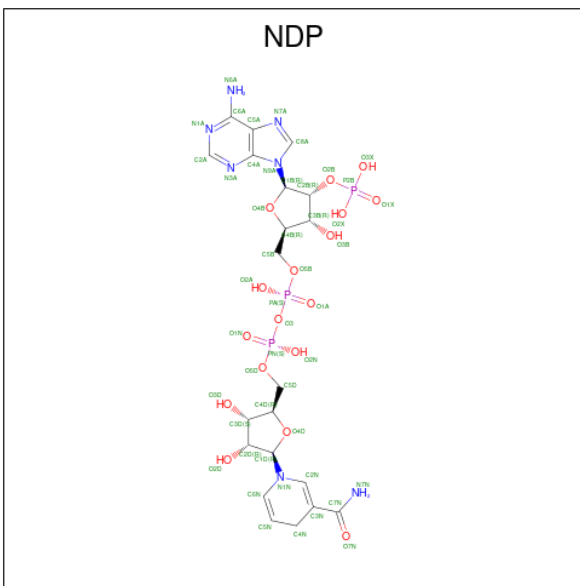
- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

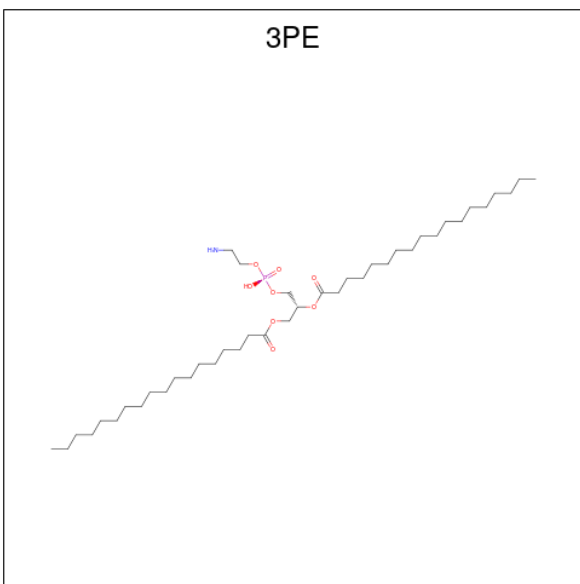
- Molecule 46 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



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

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



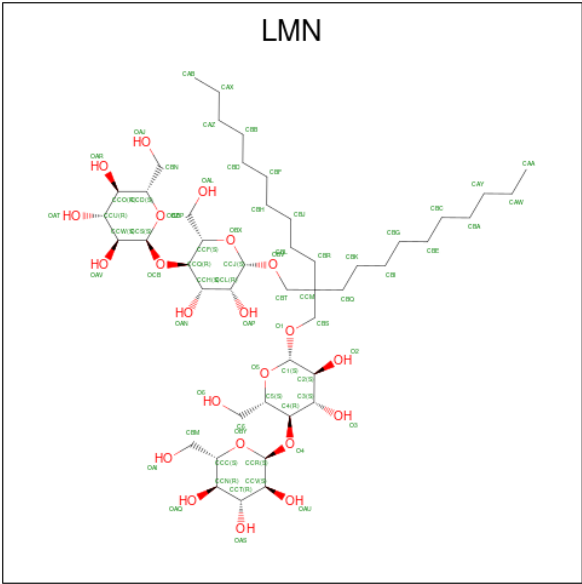
Mol	Chain	Residues	Atoms					AltConf
47	I	1	Total 51	C 41	N 1	O 8	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	J	1	Total 41	31	1	8	1	0
47	J	1	Total 44	34	1	8	1	0
47	S	1	Total 42	32	1	8	1	0
47	a	1	Total 51	41	1	8	1	0
47	b	1	Total 42	32	1	8	1	0
47	i	1	Total 42	32	1	8	1	0
47	3	1	Total 43	33	1	8	1	0
47	4	1	Total 43	33	1	8	1	0
47	4	1	Total 42	32	1	8	1	0
47	4	1	Total 51	41	1	8	1	0

- Molecule 48 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



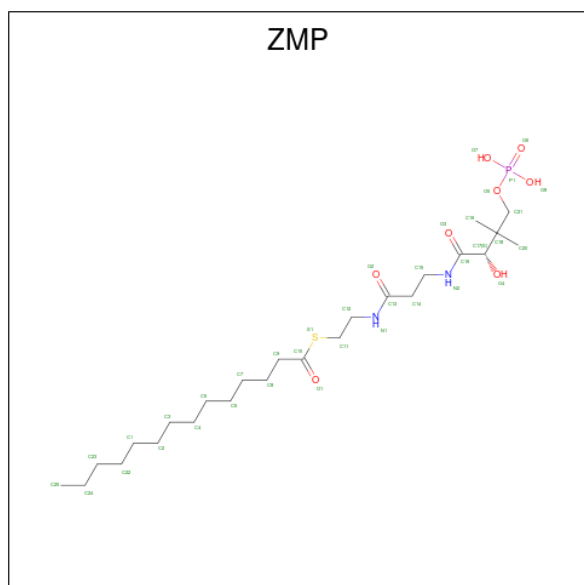
Continued from previous page...

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

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

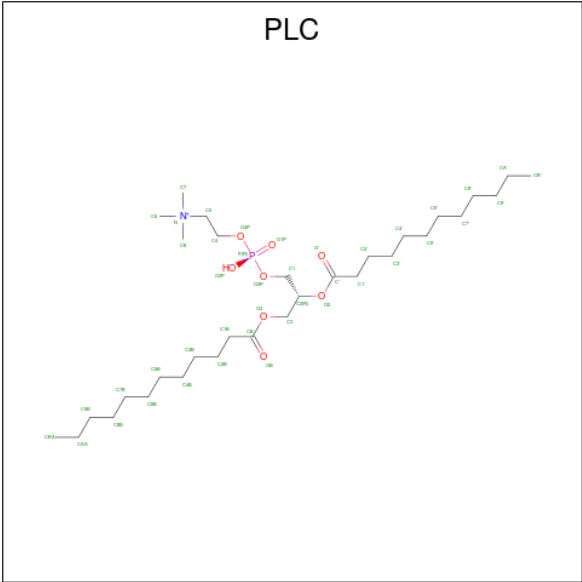
Mol	Chain	Residues	Atoms		AltConf
49	M	1	Total	Zn	0
			1	1	

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



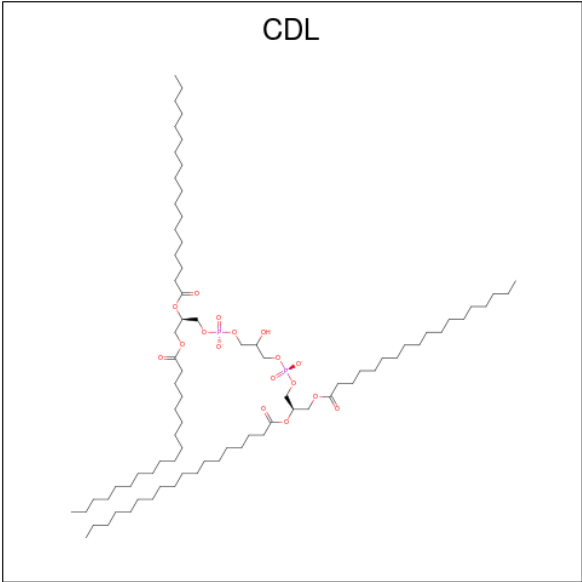
Mol	Chain	Residues	Atoms						AltConf
50	O	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	
50	Q	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	

- Molecule 51 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



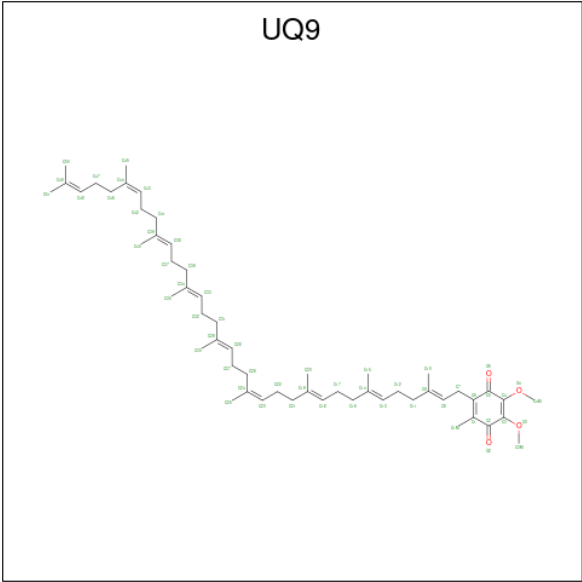
Mol	Chain	Residues	Atoms					AltConf
51	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
51	W	1	Total	C	N	O	P	0
			42	32	1	8	1	
51	1	1	Total	C	N	O	P	0
			42	32	1	8	1	
51	1	1	Total	C	N	O	P	0
			35	25	1	8	1	
51	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
51	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



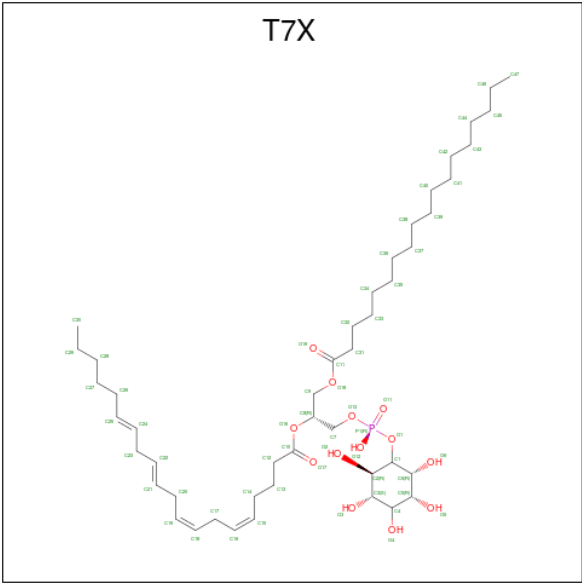
Mol	Chain	Residues	Atoms				AltConf
52	X	1	Total	C	O	P	0
			86	67	17	2	
52	Z	1	Total	C	O	P	0
			76	57	17	2	
52	2	1	Total	C	O	P	0
			83	64	17	2	
52	4	1	Total	C	O	P	0
			92	73	17	2	
52	5	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 53 is Ubiquinone-9 (CCD ID: UQ9) (formula: C₅₄H₈₂O₄).



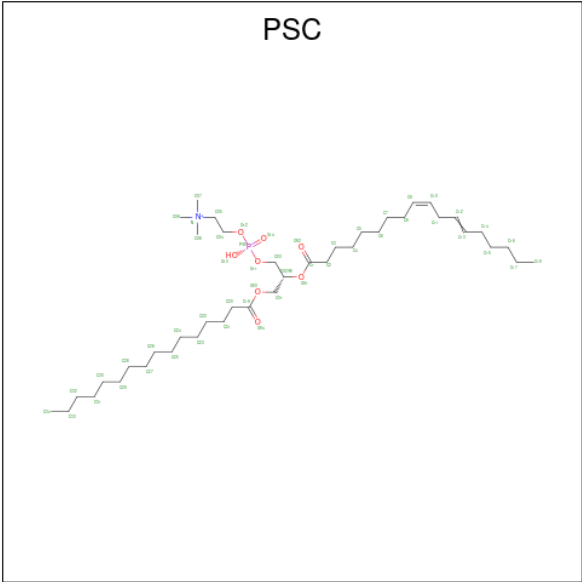
Mol	Chain	Residues	Atoms			AltConf
53	1	1	Total	C	O	0
			35	31	4	

- Molecule 54 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P).



Mol	Chain	Residues	Atoms				AltConf
54	2	1	Total	C	O	P	0
			48	34	13	1	
54	2	1	Total	C	O	P	0
			52	38	13	1	
54	3	1	Total	C	O	P	0
			49	35	13	1	
54	4	1	Total	C	O	P	0
			43	29	13	1	

- Molecule 55 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).

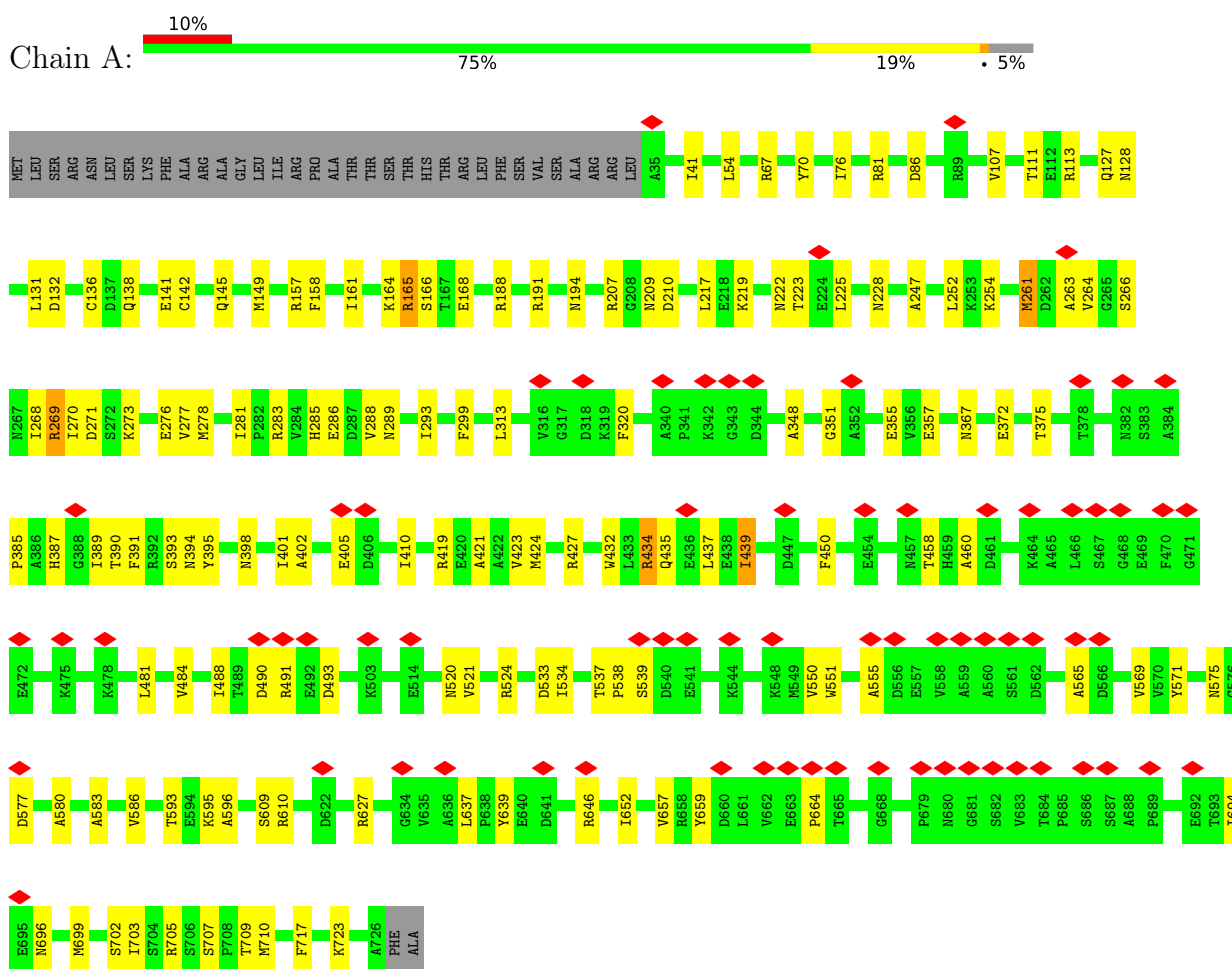


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	2	1	52	42	1	8	1	0

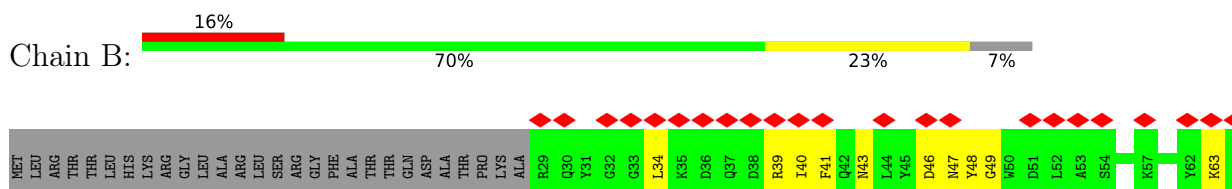
3 Residue-property plots

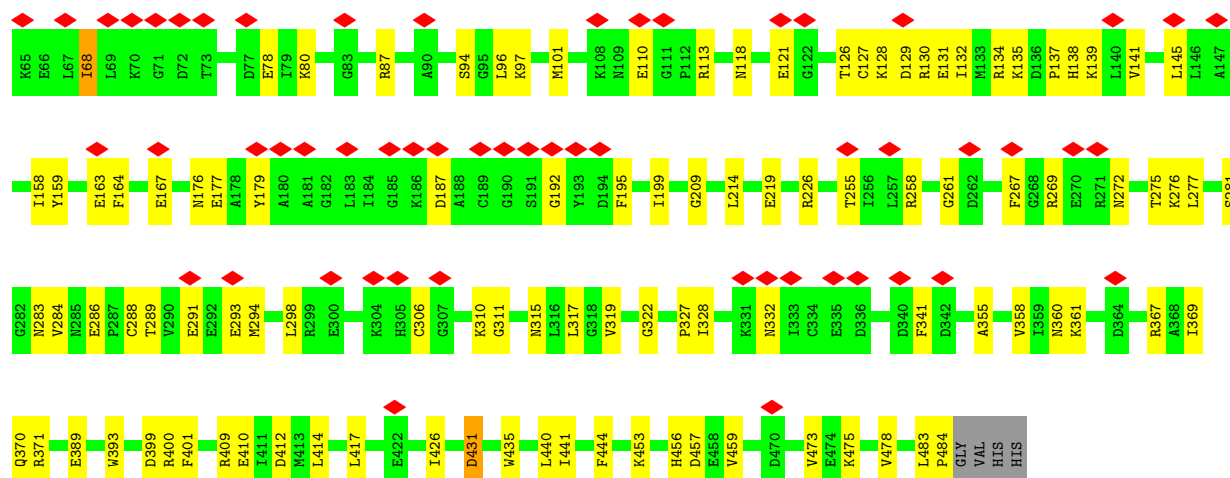
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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



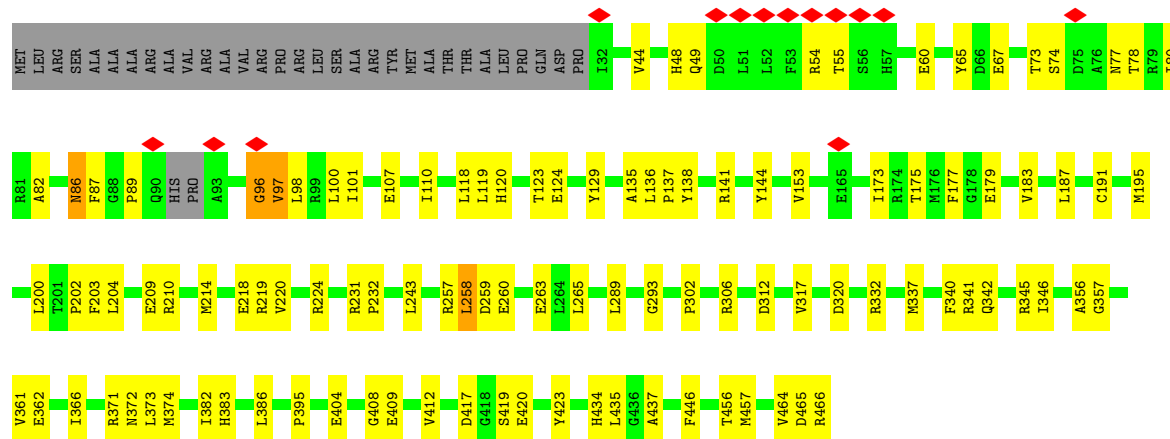
- Molecule 2: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)





• Molecule 3: Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain C: 70% 23% 7%



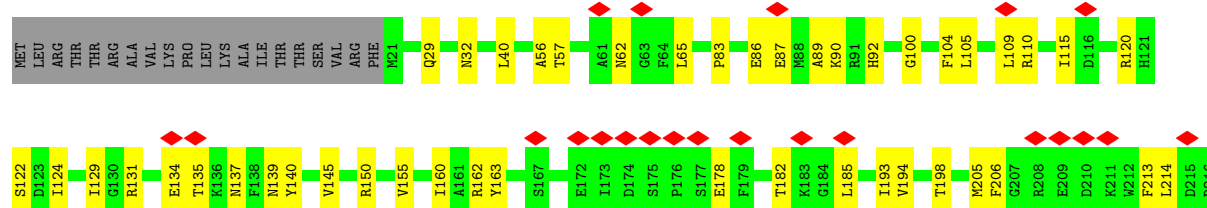
• Molecule 4: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

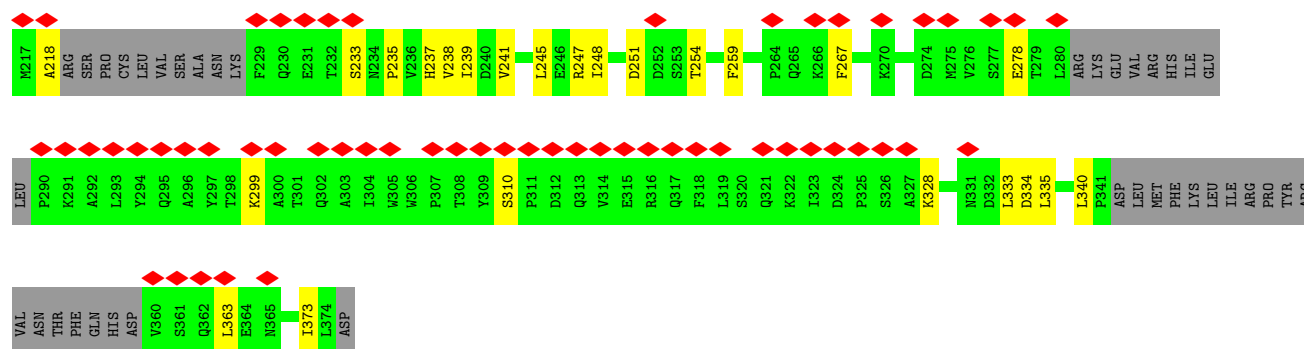
Chain D: 85% 14%



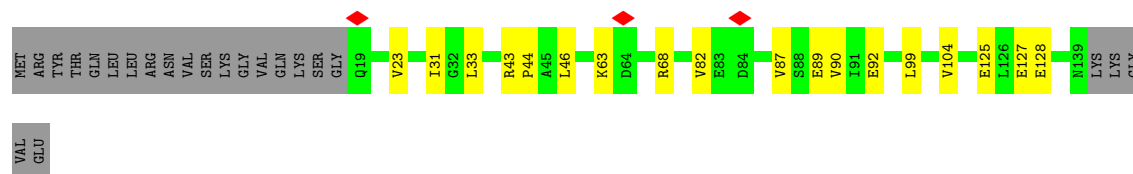
• Molecule 5: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain E: 21% 66% 18% 15%

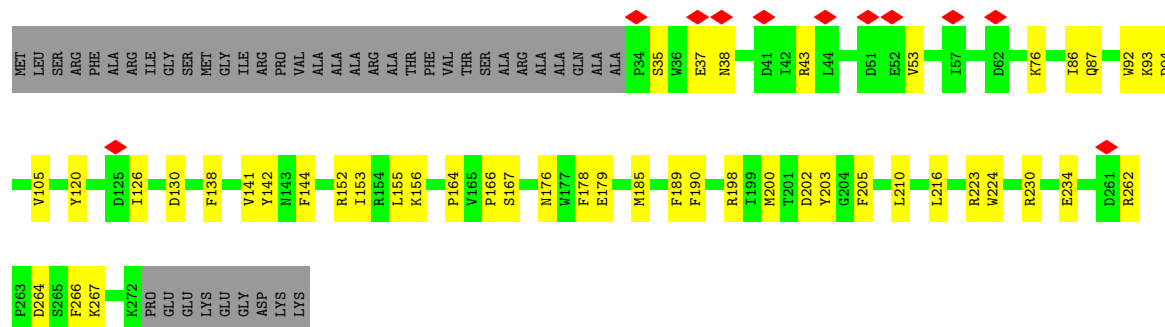




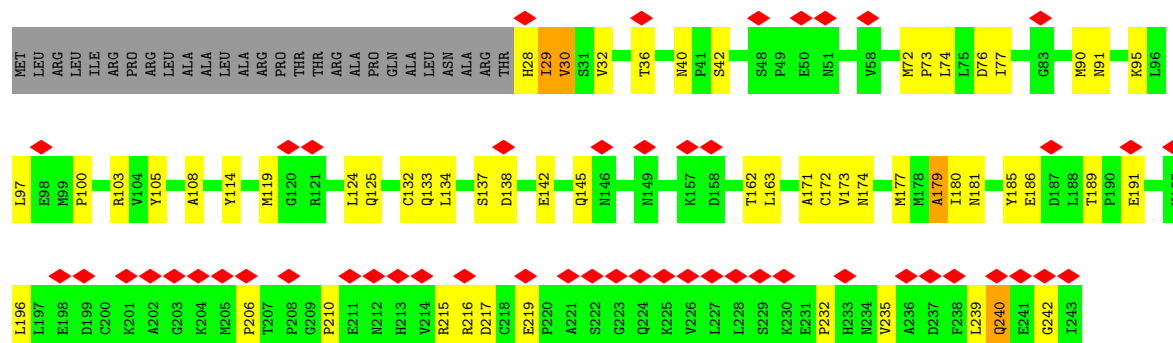
- Molecule 6: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



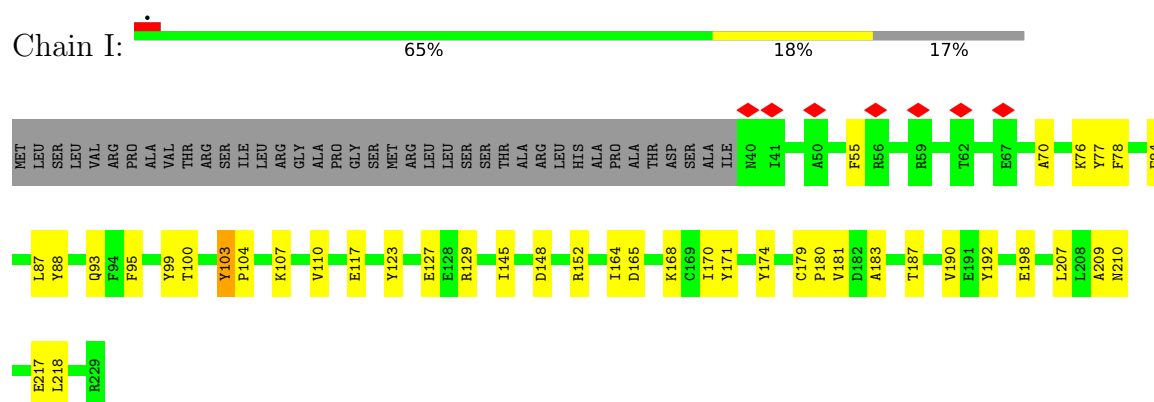
- Molecule 7: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)



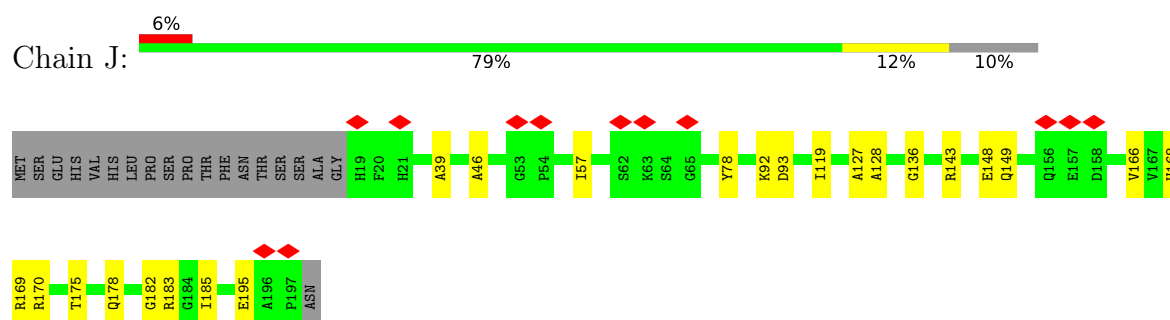
- Molecule 8: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)



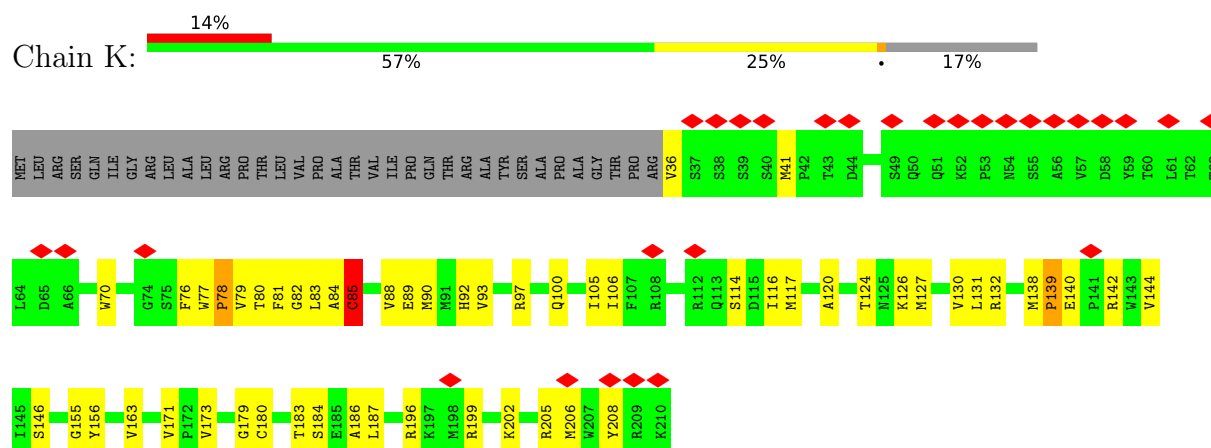
- Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)



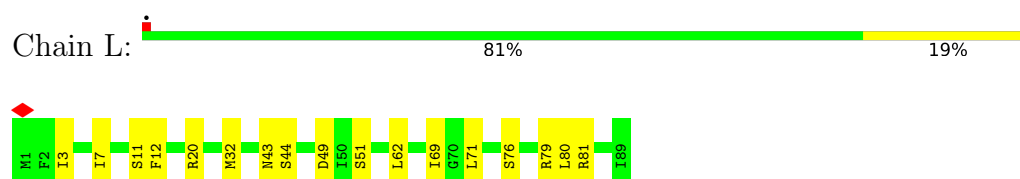
- Molecule 10: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 11: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

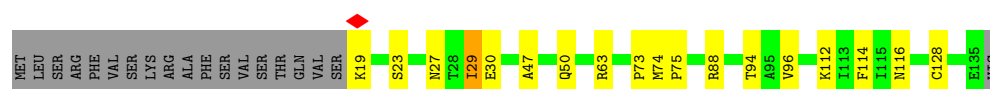


- Molecule 12: Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I)



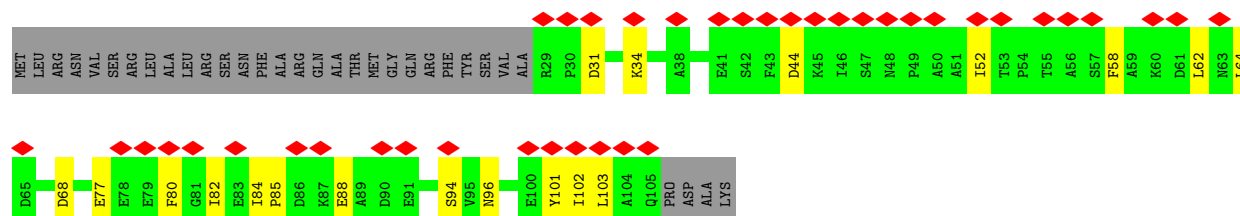
- Molecule 13: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain M: 



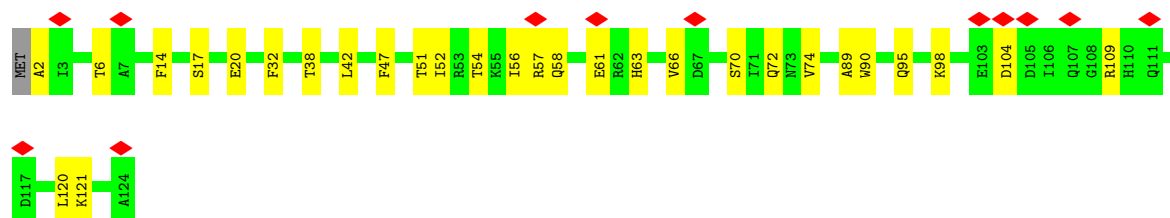
- Molecule 14: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain O: 



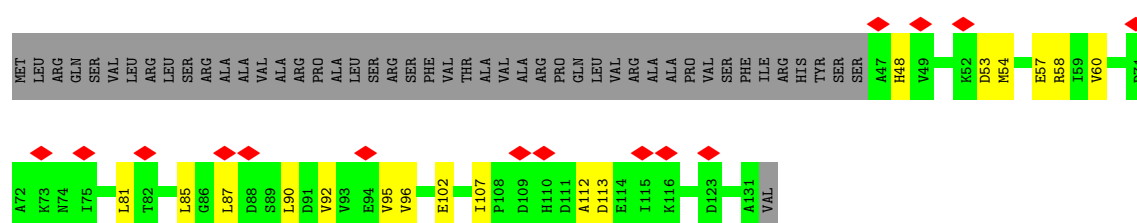
- Molecule 15: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain P: 



- Molecule 16: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Q: 

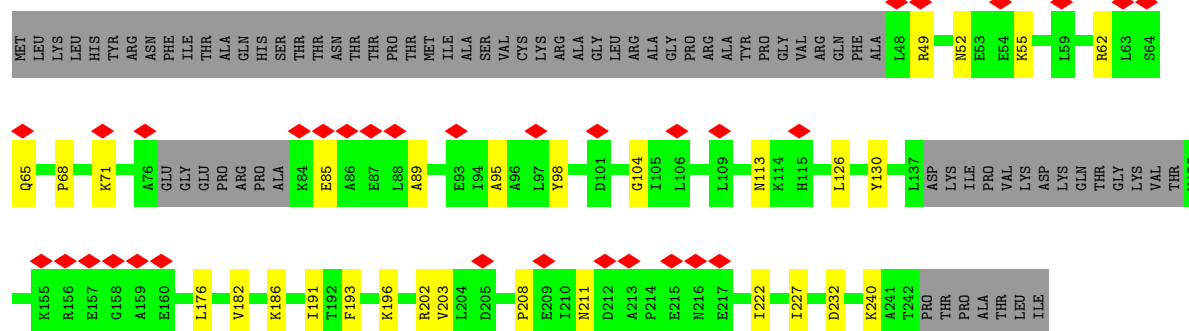


- Molecule 17: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)

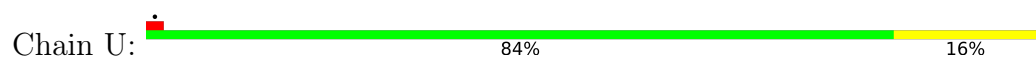
Chain R: 



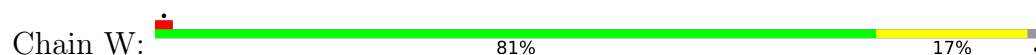
- Molecule 18: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)



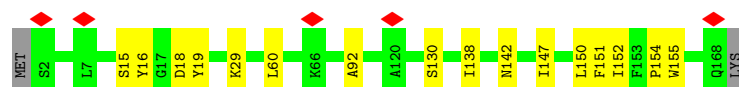
- Molecule 19: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



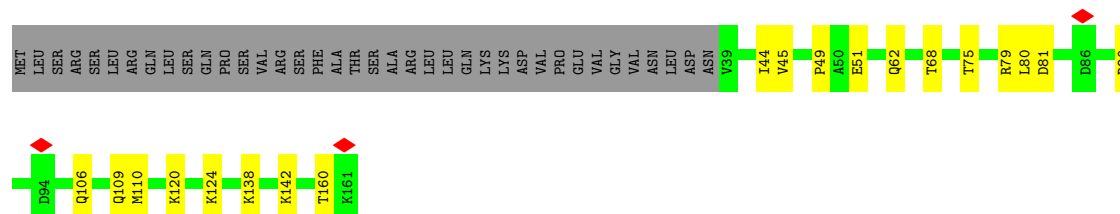
- Molecule 20: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)



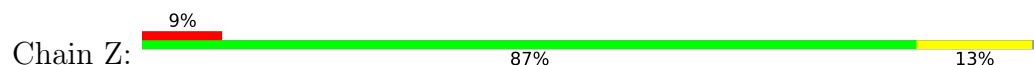
- Molecule 21: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

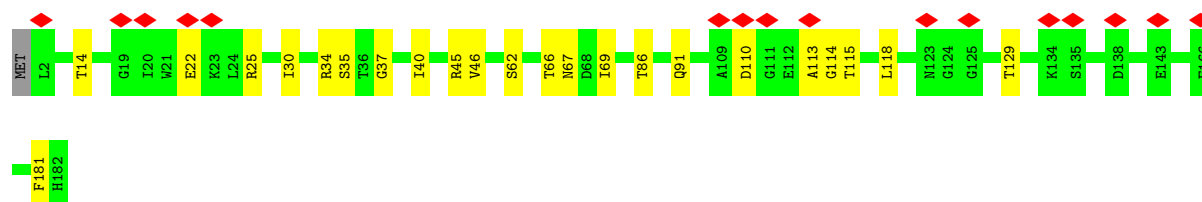


- Molecule 22: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)

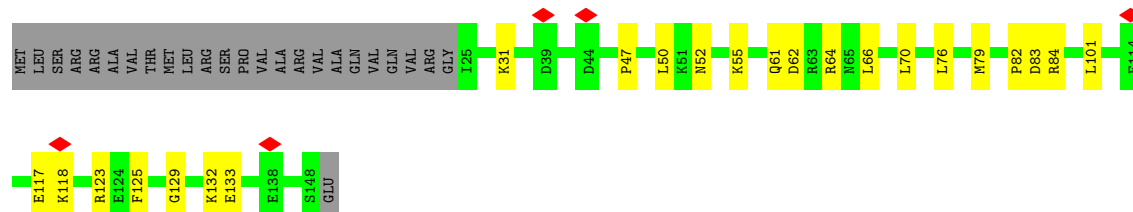


- Molecule 23: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

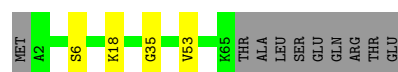
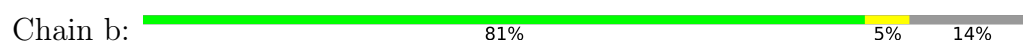




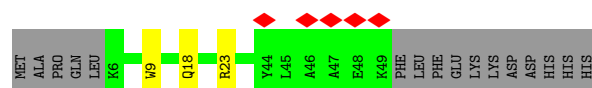
- Molecule 24: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



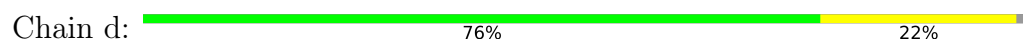
- Molecule 25: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



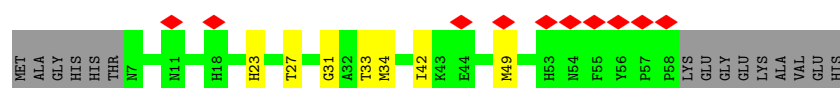
- Molecule 26: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)



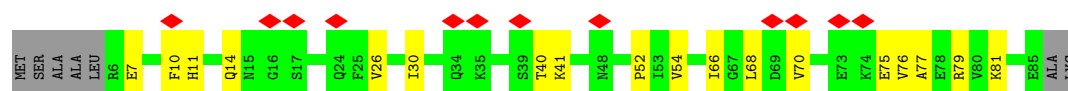
- Molecule 27: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



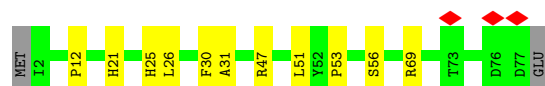
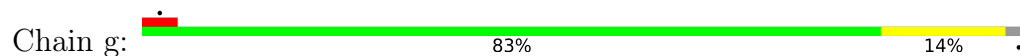
- Molecule 28: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)



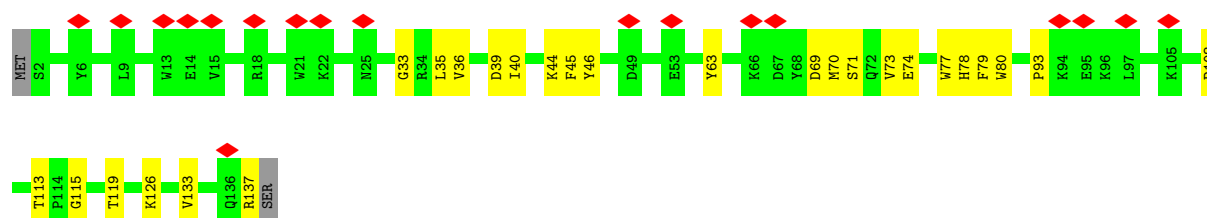
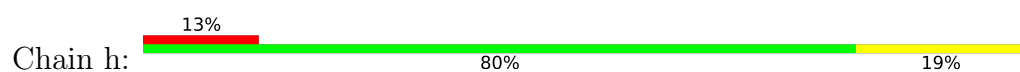
- Molecule 29: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)



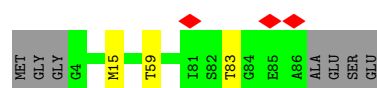
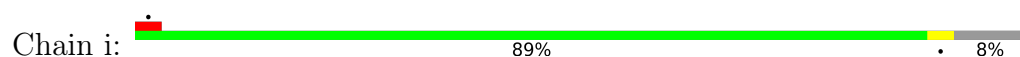
- Molecule 30: Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I)



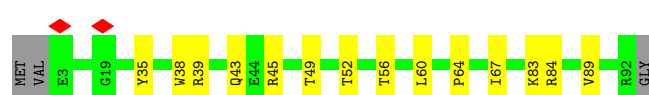
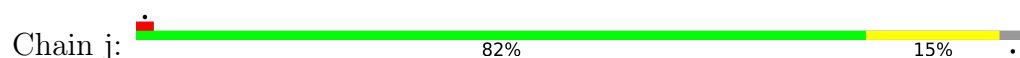
- Molecule 31: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)



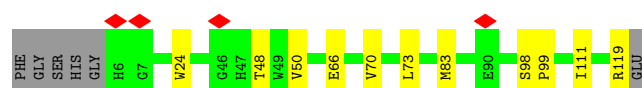
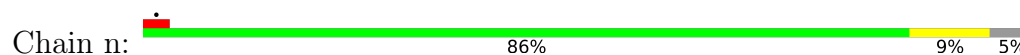
- Molecule 32: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)



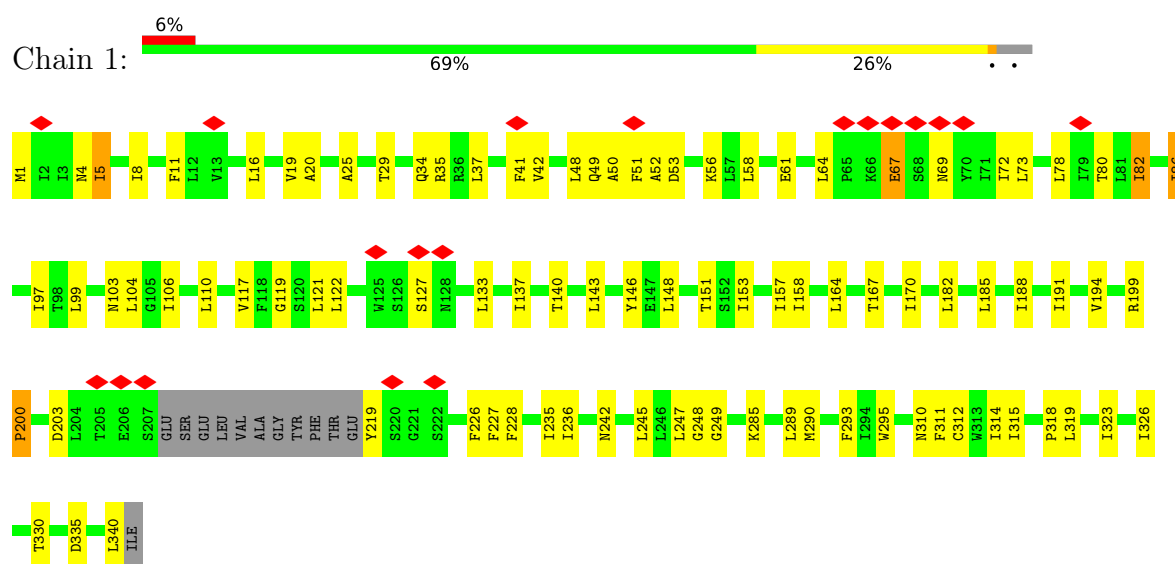
- Molecule 33: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)



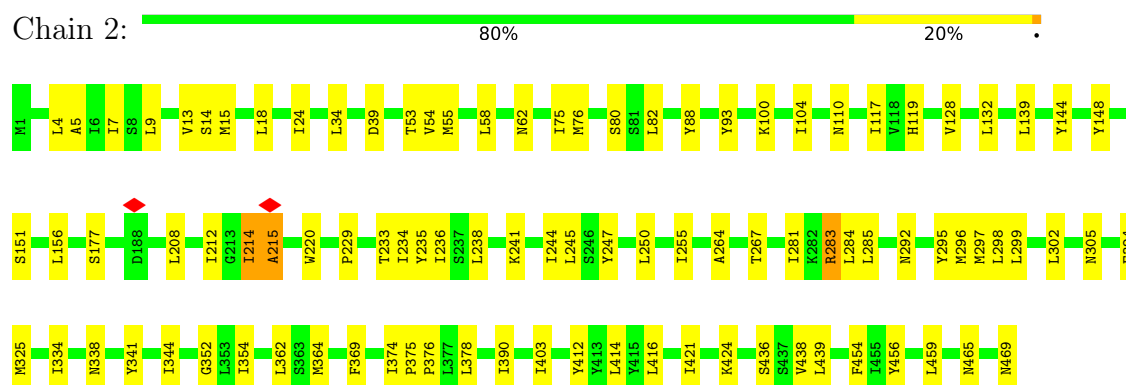
- Molecule 34: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)



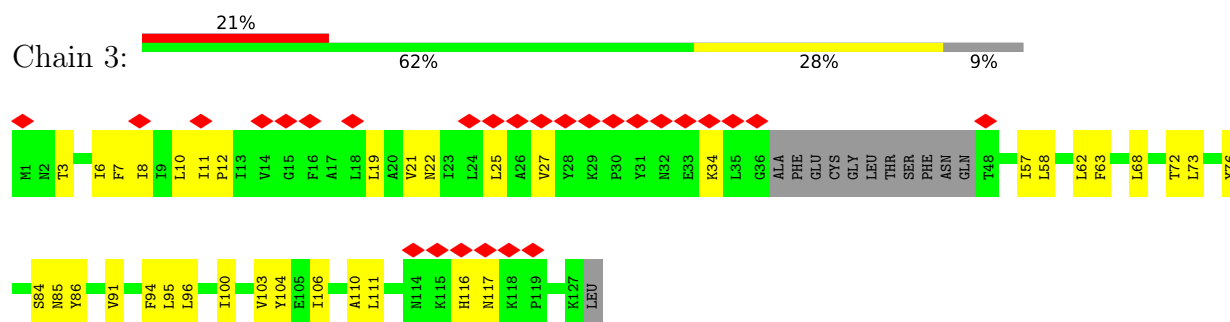
- Molecule 35: Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I)



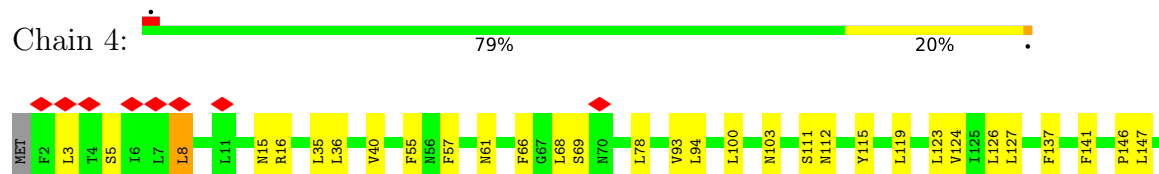
- Molecule 36: Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I)

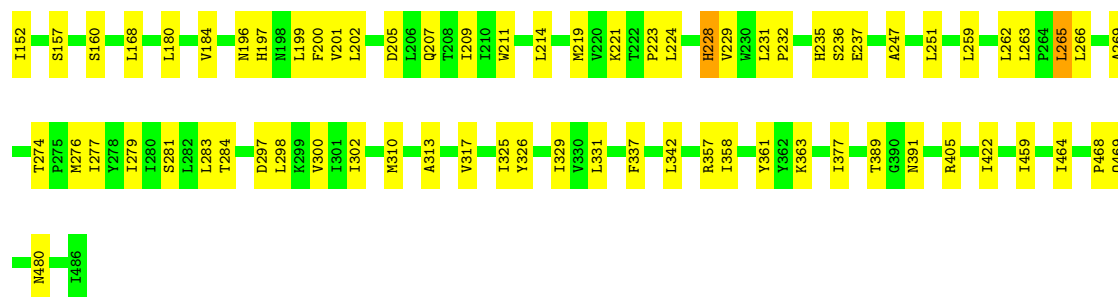


- Molecule 37: Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I)



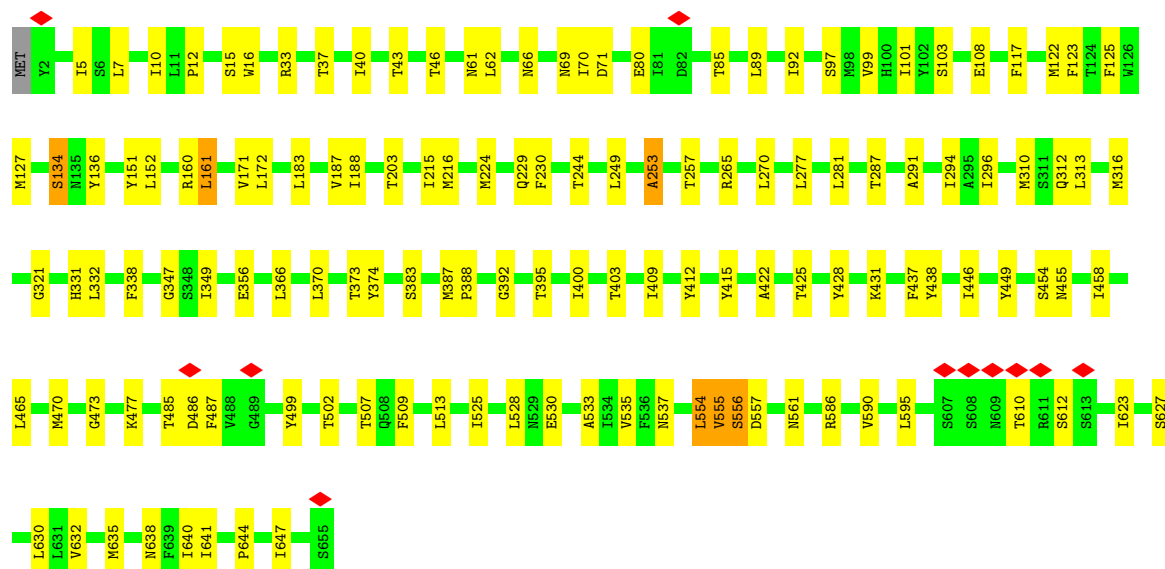
- Molecule 38: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)





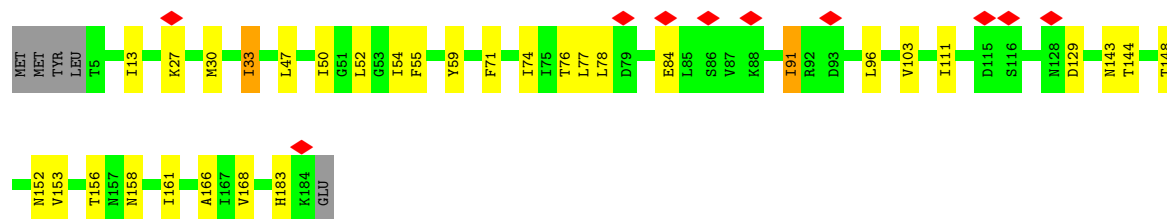
• Molecule 39: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 5: 79% 20%



• Molecule 40: Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 6: 5% 80% 16%



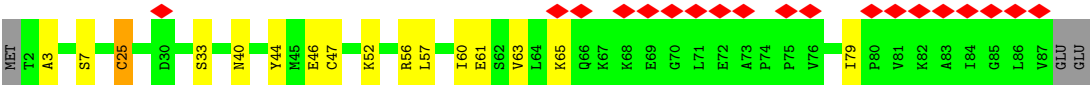
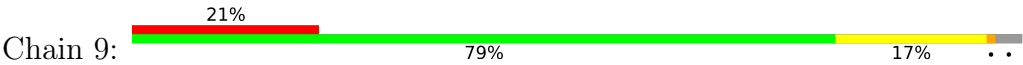
• Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 8: 15% 65% 11% 22%



LYS

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143203	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 ($e^-/\text{\AA}^2$)	51.8	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.070	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	334.80002, 334.80002, 334.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8370001, 0.8370001, 0.8370001	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UQ9, NDP, ZN, SF4, 3PE, CDL, ZMP, PSC, FES, LMN, PLC, FMN, T7X

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	0.35	0/5351	0.67	3/7262 (0.0%)
2	B	0.47	0/3605	0.84	1/4865 (0.0%)
3	C	0.52	1/3503 (0.0%)	0.80	2/4744 (0.0%)
4	D	0.45	0/697	0.73	0/940
5	E	0.54	0/2580	0.95	3/3493 (0.1%)
6	F	0.43	0/1011	0.81	0/1371
7	G	0.48	0/2040	0.78	1/2781 (0.0%)
8	H	0.46	0/1725	0.93	6/2343 (0.3%)
9	I	0.43	0/1557	0.78	1/2110 (0.0%)
10	J	0.38	0/1362	0.74	2/1855 (0.1%)
11	K	0.71	1/1415 (0.1%)	1.02	5/1925 (0.3%)
12	L	0.47	0/700	0.70	0/947
13	M	0.52	1/935 (0.1%)	0.73	0/1268
14	O	0.62	0/598	1.07	0/813
15	P	0.45	0/1054	0.84	2/1418 (0.1%)
16	Q	0.52	0/654	0.94	0/890
17	R	0.42	0/909	0.81	0/1229
18	S	0.40	0/1454	0.77	0/1960
19	U	0.48	0/1374	0.78	0/1856
20	W	0.45	0/998	0.64	0/1346
21	X	0.37	0/1335	0.64	0/1811
22	Y	0.43	0/1051	0.64	0/1420
23	Z	0.37	0/1430	0.77	2/1955 (0.1%)
24	a	0.41	0/1064	0.75	0/1439
25	b	0.32	0/503	0.56	0/679
26	c	0.34	0/364	0.66	0/491
27	d	0.42	0/776	0.70	0/1043
28	e	0.41	0/456	0.77	0/619
29	f	0.60	0/639	1.00	0/856
30	g	0.33	0/643	0.58	0/880
31	h	0.44	0/1168	0.81	2/1589 (0.1%)
32	i	0.50	0/666	0.80	0/907

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.34	0/745	0.65	0/1006
34	n	0.37	0/943	0.71	0/1279
35	1	0.48	0/2699	0.85	3/3684 (0.1%)
36	2	0.53	0/3854	0.79	6/5252 (0.1%)
37	3	0.51	0/954	0.98	2/1300 (0.2%)
38	4	0.48	0/3941	0.72	1/5382 (0.0%)
39	5	0.44	0/5327	0.75	4/7273 (0.1%)
40	6	0.48	1/1439 (0.1%)	0.90	3/1964 (0.2%)
41	8	0.53	0/657	0.99	2/879 (0.2%)
42	9	0.46	0/684	0.79	0/918
All	All	0.46	4/64860 (0.0%)	0.79	51/88042 (0.1%)

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
1	A	0	5
2	B	0	1
3	C	0	2
8	H	0	3
10	J	0	1
11	K	0	3
13	M	0	1
14	O	0	1
24	a	0	1
26	c	0	1
35	1	0	2
36	2	0	2
38	4	0	1
39	5	0	4
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	78	PRO	N-CA	17.92	1.70	1.47
13	M	74	MET	C-O	-8.86	1.19	1.23
3	C	395	PRO	CA-C	-6.92	1.48	1.51
40	6	33	ILE	CG1-CD1	-5.05	1.32	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	77	TRP	CA-C-N	15.97	139.80	119.84
11	K	77	TRP	C-N-CA	15.97	139.80	119.84
40	6	27	LYS	CA-C-N	10.35	156.47	121.27
40	6	27	LYS	C-N-CA	10.35	156.47	121.27
11	K	78	PRO	CA-N-CD	-8.11	100.65	112.00

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	247	ALA	Peptide
1	A	269	ARG	Sidechain
1	A	434	ARG	Sidechain
1	A	439	ILE	Peptide

5.2 Too-close contacts [i](#)

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	5258	0	5159	132	0
2	B	3528	0	3489	78	0
3	C	3426	0	3364	80	0
4	D	681	0	671	11	0
5	E	2527	0	2494	45	0
6	F	990	0	977	14	0
7	G	1978	0	1908	36	0
8	H	1688	0	1660	38	0
9	I	1519	0	1460	49	0
10	J	1329	0	1311	19	0
11	K	1377	0	1354	75	0
12	L	691	0	754	15	0
13	M	912	0	869	17	0
14	O	591	0	585	10	0
15	P	1030	0	1014	21	0
16	Q	648	0	636	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	R	884	0	893	17	0
18	S	1430	0	1463	19	0
19	U	1345	0	1327	20	0
20	W	974	0	987	20	0
21	X	1296	0	1268	18	0
22	Y	1021	0	984	14	0
23	Z	1389	0	1395	20	0
24	a	1030	0	967	16	0
25	b	490	0	509	3	0
26	c	353	0	343	2	0
27	d	760	0	721	21	0
28	e	436	0	426	6	0
29	f	629	0	640	14	0
30	g	617	0	597	10	0
31	h	1130	0	1084	24	0
32	i	646	0	630	3	0
33	j	724	0	706	12	0
34	n	914	0	880	12	0
35	1	2627	0	2737	86	0
36	2	3774	0	4005	75	0
37	3	933	0	1006	40	0
38	4	3847	0	4042	76	0
39	5	5197	0	5353	86	0
40	6	1415	0	1535	28	0
41	8	643	0	644	8	0
42	9	672	0	683	11	0
43	A	16	0	0	1	0
43	B	8	0	0	0	0
43	I	16	0	0	0	0
43	K	8	0	0	0	0
44	A	4	0	0	0	0
44	H	4	0	0	0	0
45	B	31	0	19	1	0
46	E	48	0	26	1	0
47	3	43	0	63	10	0
47	4	136	0	203	14	0
47	I	51	0	82	3	0
47	J	85	0	118	4	0
47	S	42	0	61	2	0
47	a	51	0	82	3	0
47	b	42	0	58	2	0
47	i	42	0	58	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	J	134	0	165	7	0
48	j	69	0	88	3	0
49	M	1	0	0	0	0
50	O	33	0	38	1	0
50	Q	33	0	38	2	0
51	1	77	0	108	4	0
51	5	73	0	100	1	0
51	W	83	0	123	7	0
52	2	83	0	116	19	0
52	4	92	0	137	4	0
52	5	78	0	103	4	0
52	X	86	0	119	14	0
52	Z	76	0	96	2	0
53	1	35	0	43	11	0
54	2	100	0	0	0	0
54	3	49	0	0	0	0
54	4	43	0	0	3	0
55	2	52	0	80	1	0
All	All	65173	0	65654	1099	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 8.

The worst 5 of 1099 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)
11:K:78:PRO:N	11:K:78:PRO:CA	1.70	1.36
11:K:81:PHE:CD2	11:K:131:LEU:HD12	1.82	1.14
1:A:264:VAL:HG12	1:A:424:MET:HE2	1.37	1.03
1:A:264:VAL:CG1	1:A:424:MET:HE2	1.89	1.01
35:1:228:PHE:CE1	53:1:402:UQ9:H12	1.95	1.01

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	690/728 (95%)	641 (93%)	49 (7%)	0	100	100
2	B	454/488 (93%)	424 (93%)	30 (7%)	0	100	100
3	C	429/466 (92%)	402 (94%)	26 (6%)	1 (0%)	43	66
4	D	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
5	E	309/375 (82%)	291 (94%)	18 (6%)	0	100	100
6	F	119/144 (83%)	112 (94%)	7 (6%)	0	100	100
7	G	237/281 (84%)	228 (96%)	8 (3%)	1 (0%)	30	53
8	H	214/243 (88%)	194 (91%)	19 (9%)	1 (0%)	24	49
9	I	188/229 (82%)	179 (95%)	9 (5%)	0	100	100
10	J	177/198 (89%)	169 (96%)	8 (4%)	0	100	100
11	K	173/210 (82%)	161 (93%)	11 (6%)	1 (1%)	21	45
12	L	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
13	M	115/136 (85%)	104 (90%)	11 (10%)	0	100	100
14	O	75/109 (69%)	69 (92%)	6 (8%)	0	100	100
15	P	121/124 (98%)	118 (98%)	3 (2%)	0	100	100
16	Q	83/132 (63%)	82 (99%)	1 (1%)	0	100	100
17	R	104/109 (95%)	96 (92%)	8 (8%)	0	100	100
18	S	168/249 (68%)	160 (95%)	8 (5%)	0	100	100
19	U	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
20	W	119/123 (97%)	114 (96%)	5 (4%)	0	100	100
21	X	165/169 (98%)	160 (97%)	5 (3%)	0	100	100
22	Y	121/161 (75%)	117 (97%)	4 (3%)	0	100	100
23	Z	179/182 (98%)	167 (93%)	12 (7%)	0	100	100
24	a	122/149 (82%)	114 (93%)	8 (7%)	0	100	100
25	b	62/74 (84%)	61 (98%)	1 (2%)	0	100	100
26	c	42/60 (70%)	37 (88%)	5 (12%)	0	100	100
27	d	88/92 (96%)	86 (98%)	2 (2%)	0	100	100
28	e	50/67 (75%)	49 (98%)	1 (2%)	0	100	100
29	f	78/87 (90%)	73 (94%)	5 (6%)	0	100	100
30	g	74/78 (95%)	70 (95%)	3 (4%)	1 (1%)	9	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	h	134/138 (97%)	126 (94%)	7 (5%)	1 (1%)	18	40
32	i	81/90 (90%)	74 (91%)	7 (9%)	0	100	100
33	j	88/93 (95%)	81 (92%)	7 (8%)	0	100	100
34	n	112/120 (93%)	102 (91%)	10 (9%)	0	100	100
35	1	325/341 (95%)	306 (94%)	19 (6%)	0	100	100
36	2	467/469 (100%)	449 (96%)	18 (4%)	0	100	100
37	3	112/128 (88%)	103 (92%)	9 (8%)	0	100	100
38	4	483/486 (99%)	464 (96%)	19 (4%)	0	100	100
39	5	652/655 (100%)	624 (96%)	26 (4%)	2 (0%)	36	59
40	6	178/185 (96%)	169 (95%)	9 (5%)	0	100	100
41	8	75/99 (76%)	71 (95%)	4 (5%)	0	100	100
42	9	84/89 (94%)	76 (90%)	8 (10%)	0	100	100
All	All	7887/8704 (91%)	7447 (94%)	432 (6%)	8 (0%)	49	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	97	VAL
7	G	94	ASP
11	K	85	CYS
39	5	555	VAL
31	h	108	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/595 (95%)	565 (100%)	0	100	100
2	B	364/389 (94%)	360 (99%)	4 (1%)	65	80
3	C	368/394 (93%)	367 (100%)	1 (0%)	86	92
4	D	68/69 (99%)	68 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	274/329 (83%)	272 (99%)	2 (1%)	76	87
6	F	109/129 (84%)	108 (99%)	1 (1%)	70	83
7	G	216/245 (88%)	216 (100%)	0	100	100
8	H	191/212 (90%)	189 (99%)	2 (1%)	68	82
9	I	156/187 (83%)	156 (100%)	0	100	100
10	J	130/147 (88%)	130 (100%)	0	100	100
11	K	152/180 (84%)	151 (99%)	1 (1%)	76	87
12	L	77/77 (100%)	76 (99%)	1 (1%)	61	78
13	M	97/115 (84%)	96 (99%)	1 (1%)	68	82
14	O	65/91 (71%)	65 (100%)	0	100	100
15	P	108/109 (99%)	108 (100%)	0	100	100
16	Q	72/111 (65%)	72 (100%)	0	100	100
17	R	97/100 (97%)	97 (100%)	0	100	100
18	S	149/211 (71%)	149 (100%)	0	100	100
19	U	147/148 (99%)	146 (99%)	1 (1%)	76	87
20	W	100/102 (98%)	100 (100%)	0	100	100
21	X	131/133 (98%)	131 (100%)	0	100	100
22	Y	105/140 (75%)	105 (100%)	0	100	100
23	Z	147/148 (99%)	147 (100%)	0	100	100
24	a	108/129 (84%)	107 (99%)	1 (1%)	70	83
25	b	50/59 (85%)	50 (100%)	0	100	100
26	c	30/45 (67%)	30 (100%)	0	100	100
27	d	83/85 (98%)	83 (100%)	0	100	100
28	e	44/55 (80%)	44 (100%)	0	100	100
29	f	69/73 (94%)	69 (100%)	0	100	100
30	g	62/64 (97%)	62 (100%)	0	100	100
31	h	121/123 (98%)	121 (100%)	0	100	100
32	i	64/68 (94%)	64 (100%)	0	100	100
33	j	71/73 (97%)	71 (100%)	0	100	100
34	n	98/102 (96%)	98 (100%)	0	100	100
35	l	292/302 (97%)	289 (99%)	3 (1%)	68	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2	433/433 (100%)	432 (100%)	1 (0%)	87	94
37	3	104/114 (91%)	104 (100%)	0	100	100
38	4	433/434 (100%)	432 (100%)	1 (0%)	87	94
39	5	579/580 (100%)	578 (100%)	1 (0%)	87	94
40	6	162/167 (97%)	160 (99%)	2 (1%)	63	79
41	8	68/76 (90%)	67 (98%)	1 (2%)	57	76
42	9	73/76 (96%)	72 (99%)	1 (1%)	59	77
All	All	6832/7419 (92%)	6807 (100%)	25 (0%)	81	92

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	a	82	PRO
35	1	86	ILE
42	9	25	CYS
35	1	82	ILE
36	2	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
21	X	157	ASN
39	5	562	HIS
33	j	73	GLN
39	5	552	GLN
38	4	480	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
43	SF4	A	801	1	0,12,12	-	-	-		
48	LMN	j	101	-	72,72,72	1.62	11 (15%)	96,98,98	1.79	19 (19%)
50	ZMP	Q	201	16	26,32,36	1.73	7 (26%)	31,39,45	2.31	8 (25%)
47	3PE	4	503	-	41,41,50	1.04	3 (7%)	44,46,55	1.26	3 (6%)
47	3PE	I	501	-	50,50,50	0.88	3 (6%)	53,55,55	1.05	3 (5%)
52	CDL	5	701	-	77,77,99	1.01	7 (9%)	83,89,111	1.25	5 (6%)
54	T7X	3	202	-	49,49,61	0.96	5 (10%)	59,61,73	1.47	7 (11%)
52	CDL	Z	201	-	75,75,99	1.00	8 (10%)	81,87,111	1.16	6 (7%)
52	CDL	2	501	-	82,82,99	0.48	0	88,94,111	0.67	3 (3%)
46	NDP	E	401	-	49,52,52	3.67	20 (40%)	66,80,80	2.13	13 (19%)
47	3PE	3	201	-	42,42,50	0.29	0	45,47,55	0.35	0
48	LMN	J	202	-	72,72,72	1.62	12 (16%)	96,98,98	1.93	28 (29%)
47	3PE	4	504	-	50,50,50	0.85	4 (8%)	53,55,55	1.19	3 (5%)
51	PLC	1	403	-	34,34,41	1.47	7 (20%)	40,42,49	1.24	3 (7%)
43	SF4	A	802	1	0,12,12	-	-	-		
47	3PE	a	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.11	3 (5%)
51	PLC	5	702	-	41,41,41	1.31	5 (12%)	47,49,49	1.13	2 (4%)
47	3PE	S	501	-	41,41,50	0.93	4 (9%)	44,46,55	1.08	1 (2%)
54	T7X	2	504	-	52,52,61	0.53	0	62,64,73	0.97	4 (6%)
52	CDL	4	502	-	91,91,99	0.92	5 (5%)	97,103,111	1.14	6 (6%)
45	FMN	B	502	-	33,33,33	2.94	14 (42%)	48,50,50	1.70	11 (22%)
47	3PE	J	203	-	43,43,50	0.95	4 (9%)	46,48,55	1.31	3 (6%)
44	FES	H	301	8	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	T7X	4	505	-	43,43,61	0.69	1 (2%)	53,55,73	1.34	8 (15%)
55	PSC	2	503	-	51,51,51	1.02	4 (7%)	57,59,59	1.07	3 (5%)
48	LMN	J	204	-	68,68,72	1.60	14 (20%)	92,94,98	1.46	14 (15%)
44	FES	A	803	1	0,4,4	-	-	-	-	-
51	PLC	5	703	-	30,30,41	1.48	5 (16%)	36,38,49	1.08	3 (8%)
51	PLC	1	401	-	41,41,41	1.32	4 (9%)	47,49,49	1.18	3 (6%)
47	3PE	J	201	-	40,40,50	0.94	3 (7%)	43,45,55	1.07	2 (4%)
54	T7X	2	502	-	48,48,61	1.00	4 (8%)	57,60,73	1.42	9 (15%)
47	3PE	4	501	-	42,42,50	0.93	4 (9%)	45,47,55	1.11	2 (4%)
47	3PE	b	201	-	41,41,50	0.93	3 (7%)	44,46,55	1.19	2 (4%)
53	UQ9	1	402	-	35,35,58	2.48	13 (37%)	42,45,73	2.10	15 (35%)
50	ZMP	O	201	14	26,32,36	1.80	5 (19%)	31,39,45	1.87	6 (19%)
43	SF4	I	502	9	0,12,12	-	-	-	-	-
43	SF4	B	501	2	0,12,12	-	-	-	-	-
43	SF4	K	301	11	0,12,12	-	-	-	-	-
47	3PE	i	101	-	41,41,50	0.95	4 (9%)	44,46,55	1.21	2 (4%)
52	CDL	X	201	-	85,85,99	0.65	1 (1%)	91,97,111	0.86	4 (4%)
51	PLC	W	201	-	40,40,41	1.32	5 (12%)	46,48,49	1.12	2 (4%)
43	SF4	I	503	9	0,12,12	-	-	-	-	-
51	PLC	W	202	-	41,41,41	1.30	4 (9%)	47,49,49	0.99	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
48	LMN	j	101	-	-	30/50/130/130	0/4/4/4
43	SF4	A	801	1	-	-	0/6/5/5
50	ZMP	Q	201	16	-	13/37/39/43	-
47	3PE	4	503	-	-	14/45/45/54	-
47	3PE	I	501	-	-	23/54/54/54	-
52	CDL	5	701	-	-	35/88/88/110	-
54	T7X	3	202	-	-	13/44/68/80	0/1/1/1
52	CDL	Z	201	-	-	32/86/86/110	-
52	CDL	2	501	-	-	26/93/93/110	-
46	NDP	E	401	-	-	11/34/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	3PE	3	201	-	-	4/46/46/54	-
48	LMN	J	202	-	-	26/50/130/130	0/4/4/4
47	3PE	4	504	-	-	25/54/54/54	-
51	PLC	1	403	-	-	8/38/38/45	-
43	SF4	A	802	1	-	-	0/6/5/5
47	3PE	a	201	-	-	10/54/54/54	-
51	PLC	5	702	-	-	21/45/45/45	-
47	3PE	S	501	-	-	18/45/45/54	-
54	T7X	2	504	-	-	14/47/71/80	0/1/1/1
52	CDL	4	502	-	-	45/102/102/110	-
45	FMN	B	502	-	-	13/18/18/18	0/3/3/3
47	3PE	J	203	-	-	21/47/47/54	-
44	FES	H	301	8	-	-	0/1/1/1
54	T7X	4	505	-	-	24/38/62/80	0/1/1/1
55	PSC	2	503	-	-	25/55/55/55	-
48	LMN	J	204	-	-	17/46/126/130	0/4/4/4
44	FES	A	803	1	-	-	0/1/1/1
51	PLC	5	703	-	-	11/34/34/45	-
51	PLC	1	401	-	-	16/45/45/45	-
47	3PE	J	201	-	-	9/44/44/54	-
54	T7X	2	502	-	-	12/43/67/80	0/1/1/1
47	3PE	4	501	-	-	8/46/46/54	-
47	3PE	b	201	-	-	13/45/45/54	-
53	UQ9	1	402	-	-	6/30/54/81	0/1/1/1
50	ZMP	O	201	14	-	5/37/39/43	-
43	SF4	B	501	2	-	-	0/6/5/5
43	SF4	I	502	9	-	-	0/6/5/5
43	SF4	K	301	11	-	-	0/6/5/5
47	3PE	i	101	-	-	20/45/45/54	-
52	CDL	X	201	-	-	41/96/96/110	-
51	PLC	W	201	-	-	16/44/44/45	-
43	SF4	I	503	9	-	-	0/6/5/5
51	PLC	W	202	-	-	18/45/45/45	-

The worst 5 of 197 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	E	401	NDP	C6N-C5N	12.29	1.55	1.33
53	1	402	UQ9	C6-C1	9.45	1.52	1.35
46	E	401	NDP	O4B-C1B	7.91	1.60	1.42
46	E	401	NDP	O4D-C1D	7.86	1.60	1.42
45	B	502	FMN	C4A-N5	7.84	1.46	1.30

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Q	201	ZMP	C14-C15-N2	-8.64	94.46	111.90
48	j	101	LMN	CBR-CBL-CBJ	7.32	134.98	113.19
48	J	202	LMN	CBM-CCC-CCN	-6.71	97.30	113.00
48	J	204	LMN	CBR-CBL-CBJ	6.27	131.88	113.19
46	E	401	NDP	N6A-C6A-N1A	-6.23	104.71	118.35

There are no chirality outliers.

5 of 643 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	502	FMN	N10-C1'-C2'-O2'
45	B	502	FMN	N10-C1'-C2'-C3'
45	B	502	FMN	C1'-C2'-C3'-O3'
45	B	502	FMN	C1'-C2'-C3'-C4'
45	B	502	FMN	O3'-C3'-C4'-O4'

There are no ring outliers.

32 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	A	801	SF4	1	0
48	j	101	LMN	3	0
50	Q	201	ZMP	2	0
47	4	503	3PE	3	0
47	I	501	3PE	3	0
52	5	701	CDL	4	0
52	Z	201	CDL	2	0
52	2	501	CDL	19	0
46	E	401	NDP	1	0
47	3	201	3PE	10	0
48	J	202	LMN	3	0
47	4	504	3PE	9	0
51	1	403	PLC	1	0

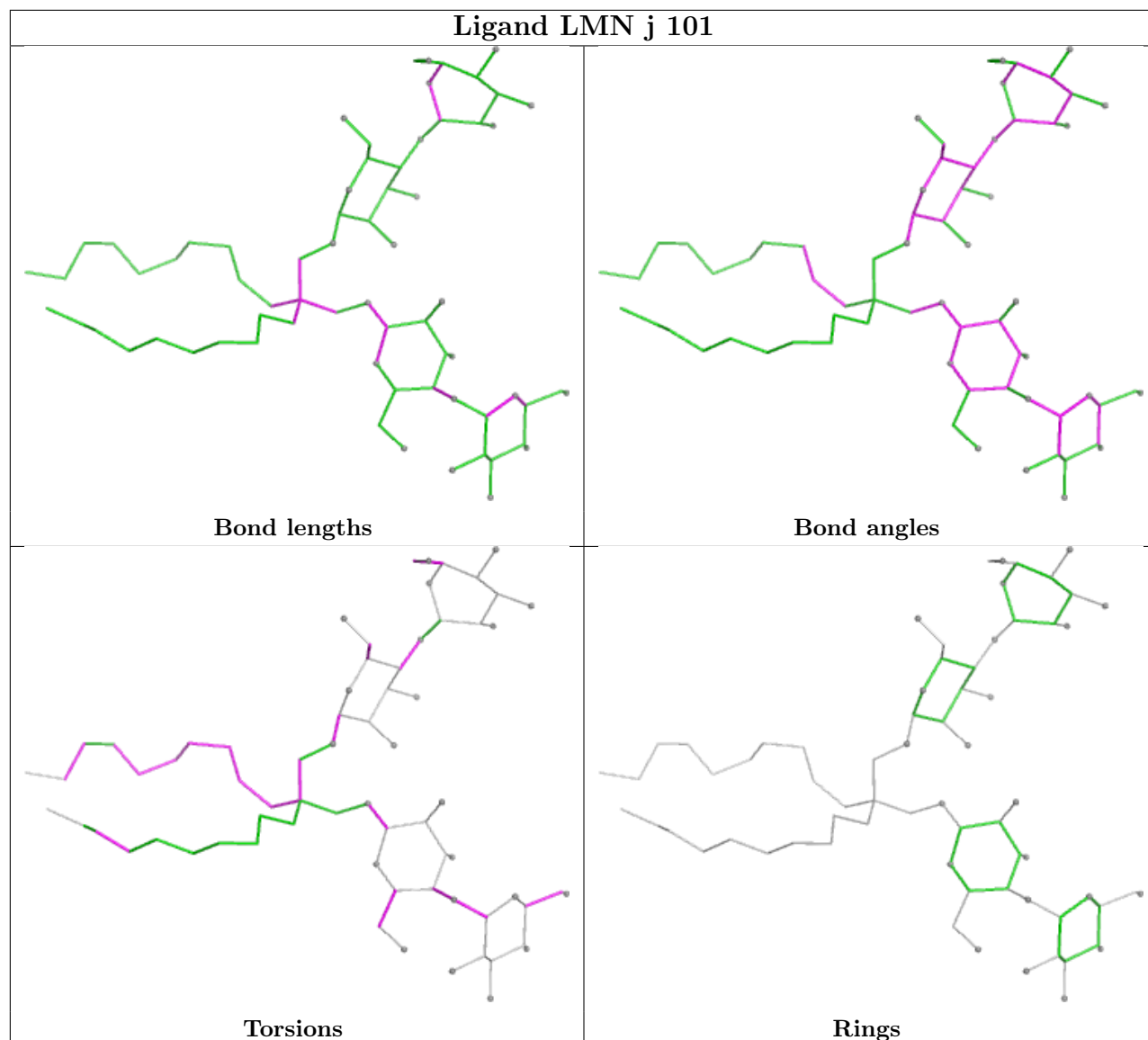
Continued on next page...

Continued from previous page...

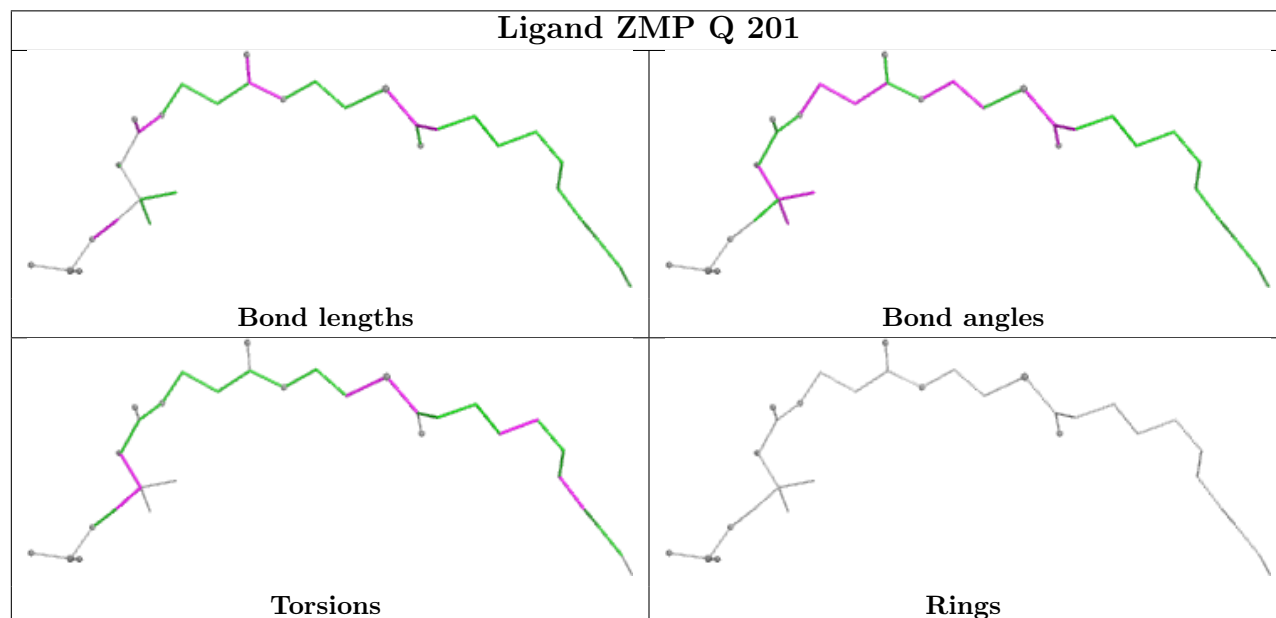
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	a	201	3PE	3	0
51	5	702	PLC	1	0
47	S	501	3PE	2	0
52	4	502	CDL	4	0
45	B	502	FMN	1	0
47	J	203	3PE	2	0
54	4	505	T7X	3	0
55	2	503	PSC	1	0
48	J	204	LMN	4	0
51	1	401	PLC	3	0
47	J	201	3PE	2	0
47	4	501	3PE	3	0
47	b	201	3PE	2	0
53	1	402	UQ9	11	0
50	O	201	ZMP	1	0
47	i	101	3PE	2	0
52	X	201	CDL	14	0
51	W	201	PLC	5	0
51	W	202	PLC	4	0

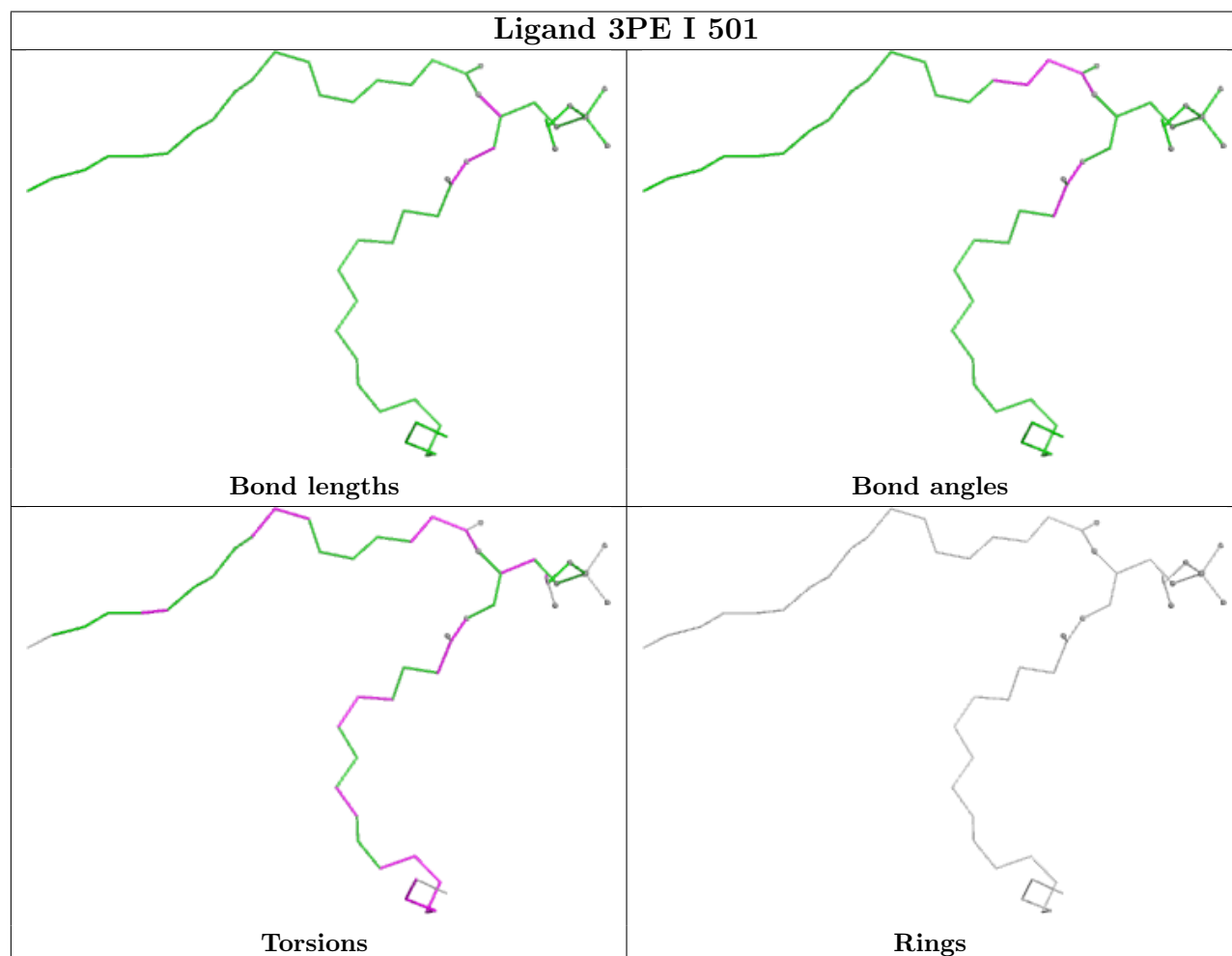
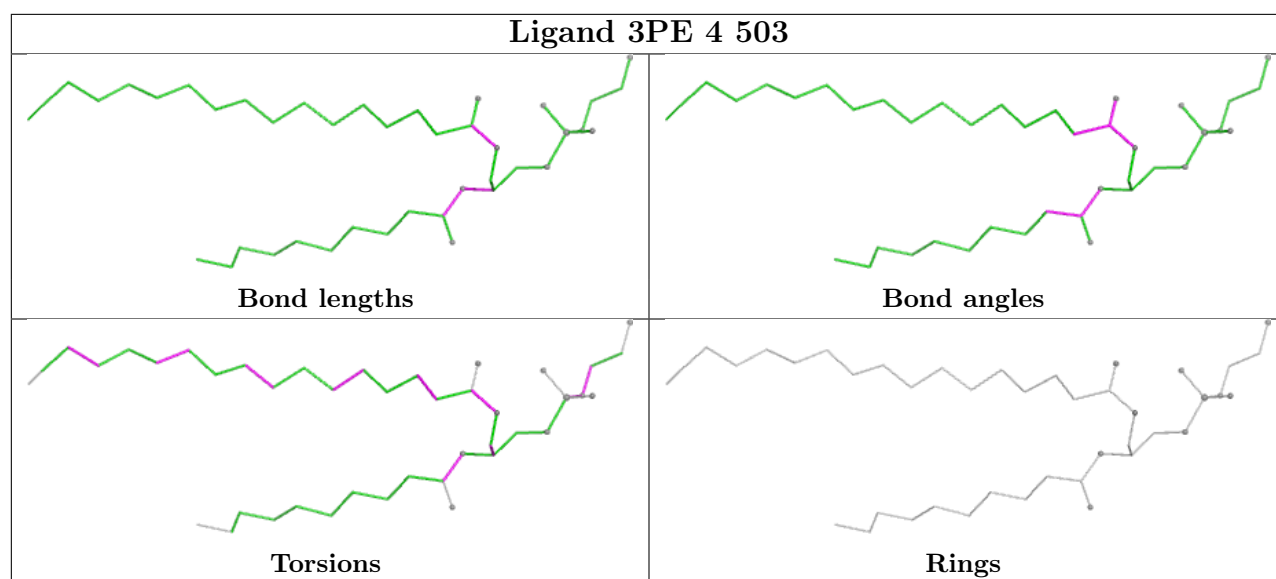
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

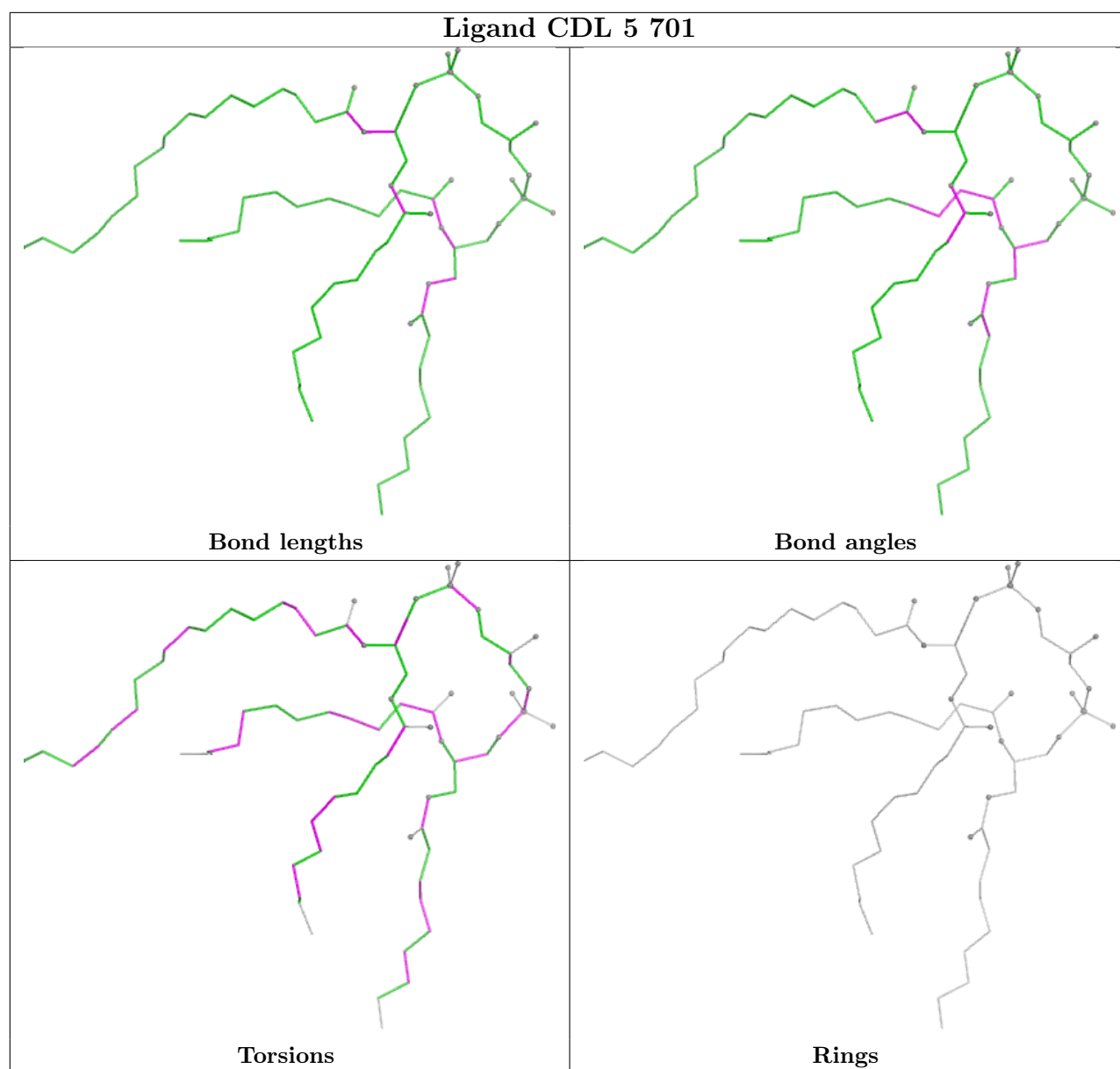
Ligand LMN j 101

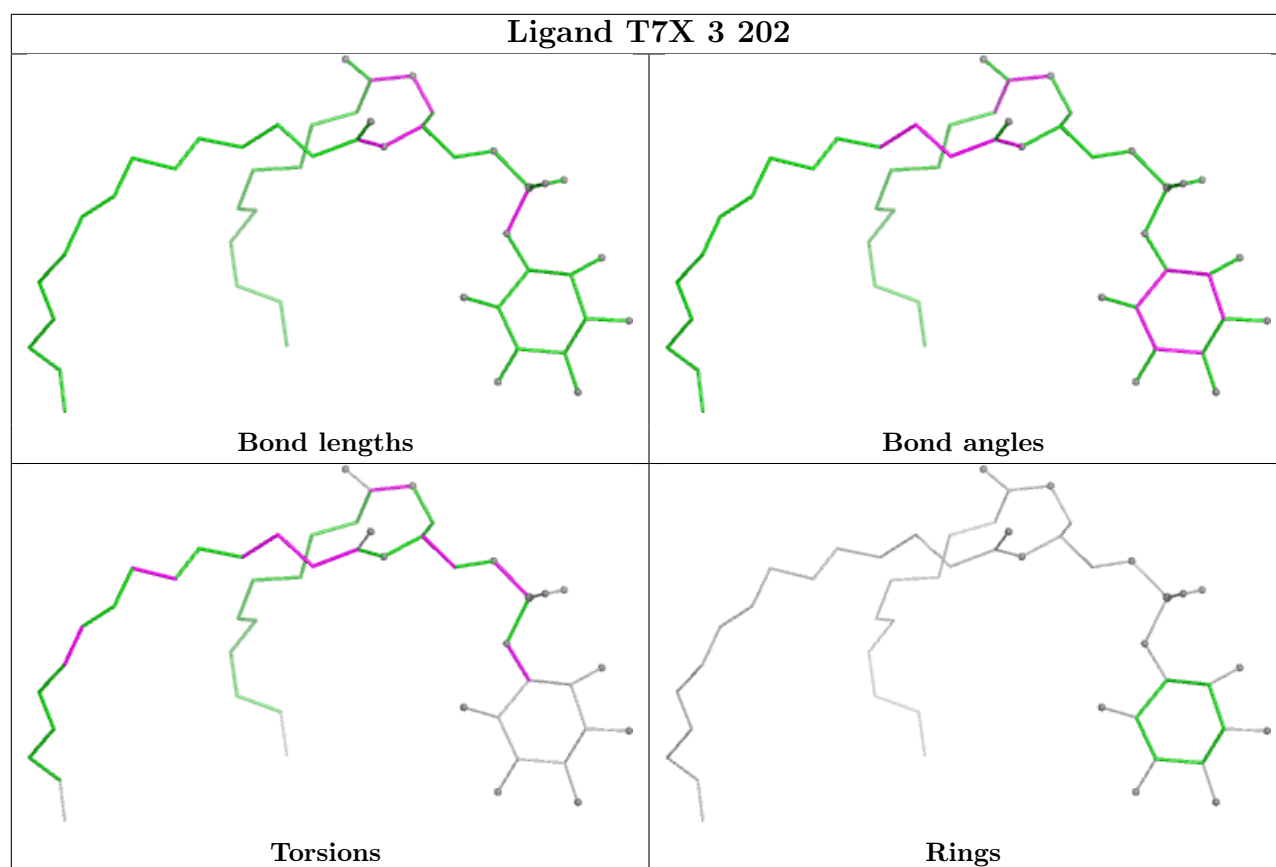


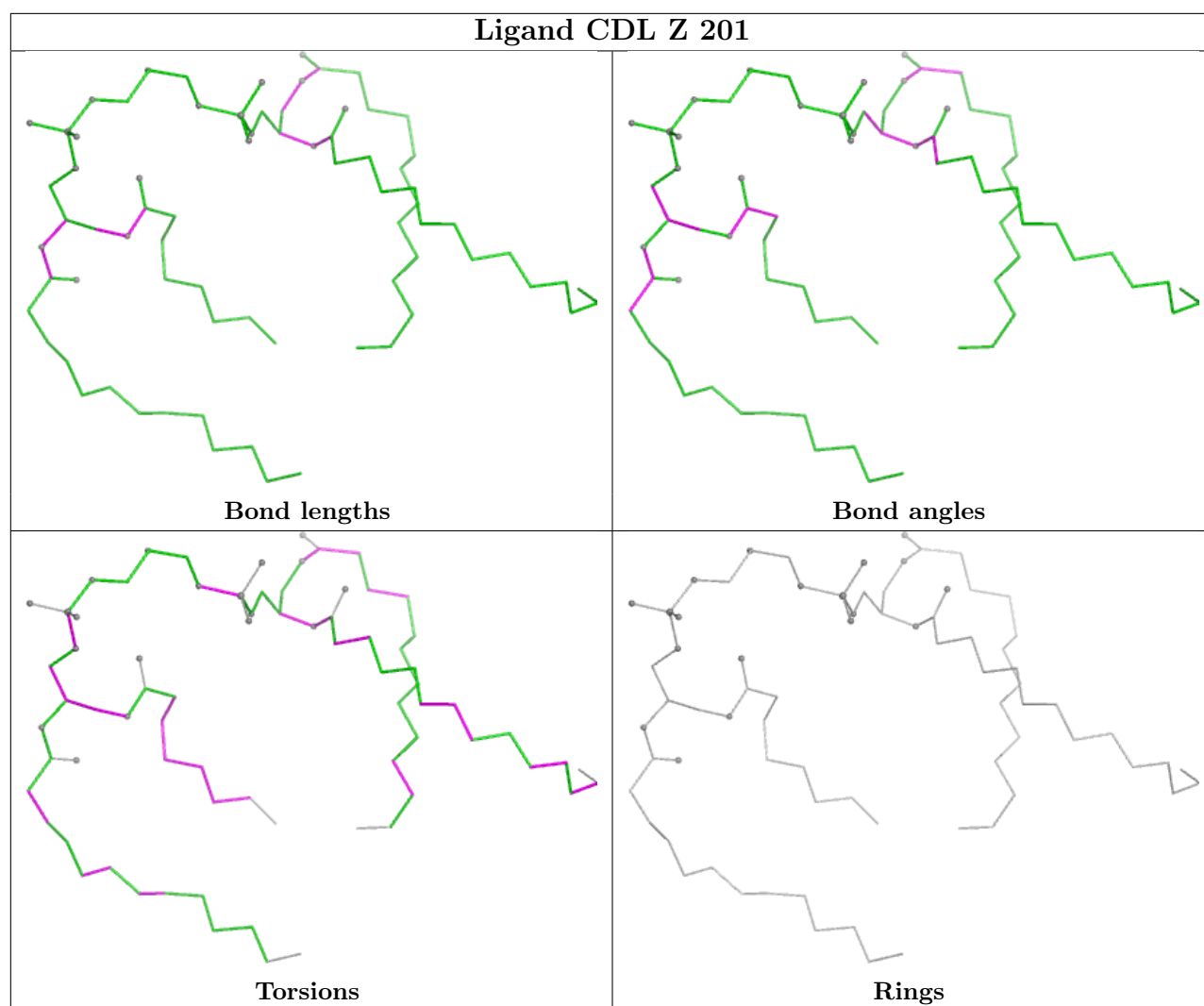
Ligand ZMP Q 201

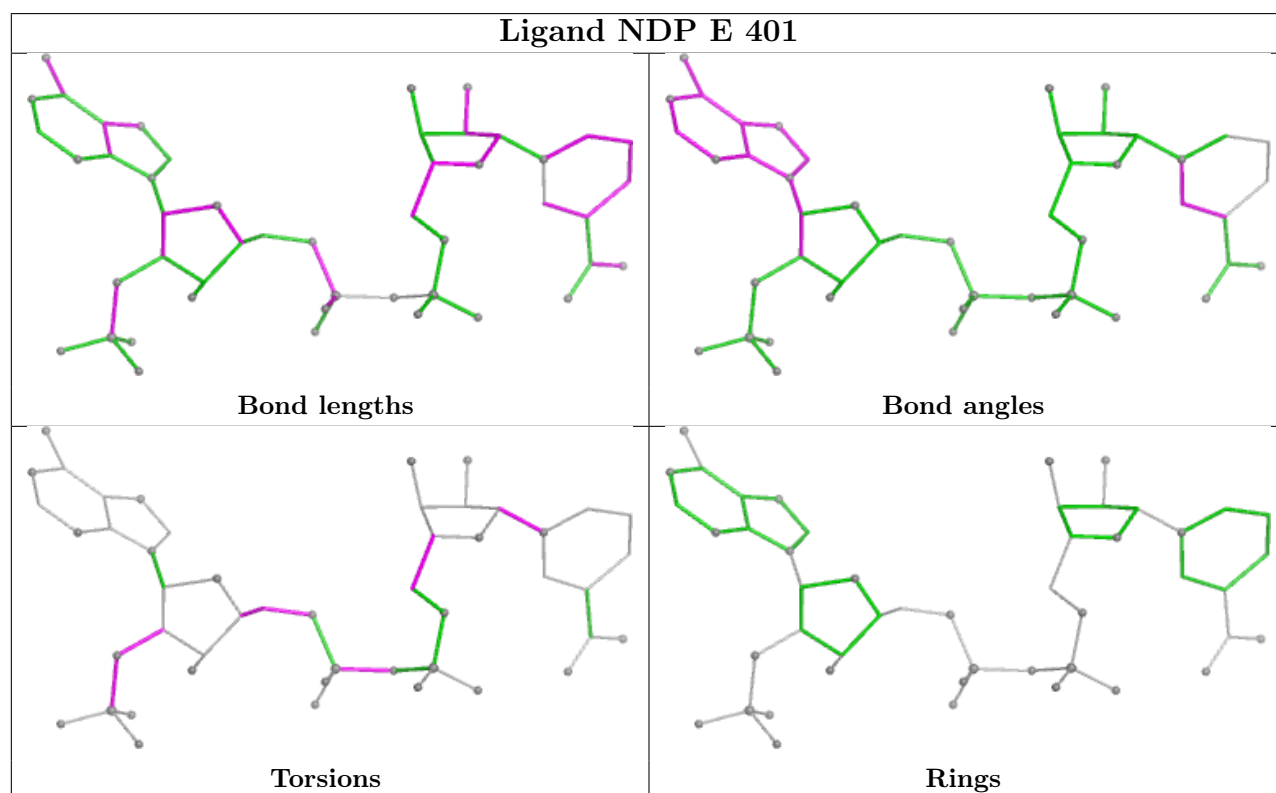
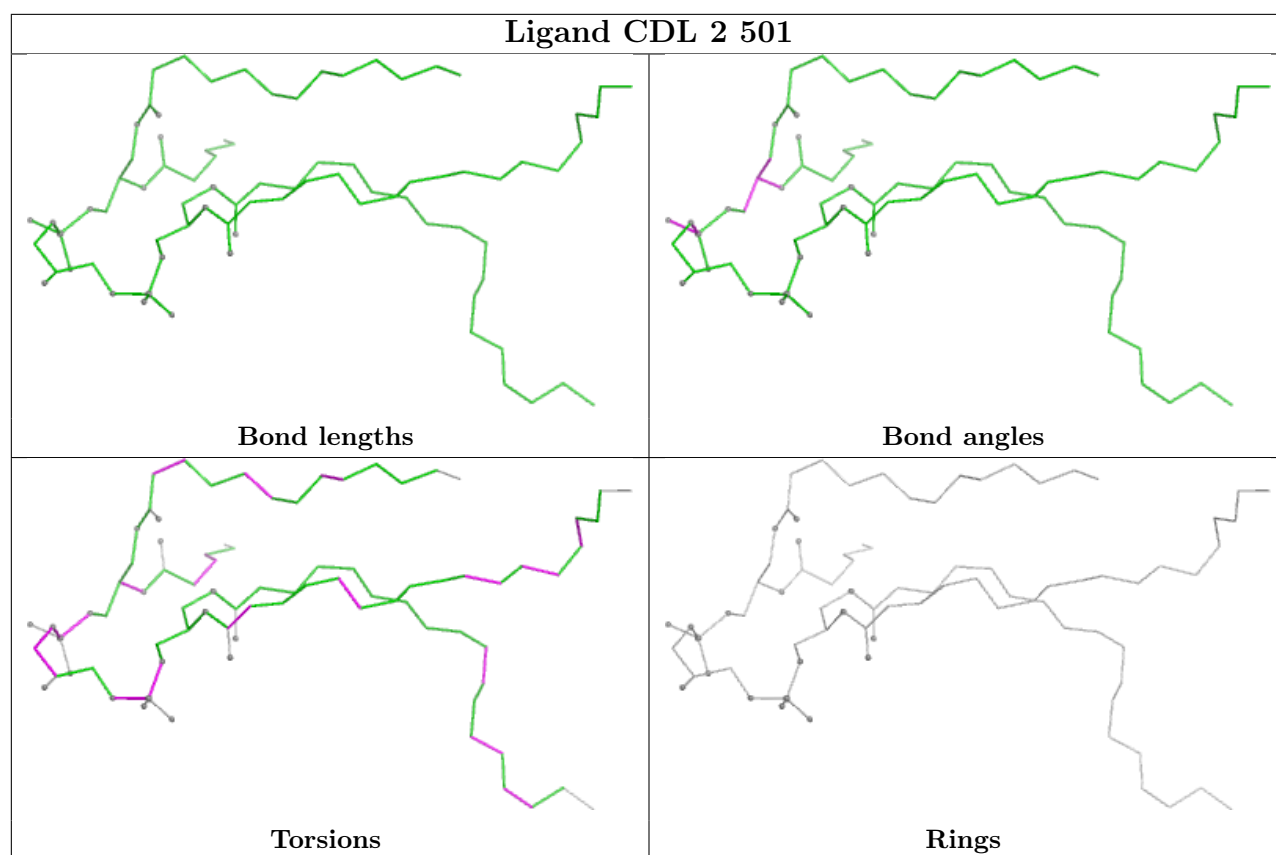


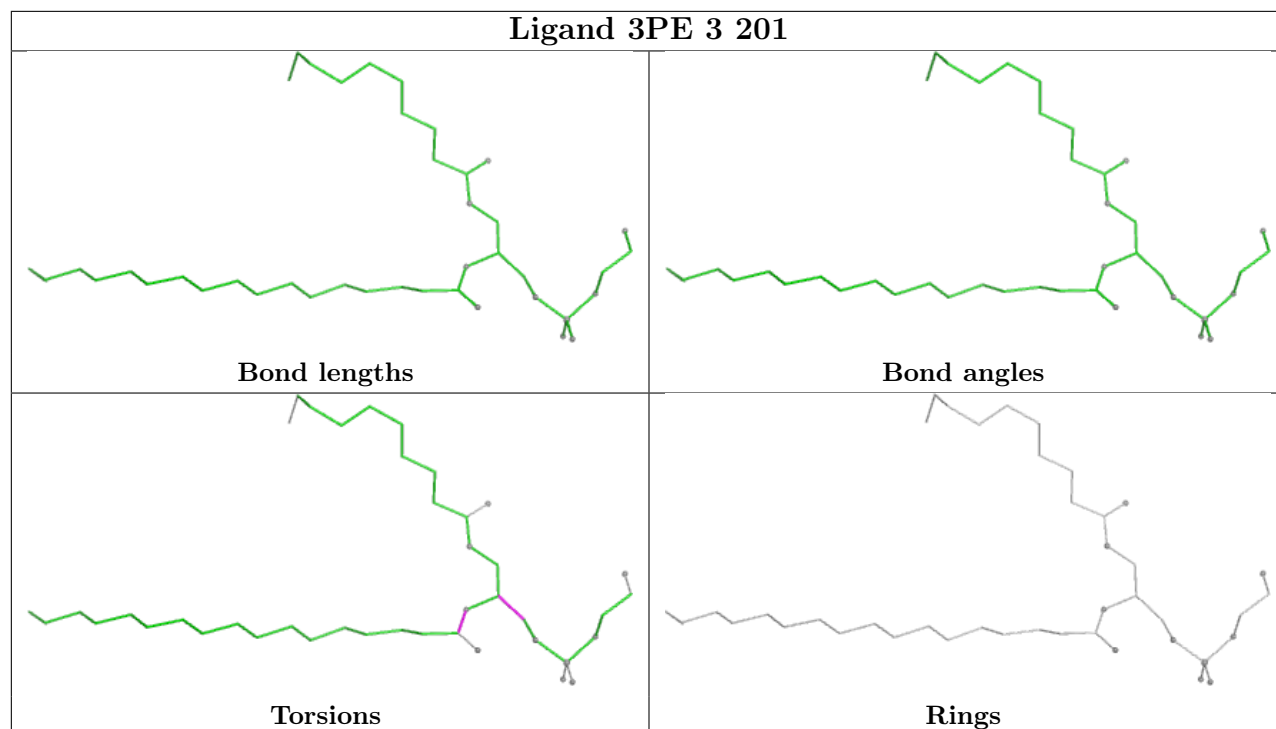


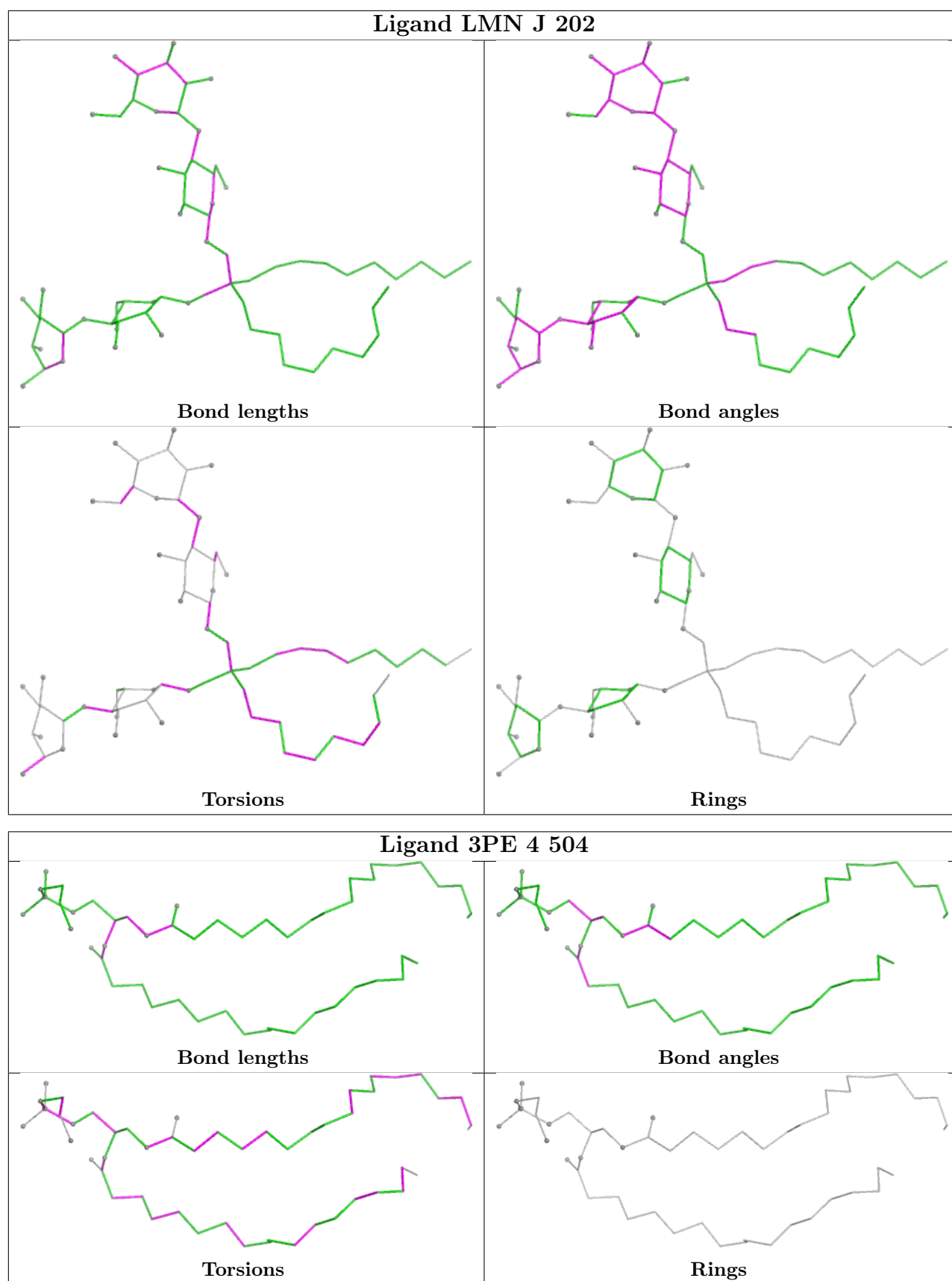


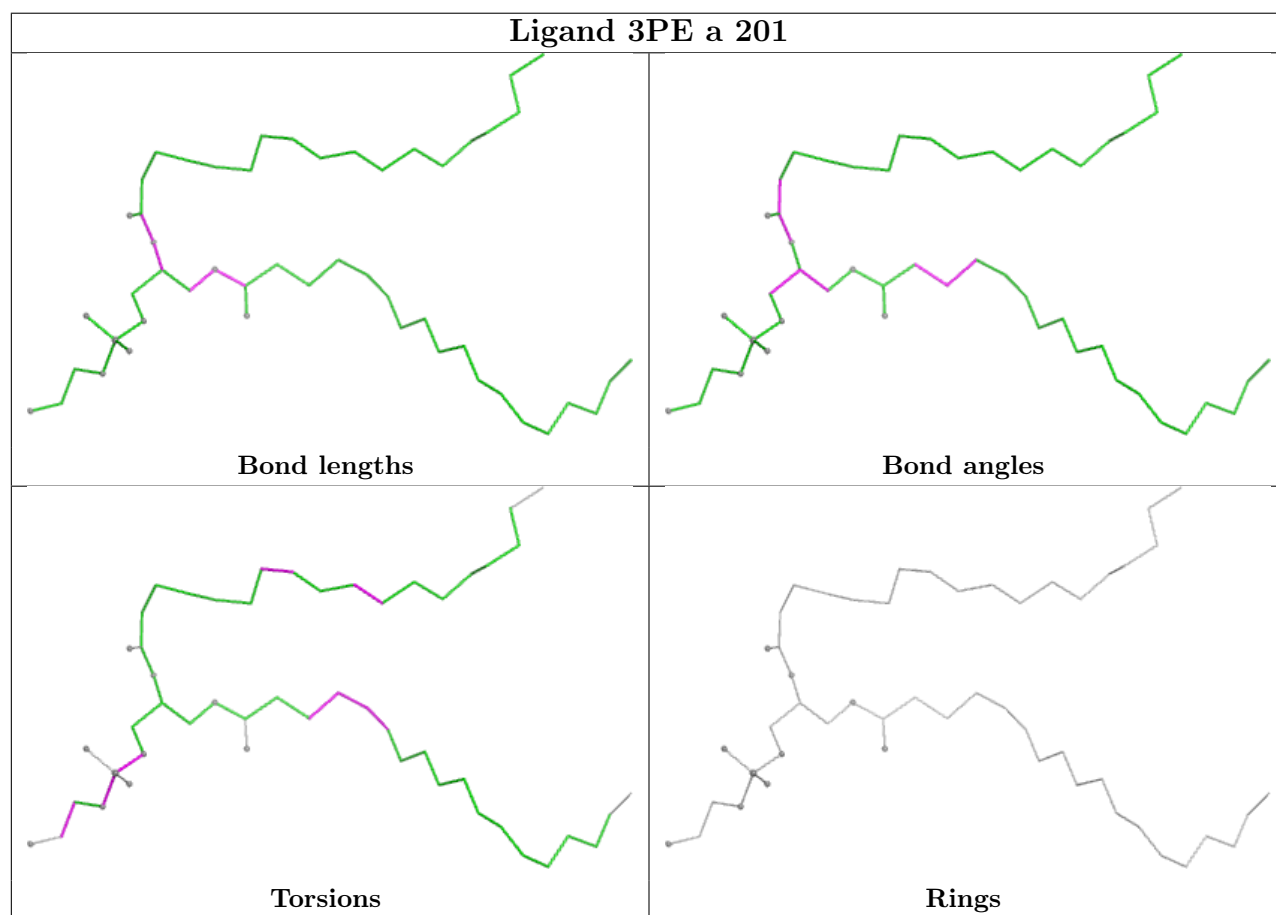
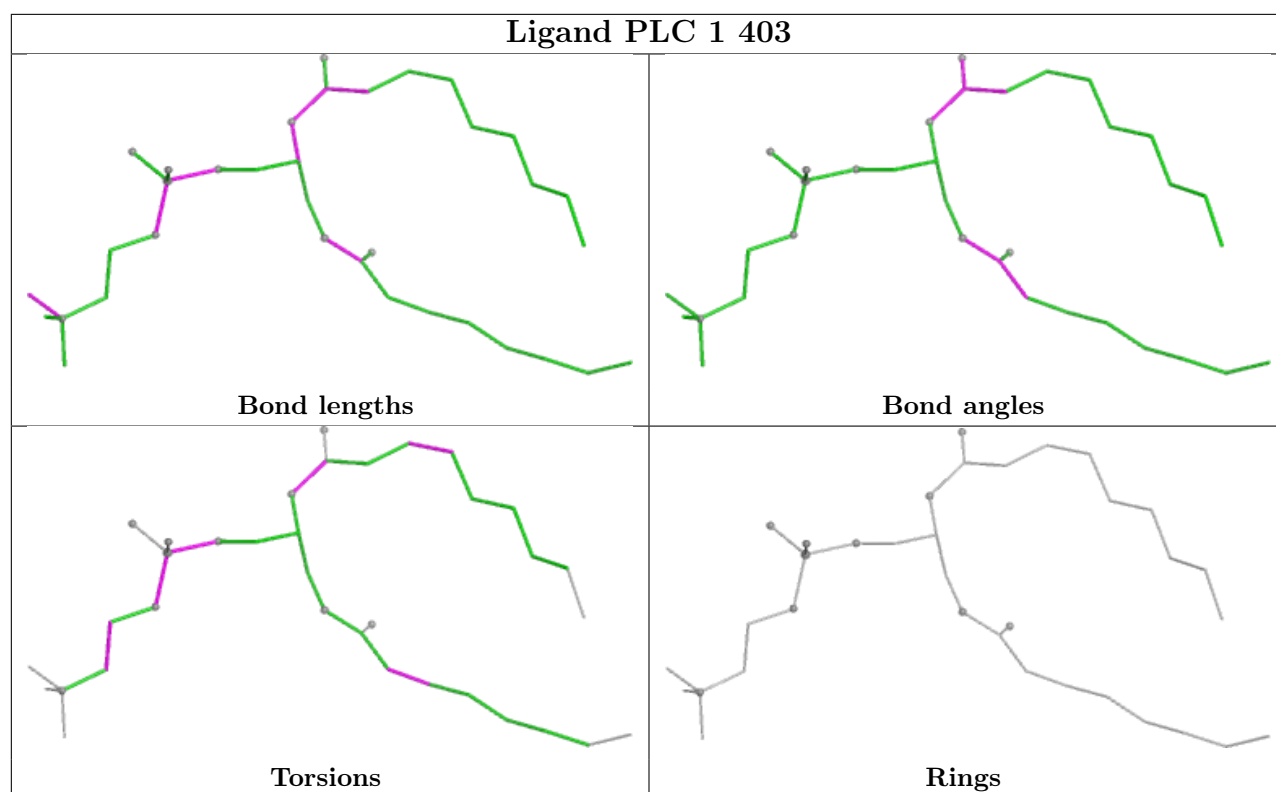


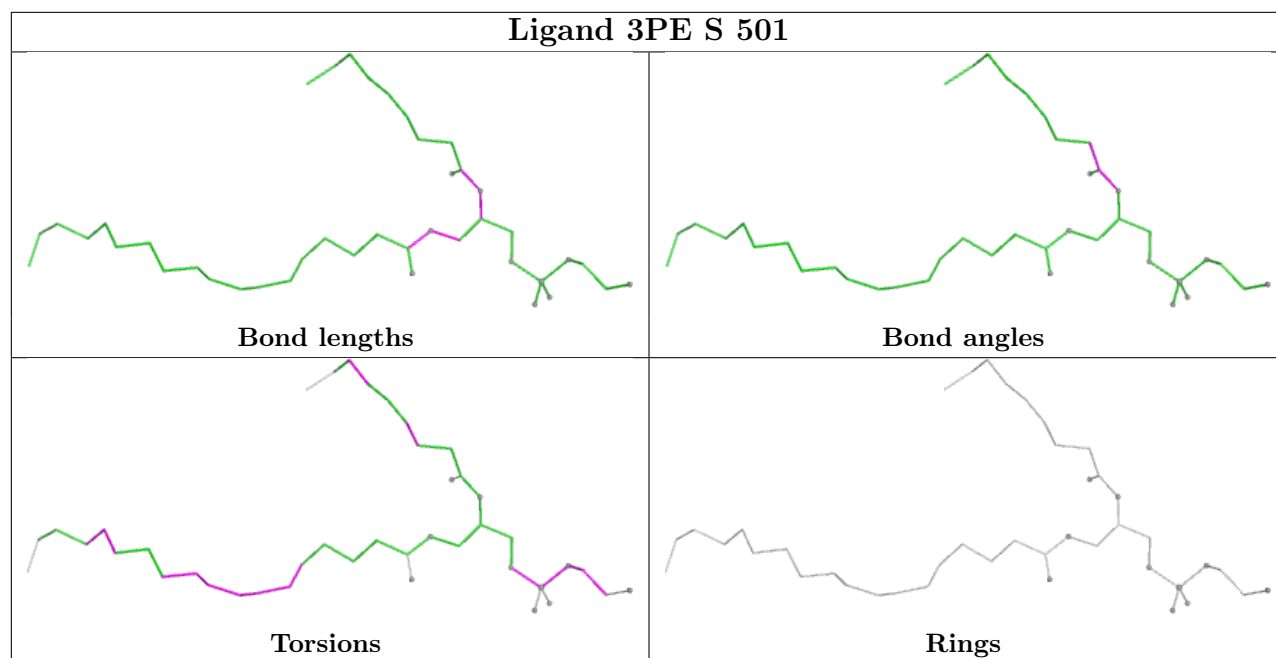
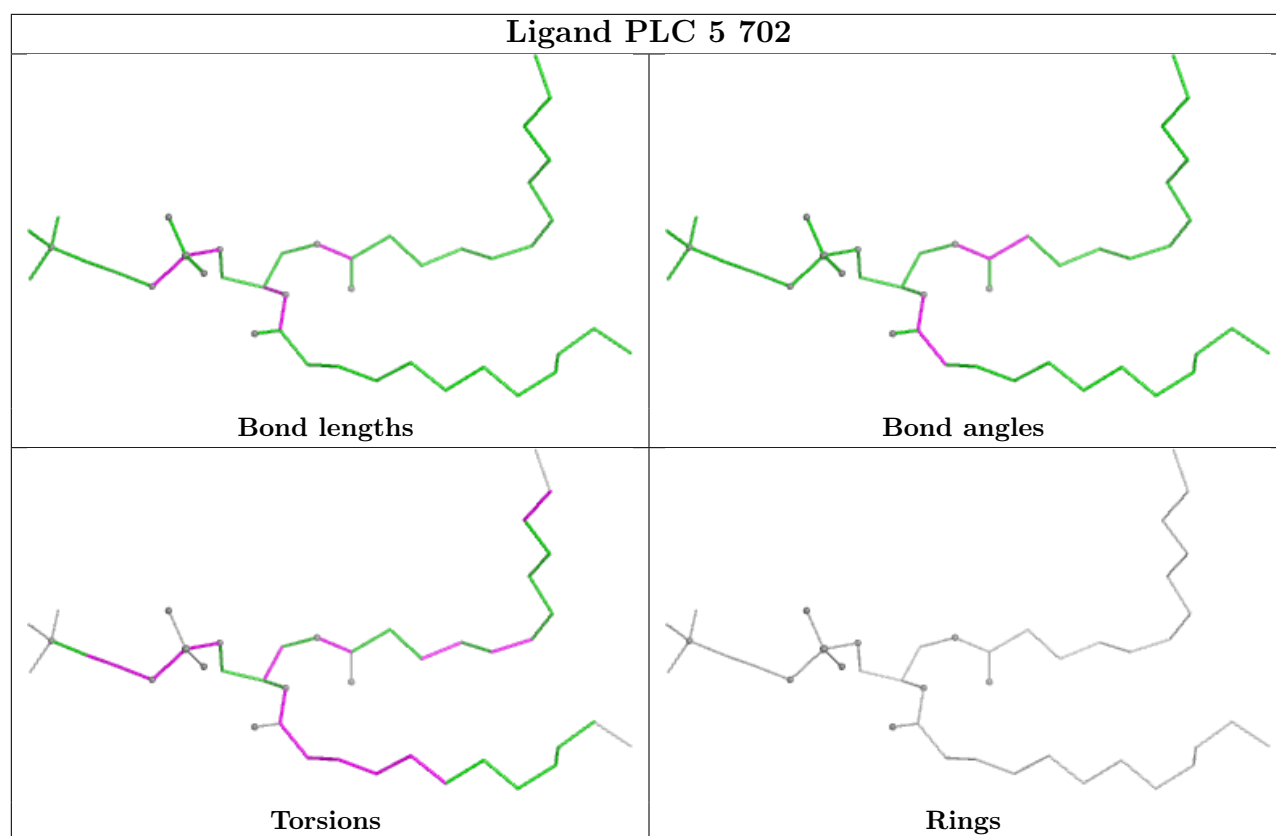


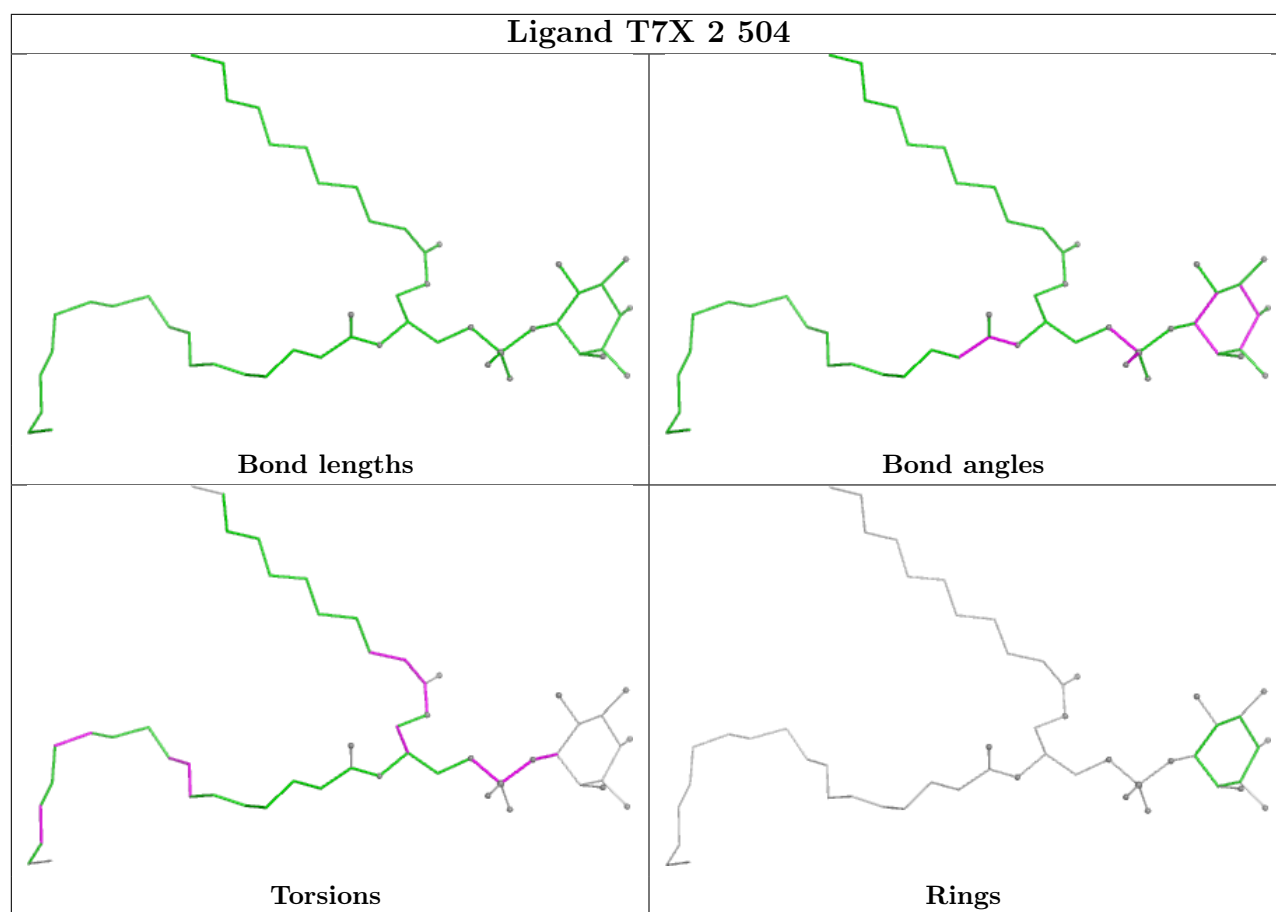


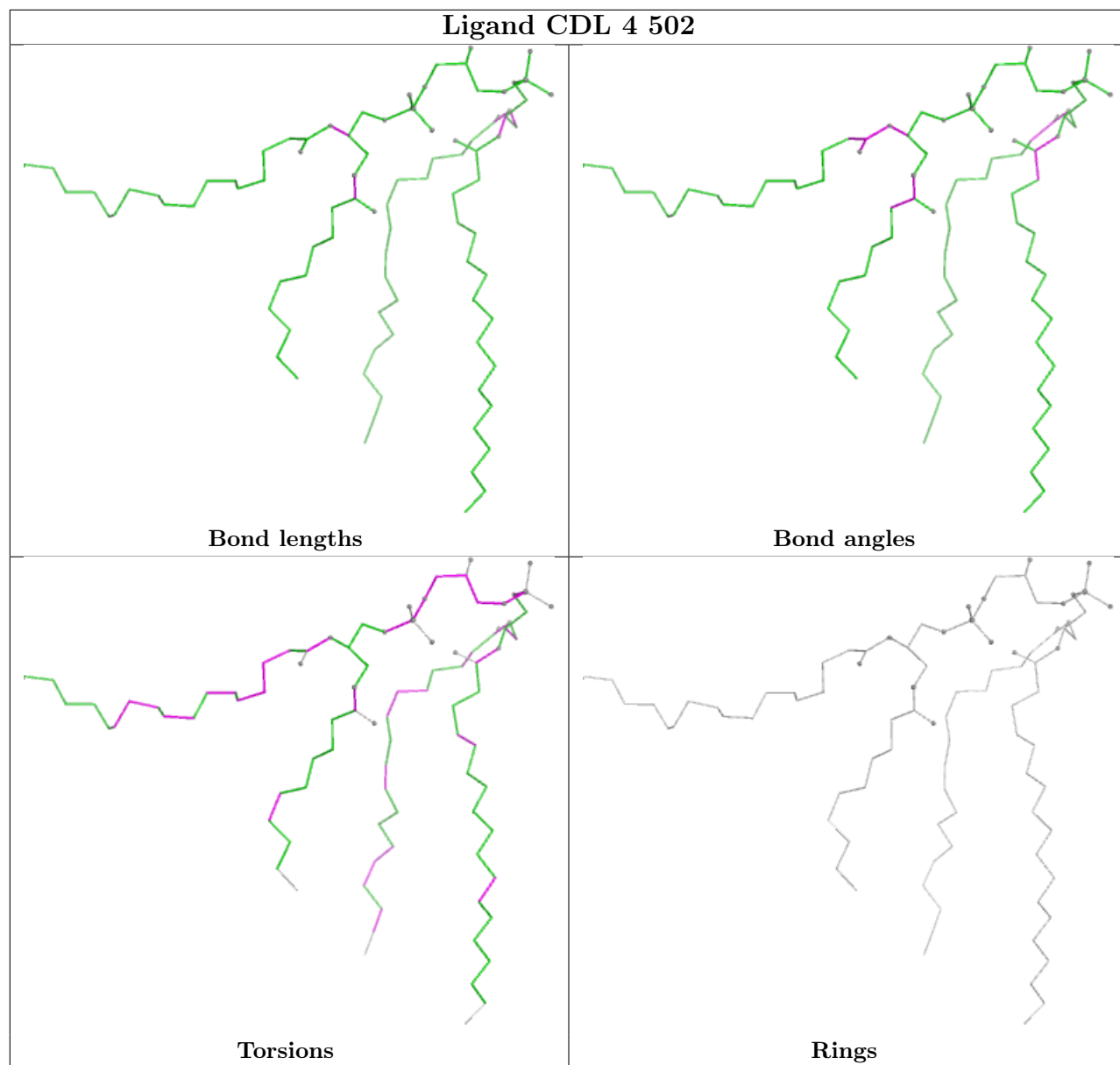


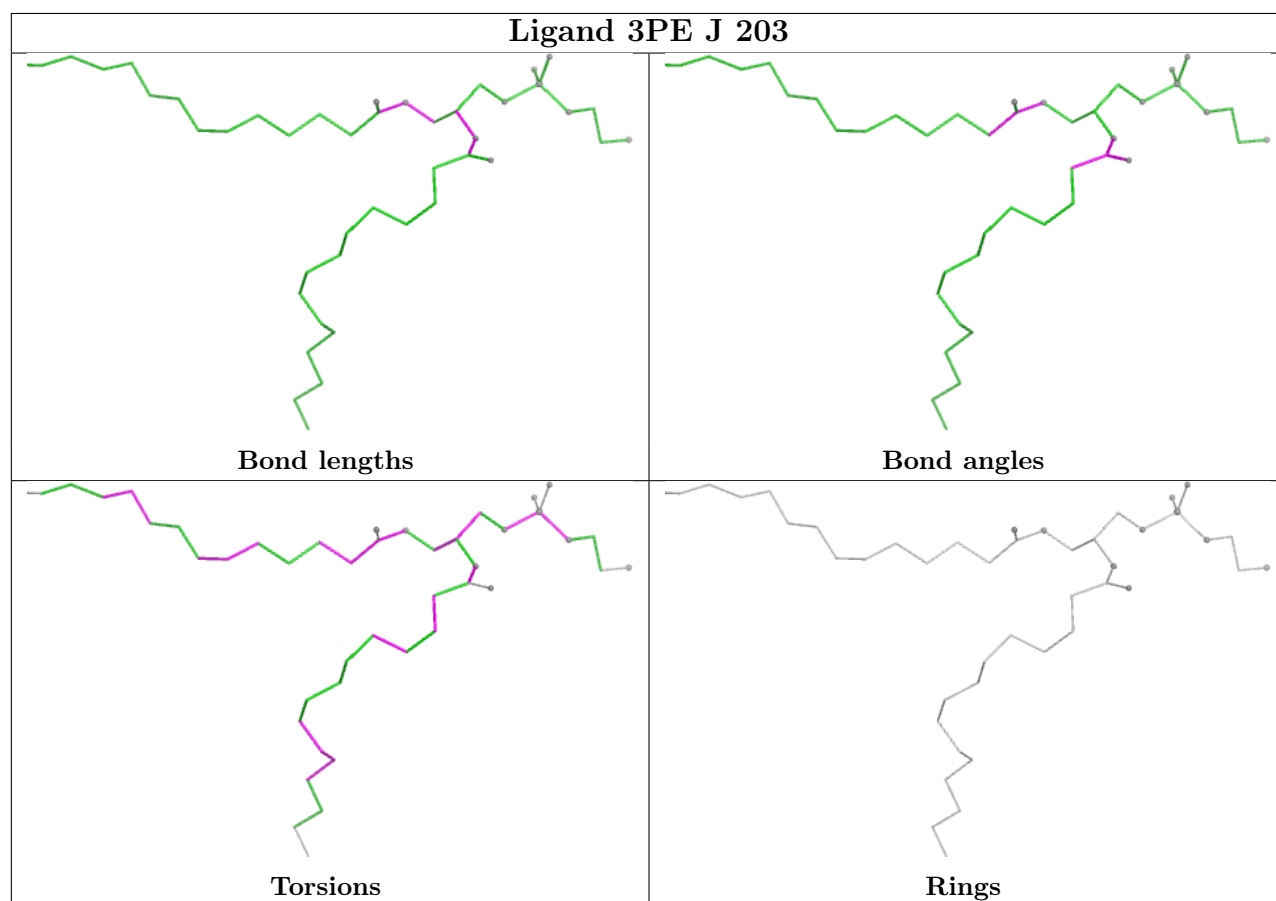
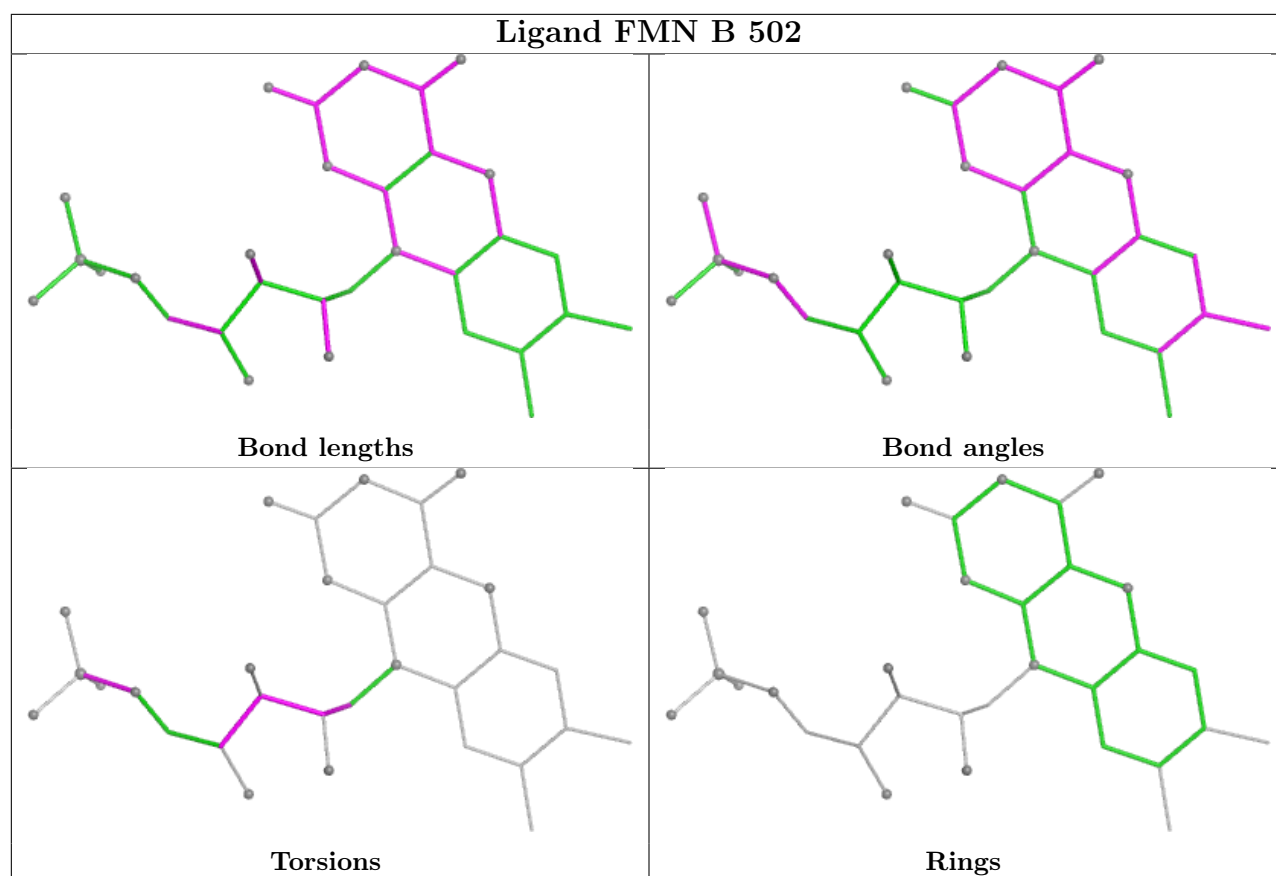


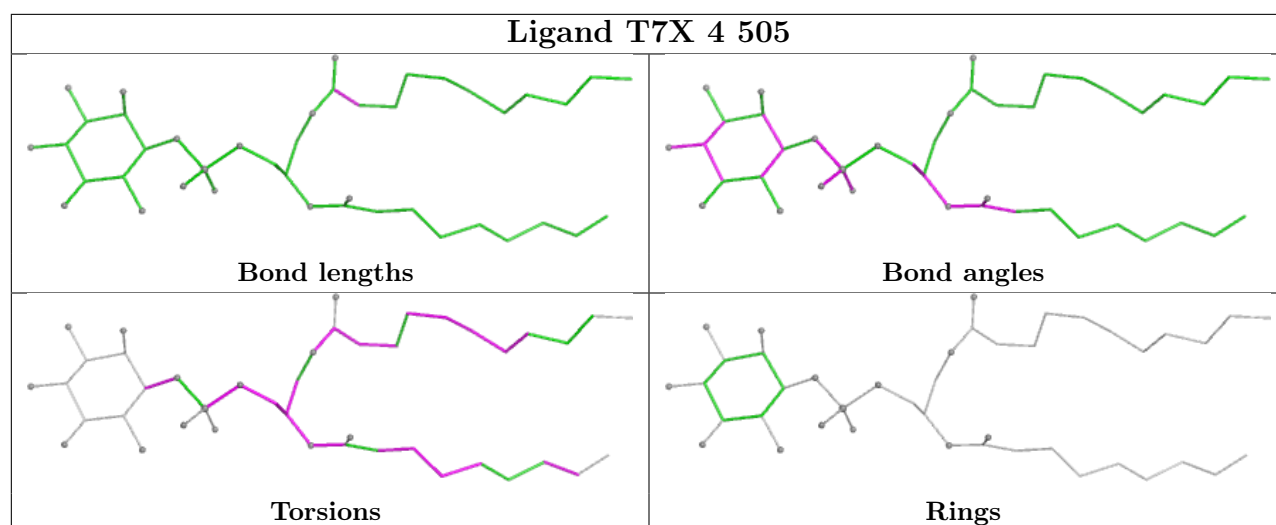


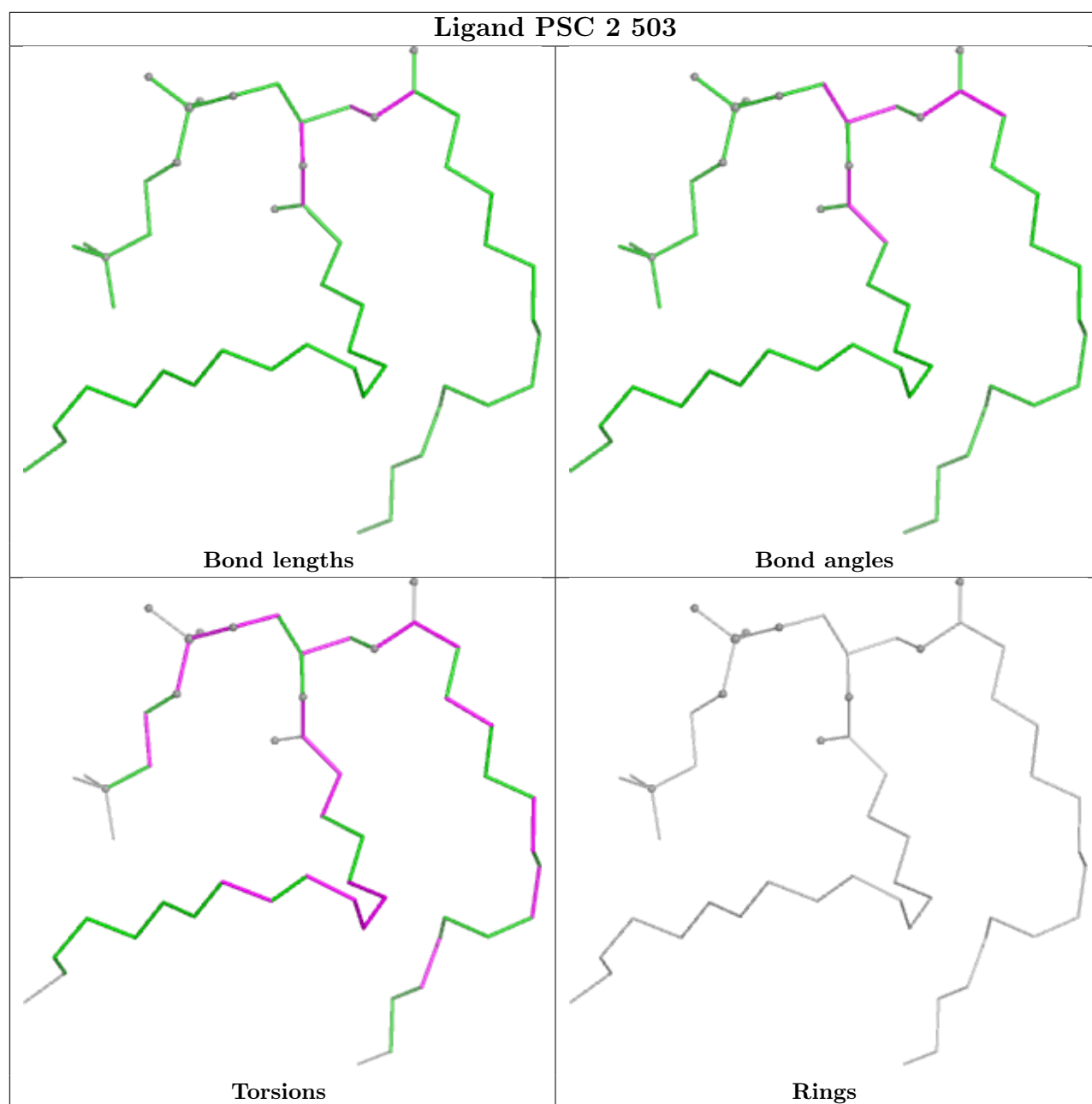


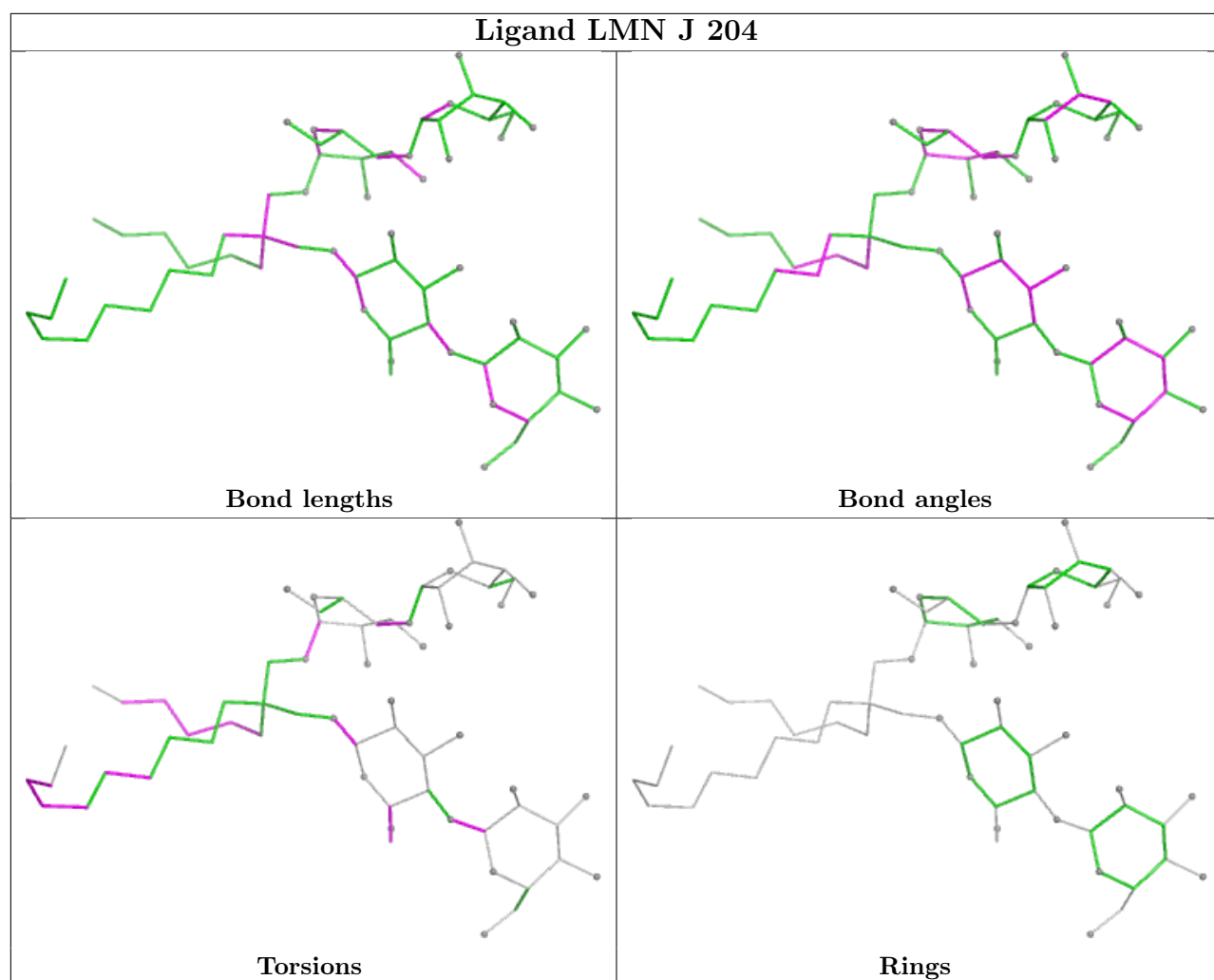


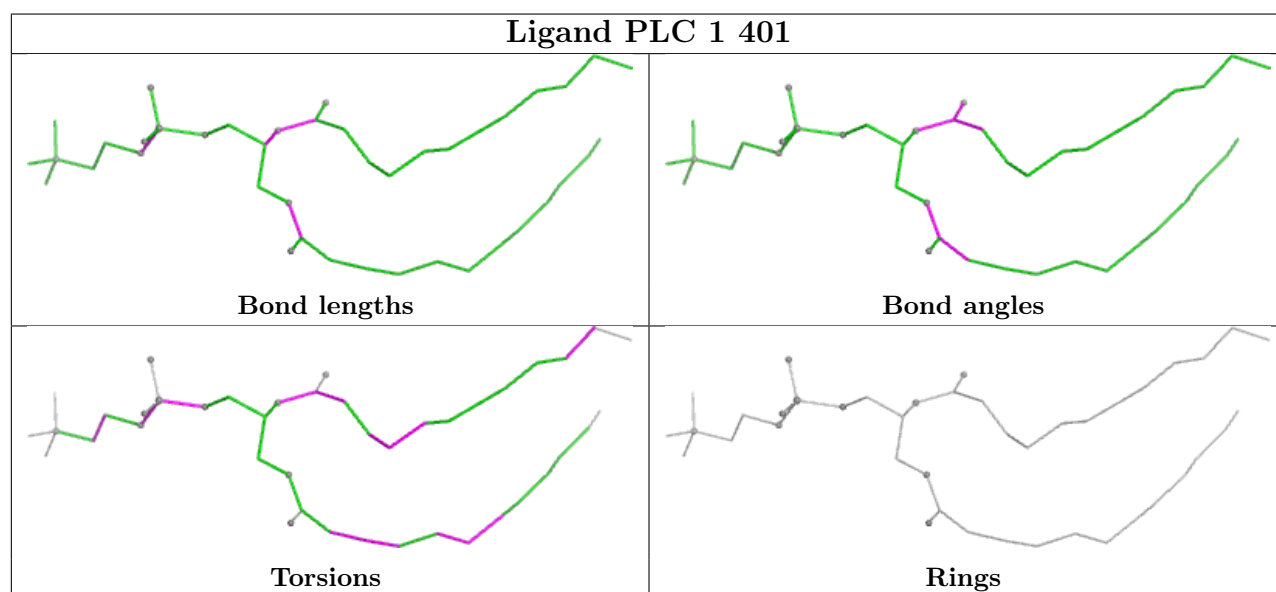
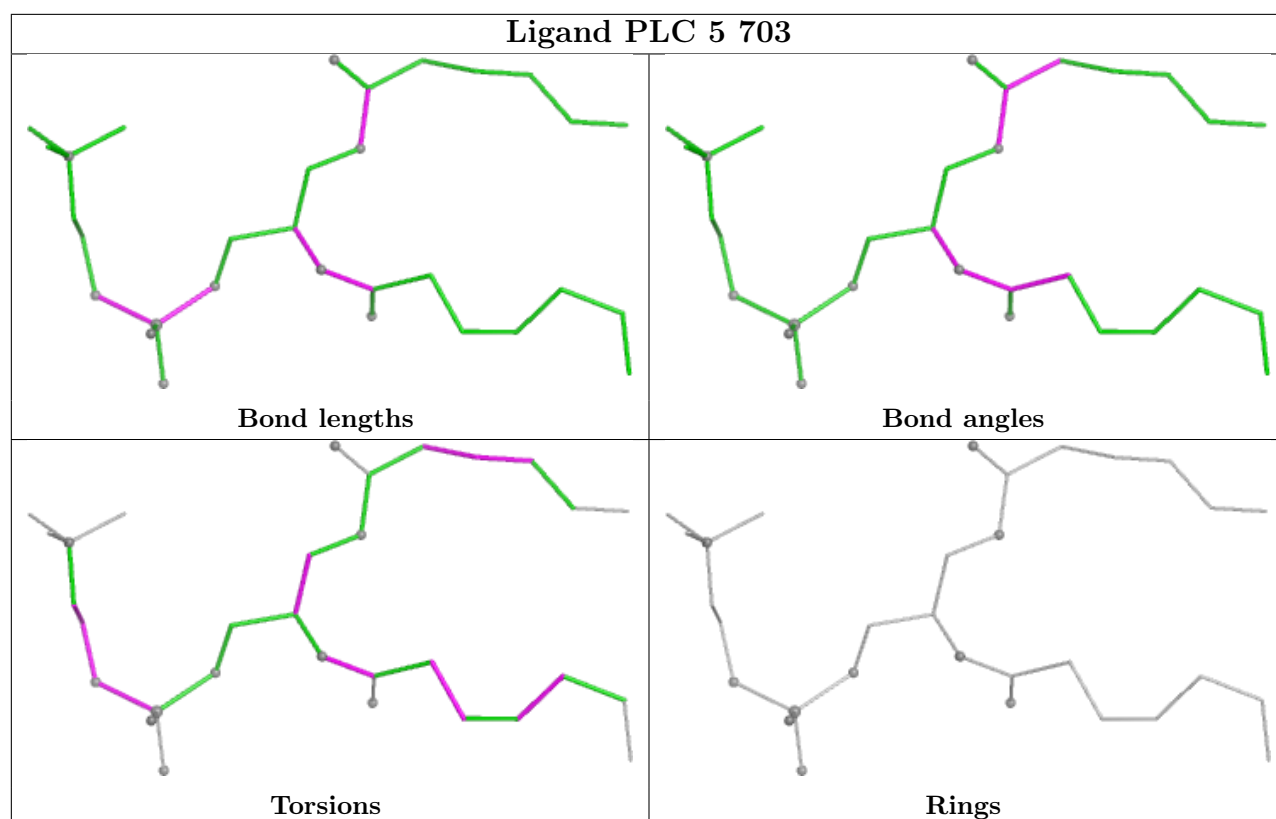


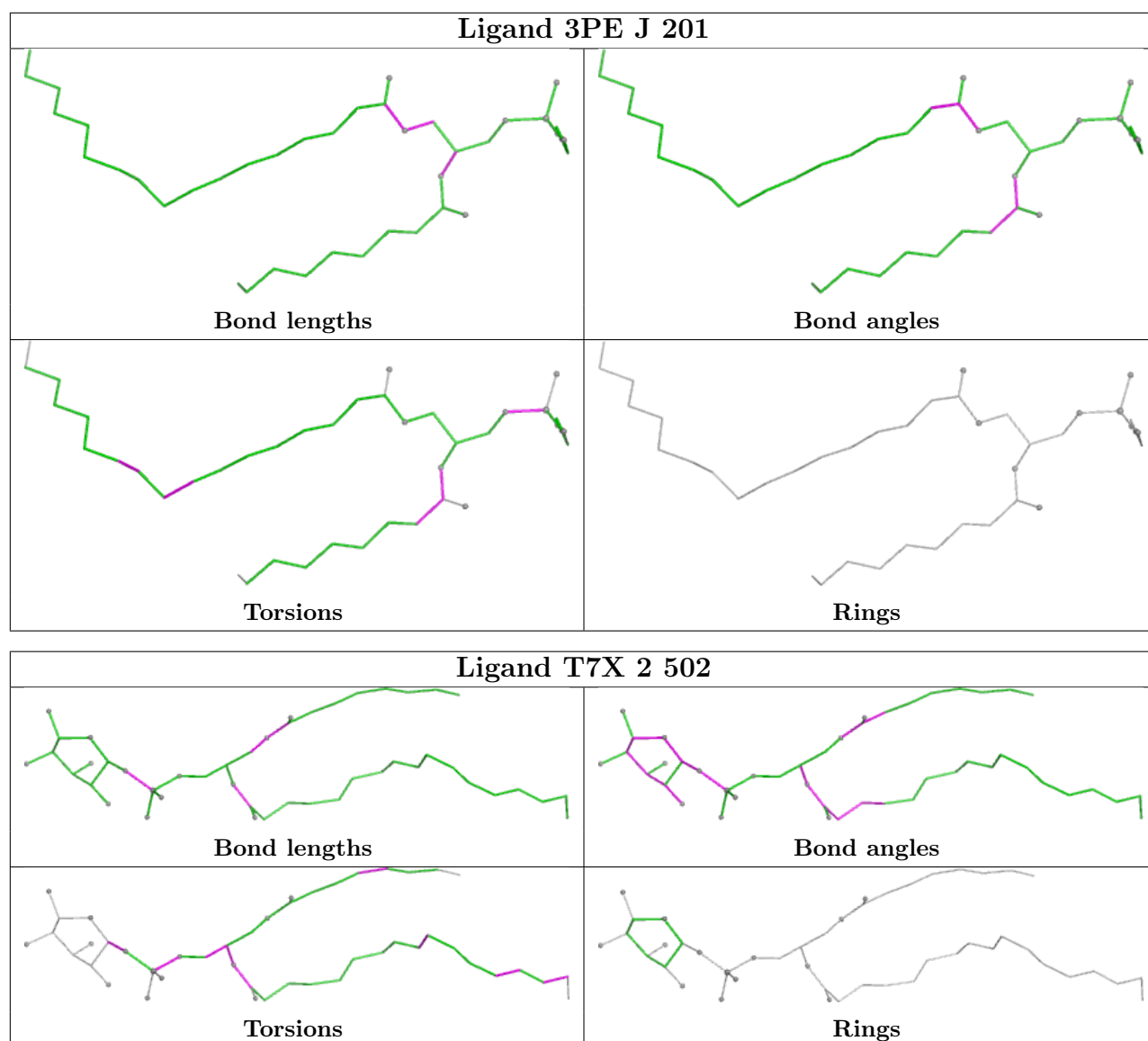


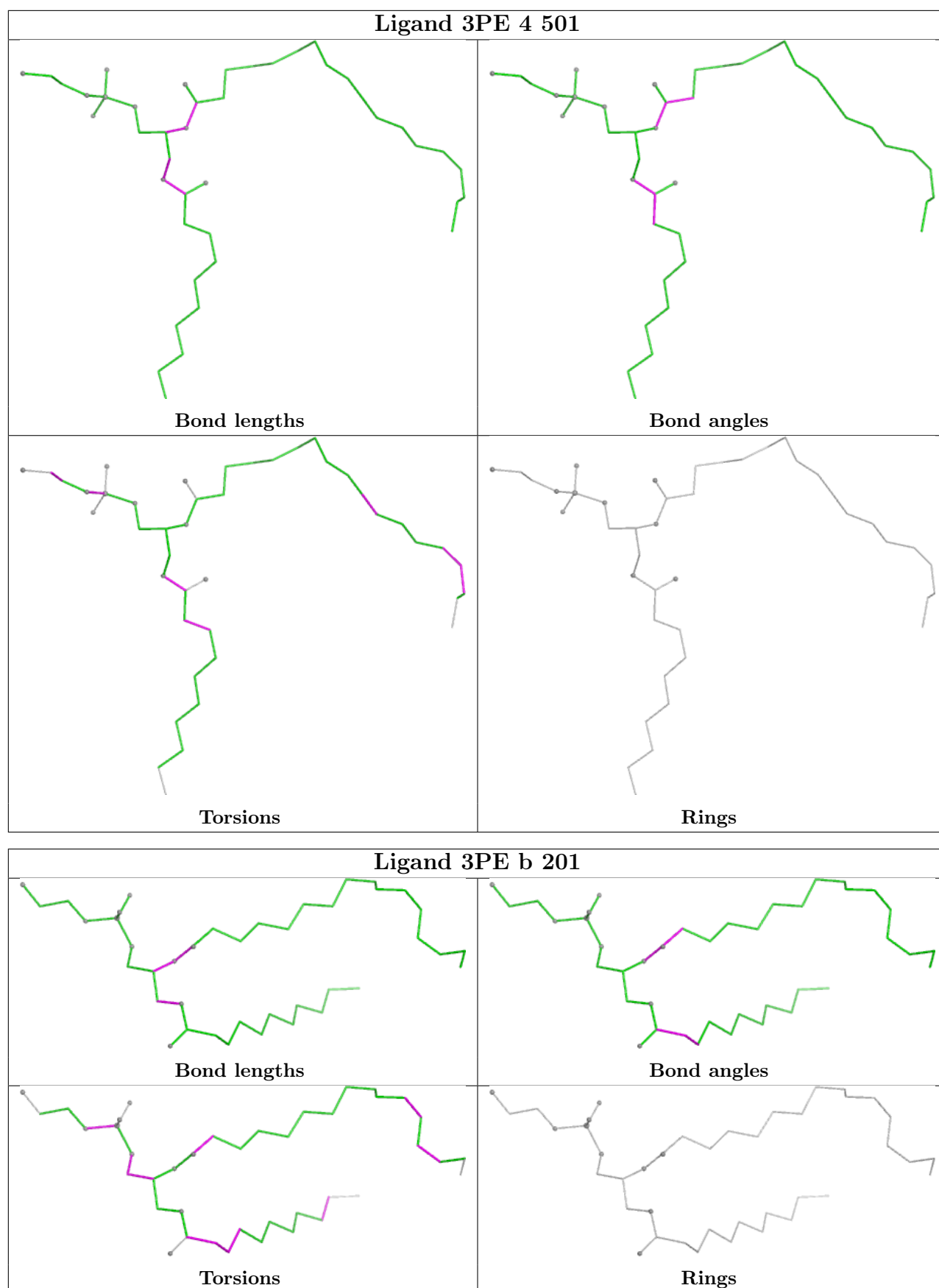


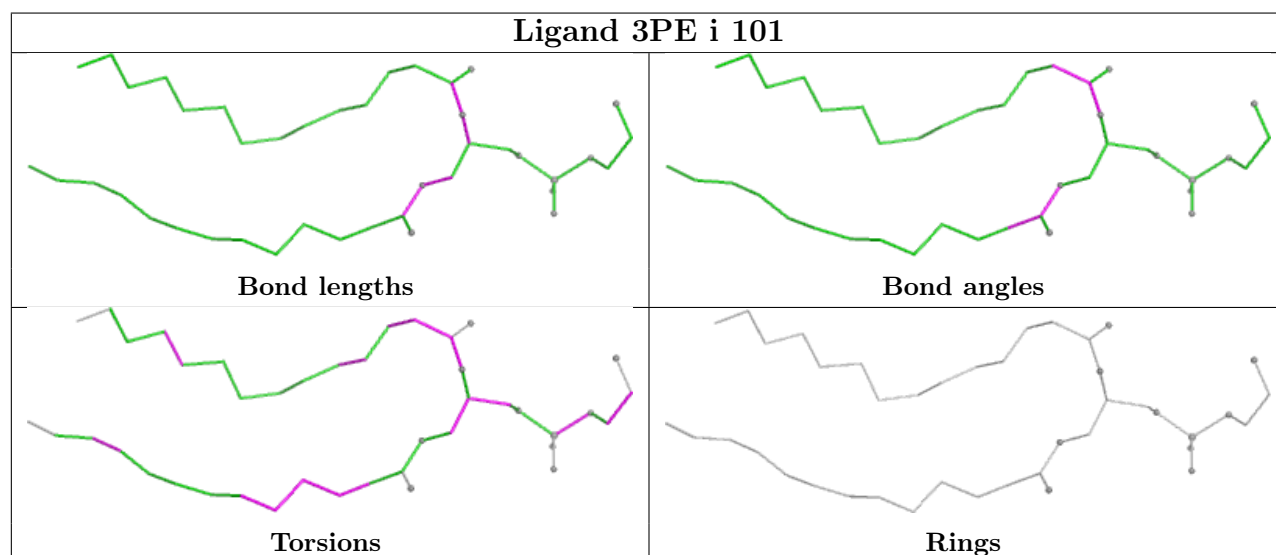
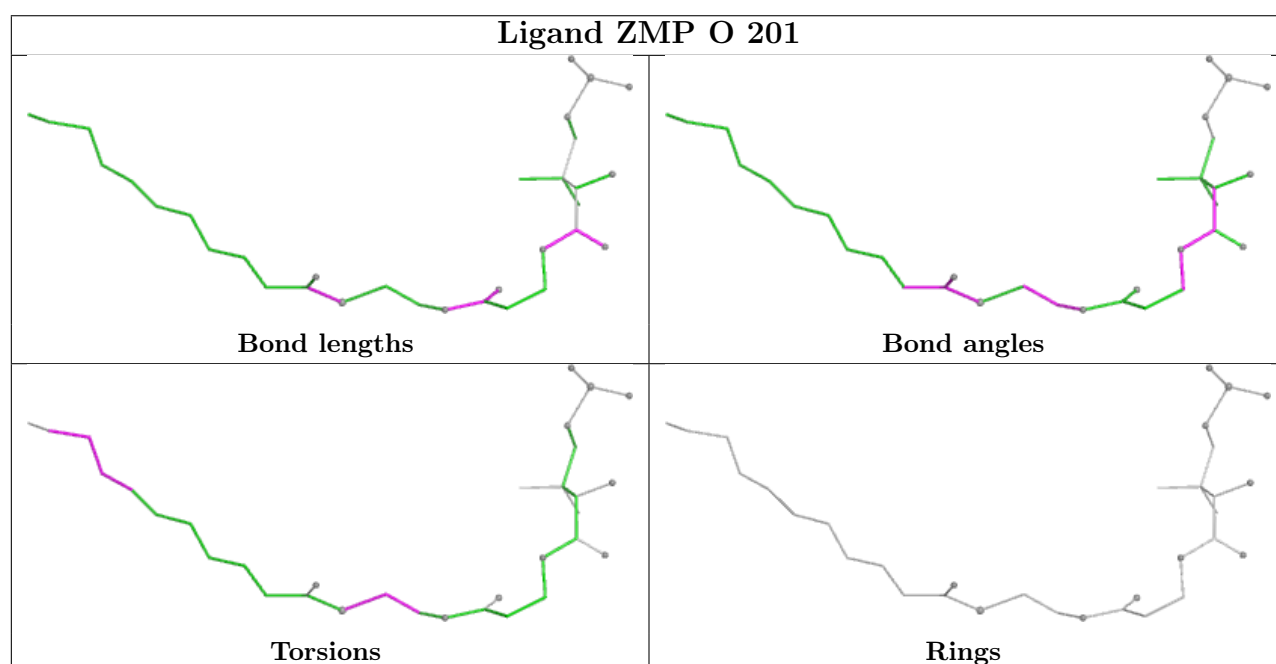
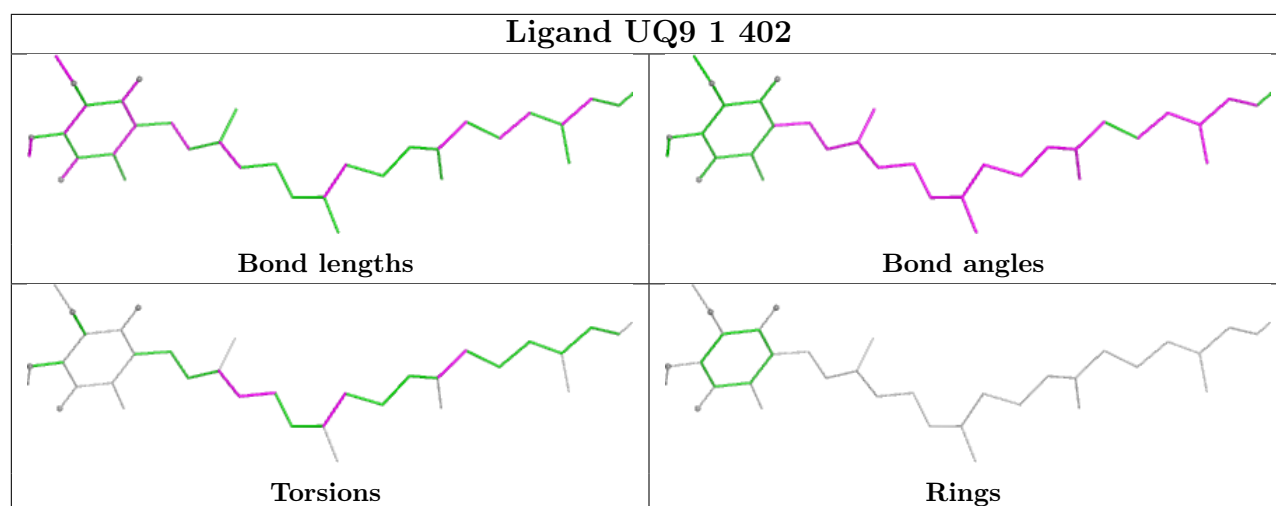


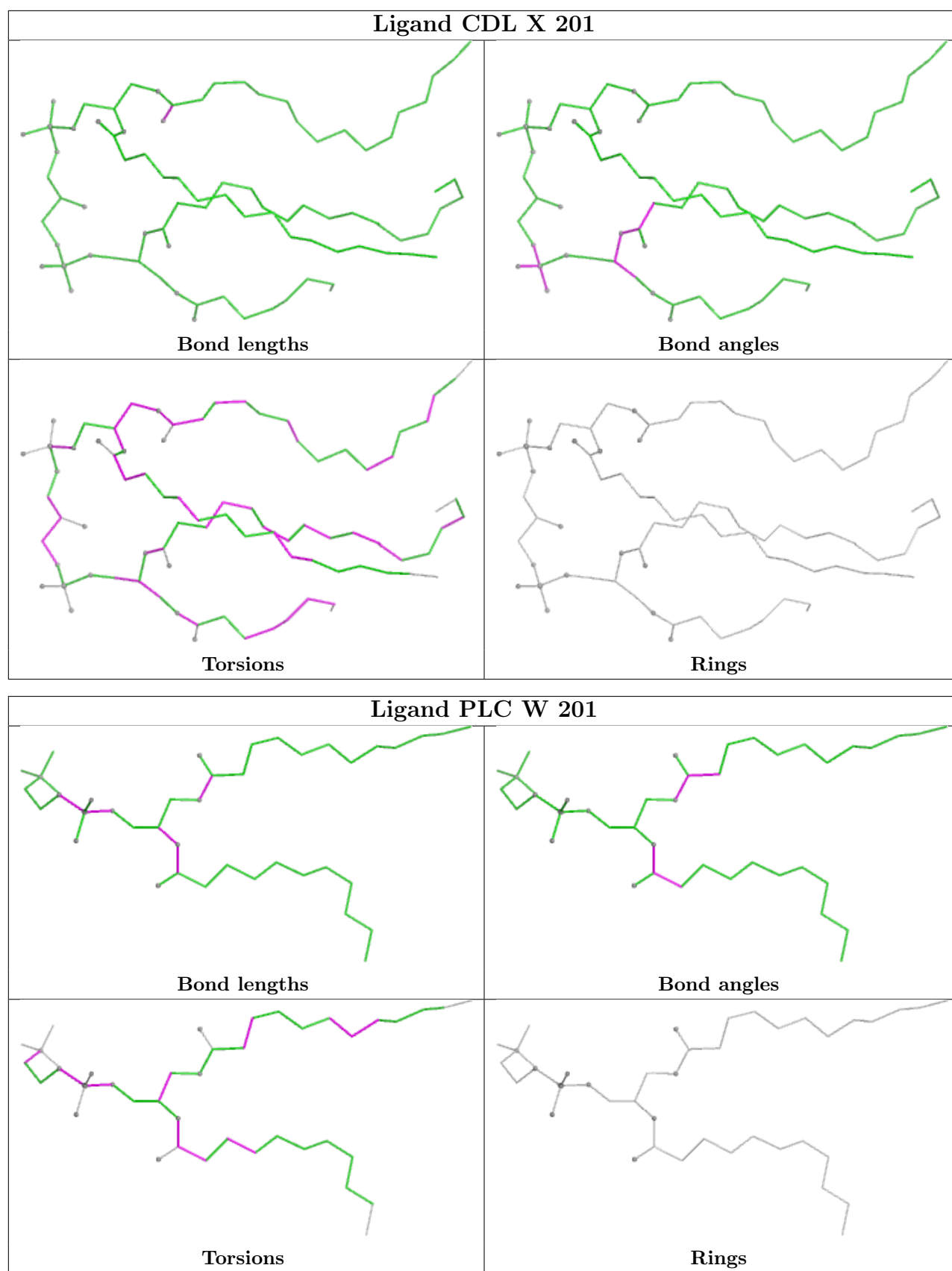


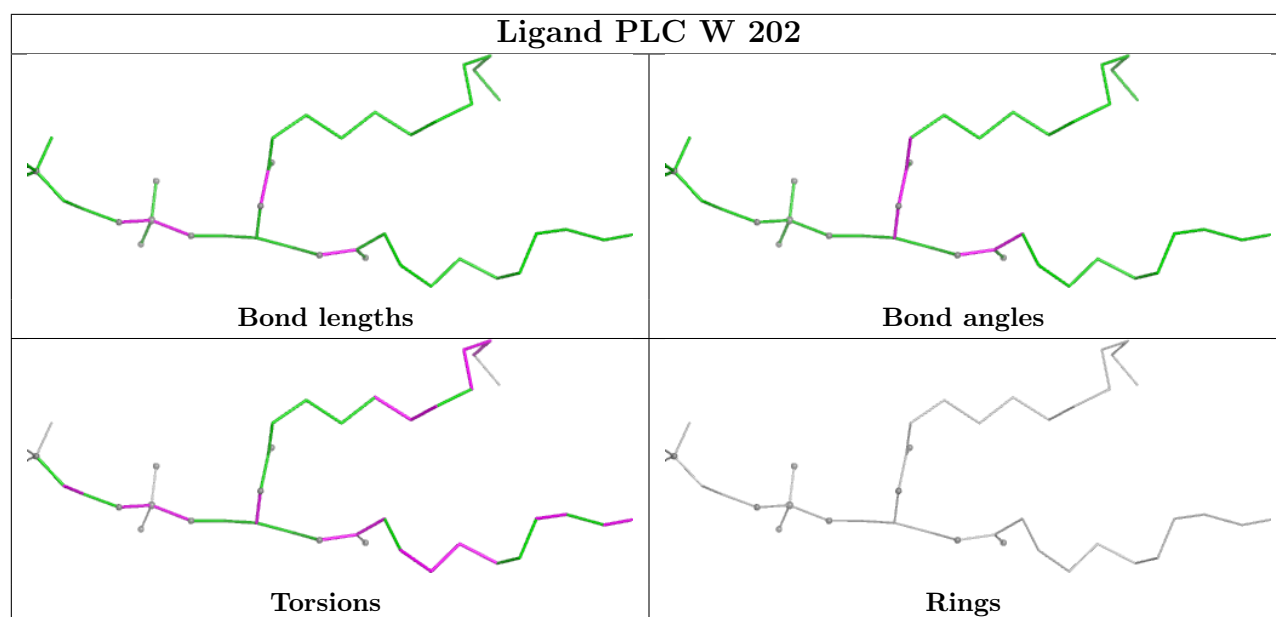












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

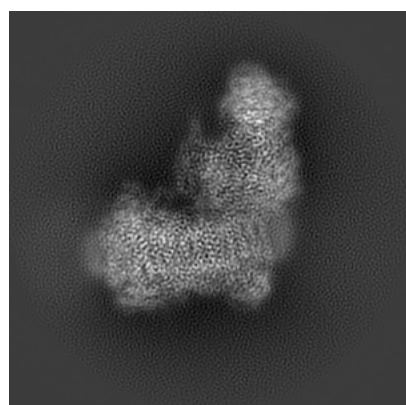
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10711. These allow visual inspection of the internal detail of the map and identification of artifacts.

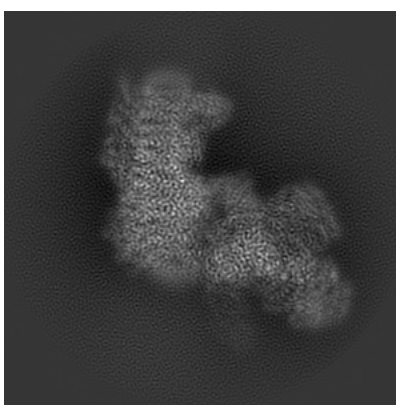
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

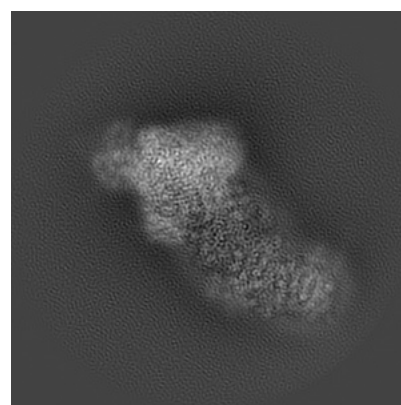
6.1.1 Primary map



X



Y

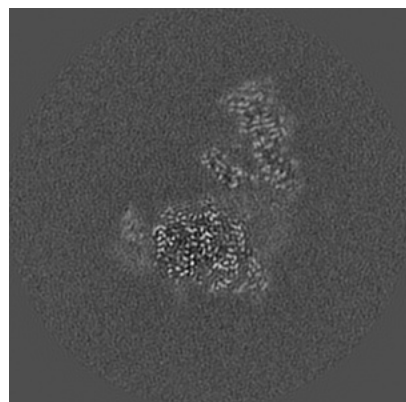


Z

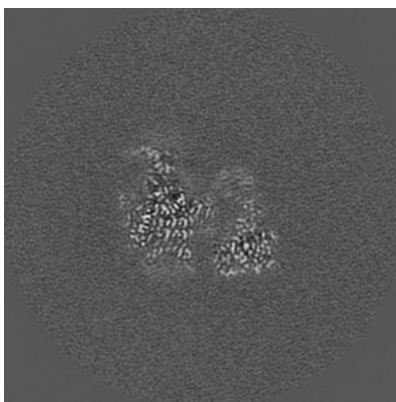
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

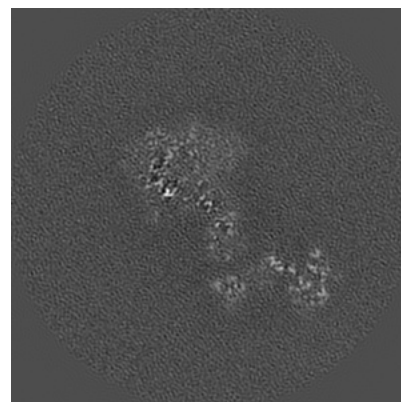
6.2.1 Primary map



X Index: 200



Y Index: 200

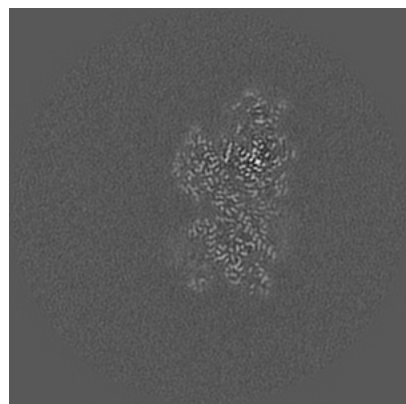


Z Index: 200

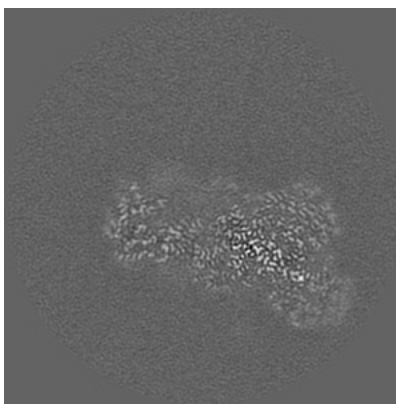
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

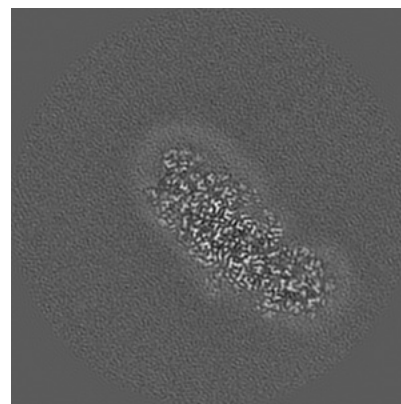
6.3.1 Primary map



X Index: 159



Y Index: 244

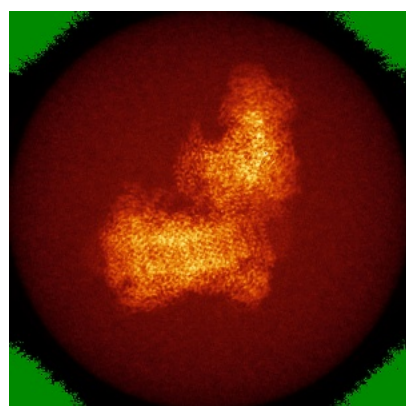


Z Index: 174

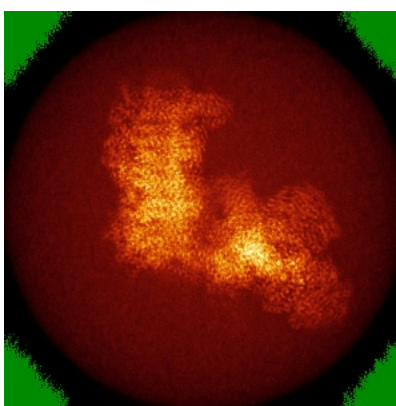
The images above show the largest variance slices of the map in three orthogonal directions.

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

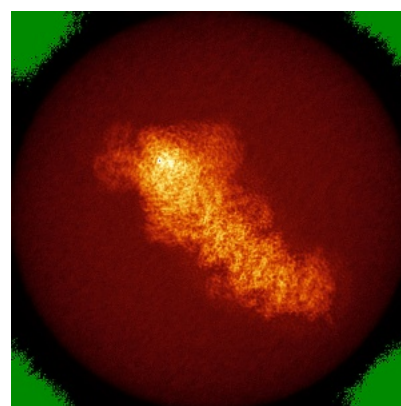
6.4.1 Primary map



X



Y

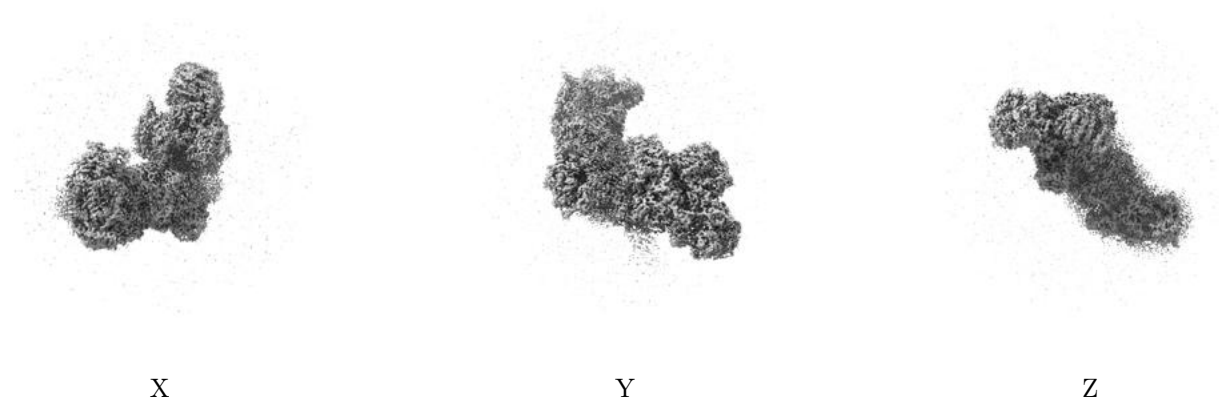


Z

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 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

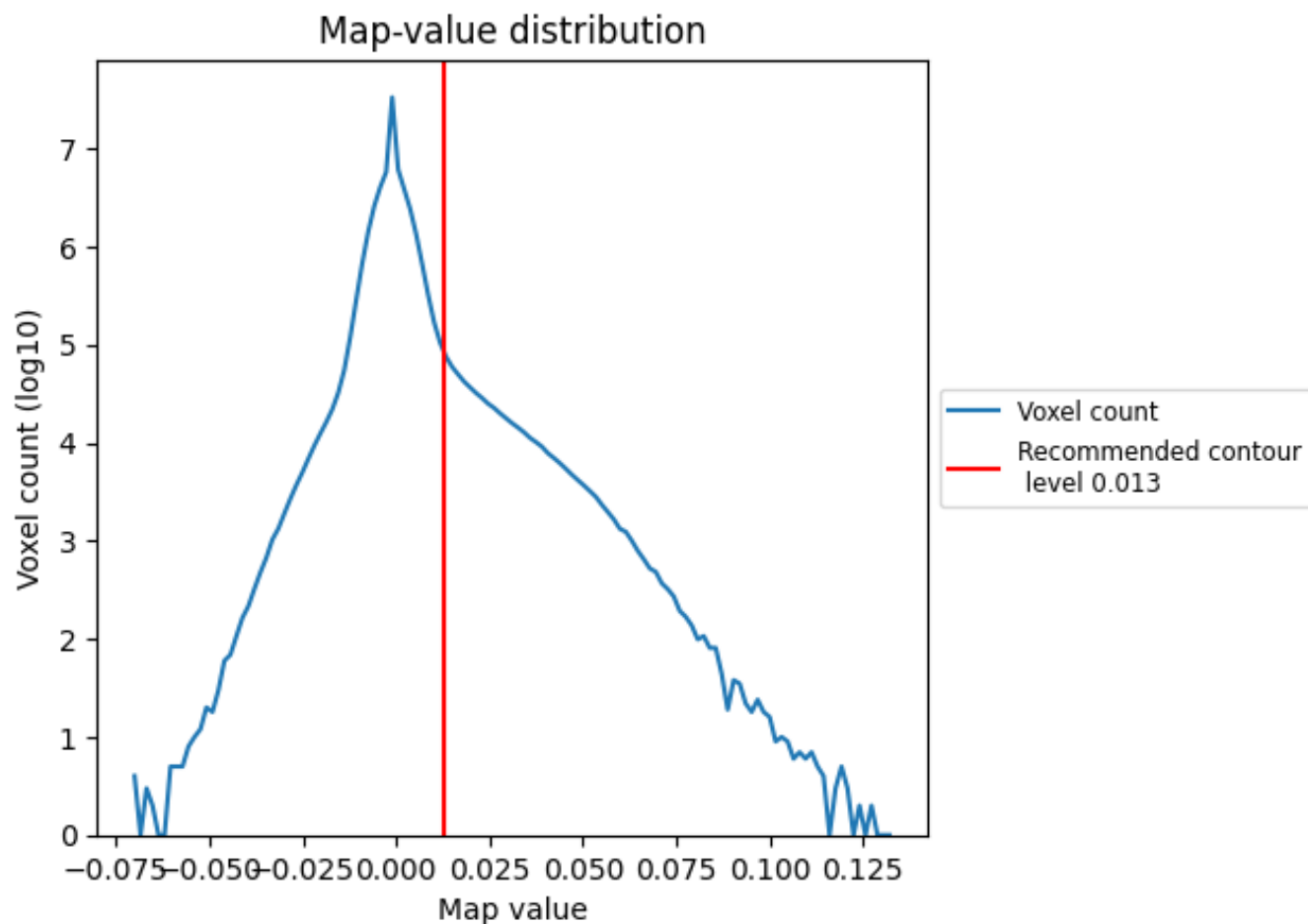
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

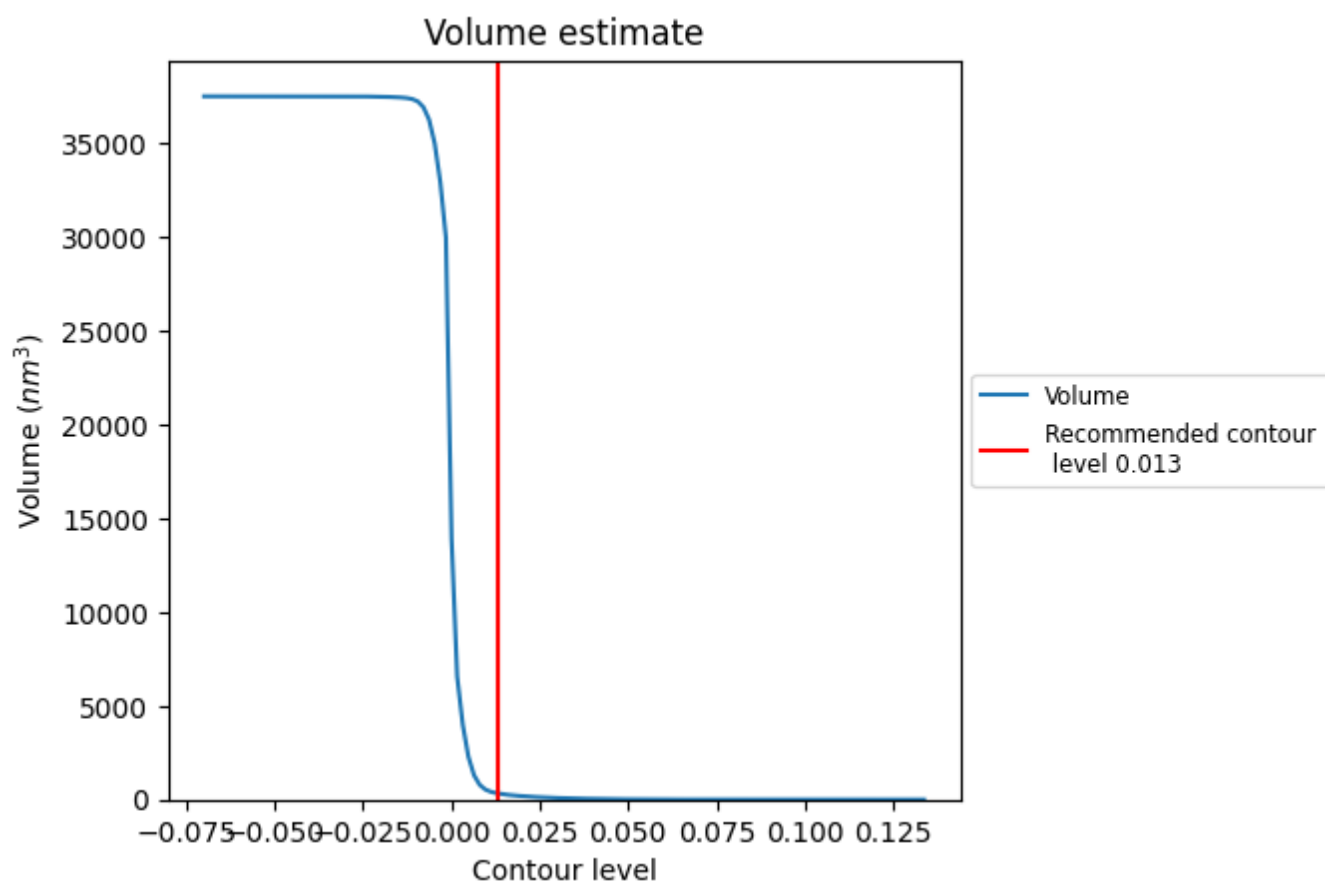
This section contains the results of statistical analysis of the map.

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.

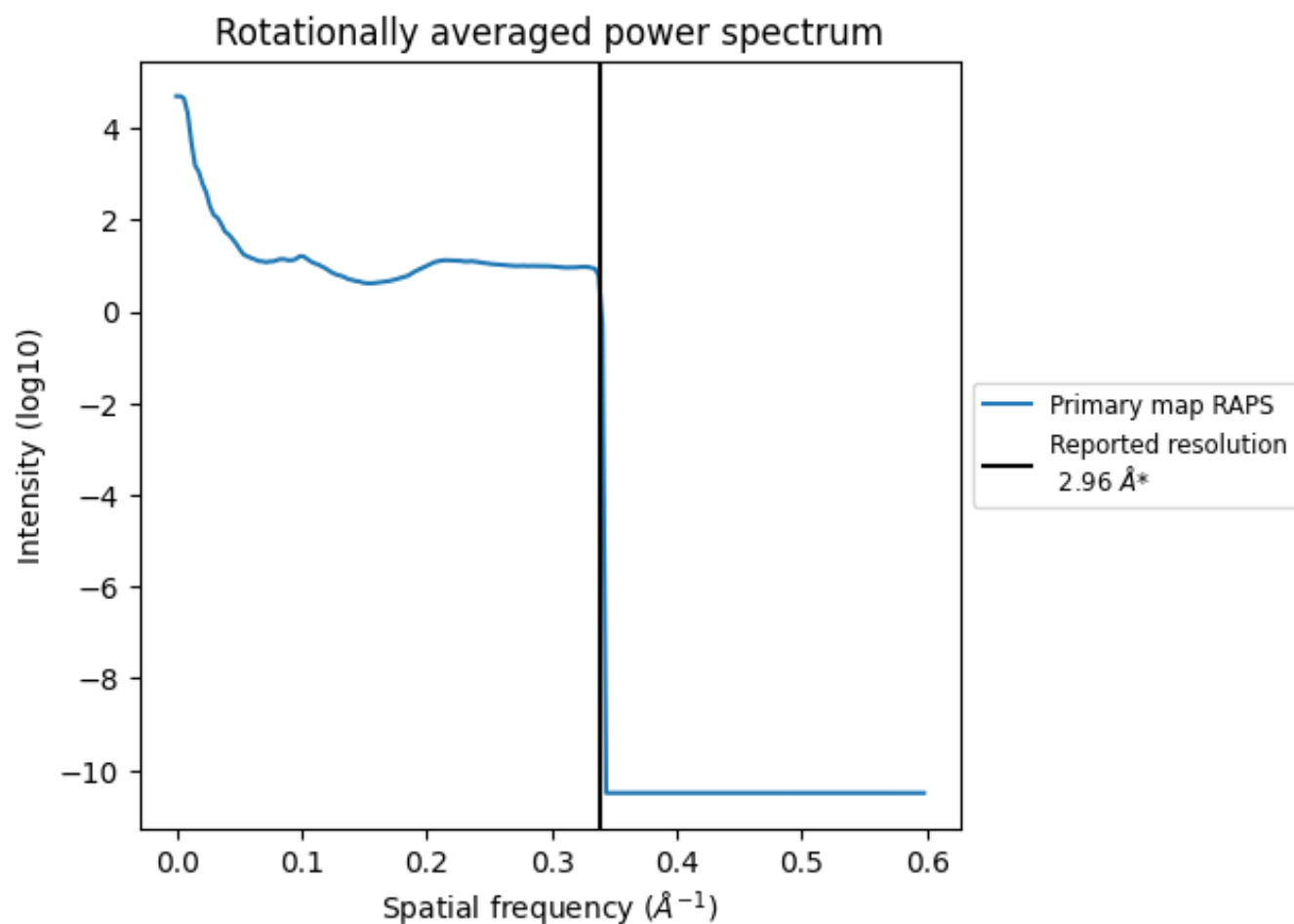
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm^3 ; this corresponds to an approximate mass of 301 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 ⓘ

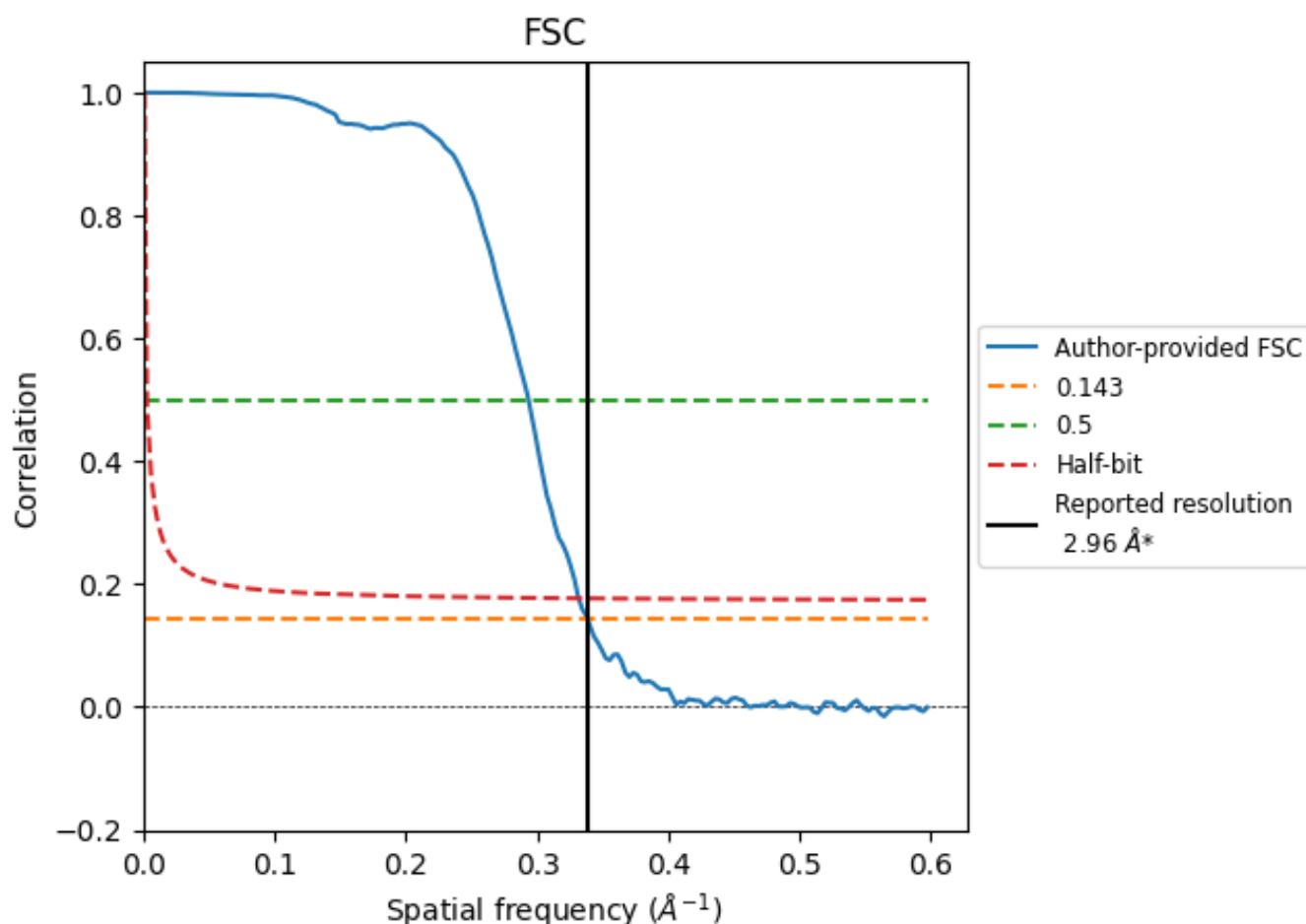


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

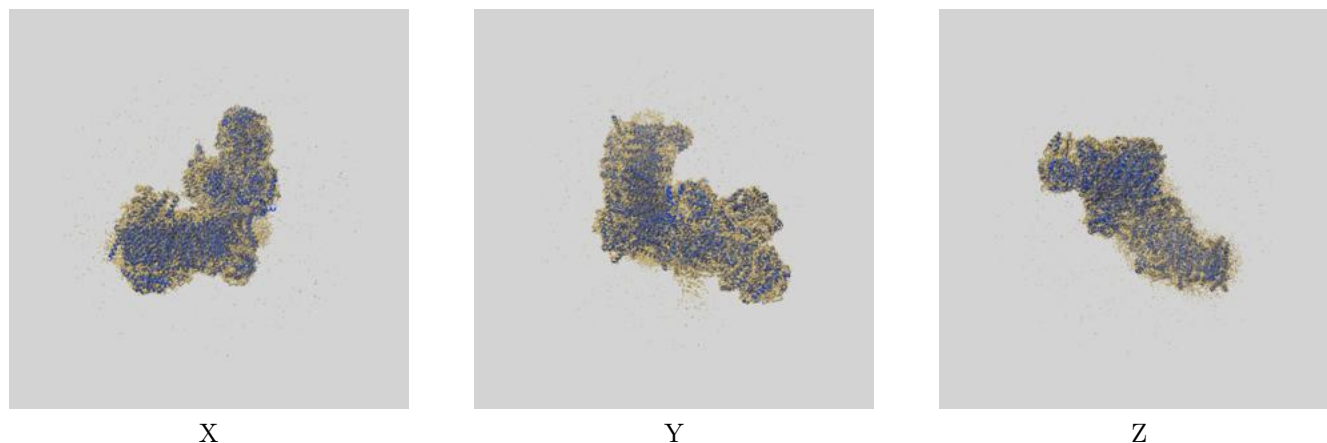
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.95	3.41	3.01
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

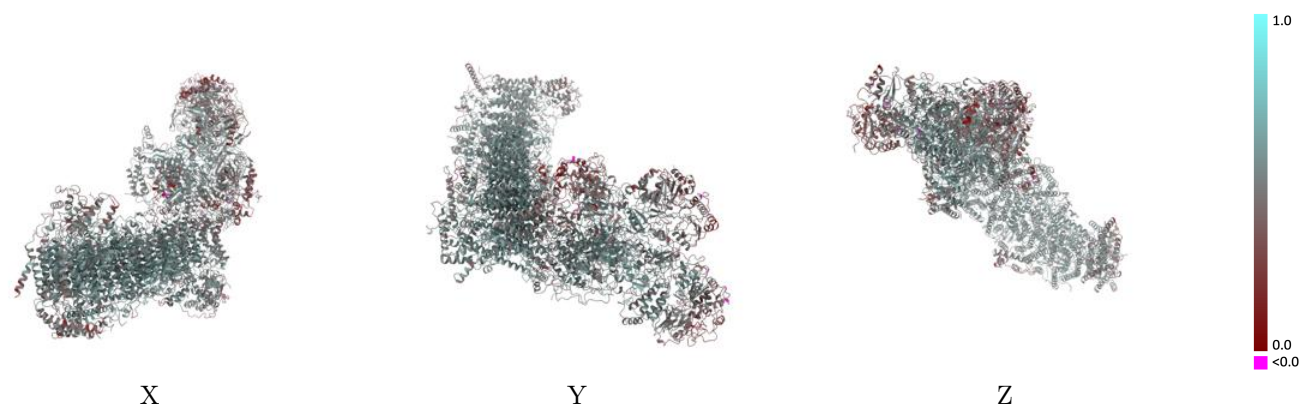
This section contains information regarding the fit between EMDB map EMD-10711 and PDB model 6Y79. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



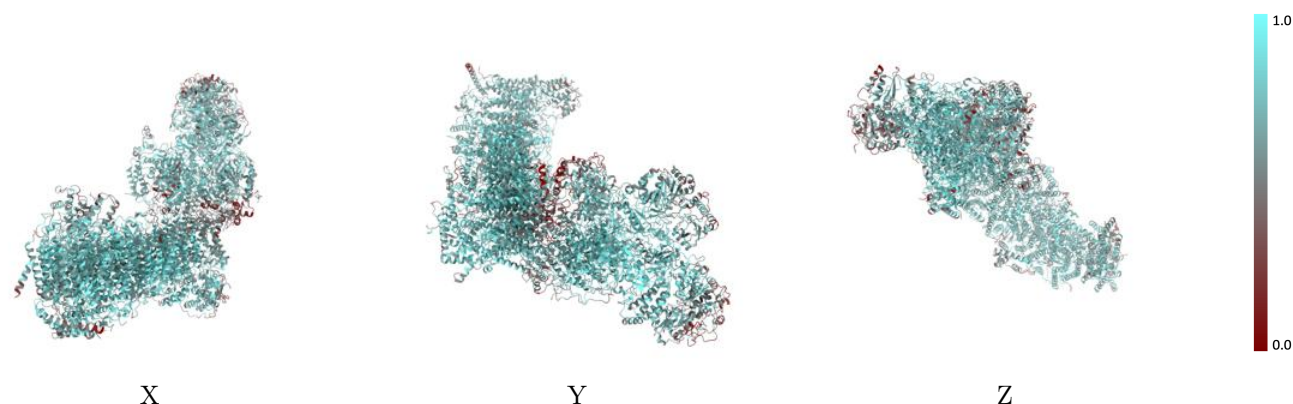
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



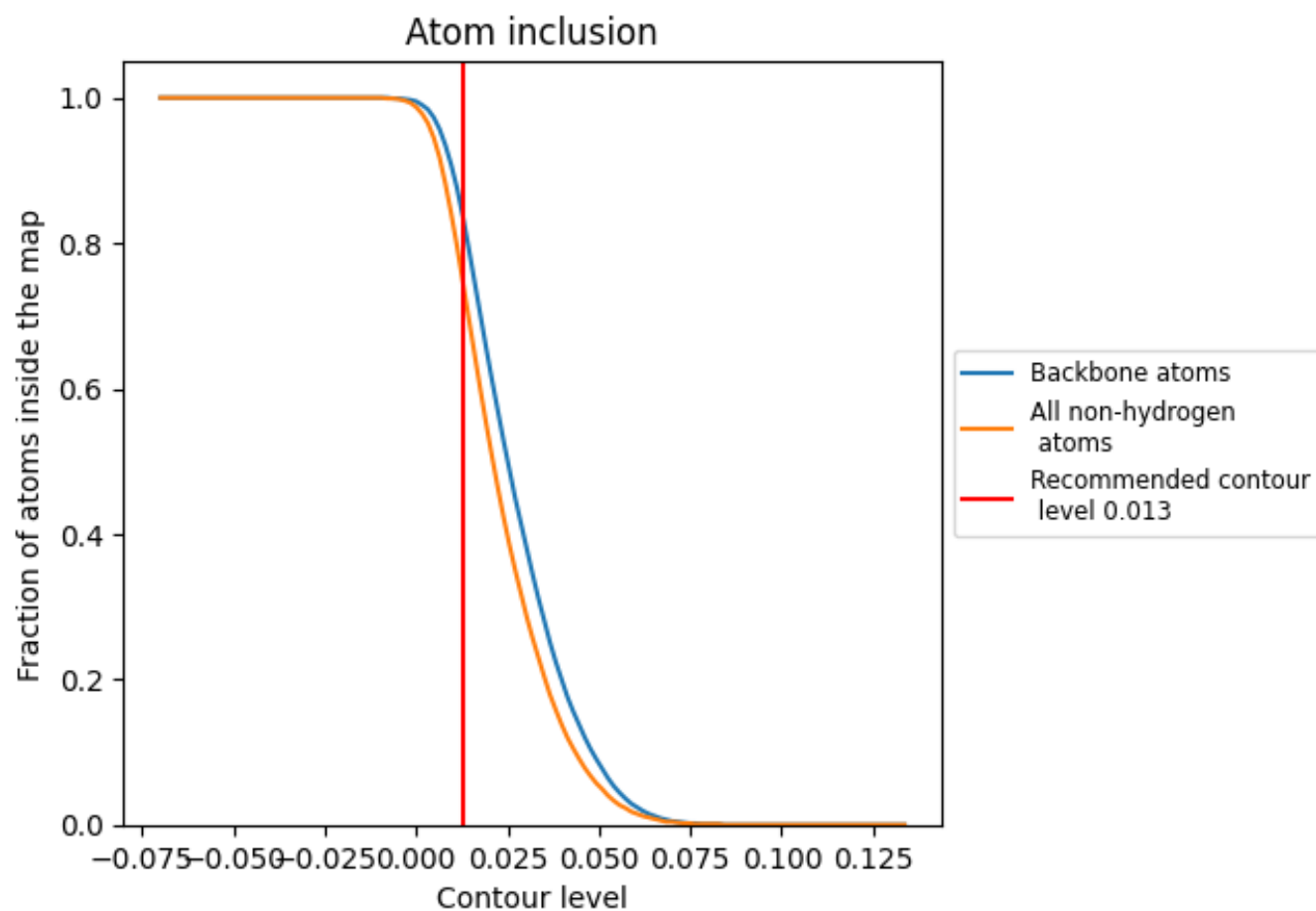
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 74% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5050
1	 0.7210	 0.5160
2	 0.8890	 0.5870
3	 0.6210	 0.4840
4	 0.8670	 0.5810
5	 0.8030	 0.5500
6	 0.7540	 0.5340
8	 0.6170	 0.4360
9	 0.6450	 0.4770
A	 0.7030	 0.4450
B	 0.6200	 0.4310
C	 0.8330	 0.5500
D	 0.7470	 0.5110
E	 0.5740	 0.4060
F	 0.7460	 0.5090
G	 0.8300	 0.5570
H	 0.5820	 0.4270
I	 0.8120	 0.5120
J	 0.7430	 0.5310
K	 0.6780	 0.4590
L	 0.8270	 0.5580
M	 0.7830	 0.5100
O	 0.4220	 0.3240
P	 0.7230	 0.4990
Q	 0.5620	 0.4290
R	 0.6780	 0.4640
S	 0.6360	 0.4490
U	 0.7360	 0.5100
W	 0.7480	 0.5200
X	 0.8200	 0.5570
Y	 0.8030	 0.5380
Z	 0.6960	 0.5090
a	 0.7230	 0.5080
b	 0.8610	 0.5740
c	 0.6370	 0.4420



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.8080	 0.5300
e	 0.5860	 0.4580
f	 0.5880	 0.4050
g	 0.7940	 0.5220
h	 0.6840	 0.5010
i	 0.7750	 0.5190
j	 0.7590	 0.5210
n	 0.7520	 0.5140