



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:47 AM UTC

PDB ID : 6RFQ / pdb_00006rfq
EMDB ID : EMD-4872
Title : Cryo-EM structure of a respiratory complex I assembly intermediate with ND-UFAF2
Authors : Parey, K.; Vonck, J.
Deposited on : 2019-04-16
Resolution : 3.30 Å(reported)

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:

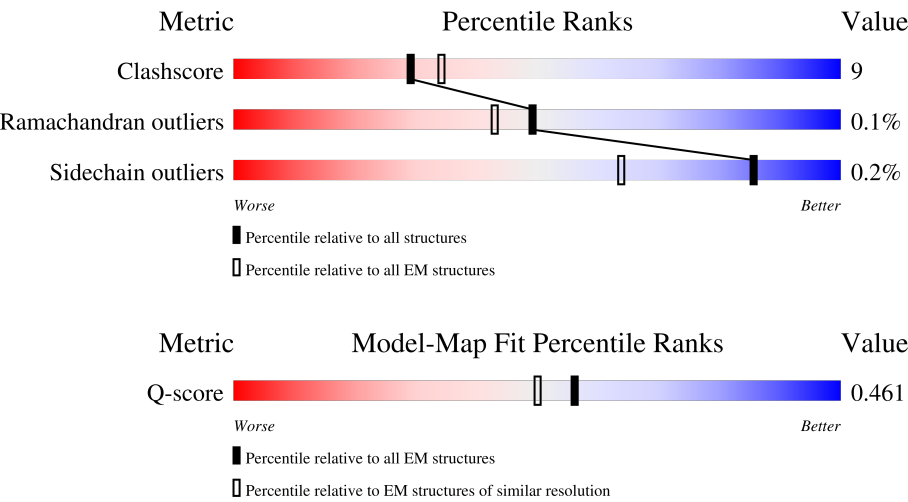
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	

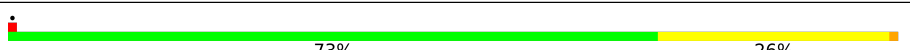
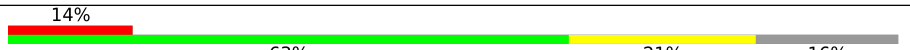
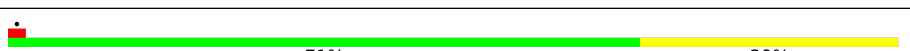
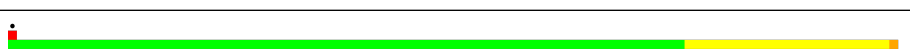
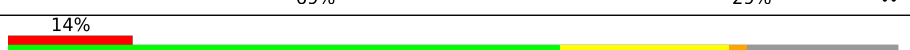
Continued on next page...

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	O	109	
14	P	124	
15	Q	132	
16	R	109	
17	S	249	
18	U	172	
19	W	123	
20	X	169	
21	Y	161	
22	Z	182	
23	a	149	
24	b	74	
25	c	60	
26	d	92	
27	e	67	
28	f	87	
29	g	78	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	i	90	
31	j	93	
32	k	237	
33	n	120	
34	1	341	
35	2	469	
36	3	128	
37	4	486	
38	5	655	
39	6	185	
40	8	99	
41	9	89	

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
48	CDL	J	204	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 62052 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	694	Total	C	N	O	S	0	0
			5274	3275	928	1042	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	441	Total	C	N	O	S	0	0
			3421	2161	601	635	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	430	Total	C	N	O	S	0	0
			3415	2170	583	640	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	263	Total	C	N	O	S	0	0
			2075	1315	362	390	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	210	Total	C	N	O	S	0	0
			1739	1119	297	319	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	215	Total	C	N	O	S	0	0
			1680	1054	283	325	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	153	Total	C	N	O	S	0	0
			1190	756	206	214	14		

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

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

- Molecule 14 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

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

- Molecule 15 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

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

- Molecule 16 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

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

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

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

- Molecule 19 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	119	Total	C	N	O	S	0	0
			961	615	176	165	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	120	Total	C	N	O	S	0	0
			922	589	158	174	1		

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

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

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

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

- Molecule 25 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

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

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

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

- Molecule 28 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	79	Total	C	N	O	S	0	0
			620	389	118	112	1		

- Molecule 29 is a protein called Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
29	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 30 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

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

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

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

- Molecule 32 is a protein called Subunit N7BML assembly factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	98	Total	C	N	O		0	0
			828	538	148	142			

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

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

- Molecule 34 is a protein called Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	318	Total	C	N	O	S	0	0
			2540	1738	369	426	7		

- Molecule 35 is a protein called Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	469	Total	C	N	O	S	0	0
			3774	2557	550	655	12		

- Molecule 36 is a protein called Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	108	Total	C	N	O	S	0	0
			869	600	127	140	2		

- Molecule 37 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	486	Total	C	N	O	S	0	0
			3855	2600	586	654	15		

- Molecule 38 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	654	Total	C	N	O	S	0	0
			5197	3479	785	905	28		

- Molecule 39 is a protein called Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	6	183	Total	C	N	O	S	0	0
			1443	979	207	249	8		

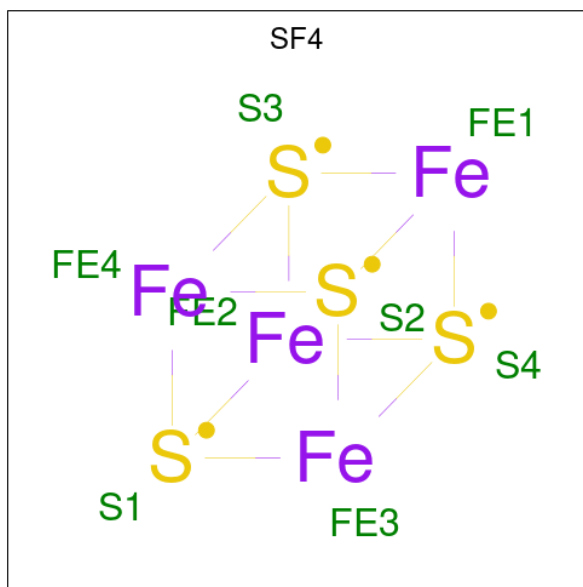
- Molecule 40 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	8	82	Total	C	N	O	S	0	0
			672	426	122	116	8		

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

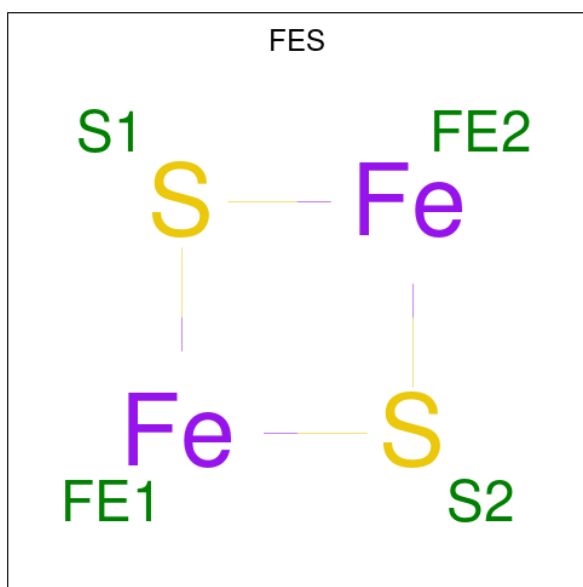
Mol	Chain	Residues	Atoms					AltConf	Trace
41	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 42 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



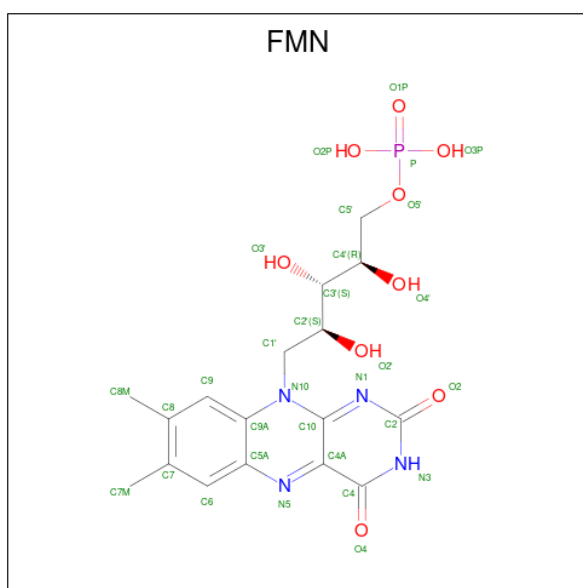
Mol	Chain	Residues	Atoms			AltConf
42	A	1	Total	Fe	S	0
			8	4	4	
42	A	1	Total	Fe	S	0
			8	4	4	
42	B	1	Total	Fe	S	0
			8	4	4	
42	I	1	Total	Fe	S	0
			8	4	4	
42	I	1	Total	Fe	S	0
			8	4	4	
42	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 43 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

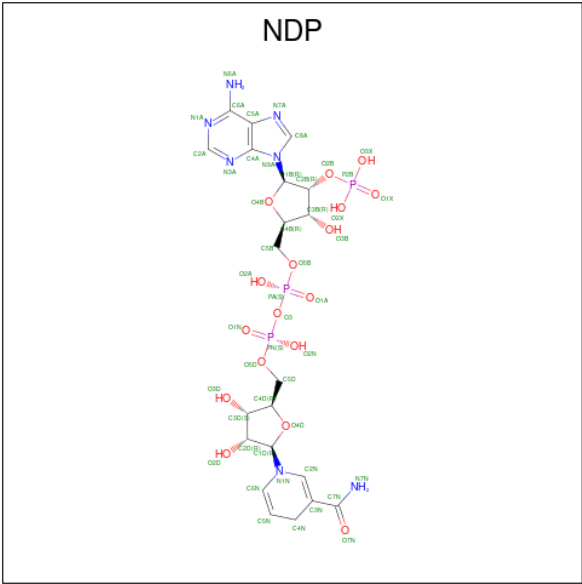
- Molecule 44 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

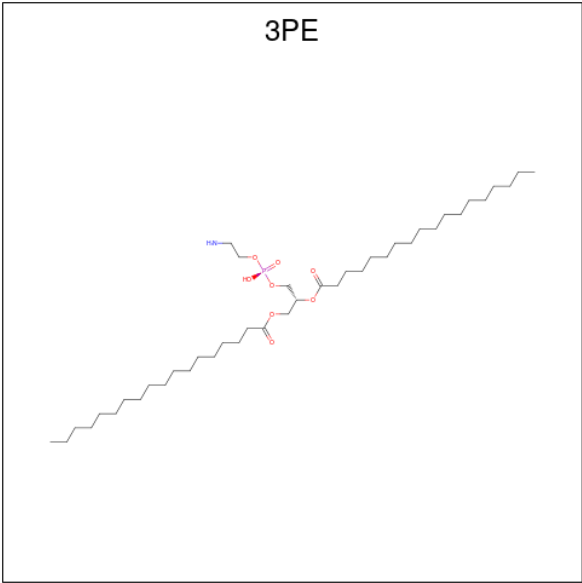
- Molecule 45 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



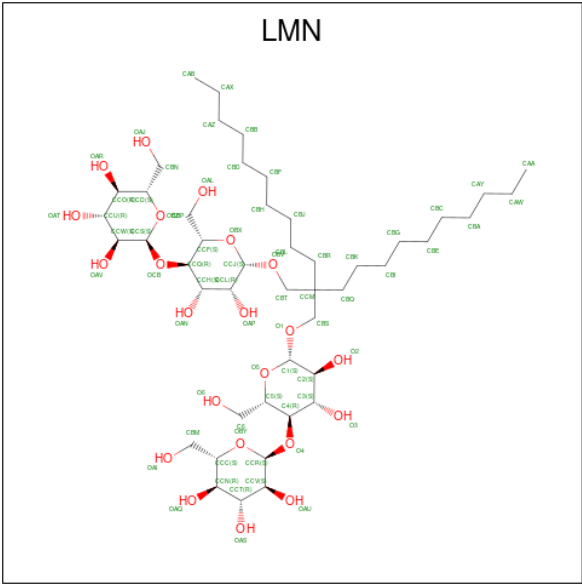
Mol	Chain	Residues	Atoms					AltConf
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	

Continued on next page...

Continued from previous page...

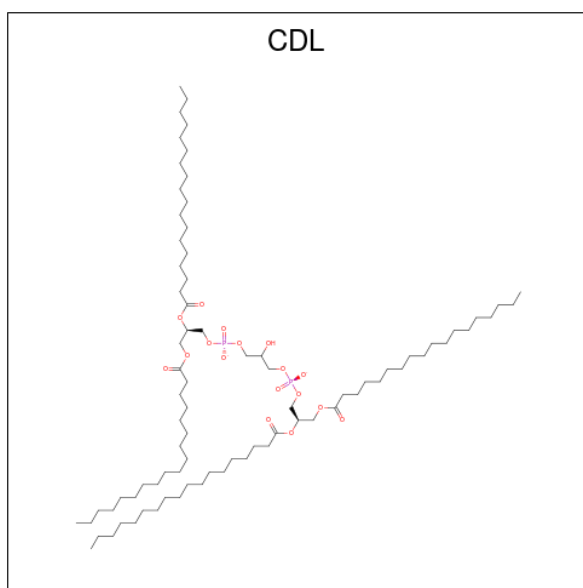
Mol	Chain	Residues	Atoms					AltConf
46	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	4	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	5	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 47 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



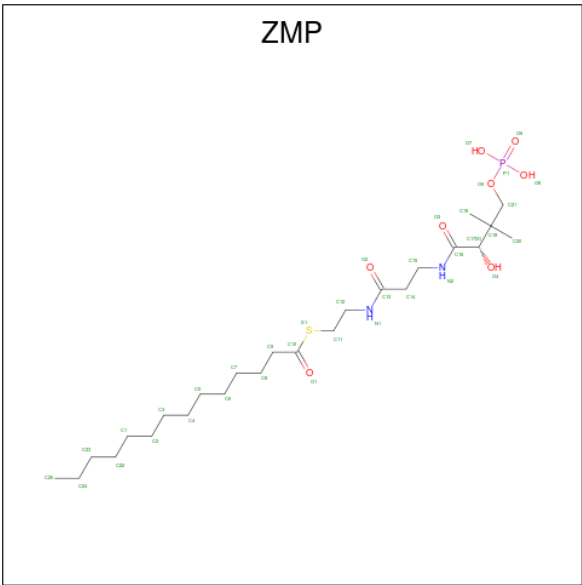
Mol	Chain	Residues	Atoms			AltConf
47	J	1	Total	C	O	0
			69	47	22	
47	j	1	Total	C	O	0
			65	43	22	

- Molecule 48 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



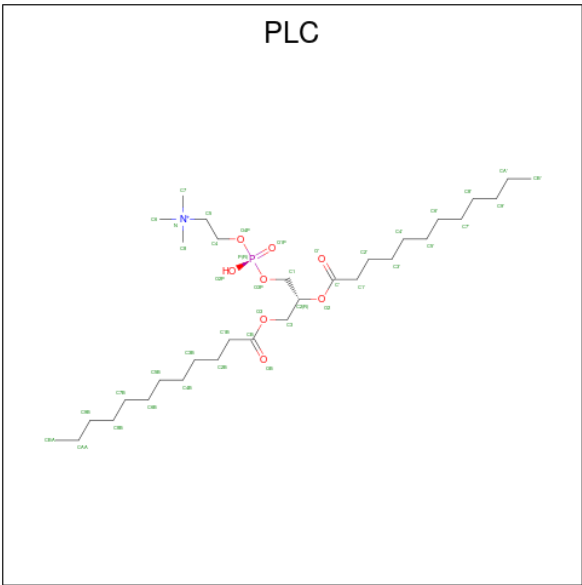
Mol	Chain	Residues	Atoms				AltConf
48	J	1	Total	C	O	P	0
			78	59	17	2	
48	X	1	Total	C	O	P	0
			82	63	17	2	
48	g	1	Total	C	O	P	0
			83	64	17	2	
48	4	1	Total	C	O	P	0
			92	73	17	2	

- Molecule 49 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



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

- Molecule 50 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



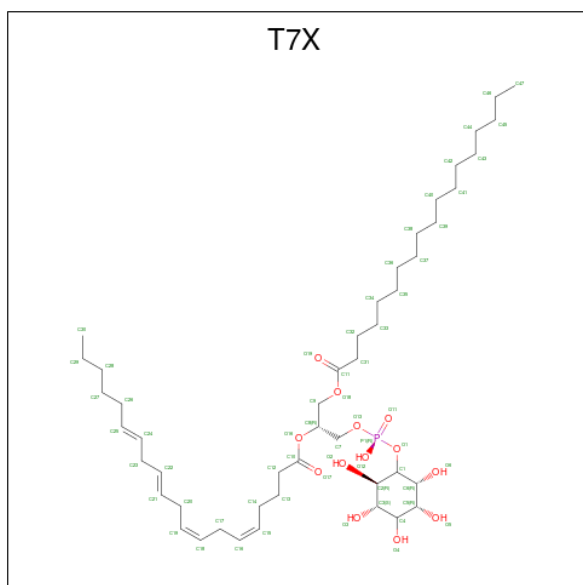
Mol	Chain	Residues	Atoms					AltConf
50	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
50	W	1	Total	C	N	O	P	0
			42	32	1	8	1	

Continued on next page...

Continued from previous page...

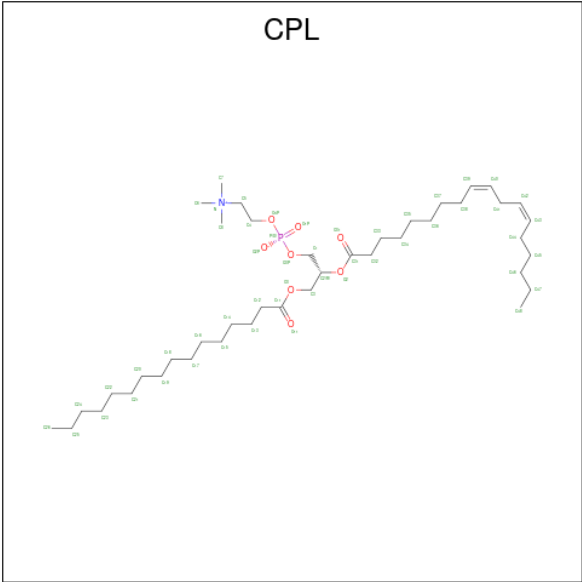
Mol	Chain	Residues	Atoms					AltConf
50	n	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

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



Mol	Chain	Residues	Atoms					AltConf
51	2	1	Total	C	O	P		0
			48	34	13	1		
51	2	1	Total	C	O	P		0
			52	38	13	1		
51	4	1	Total	C	O	P		0
			43	29	13	1		

- Molecule 52 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: $C_{42}H_{80}NO_8P$).

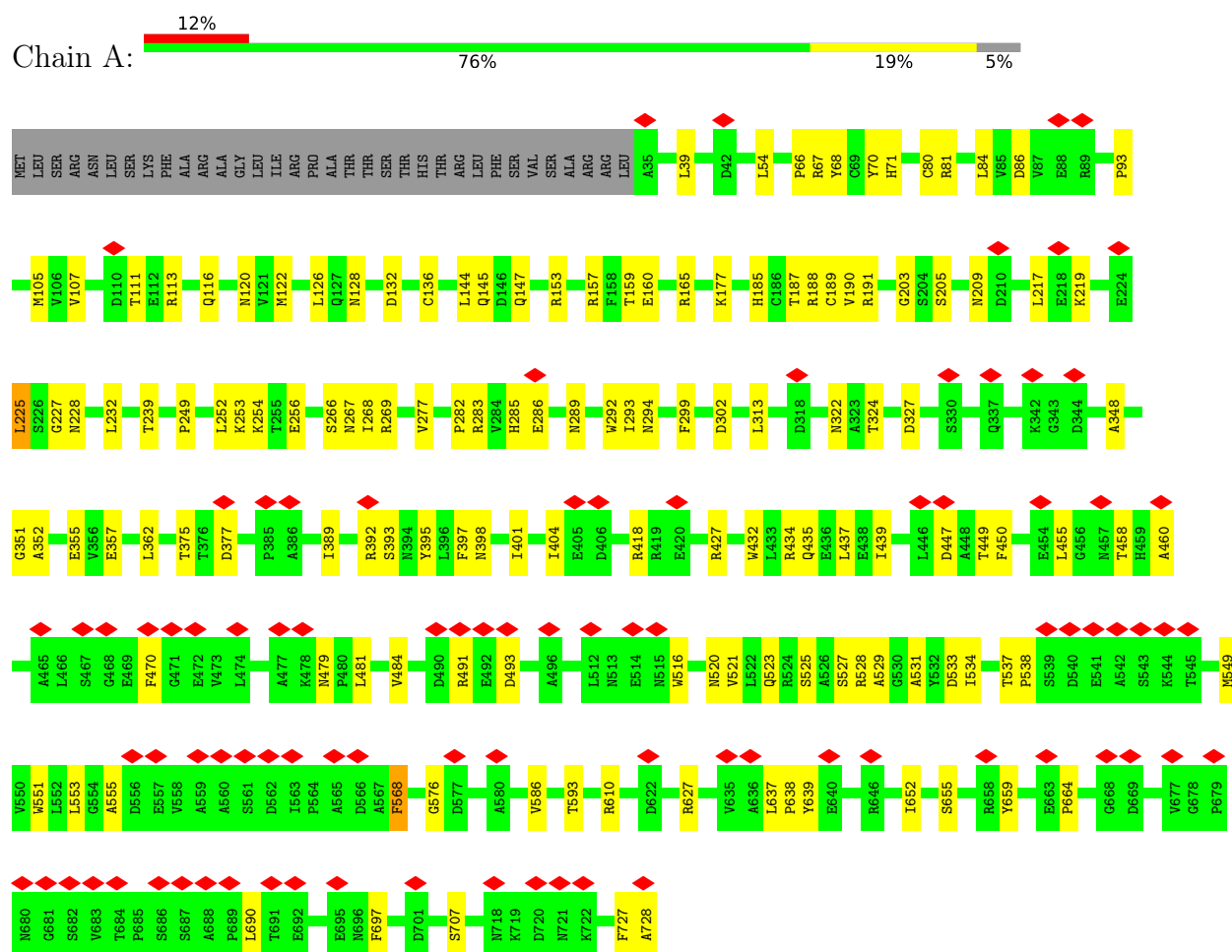


Mol	Chain	Residues	Atoms					AltConf
52	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

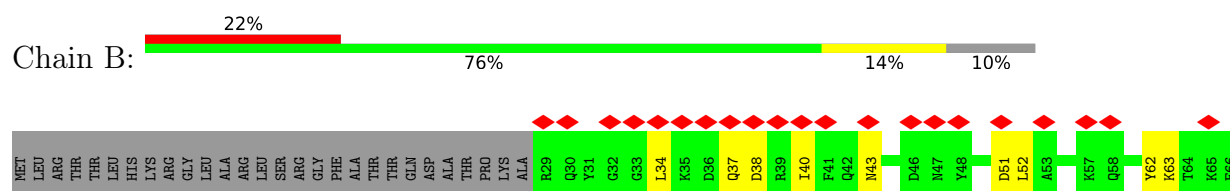
3 Residue-property plots

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.

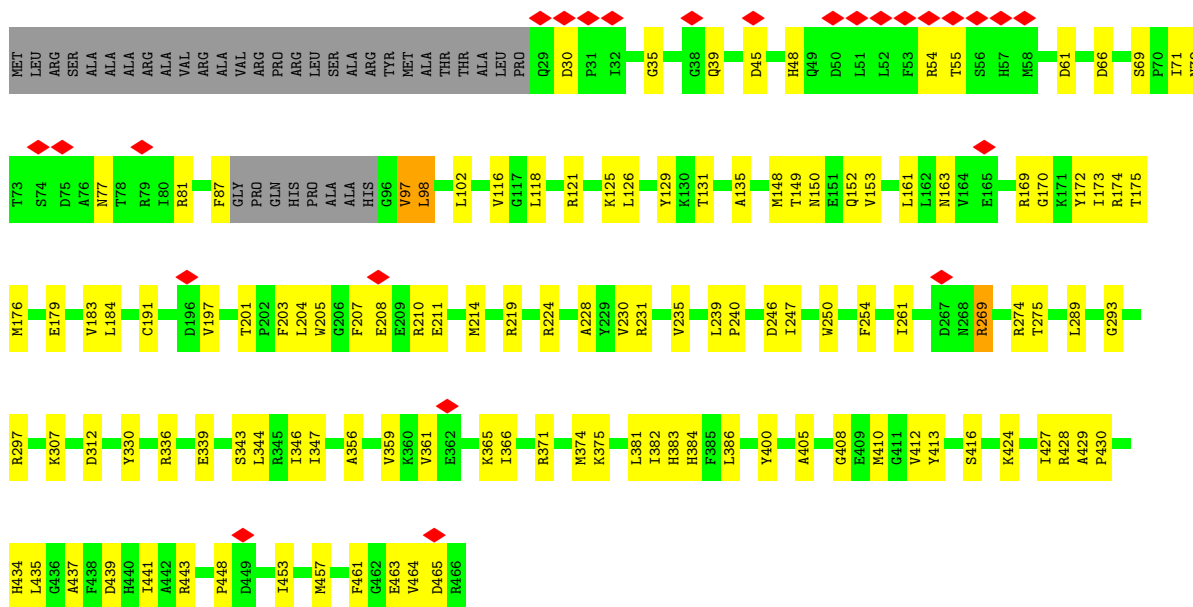
- Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)



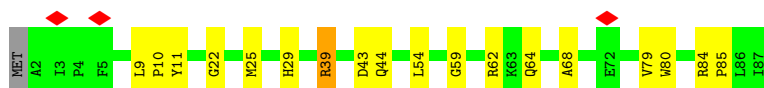
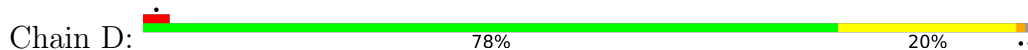
- Molecule 2: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)



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

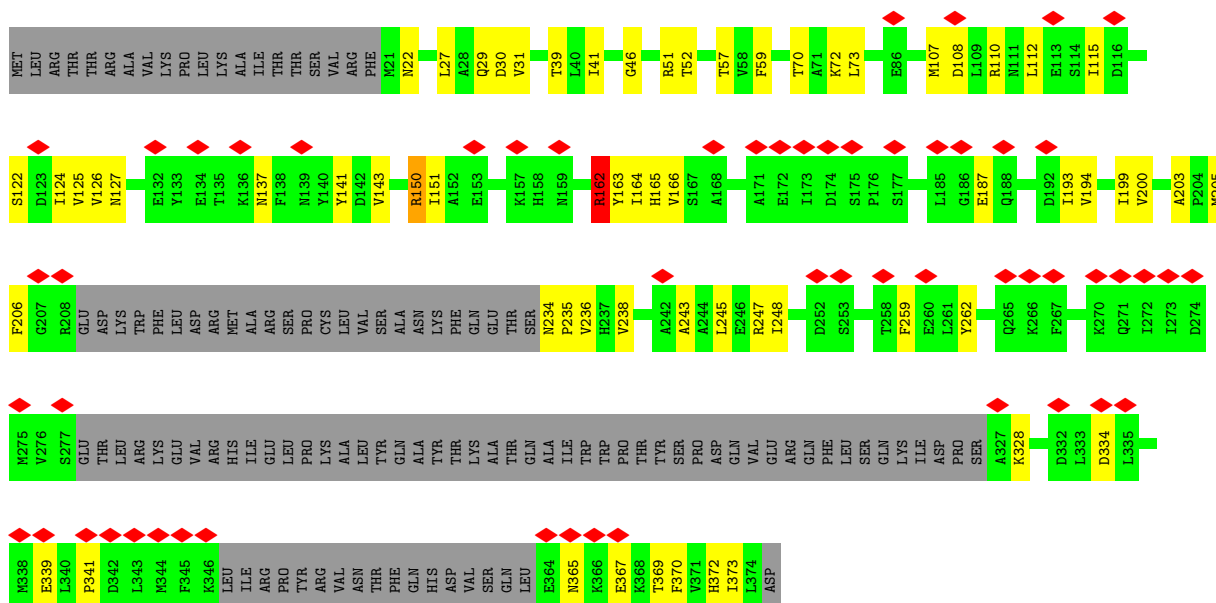


- Molecule 4: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

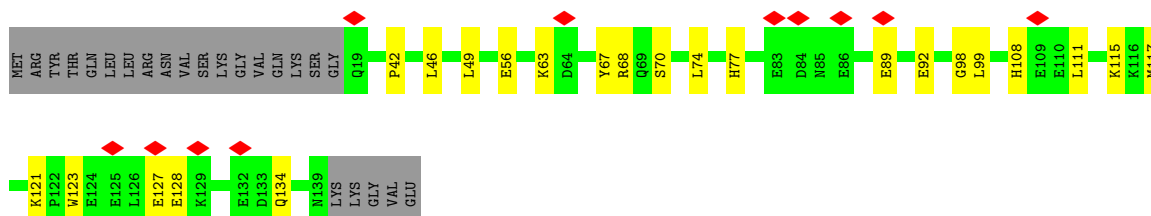


- Molecule 5: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

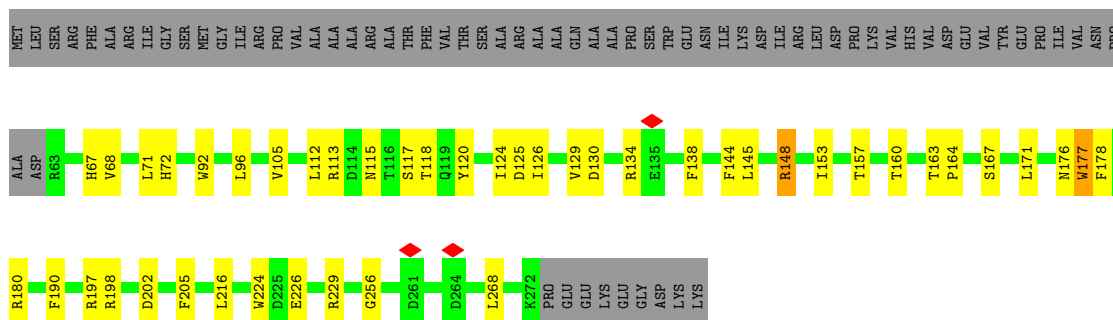




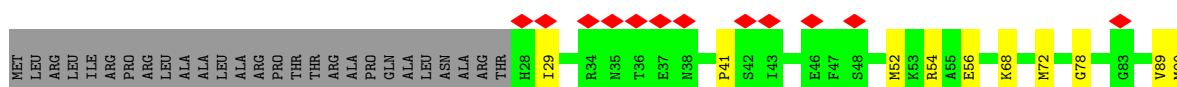
- Molecule 6: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)

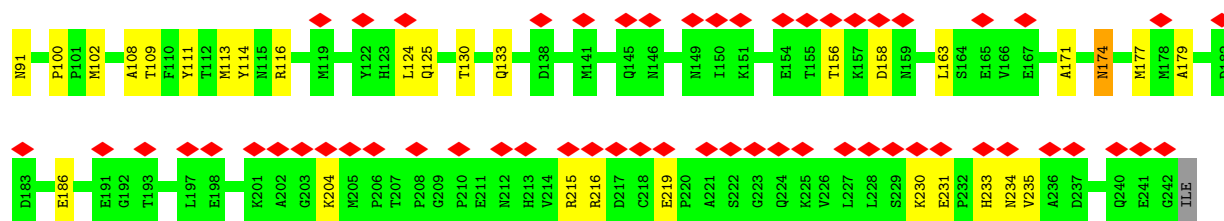


- Molecule 7: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)

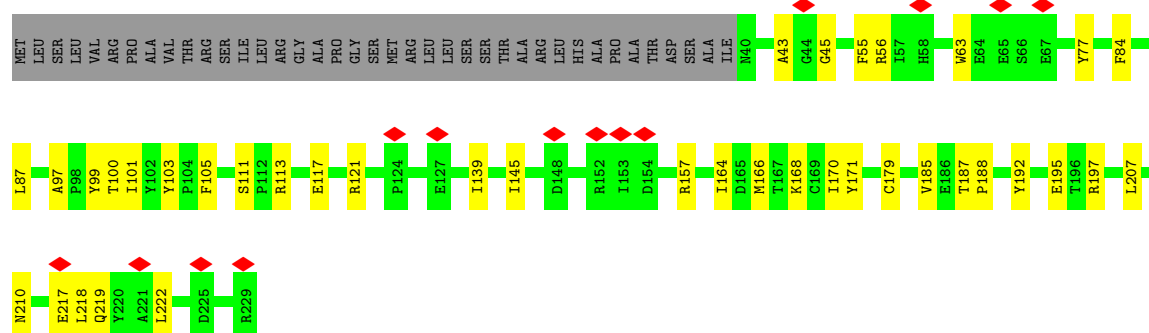


- Molecule 8: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

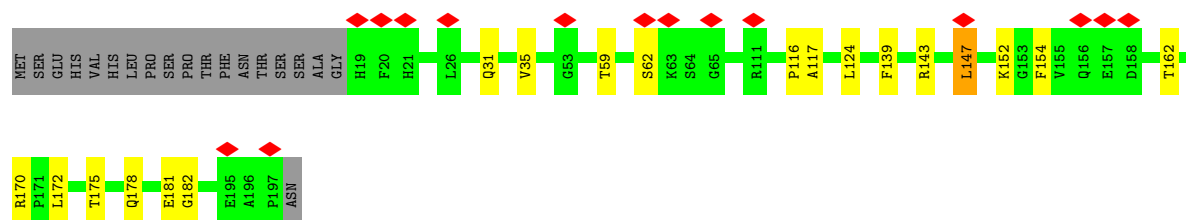
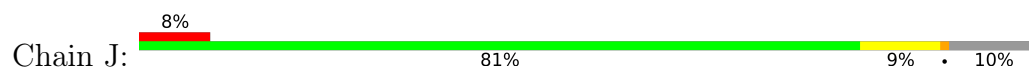




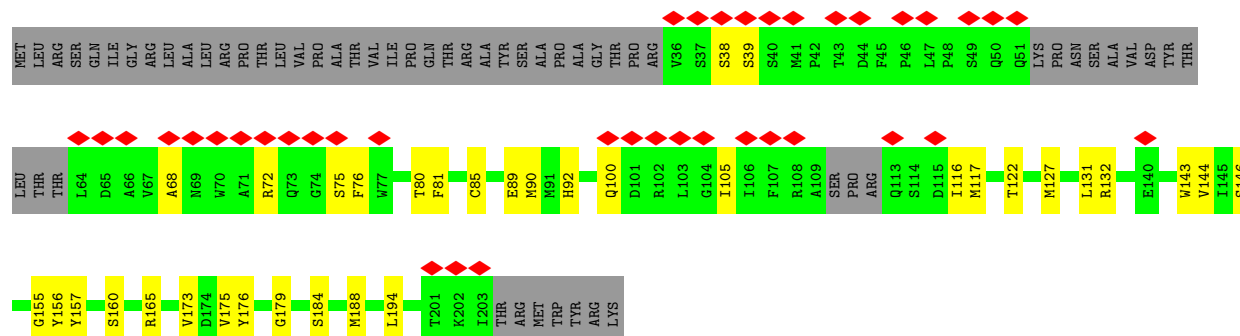
- Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)



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



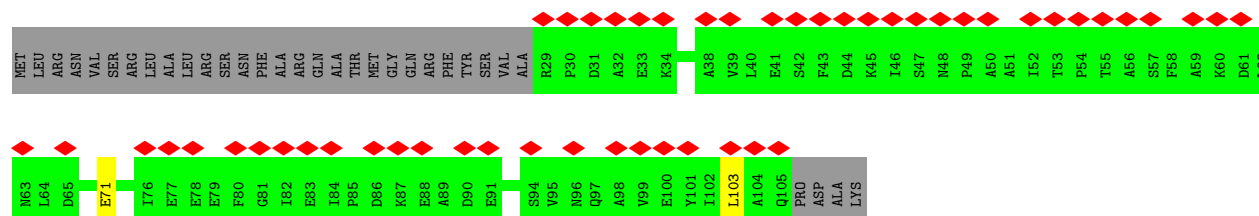
- Molecule 11: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)



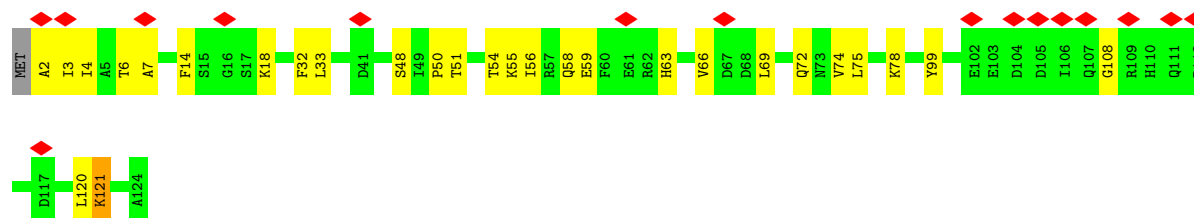
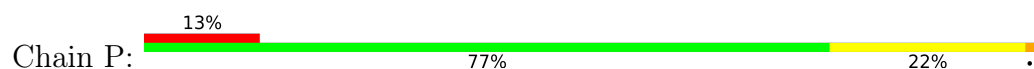
- Molecule 12: Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I)



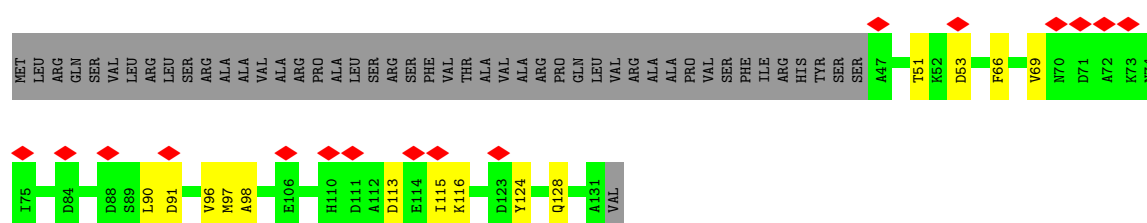
- Molecule 13: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)



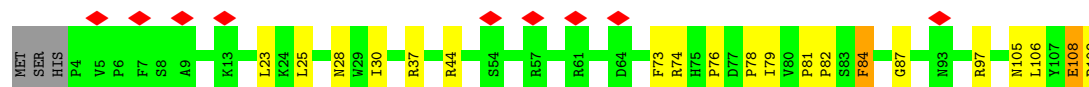
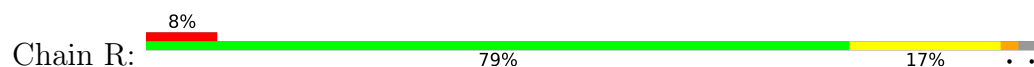
- Molecule 14: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



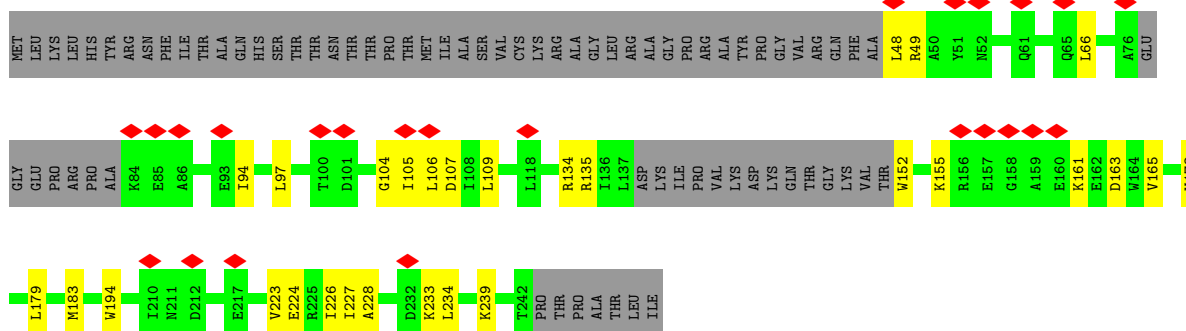
- Molecule 15: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)



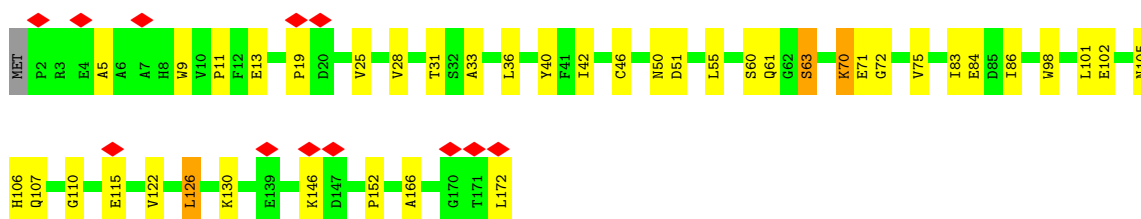
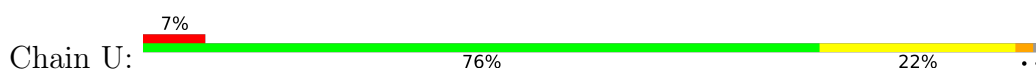
- Molecule 16: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)



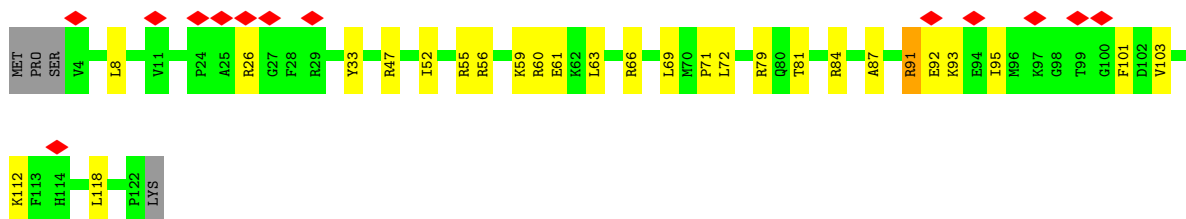
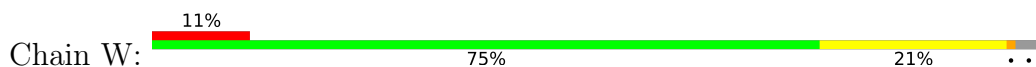
- Molecule 17: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)



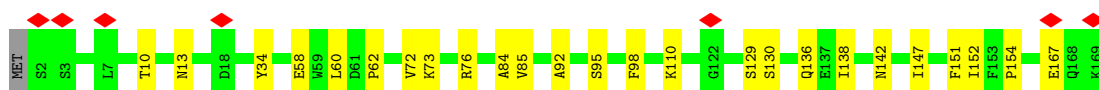
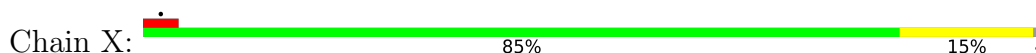
• Molecule 18: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



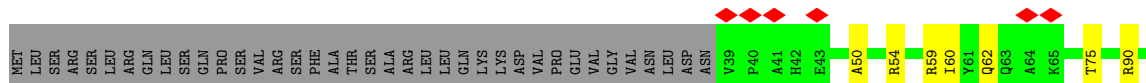
• Molecule 19: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

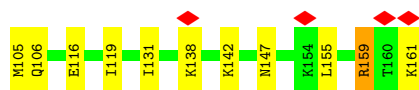


• Molecule 20: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

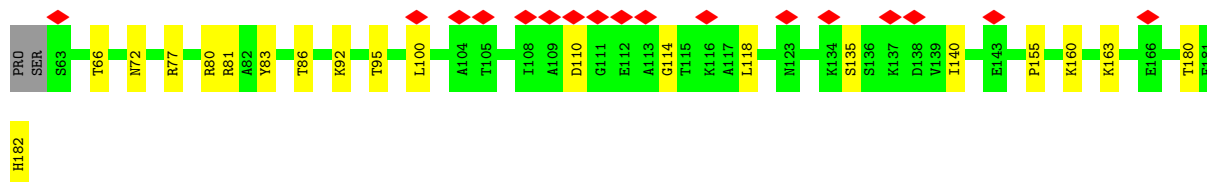
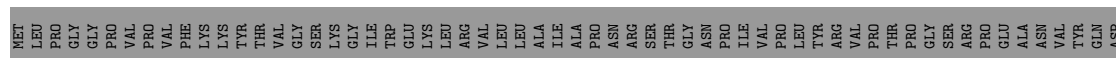


• Molecule 21: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)

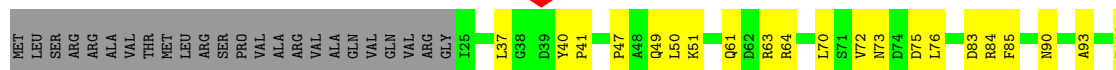




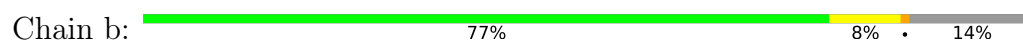
- Molecule 22: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)



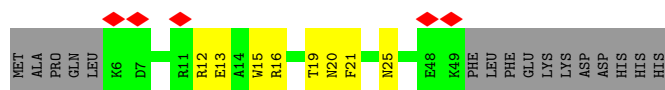
- Molecule 23: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



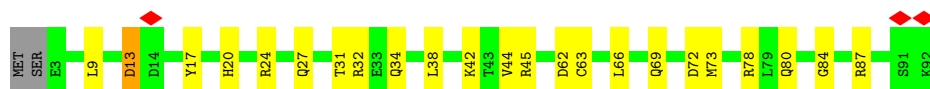
- Molecule 24: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 25: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)

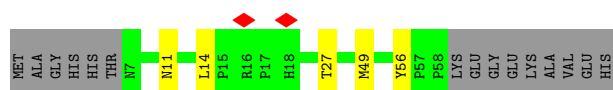


- Molecule 26: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



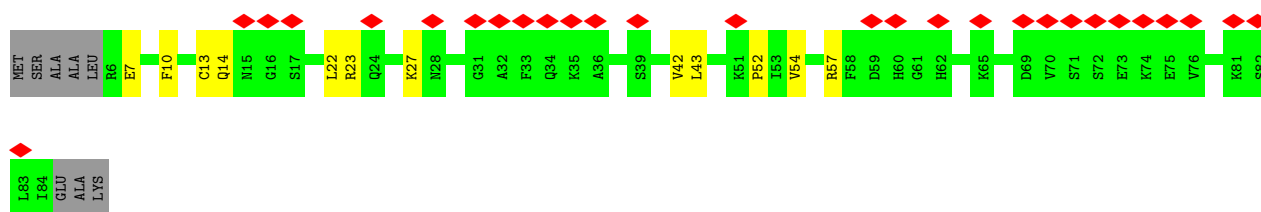
- Molecule 27: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain e:  70% 7% 22%



- Molecule 28: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain f:  32% 77% 14% 9%



- Molecule 29: Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain g:  83% 14%



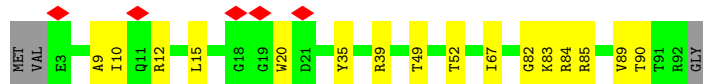
- Molecule 30: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain i:  77% 16% 8%



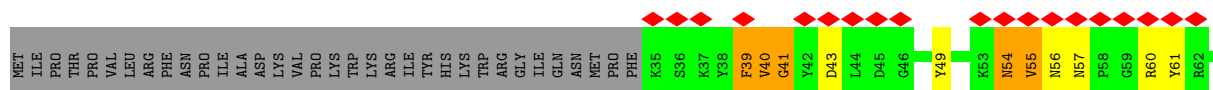
- Molecule 31: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

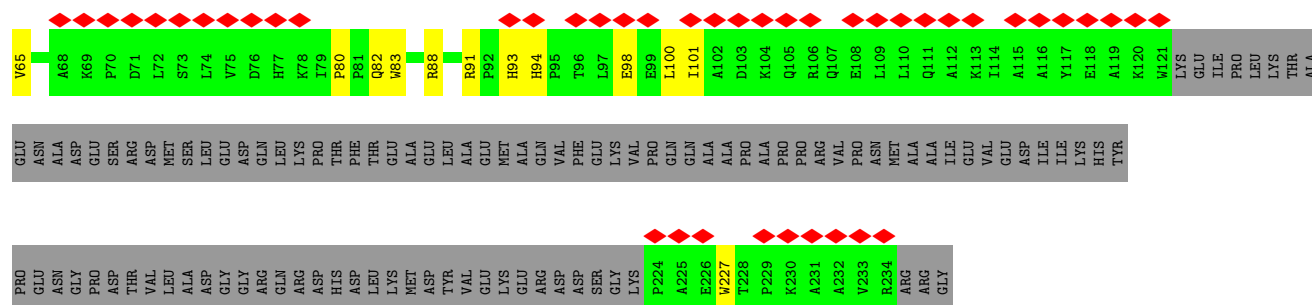
Chain j:  5% 80% 17%



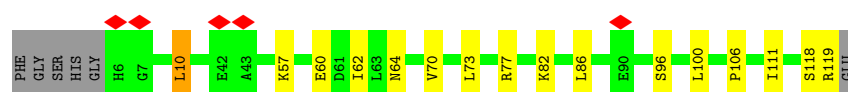
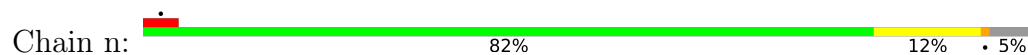
- Molecule 32: Subunit N7BML assembly factor

Chain k:  27% 32% 8% 59%

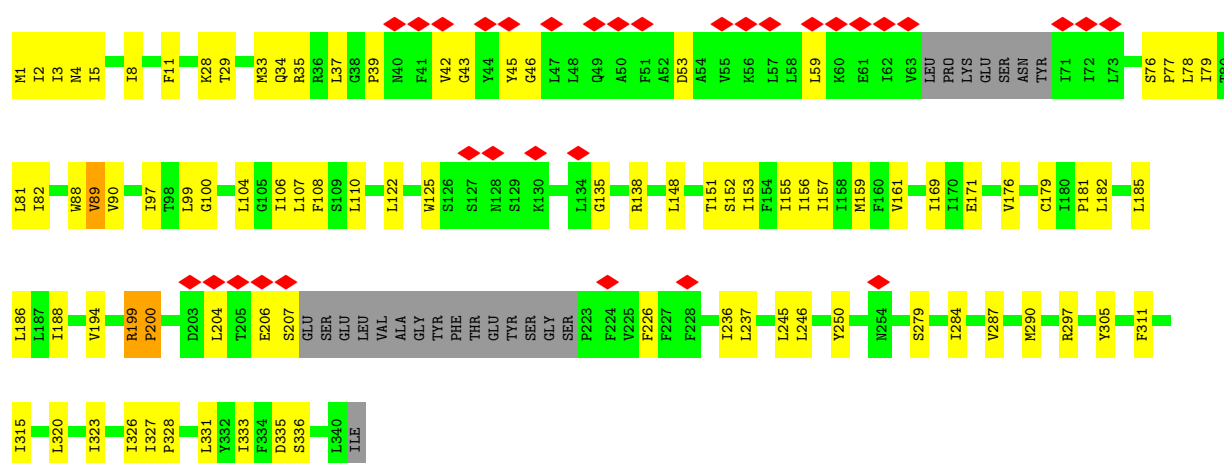




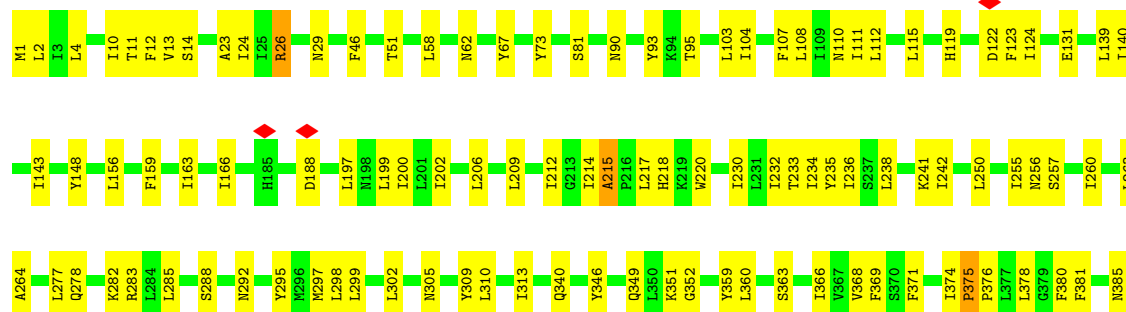
- Molecule 33: Subunit NUM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 34: Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I)

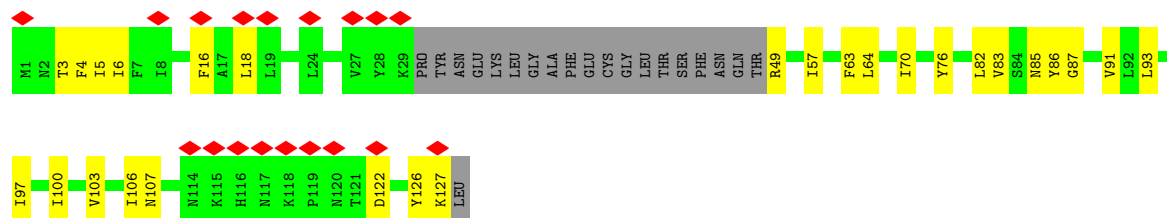


- Molecule 35: Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I)

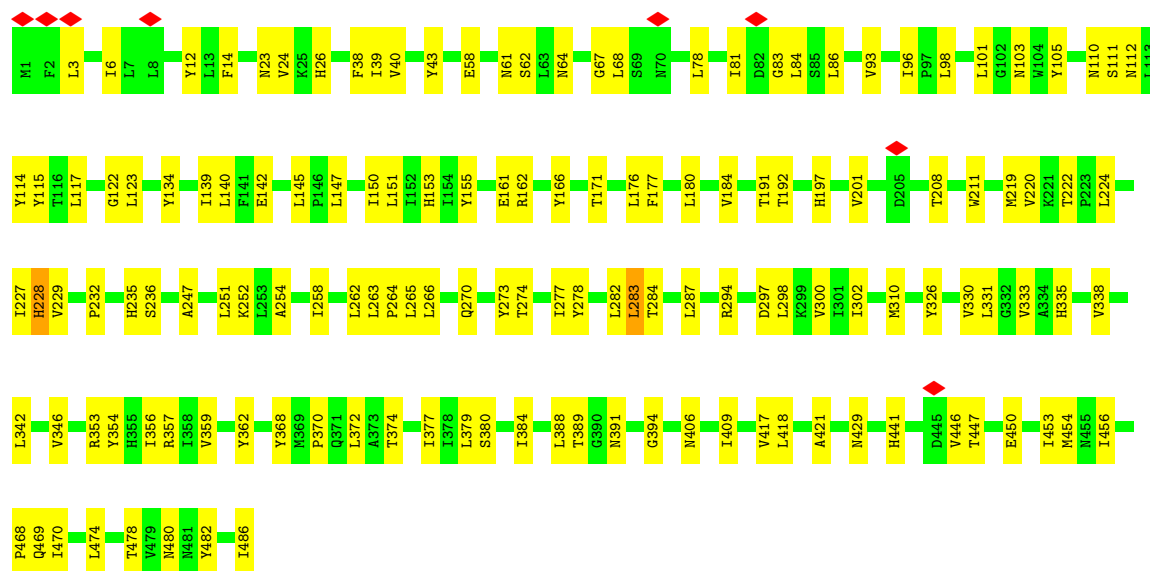




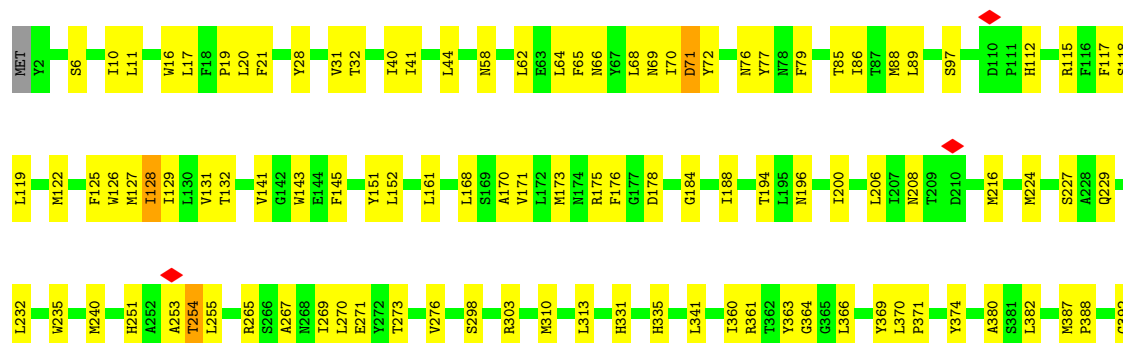
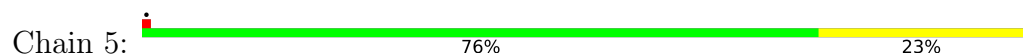
- Molecule 36: Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I)

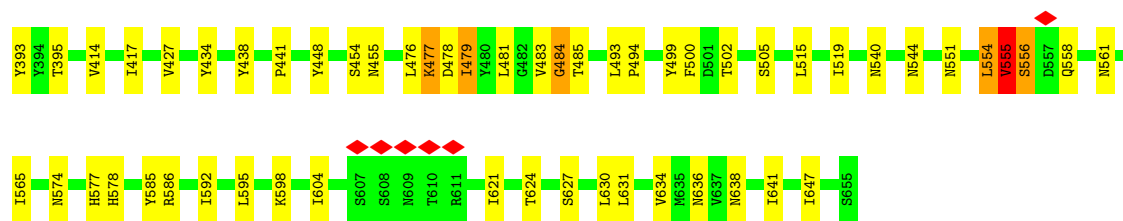


- Molecule 37: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)

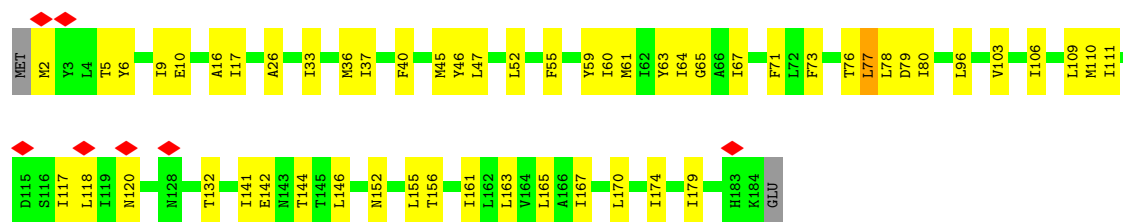


- Molecule 38: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

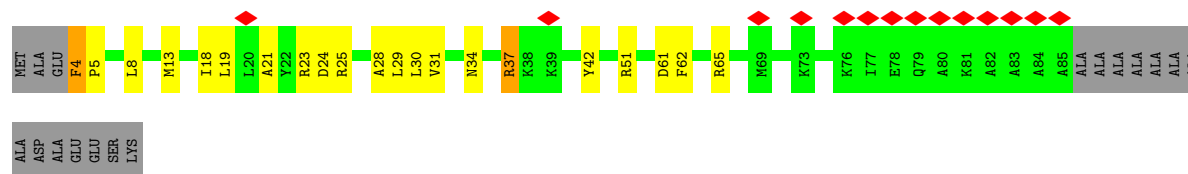




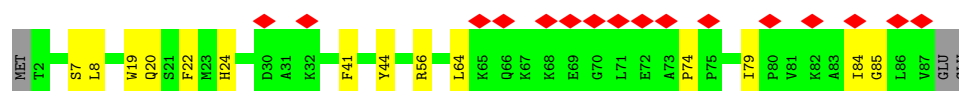
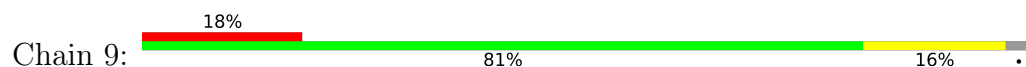
- Molecule 39: Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 40: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 41: 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	112418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	46425	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.202	Depositor
Minimum map value	-0.072	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	491.112, 491.112, 491.112	wwPDB
Map dimensions	456, 456, 456	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.44	0/5368	0.69	3/7285 (0.0%)
2	B	0.54	4/3496 (0.1%)	0.72	5/4717 (0.1%)
3	C	0.56	0/3492	0.81	2/4729 (0.0%)
4	D	0.50	0/697	0.70	1/940 (0.1%)
5	E	0.43	0/2113	0.71	2/2854 (0.1%)
6	F	0.38	0/1011	0.77	0/1371
7	G	0.55	0/1793	0.80	1/2441 (0.0%)
8	H	0.38	1/1717 (0.1%)	0.72	1/2332 (0.0%)
9	I	0.53	0/1557	0.77	1/2110 (0.0%)
10	J	0.45	0/1362	0.73	2/1855 (0.1%)
11	K	0.55	0/1220	0.80	0/1656
12	L	0.57	0/700	0.81	0/947
13	O	0.25	0/598	0.56	0/813
14	P	0.43	0/1061	0.73	2/1427 (0.1%)
15	Q	0.33	0/654	0.61	0/890
16	R	0.46	0/909	0.76	0/1229
17	S	0.41	0/1454	0.66	0/1960
18	U	0.46	0/1374	0.80	2/1856 (0.1%)
19	W	0.44	0/984	0.68	0/1327
20	X	0.48	0/1344	0.67	0/1822
21	Y	0.47	1/1051 (0.1%)	0.64	1/1420 (0.1%)
22	Z	0.40	0/947	0.65	0/1291
23	a	0.50	0/1064	0.76	0/1439
24	b	0.44	0/503	0.65	1/679 (0.1%)
25	c	0.39	0/364	0.55	0/491
26	d	0.57	0/776	0.75	0/1043
27	e	0.36	0/456	0.65	0/619
28	f	0.32	0/630	0.67	0/844
29	g	0.39	0/643	0.64	1/880 (0.1%)
30	i	0.48	0/666	0.65	0/907
31	j	0.43	0/745	0.66	0/1006
32	k	0.42	0/856	0.82	2/1163 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	n	0.48	0/943	0.71	2/1279 (0.2%)
34	1	0.60	0/2608	0.88	1/3558 (0.0%)
35	2	0.71	1/3854 (0.0%)	0.89	4/5252 (0.1%)
36	3	0.51	0/888	0.86	0/1210
37	4	0.66	0/3949	0.84	0/5392
38	5	0.62	2/5327 (0.0%)	0.86	8/7273 (0.1%)
39	6	0.55	0/1468	0.83	1/2003 (0.0%)
40	8	0.50	1/686 (0.1%)	0.77	2/918 (0.2%)
41	9	0.47	0/684	0.66	0/918
All	All	0.52	10/62012 (0.0%)	0.77	45/84146 (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	1
3	C	0	2
5	E	0	1
7	G	0	1
8	H	0	5
16	R	0	2
17	S	0	1
18	U	0	3
19	W	0	1
22	Z	0	1
26	d	0	1
31	j	0	1
32	k	0	2
34	1	0	2
37	4	0	3
38	5	0	5
40	8	0	1
All	All	0	33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	113	ARG	NE-CZ	16.13	1.50	1.33
2	B	113	ARG	CZ-NH2	-9.30	1.21	1.33
2	B	113	ARG	CD-NE	-8.35	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	100	PRO	CA-C	-6.94	1.47	1.52
2	B	113	ARG	CZ-NH1	6.52	1.41	1.32

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	ARG	NE-CZ-NH1	9.93	131.43	121.50
38	5	254	THR	N-CA-C	7.11	118.72	110.97
3	C	381	LEU	CA-CB-CG	7.10	141.14	116.30
38	5	128	ILE	CG1-CB-CG2	-7.00	89.71	110.70
5	E	162	ARG	N-CA-C	6.76	120.73	111.54

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	568	PHE	Peptide
3	C	269	ARG	Sidechain
3	C	336	ARG	Sidechain
5	E	51	ARG	Sidechain
7	G	148	ARG	Sidechain

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	5274	0	5173	99	0
2	B	3421	0	3372	44	0
3	C	3415	0	3353	111	0
4	D	681	0	671	20	0
5	E	2075	0	2064	46	0
6	F	990	0	977	15	0
7	G	1739	0	1678	38	0
8	H	1680	0	1649	28	0
9	I	1519	0	1460	40	0
10	J	1329	0	1311	27	0
11	K	1190	0	1163	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	691	0	754	26	0
13	O	591	0	585	4	0
14	P	1036	0	1018	21	0
15	Q	648	0	636	10	0
16	R	884	0	893	25	0
17	S	1430	0	1463	27	0
18	U	1345	0	1327	30	0
19	W	961	0	974	26	0
20	X	1305	0	1281	27	0
21	Y	1021	0	984	13	0
22	Z	922	0	908	17	0
23	a	1030	0	967	27	0
24	b	490	0	509	6	0
25	c	353	0	343	7	0
26	d	760	0	721	21	0
27	e	436	0	426	5	0
28	f	620	0	634	8	0
29	g	617	0	597	15	0
30	i	646	0	630	15	0
31	j	724	0	706	14	0
32	k	828	0	815	22	0
33	n	914	0	880	14	0
34	1	2540	0	2658	69	0
35	2	3774	0	4005	106	0
36	3	869	0	944	31	0
37	4	3855	0	4054	105	0
38	5	5197	0	5353	147	0
39	6	1443	0	1565	49	0
40	8	672	0	677	20	0
41	9	672	0	683	14	0
42	A	16	0	0	0	0
42	B	8	0	0	0	0
42	I	16	0	0	0	0
42	K	8	0	0	1	0
43	A	4	0	0	0	0
43	H	4	0	0	0	0
44	B	31	0	19	2	0
45	E	48	0	26	1	0
46	4	136	0	203	13	0
46	5	93	0	140	7	0
46	6	36	0	46	5	0
46	I	51	0	82	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	J	85	0	118	4	0
46	g	43	0	63	2	0
47	J	69	0	88	5	0
47	j	65	0	77	2	0
48	4	92	0	137	6	0
48	J	78	0	103	22	0
48	X	82	0	108	4	0
48	g	83	0	116	7	0
49	O	33	0	38	1	0
49	Q	33	0	38	0	0
50	5	31	0	36	1	0
50	W	83	0	123	3	0
50	n	42	0	64	1	0
51	2	100	0	0	0	0
51	4	43	0	0	1	0
52	2	52	0	80	4	0
All	All	62052	0	62566	1160	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 9.

The worst 5 of 1160 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)
38:5:79:PHE:HE1	38:5:129:ILE:HG23	1.19	1.07
3:C:172:TYR:O	3:C:175:THR:HG22	1.56	1.05
1:A:375:THR:HG22	1:A:538:PRO:HG3	1.39	1.04
35:2:202:ILE:HG22	35:2:206:LEU:HD13	1.39	1.04
10:J:117:ALA:HA	48:J:204:CDL:HA4	1.45	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	692/728 (95%)	642 (93%)	50 (7%)	0	100	100
2	B	439/488 (90%)	409 (93%)	30 (7%)	0	100	100
3	C	426/466 (91%)	396 (93%)	30 (7%)	0	100	100
4	D	84/87 (97%)	79 (94%)	5 (6%)	0	100	100
5	E	255/375 (68%)	241 (94%)	14 (6%)	0	100	100
6	F	119/144 (83%)	109 (92%)	10 (8%)	0	100	100
7	G	208/281 (74%)	195 (94%)	13 (6%)	0	100	100
8	H	213/243 (88%)	191 (90%)	22 (10%)	0	100	100
9	I	188/229 (82%)	176 (94%)	12 (6%)	0	100	100
10	J	177/198 (89%)	164 (93%)	13 (7%)	0	100	100
11	K	147/210 (70%)	136 (92%)	11 (8%)	0	100	100
12	L	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
13	O	75/109 (69%)	71 (95%)	4 (5%)	0	100	100
14	P	121/124 (98%)	113 (93%)	8 (7%)	0	100	100
15	Q	83/132 (63%)	80 (96%)	3 (4%)	0	100	100
16	R	104/109 (95%)	93 (89%)	11 (11%)	0	100	100
17	S	168/249 (68%)	156 (93%)	12 (7%)	0	100	100
18	U	169/172 (98%)	153 (90%)	15 (9%)	1 (1%)	21	52
19	W	117/123 (95%)	112 (96%)	5 (4%)	0	100	100
20	X	166/169 (98%)	156 (94%)	10 (6%)	0	100	100
21	Y	121/161 (75%)	113 (93%)	8 (7%)	0	100	100
22	Z	118/182 (65%)	107 (91%)	11 (9%)	0	100	100
23	a	122/149 (82%)	109 (89%)	13 (11%)	0	100	100
24	b	62/74 (84%)	60 (97%)	2 (3%)	0	100	100
25	c	42/60 (70%)	38 (90%)	4 (10%)	0	100	100
26	d	88/92 (96%)	82 (93%)	5 (6%)	1 (1%)	11	39
27	e	50/67 (75%)	49 (98%)	1 (2%)	0	100	100
28	f	77/87 (88%)	67 (87%)	10 (13%)	0	100	100
29	g	74/78 (95%)	64 (86%)	10 (14%)	0	100	100
30	i	81/90 (90%)	77 (95%)	4 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	j	88/93 (95%)	81 (92%)	6 (7%)	1 (1%)	11	39
32	k	94/237 (40%)	86 (92%)	6 (6%)	2 (2%)	5	26
33	n	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	14	43
34	1	312/341 (92%)	292 (94%)	20 (6%)	0	100	100
35	2	467/469 (100%)	436 (93%)	30 (6%)	1 (0%)	43	71
36	3	104/128 (81%)	98 (94%)	6 (6%)	0	100	100
37	4	484/486 (100%)	455 (94%)	28 (6%)	1 (0%)	43	71
38	5	652/655 (100%)	605 (93%)	44 (7%)	3 (0%)	24	55
39	6	181/185 (98%)	166 (92%)	15 (8%)	0	100	100
40	8	80/99 (81%)	75 (94%)	5 (6%)	0	100	100
41	9	84/89 (94%)	78 (93%)	6 (7%)	0	100	100
All	All	7531/8667 (87%)	6990 (93%)	530 (7%)	11 (0%)	49	75

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	k	40	VAL
32	k	55	VAL
38	5	555	VAL
38	5	556	SER
35	2	188	ASP

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	566/595 (95%)	565 (100%)	1 (0%)	87	88
2	B	353/389 (91%)	353 (100%)	0	100	100
3	C	369/394 (94%)	367 (100%)	2 (0%)	81	83
4	D	68/69 (99%)	68 (100%)	0	100	100
5	E	225/329 (68%)	224 (100%)	1 (0%)	84	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	109/129 (84%)	108 (99%)	1 (1%)	70	78
7	G	188/245 (77%)	188 (100%)	0	100	100
8	H	190/212 (90%)	190 (100%)	0	100	100
9	I	156/187 (83%)	156 (100%)	0	100	100
10	J	130/147 (88%)	130 (100%)	0	100	100
11	K	131/180 (73%)	131 (100%)	0	100	100
12	L	77/77 (100%)	77 (100%)	0	100	100
13	O	65/91 (71%)	65 (100%)	0	100	100
14	P	109/110 (99%)	109 (100%)	0	100	100
15	Q	72/111 (65%)	72 (100%)	0	100	100
16	R	97/100 (97%)	96 (99%)	1 (1%)	68	76
17	S	149/211 (71%)	148 (99%)	1 (1%)	76	80
18	U	147/148 (99%)	147 (100%)	0	100	100
19	W	98/102 (96%)	98 (100%)	0	100	100
20	X	132/133 (99%)	132 (100%)	0	100	100
21	Y	105/140 (75%)	105 (100%)	0	100	100
22	Z	95/148 (64%)	95 (100%)	0	100	100
23	a	108/129 (84%)	108 (100%)	0	100	100
24	b	50/59 (85%)	50 (100%)	0	100	100
25	c	30/45 (67%)	30 (100%)	0	100	100
26	d	83/85 (98%)	82 (99%)	1 (1%)	63	75
27	e	44/55 (80%)	44 (100%)	0	100	100
28	f	68/73 (93%)	68 (100%)	0	100	100
29	g	62/64 (97%)	62 (100%)	0	100	100
30	i	64/68 (94%)	64 (100%)	0	100	100
31	j	71/73 (97%)	71 (100%)	0	100	100
32	k	86/207 (42%)	86 (100%)	0	100	100
33	n	98/102 (96%)	98 (100%)	0	100	100
34	1	282/302 (93%)	280 (99%)	2 (1%)	76	80
35	2	433/433 (100%)	433 (100%)	0	100	100
36	3	97/114 (85%)	97 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	4	434/434 (100%)	434 (100%)	0	100	100
38	5	579/580 (100%)	578 (100%)	1 (0%)	87	88
39	6	165/167 (99%)	165 (100%)	0	100	100
40	8	69/76 (91%)	69 (100%)	0	100	100
41	9	73/76 (96%)	73 (100%)	0	100	100
All	All	6527/7389 (88%)	6516 (100%)	11 (0%)	85	88

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	d	13	ASP
34	1	3	ILE
38	5	477	LYS
34	1	89	VAL
6	F	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
26	d	77	HIS
35	2	185	HIS
38	5	636	ASN
28	f	11	HIS
32	k	93	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

36 ligands 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$
46	3PE	J	203	-	43,43,50	0.92	3 (6%)	46,48,55	1.17	2 (4%)
49	ZMP	Q	201	15	27,32,36	1.78	6 (22%)	31,39,45	2.00	8 (25%)
48	CDL	X	201	-	81,81,99	0.98	7 (8%)	87,93,111	1.20	5 (5%)
51	T7X	2	501	-	48,48,61	0.96	4 (8%)	57,60,73	1.30	6 (10%)
50	PLC	W	401	-	40,40,41	1.37	6 (15%)	46,48,49	1.22	3 (6%)
50	PLC	n	1101	-	41,41,41	1.34	6 (14%)	47,49,49	1.06	2 (4%)
42	SF4	A	801	1	0,12,12	-	-	-	-	-
48	CDL	J	204	-	77,77,99	1.04	4 (5%)	83,89,111	1.15	9 (10%)
43	FES	A	803	1	0,4,4	-	-	-	-	-
43	FES	H	301	8	0,4,4	-	-	-	-	-
46	3PE	I	303	-	50,50,50	0.89	4 (8%)	53,55,55	1.37	3 (5%)
46	3PE	g	202	-	42,42,50	0.92	3 (7%)	45,47,55	1.32	2 (4%)
48	CDL	g	201	-	82,82,99	0.96	6 (7%)	88,94,111	1.26	5 (5%)
45	NDP	E	401	-	51,52,52	3.57	21 (41%)	71,80,80	2.20	18 (25%)
46	3PE	J	201	-	40,40,50	1.00	3 (7%)	43,45,55	1.30	3 (6%)
46	3PE	6	301	-	35,35,50	1.03	4 (11%)	38,40,55	1.13	2 (5%)
51	T7X	2	503	-	52,52,61	0.94	4 (7%)	61,64,73	1.29	7 (11%)
42	SF4	A	802	1	0,12,12	-	-	-	-	-
46	3PE	4	505	-	50,50,50	0.83	3 (6%)	53,55,55	1.21	4 (7%)
47	LMN	j	101	-	68,68,72	1.61	12 (17%)	88,94,98	1.54	17 (19%)
46	3PE	5	901	-	41,41,50	1.00	3 (7%)	44,46,55	1.20	3 (6%)
51	T7X	4	504	-	43,43,61	0.97	4 (9%)	52,55,73	1.39	4 (7%)
48	CDL	4	502	-	91,91,99	0.96	8 (8%)	97,103,111	1.20	6 (6%)
49	ZMP	O	201	13	27,32,36	1.65	5 (18%)	31,39,45	1.87	8 (25%)
42	SF4	I	302	9	0,12,12	-	-	-	-	-
46	3PE	5	903	-	50,50,50	0.90	4 (8%)	53,55,55	1.18	2 (3%)
42	SF4	K	301	11	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	CPL	2	502	-	51,51,51	1.00	4 (7%)	57,59,59	1.11	3 (5%)
50	PLC	5	902	-	30,30,41	1.51	6 (20%)	36,38,49	1.05	3 (8%)
44	FMN	B	502	-	33,33,33	2.88	12 (36%)	48,50,50	1.64	9 (18%)
42	SF4	I	301	9	0,12,12	-	-	-	-	-
47	LMN	J	202	-	72,72,72	1.51	8 (11%)	92,98,98	1.62	18 (19%)
46	3PE	4	503	-	41,41,50	0.94	4 (9%)	44,46,55	1.14	3 (6%)
42	SF4	B	501	2	0,12,12	-	-	-	-	-
46	3PE	4	501	-	42,42,50	0.96	3 (7%)	45,47,55	1.24	3 (6%)
50	PLC	W	402	-	41,41,41	1.31	5 (12%)	47,49,49	1.22	2 (4%)

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
46	3PE	J	203	-	-	23/47/47/54	-
49	ZMP	Q	201	15	-	7/37/39/43	-
48	CDL	X	201	-	-	27/92/92/110	-
51	T7X	2	501	-	-	14/43/67/80	0/1/1/1
50	PLC	W	401	-	-	20/44/44/45	-
50	PLC	n	1101	-	-	11/45/45/45	-
48	CDL	J	204	-	-	21/88/88/110	-
42	SF4	A	801	1	-	-	0/6/5/5
43	FES	A	803	1	-	-	0/1/1/1
43	FES	H	301	8	-	-	0/1/1/1
46	3PE	I	303	-	-	23/54/54/54	-
46	3PE	g	202	-	-	20/46/46/54	-
48	CDL	g	201	-	-	37/93/93/110	-
45	NDP	E	401	-	-	14/34/77/77	0/5/5/5
46	3PE	J	201	-	-	21/44/44/54	-
46	3PE	6	301	-	-	20/39/39/54	-
51	T7X	2	503	-	-	20/47/71/80	0/1/1/1
42	SF4	A	802	1	-	-	0/6/5/5
46	3PE	4	505	-	-	23/54/54/54	-
47	LMN	j	101	-	-	20/46/126/130	0/4/4/4
46	3PE	5	901	-	-	20/45/45/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	T7X	4	504	-	-	26/38/62/80	0/1/1/1
48	CDL	4	502	-	-	50/102/102/110	-
49	ZMP	O	201	13	-	13/37/39/43	-
42	SF4	I	302	9	-	-	0/6/5/5
46	3PE	5	903	-	-	18/54/54/54	-
42	SF4	K	301	11	-	-	0/6/5/5
52	CPL	2	502	-	-	26/55/55/55	-
50	PLC	5	902	-	-	17/34/34/45	-
44	FMN	B	502	-	-	10/18/18/18	0/3/3/3
42	SF4	I	301	9	-	-	0/6/5/5
47	LMN	J	202	-	-	26/50/130/130	0/4/4/4
46	3PE	4	503	-	-	20/45/45/54	-
42	SF4	B	501	2	-	-	0/6/5/5
46	3PE	4	501	-	-	22/46/46/54	-
50	PLC	W	402	-	-	22/45/45/45	-

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	E	401	NDP	C2B-C1B	-8.24	1.32	1.53
45	E	401	NDP	O4B-C1B	7.76	1.59	1.42
45	E	401	NDP	O4D-C1D	7.75	1.59	1.42
45	E	401	NDP	C2D-C1D	-7.40	1.30	1.53
45	E	401	NDP	C6N-C5N	7.17	1.55	1.33

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	E	401	NDP	N6A-C6A-N1A	-6.68	103.49	118.38
45	E	401	NDP	C4A-N9A-C1B	-6.48	111.49	126.63
49	Q	201	ZMP	C9-C10-S1	6.17	120.75	113.40
45	E	401	NDP	N3A-C2A-N1A	-6.16	119.25	128.58
45	E	401	NDP	C1B-N9A-C8A	6.06	140.54	127.09

There are no chirality outliers.

5 of 591 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	502	FMN	N10-C1'-C2'-O2'

Continued on next page...

Continued from previous page...

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

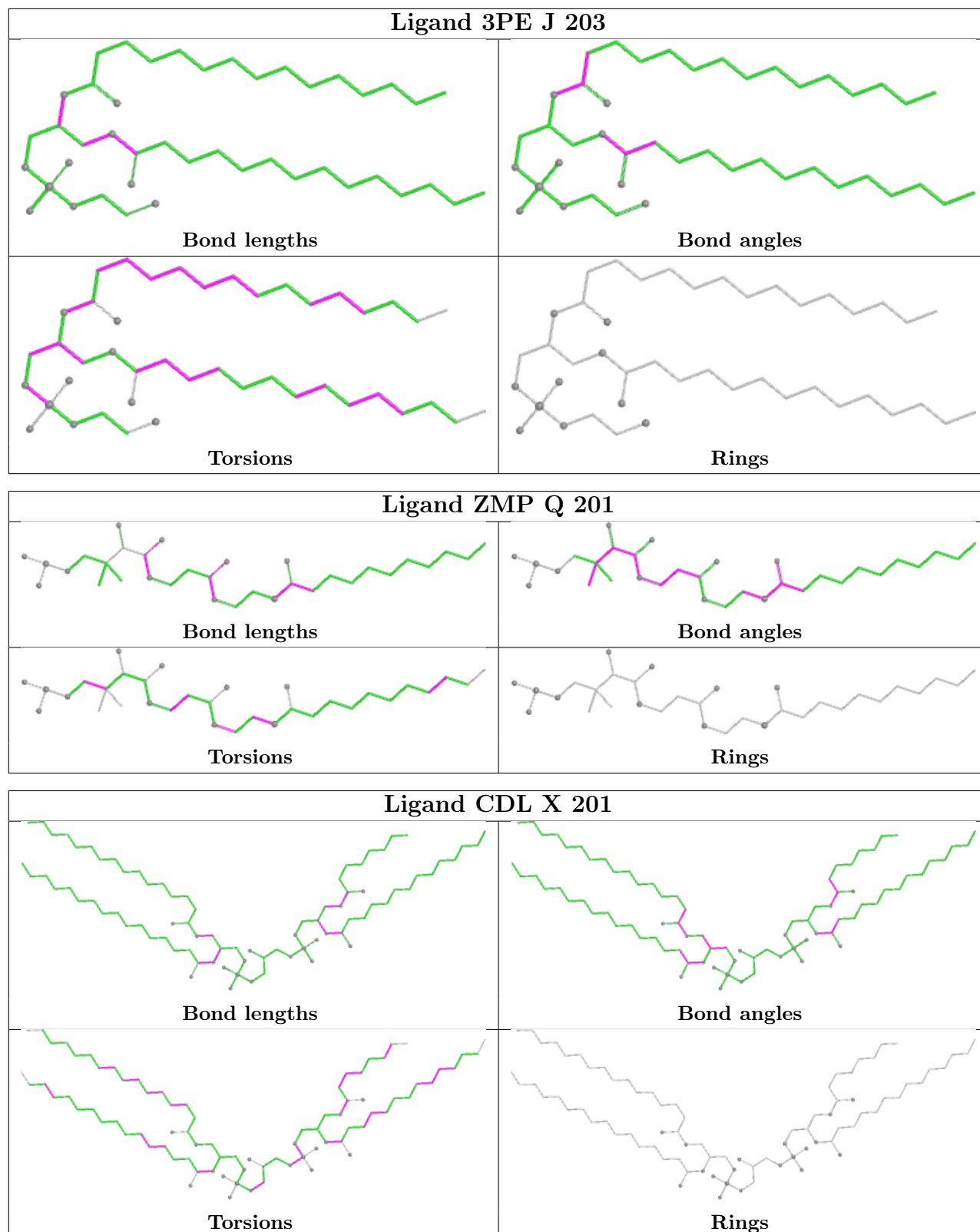
There are no ring outliers.

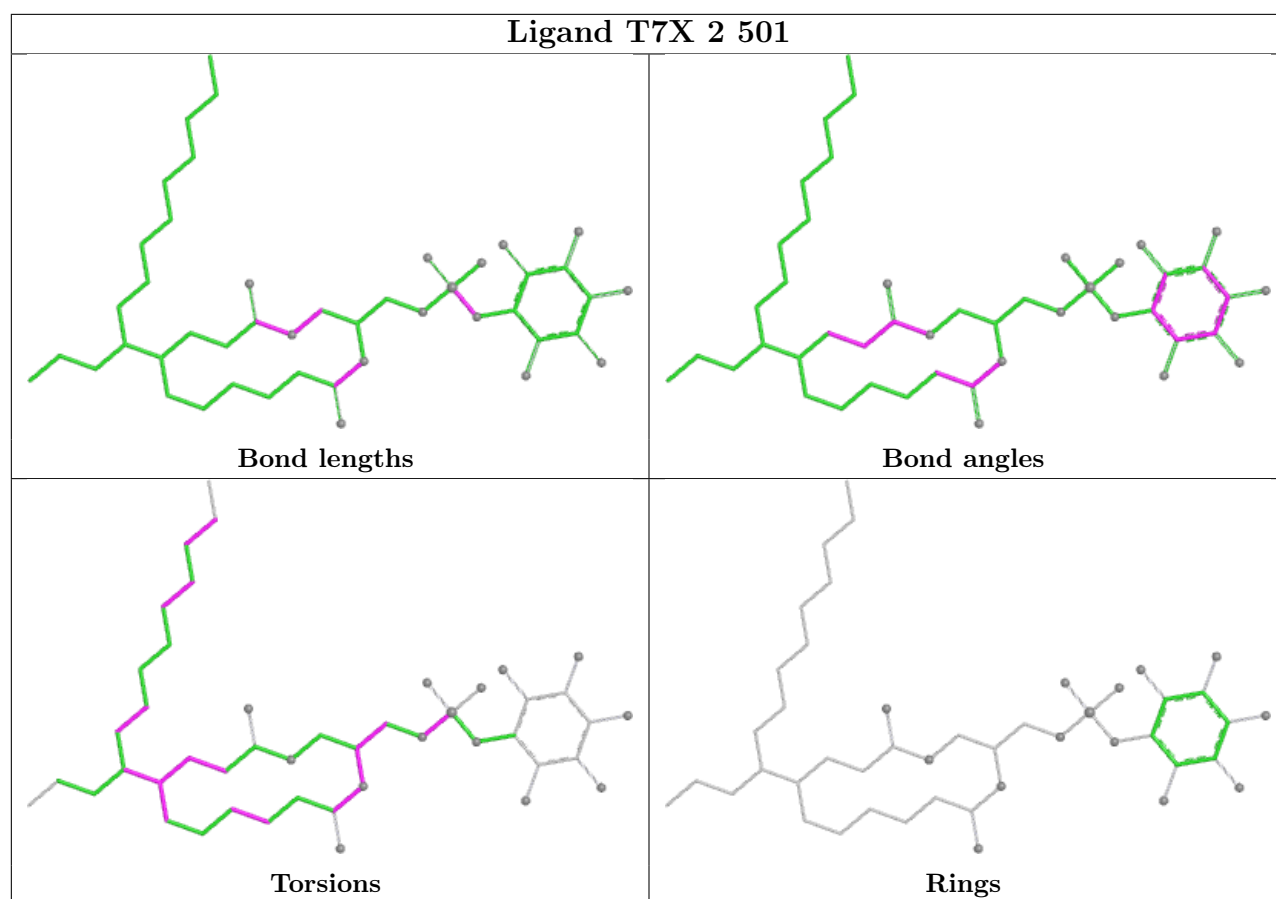
23 monomers are involved in 89 short contacts:

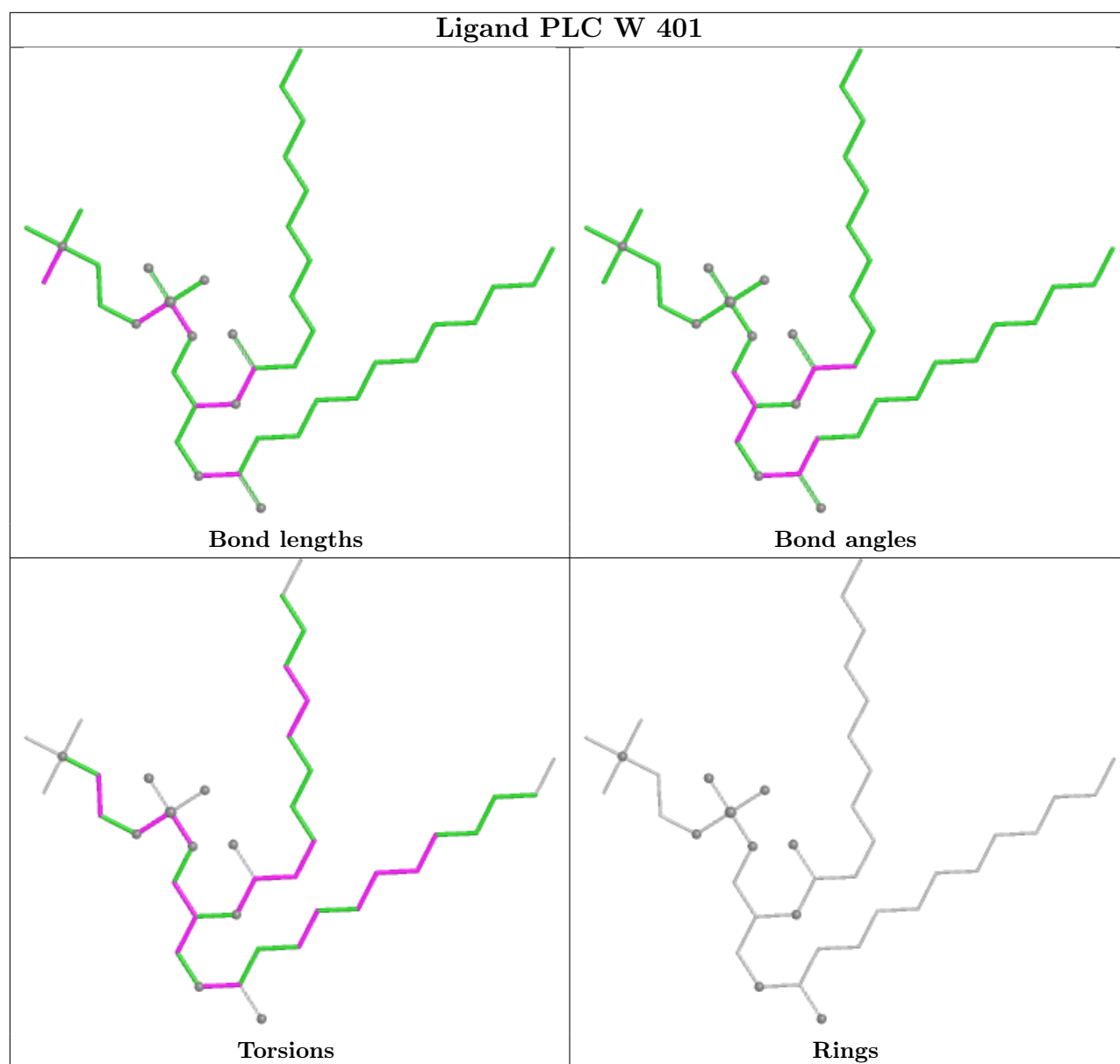
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	J	203	3PE	4	0
48	X	201	CDL	4	0
50	W	401	PLC	2	0
50	n	1101	PLC	1	0
48	J	204	CDL	22	0
46	g	202	3PE	2	0
48	g	201	CDL	7	0
45	E	401	NDP	1	0
46	6	301	3PE	5	0
46	4	505	3PE	4	0
47	j	101	LMN	2	0
46	5	901	3PE	7	0
51	4	504	T7X	1	0
48	4	502	CDL	6	0
49	O	201	ZMP	1	0
42	K	301	SF4	1	0
52	2	502	CPL	4	0
50	5	902	PLC	1	0
44	B	502	FMN	2	0
47	J	202	LMN	5	0
46	4	503	3PE	2	0
46	4	501	3PE	7	0
50	W	402	PLC	1	0

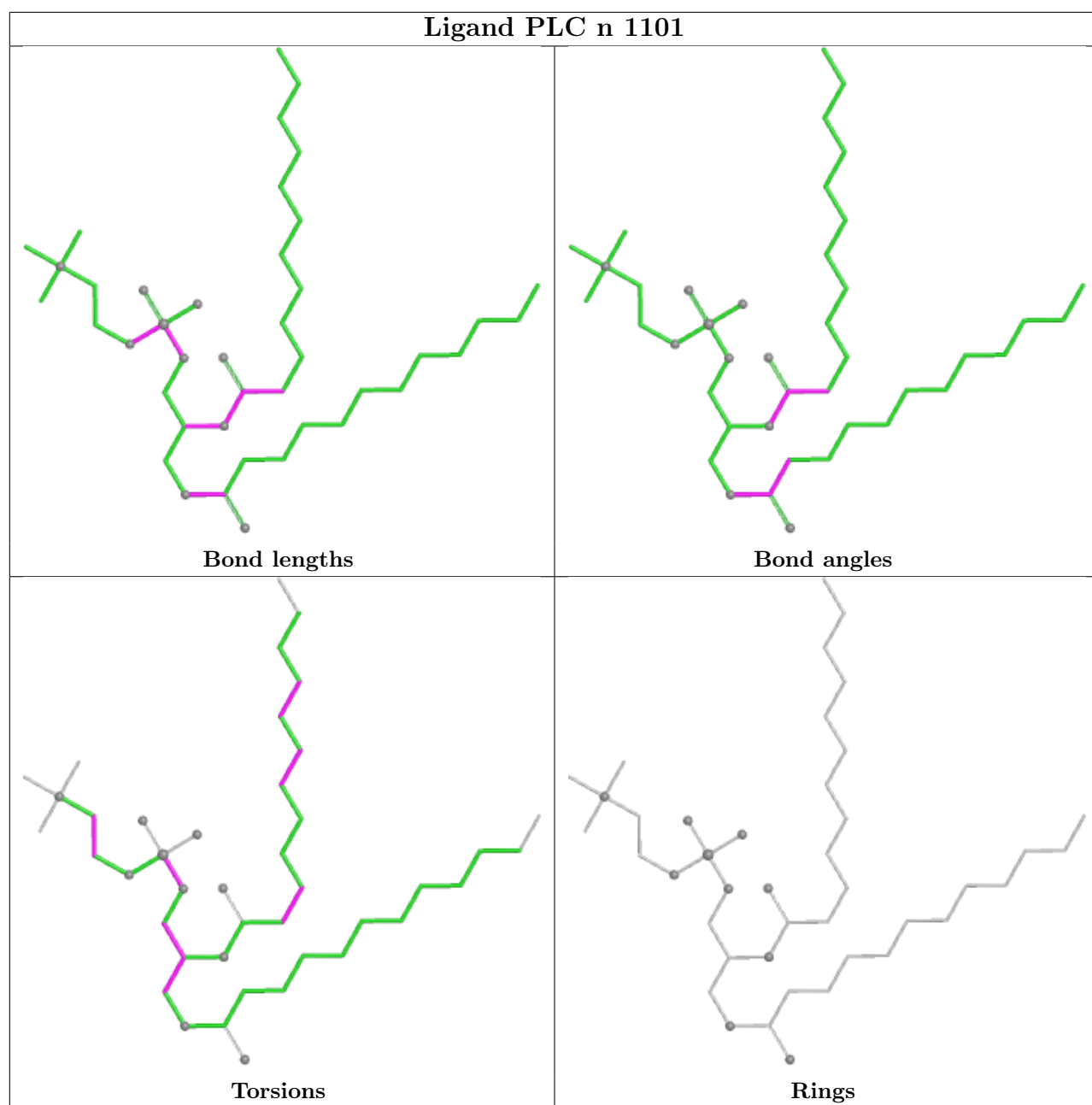
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

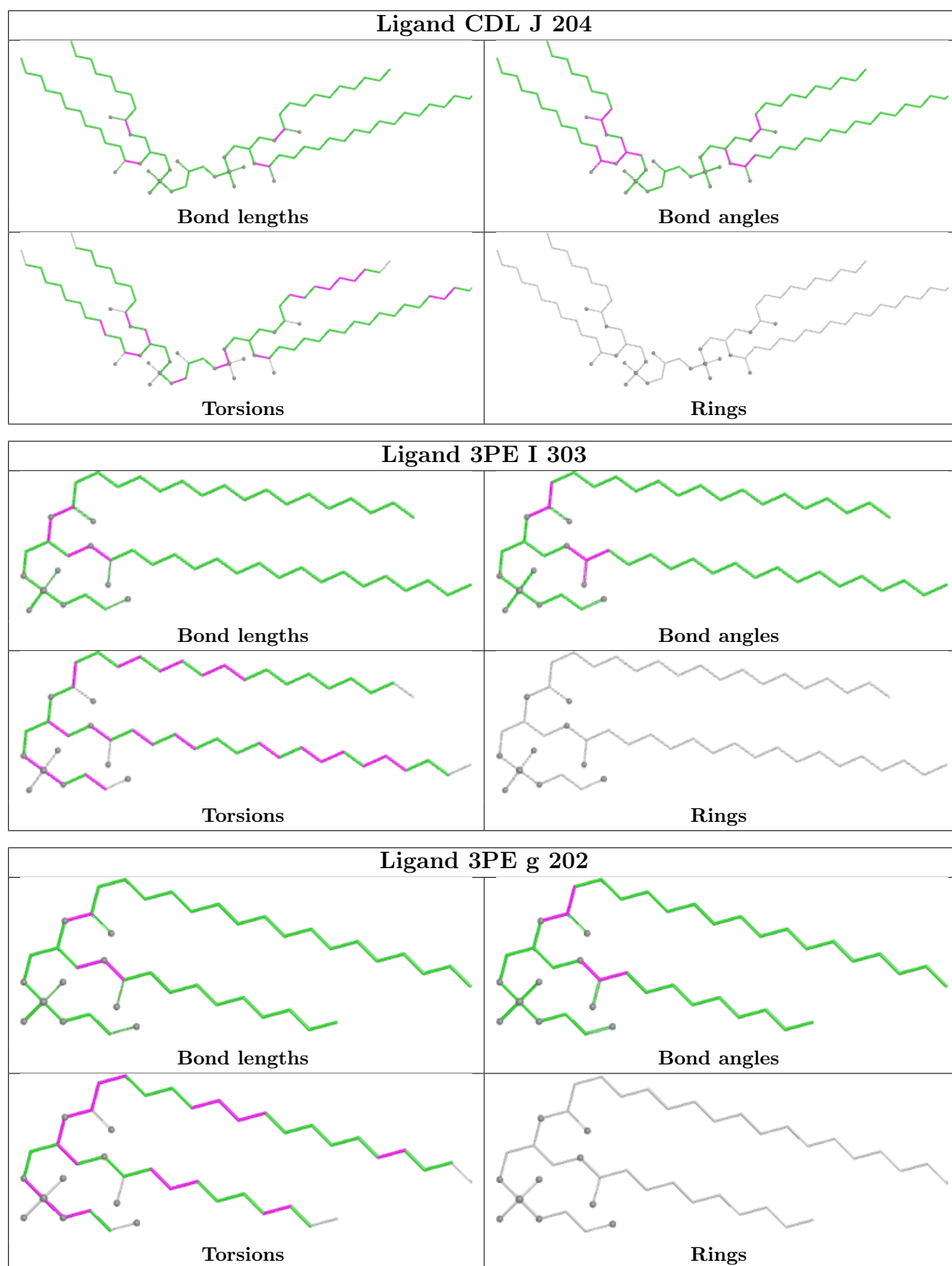
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

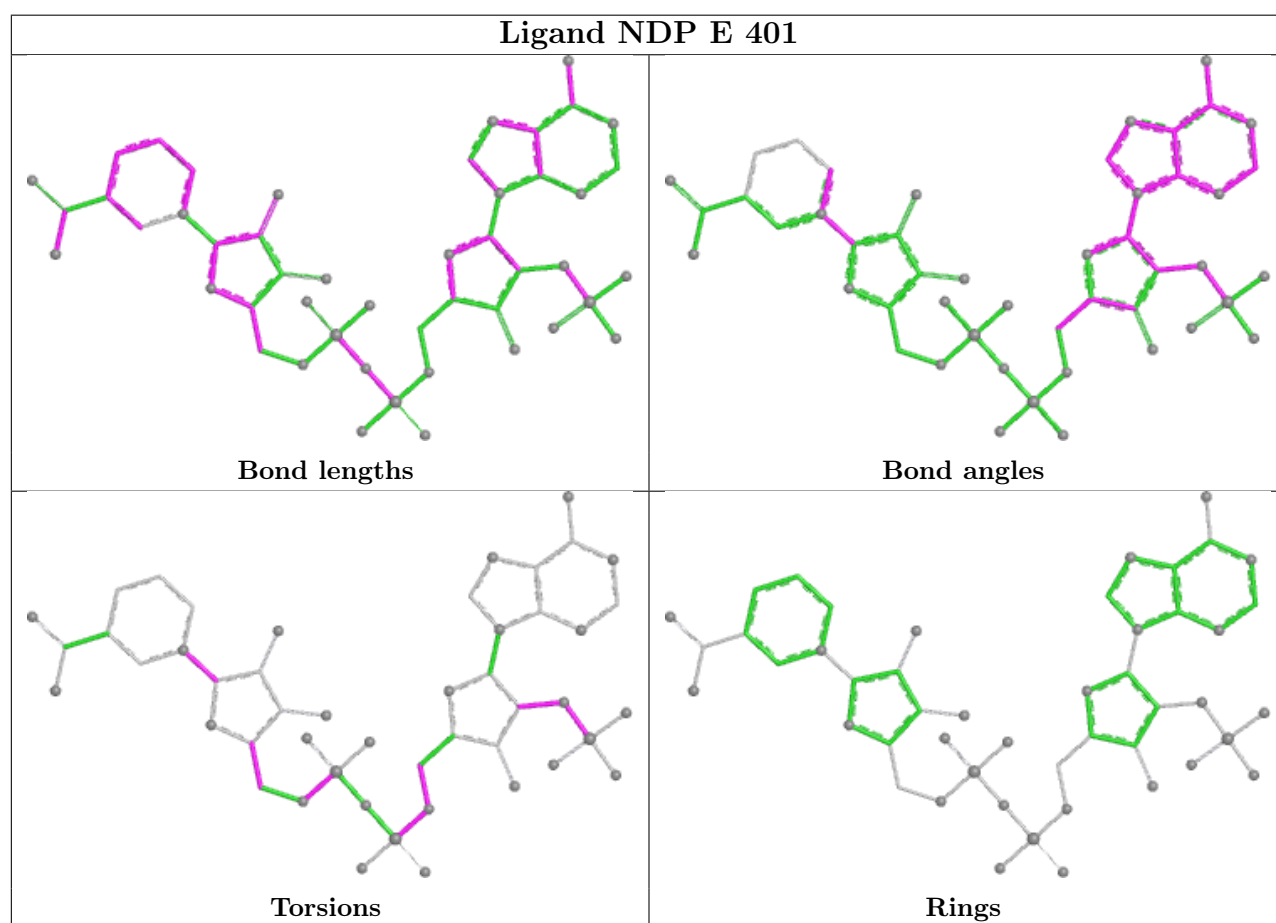
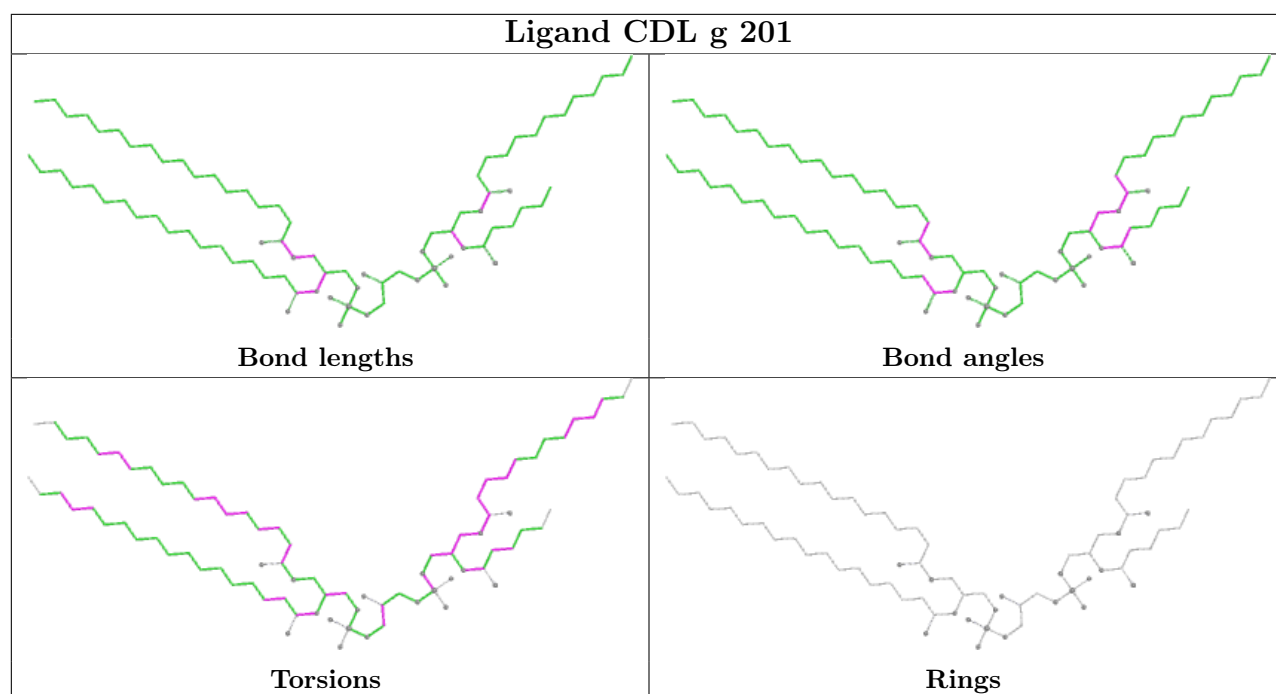


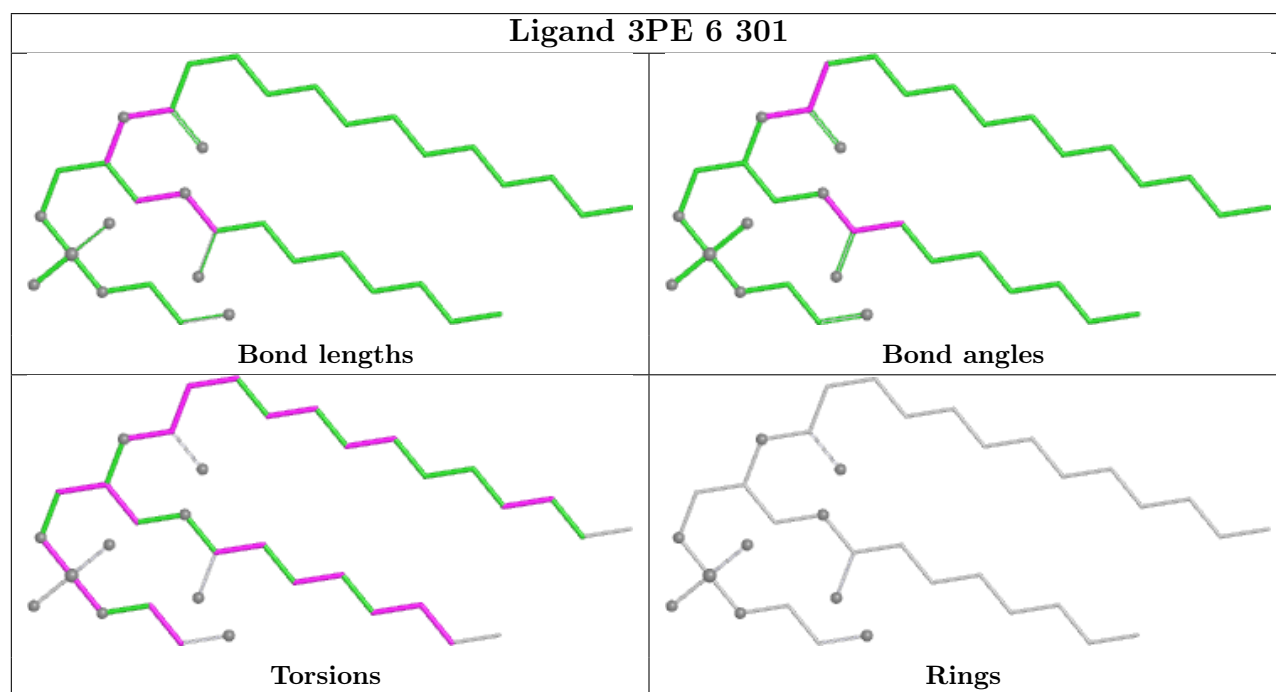
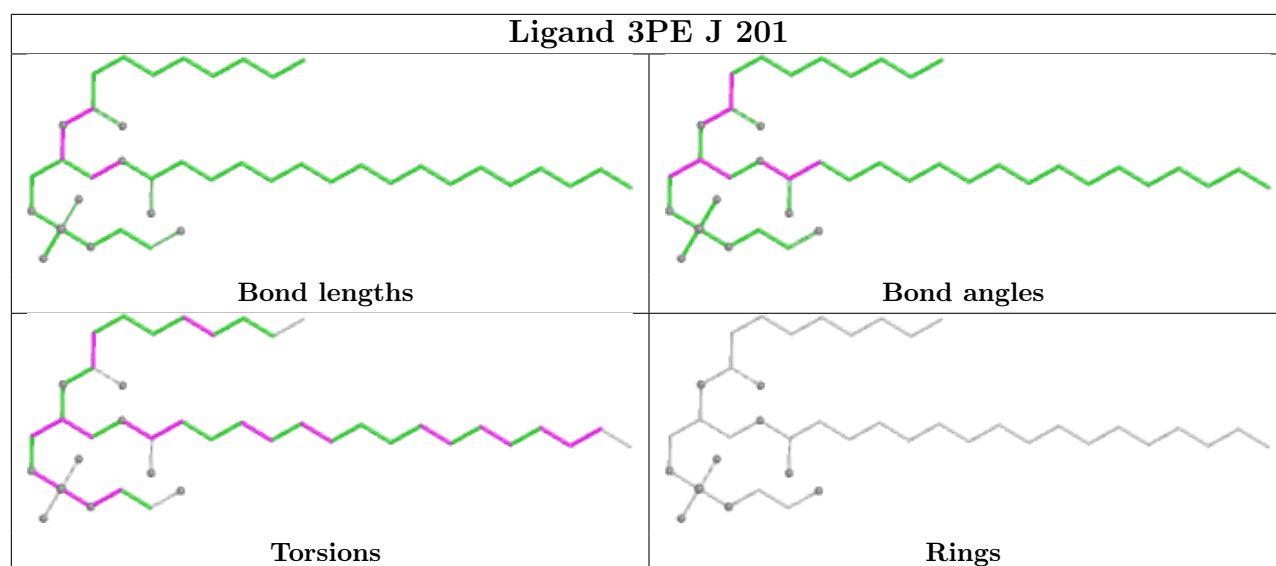


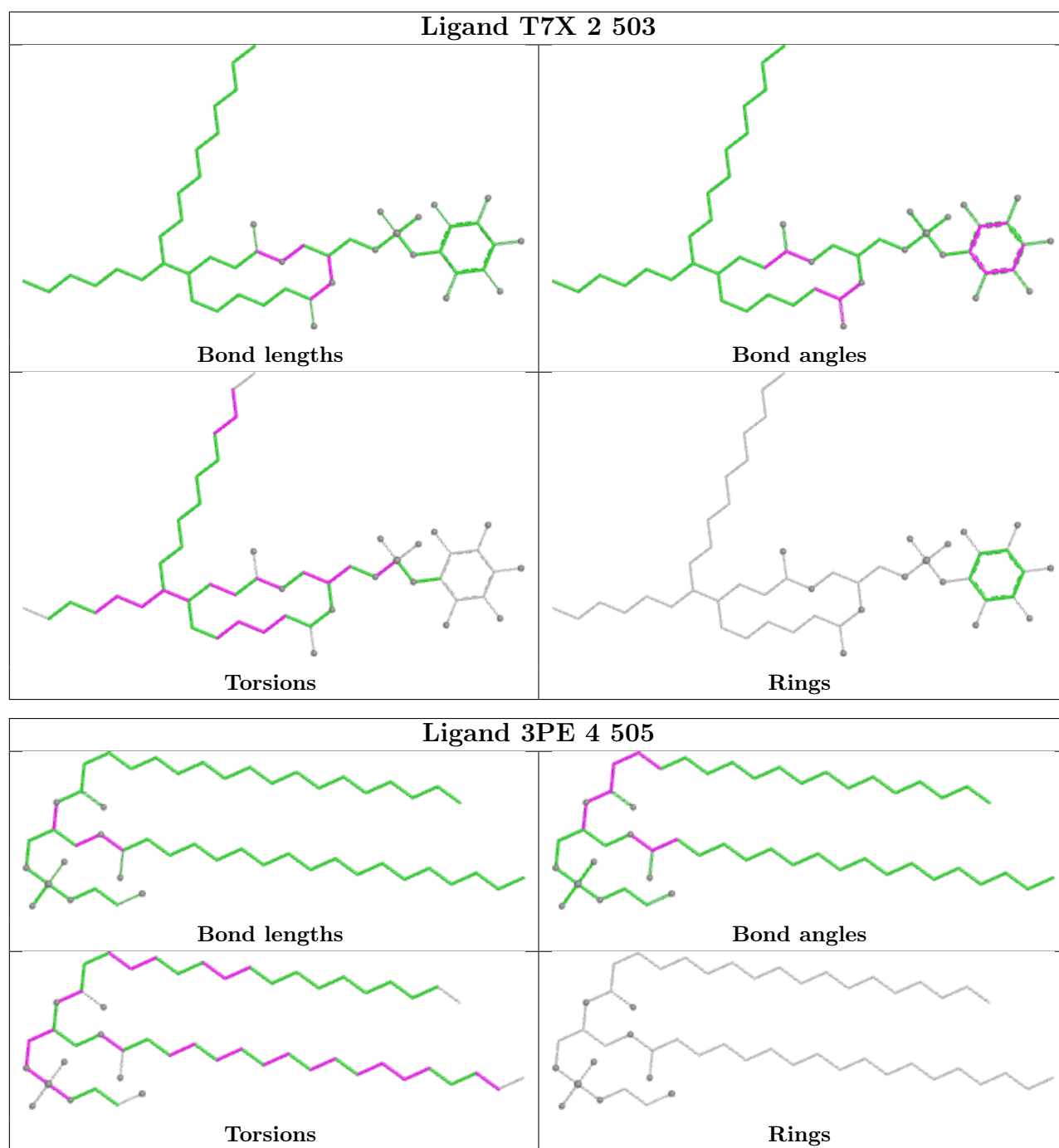


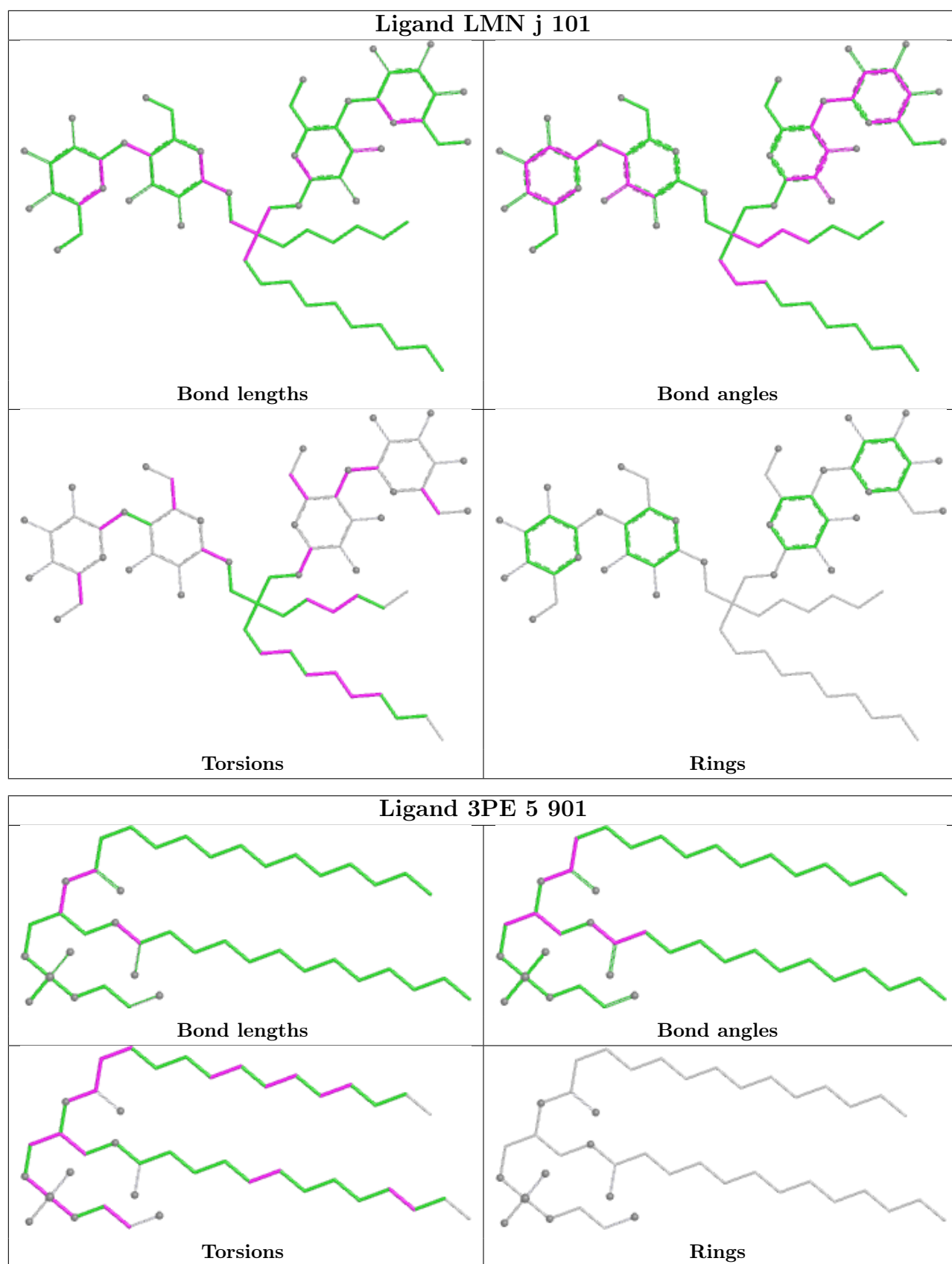


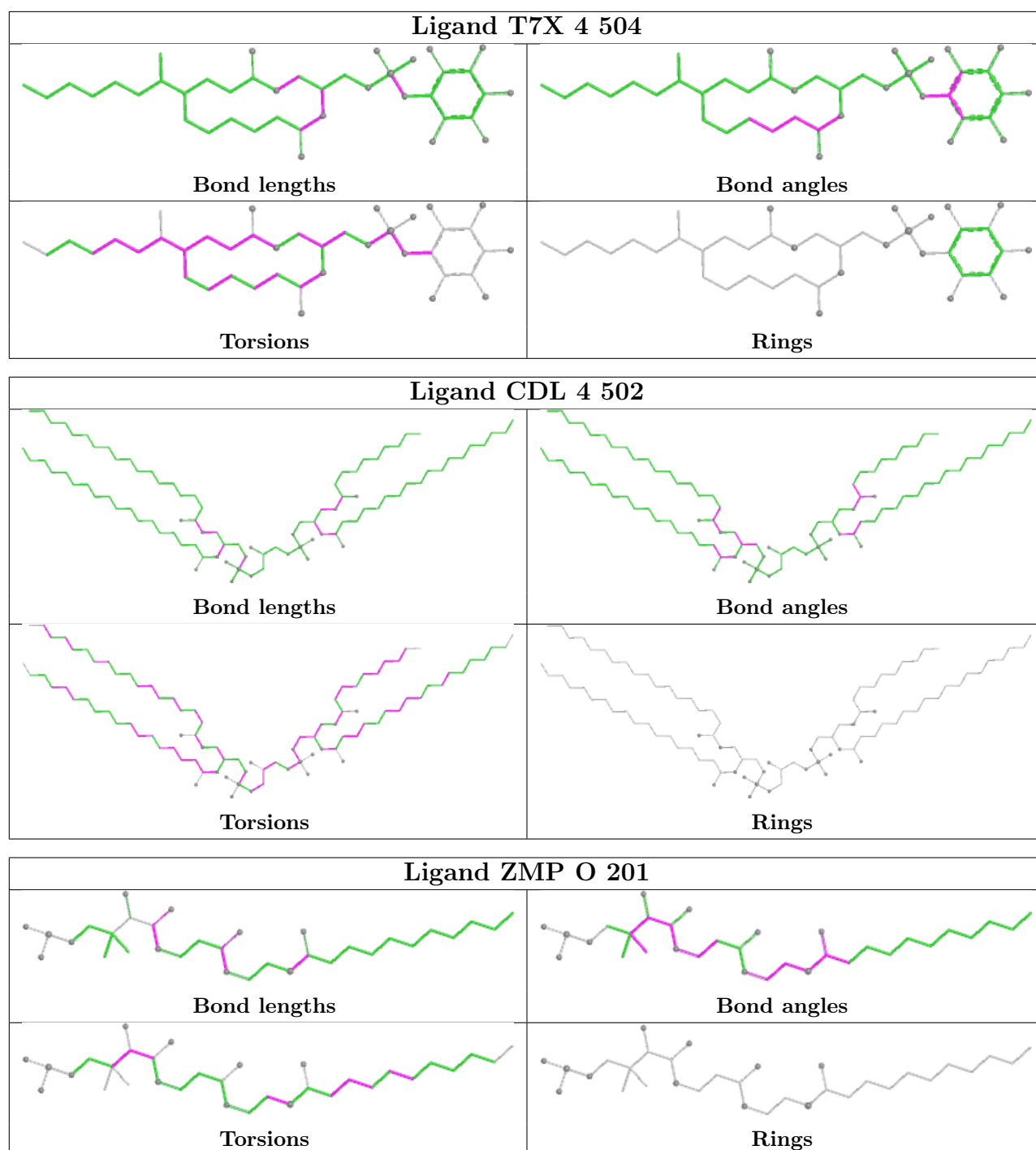


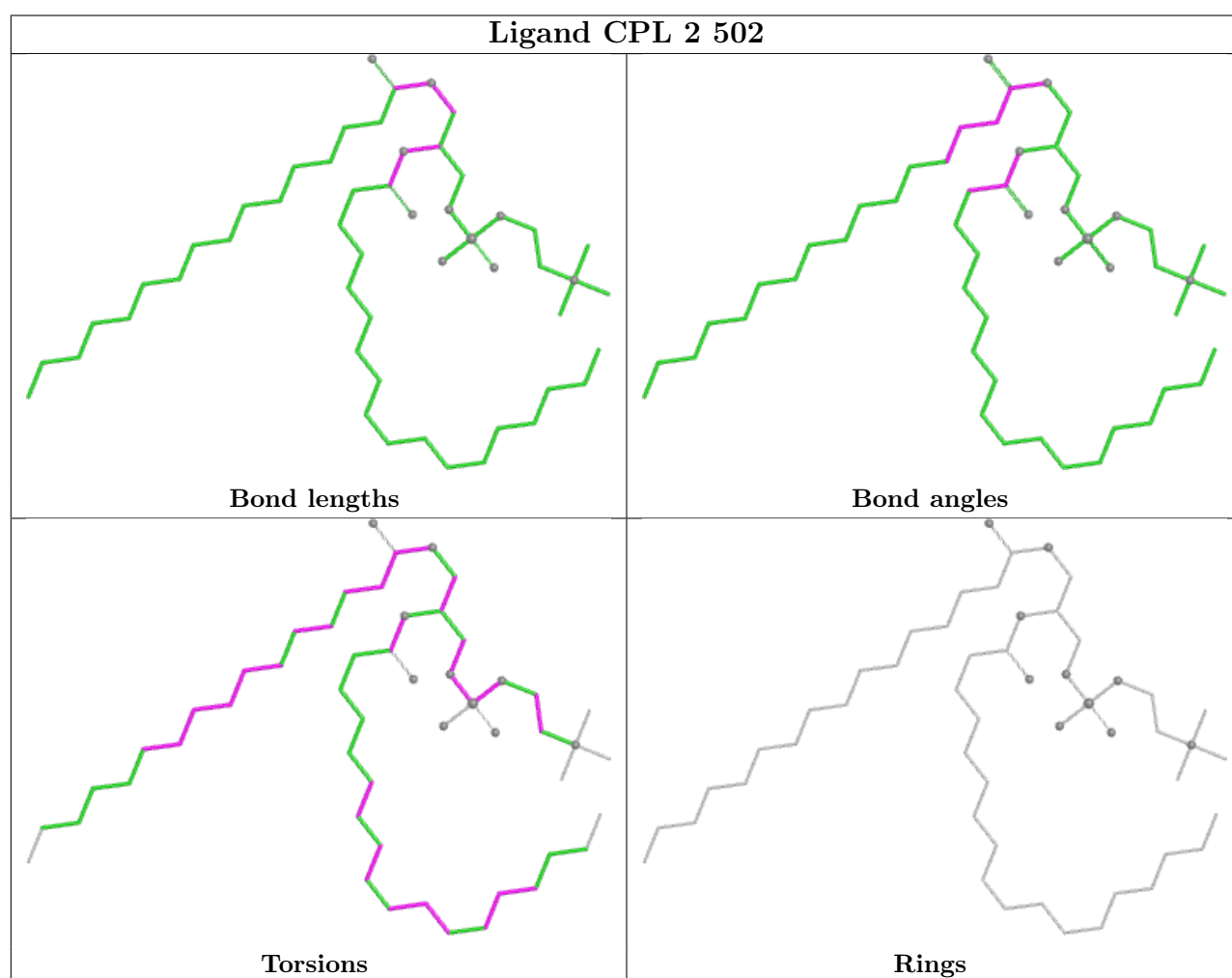
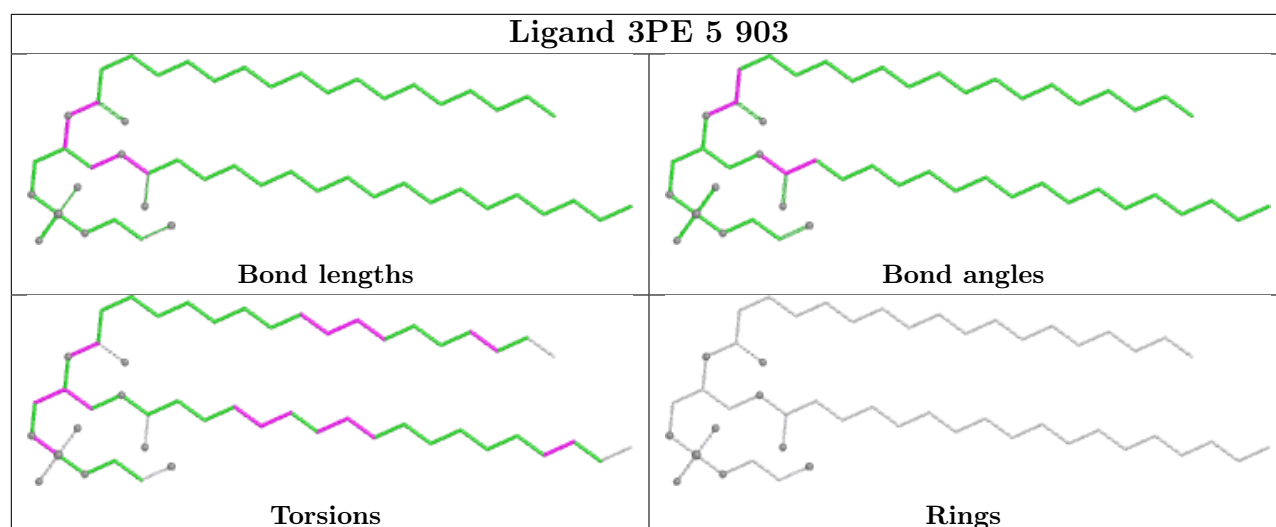




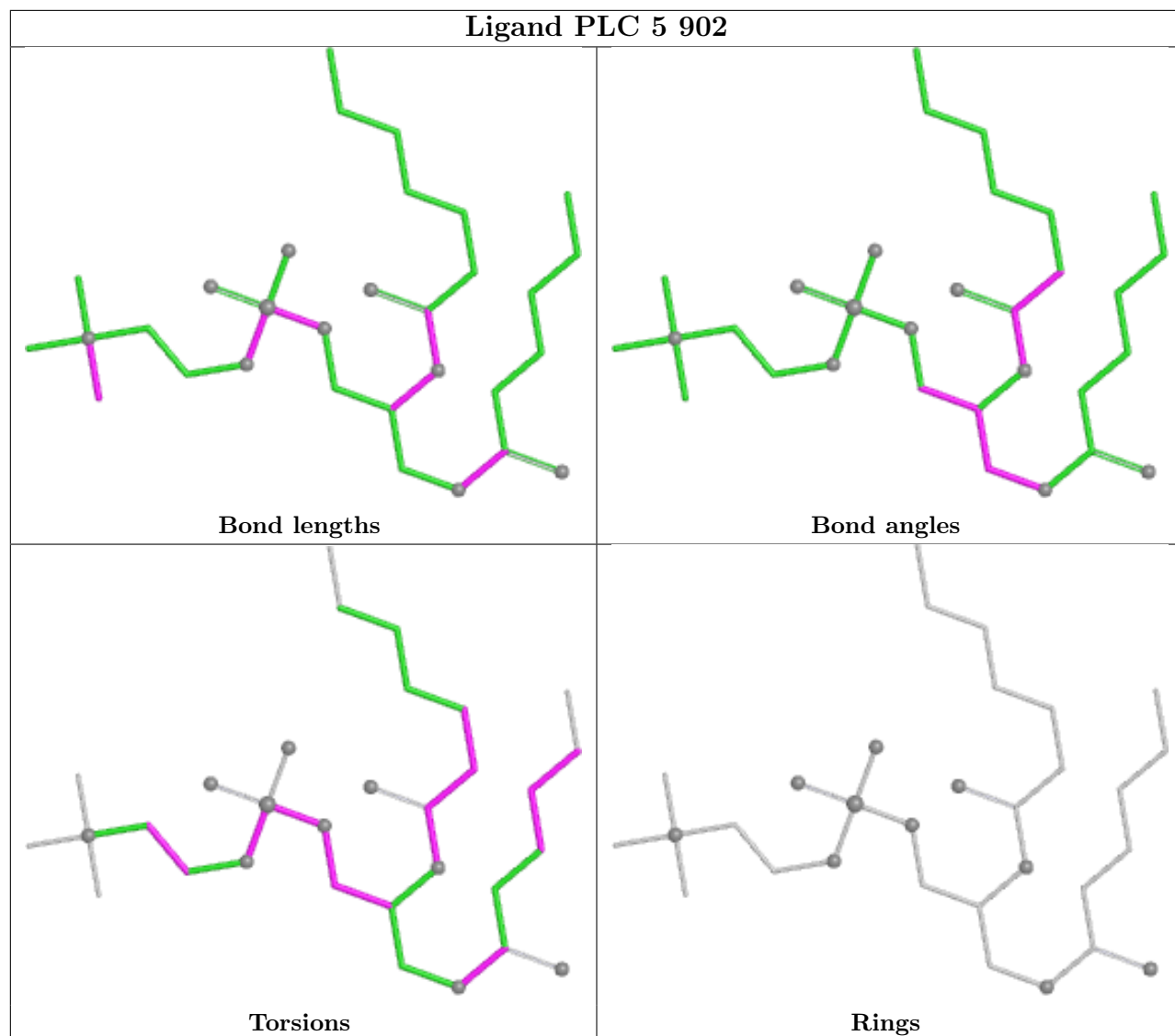


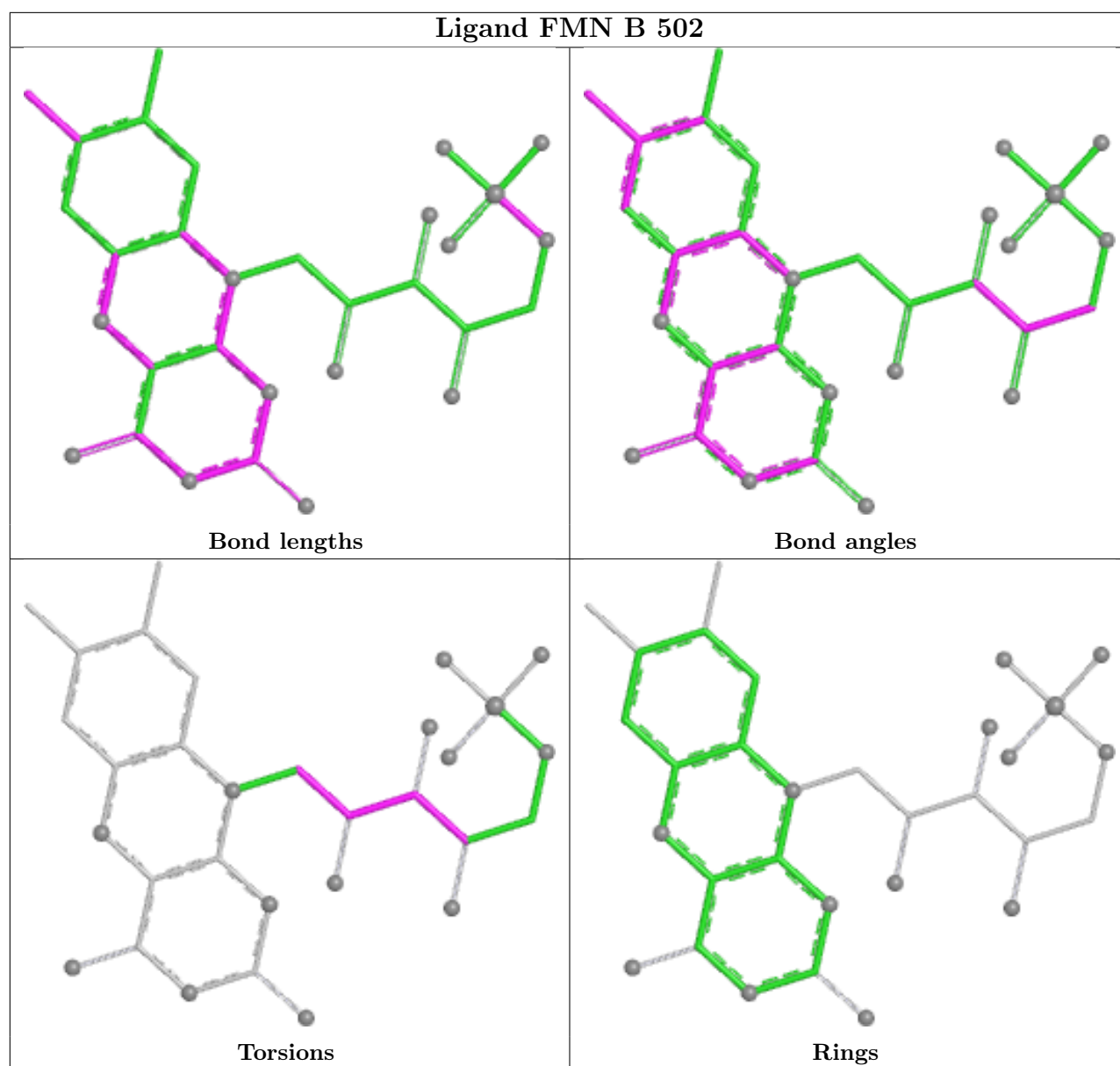


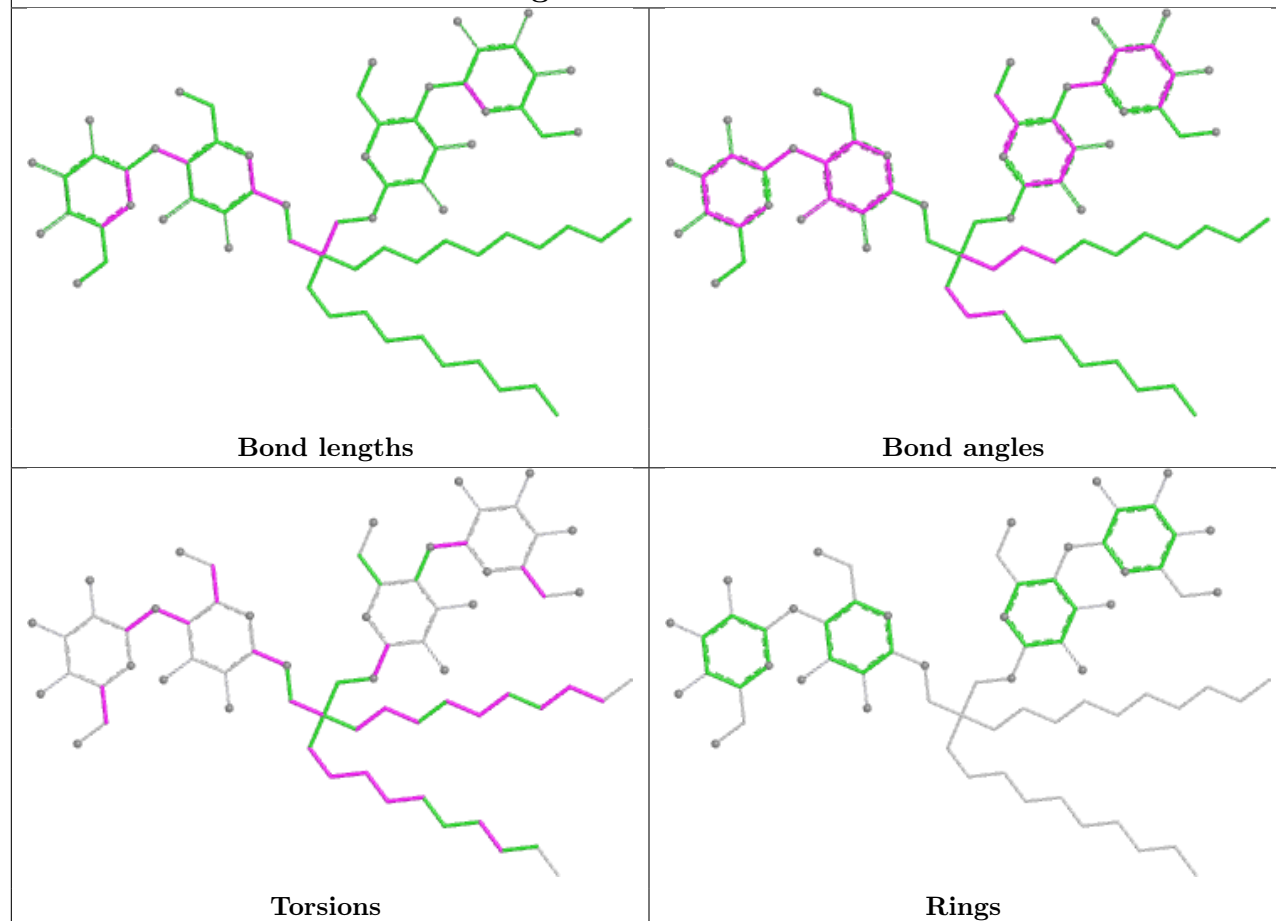
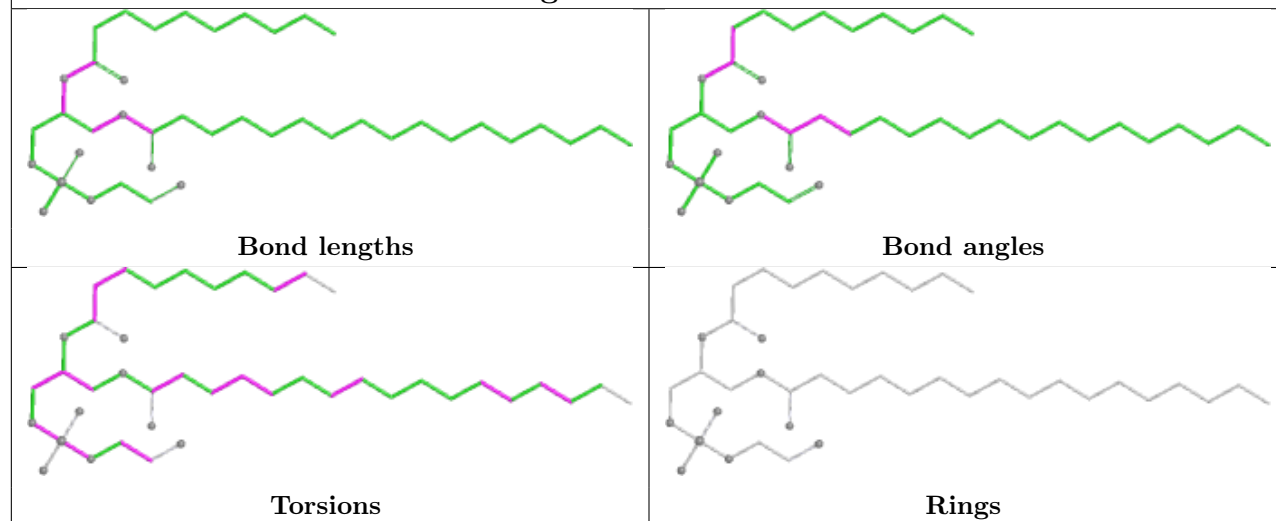


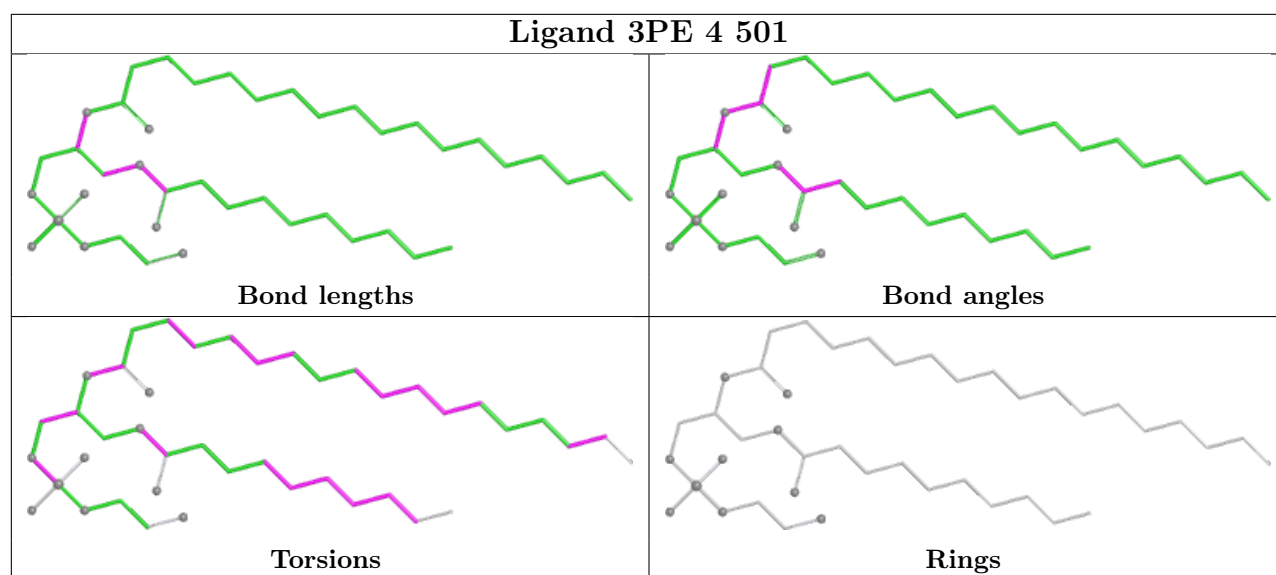


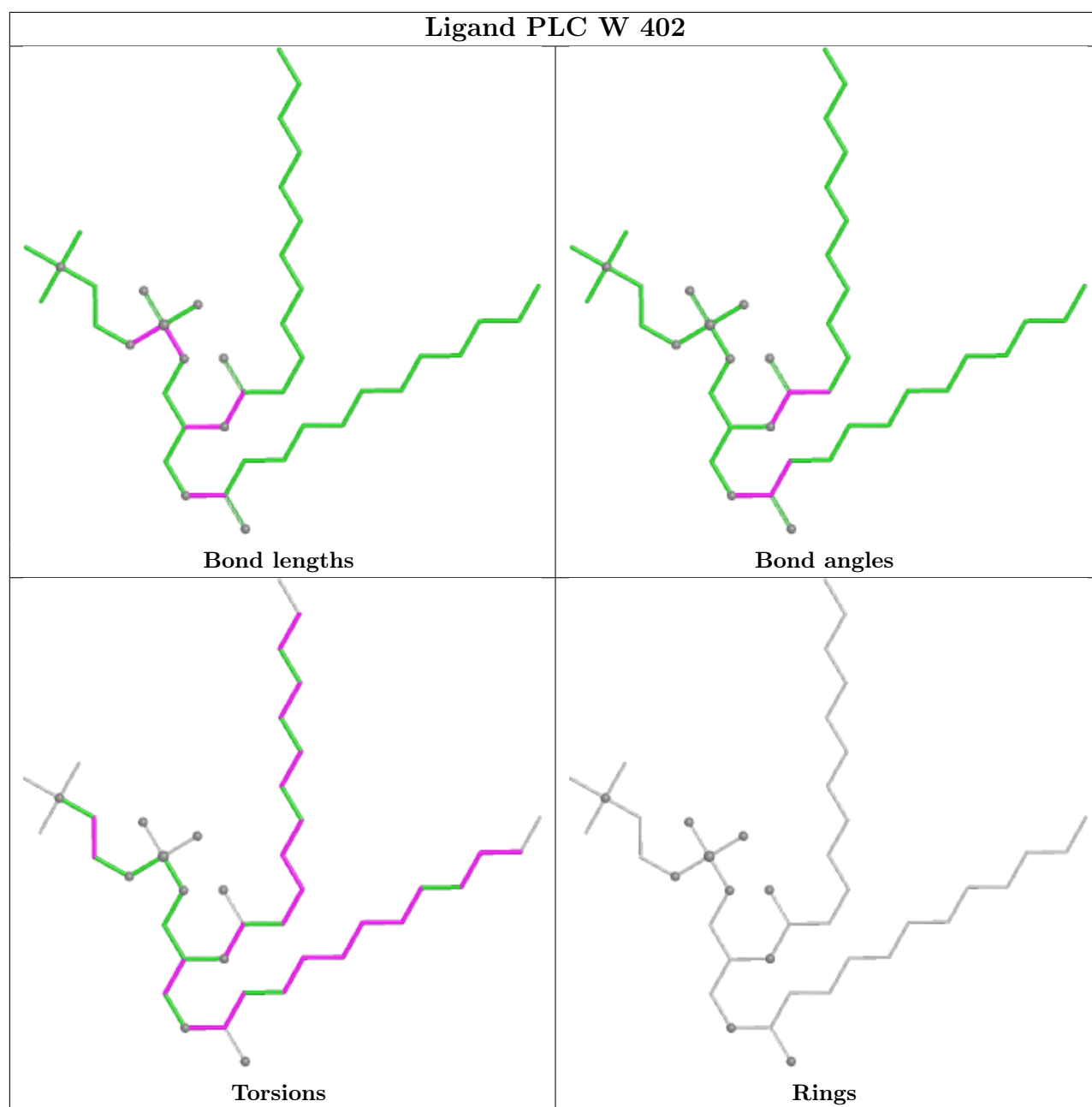
Ligand PLC 5 902





Ligand LMN J 202**Ligand 3PE 4 503**





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.

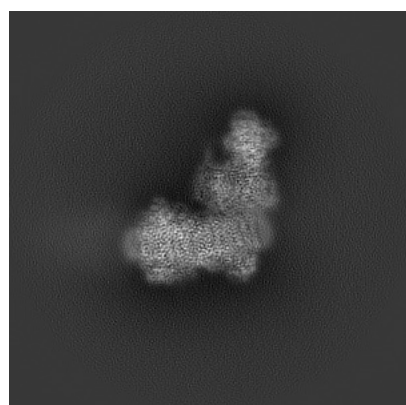
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4872. These allow visual inspection of the internal detail of the map and identification of artifacts.

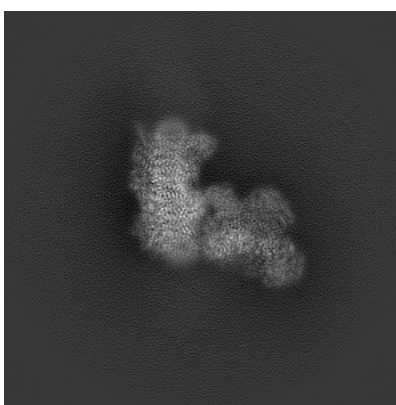
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

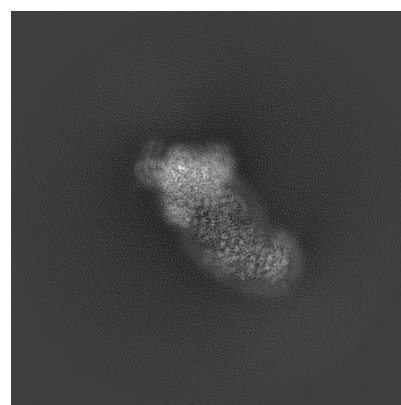
6.1.1 Primary map



X



Y

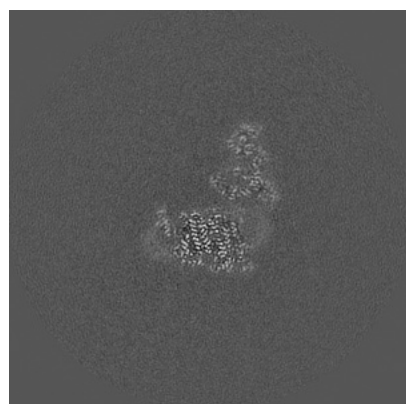


Z

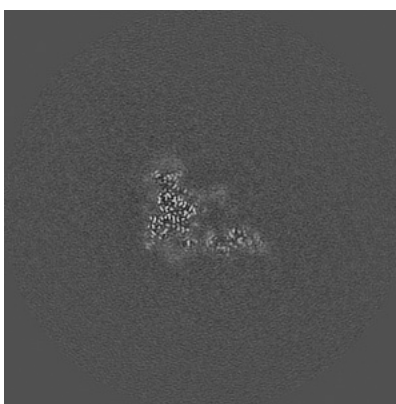
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

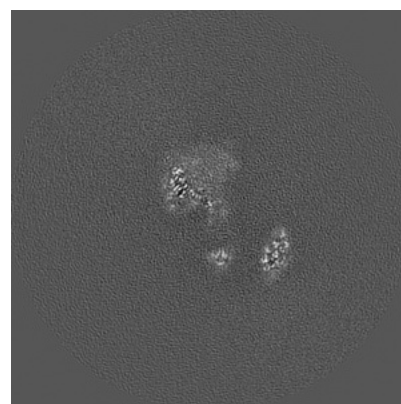
6.2.1 Primary map



X Index: 228



Y Index: 228

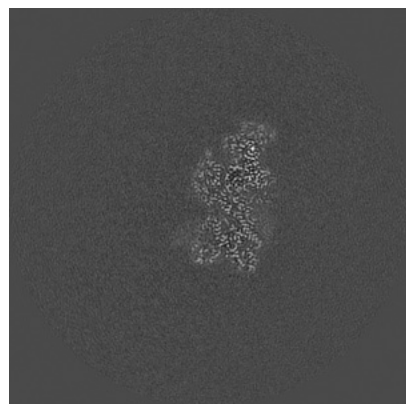


Z Index: 228

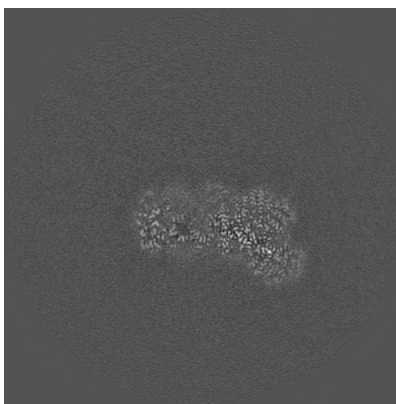
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

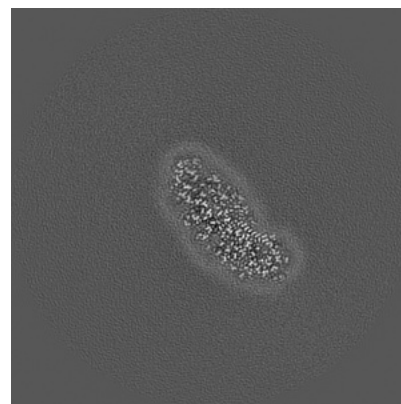
6.3.1 Primary map



X Index: 193



Y Index: 272

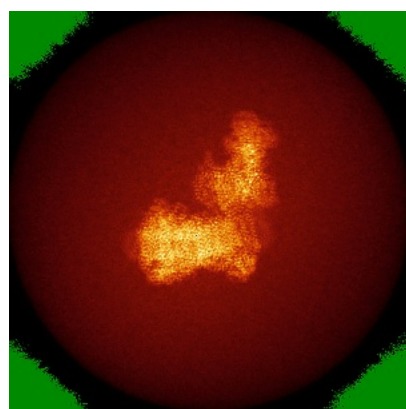


Z Index: 196

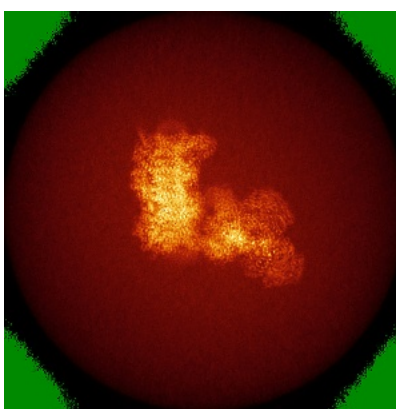
The images above show the largest variance slices of the map in three orthogonal directions.

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

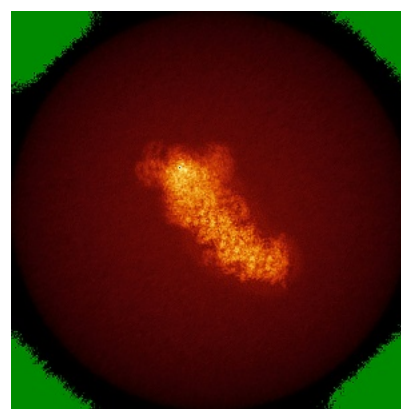
6.4.1 Primary map



X



Y

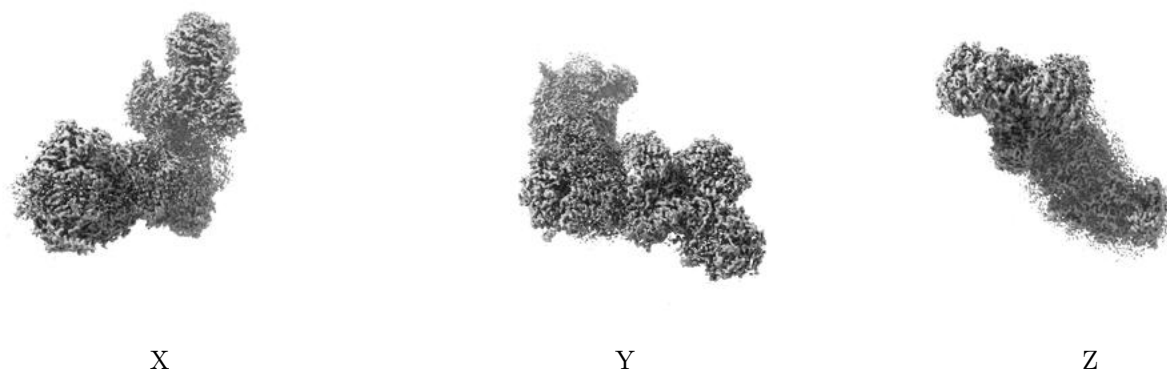


Z

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

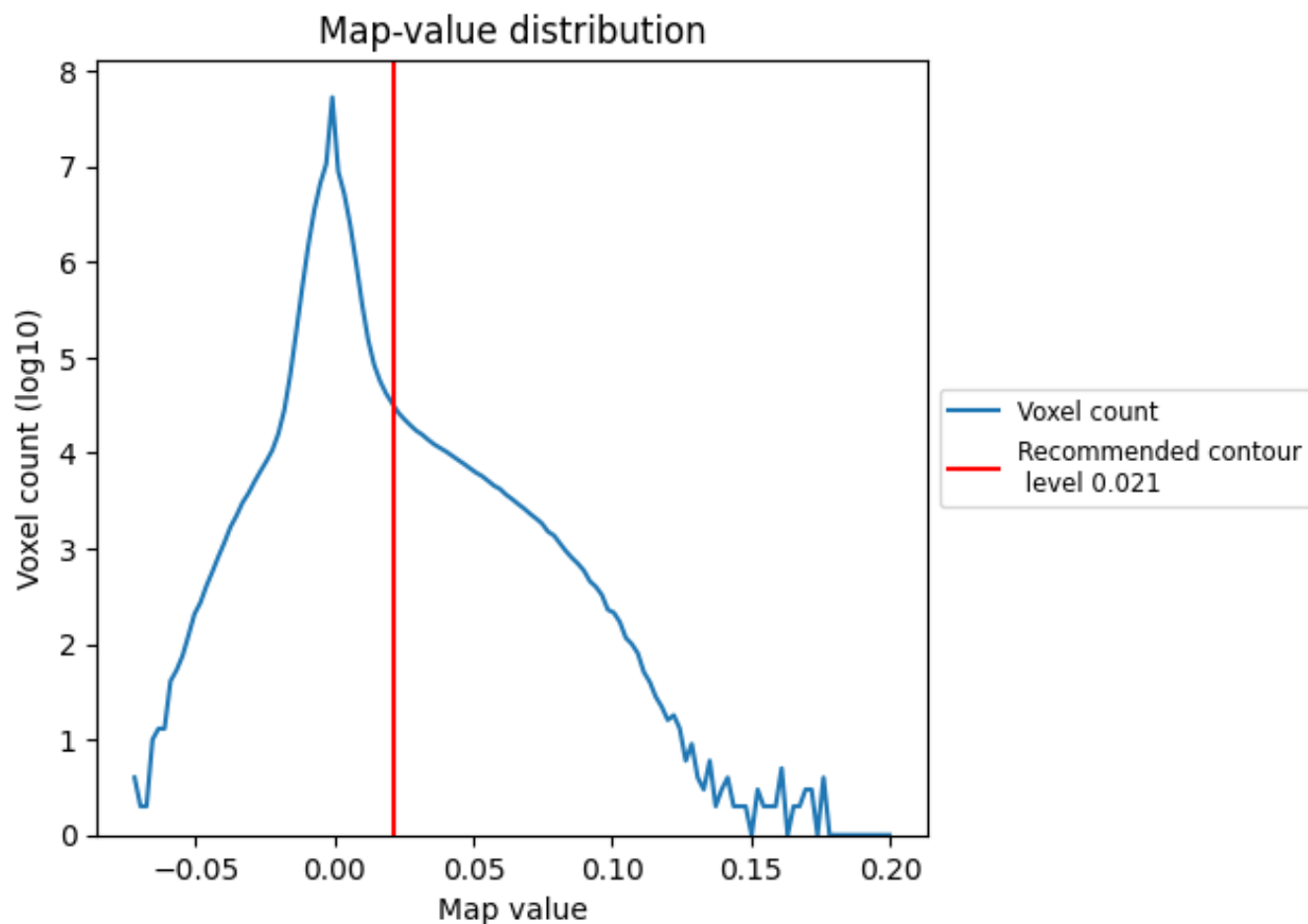
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

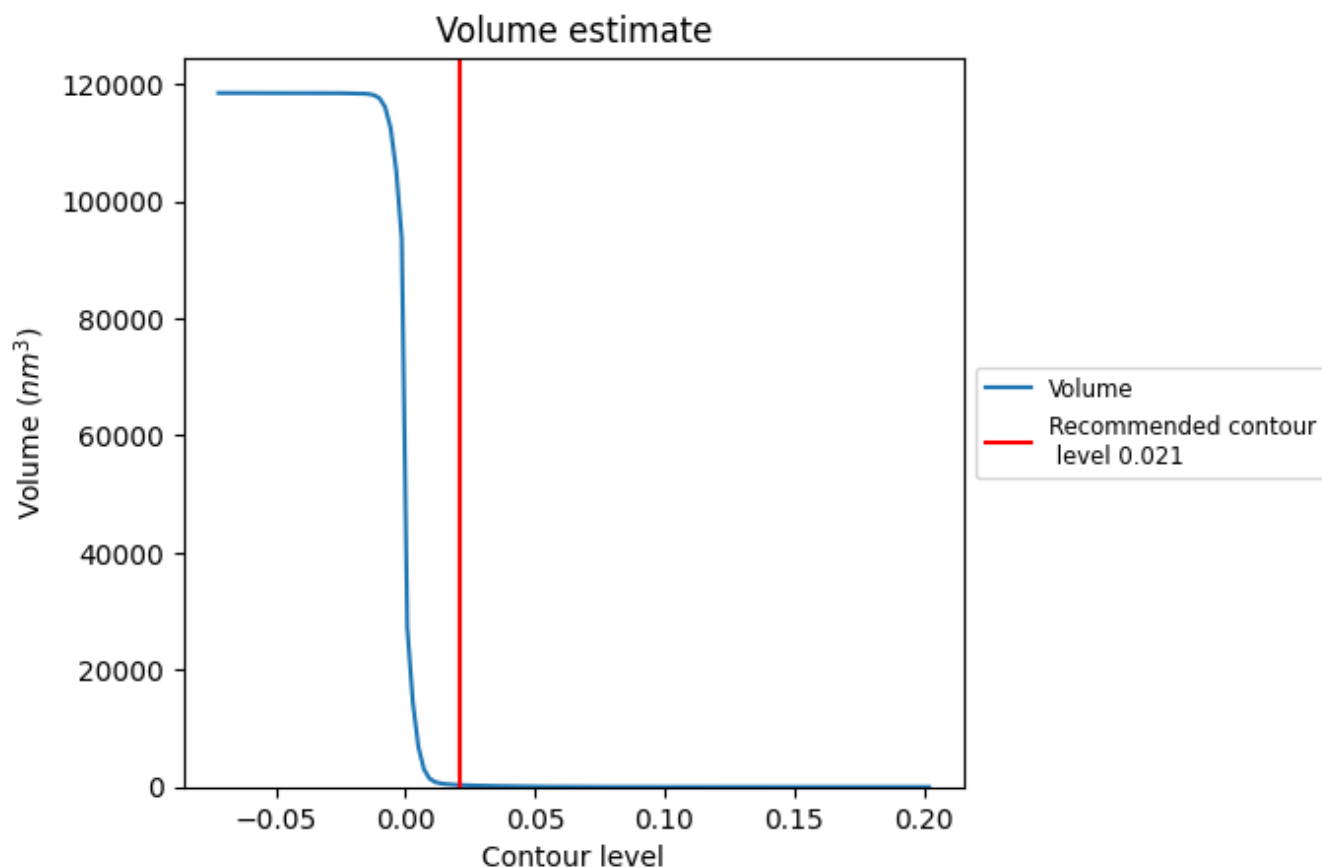
This section contains the results of statistical analysis of the map.

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.

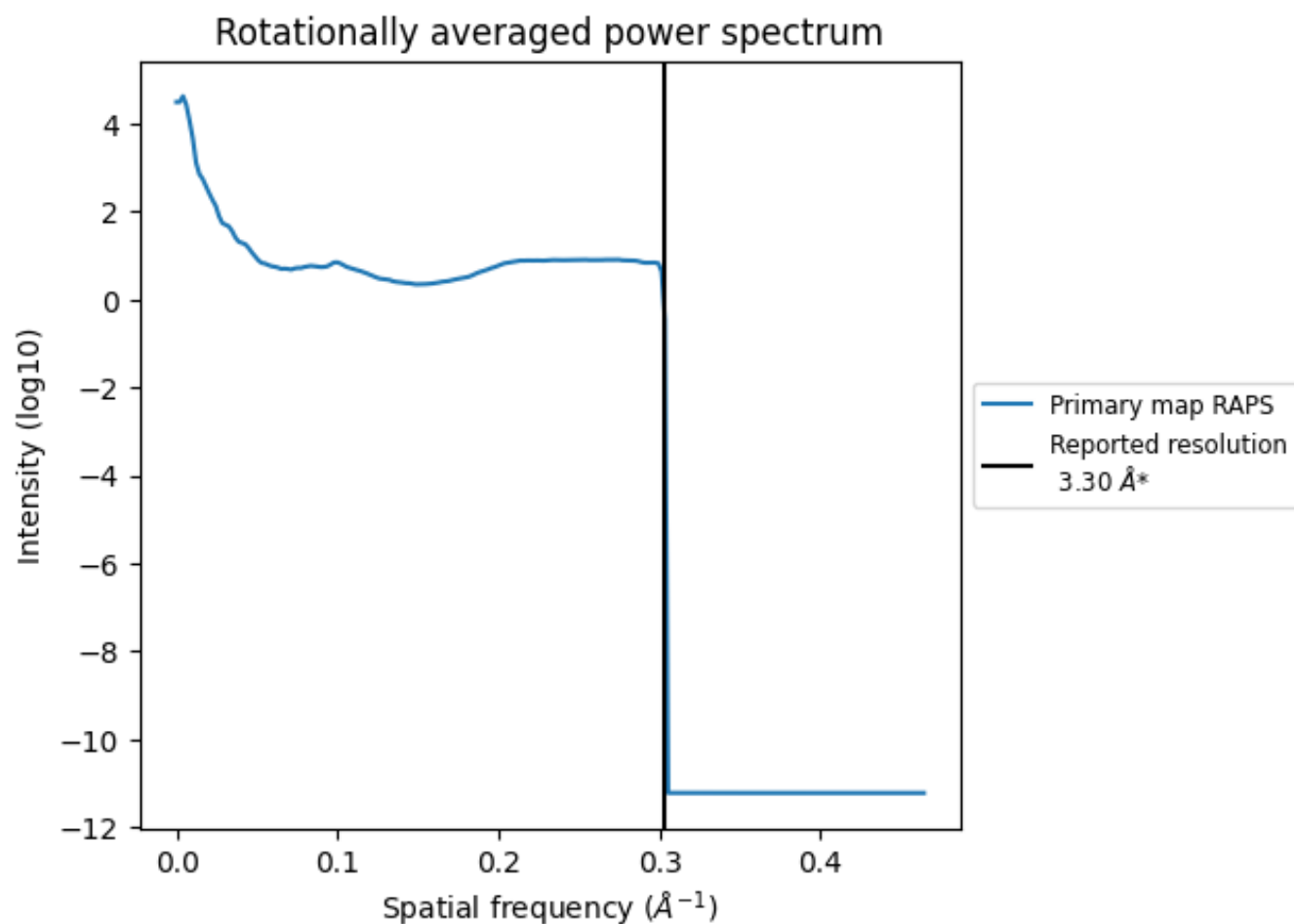
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm^3 ; this corresponds to an approximate mass of 300 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 ⓘ

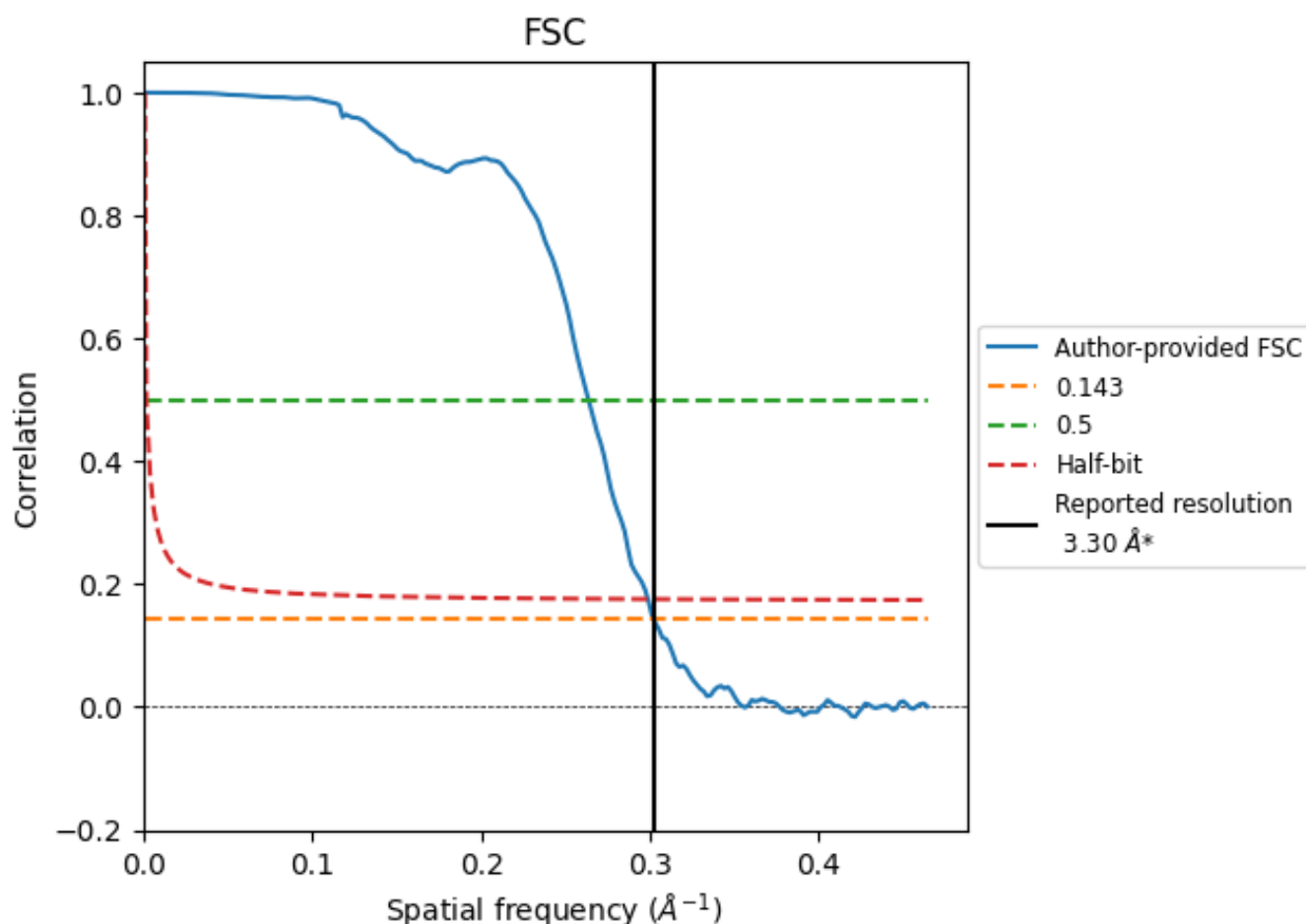


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

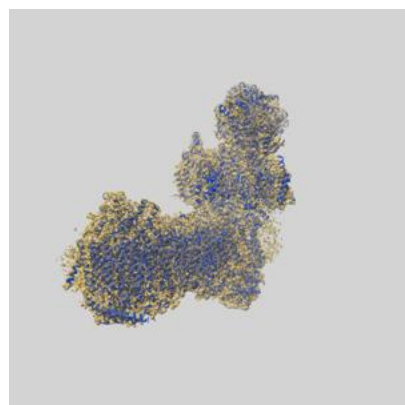
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.79	3.35
Unmasked-calculated*	-	-	-

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

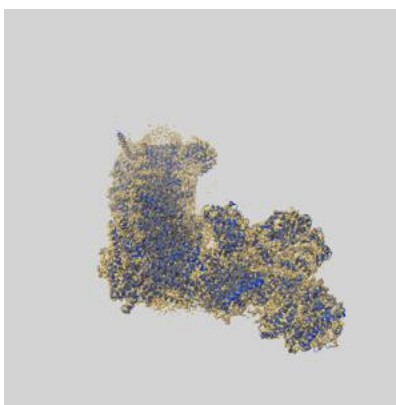
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4872 and PDB model 6RFQ. Per-residue inclusion information can be found in section 3 on page 20.

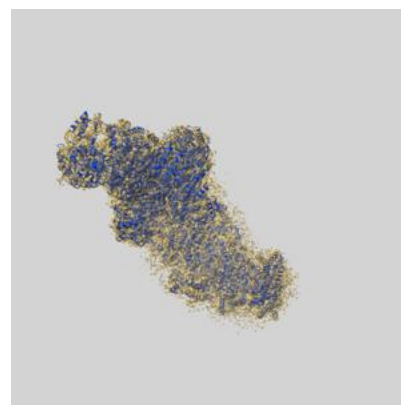
9.1 Map-model overlay [i](#)



X



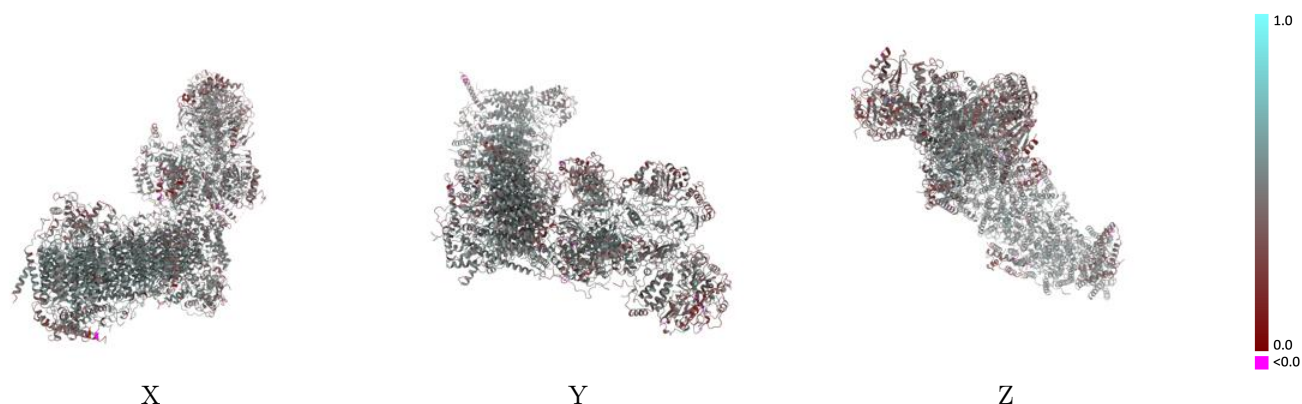
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

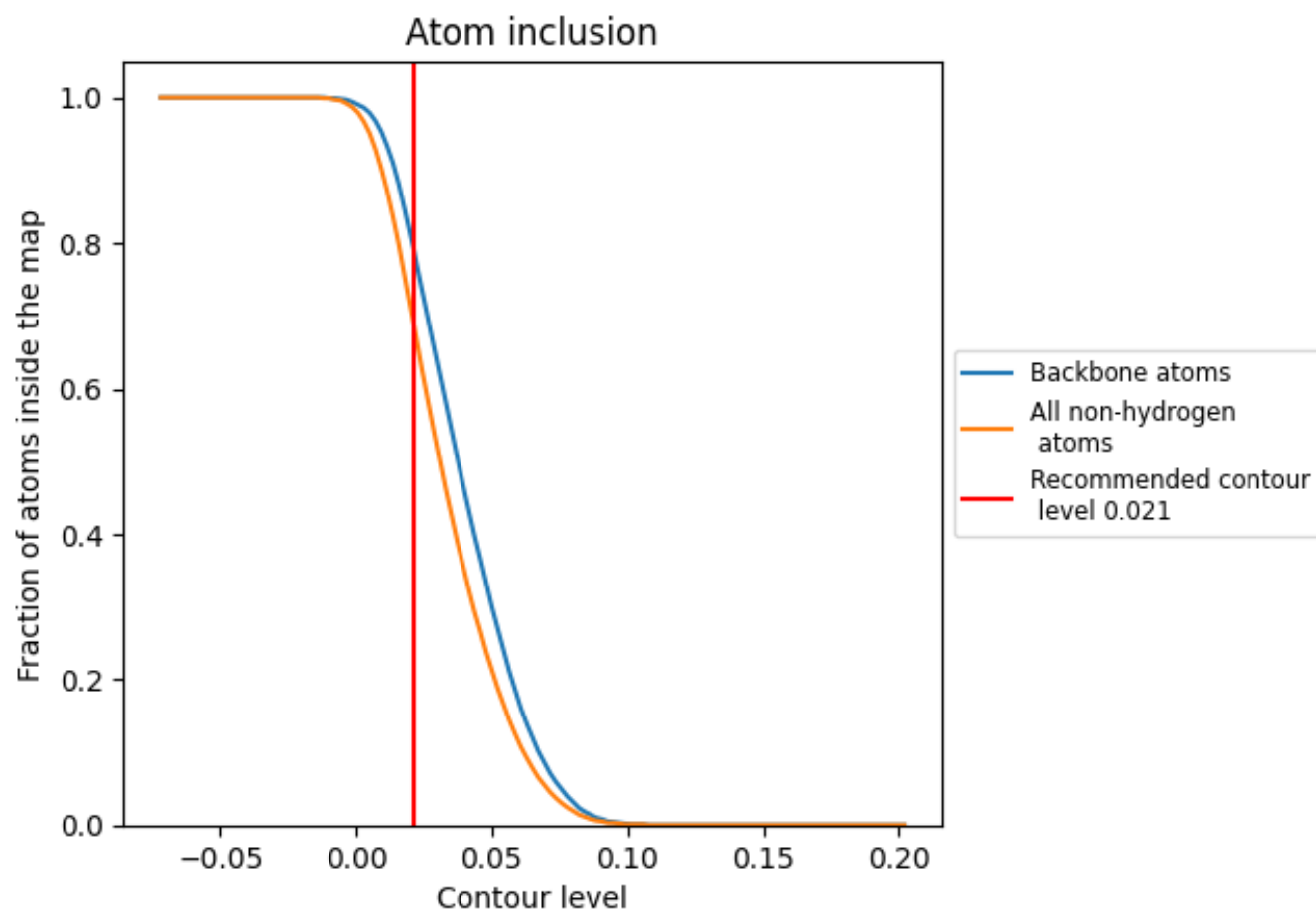


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.4610
1	 0.6690	 0.4590
2	 0.8160	 0.5260
3	 0.6280	 0.4540
4	 0.7960	 0.5180
5	 0.7880	 0.5070
6	 0.6860	 0.4790
8	 0.6240	 0.3730
9	 0.6450	 0.4420
A	 0.6570	 0.4430
B	 0.5670	 0.4070
C	 0.7390	 0.4810
D	 0.7270	 0.4740
E	 0.5790	 0.4320
F	 0.6790	 0.4350
G	 0.7890	 0.5030
H	 0.5090	 0.3680
I	 0.7490	 0.4830
J	 0.7240	 0.4610
K	 0.6240	 0.4520
L	 0.7550	 0.4760
O	 0.3310	 0.3060
P	 0.6350	 0.4270
Q	 0.5900	 0.3990
R	 0.6970	 0.4260
S	 0.6480	 0.3910
U	 0.6920	 0.4590
W	 0.6840	 0.4630
X	 0.7590	 0.4860
Y	 0.7060	 0.4810
Z	 0.6550	 0.4430
a	 0.7480	 0.4430
b	 0.7930	 0.5000
c	 0.6870	 0.4150
d	 0.7840	 0.4840



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.6990	 0.4640
f	 0.4840	 0.3600
g	 0.7760	 0.5230
i	 0.7540	 0.4620
j	 0.7250	 0.4790
k	 0.3270	 0.3570
n	 0.7130	 0.4680