



wwPDB EM Validation Summary Report ⓘ

May 6, 2025 – 04:08 AM EDT

PDB ID : 8ESZ / pdb_00008esz
EMDB ID : EMD-28582
Title : Structure of mitochondrial complex I from *Drosophila melanogaster*, Helix-locked state
Authors : Padavannil, A.; Letts, J.A.
Deposited on : 2022-10-15
Resolution : 3.40 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

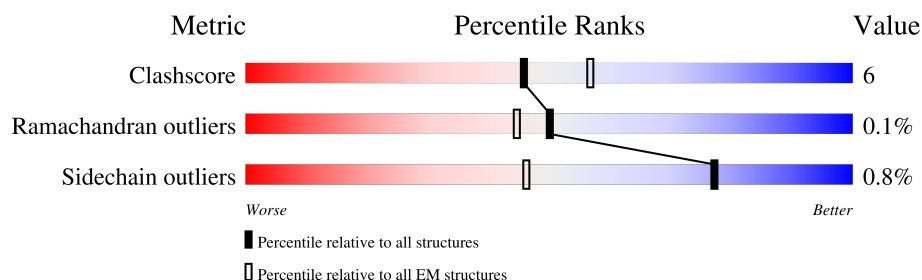
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	AN	142	<div> <div>12%</div> <div>80%</div> <div>15%</div> <div>• •</div> </div>
2	S6	126	<div> <div>•</div> <div>63%</div> <div>7%</div> <div>29%</div> </div>
3	S1	731	<div> <div>8%</div> <div>80%</div> <div>13%</div> <div>7%</div> </div>
4	S3	265	<div> <div>•</div> <div>64%</div> <div>14%</div> <div>23%</div> </div>
5	V2	242	<div> <div>14%</div> <div>78%</div> <div>10%</div> <div>12%</div> </div>
6	S7	221	<div> <div>•</div> <div>61%</div> <div>21%</div> <div>•</div> <div>18%</div> </div>
7	S8	217	<div> <div>•</div> <div>72%</div> <div>14%</div> <div>14%</div> </div>
8	1	315	<div> <div>79%</div> <div>20%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	4	446	
10	5	577	
11	A8	175	
12	A1	123	
13	AO	154	
14	S5	101	
15	AM	170	
16	BL	159	
17	B6	167	
18	B4	113	
19	B7	117	
20	B5	186	
21	B9	144	
22	BM	150	
23	B8	175	
24	B3	110	
25	AB	152	
25	AC	152	
26	C2	116	
27	B1	56	
28	S4	183	
29	A9	416	
30	B2	94	
31	S2	468	
32	V3	37	

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Mol	Chain	Length	Quality of chain
33	V1	474	
34	2	341	
35	A7	103	
36	A3	77	
37	4L	96	
38	6	174	
39	3	117	
40	A5	124	
41	AL	407	
42	A6	124	

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
46	SF4	S7	301	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 67757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AN	136	Total	C	N	O	S	0	0
			1145	747	191	202	5		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S6	89	Total	C	N	O	S	0	0
			716	453	130	129	4		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S1	683	Total	C	N	O	S	0	0
			5181	3246	919	987	29		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S3	205	Total	C	N	O	S	0	0
			1699	1086	298	310	5		

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V2	214	Total	C	N	O	S	0	0
			1680	1062	285	321	12		

- Molecule 6 is a protein called LD31474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	182	Total	C	N	O	S	0	0
			1435	920	251	250	14		

- Molecule 7 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	186	Total	C	N	O	S	0	0
			1485	935	251	287	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	315	Total	C	N	O	S	0	0
			2571	1764	367	418	22		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4	446	Total	C	N	O	S	0	0
			3606	2450	533	581	42		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	577	Total	C	N	O	S	0	0
			4606	3092	680	774	60		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A8	174	Total	C	N	O	S	0	0
			1384	867	240	267	10		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A1	70	Total	C	N	O	S	0	0
			581	375	97	103	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AO	146	Total	C	N	O	S	0	0
			1202	787	203	210	2		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S5	100	Total	C	N	O	S	0	0
			828	523	145	149	11		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	168	Total	C	N	O	S	0	0
			1281	832	212	230	7		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	151	Total	C	N	O	S	0	0
			1266	794	232	230	10		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B6	161	Total	C	N	O	S	0	0
			1302	829	242	226	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B4	107	Total	C	N	O	S	0	0
			884	566	162	155	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B7	117	Total	C	N	O	S	0	0
			972	617	170	175	10		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B5	143	Total	C	N	O	S	0	0
			1221	787	209	222	3		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B9	134	Total	C	N	O	S	0	0
			1148	732	217	196	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BM	106	Total	C	N	O	S	0	0
			871	560	140	170	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B8	144	Total	C	N	O	S	0	0
			1201	783	191	223	4		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B3	81	Total	C	N	O	S	0	0
			646	421	113	111	1		

- Molecule 25 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AC	85	Total	C	N	O	S	0	0
			680	438	103	137	2		
25	AB	84	Total	C	N	O	S	0	0
			670	433	102	133	2		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C2	115	Total	C	N	O	S	0	0
			908	590	159	158	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B1	55	Total	C	N	O	S	0	0
			430	278	76	74	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S4	151	Total	C	N	O	S	0	0
			1214	756	227	227	4		

- Molecule 29 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A9	377	Total	C	N	O	S	0	0
			3030	1931	546	543	10		

- Molecule 30 is a protein called GEO11417p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B2	60	Total	C	N	O	S	0	0
			495	323	88	83	1		

- Molecule 31 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S2	429	Total	C	N	O	S	0	0
			3427	2197	578	629	23		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	V3	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochond-

drial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V1	438	Total	C	N	O	S	0	0
			3361	2121	599	615	26		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2	341	Total	C	N	O	S	0	0
			2797	1893	411	459	34		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A7	91	Total	C	N	O	S	0	0
			736	463	138	134	1		

- Molecule 36 is a protein called RH45008p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	A3	66	Total	C	N	O	S	0	0
			519	327	95	96	1		

- Molecule 37 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4L	96	Total	C	N	O	S	0	0
			794	540	113	128	13		

- Molecule 38 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6	174	Total	C	N	O	S	0	0
			1404	949	202	236	17		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3	117	Total	C	N	O	S	0	0
			956	652	141	156	7		

- Molecule 40 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A5	117	Total	C	N	O	S	0	0
			914	584	161	165	4		

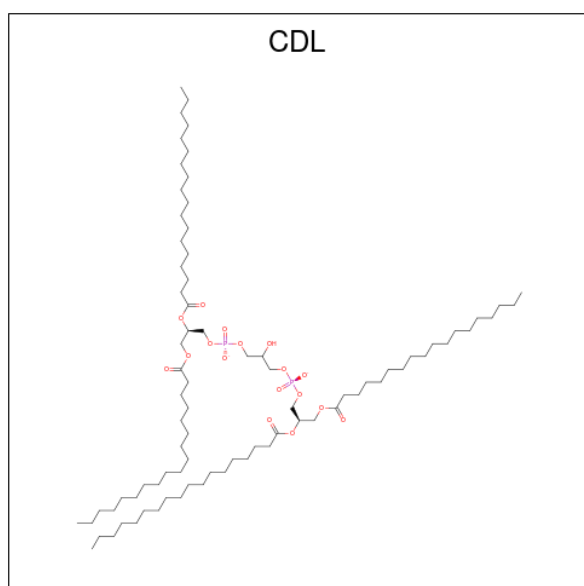
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AL	368	Total	C	N	O	S	0	0
			3008	1927	504	561	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	A6	115	Total	C	N	O	S	0	0
			977	624	174	173	6		

- Molecule 43 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



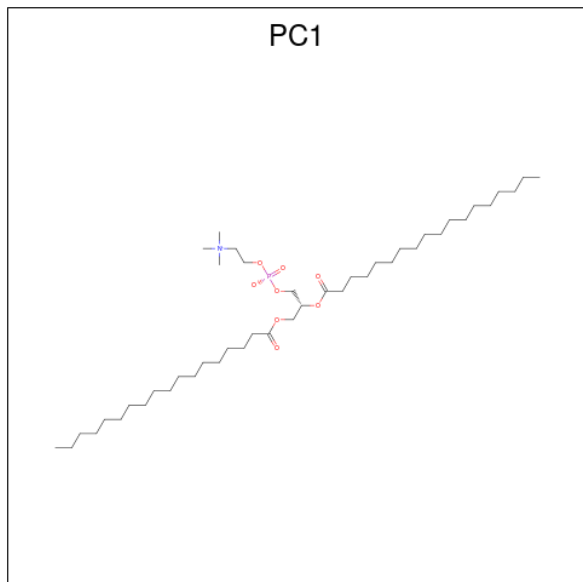
Mol	Chain	Residues	Atoms				AltConf
43	AN	1	Total	C	O	P	0
			67	48	17	2	
43	AM	1	Total	C	O	P	0
			76	57	17	2	
43	B6	1	Total	C	O	P	0
			47	28	17	2	

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Mol	Chain	Residues	Atoms				AltConf
43	B5	1	Total	C	O	P	0
			76	57	17	2	
43	B5	1	Total	C	O	P	0
			66	47	17	2	
43	2	1	Total	C	O	P	0
			45	27	16	2	
43	6	1	Total	C	O	P	0
			86	67	17	2	
43	3	1	Total	C	O	P	0
			54	35	17	2	

- Molecule 44 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
44	AN	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	S7	1	Total	C	N	O	P	0
			46	36	1	8	1	
44	1	1	Total	C	N	O	P	0
			54	44	1	8	1	
44	4	1	Total	C	N	O	P	0
			39	29	1	8	1	
44	4	1	Total	C	N	O	P	0
			39	29	1	8	1	
44	5	1	Total	C	N	O	P	0
			34	24	1	8	1	

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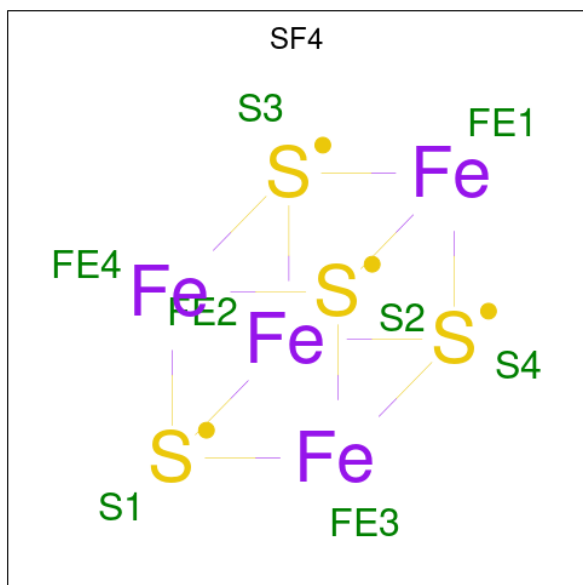
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Mol	Chain	Residues	Atoms					AltConf
44	AM	1	Total	C	N	O	P	0
			37	27	1	8	1	
44	AM	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	AM	1	Total	C	N	O	P	0
			32	22	1	8	1	
44	B6	1	Total	C	N	O	P	0
			37	27	1	8	1	
44	A9	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	2	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
45	S6	1	Total	Zn	0
			1	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



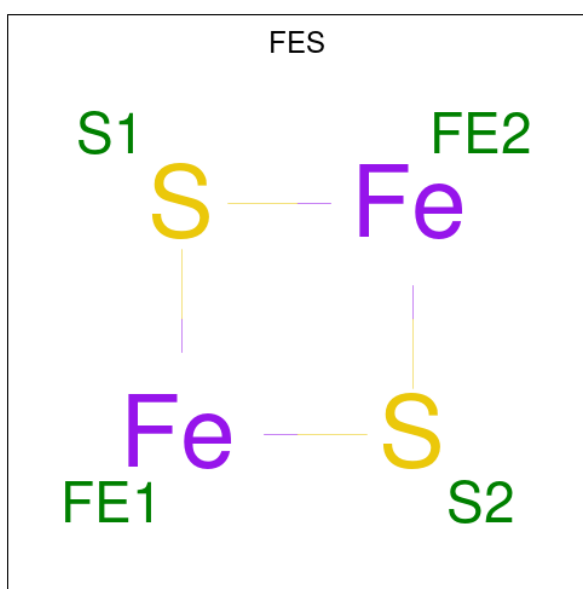
Mol	Chain	Residues	Atoms			AltConf
46	S1	1	Total	Fe	S	0
			8	4	4	
46	S1	1	Total	Fe	S	0
			8	4	4	

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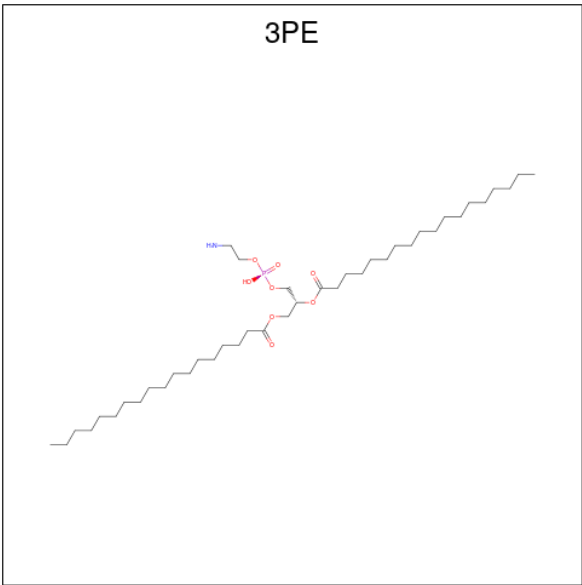
Mol	Chain	Residues	Atoms			AltConf
46	S7	1	Total	Fe	S	0
			8	4	4	
46	S8	1	Total	Fe	S	0
			8	4	4	
46	S8	1	Total	Fe	S	0
			8	4	4	
46	V1	1	Total	Fe	S	0
			8	4	4	

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



Mol	Chain	Residues	Atoms			AltConf
47	S1	1	Total	Fe	S	0
			4	2	2	
47	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$).



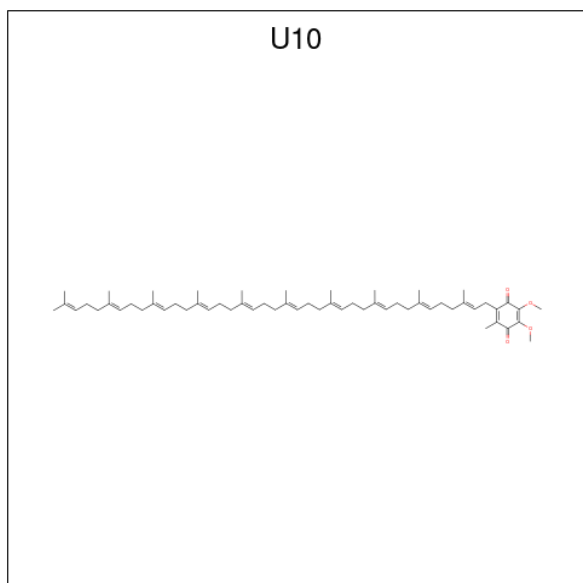
Mol	Chain	Residues	Atoms					AltConf
48	S7	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	S7	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	1	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	4	1	Total	C	N	O	P	0
			32	22	1	8	1	
48	4	1	Total	C	N	O	P	0
			45	35	1	8	1	
48	4	1	Total	C	N	O	P	0
			36	26	1	8	1	
48	4	1	Total	C	N	O	P	0
			39	29	1	8	1	
48	5	1	Total	C	O	P		0
			32	23	8	1		
48	5	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	5	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	5	1	Total	C	N	O	P	0
			30	20	1	8	1	
48	5	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	5	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	5	1	Total	C	N	O	P	0
			45	35	1	8	1	

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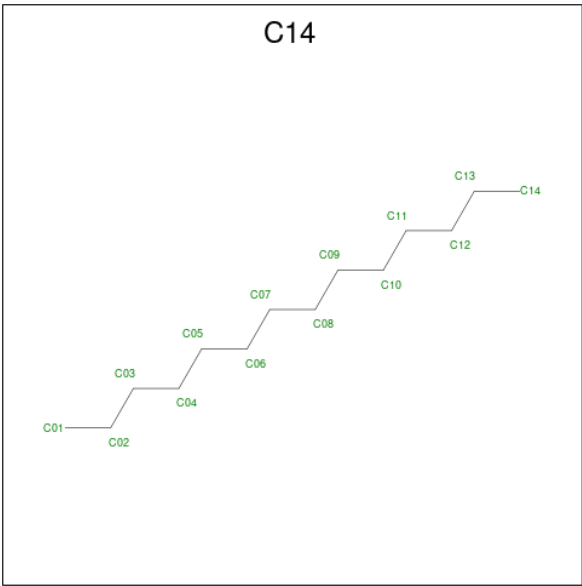
Mol	Chain	Residues	Atoms					AltConf
48	AM	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	AM	1	Total	C	N	O	P	0
			31	21	1	8	1	
48	B6	1	Total	C	O	P		0
			48	39	8	1		
48	B4	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	C2	1	Total	C	N	O	P	0
			45	35	1	8	1	
48	B1	1	Total	C	N	O	P	0
			37	27	1	8	1	
48	2	1	Total	C	N	O	P	0
			30	20	1	8	1	
48	6	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	3	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	3	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 49 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



Mol	Chain	Residues	Atoms			AltConf
49	1	1	Total	C	O	0
			63	59	4	

- Molecule 50 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).



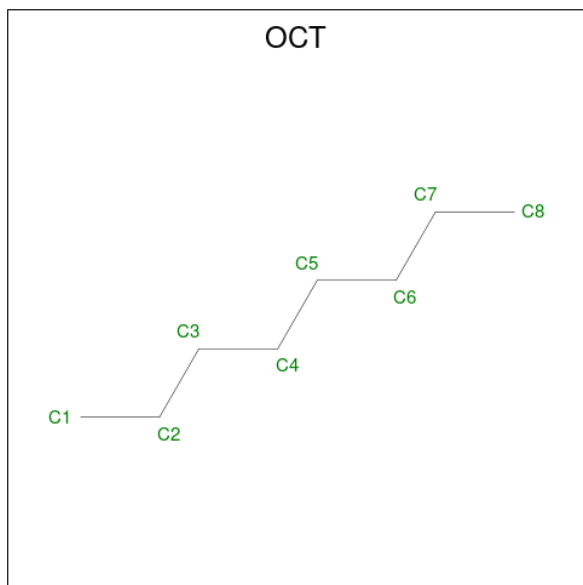
Mol	Chain	Residues	Atoms	AltConf
50	AO	1	Total C 14 14	0
50	B5	1	Total C 14 14	0
50	C2	1	Total C 14 14	0

- Molecule 51 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



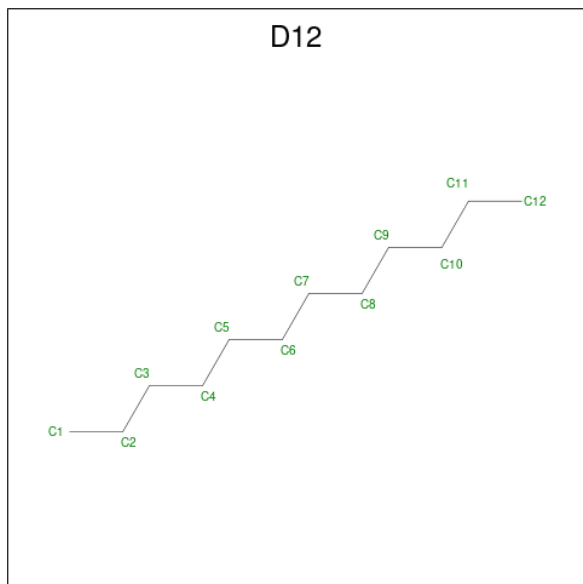
Mol	Chain	Residues	Atoms						AltConf
51	AC	1	Total 34	C 23	N 2	O 7	P 1	S 1	0
51	AB	1	Total 32	C 21	N 2	O 7	P 1	S 1	0

- Molecule 52 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



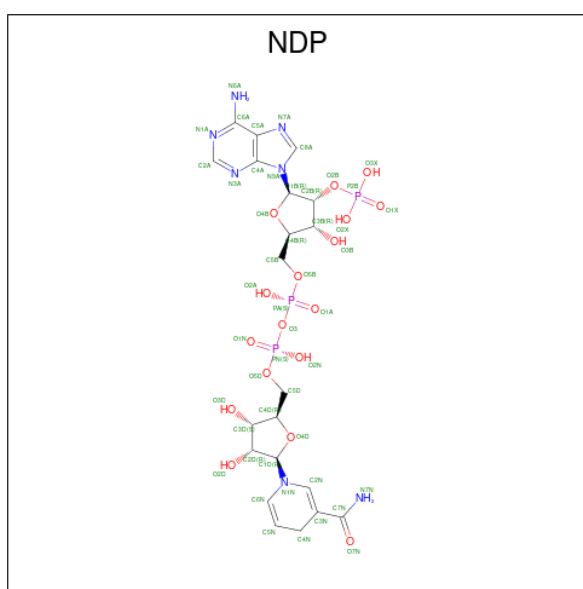
Mol	Chain	Residues	Atoms		AltConf
52	B1	1	Total	C	0
			8	8	

- Molecule 53 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



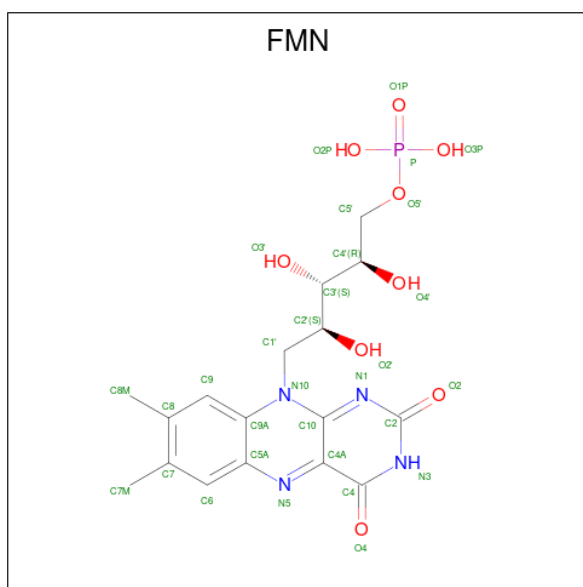
Mol	Chain	Residues	Atoms	AltConf
53	B1	1	Total C 12 12	0
53	A9	1	Total C 12 12	0
53	A9	1	Total C 12 12	0
53	A3	1	Total C 12 12	0

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



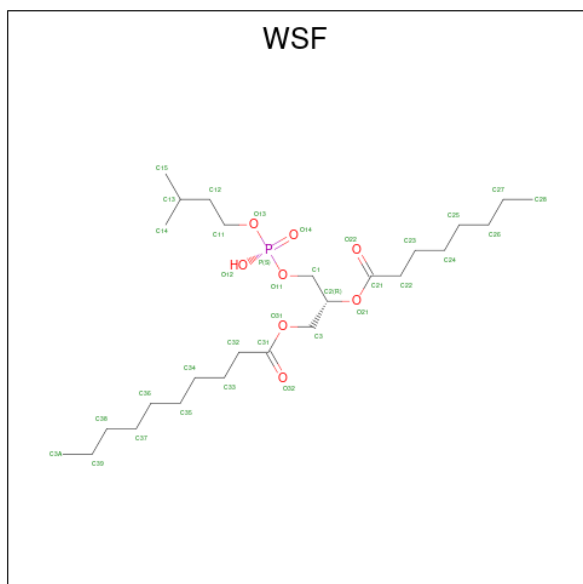
Mol	Chain	Residues	Atoms					AltConf
54	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 55 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



Mol	Chain	Residues	Atoms					AltConf
55	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 56 is (2R)-3-{[(S)-hydroxy(3-methylbutoxy)phosphoryl]oxy}-2-(octanoyloxy)propyl decanoate (CCD ID: WSF) (formula: $C_{26}H_{51}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
56	6	1	Total	C	O	P	0
			35	26	8	1	

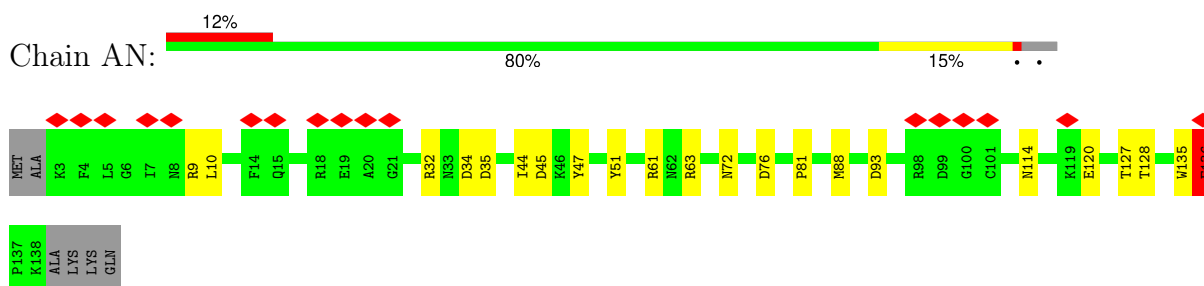
- Molecule 57 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



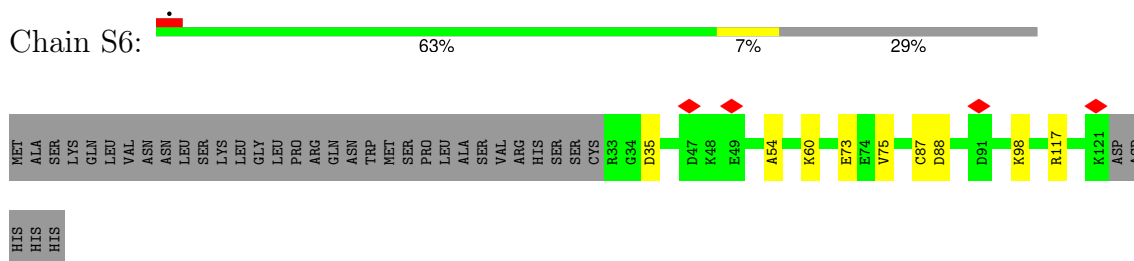
3 Residue-property plots [i](#)

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

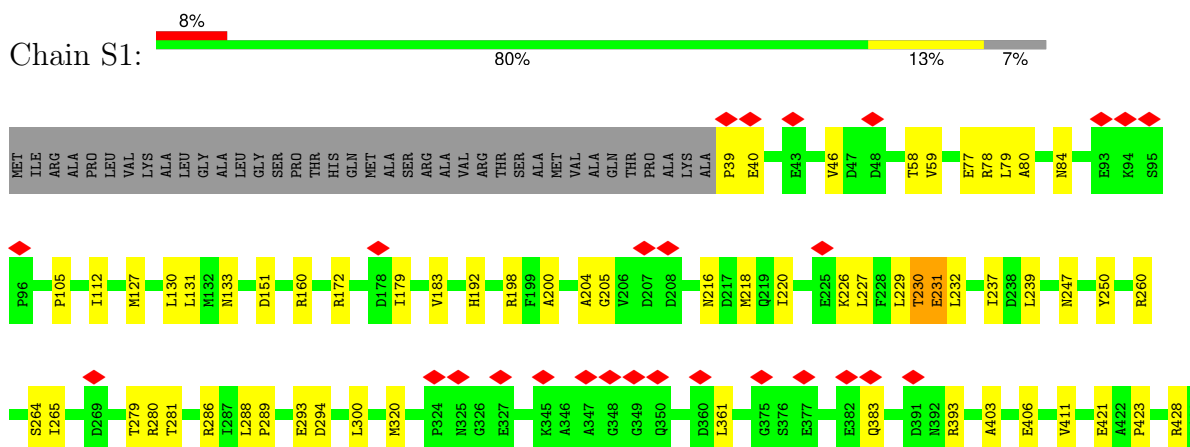
- Molecule 1: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

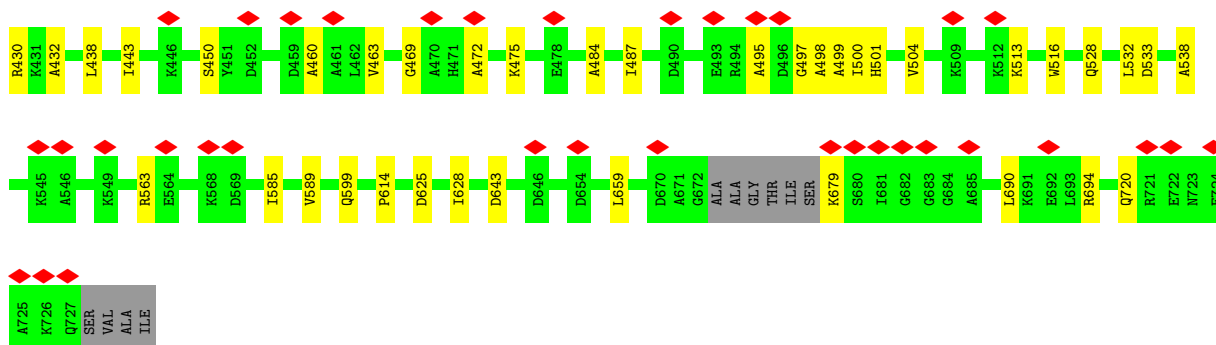


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

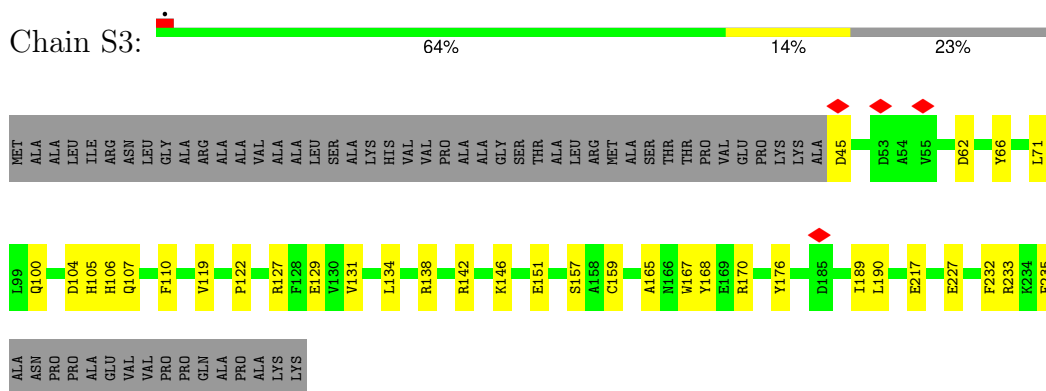


- Molecule 3: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

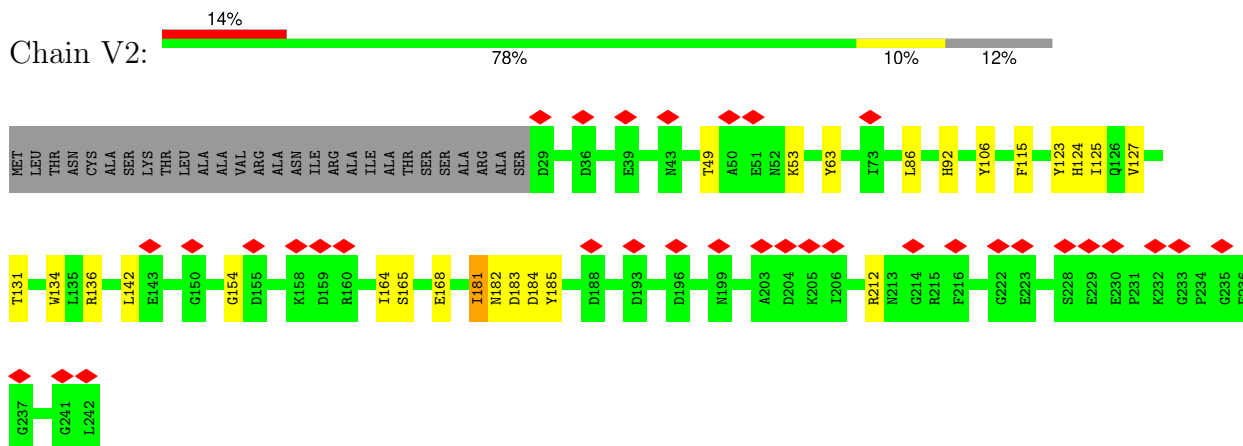




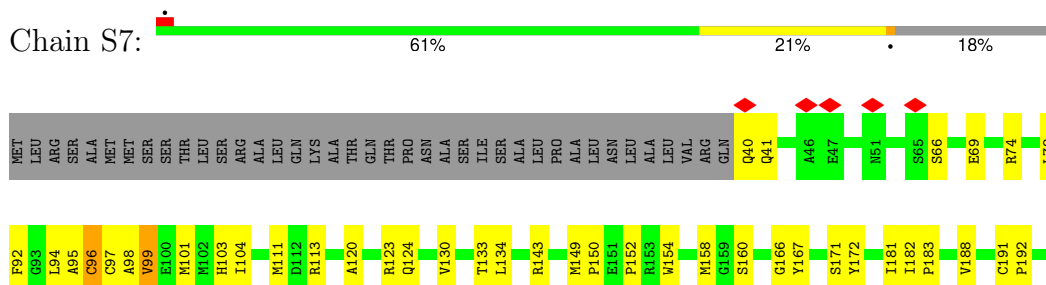
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A



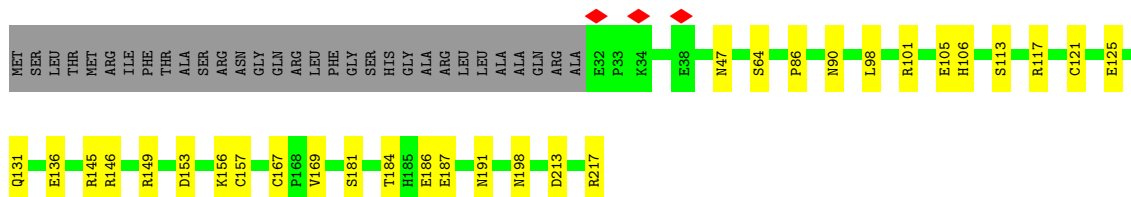
- Molecule 6: LD31474p





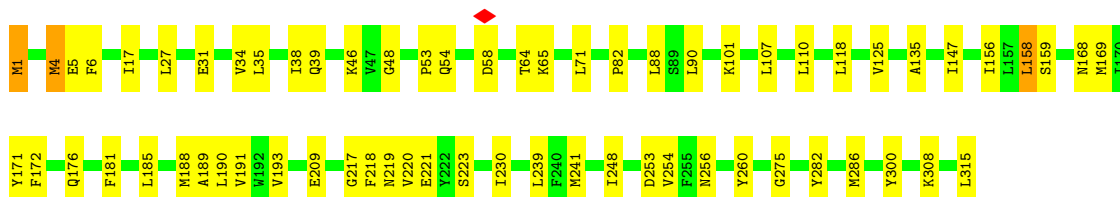
- Molecule 7: NADH dehydrogenase (ubiquinone) 23 kDa subunit

Chain S8: 72% 14% 14%



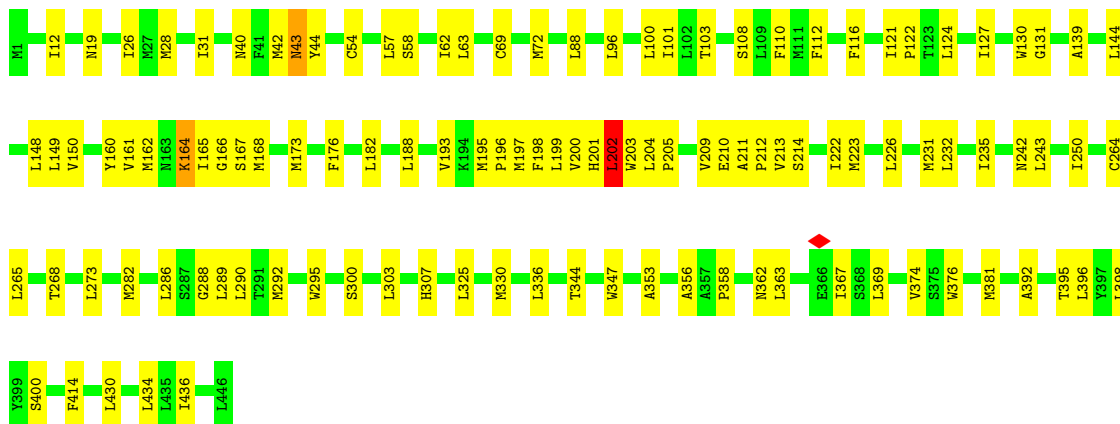
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1: 79% 20%



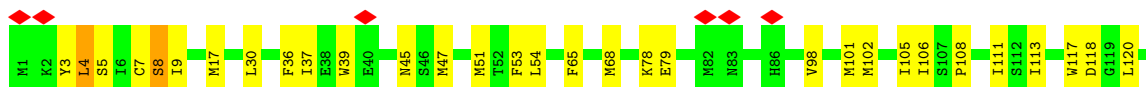
- Molecule 9: NADH-ubiquinone oxidoreductase chain 4

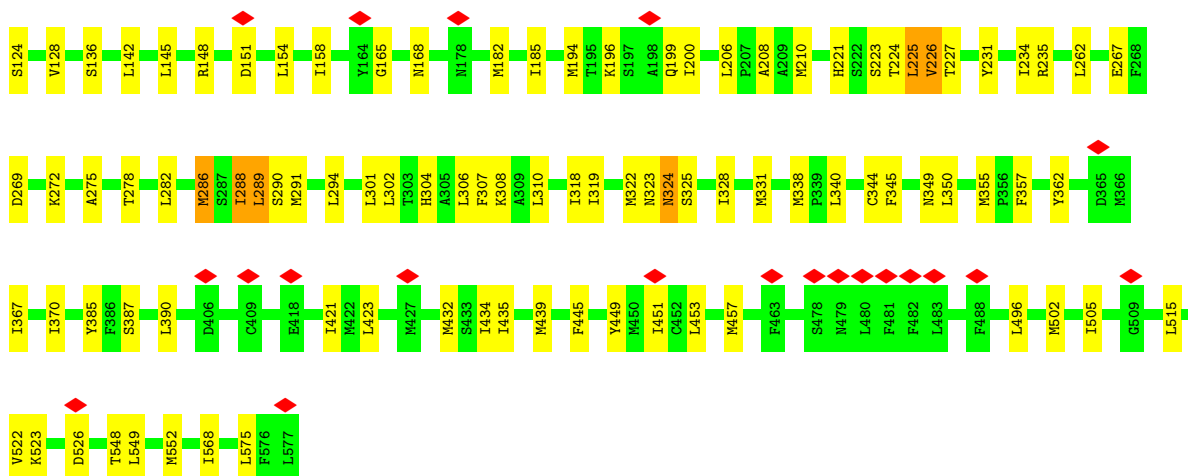
Chain 4: 75% 25%



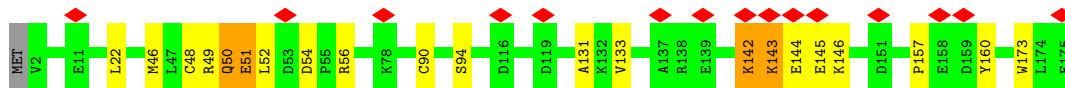
- Molecule 10: NADH-ubiquinone oxidoreductase chain 5

Chain 5: 5% 78% 20%

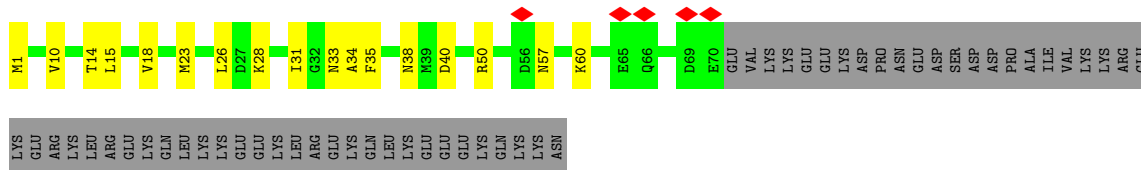




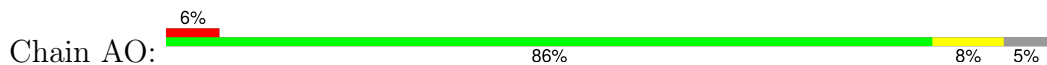
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



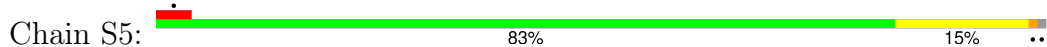
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



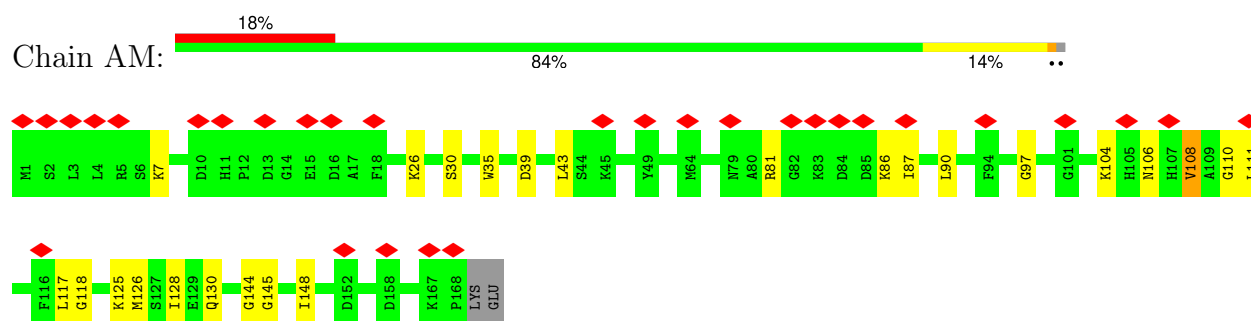
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



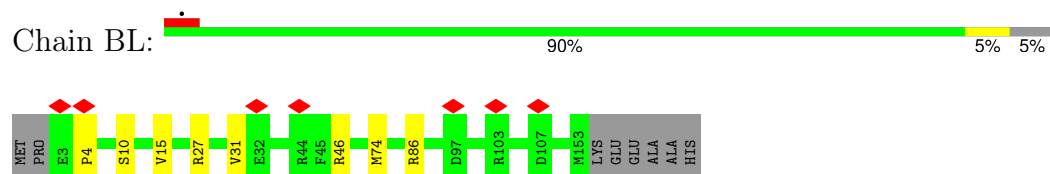
- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



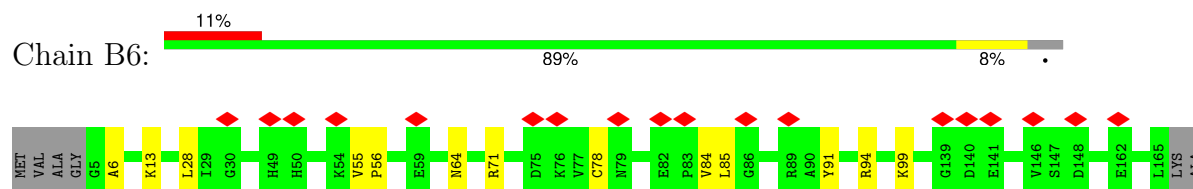
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



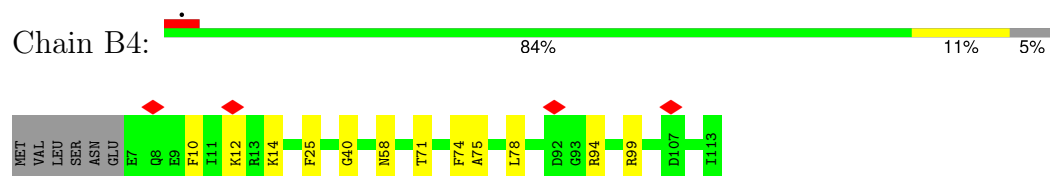
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



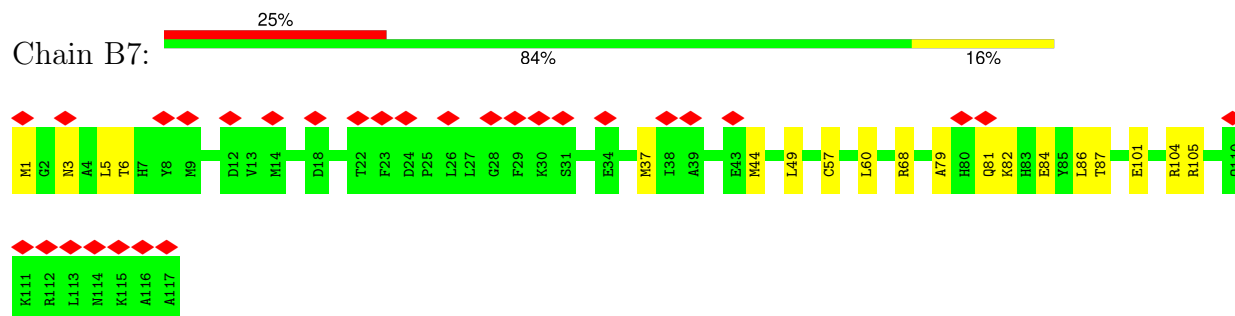
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

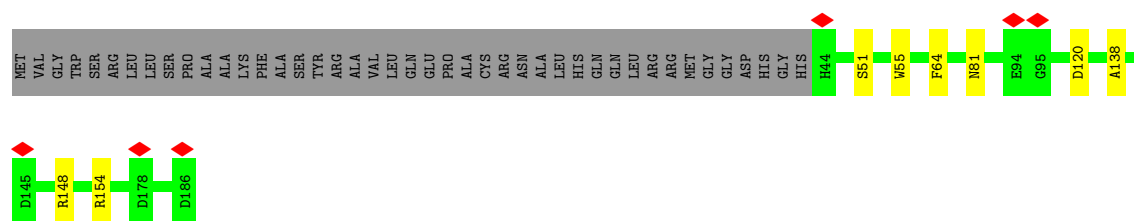


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

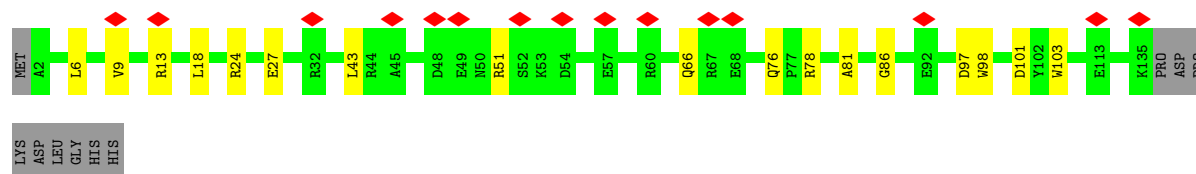
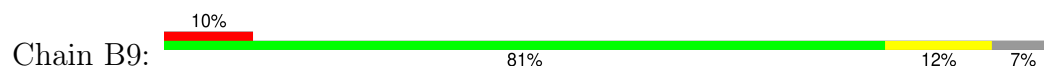


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

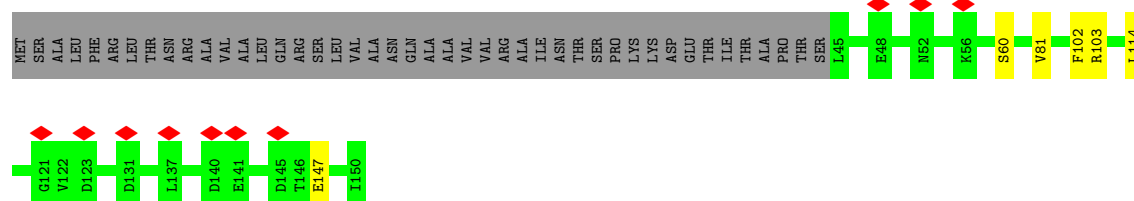




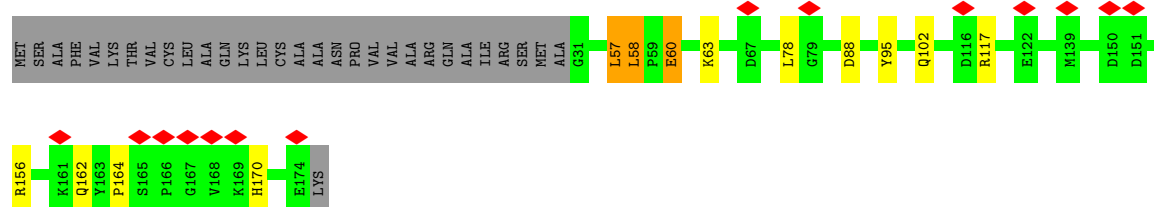
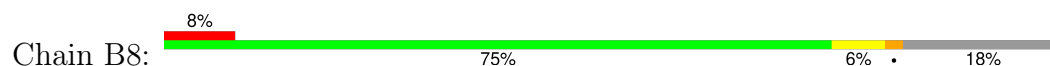
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



HIS
GLU
GLU
HIS
GLY
ASP
LYS
GLY
HIS
HIS

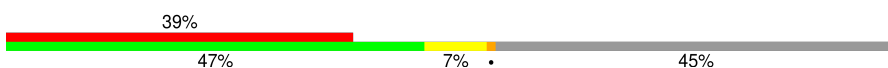
- Molecule 25: Acyl carrier protein, mitochondrial

Chain AC: 

MET SER PHE THR GLN ILE ALA ARG SER CYS SER ARG LEU LEU ALA ALA THR LEU LEU PRO ARG ARG VAL VAL VAL SER GLY ILE LEU LEU ILE ILE GLN SER SER GLN ALA SER ARG MET MET HIS ARG ILE ALA VAL PRO SER MET THR SER GLN LEU SER GLN GLU ARG CYS GLY ARG TRP GLN THR LEU

VAL ARG LYS TYR SER ALA LYS P68 P69 L86 L88 D87 D90 P91 S92 K93 L94 N95 V96 E97 F100 I101 N102 D103 L104 G105 L106 D107 D110 E119 D120 D128 A131 L134 P137 A138 D139 I140 Y143 K147 E148 E152

- Molecule 25: Acyl carrier protein, mitochondrial

Chain AB: 

MET SER PHE THR GLN ILE ALA ARG SER CYS SER ARG LEU LEU ALA ALA THR LEU LEU PRO ARG ARG VAL VAL VAL SER GLY ILE LEU LEU ILE ILE GLN SER SER GLN ALA SER ARG MET MET HIS ARG ILE ALA VAL PRO SER MET THR SER GLN LEU SER GLN GLU CYS ARG GLY ARG TRP GLN THR LEU

VAL ARG LYS TYR SER ALA LYS P68 P69 L70 S71 L72 K73 L74 E77 R78 V79 L80 L81 V82 L83 K84 L85 Y86 D87 K88 I89 D90 P91 S92 K93 L94 N95 V96 E97 S98 H99 F100 I101 N102 D103 L104 G105 L106 D107 D110 H111 V112 I115 E119 D120 G123 F124 E125 I126


P127 D128 S129 D130 A131 E132 K133 L134 L135 K136 P137 A138 D139 I140 I141 K142 Y143 V144 A145 D146 K147 E148 D149 V150 Y151 GLU

- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain C2: 


MET S2 D6 E9 K14 S23 G45 P49 S52 D95 D96 V115 K116

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

Chain B1: 

MET V2 L3 D6 K7 R8 R37 D38 G44 R45 P46 A47 G48 S49 E50 G51 K52 A53 V56

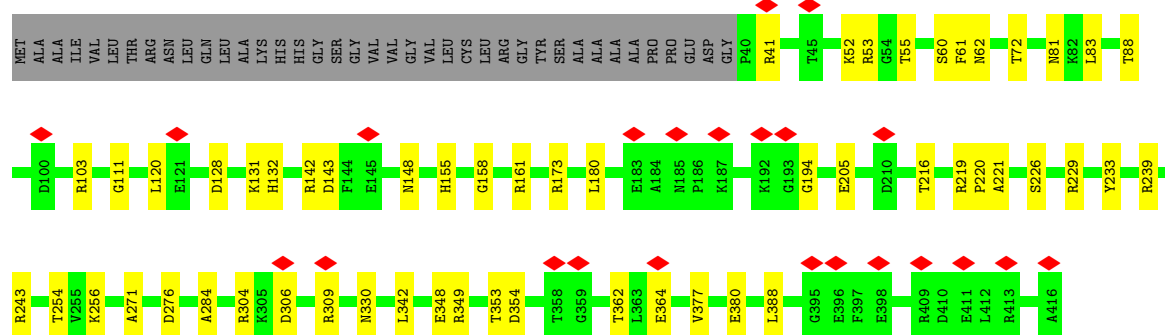
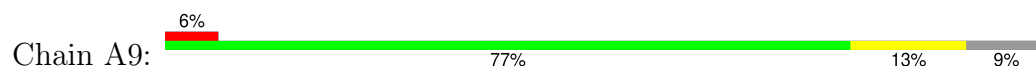
- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4: 

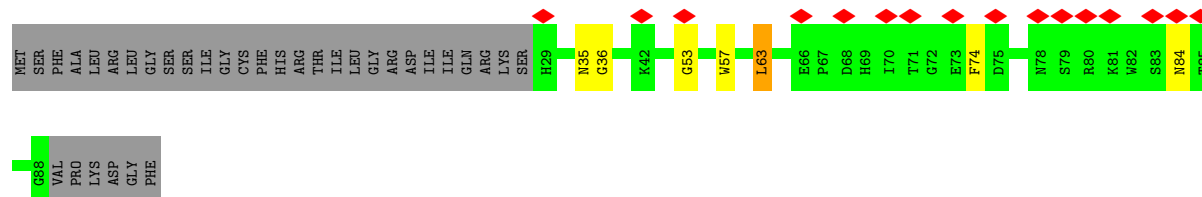
MET SER ALA LEU GLN MET CYS ARG THR SER ALA SER LEU GLN LEU LEU TYR GLN ALA ASN ARG ALA ALA ALA ARG TRP TRP SER THR ALA T33 D34 G35 D39 P40 K41 R46 P47 E48 E49 L50 E51 U52 R53 E77 E81 R82 R85 R86 Q95 I106



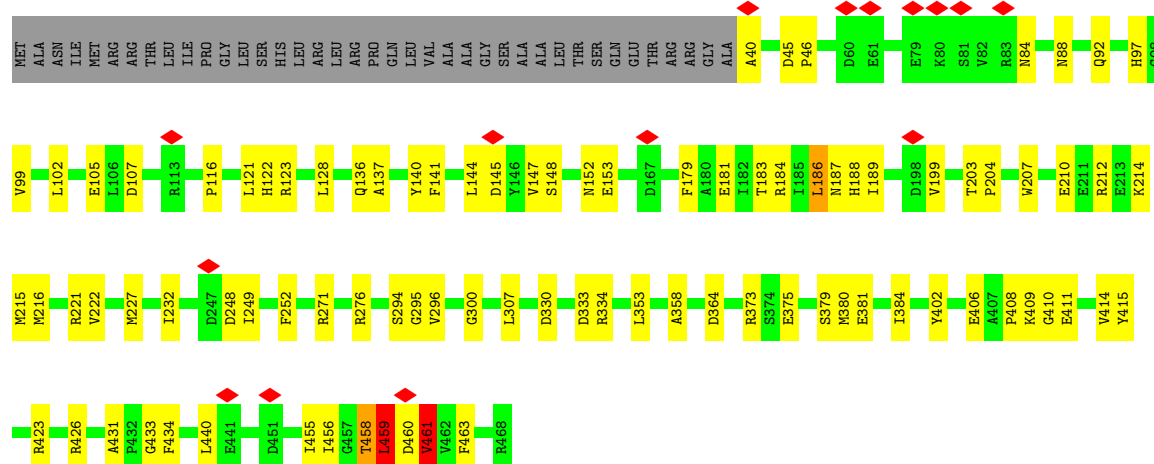
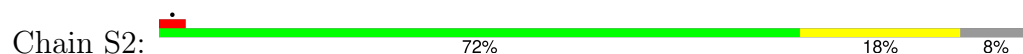
- Molecule 29: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A



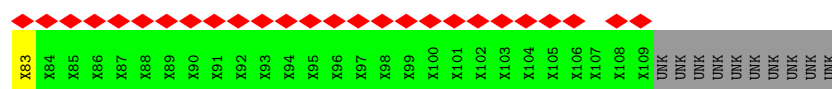
- Molecule 30: GEO11417p1



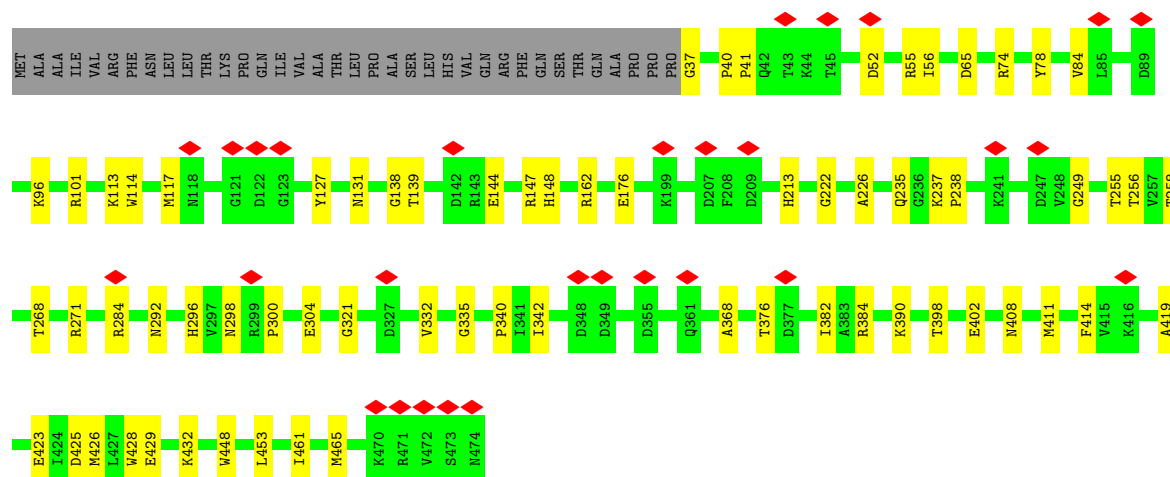
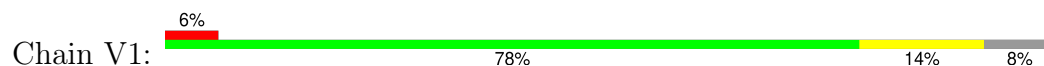
- Molecule 31: Complex I-49kD



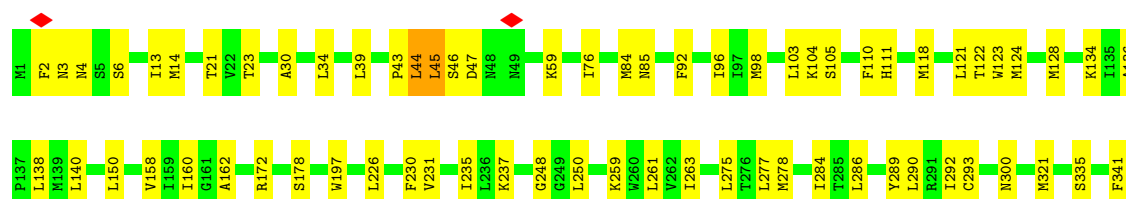
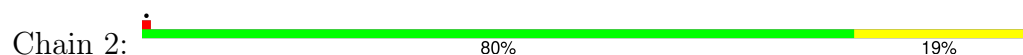
- Molecule 32: NADH dehydrogenase [ubiquinone] flavoprotein 3



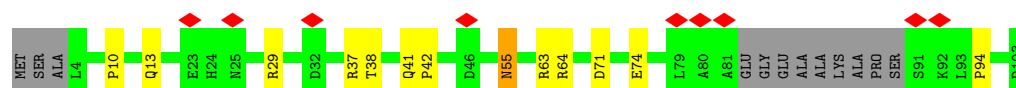
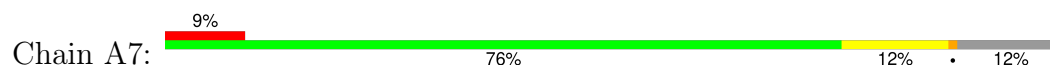
- Molecule 33: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



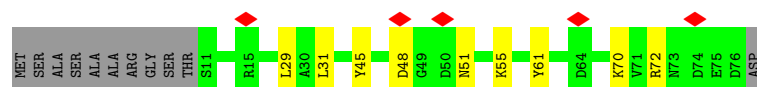
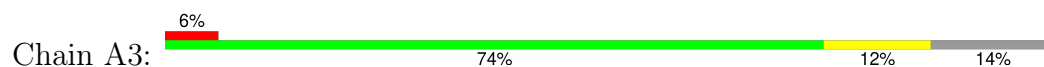
- Molecule 34: NADH-ubiquinone oxidoreductase chain 2



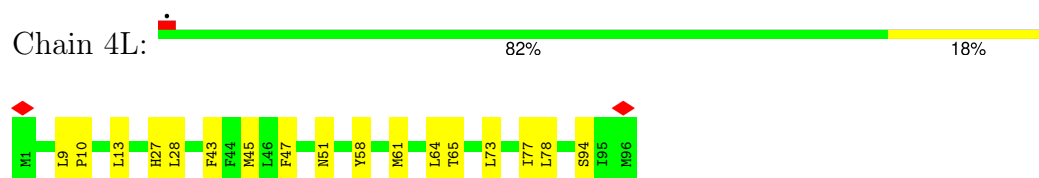
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



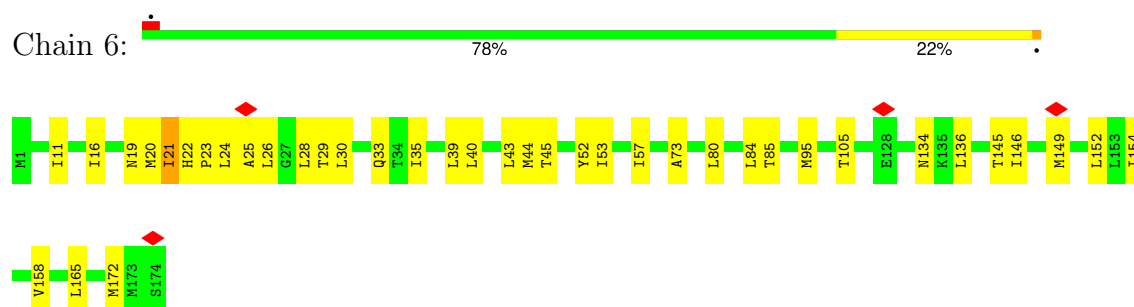
- Molecule 36: RH45008p



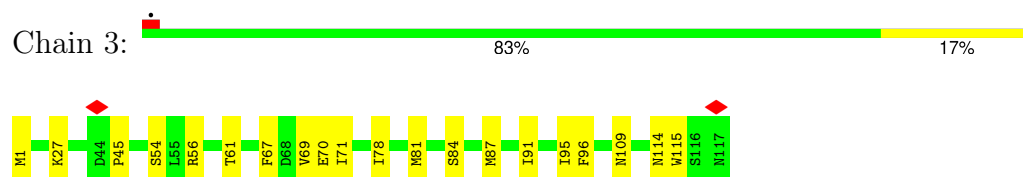
- Molecule 37: NADH-ubiquinone oxidoreductase chain 4L



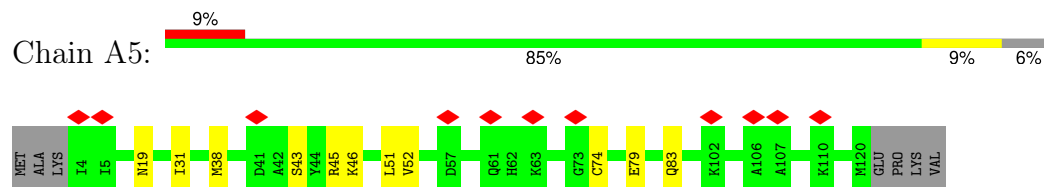
- Molecule 38: NADH-ubiquinone oxidoreductase chain 6



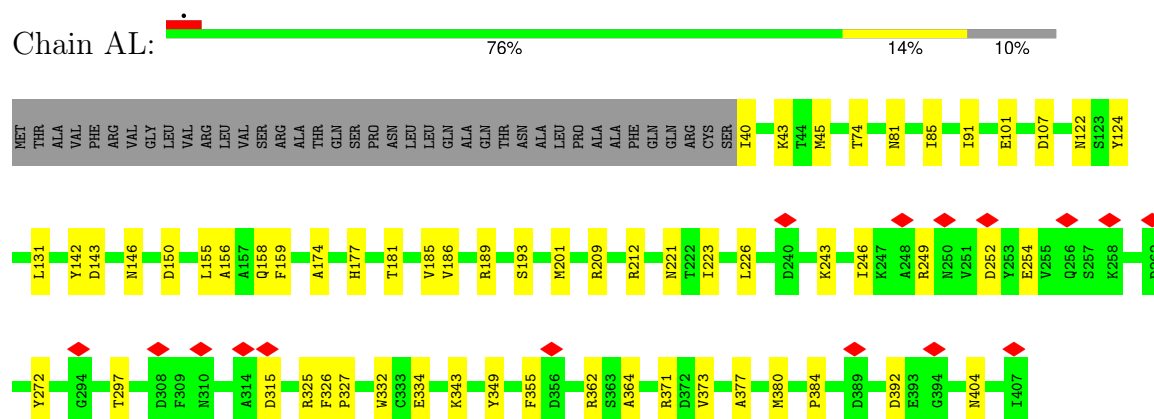
- Molecule 39: NADH-ubiquinone oxidoreductase chain 3



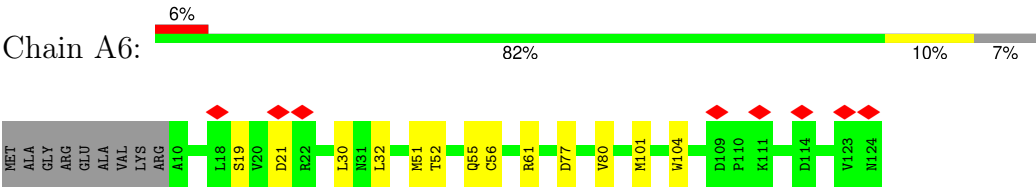
- Molecule 40: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	293389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.876	Depositor
Minimum map value	-1.949	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.55	Depositor
Map size (\AA)	450.56, 450.56, 450.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.88, 0.88, 0.88	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, NDP, OCT, SF4, U10, DGT, FMN, ZMP, C14, FES, D12, ZN, CDL, WSF, 3PE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AN	0.26	0/1185	0.54	0/1605
2	S6	0.13	0/733	0.33	0/987
3	S1	0.21	0/5264	0.52	1/7133 (0.0%)
4	S3	0.21	0/1745	0.49	0/2370
5	V2	0.24	0/1719	0.56	0/2328
6	S7	0.34	0/1473	0.66	1/1997 (0.1%)
7	S8	0.22	0/1518	0.50	0/2050
8	1	0.32	0/2651	0.62	0/3593
9	4	0.35	1/3711 (0.0%)	0.69	1/5029 (0.0%)
10	5	0.38	0/4726	0.71	1/6396 (0.0%)
11	A8	0.32	0/1417	0.57	0/1911
12	A1	0.24	0/594	0.57	0/801
13	AO	0.24	0/1240	0.47	0/1682
14	S5	0.22	0/846	0.54	0/1128
15	AM	0.27	0/1318	0.53	0/1790
16	BL	0.25	0/1299	0.57	0/1754
17	B6	0.21	0/1338	0.52	0/1808
18	B4	0.23	0/905	0.50	0/1210
19	B7	0.27	0/995	0.58	0/1336
20	B5	0.19	0/1255	0.44	0/1694
21	B9	0.21	0/1181	0.43	0/1593
22	BM	0.19	0/896	0.44	0/1222
23	B8	0.28	0/1250	0.53	0/1701
24	B3	0.17	0/665	0.41	0/903
25	AB	0.23	0/680	0.62	2/919 (0.2%)
25	AC	0.24	0/690	0.67	2/931 (0.2%)
26	C2	0.24	0/936	0.46	0/1271
27	B1	0.19	0/441	0.47	0/590
28	S4	0.24	0/1245	0.54	0/1687
29	A9	0.20	0/3105	0.49	2/4200 (0.0%)
30	B2	0.20	0/519	0.47	0/713
31	S2	0.29	0/3512	0.63	5/4761 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	V1	0.24	0/3438	0.54	0/4643
34	2	0.26	0/2876	0.60	3/3890 (0.1%)
35	A7	0.18	0/752	0.45	0/1018
36	A3	0.18	0/528	0.43	0/714
37	4L	0.26	0/815	0.57	0/1095
38	6	0.34	0/1431	0.69	0/1933
39	3	0.33	0/979	0.69	2/1325 (0.2%)
40	A5	0.20	0/933	0.48	0/1265
41	AL	0.20	0/3083	0.46	0/4168
42	A6	0.25	0/997	0.56	0/1340
All	All	0.27	1/66884 (0.0%)	0.57	20/90484 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S7	0	1
16	BL	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	4	12	ILE	C-N	5.66	1.39	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	44	LEU	N-CA-C	-7.79	98.96	110.48
25	AC	69	PRO	N-CA-CB	7.42	111.04	103.25
25	AB	69	PRO	N-CA-CB	7.24	110.85	103.25
25	AC	68	PRO	N-CA-CB	6.75	110.42	103.00
25	AB	68	PRO	N-CA-CB	6.74	110.42	103.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	BL	86	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	S7	191	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	1145	0	1102	20	0
2	S6	716	0	700	7	0
3	S1	5181	0	5227	62	0
4	S3	1699	0	1648	26	0
5	V2	1680	0	1657	15	0
6	S7	1435	0	1448	42	0
7	S8	1485	0	1422	24	0
8	1	2571	0	2628	52	0
9	4	3606	0	3740	82	0
10	5	4606	0	4742	90	0
11	A8	1384	0	1324	13	0
12	A1	581	0	582	12	0
13	AO	1202	0	1211	12	0
14	S5	828	0	807	12	0
15	AM	1281	0	1267	19	0
16	BL	1266	0	1205	5	0
17	B6	1302	0	1295	11	0
18	B4	884	0	879	12	0
19	B7	972	0	959	13	0
20	B5	1221	0	1186	8	0
21	B9	1148	0	1113	12	0
22	BM	871	0	822	6	0
23	B8	1201	0	1107	12	0
24	B3	646	0	641	4	0
25	AB	670	0	669	7	0
25	AC	680	0	675	8	0
26	C2	908	0	896	7	0
27	B1	430	0	436	5	0
28	S4	1214	0	1186	10	0
29	A9	3030	0	3032	38	0
30	B2	495	0	457	5	0
31	S2	3427	0	3399	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	V3	135	0	30	1	0
33	V1	3361	0	3339	41	0
34	2	2797	0	2879	49	0
35	A7	736	0	737	10	0
36	A3	519	0	517	7	0
37	4L	794	0	818	16	0
38	6	1404	0	1517	34	0
39	3	956	0	1030	18	0
40	A5	914	0	944	8	0
41	AL	3008	0	2945	39	0
42	A6	977	0	997	8	0
43	2	45	0	34	1	0
43	3	54	0	52	0	0
43	6	86	0	122	4	0
43	AM	76	0	96	5	0
43	AN	67	0	78	3	0
43	B5	142	0	172	7	0
43	B6	47	0	38	2	0
44	1	54	0	88	2	0
44	2	45	0	67	1	0
44	4	78	0	104	4	0
44	5	34	0	41	3	0
44	A9	44	0	62	3	0
44	AM	113	0	151	5	0
44	AN	44	0	62	2	0
44	B6	37	0	48	1	0
44	S7	46	0	69	0	0
45	S6	1	0	0	0	0
46	S1	16	0	0	0	0
46	S7	8	0	0	7	0
46	S8	16	0	0	0	0
46	V1	8	0	0	0	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	1	51	0	82	1	0
48	2	30	0	34	2	0
48	3	92	0	141	3	0
48	4	152	0	203	3	0
48	5	275	0	377	9	0
48	6	35	0	43	2	0
48	AM	72	0	95	3	0
48	B1	37	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	B4	47	0	71	0	0
48	B6	48	0	75	2	0
48	C2	45	0	67	1	0
48	S7	66	0	80	3	0
49	1	63	0	87	3	0
50	AO	14	0	30	0	0
50	B5	14	0	30	0	0
50	C2	14	0	30	0	0
51	AB	32	0	36	0	0
51	AC	34	0	40	1	0
52	B1	8	0	18	0	0
53	A3	12	0	26	0	0
53	A9	24	0	52	0	0
53	B1	12	0	26	0	0
54	A9	48	0	26	0	0
55	V1	31	0	19	2	0
56	6	35	0	0	8	0
57	AL	31	0	12	5	0
All	All	67757	0	68247	819	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 6.

The worst 5 of 819 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)
6:S7:97:CYS:SG	46:S7:301:SF4:FE1	1.46	1.06
31:S2:186:LEU:HD12	31:S2:212:ARG:HG3	1.42	1.02
38:6:20:MET:HE3	38:6:25:ALA:HB1	1.43	0.97
56:6:201:WSF:C13	56:6:201:WSF:C15	2.43	0.96
56:6:201:WSF:C15	56:6:201:WSF:C14	2.44	0.96

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	AN	134/142 (94%)	130 (97%)	3 (2%)	1 (1%)	19	47
2	S6	87/126 (69%)	87 (100%)	0	0	100	100
3	S1	679/731 (93%)	660 (97%)	19 (3%)	0	100	100
4	S3	203/265 (77%)	196 (97%)	7 (3%)	0	100	100
5	V2	212/242 (88%)	208 (98%)	4 (2%)	0	100	100
6	S7	180/221 (81%)	168 (93%)	12 (7%)	0	100	100
7	S8	184/217 (85%)	179 (97%)	5 (3%)	0	100	100
8	1	313/315 (99%)	300 (96%)	13 (4%)	0	100	100
9	4	444/446 (100%)	421 (95%)	21 (5%)	2 (0%)	25	54
10	5	575/577 (100%)	552 (96%)	22 (4%)	1 (0%)	44	72
11	A8	172/175 (98%)	164 (95%)	8 (5%)	0	100	100
12	A1	68/123 (55%)	68 (100%)	0	0	100	100
13	AO	144/154 (94%)	140 (97%)	4 (3%)	0	100	100
14	S5	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
15	AM	166/170 (98%)	161 (97%)	5 (3%)	0	100	100
16	BL	149/159 (94%)	148 (99%)	1 (1%)	0	100	100
17	B6	159/167 (95%)	155 (98%)	4 (2%)	0	100	100
18	B4	105/113 (93%)	101 (96%)	4 (4%)	0	100	100
19	B7	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
20	B5	141/186 (76%)	139 (99%)	2 (1%)	0	100	100
21	B9	132/144 (92%)	131 (99%)	1 (1%)	0	100	100
22	BM	104/150 (69%)	100 (96%)	4 (4%)	0	100	100
23	B8	142/175 (81%)	134 (94%)	8 (6%)	0	100	100
24	B3	79/110 (72%)	75 (95%)	4 (5%)	0	100	100
25	AB	82/152 (54%)	78 (95%)	3 (4%)	1 (1%)	11	35
25	AC	83/152 (55%)	79 (95%)	3 (4%)	1 (1%)	11	35
26	C2	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
27	B1	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
28	S4	149/183 (81%)	145 (97%)	4 (3%)	0	100	100
29	A9	375/416 (90%)	366 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	B2	58/94 (62%)	57 (98%)	1 (2%)	0	100	100
31	S2	427/468 (91%)	418 (98%)	8 (2%)	1 (0%)	44	72
33	V1	436/474 (92%)	421 (97%)	15 (3%)	0	100	100
34	2	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
35	A7	87/103 (84%)	85 (98%)	2 (2%)	0	100	100
36	A3	64/77 (83%)	64 (100%)	0	0	100	100
37	4L	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
38	6	172/174 (99%)	172 (100%)	0	0	100	100
39	3	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
40	A5	115/124 (93%)	114 (99%)	1 (1%)	0	100	100
41	AL	366/407 (90%)	354 (97%)	12 (3%)	0	100	100
42	A6	113/124 (91%)	107 (95%)	6 (5%)	0	100	100
All	All	8026/9000 (89%)	7779 (97%)	240 (3%)	7 (0%)	50	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	4	43	ASN
9	4	202	LEU
10	5	324	ASN
25	AB	69	PRO
25	AC	69	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	AN	118/122 (97%)	116 (98%)	2 (2%)	56	74
2	S6	77/111 (69%)	77 (100%)	0	100	100
3	S1	549/582 (94%)	545 (99%)	4 (1%)	81	88
4	S3	184/225 (82%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	V2	185/205 (90%)	182 (98%)	3 (2%)	58	75
6	S7	152/184 (83%)	150 (99%)	2 (1%)	65	78
7	S8	159/182 (87%)	159 (100%)	0	100	100
8	1	282/282 (100%)	278 (99%)	4 (1%)	62	77
9	4	403/404 (100%)	400 (99%)	3 (1%)	81	88
10	5	518/518 (100%)	505 (98%)	13 (2%)	42	65
11	A8	150/151 (99%)	144 (96%)	6 (4%)	27	52
12	A1	63/115 (55%)	63 (100%)	0	100	100
13	AO	128/134 (96%)	128 (100%)	0	100	100
14	S5	88/89 (99%)	87 (99%)	1 (1%)	70	81
15	AM	129/131 (98%)	128 (99%)	1 (1%)	79	87
16	BL	135/141 (96%)	135 (100%)	0	100	100
17	B6	133/136 (98%)	133 (100%)	0	100	100
18	B4	88/94 (94%)	88 (100%)	0	100	100
19	B7	104/104 (100%)	104 (100%)	0	100	100
20	B5	129/162 (80%)	129 (100%)	0	100	100
21	B9	116/126 (92%)	116 (100%)	0	100	100
22	BM	95/131 (72%)	95 (100%)	0	100	100
23	B8	121/145 (83%)	117 (97%)	4 (3%)	33	58
24	B3	66/84 (79%)	66 (100%)	0	100	100
25	AB	76/136 (56%)	76 (100%)	0	100	100
25	AC	77/136 (57%)	77 (100%)	0	100	100
26	C2	93/94 (99%)	93 (100%)	0	100	100
27	B1	42/43 (98%)	42 (100%)	0	100	100
28	S4	131/154 (85%)	131 (100%)	0	100	100
29	A9	319/346 (92%)	319 (100%)	0	100	100
30	B2	51/80 (64%)	50 (98%)	1 (2%)	50	70
31	S2	368/398 (92%)	363 (99%)	5 (1%)	62	77
33	V1	350/381 (92%)	350 (100%)	0	100	100
34	2	317/317 (100%)	314 (99%)	3 (1%)	75	86
35	A7	79/86 (92%)	78 (99%)	1 (1%)	65	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	A3	52/59 (88%)	52 (100%)	0	100	100
37	4L	91/91 (100%)	91 (100%)	0	100	100
38	6	167/167 (100%)	164 (98%)	3 (2%)	54	73
39	3	110/110 (100%)	110 (100%)	0	100	100
40	A5	96/102 (94%)	96 (100%)	0	100	100
41	AL	324/356 (91%)	324 (100%)	0	100	100
42	A6	108/114 (95%)	108 (100%)	0	100	100
All	All	7023/7728 (91%)	6967 (99%)	56 (1%)	77	87

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	5	291	MET
38	6	43	LEU
11	A8	145	GLU
38	6	40	LEU
34	2	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
34	2	318	ASN
41	AL	176	GLN
37	4L	24	ASN
40	A5	19	ASN
41	AL	404	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 1 is monoatomic - leaving 67 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	CDL	B6	203	-	46,46,99	0.41	0	52,58,111	0.39	0
43	CDL	6	203	-	85,85,99	0.32	0	91,97,111	0.29	0
55	FMN	V1	501	-	33,33,33	0.31	0	48,50,50	0.43	0
48	3PE	5	603	-	32,32,50	0.40	0	35,37,55	0.69	1 (2%)
56	WSF	6	201	-	34,34,34	4.99	3 (8%)	37,40,40	2.85	4 (10%)
44	PC1	AM	201	-	36,36,53	0.34	0	42,44,61	0.36	0
43	CDL	B5	202	-	65,65,99	0.36	0	71,77,111	0.31	0
47	FES	V2	301	5	0,4,4	-	-	-	-	-
44	PC1	AN	202	-	43,43,53	0.33	0	49,51,61	0.30	0
44	PC1	5	606	-	33,33,53	0.38	0	39,41,61	0.39	0
52	OCT	B1	101	-	7,7,7	0.12	0	6,6,6	0.05	0
44	PC1	2	402	-	44,44,53	0.31	0	50,52,61	0.32	0
48	3PE	B4	201	-	46,46,50	0.31	0	49,51,55	0.28	0
48	3PE	B6	201	-	47,47,50	0.38	0	50,52,55	0.39	1 (2%)
48	3PE	4	503	-	44,44,50	0.31	0	47,49,55	0.27	0
44	PC1	A9	501	-	43,43,53	0.31	0	49,51,61	0.30	0
48	3PE	5	608	-	44,44,50	0.34	0	47,49,55	0.59	1 (2%)
44	PC1	1	401	-	53,53,53	0.33	0	59,61,61	0.55	1 (1%)
48	3PE	4	502	-	31,31,50	0.37	0	34,36,55	0.33	0
48	3PE	5	605	-	32,32,50	0.37	0	35,37,55	0.32	0
43	CDL	B5	201	-	75,75,99	0.34	0	81,87,111	0.31	0
44	PC1	AM	206	-	31,31,53	0.39	0	37,39,61	0.41	0
48	3PE	5	602	-	50,50,50	0.31	0	53,55,55	0.32	0
51	ZMP	AC	201	-	28,33,36	0.81	1 (3%)	32,40,45	3.27	6 (18%)
50	C14	AO	201	-	13,13,13	0.11	0	12,12,12	0.07	0
50	C14	B5	203	-	13,13,13	0.11	0	12,12,12	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	D12	B1	102	-	11,11,11	0.10	0	10,10,10	0.06	0
48	3PE	S7	303	-	32,32,50	0.37	0	35,37,55	0.34	0
43	CDL	AM	204	-	75,75,99	0.36	0	81,87,111	0.49	1 (1%)
48	3PE	B1	103	-	36,36,50	0.37	0	39,41,55	0.64	1 (2%)
44	PC1	B6	202	-	36,36,53	0.36	0	42,44,61	0.64	1 (2%)
48	3PE	5	607	-	50,50,50	0.29	0	53,55,55	0.30	0
44	PC1	S7	304	-	45,45,53	0.33	0	51,53,61	0.33	0
48	3PE	5	601	-	31,31,50	0.38	0	34,36,55	0.34	0
46	SF4	V1	502	33	0,12,12	-	-	-		
48	3PE	4	504	-	35,35,50	0.35	0	38,40,55	0.34	0
48	3PE	4	506	-	38,38,50	0.36	0	41,43,55	0.63	1 (2%)
48	3PE	AM	202	-	40,40,50	0.33	0	43,45,55	0.35	0
54	NDP	A9	502	-	47,52,52	0.54	0	61,80,80	0.54	1 (1%)
44	PC1	AM	205	-	43,43,53	0.32	0	49,51,61	0.44	0
46	SF4	S8	302	7	0,12,12	-	-	-		
48	3PE	1	403	-	50,50,50	0.30	0	53,55,55	0.31	0
44	PC1	4	505	-	38,38,53	0.33	0	44,46,61	0.34	0
48	3PE	5	604	-	29,29,50	0.39	0	32,34,55	0.35	0
46	SF4	S1	801	3	0,12,12	-	-	-		
48	3PE	AM	203	-	30,30,50	0.38	0	33,35,55	0.35	0
47	FES	S1	803	3	0,4,4	-	-	-		
43	CDL	AN	201	-	66,66,99	0.36	0	72,78,111	0.38	0
48	3PE	C2	201	-	44,44,50	0.32	0	47,49,55	0.35	0
48	3PE	6	202	-	34,34,50	0.37	0	37,39,55	0.34	0
50	C14	C2	202	-	13,13,13	0.10	0	12,12,12	0.07	0
53	D12	A3	101	-	11,11,11	0.11	0	10,10,10	0.06	0
57	DGT	AL	501	-	29,33,33	0.96	3 (10%)	37,52,52	0.70	1 (2%)
48	3PE	3	202	-	50,50,50	0.30	0	53,55,55	0.37	0
46	SF4	S1	802	3	0,12,12	-	-	-		
53	D12	A9	503	-	11,11,11	0.11	0	10,10,10	0.05	0
43	CDL	2	403	-	43,43,99	0.60	1 (2%)	47,54,111	0.63	1 (2%)
49	U10	1	402	-	63,63,63	2.26	25 (39%)	78,79,79	1.48	19 (24%)
46	SF4	S8	301	7	0,12,12	-	-	-		
48	3PE	S7	302	-	32,32,50	0.37	0	35,37,55	0.31	0
48	3PE	2	401	-	29,29,50	0.38	0	32,34,55	0.36	0
46	SF4	S7	301	6	0,12,12	-	-	-		
53	D12	A9	504	-	11,11,11	0.11	0	10,10,10	0.07	0
44	PC1	4	501	-	38,38,53	0.35	0	44,46,61	0.37	0
51	ZMP	AB	201	-	26,31,36	0.77	1 (3%)	30,38,45	3.45	6 (20%)
48	3PE	3	203	-	40,40,50	0.36	0	43,45,55	0.60	1 (2%)
43	CDL	3	201	-	53,53,99	0.40	0	59,65,111	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CDL	B6	203	-	-	21/56/56/110	-
43	CDL	6	203	-	-	16/96/96/110	-
55	FMN	V1	501	-	-	10/18/18/18	0/3/3/3
48	3PE	5	603	-	-	9/36/36/54	-
56	WSF	6	201	-	-	5/38/38/38	-
44	PC1	AM	201	-	-	5/40/40/57	-
43	CDL	B5	202	-	-	16/76/76/110	-
47	FES	V2	301	5	-	-	0/1/1/1
44	PC1	AN	202	-	-	6/47/47/57	-
44	PC1	5	606	-	-	9/37/37/57	-
52	OCT	B1	101	-	-	0/5/5/5	-
46	SF4	S8	302	7	-	-	0/6/5/5
44	PC1	2	402	-	-	6/48/48/57	-
48	3PE	B4	201	-	-	9/50/50/54	-
48	3PE	B6	201	-	-	6/49/49/54	-
48	3PE	4	503	-	-	5/48/48/54	-
44	PC1	A9	501	-	-	6/47/47/57	-
48	3PE	5	608	-	-	11/48/48/54	-
44	PC1	1	401	-	-	13/57/57/57	-
48	3PE	4	502	-	-	8/35/35/54	-
48	3PE	5	605	-	-	7/36/36/54	-
43	CDL	B5	201	-	-	18/86/86/110	-
44	PC1	AM	206	-	-	14/35/35/57	-
48	3PE	5	602	-	-	5/54/54/54	-
51	ZMP	AC	201	-	-	13/38/40/43	-
50	C14	AO	201	-	-	0/11/11/11	-
50	C14	B5	203	-	-	0/11/11/11	-
53	D12	B1	102	-	-	0/9/9/9	-
48	3PE	S7	303	-	-	6/36/36/54	-
43	CDL	AM	204	-	-	23/86/86/110	-
48	3PE	B1	103	-	-	7/40/40/54	-
44	PC1	B6	202	-	-	10/40/40/57	-
48	3PE	5	607	-	-	12/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	PC1	S7	304	-	-	14/49/49/57	-
48	3PE	5	601	-	-	8/35/35/54	-
48	3PE	4	504	-	-	12/39/39/54	-
48	3PE	AM	202	-	-	6/44/44/54	-
48	3PE	4	506	-	-	11/42/42/54	-
54	NDP	A9	502	-	-	2/30/77/77	0/5/5/5
46	SF4	V1	502	33	-	-	0/6/5/5
44	PC1	AM	205	-	-	9/47/47/57	-
48	3PE	1	403	-	-	9/54/54/54	-
48	3PE	5	604	-	-	8/33/33/54	-
44	PC1	4	505	-	-	6/42/42/57	-
48	3PE	AM	203	-	-	6/34/34/54	-
48	3PE	C2	201	-	-	8/48/48/54	-
48	3PE	6	202	-	-	11/38/38/54	-
46	SF4	S1	801	3	-	-	0/6/5/5
43	CDL	AN	201	-	-	28/77/77/110	-
50	C14	C2	202	-	-	1/11/11/11	-
53	D12	A3	101	-	-	0/9/9/9	-
57	DGT	AL	501	-	-	3/18/34/34	0/3/3/3
47	FES	S1	803	3	-	-	0/1/1/1
48	3PE	3	202	-	-	12/54/54/54	-
46	SF4	S1	802	3	-	-	0/6/5/5
53	D12	A9	503	-	-	0/9/9/9	-
43	CDL	2	403	-	-	20/53/53/110	-
49	U10	1	402	-	-	19/63/87/87	0/1/1/1
48	3PE	S7	302	-	-	6/36/36/54	-
46	SF4	S8	301	7	-	-	0/6/5/5
48	3PE	2	401	-	-	8/33/33/54	-
46	SF4	S7	301	6	-	-	0/6/5/5
53	D12	A9	504	-	-	0/9/9/9	-
44	PC1	4	501	-	-	17/42/42/57	-
51	ZMP	AB	201	-	-	5/36/38/43	-
48	3PE	3	203	-	-	12/44/44/54	-
43	CDL	3	201	-	-	17/64/64/110	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	6	201	WSF	C14-C13	17.63	2.43	1.51
56	6	201	WSF	C15-C13	17.59	2.43	1.51
56	6	201	WSF	C12-C13	14.87	2.46	1.51
49	1	402	U10	C6-C1	10.61	1.54	1.35
49	1	402	U10	C4-C3	4.81	1.53	1.36

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	6	201	WSF	C15-C13-C14	-11.30	60.13	110.53
51	AB	201	ZMP	C19-C18-C17	-10.47	90.92	108.77
51	AC	201	ZMP	C20-C18-C17	-9.61	92.38	108.77
51	AC	201	ZMP	C19-C18-C17	-9.44	92.67	108.77
51	AB	201	ZMP	C20-C18-C17	-9.25	92.99	108.77

There are no chirality outliers.

5 of 534 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	AN	201	CDL	CA2-OA2-PA1-OA3
43	AN	201	CDL	CA2-OA2-PA1-OA4
43	AN	201	CDL	CA2-OA2-PA1-OA5
43	AN	201	CDL	CA3-OA5-PA1-OA2
43	AN	201	CDL	OA5-CA3-CA4-OA6

There are no ring outliers.

43 monomers are involved in 91 short contacts:

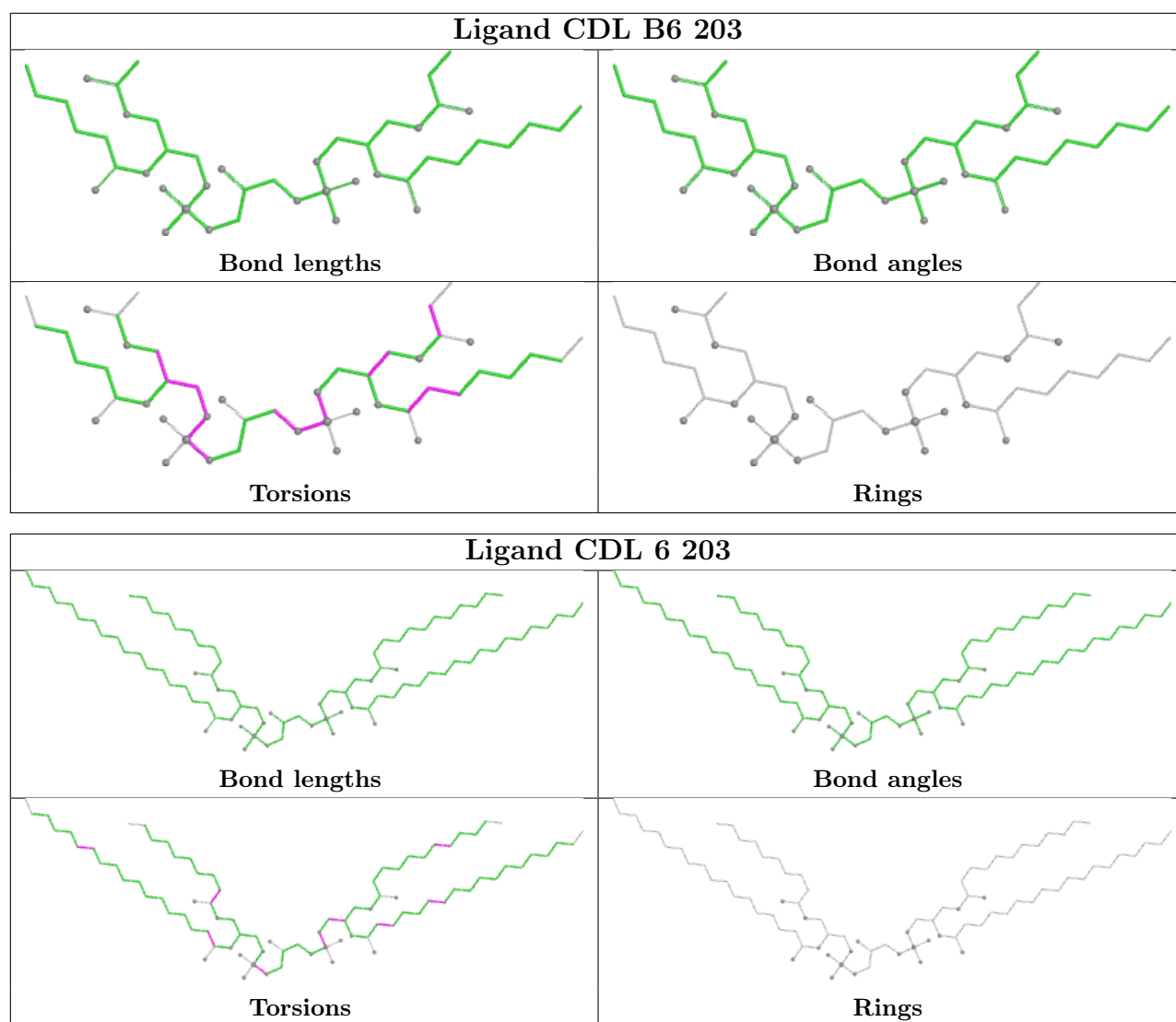
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	B6	203	CDL	2	0
43	6	203	CDL	4	0
55	V1	501	FMN	2	0
48	5	603	3PE	1	0
56	6	201	WSF	8	0
43	B5	202	CDL	1	0
44	AN	202	PC1	2	0
44	5	606	PC1	3	0
44	2	402	PC1	1	0
48	B6	201	3PE	2	0
44	A9	501	PC1	3	0
48	5	608	3PE	2	0
44	1	401	PC1	2	0

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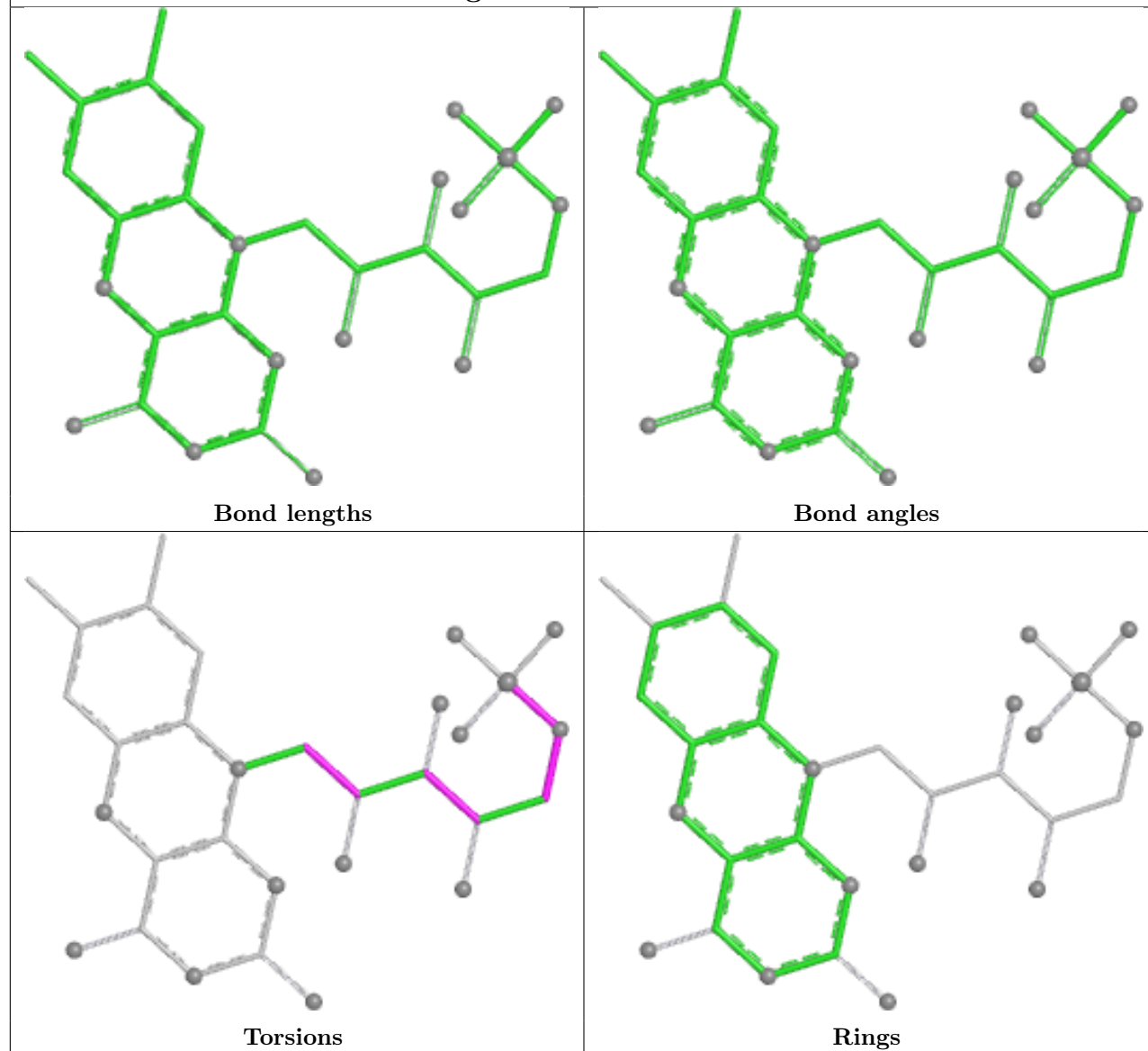
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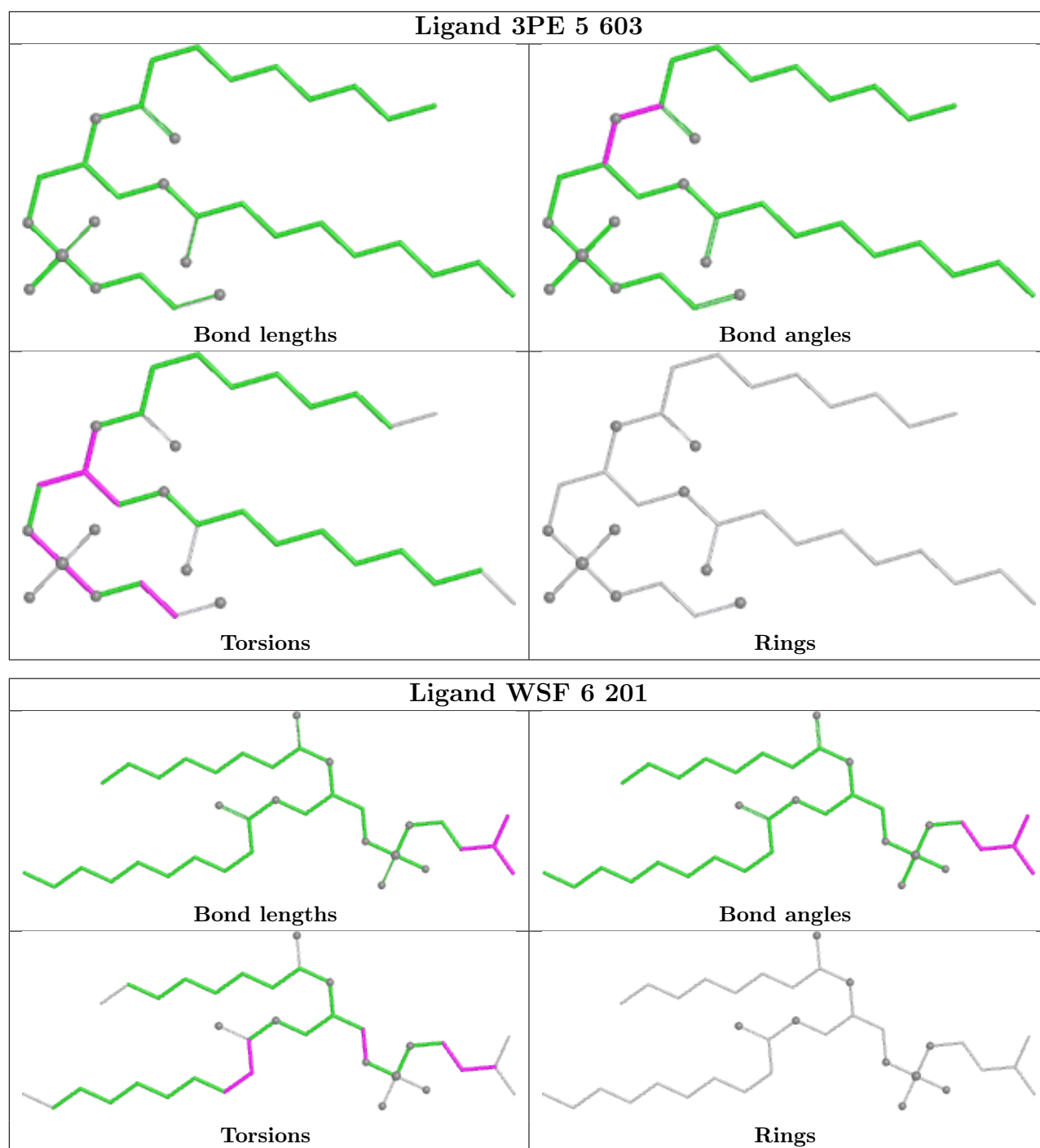
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	4	502	3PE	1	0
48	5	605	3PE	1	0
43	B5	201	CDL	6	0
44	AM	206	PC1	1	0
48	5	602	3PE	1	0
51	AC	201	ZMP	1	0
48	S7	303	3PE	2	0
43	AM	204	CDL	5	0
44	B6	202	PC1	1	0
48	5	607	3PE	2	0
48	5	601	3PE	1	0
48	4	504	3PE	2	0
48	AM	202	3PE	2	0
44	AM	205	PC1	4	0
48	1	403	3PE	1	0
44	4	505	PC1	2	0
48	5	604	3PE	1	0
48	AM	203	3PE	1	0
43	AN	201	CDL	3	0
48	C2	201	3PE	1	0
48	6	202	3PE	2	0
57	AL	501	DGT	5	0
48	3	202	3PE	1	0
43	2	403	CDL	1	0
49	1	402	U10	3	0
48	S7	302	3PE	1	0
48	2	401	3PE	2	0
46	S7	301	SF4	7	0
44	4	501	PC1	2	0
48	3	203	3PE	2	0

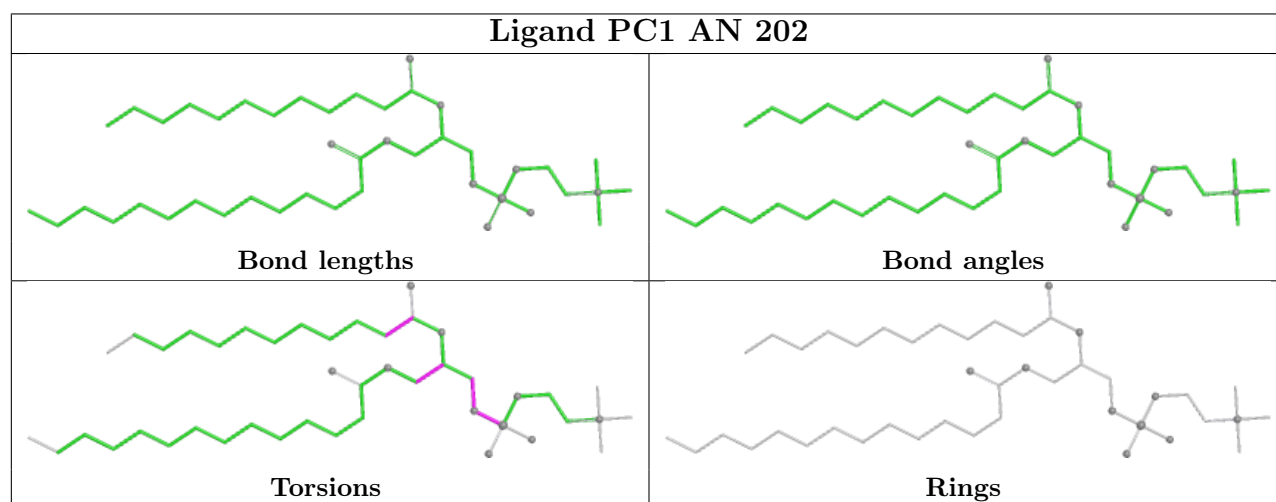
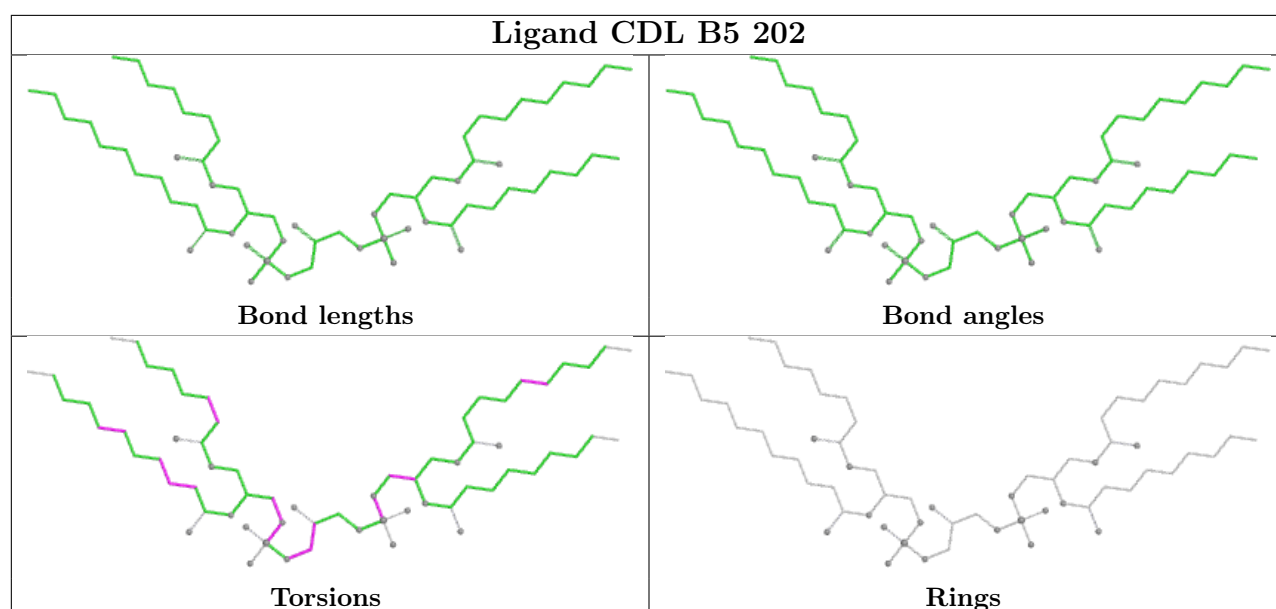
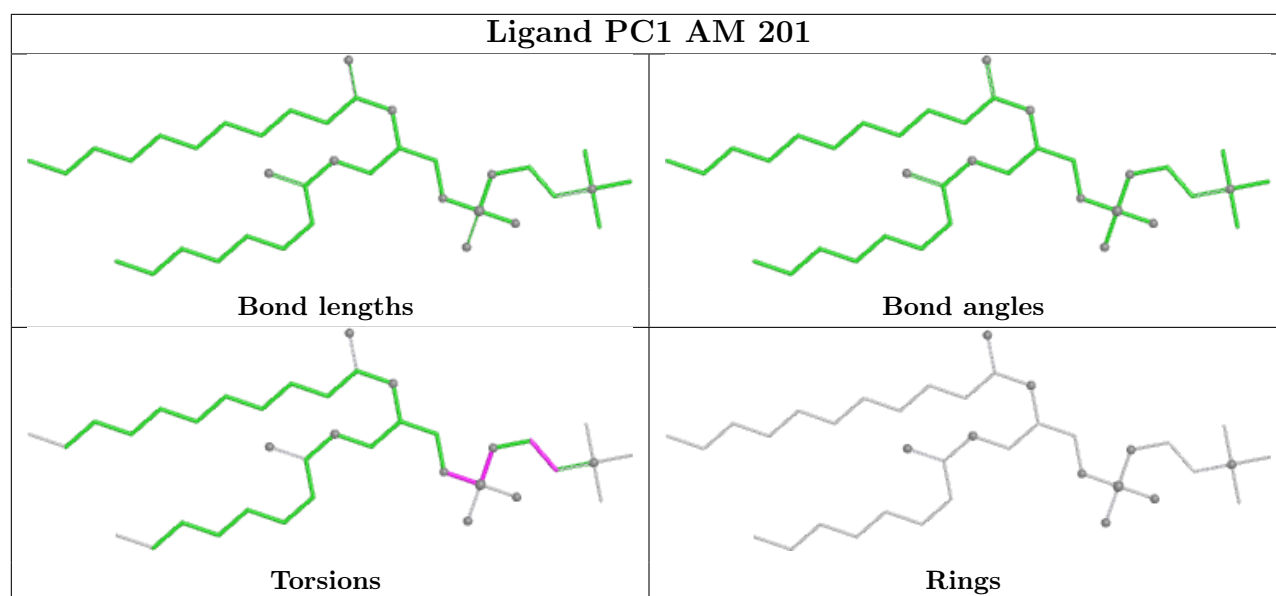
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

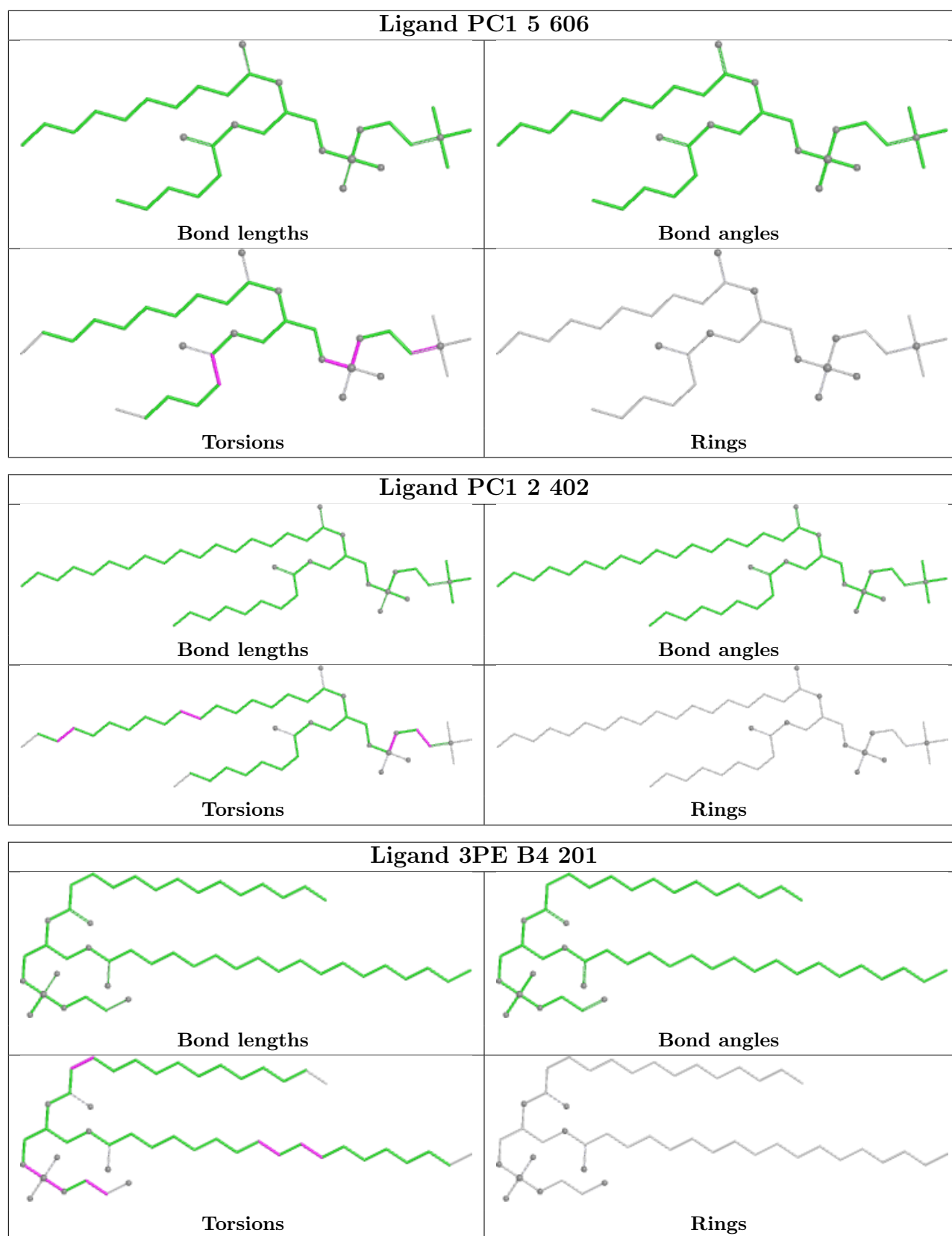


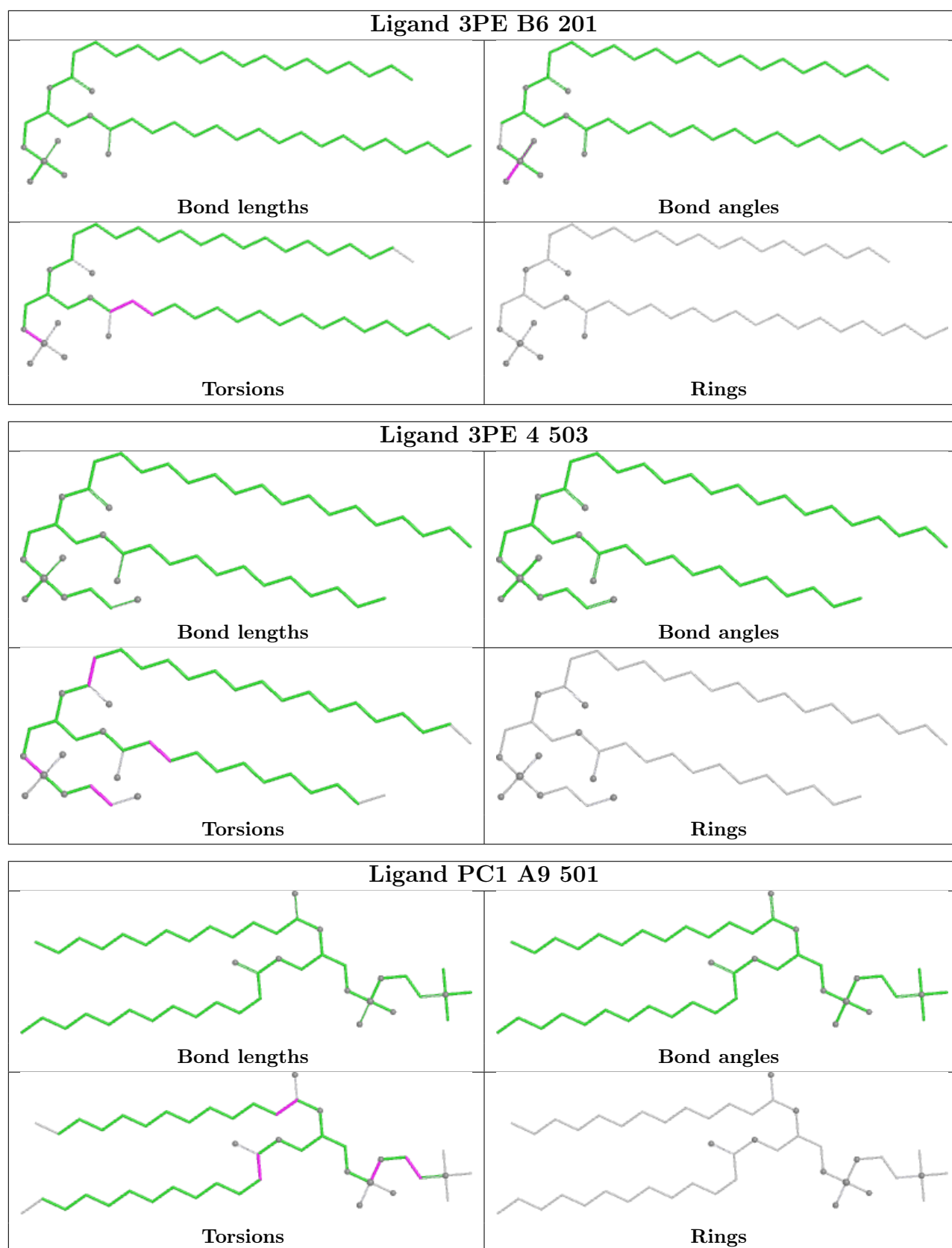
Ligand FMN V1 501

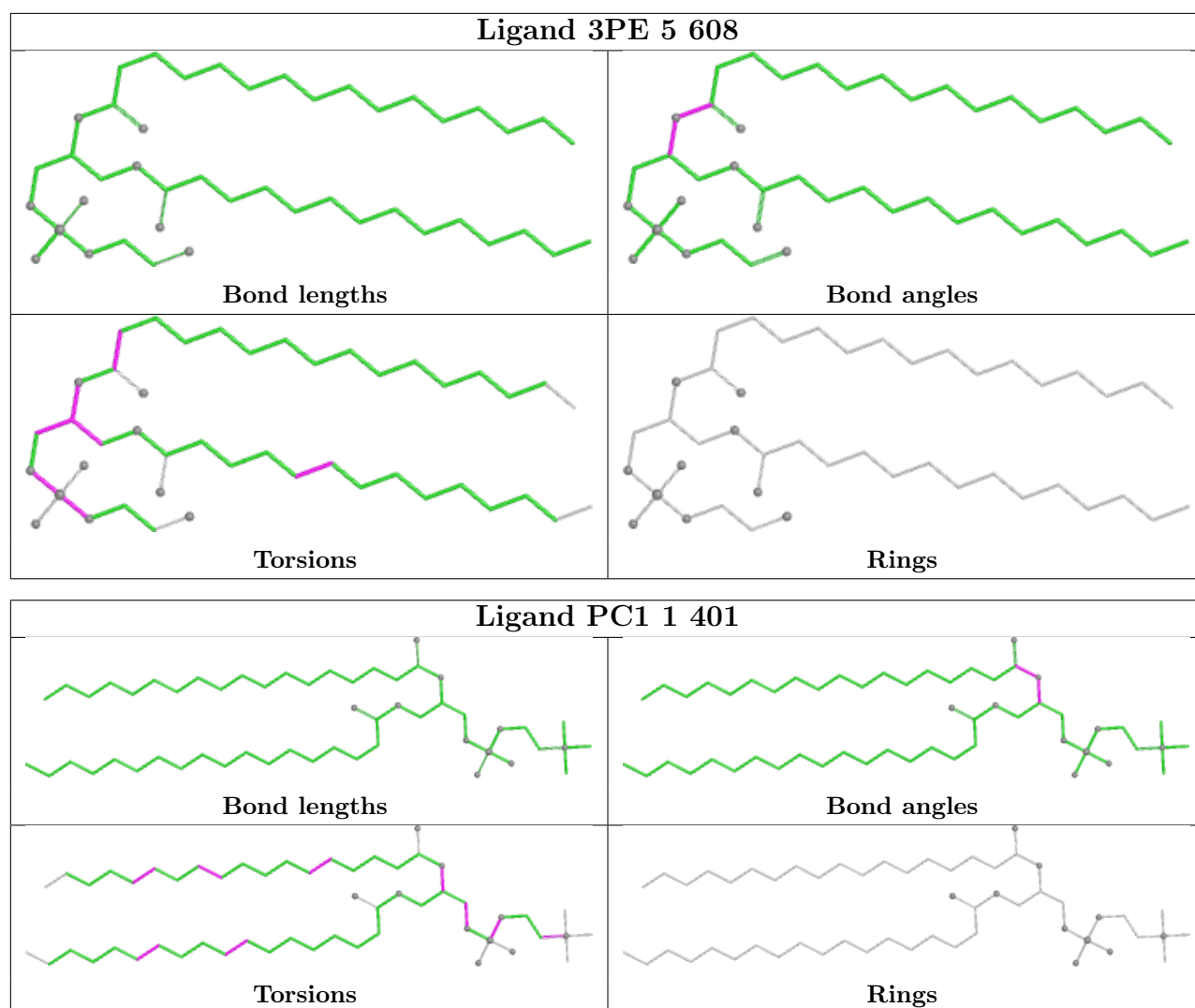


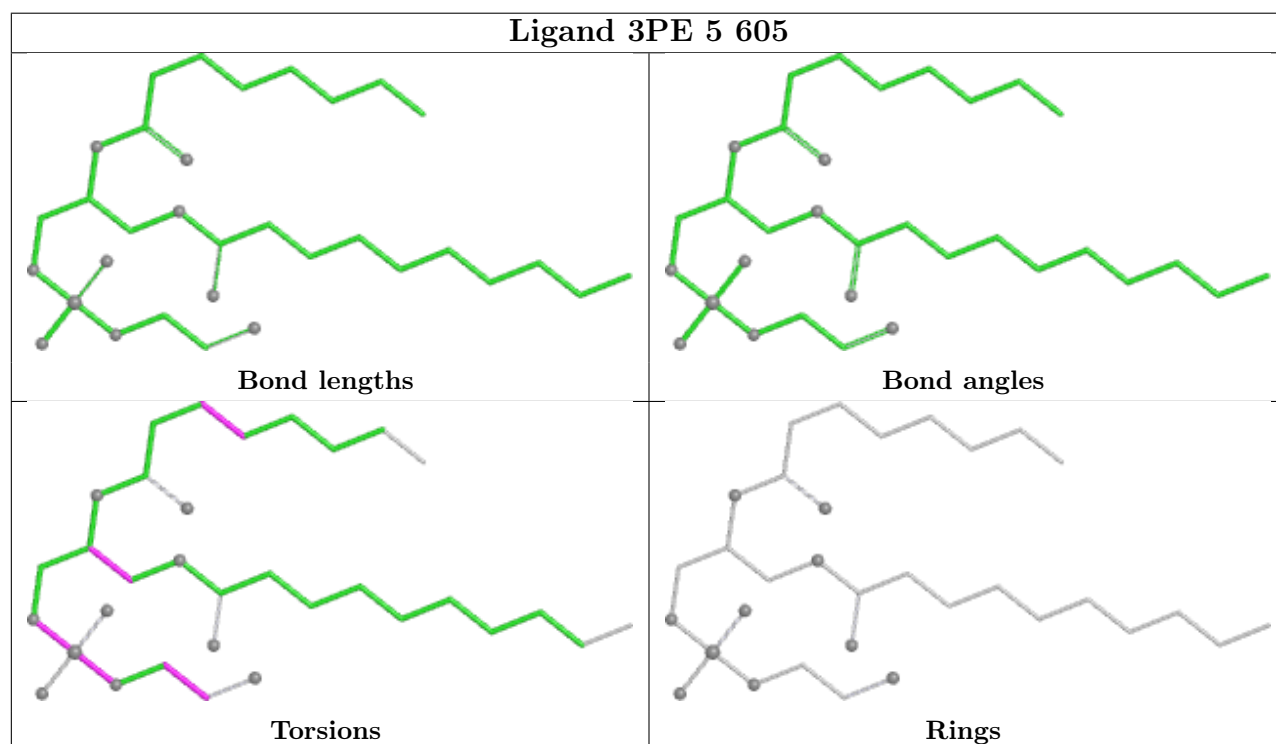
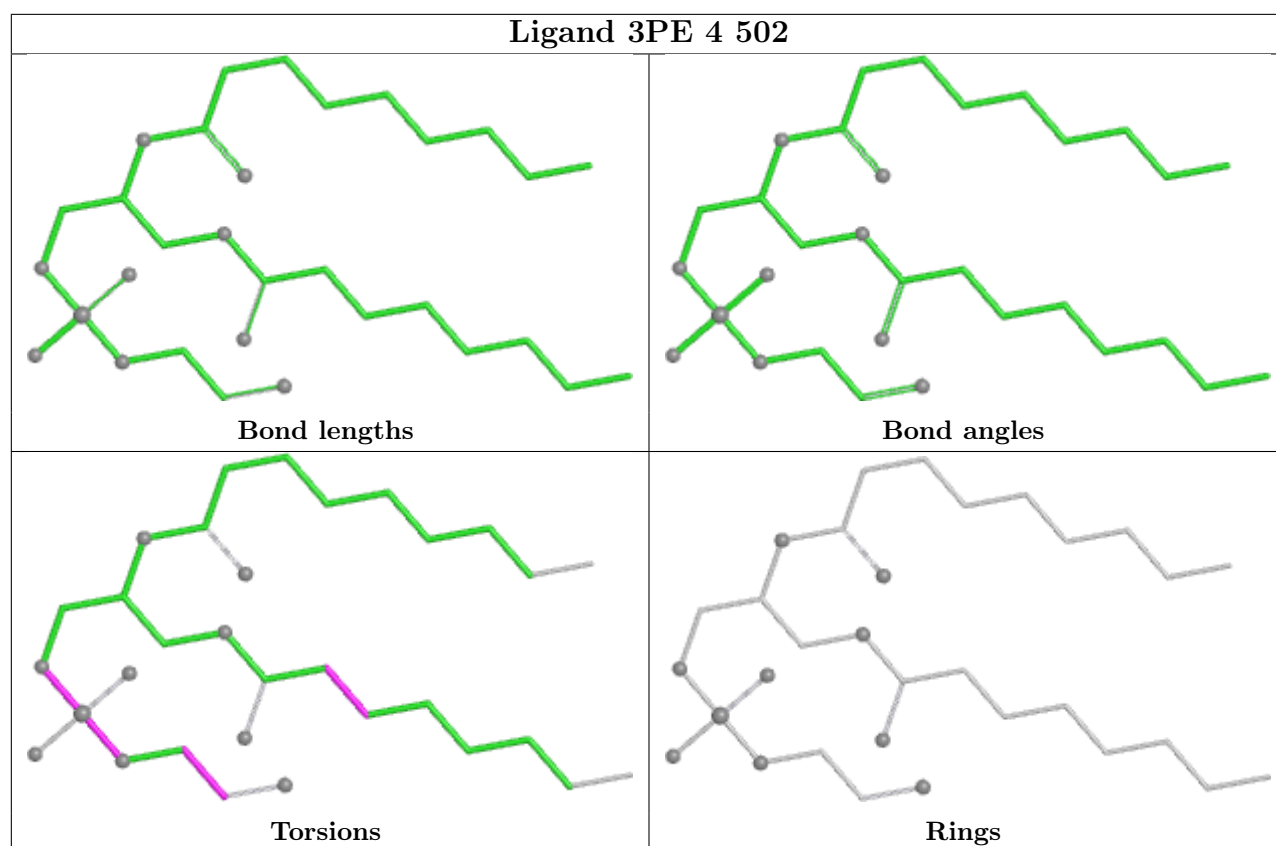


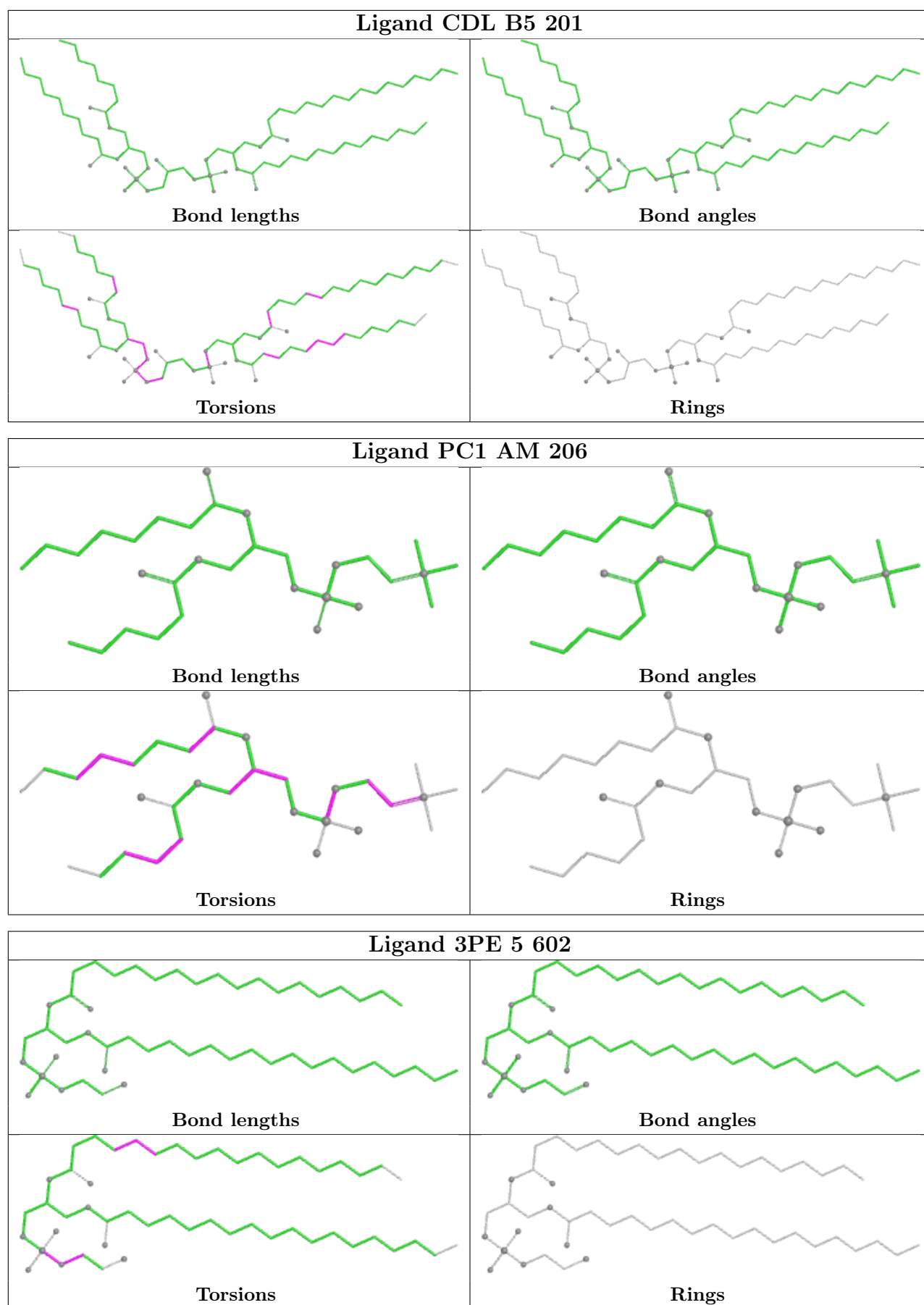


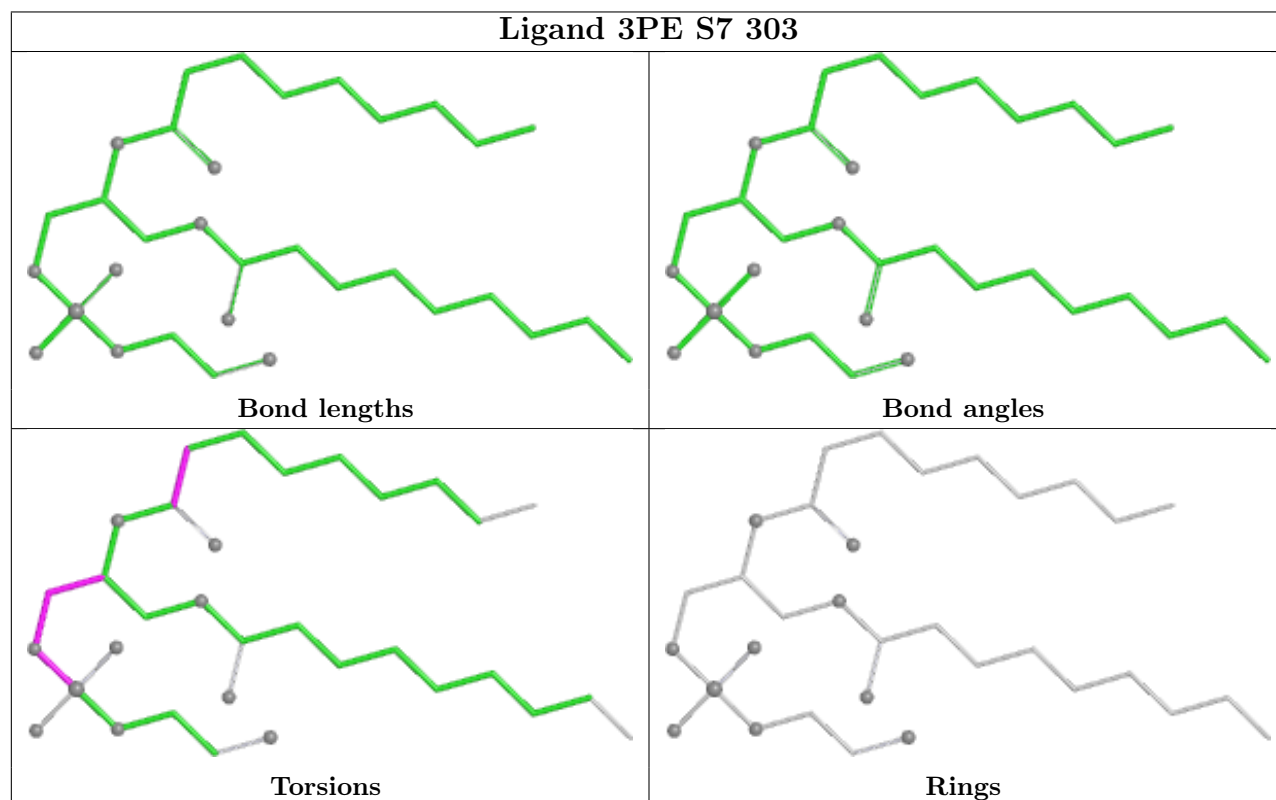
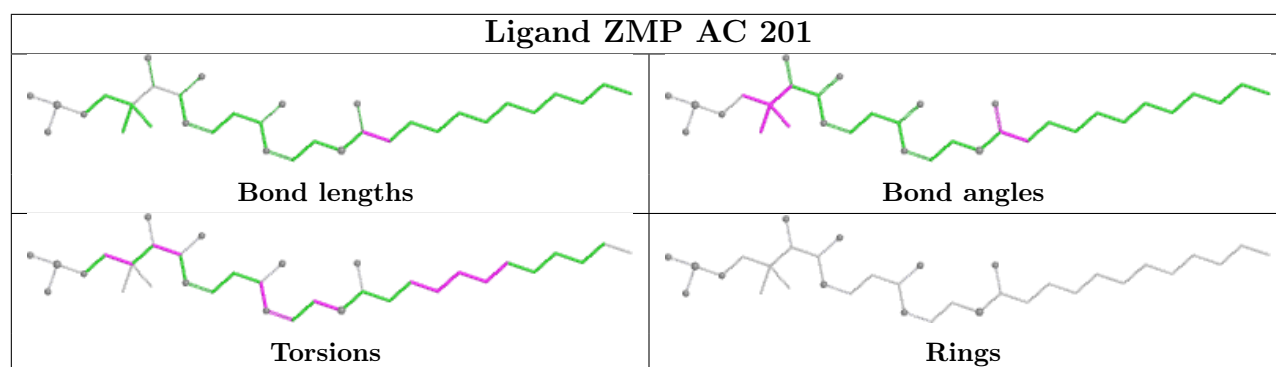


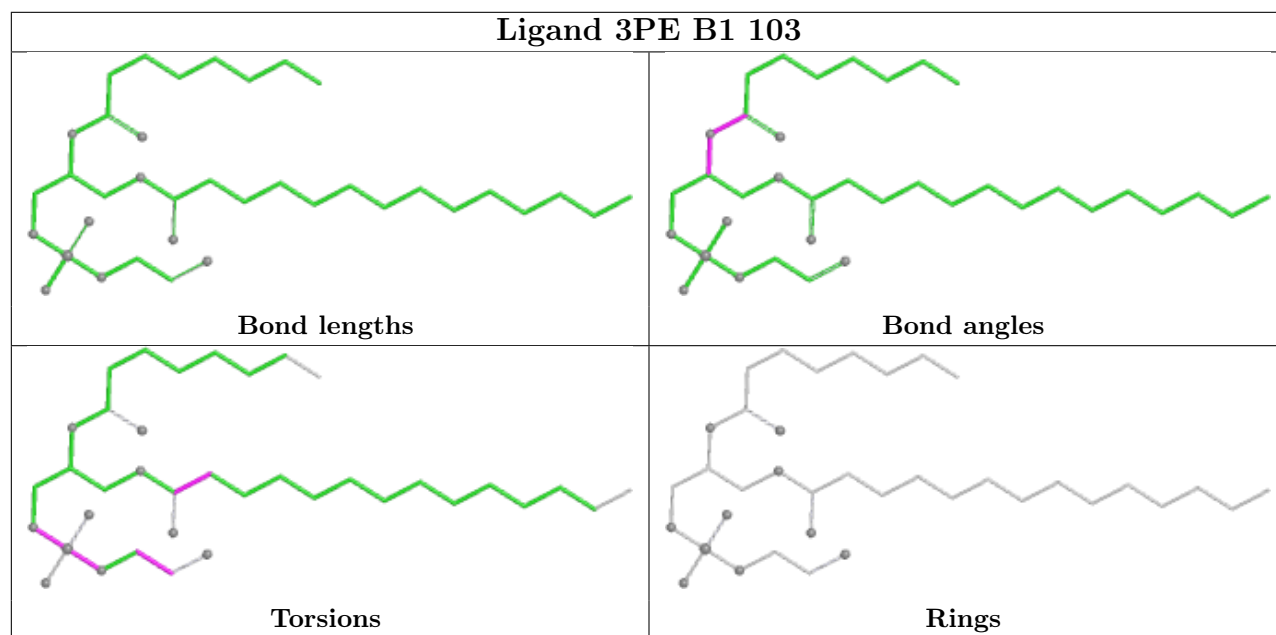
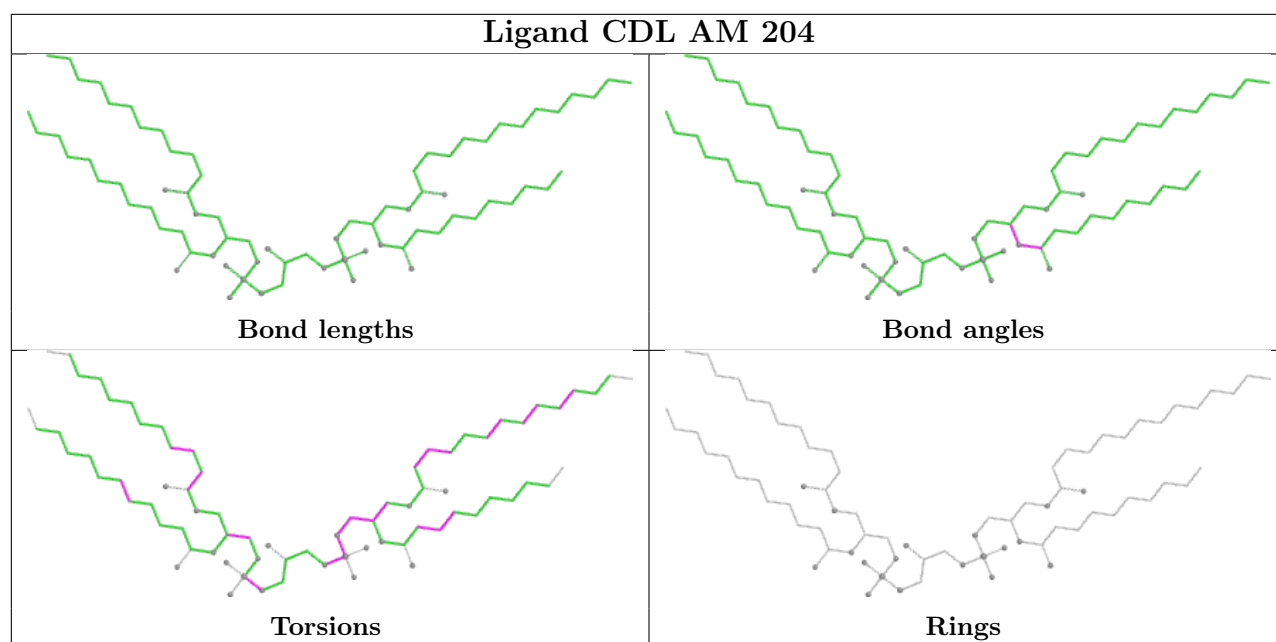


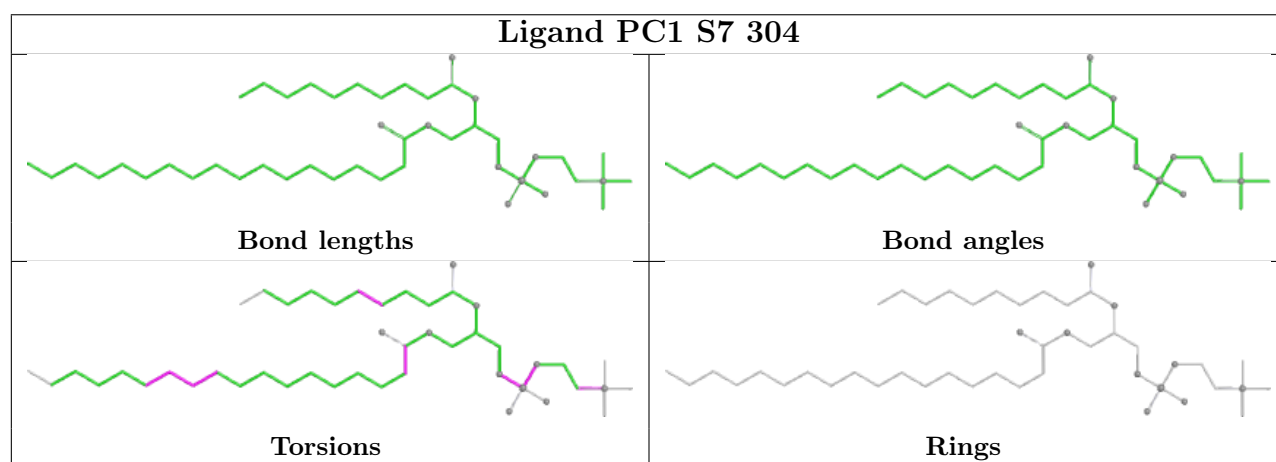
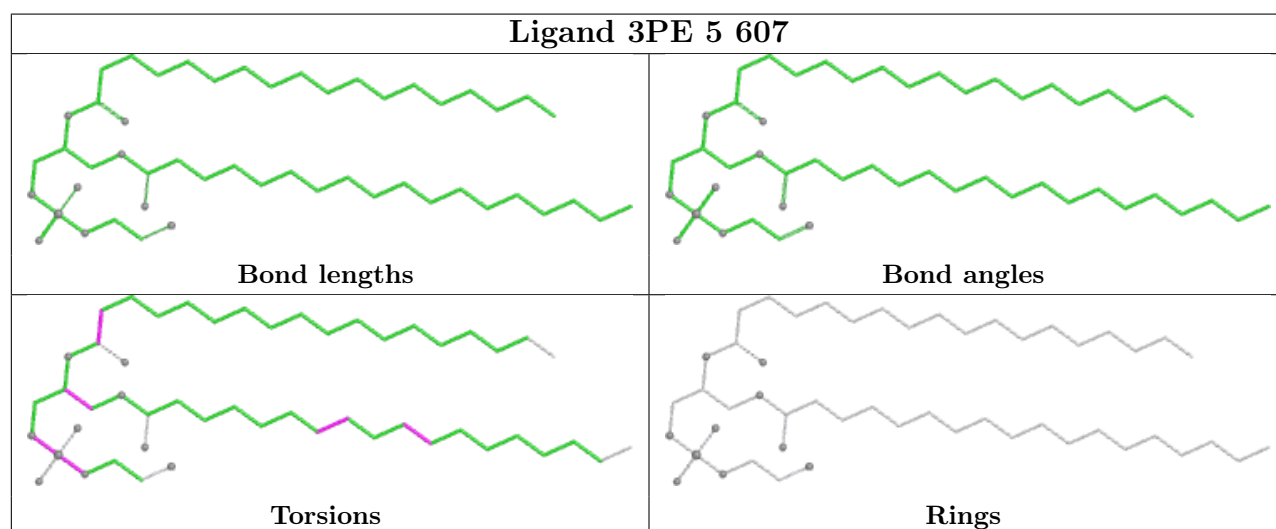
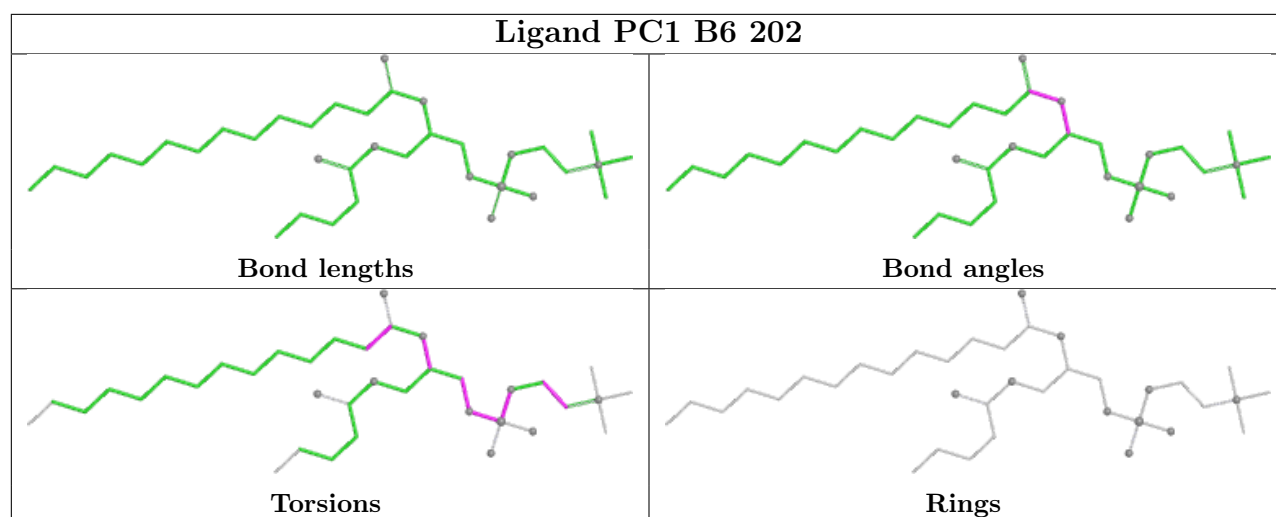


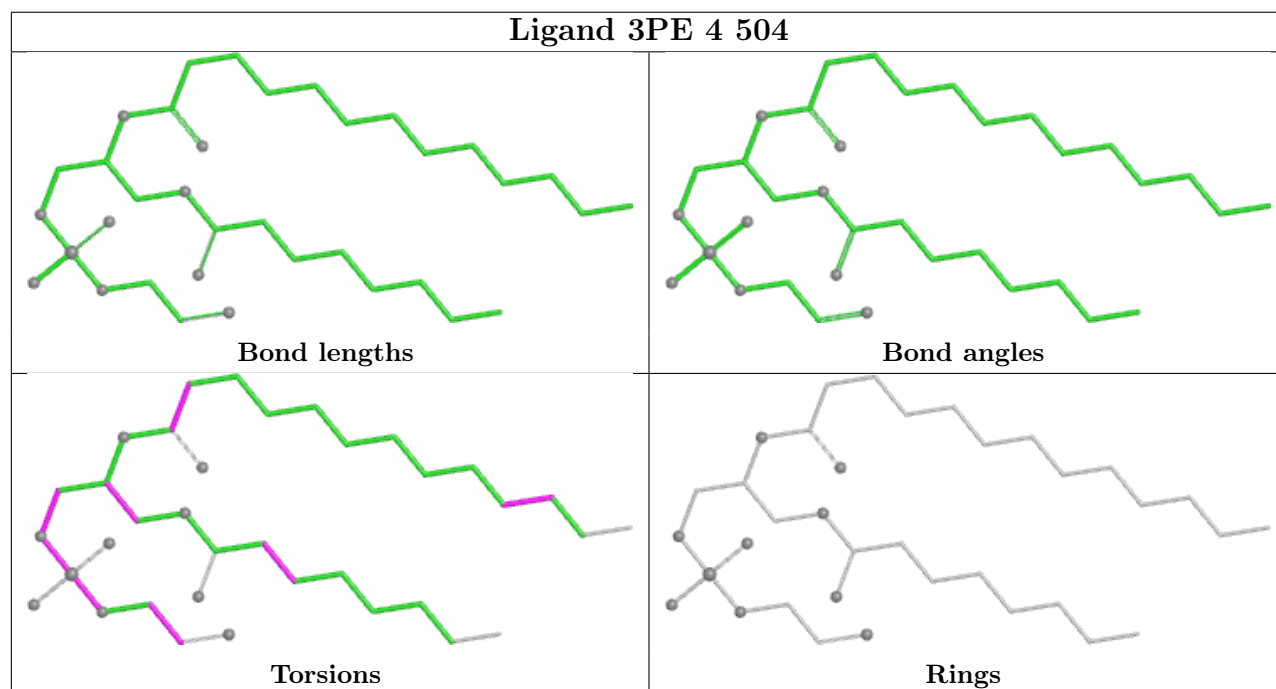
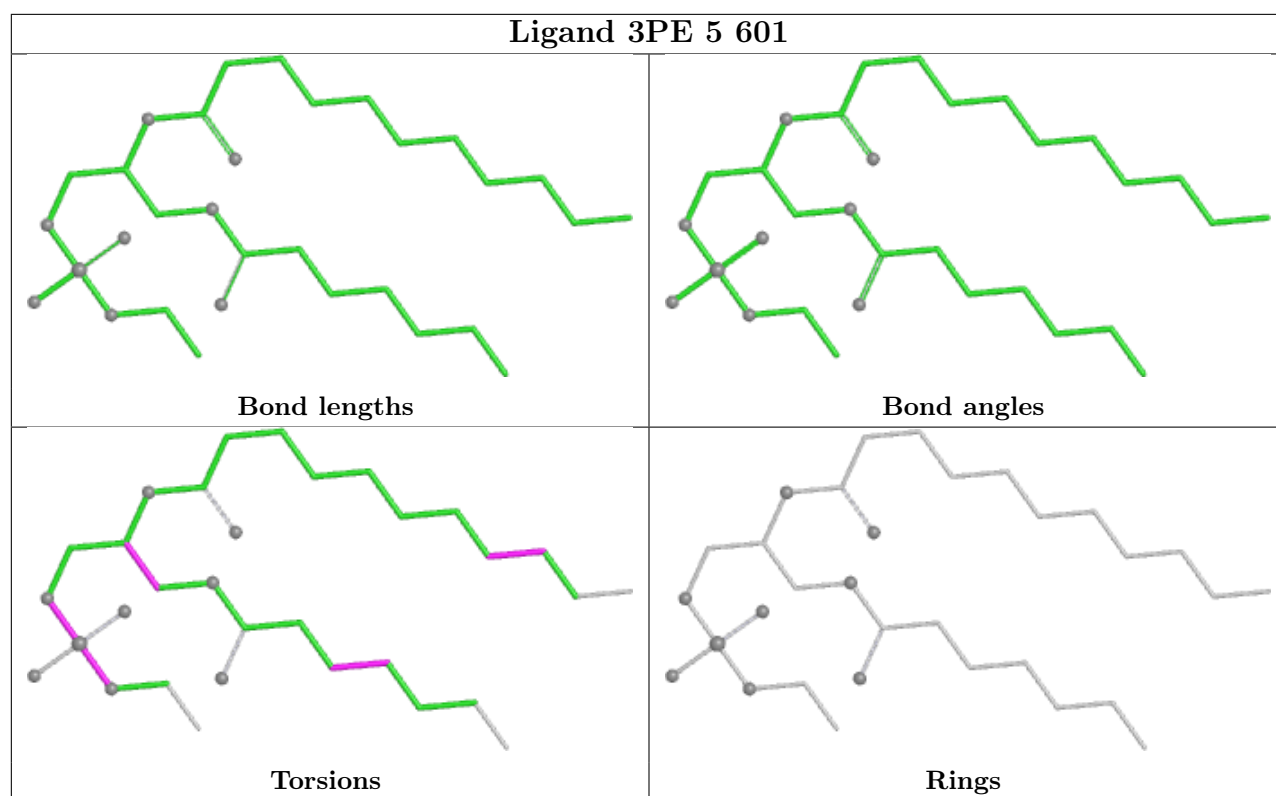


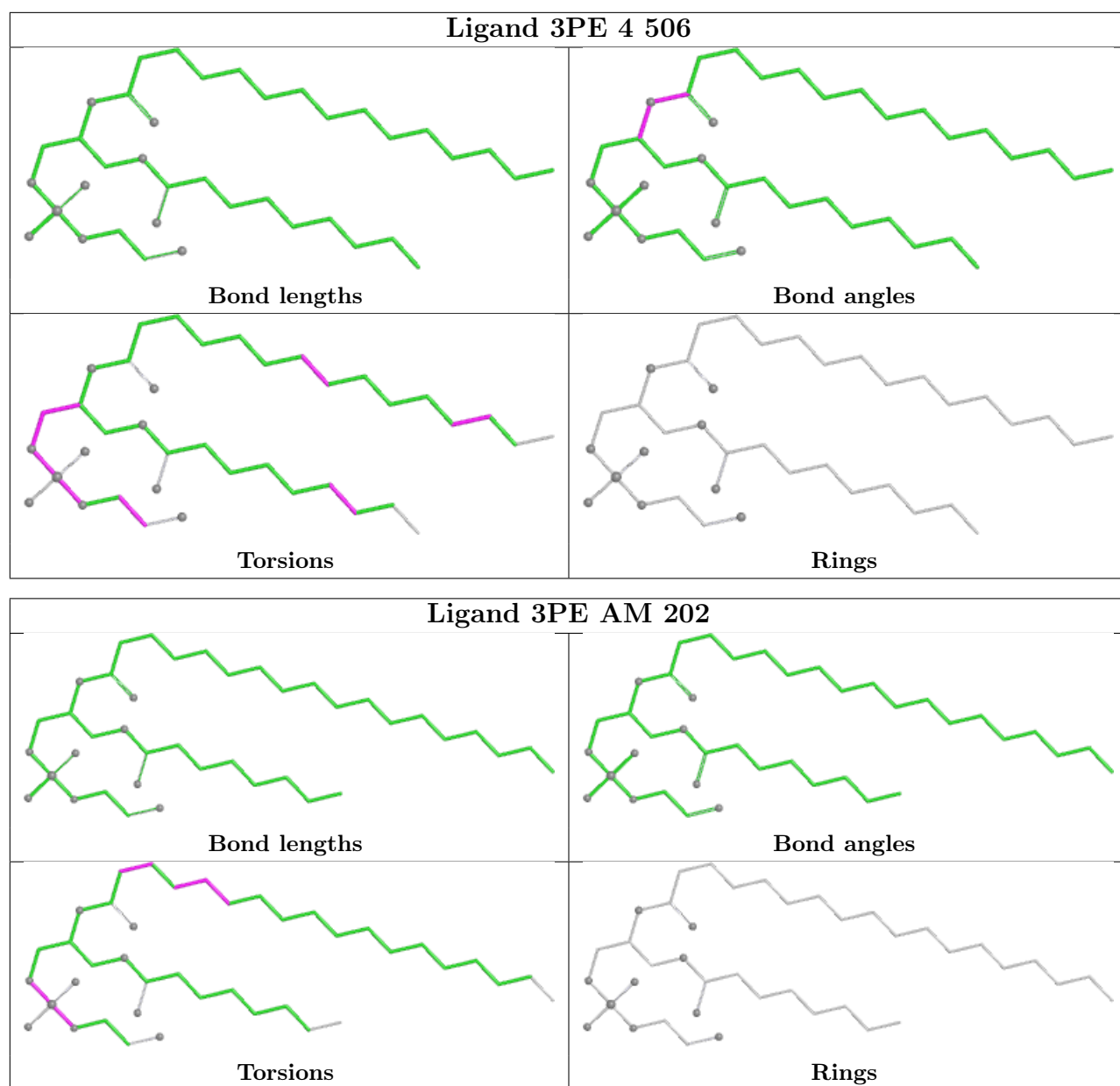




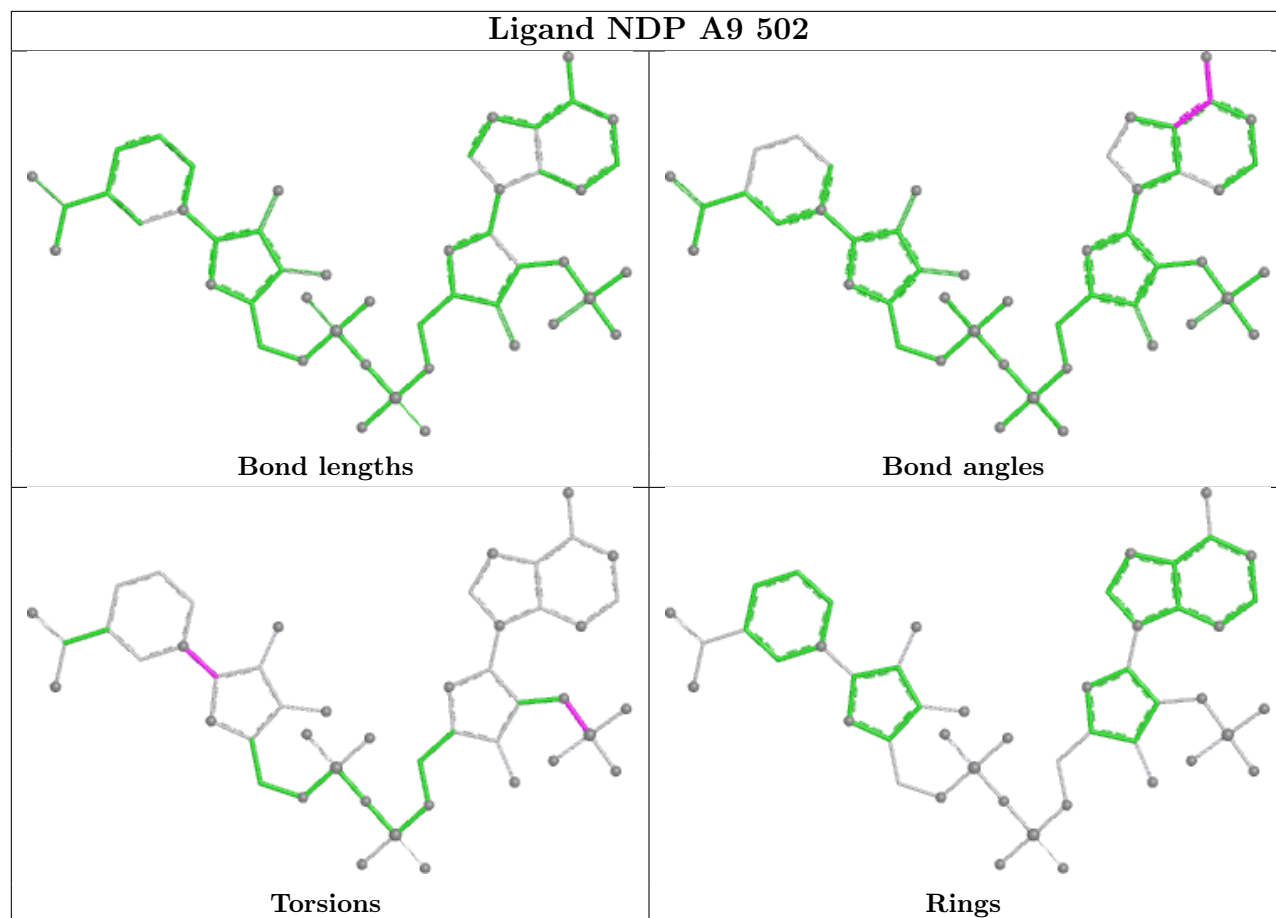




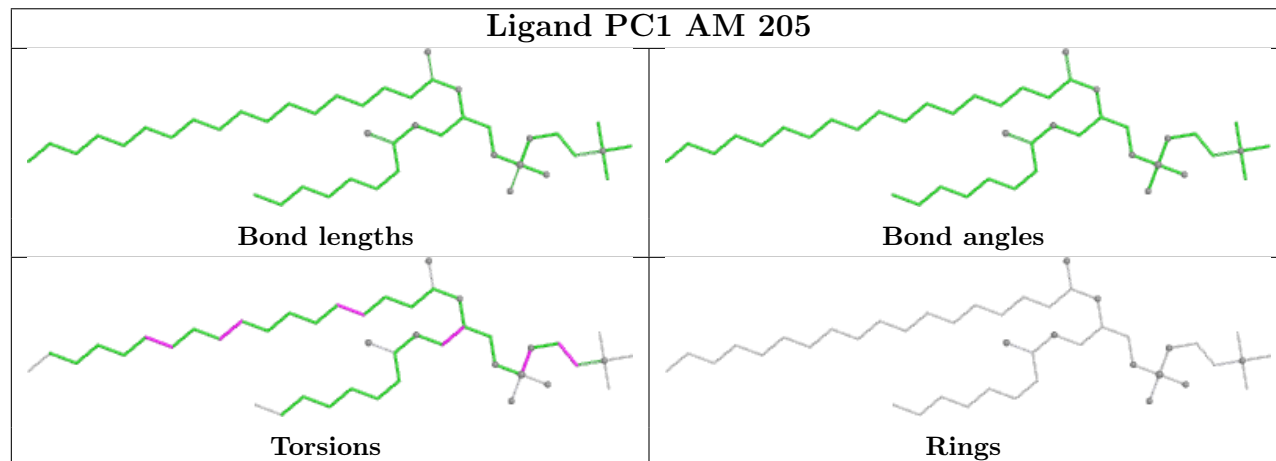


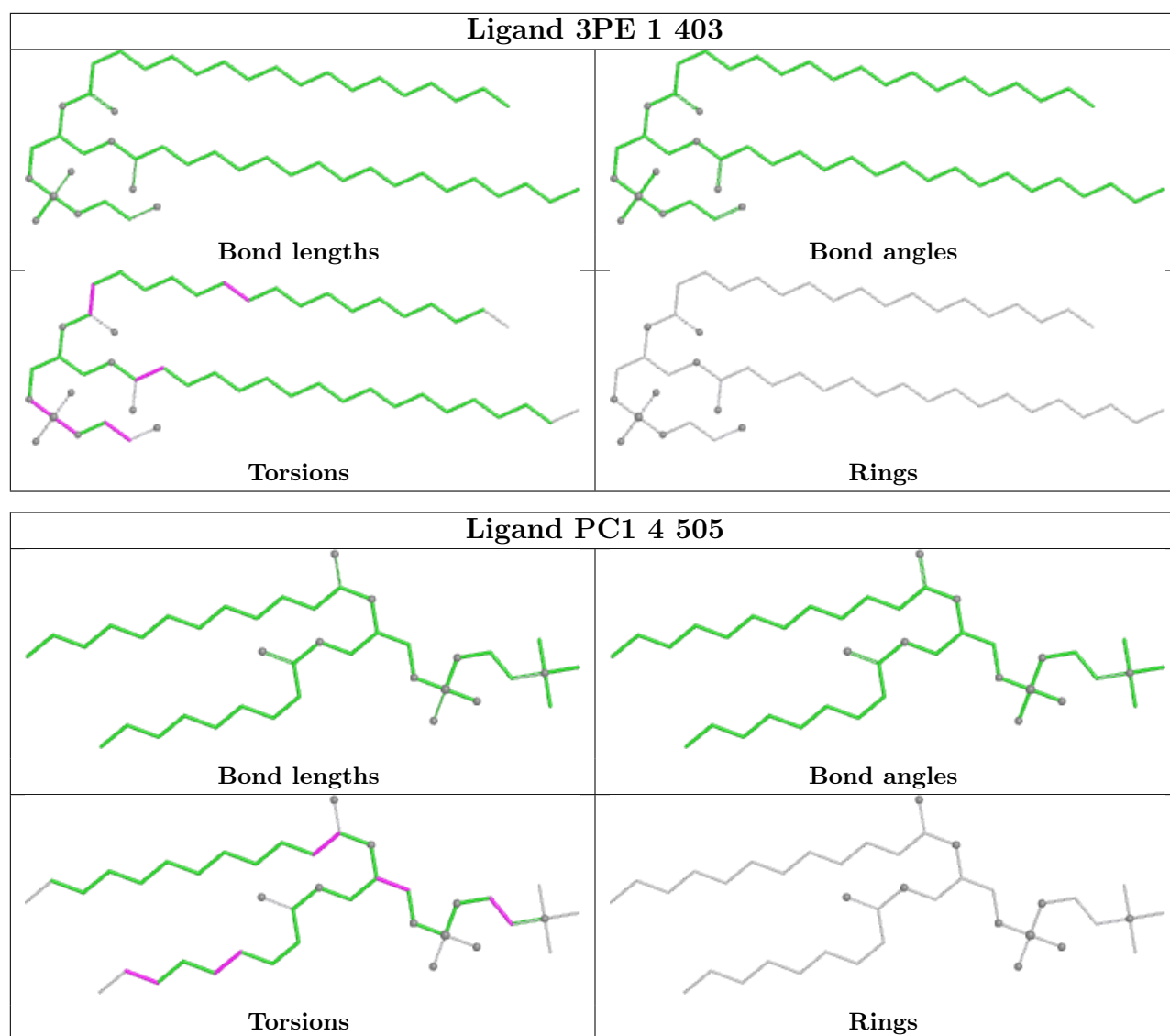


Ligand NDP A9 502

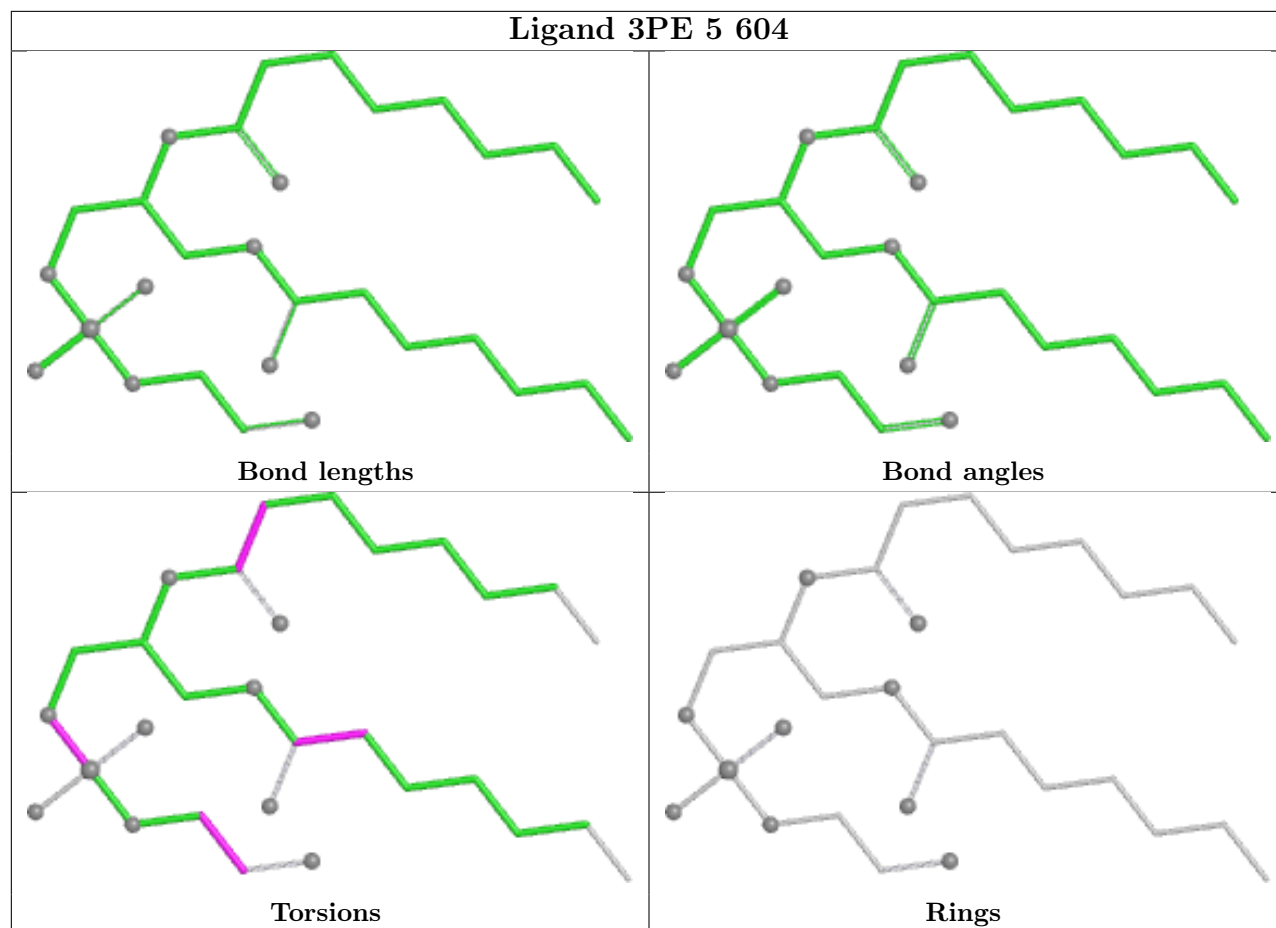


Ligand PC1 AM 205

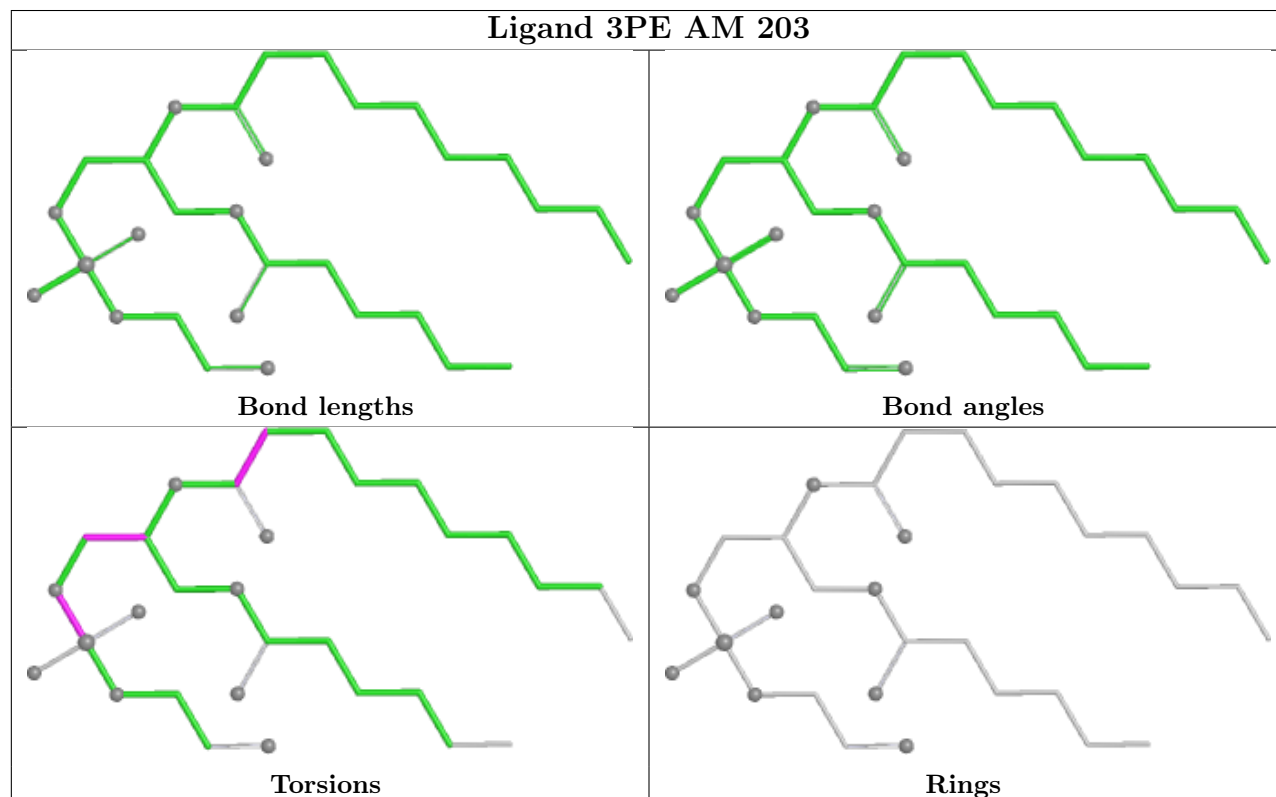


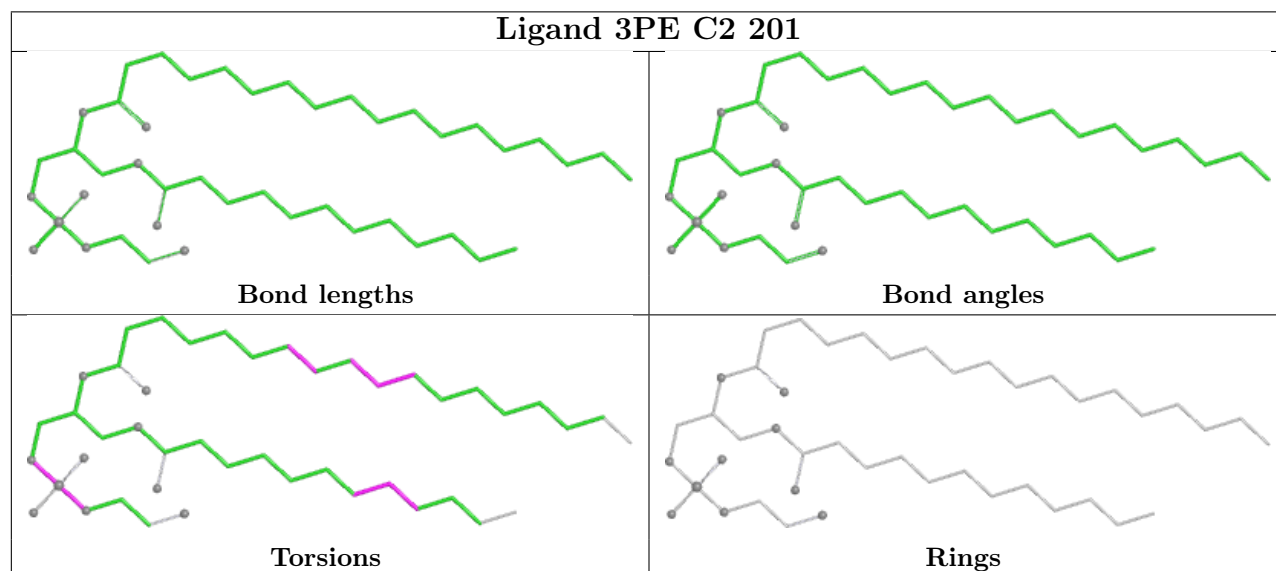
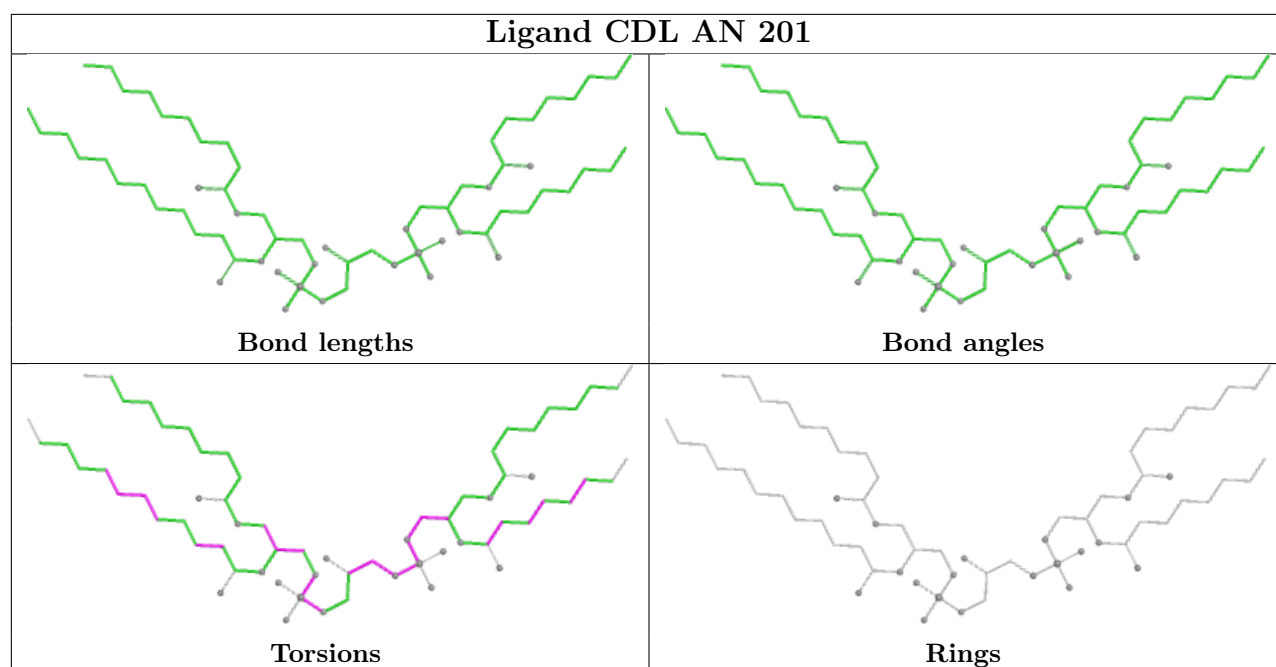


Ligand 3PE 5 604

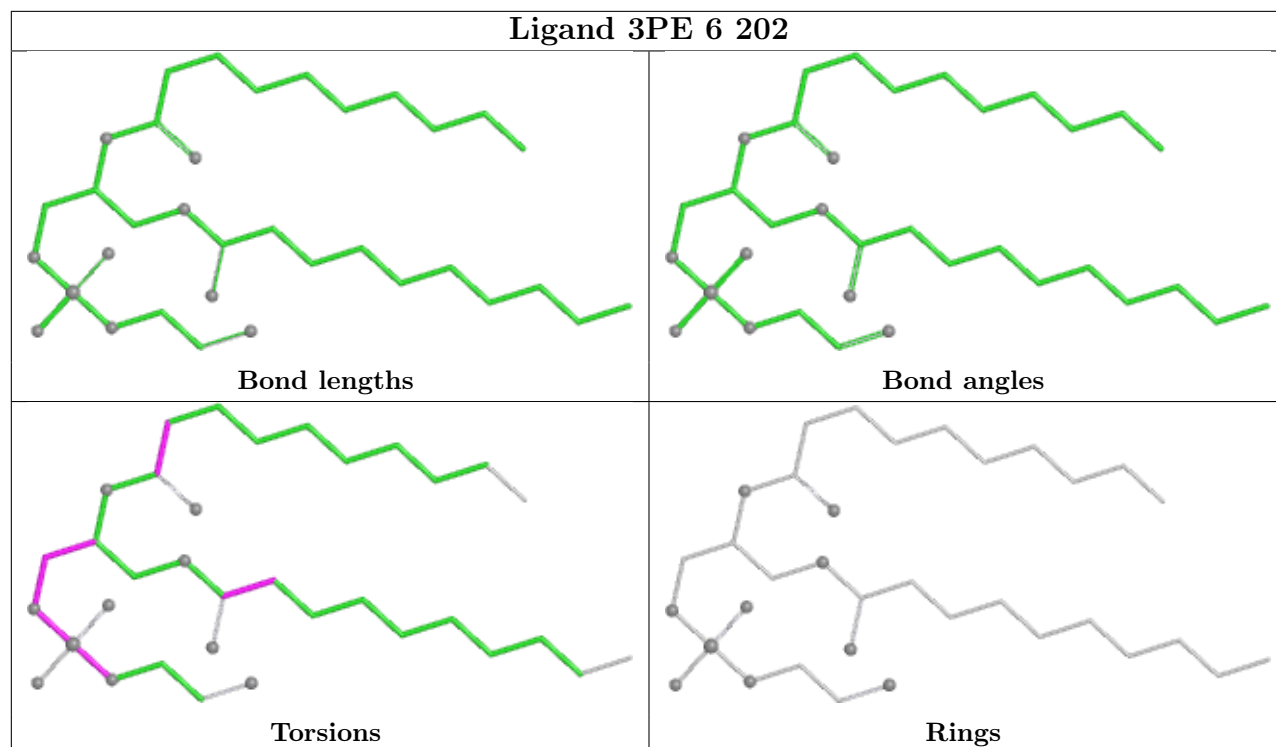


Ligand 3PE AM 203

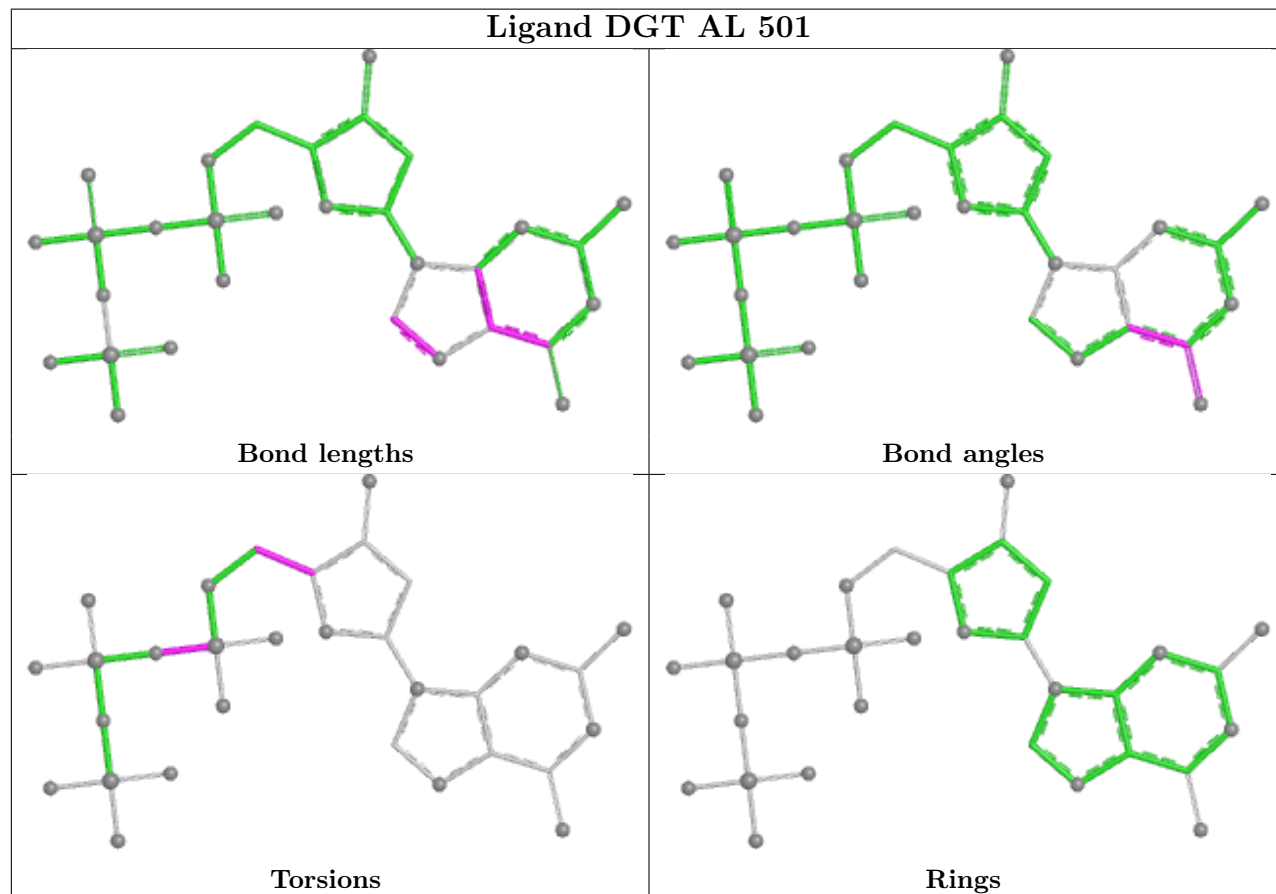


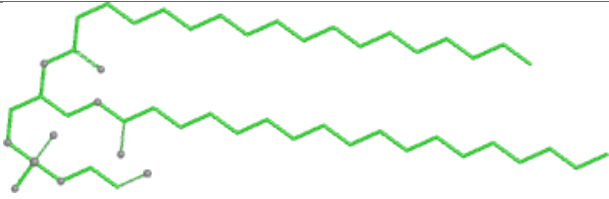
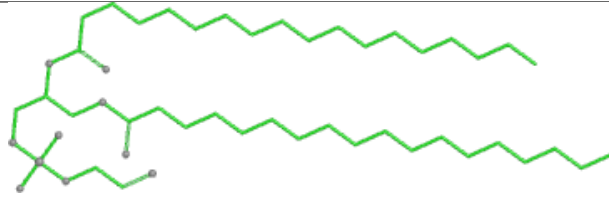
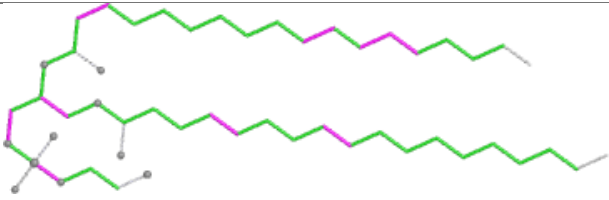
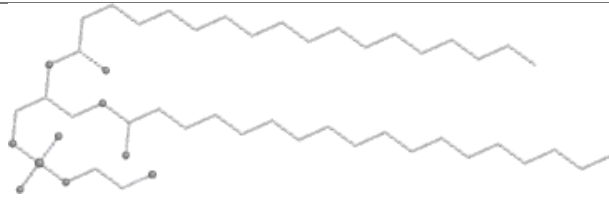


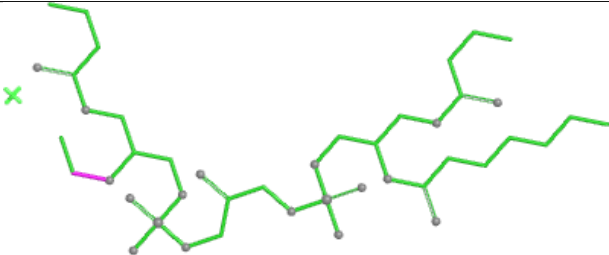
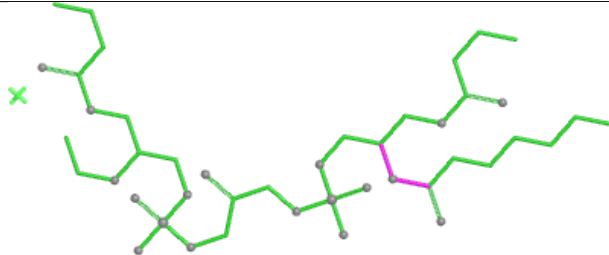
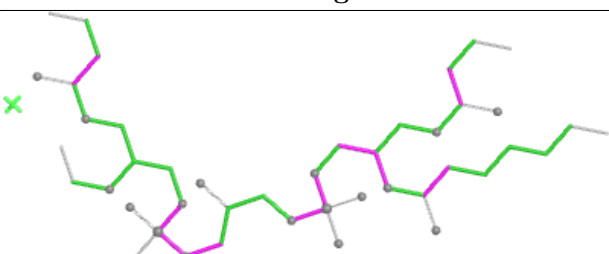
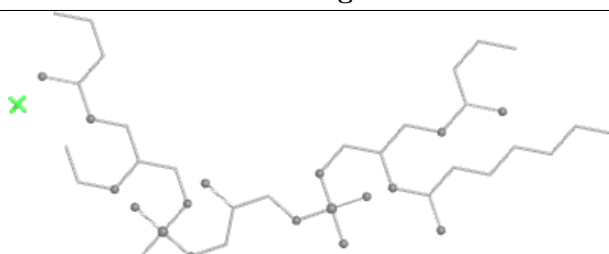
Ligand 3PE 6 202

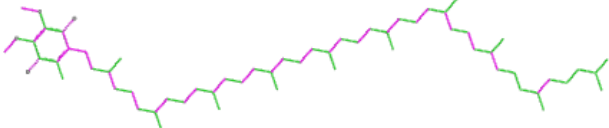
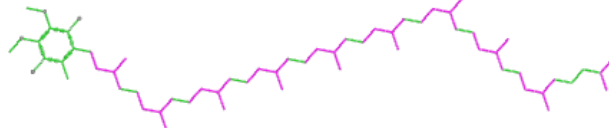
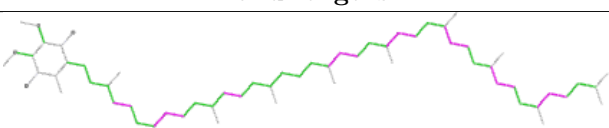
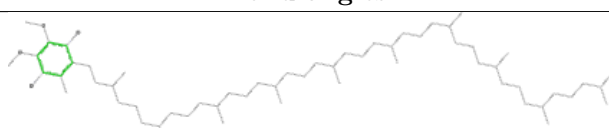


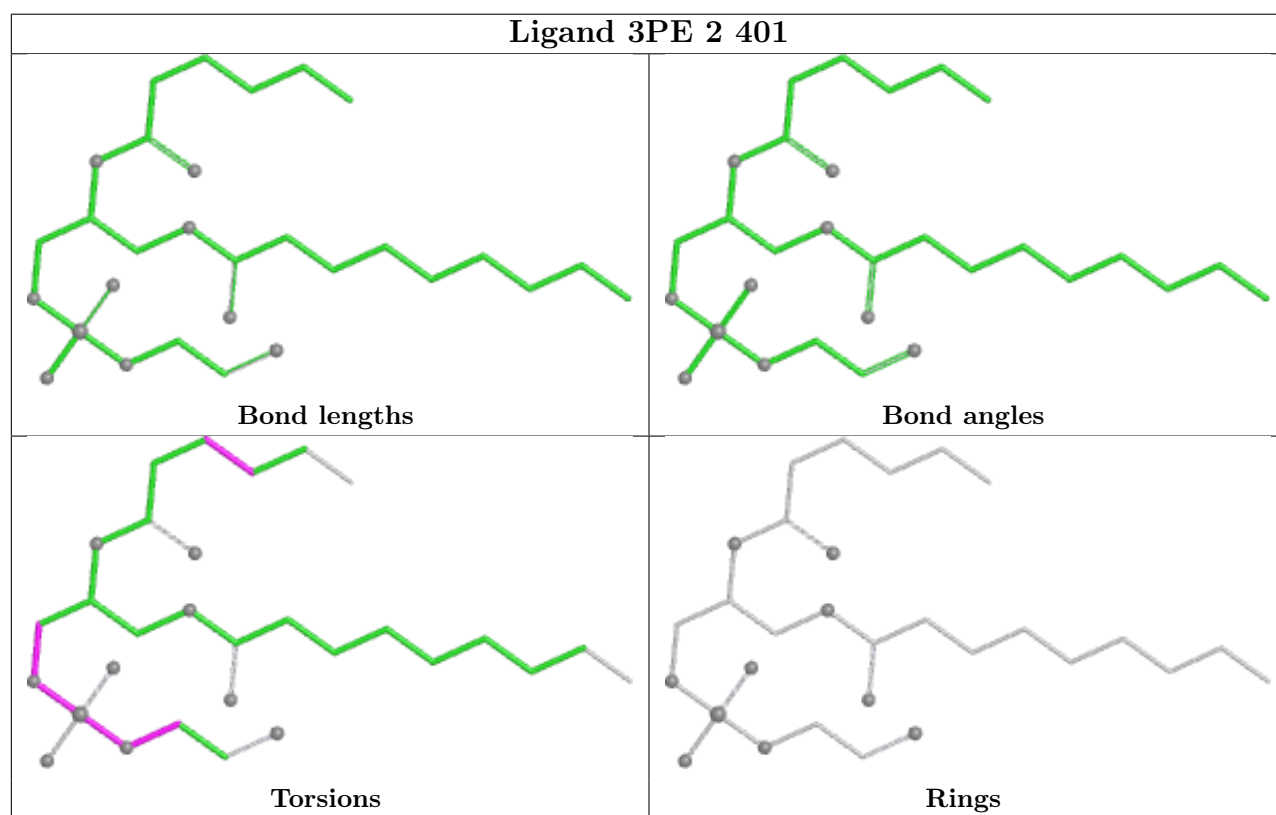
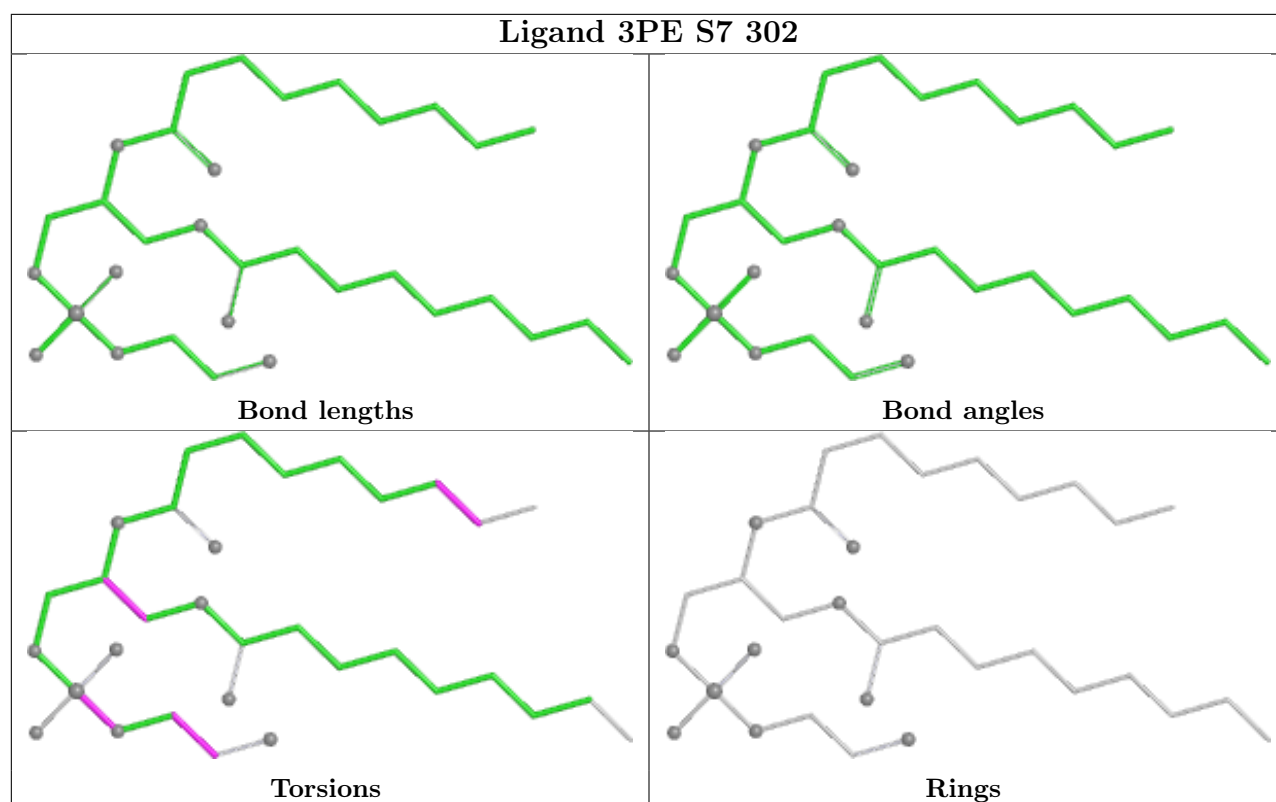
Ligand DGT AL 501

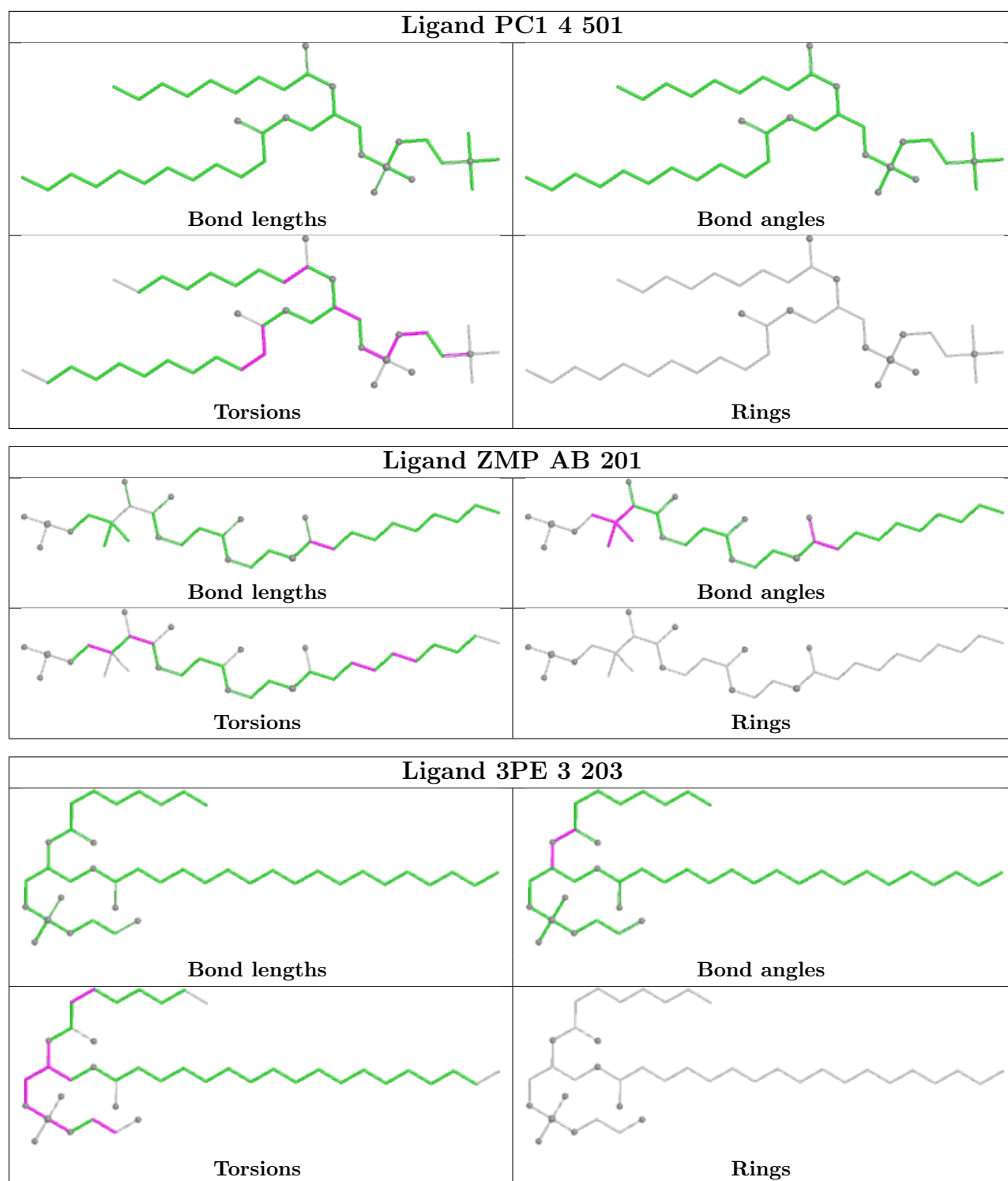


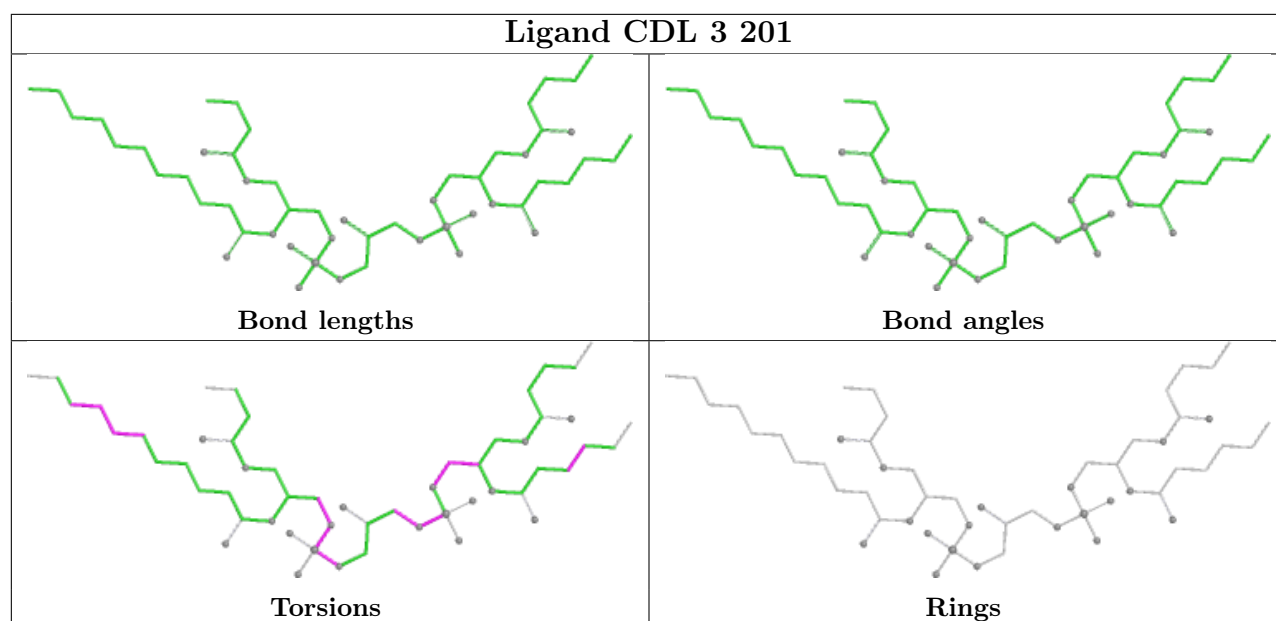
Ligand 3PE 3 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CDL 2 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand U10 1 402	
	
Bond lengths	Bond angles
	
Torsions	Rings







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.

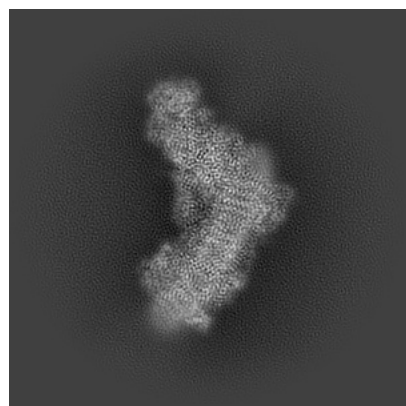
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28582. These allow visual inspection of the internal detail of the map and identification of artifacts.

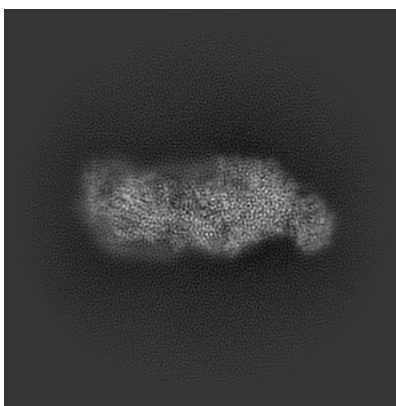
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

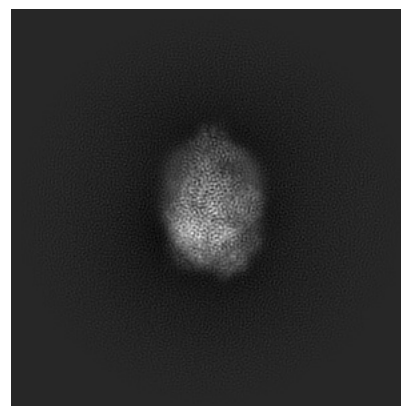
6.1.1 Primary map



X

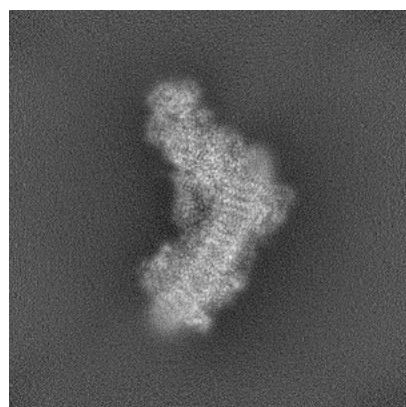


Y

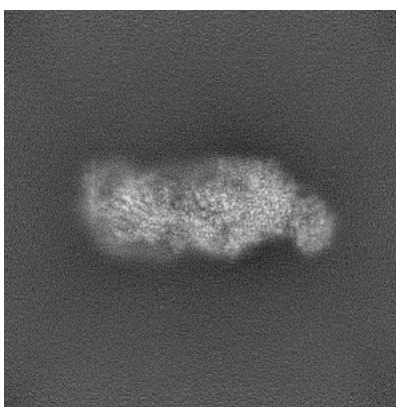


Z

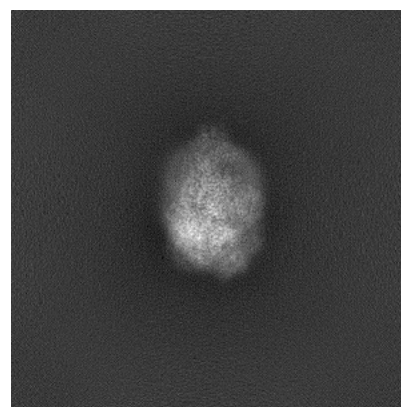
6.1.2 Raw map



X



Y

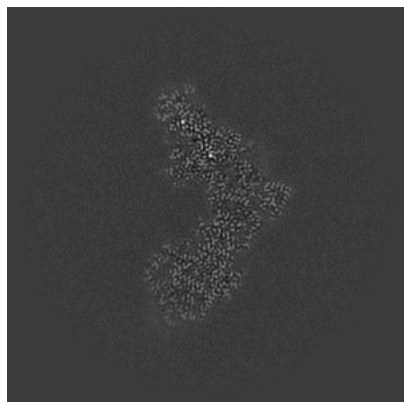


Z

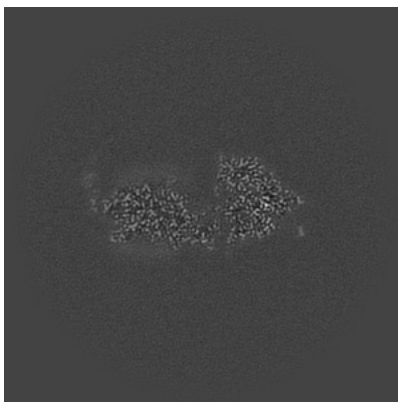
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

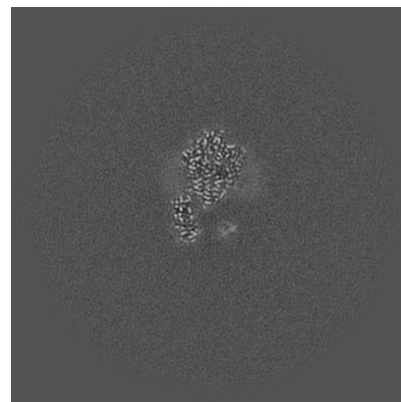
6.2.1 Primary map



X Index: 256

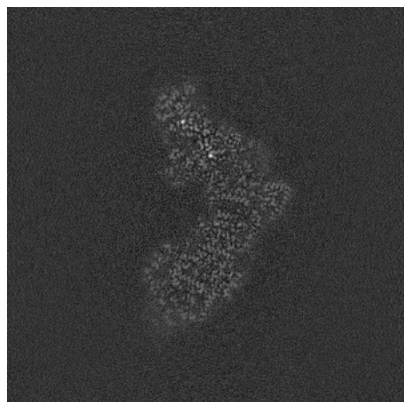


Y Index: 256

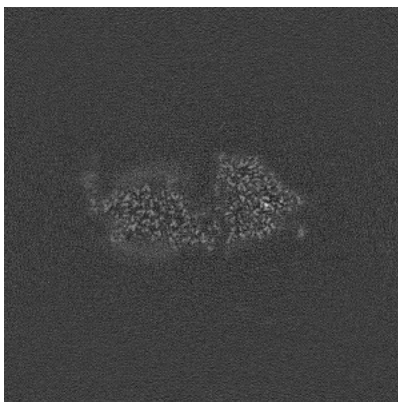


Z Index: 256

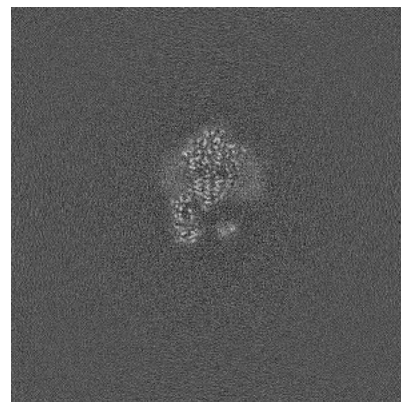
6.2.2 Raw map



X Index: 256



Y Index: 256

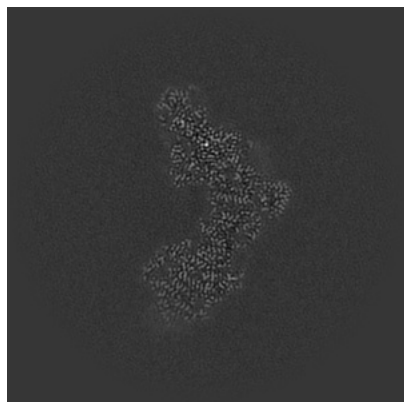


Z Index: 256

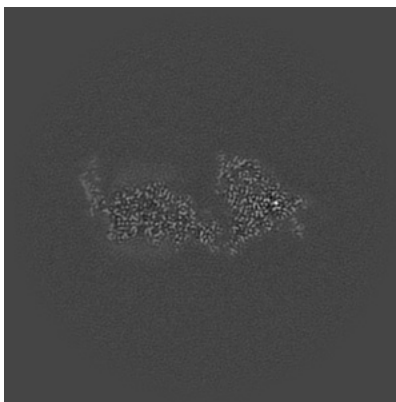
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

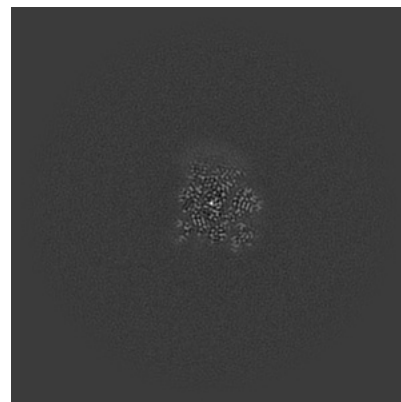
6.3.1 Primary map



X Index: 258

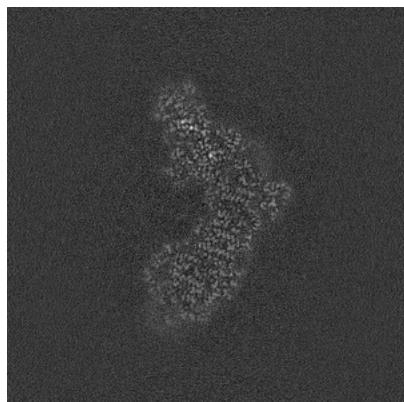


Y Index: 251

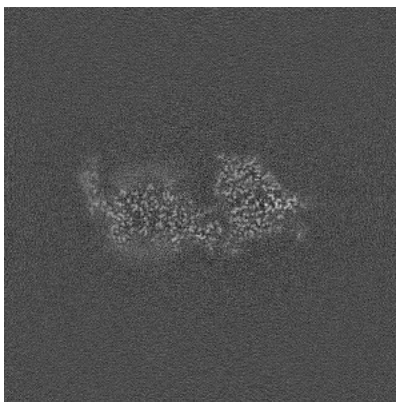


Z Index: 321

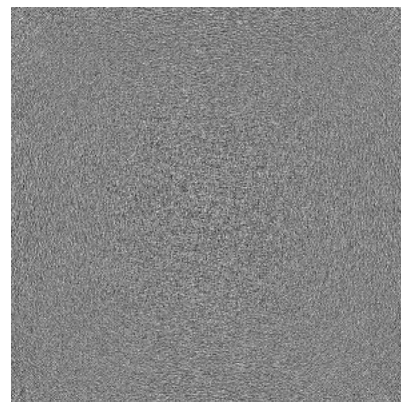
6.3.2 Raw map



X Index: 255



Y Index: 253

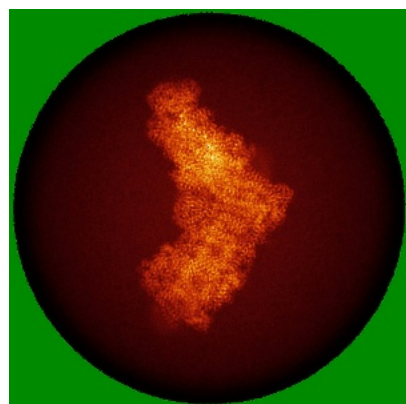


Z Index: 0

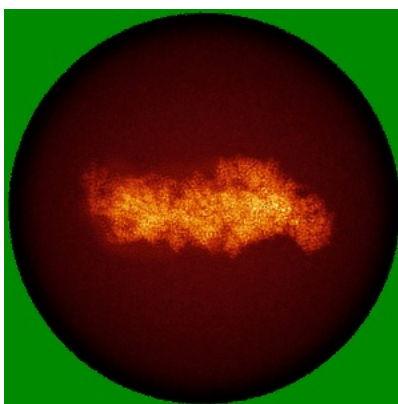
The images above show the largest variance slices of the map in three orthogonal directions.

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

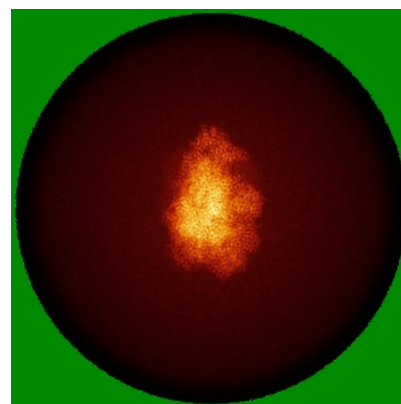
6.4.1 Primary map



X

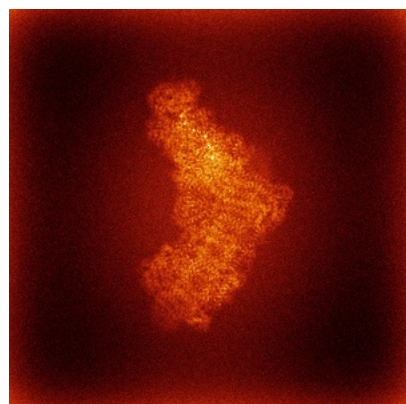


Y

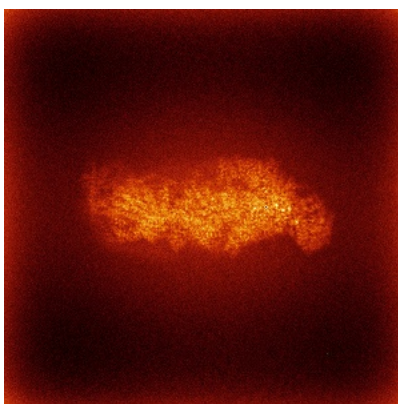


Z

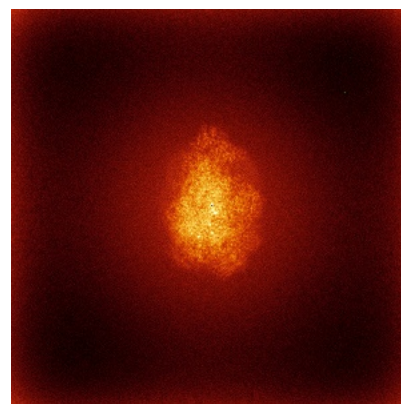
6.4.2 Raw map



X



Y

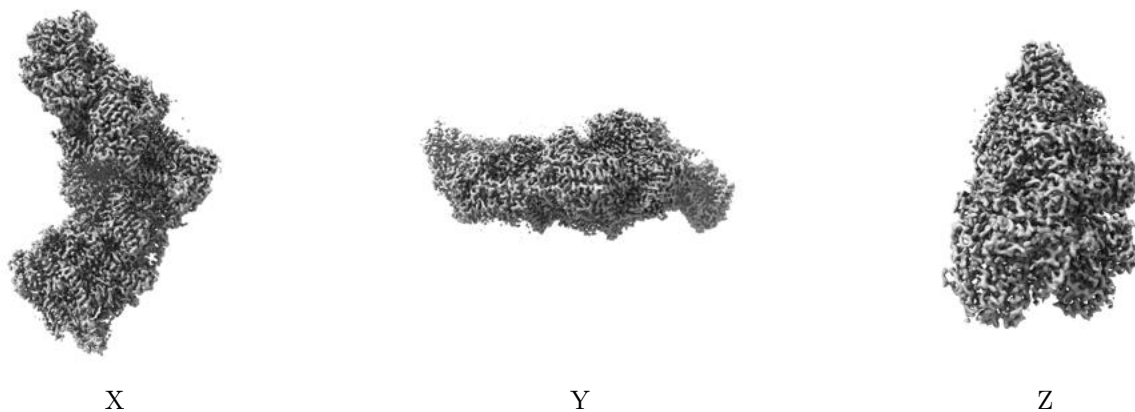


Z

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

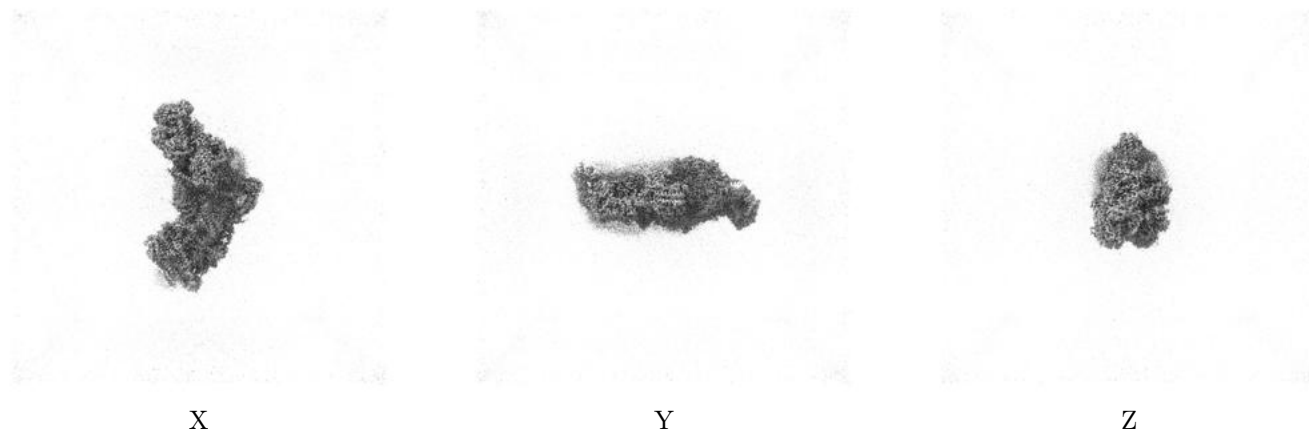
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

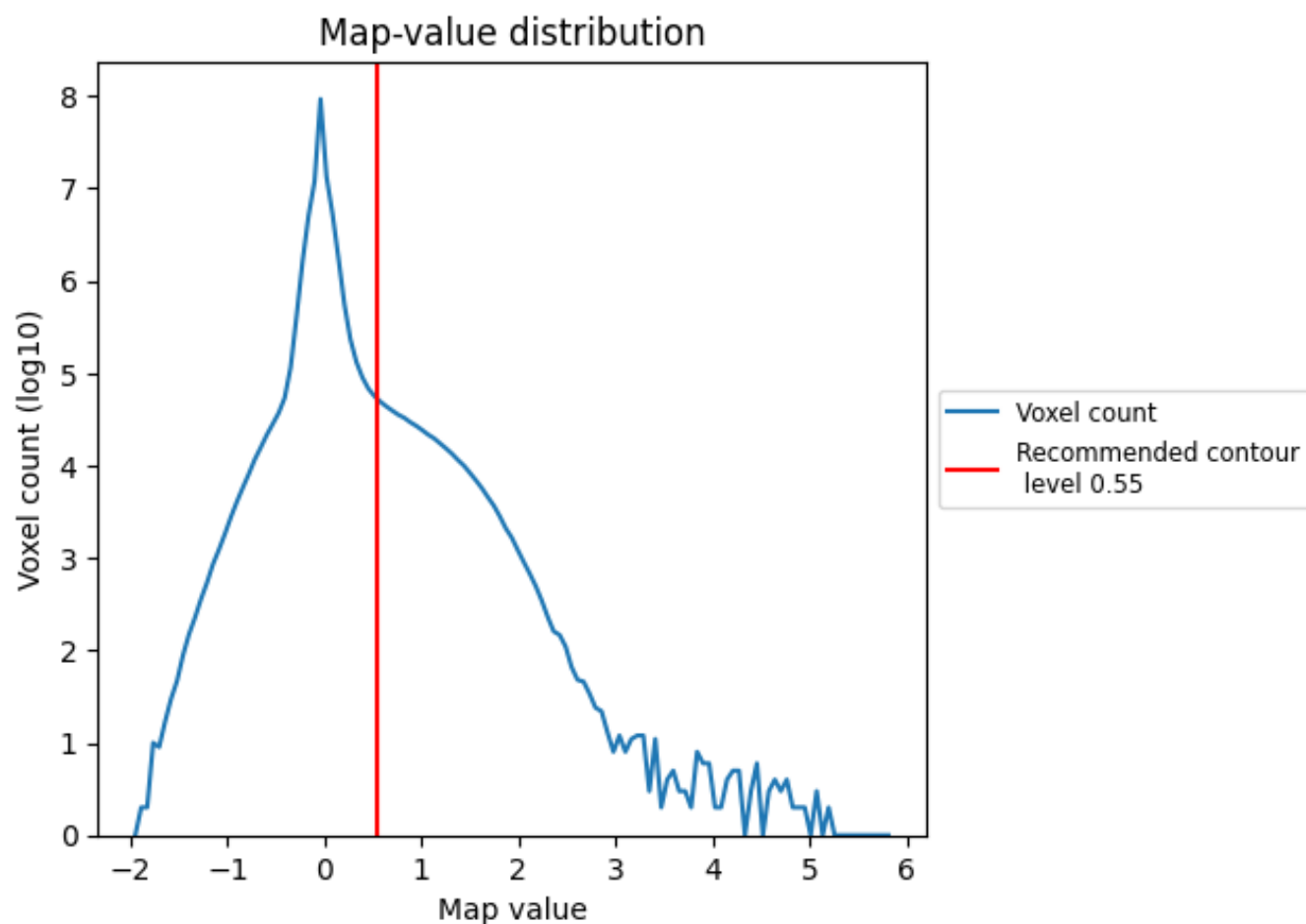
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

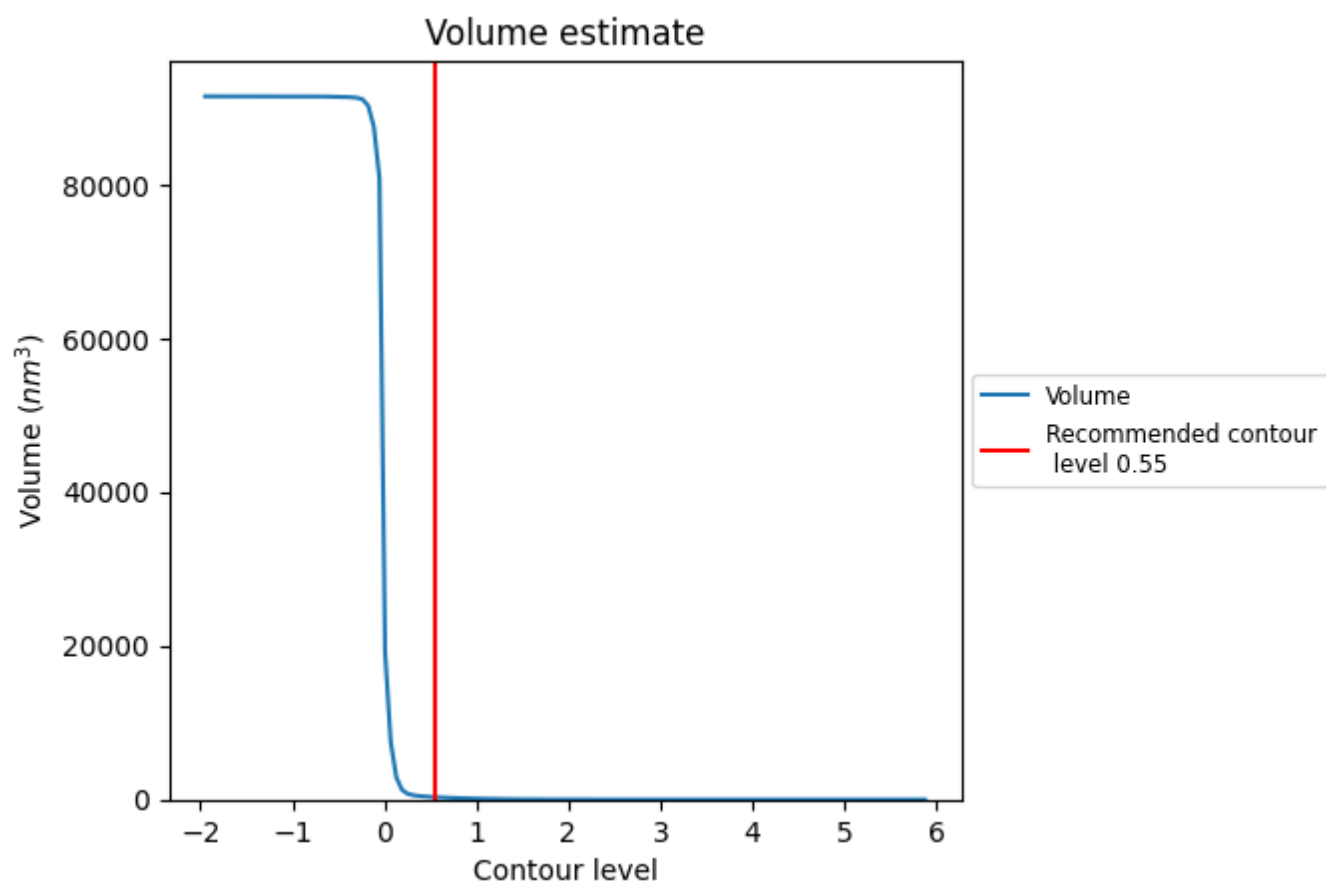
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

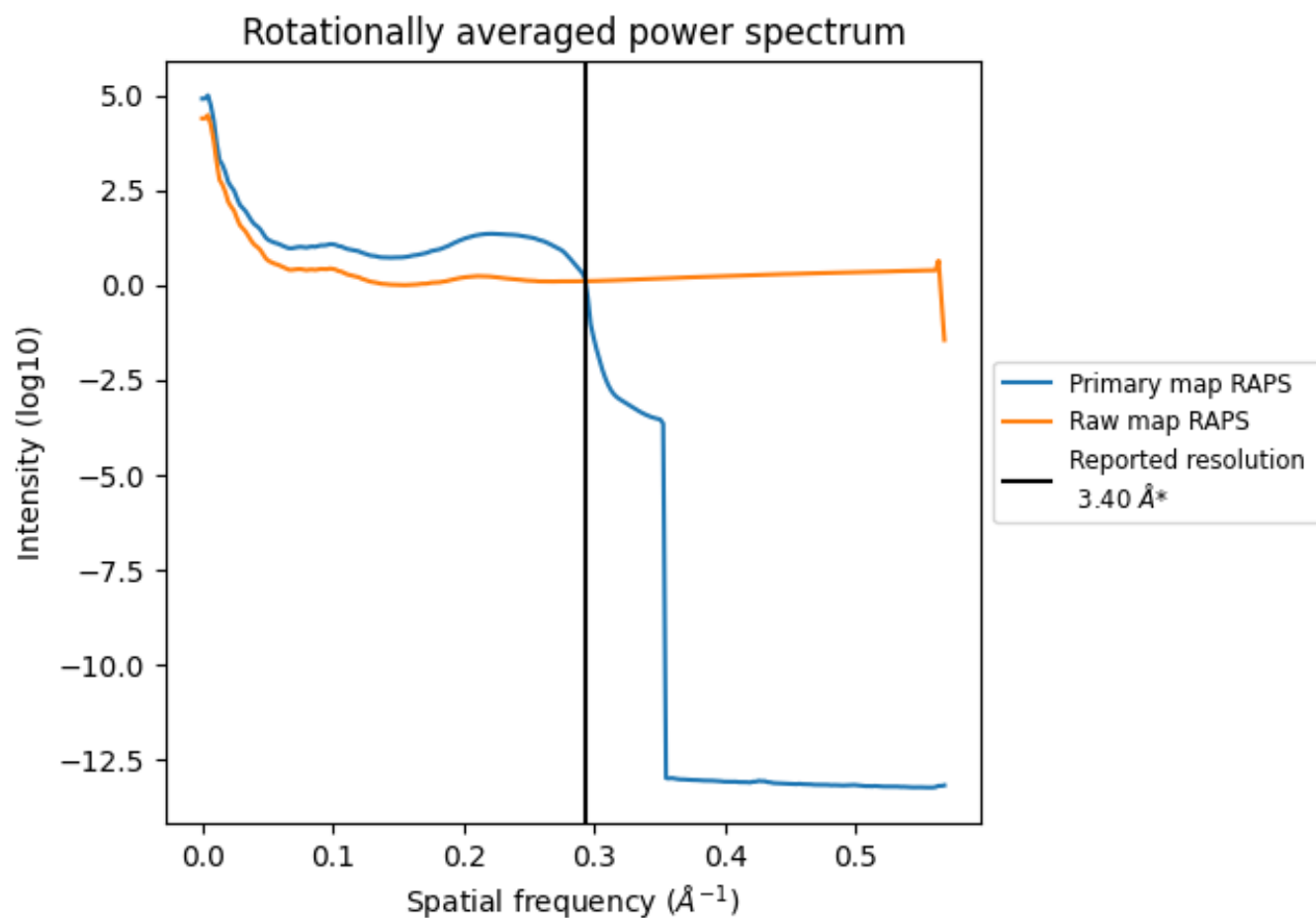
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm^3 ; this corresponds to an approximate mass of 281 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 ⓘ

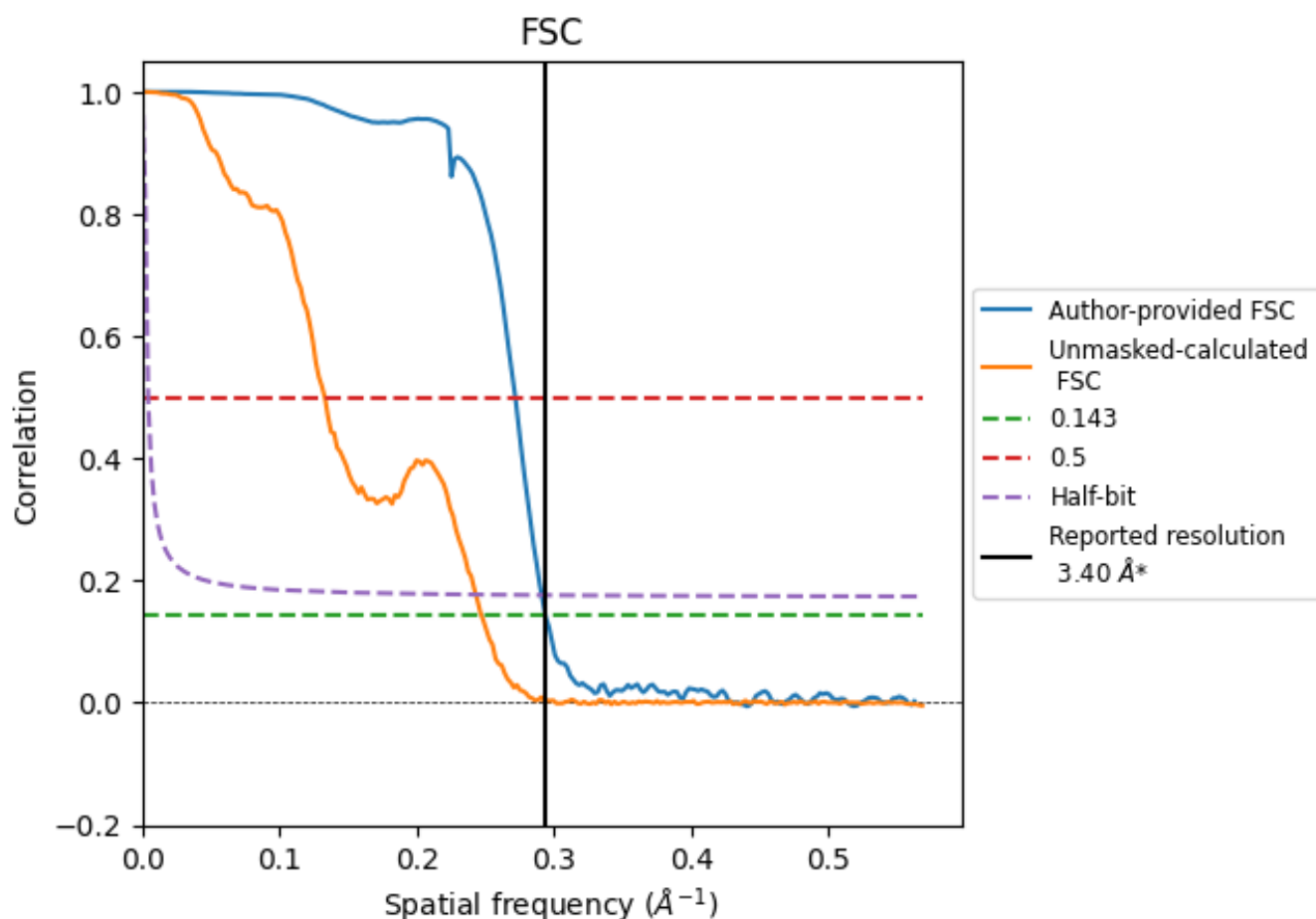


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

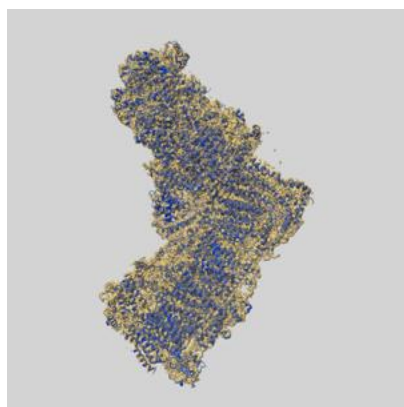
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.68	3.44
Unmasked-calculated*	4.05	7.52	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.4 by more than 10 %

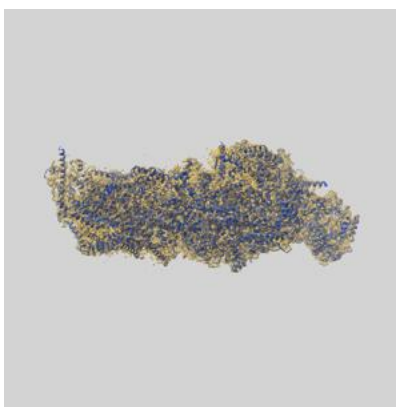
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28582 and PDB model 8ESZ. Per-residue inclusion information can be found in section [3](#) on page [22](#).

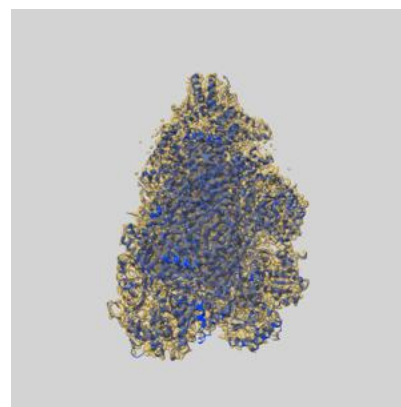
9.1 Map-model overlay [i](#)



X



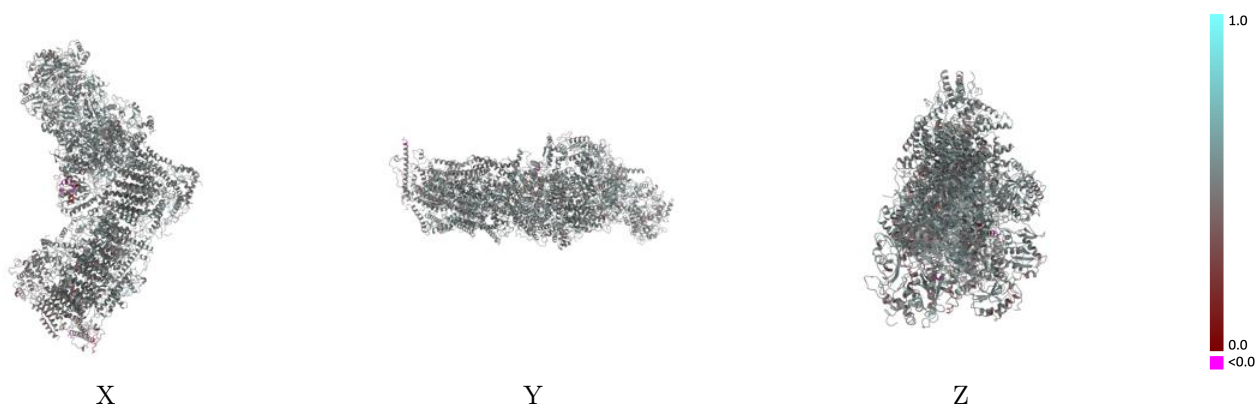
Y



Z

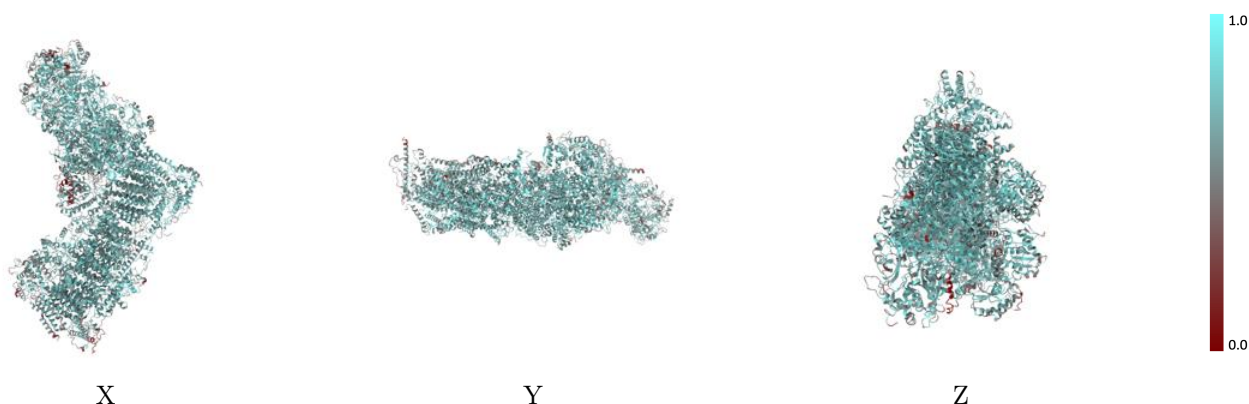
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



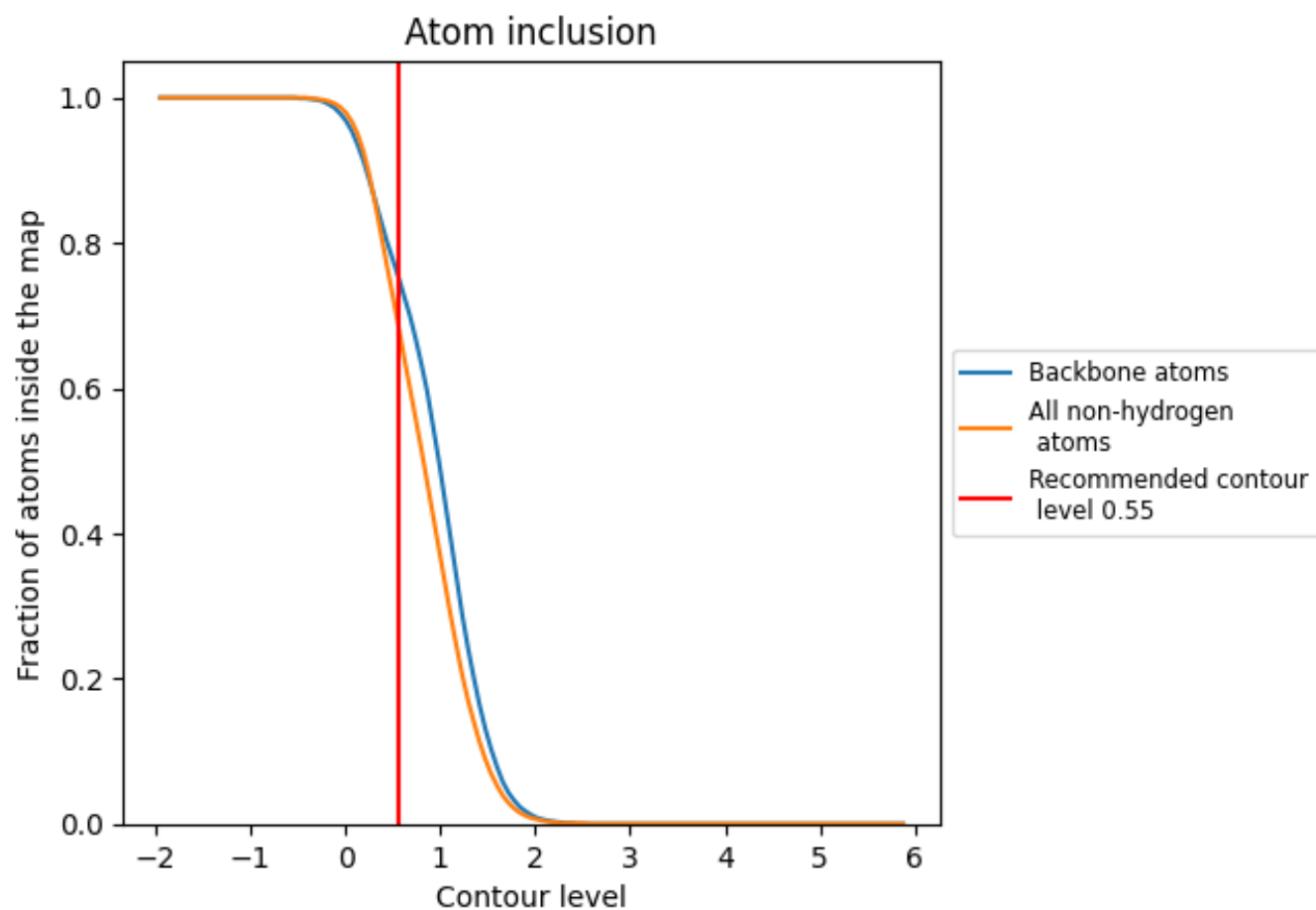
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6920	 0.4980
1	 0.7330	 0.5050
2	 0.7390	 0.5110
3	 0.6850	 0.4990
4	 0.7440	 0.5130
4L	 0.7090	 0.4980
5	 0.6680	 0.4840
6	 0.6760	 0.4990
A1	 0.7160	 0.4930
A3	 0.6920	 0.5070
A5	 0.6810	 0.5030
A6	 0.6790	 0.4900
A7	 0.6730	 0.5000
A8	 0.6810	 0.4930
A9	 0.7240	 0.5140
AB	 0.3060	 0.3330
AC	 0.5680	 0.4610
AL	 0.7260	 0.5090
AM	 0.5800	 0.4840
AN	 0.6500	 0.4960
AO	 0.7240	 0.5040
B1	 0.5950	 0.4860
B2	 0.5740	 0.4560
B3	 0.5400	 0.4410
B4	 0.6930	 0.4910
B5	 0.7390	 0.5250
B6	 0.6420	 0.4920
B7	 0.5390	 0.4190
B8	 0.6740	 0.4870
B9	 0.6740	 0.4870
BL	 0.7320	 0.5060
BM	 0.6830	 0.4900
C2	 0.7030	 0.5130
S1	 0.7020	 0.5040
S2	 0.7440	 0.5120



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Chain	Atom inclusion	Q-score
S3	 0.7680	 0.5300
S4	 0.6750	 0.5070
S5	 0.7370	 0.5150
S6	 0.7240	 0.5330
S7	 0.7450	 0.5060
S8	 0.7760	 0.5190
V1	 0.6850	 0.4880
V2	 0.6370	 0.4870
V3	 0.1480	 0.3400