



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:13 AM UTC

PDB ID : 7W1U / pdb_00007w1u
EMDB ID : EMD-32256
Title : Active state CI from Rotenone dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-20
Resolution : 3.20 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

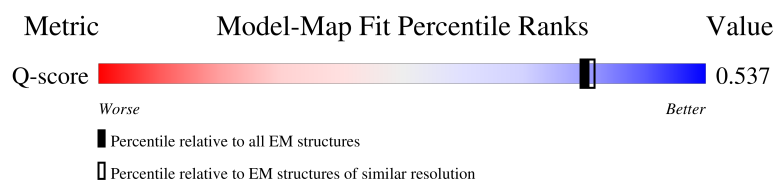
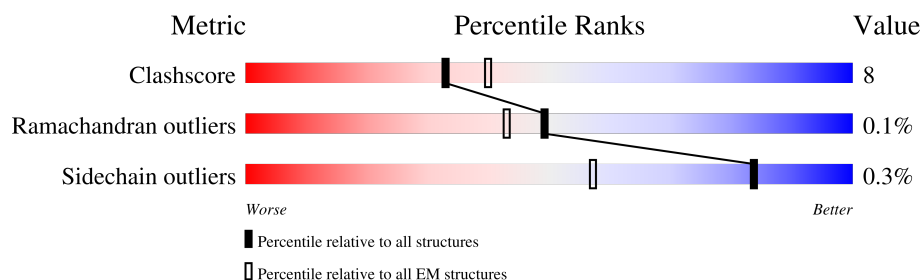
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	433	6% 81% 19%
2	B	176	82% 18%
3	C	156	75% 25%
4	E	115	10% 83% 17%

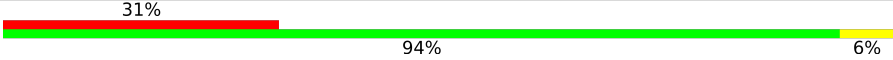
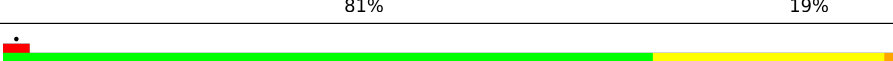
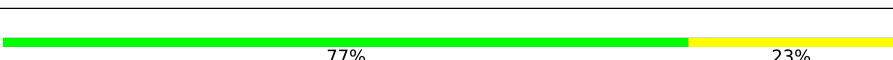
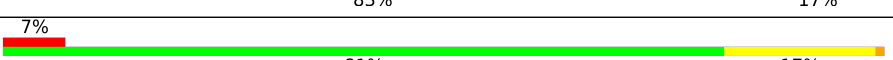
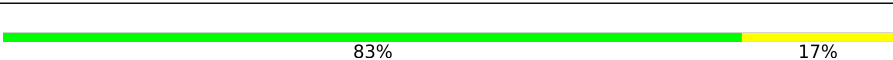
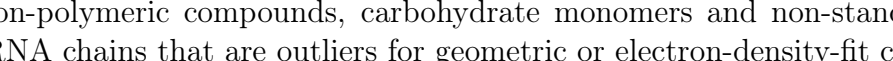
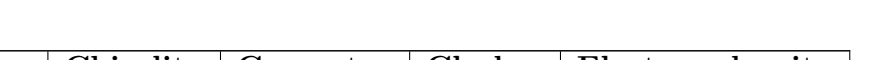
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156	
27	d	175	
28	e	104	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	121	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

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
45	SF4	A	501	-	-	X	-
45	SF4	C	301	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 67815 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] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3324	2100	590	614	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1392	875	239	267	11		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1247	794	227	212	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			687	432	129	124	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			690	446	102	137	5		
6	X	88	Total	C	N	O	S	0	0
			699	450	103	141	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 9 is a protein called NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5292	3318	923	1012	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3450	2206	591	629	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			566	364	103	94	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			639	414	109	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			819	537	144	137	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			377	246	65	66		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1290	862	188	227	13		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O		0	0
			1062	691	182	189			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2498	1673	382	422	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

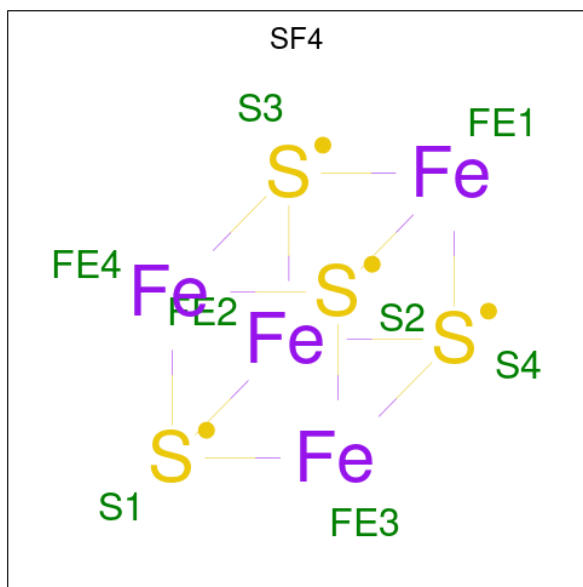
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

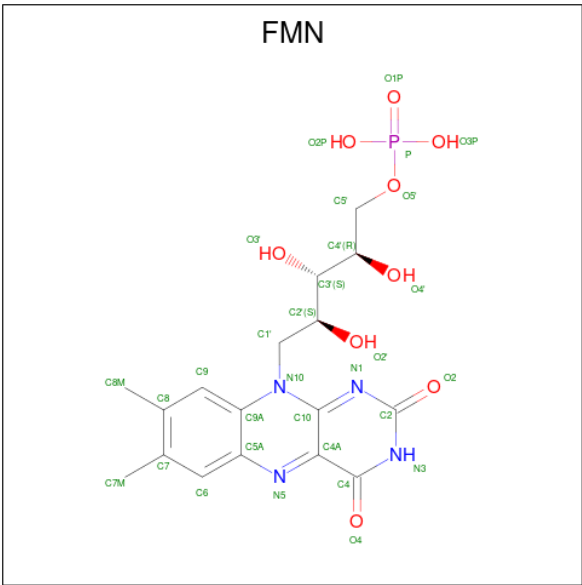
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1644	438	490	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



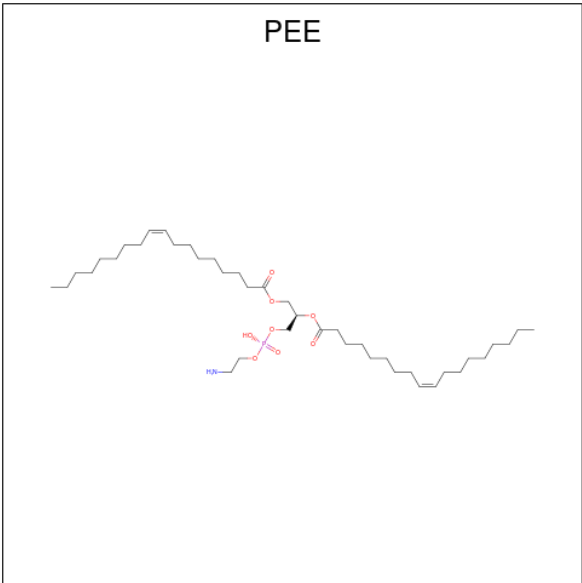
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



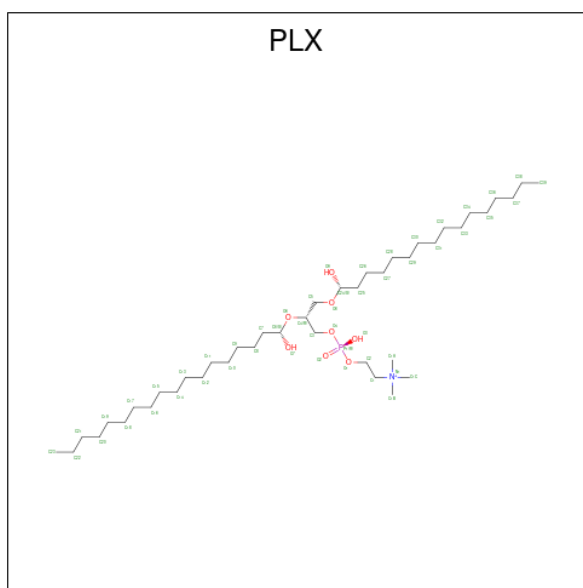
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	W	1	Total	C	N	O	P	0
			41	31	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
47	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
47	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	s	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 48 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



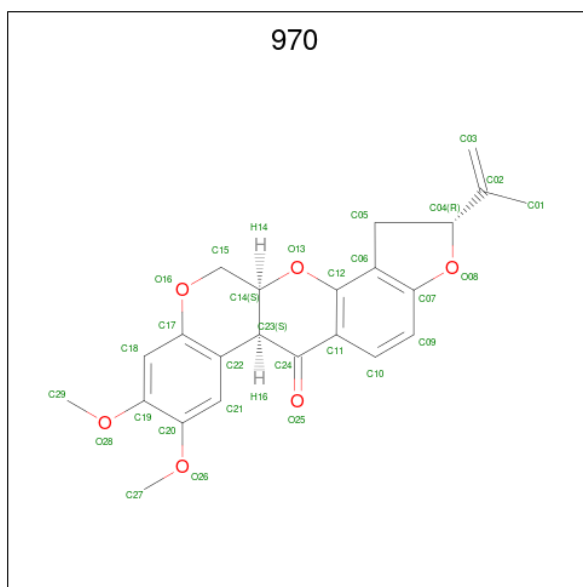
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	

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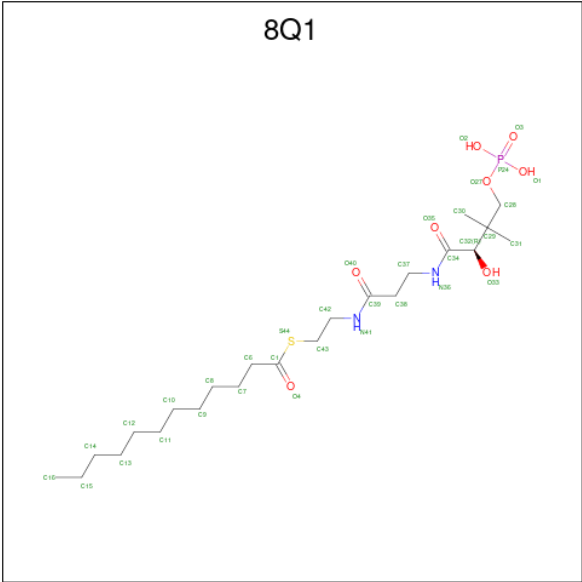
Mol	Chain	Residues	Atoms					AltConf
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



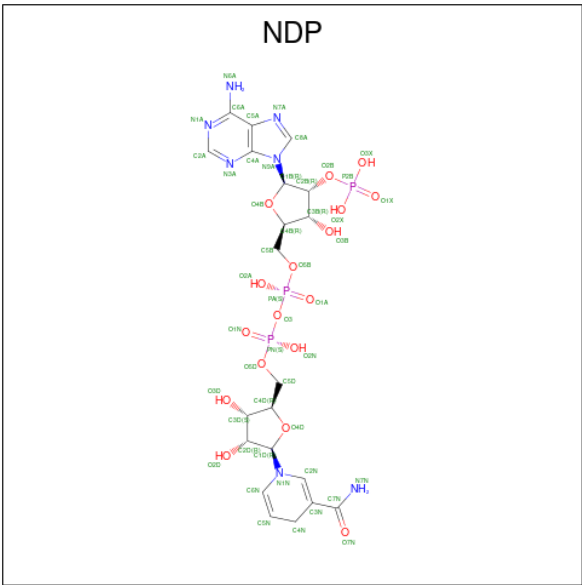
Mol	Chain	Residues	Atoms			AltConf
49	C	1	Total	C	O	0
			29	23	6	

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



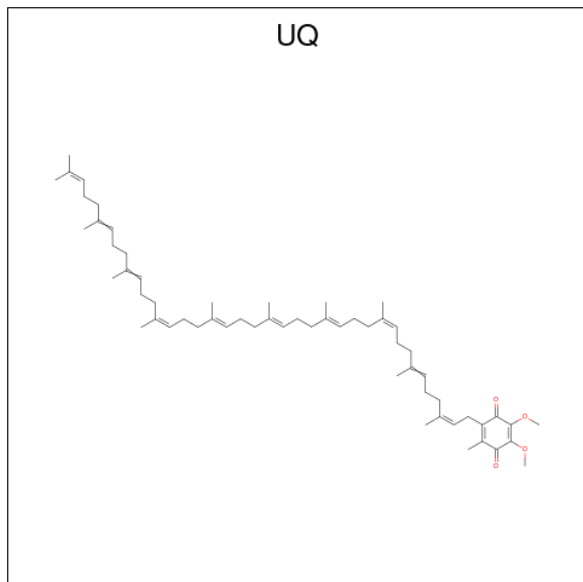
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



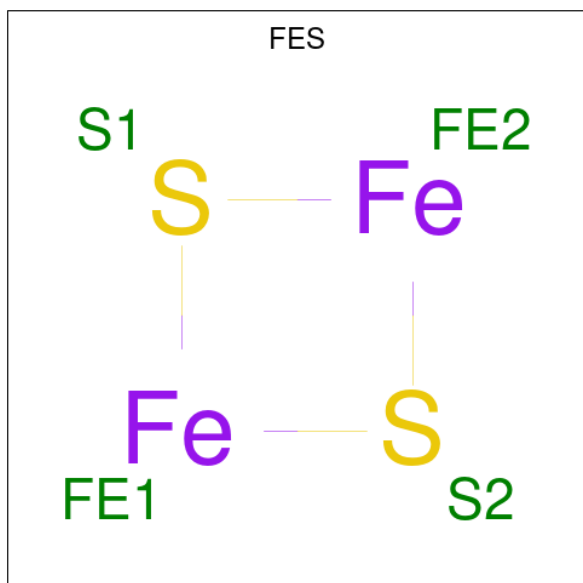
Mol	Chain	Residues	Atoms					AltConf
51	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 52 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
52	J	1	Total	C	O	0
			33	29	4	
52	s	1	Total	C	O	0
			38	34	4	

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

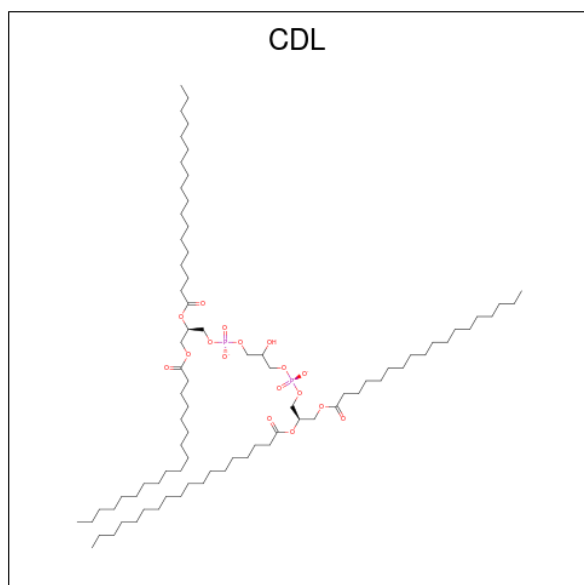


Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	Fe	S	0
			4	2	2	
53	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
54	M	1	Total	Mg	0
			1	1	

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
55	S	1	Total	C	O	P	0
			51	32	17	2	
55	V	1	Total	C	O	P	0
			94	75	17	2	
55	V	1	Total	C	O	P	0
			100	81	17	2	
55	a	1	Total	C	O	P	0
			100	81	17	2	
55	l	1	Total	C	O	P	0
			99	80	17	2	
55	l	1	Total	C	O	P	0
			100	81	17	2	

Continued on next page...

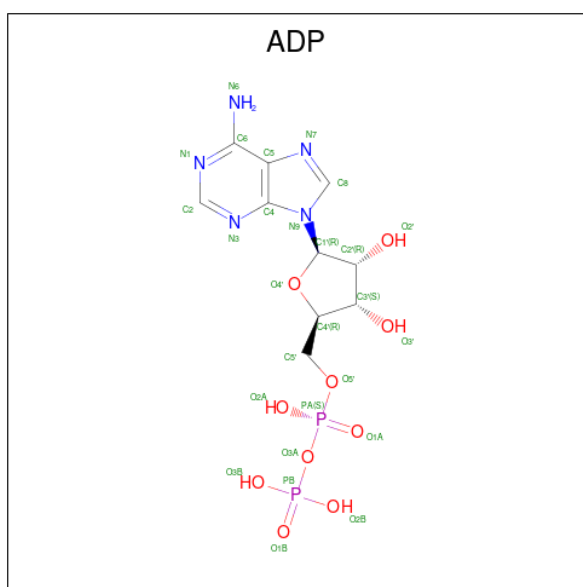
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
55	n	1	Total	C	O	P	0
			55	36	17	2	
55	r	1	Total	C	O	P	0
			99	80	17	2	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
56	T	1	Total	Zn	0
			1	1	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

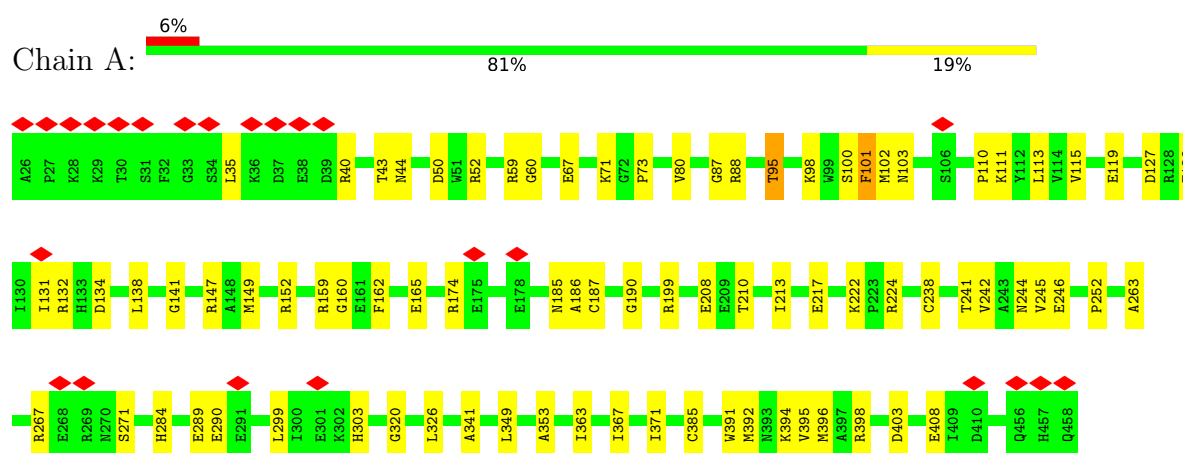


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

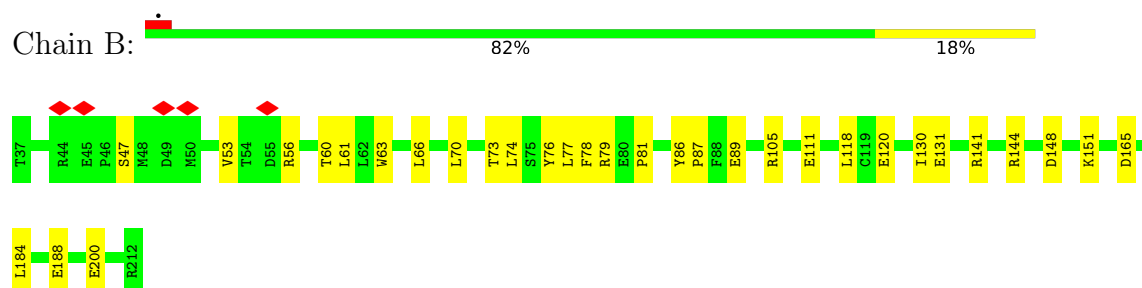
3 Residue-property plots

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.

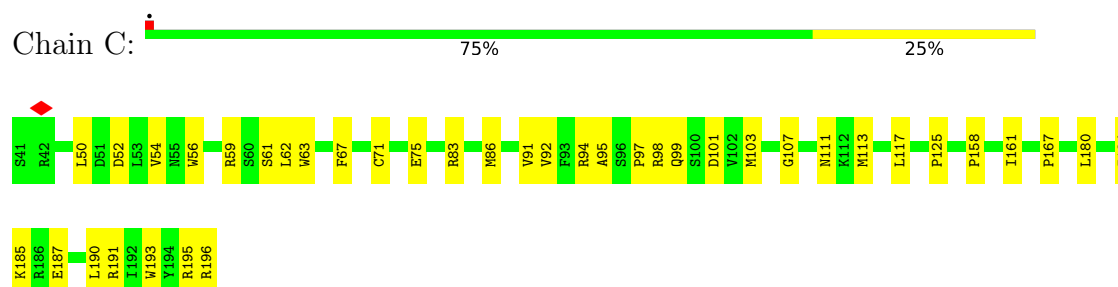
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



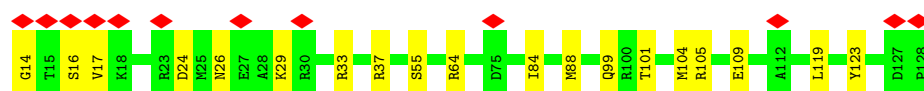
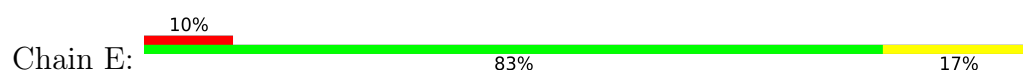
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



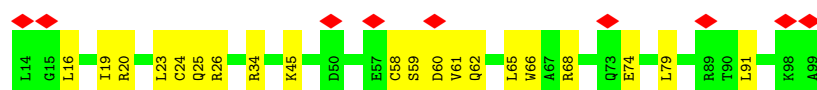
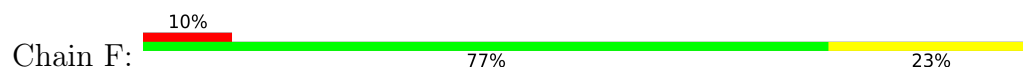
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



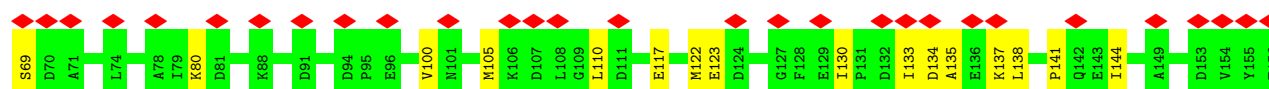
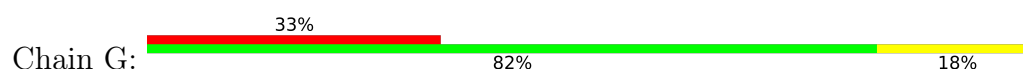
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



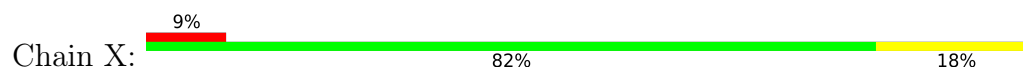
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



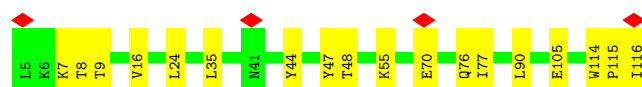
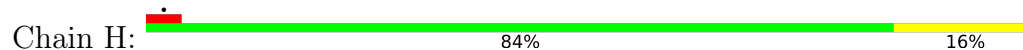
- Molecule 6: Acyl carrier protein



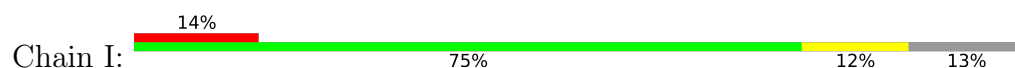
- Molecule 6: Acyl carrier protein



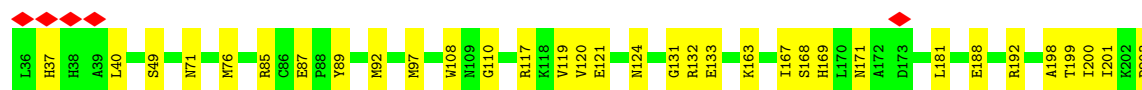
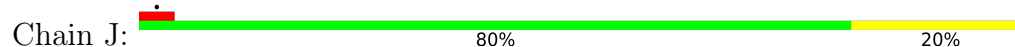
- Molecule 7: Complex I subunit B13

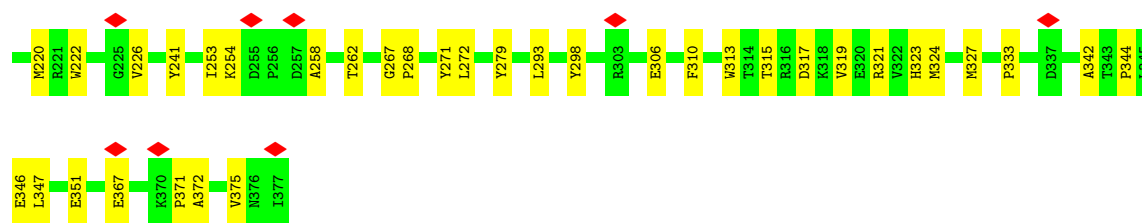


- Molecule 8: Complex I-B14.5a

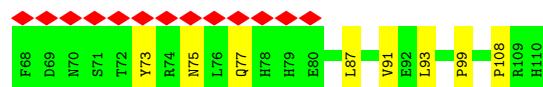
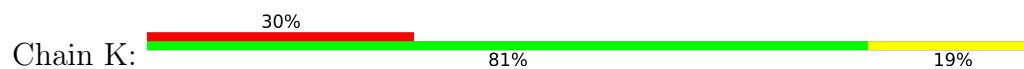


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

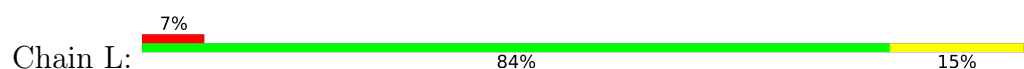




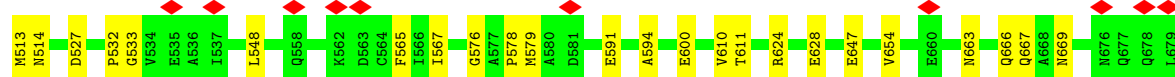
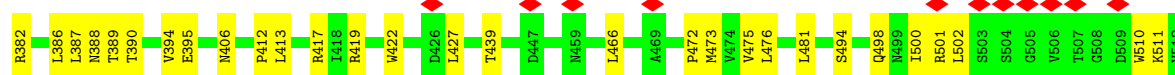
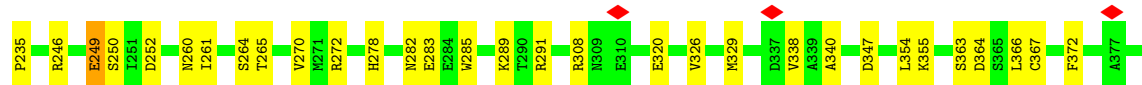
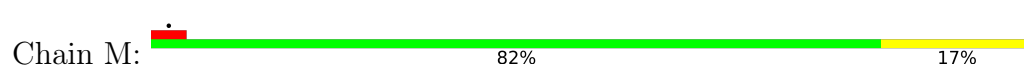
- Molecule 10: Complex I-9kD



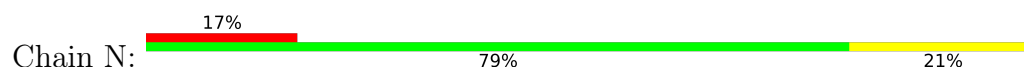
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

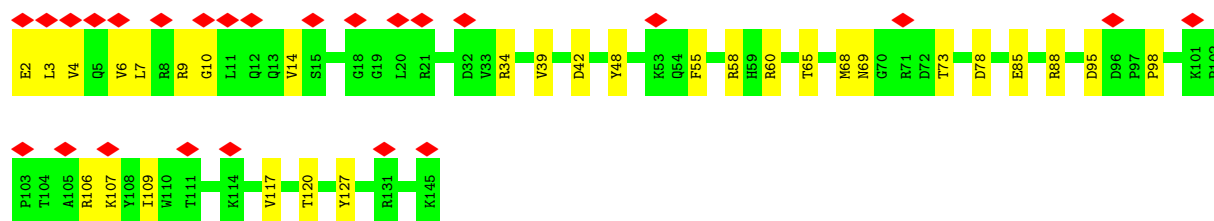


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

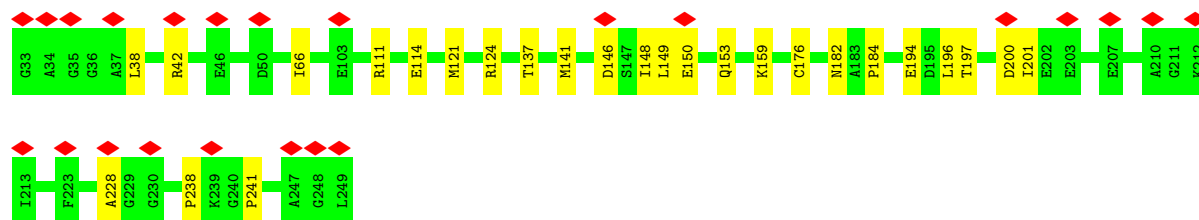
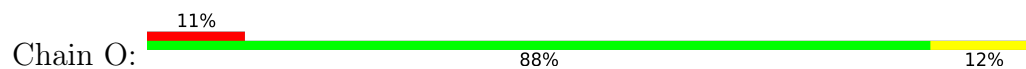


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

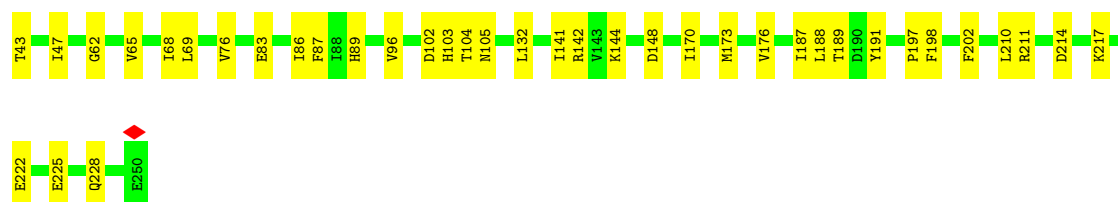
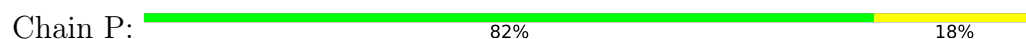




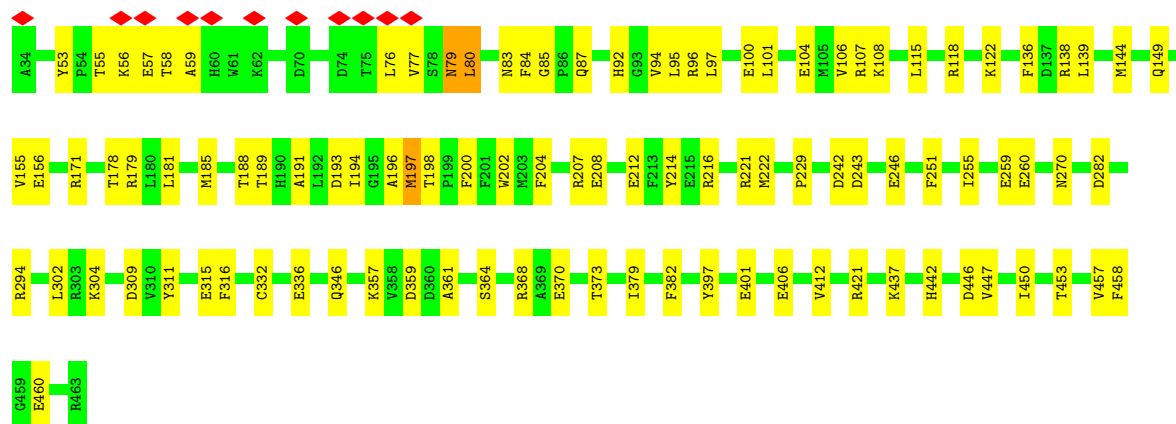
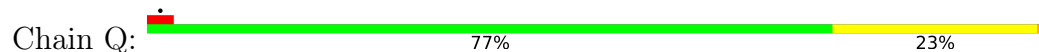
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: Complex I-30kD

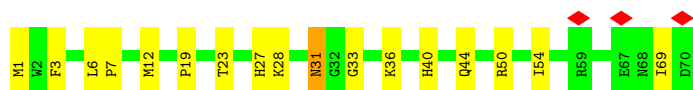


- Molecule 16: Complex I-49kD

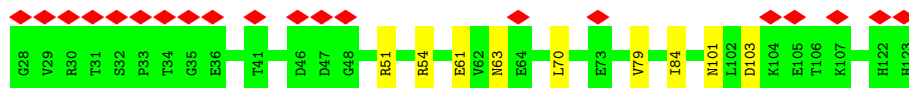
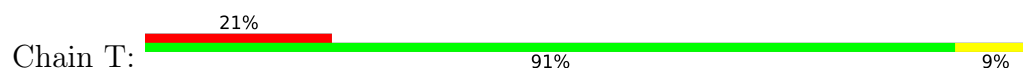


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

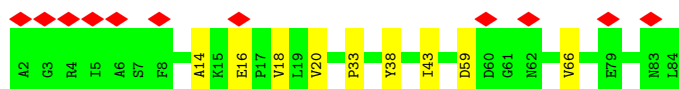
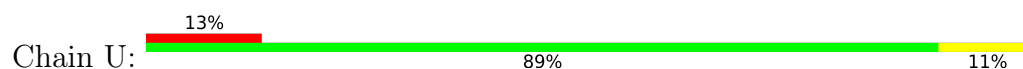




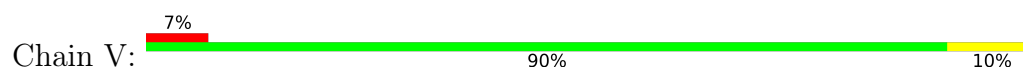
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



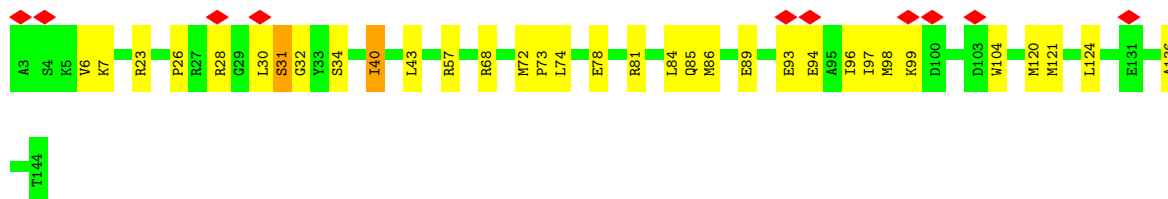
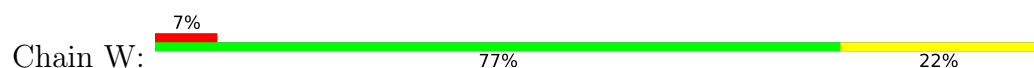
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



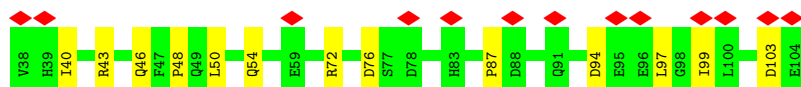
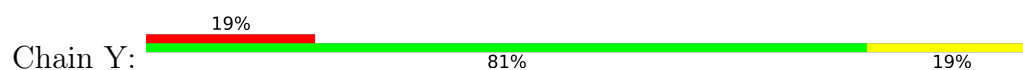
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 21: Complex I-B16.6



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

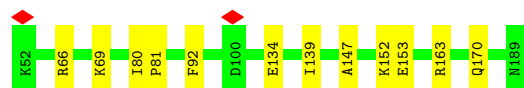
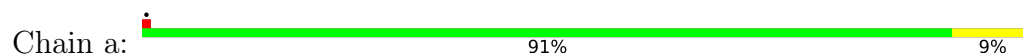


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

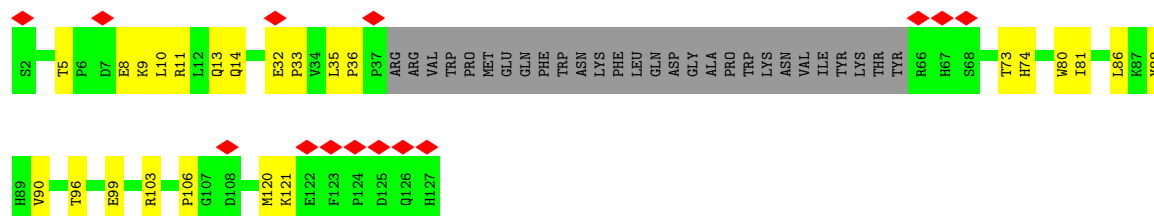




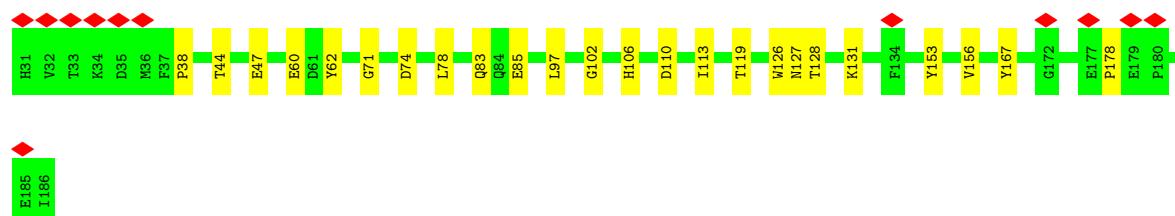
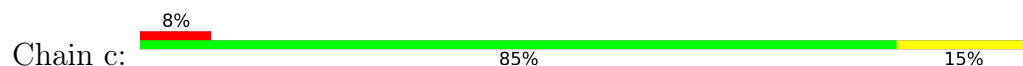
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



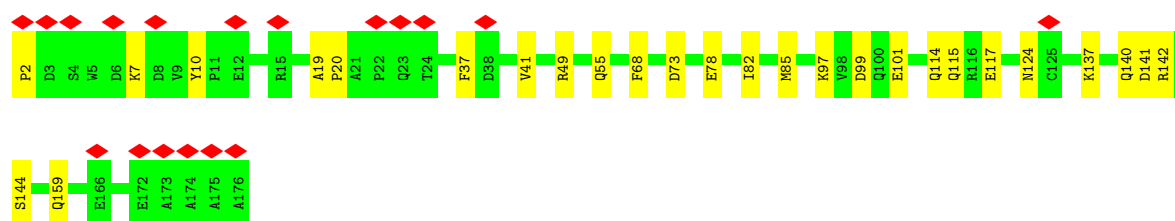
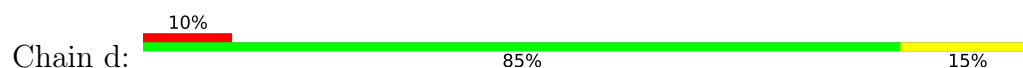
- Molecule 25: Complex I-B17



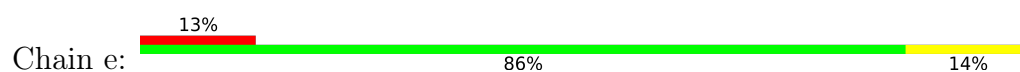
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



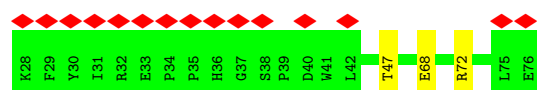
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



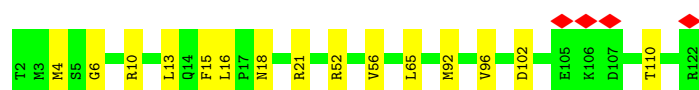
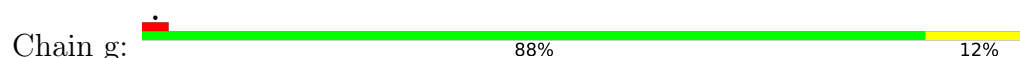
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



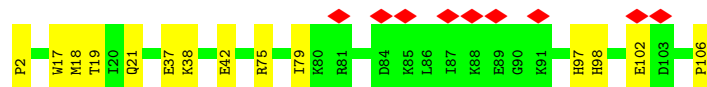
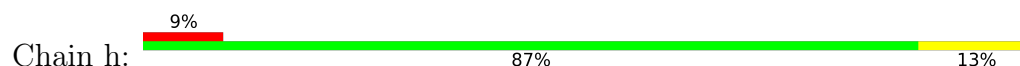
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



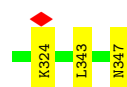
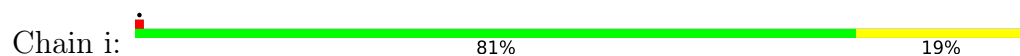
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

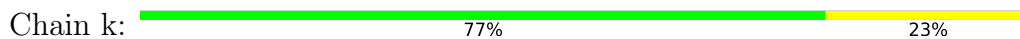


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

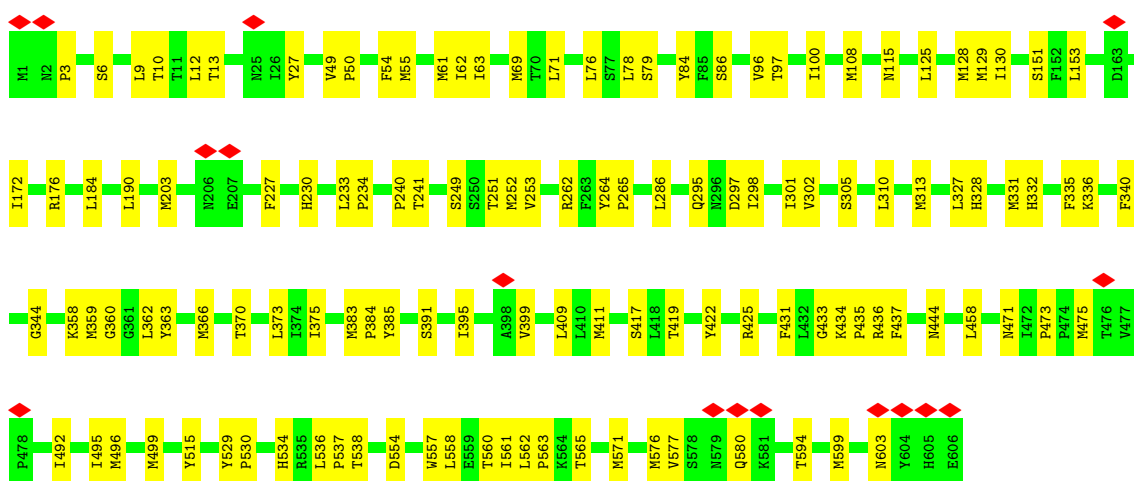
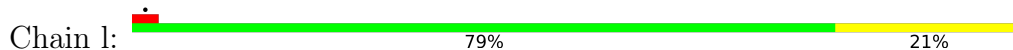




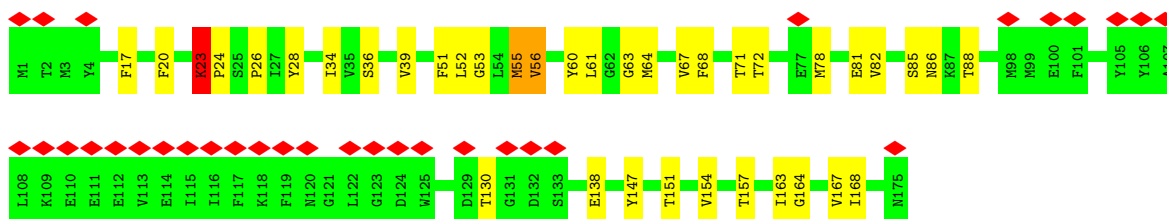
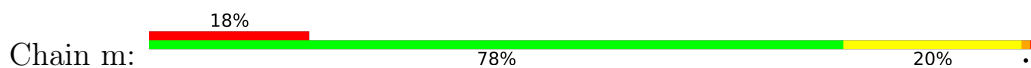
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



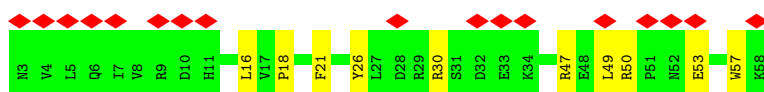
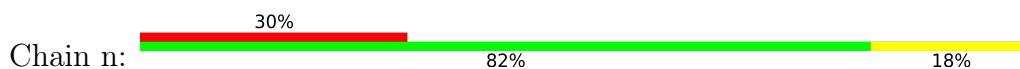
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



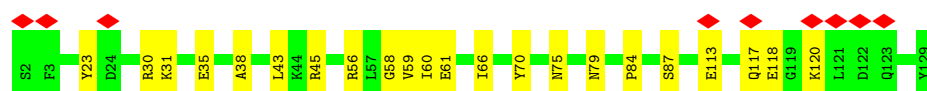
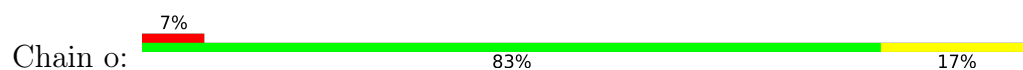
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



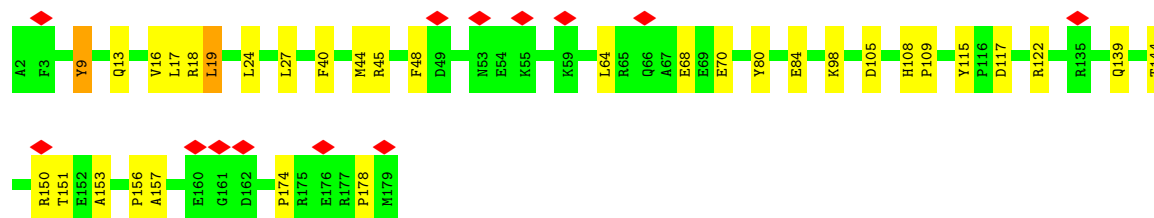
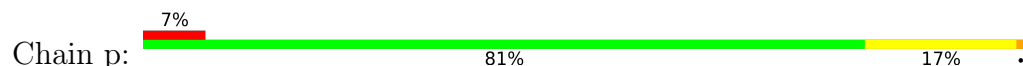
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



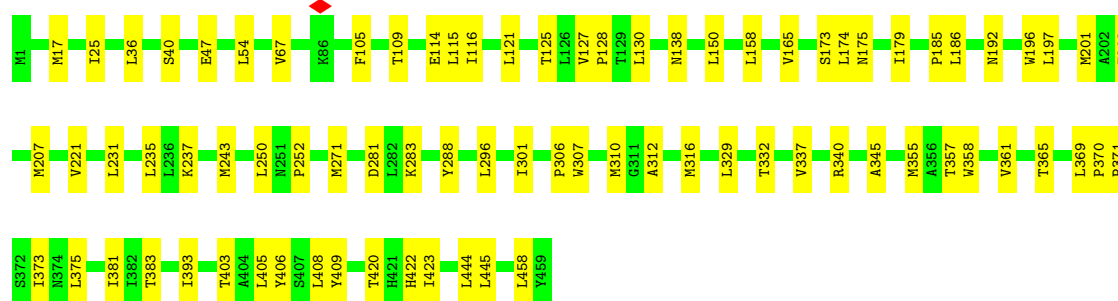
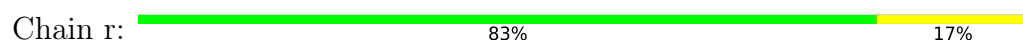
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



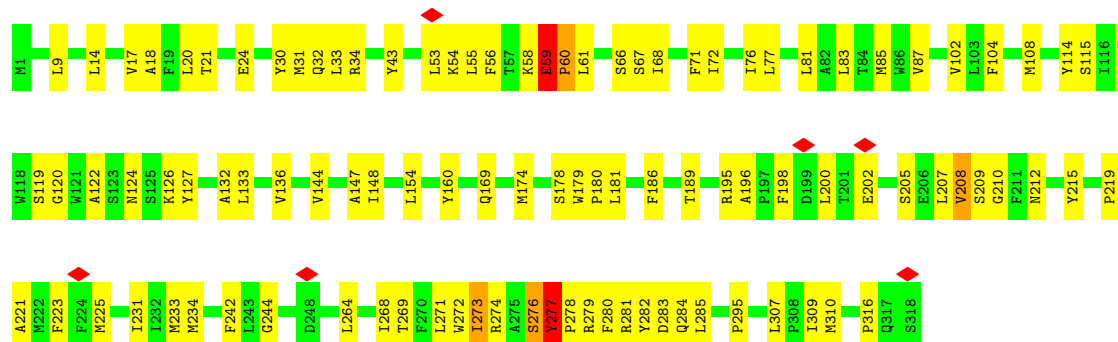
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



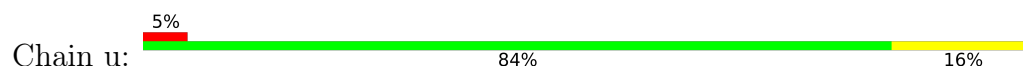
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

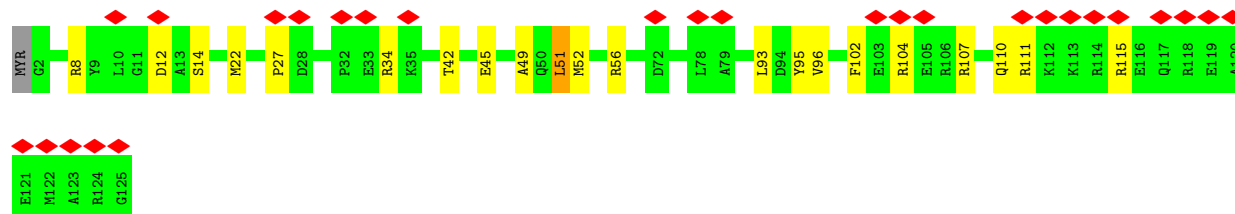
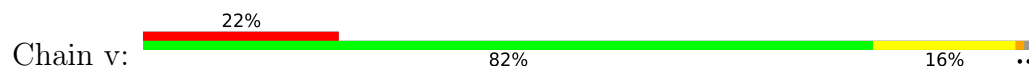


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

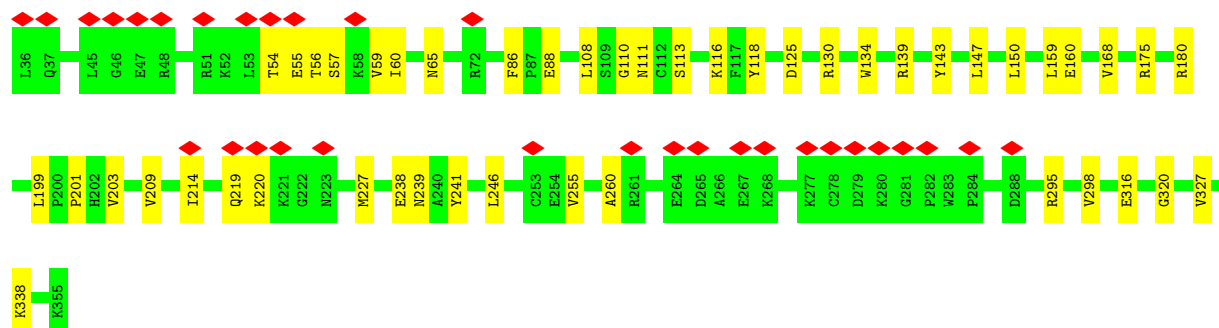
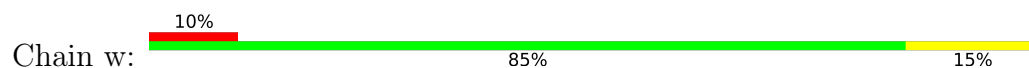




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39380	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 970, FMN, 8Q1, 2MR, ADP, ZN, UQ, PEE, NDP, MG, SF4, CDL, FES, PLX

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	0.16	0/3400	0.35	0/4596
2	B	0.19	0/1423	0.39	0/1930
3	C	0.23	0/1278	0.45	0/1729
4	E	0.15	0/995	0.35	0/1340
5	F	0.20	0/698	0.44	0/940
6	G	0.15	0/702	0.41	0/952
6	X	0.12	0/711	0.28	0/963
7	H	0.17	0/929	0.39	0/1258
8	I	0.14	0/798	0.35	0/1079
9	J	0.16	0/2828	0.36	2/3834 (0.1%)
10	K	0.12	0/377	0.27	0/509
11	L	0.16	0/1039	0.34	0/1403
12	M	0.16	0/5380	0.36	0/7290
13	N	0.12	0/1245	0.31	0/1694
14	O	0.15	0/1711	0.36	0/2328
15	P	0.18	0/1789	0.37	0/2436
16	Q	0.22	0/3528	0.44	1/4784 (0.0%)
17	S	0.15	0/581	0.39	0/781
18	T	0.12	0/755	0.28	0/1018
19	U	0.12	0/660	0.28	0/908
20	V	0.13	0/1042	0.26	0/1411
21	W	0.19	0/1198	0.43	0/1617
22	Y	0.13	0/610	0.31	0/836
23	Z	0.11	0/660	0.28	0/892
24	a	0.13	0/1184	0.30	0/1603
25	b	0.16	0/844	0.38	0/1149
26	c	0.13	0/1371	0.32	0/1875
27	d	0.14	0/1494	0.29	0/2015
28	e	0.13	0/891	0.29	0/1210
29	f	0.11	0/385	0.25	0/522
30	g	0.14	0/1031	0.31	0/1394
31	h	0.14	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.17	0/2773	0.35	0/3768
33	j	0.27	0/938	0.64	2/1281 (0.2%)
34	k	0.18	0/759	0.40	0/1029
35	l	0.16	0/4947	0.34	0/6728
36	m	0.22	0/1323	0.52	2/1797 (0.1%)
37	n	0.14	0/491	0.29	0/663
38	o	0.14	0/1092	0.31	0/1481
39	p	0.16	0/1590	0.34	0/2155
40	r	0.17	0/3723	0.34	0/5078
41	s	0.24	0/2571	0.61	7/3517 (0.2%)
42	u	0.14	0/1436	0.34	0/1938
43	v	0.12	0/1052	0.35	2/1411 (0.1%)
44	w	0.14	0/2642	0.30	0/3579
All	All	0.17	0/67763	0.37	16/91911 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	s	277	TYR	CA-C-N	10.70	130.66	119.85
41	s	277	TYR	C-N-CA	10.70	130.66	119.85
41	s	276	SER	N-CA-C	8.35	120.39	111.28
36	m	23	LYS	CA-C-N	6.95	128.53	119.84
36	m	23	LYS	C-N-CA	6.95	128.53	119.84

There are no chirality outliers.

There are no planarity outliers.

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	3324	0	3281	63	0
2	B	1392	0	1323	41	0
3	C	1247	0	1251	48	0
4	E	971	0	975	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	687	0	700	15	0
6	G	690	0	669	17	0
6	X	699	0	682	12	0
7	H	910	0	950	14	0
8	I	780	0	808	20	0
9	J	2751	0	2773	47	0
10	K	366	0	338	11	0
11	L	1016	0	1016	22	0
12	M	5292	0	5322	76	0
13	N	1204	0	1162	21	0
14	O	1671	0	1673	19	0
15	P	1738	0	1693	28	0
16	Q	3450	0	3380	96	0
17	S	566	0	561	22	0
18	T	741	0	702	7	0
19	U	639	0	631	9	0
20	V	1021	0	1025	9	0
21	W	1167	0	1155	28	0
22	Y	584	0	529	11	0
23	Z	641	0	620	6	0
24	a	1151	0	1164	10	0
25	b	819	0	835	21	0
26	c	1315	0	1208	16	0
27	d	1461	0	1429	22	0
28	e	867	0	817	12	0
29	f	377	0	353	4	0
30	g	1000	0	994	15	0
31	h	867	0	871	14	0
32	i	2710	0	2874	48	0
33	j	914	0	951	60	0
34	k	748	0	799	34	0
35	l	4816	0	4955	94	0
36	m	1290	0	1256	55	0
37	n	479	0	486	8	0
38	o	1062	0	1072	22	0
39	p	1534	0	1470	33	0
40	r	3631	0	3839	61	0
41	s	2498	0	2592	113	0
42	u	1398	0	1374	21	0
43	v	1028	0	982	15	0
44	w	2582	0	2536	30	0
45	A	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B	16	0	0	0	0
45	C	8	0	0	3	0
45	M	16	0	0	0	0
46	A	31	0	19	5	0
47	B	51	0	82	7	0
47	W	41	0	59	3	0
47	j	51	0	82	3	0
47	l	136	0	200	10	0
47	r	51	0	82	5	0
47	s	47	0	71	11	0
48	C	52	0	88	10	0
48	a	52	0	88	2	0
48	e	52	0	88	6	0
48	g	52	0	88	7	0
48	j	52	0	88	2	0
48	r	52	0	88	5	0
49	C	29	0	0	0	0
50	G	35	0	0	1	0
50	X	35	0	0	1	0
51	J	48	0	24	3	0
52	J	33	0	39	4	0
52	s	38	0	47	7	0
53	M	4	0	0	0	0
53	O	4	0	0	1	0
54	M	1	0	0	0	0
55	S	51	0	46	15	0
55	V	194	0	294	15	0
55	a	100	0	156	3	0
55	l	199	0	307	18	0
55	n	55	0	54	1	0
55	r	99	0	151	4	0
56	T	1	0	0	0	0
57	w	27	0	11	1	0
All	All	67815	0	68328	1140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1140 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)
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.20
33:j:27:LEU:CD2	41:s:60:PRO:HD2	1.73	1.18
33:j:27:LEU:HD21	41:s:60:PRO:HD2	1.17	1.13
11:L:78:ARG:NH2	12:M:249:GLU:HG3	1.64	1.12
36:m:55:MET:HE3	36:m:55:MET:HA	1.30	1.09

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	431/433 (100%)	417 (97%)	12 (3%)	2 (0%)	24	59
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	14	47
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	660 (96%)	28 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	427/430 (99%)	410 (96%)	17 (4%)	0	100	100
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
21	W	140/142 (99%)	129 (92%)	8 (6%)	3 (2%)	5	31
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
26	c	154/156 (99%)	143 (93%)	11 (7%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	332 (96%)	13 (4%)	0	100	100
33	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	582 (96%)	22 (4%)	0	100	100
36	m	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	5 (3%)	1 (1%)	21	56
40	r	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
41	s	316/318 (99%)	309 (98%)	5 (2%)	2 (1%)	21	56
42	u	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	21	56
43	v	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8174/8313 (98%)	7858 (96%)	306 (4%)	10 (0%)	49	79

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	PHE
21	W	32	GLY
1	A	186	ALA
21	W	31	SER
7	H	77	ILE

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	345/346 (100%)	344 (100%)	1 (0%)	86	88
2	B	146/151 (97%)	146 (100%)	0	100	100
3	C	131/132 (99%)	131 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	78/81 (96%)	78 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	295 (100%)	1 (0%)	86	88
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	81
12	M	579/580 (100%)	577 (100%)	2 (0%)	86	88
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	368/370 (100%)	365 (99%)	3 (1%)	73	82
17	S	57/58 (98%)	56 (98%)	1 (2%)	51	74
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	68/69 (99%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	118 (97%)	4 (3%)	33	65
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	311 (100%)	0	100	100
33	j	100/100 (100%)	99 (99%)	1 (1%)	68	80
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	540/540 (100%)	540 (100%)	0	100	100
36	m	128/141 (91%)	125 (98%)	3 (2%)	44	70
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	157 (99%)	2 (1%)	61	78
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	273/275 (99%)	271 (99%)	2 (1%)	76	83
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7144/7240 (99%)	7123 (100%)	21 (0%)	84	88

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	m	23	LYS
39	p	9	TYR
41	s	277	TYR

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Mol	Chain	Res	Type
39	p	19	LEU
36	m	56	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
40	r	175	ASN
41	s	250	HIS
44	w	188	ASN
15	P	124	ASN
15	P	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	2.03	1 (10%)	5,13,15	6.07	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.71	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.38	130.83	119.48
16	Q	118	2MR	CD-NE-CZ	4.25	131.35	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.20	130.51	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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	$\# Z > 2$
55	CDL	1	702	-	98,98,99	1.11	8 (8%)	104,110,111	0.91	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	UQ	J	402	-	33,33,63	3.53	9 (27%)	42,43,79	2.78	15 (35%)
48	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.65	1 (1%)
47	PEE	l	701	-	39,39,50	1.33	6 (15%)	42,44,55	1.11	3 (7%)
47	PEE	l	705	-	45,45,50	1.24	6 (13%)	48,50,55	0.97	2 (4%)
50	8Q1	G	201	6	32,34,34	1.62	6 (18%)	39,43,43	1.68	5 (12%)
55	CDL	r	503	-	98,98,99	1.11	8 (8%)	104,110,111	0.87	4 (3%)
47	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.04	2 (4%)
47	PEE	s	401	-	46,46,50	1.23	6 (13%)	49,51,55	1.00	2 (4%)
55	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
48	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
55	CDL	S	101	-	50,50,99	1.43	9 (18%)	56,62,111	1.20	4 (7%)
49	970	C	303	-	33,33,33	4.89	16 (48%)	48,50,50	2.95	22 (45%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
45	SF4	B	302	2	0,12,12	-	-	-	-	-
53	FES	O	301	14	0,4,4	-	-	-	-	-
48	PLX	C	302	-	51,51,51	0.61	0	53,59,59	0.74	1 (1%)
47	PEE	l	704	-	49,49,50	1.19	6 (12%)	52,54,55	0.95	2 (3%)
46	FMN	A	502	-	33,33,33	1.43	6 (18%)	48,50,50	1.30	8 (16%)
48	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
53	FES	M	803	12	0,4,4	-	-	-	-	-
55	CDL	n	101	-	54,54,99	1.38	9 (16%)	60,66,111	1.10	4 (6%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
55	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.89	4 (4%)
55	CDL	V	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
55	CDL	l	703	-	99,99,99	1.11	8 (8%)	105,111,111	0.88	4 (3%)
47	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.96	2 (3%)
48	PLX	e	201	-	51,51,51	1.21	5 (9%)	53,59,59	0.55	1 (1%)
47	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
48	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.61	1 (1%)
50	8Q1	X	201	-	32,34,34	1.61	6 (18%)	39,43,43	1.60	6 (15%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
51	NDP	J	401	-	51,52,52	4.28	25 (49%)	71,80,80	2.22	14 (19%)
47	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	1.01	2 (3%)
52	UQ	s	402	-	38,38,63	3.63	11 (28%)	48,49,79	2.75	17 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.91	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CDL	l	702	-	-	54/109/109/110	-
52	UQ	J	402	-	-	11/27/51/87	0/1/1/1
48	PLX	g	201	-	-	36/55/55/55	-
47	PEE	l	701	-	-	24/43/43/54	-
47	PEE	l	705	-	-	26/49/49/54	-
50	8Q1	G	201	6	-	17/41/41/41	-
55	CDL	r	503	-	-	55/109/109/110	-
47	PEE	W	201	-	-	25/44/44/54	-
47	PEE	s	401	-	-	24/50/50/54	-
55	CDL	a	201	-	-	58/110/110/110	-
48	PLX	j	202	-	-	31/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
55	CDL	S	101	-	-	33/61/61/110	-
49	970	C	303	-	-	4/8/41/41	0/5/5/5
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
53	FES	O	301	14	-	-	0/1/1/1
48	PLX	C	302	-	-	20/55/55/55	-
47	PEE	l	704	-	-	28/53/53/54	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
48	PLX	a	202	-	-	30/55/55/55	-
53	FES	M	803	12	-	-	0/1/1/1
55	CDL	n	101	-	-	29/65/65/110	-
45	SF4	B	301	2	-	-	0/6/5/5
55	CDL	V	201	-	-	61/104/104/110	-
55	CDL	V	202	-	-	59/110/110/110	-
55	CDL	l	703	-	-	47/110/110/110	-
47	PEE	j	201	-	-	24/54/54/54	-
48	PLX	e	201	-	-	30/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	r	501	-	-	25/54/54/54	-
45	SF4	C	301	3	-	-	0/6/5/5
48	PLX	r	502	-	-	22/55/55/55	-
50	8Q1	X	201	-	-	21/41/41/41	-
45	SF4	M	802	12	-	-	0/6/5/5
51	NDP	J	401	-	-	9/34/77/77	0/5/5/5
47	PEE	B	303	-	-	22/54/54/54	-
52	UQ	s	402	-	-	12/33/57/87	0/1/1/1
57	ADP	w	401	-	-	6/16/32/32	0/3/3/3

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	303	970	O16-C17	17.54	1.57	1.37
51	J	401	NDP	C3B-C2B	-13.17	1.24	1.53
49	C	303	970	O25-C24	11.48	1.37	1.22
51	J	401	NDP	O4D-C4D	10.76	1.68	1.45
52	s	402	UQ	C18-C19	10.04	1.56	1.33

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C	303	970	O25-C24-C23	-8.98	108.57	120.99
49	C	303	970	O25-C24-C11	-8.64	108.82	122.18
52	s	402	UQ	C7-C8-C9	-8.03	113.00	126.83
52	J	402	UQ	C7-C8-C9	-7.88	113.26	126.83
51	J	401	NDP	C3N-C2N-N1N	-7.83	111.70	123.20

There are no chirality outliers.

5 of 850 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
47	B	303	PEE	C11-C10-O2-C2

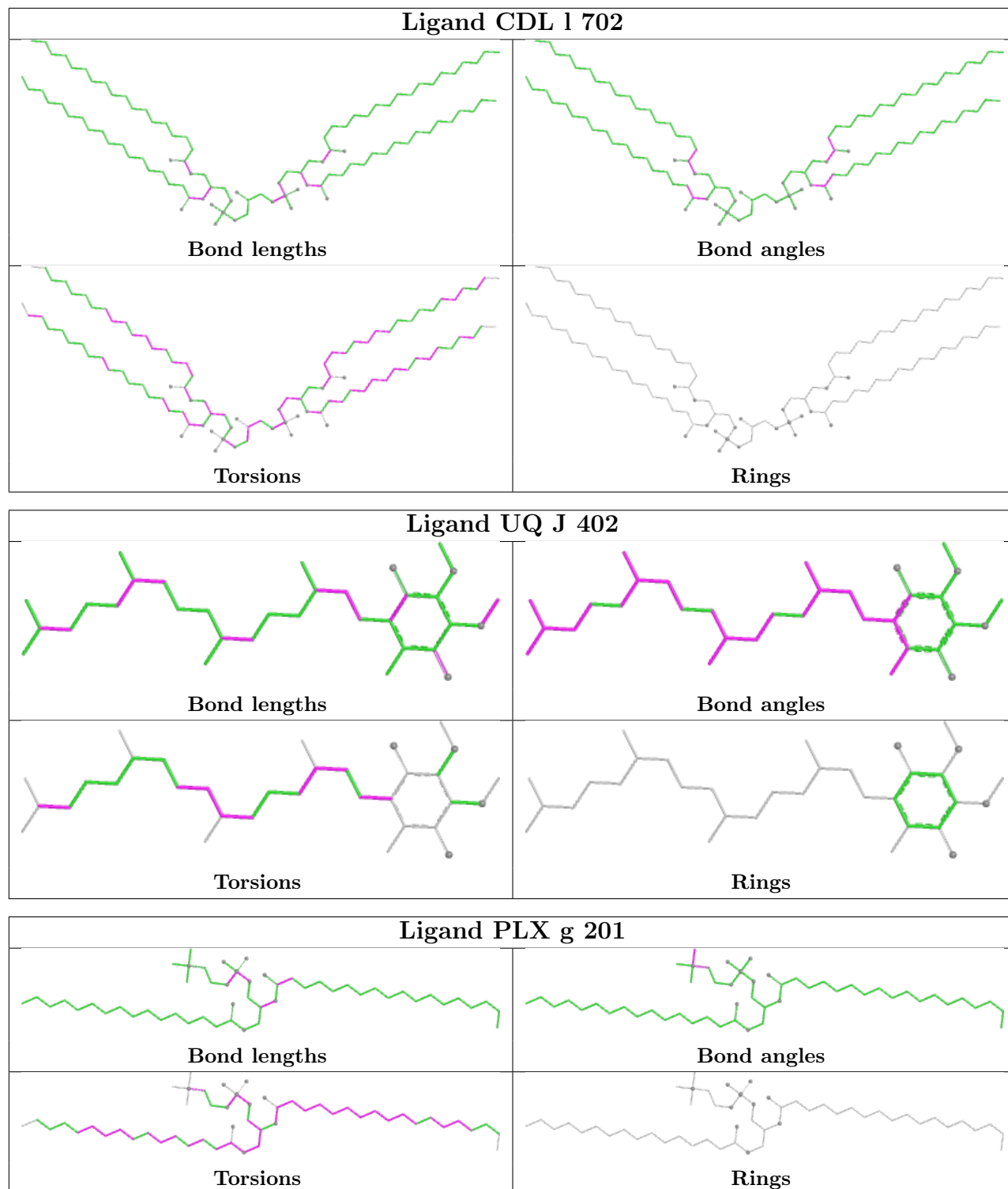
There are no ring outliers.

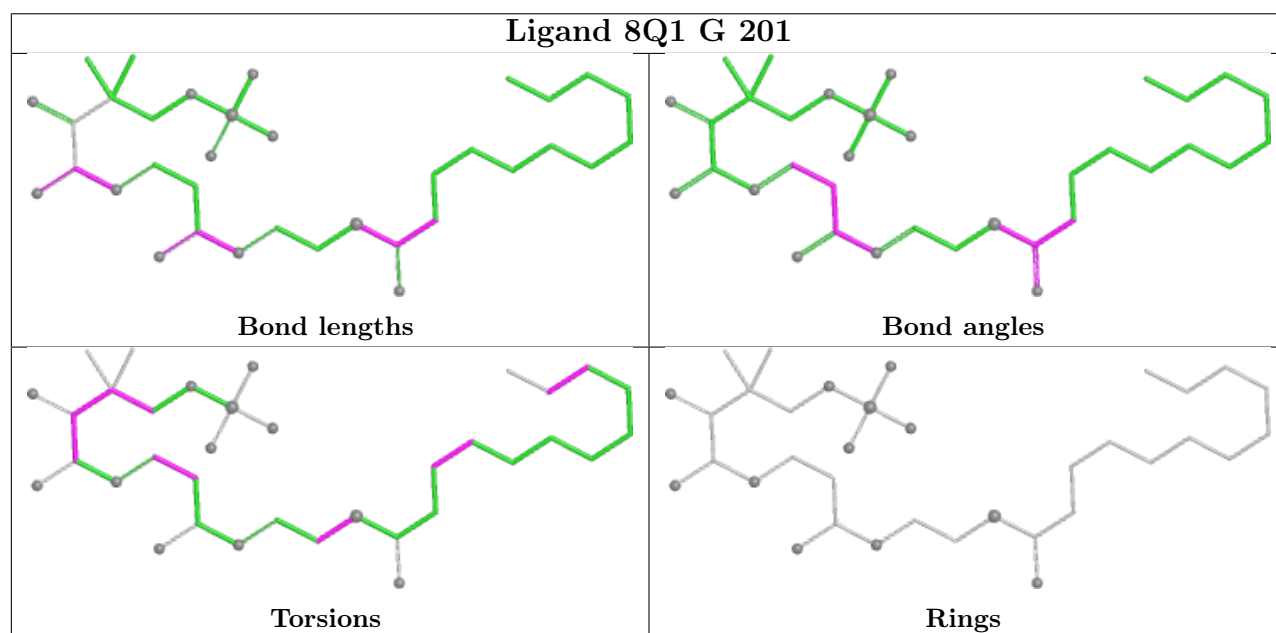
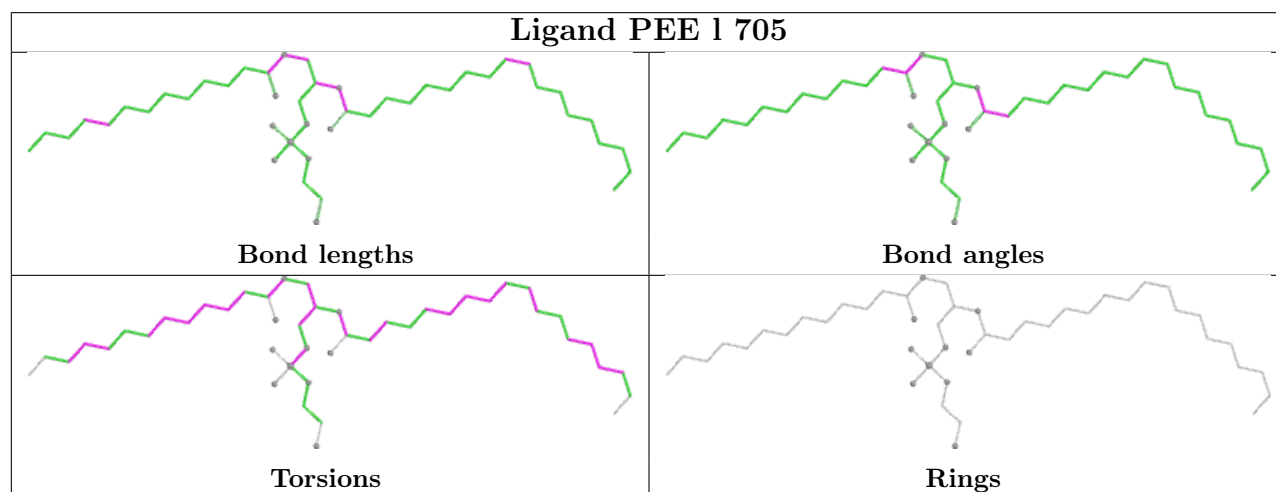
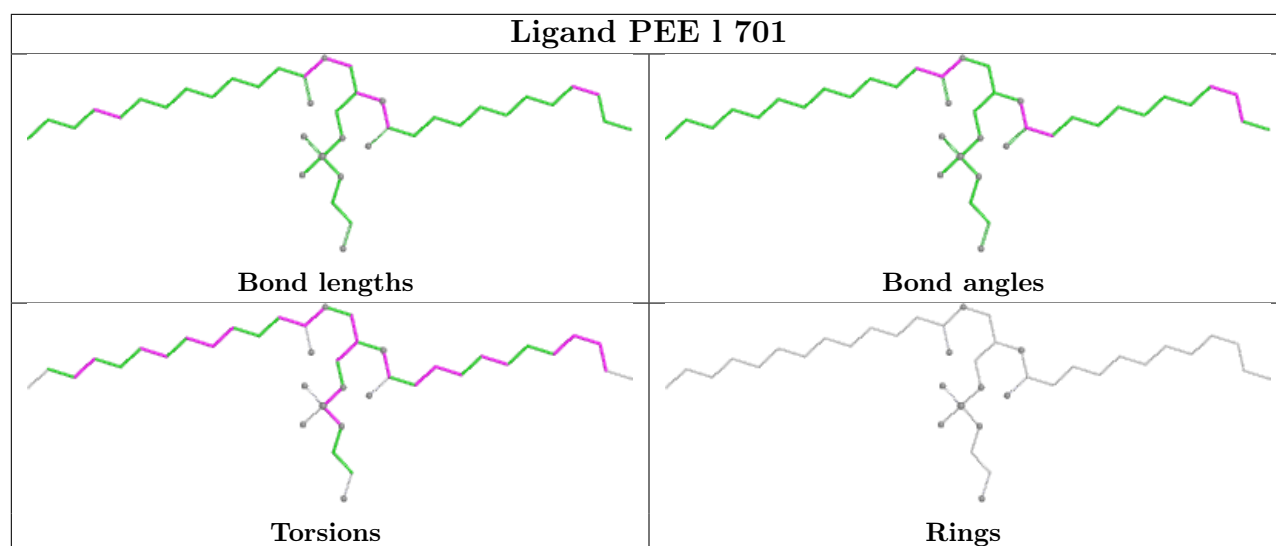
32 monomers are involved in 149 short contacts:

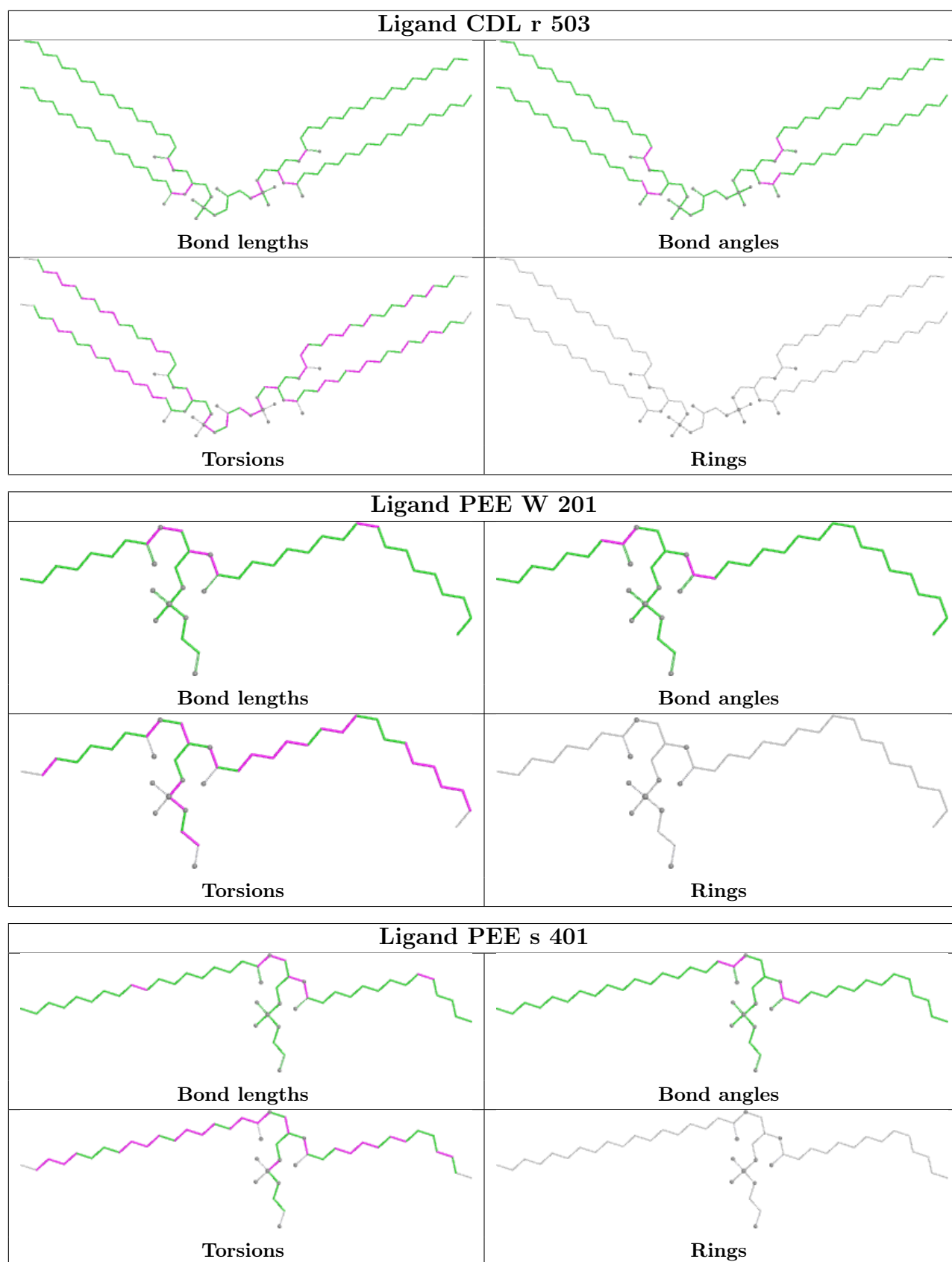
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	l	702	CDL	12	0
52	J	402	UQ	4	0
48	g	201	PLX	7	0
47	l	701	PEE	1	0
47	l	705	PEE	4	0
50	G	201	8Q1	1	0
55	r	503	CDL	4	0
47	W	201	PEE	3	0
47	s	401	PEE	11	0
55	a	201	CDL	3	0
48	j	202	PLX	2	0
55	S	101	CDL	15	0
45	A	501	SF4	2	0
53	O	301	FES	1	0
48	C	302	PLX	10	0
47	l	704	PEE	5	0
46	A	502	FMN	5	0
48	a	202	PLX	2	0
55	n	101	CDL	1	0
55	V	201	CDL	8	0
55	V	202	CDL	7	0
55	l	703	CDL	6	0
47	j	201	PEE	3	0
48	e	201	PLX	6	0
47	r	501	PEE	5	0
45	C	301	SF4	3	0
48	r	502	PLX	5	0
50	X	201	8Q1	1	0
51	J	401	NDP	3	0
47	B	303	PEE	7	0
52	s	402	UQ	7	0
57	w	401	ADP	1	0

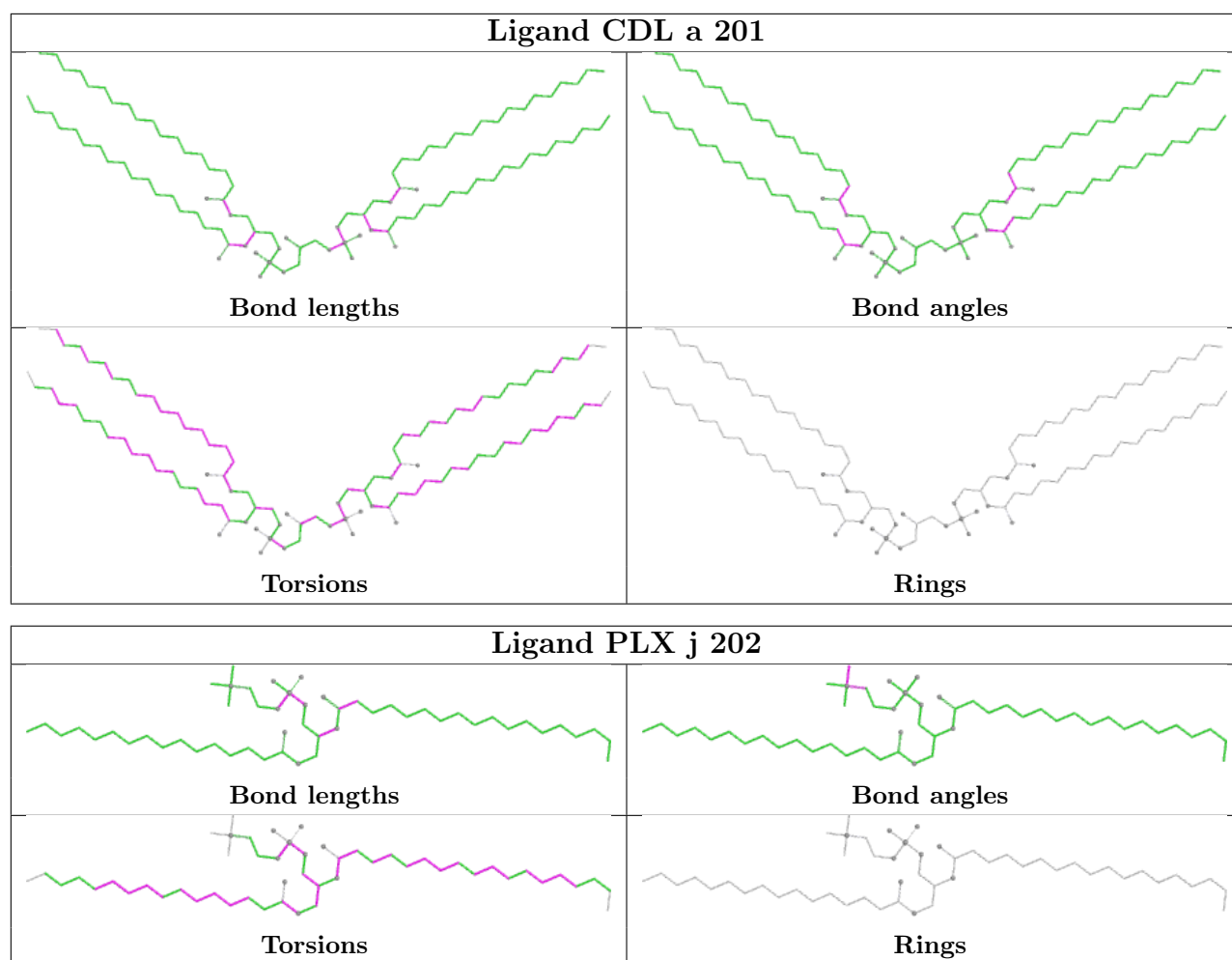
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

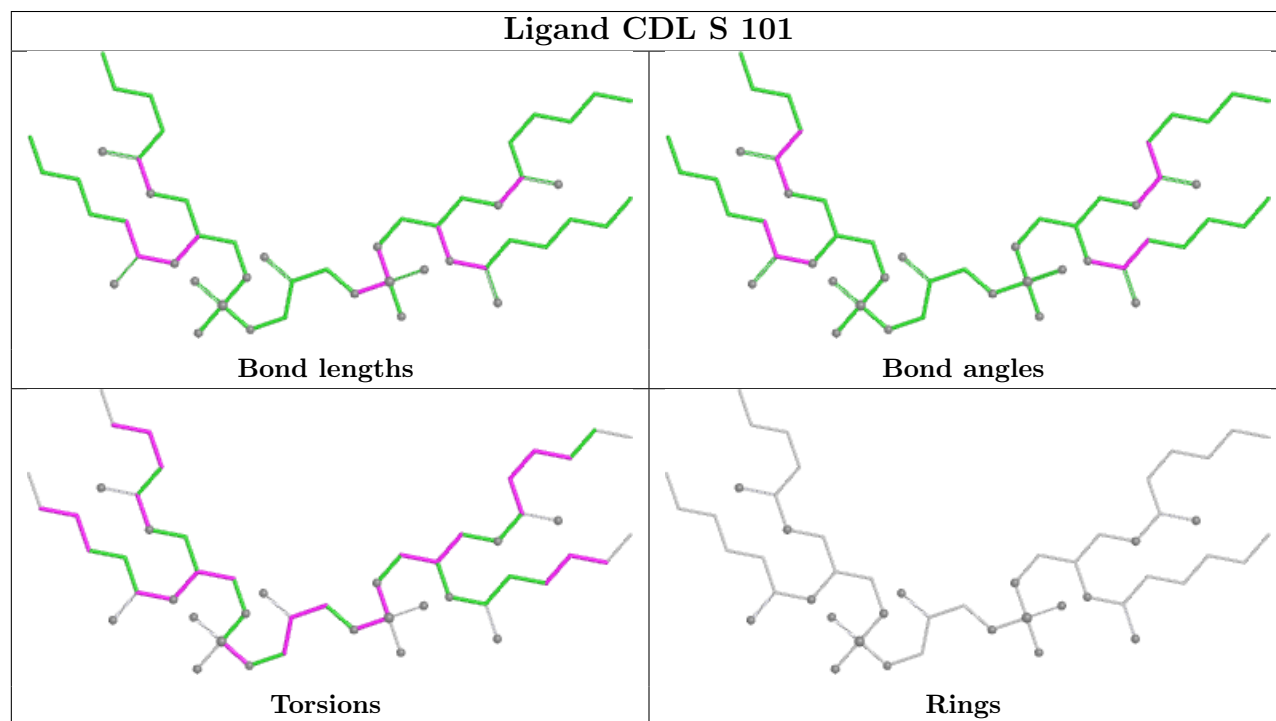
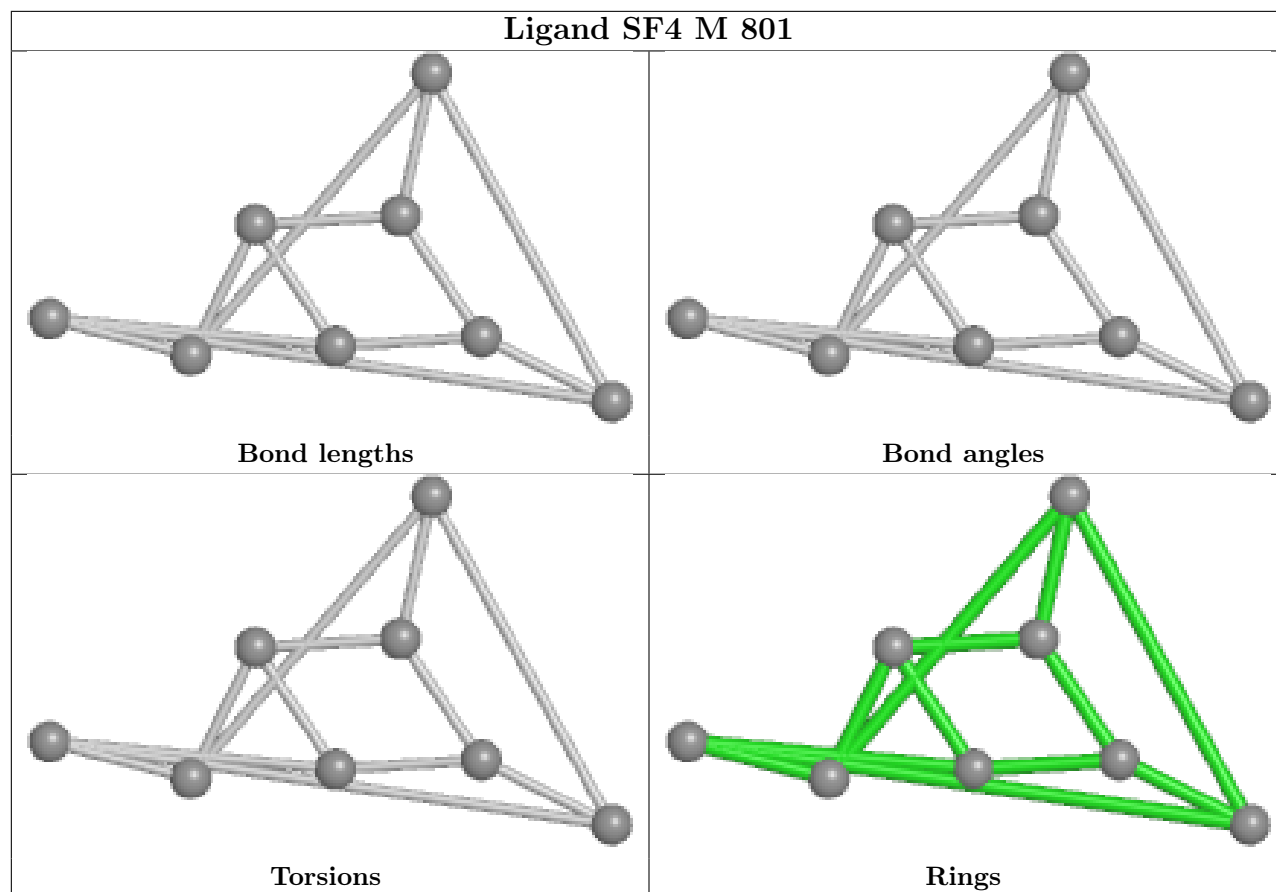
equivalents in the CSD to analyse the geometry.

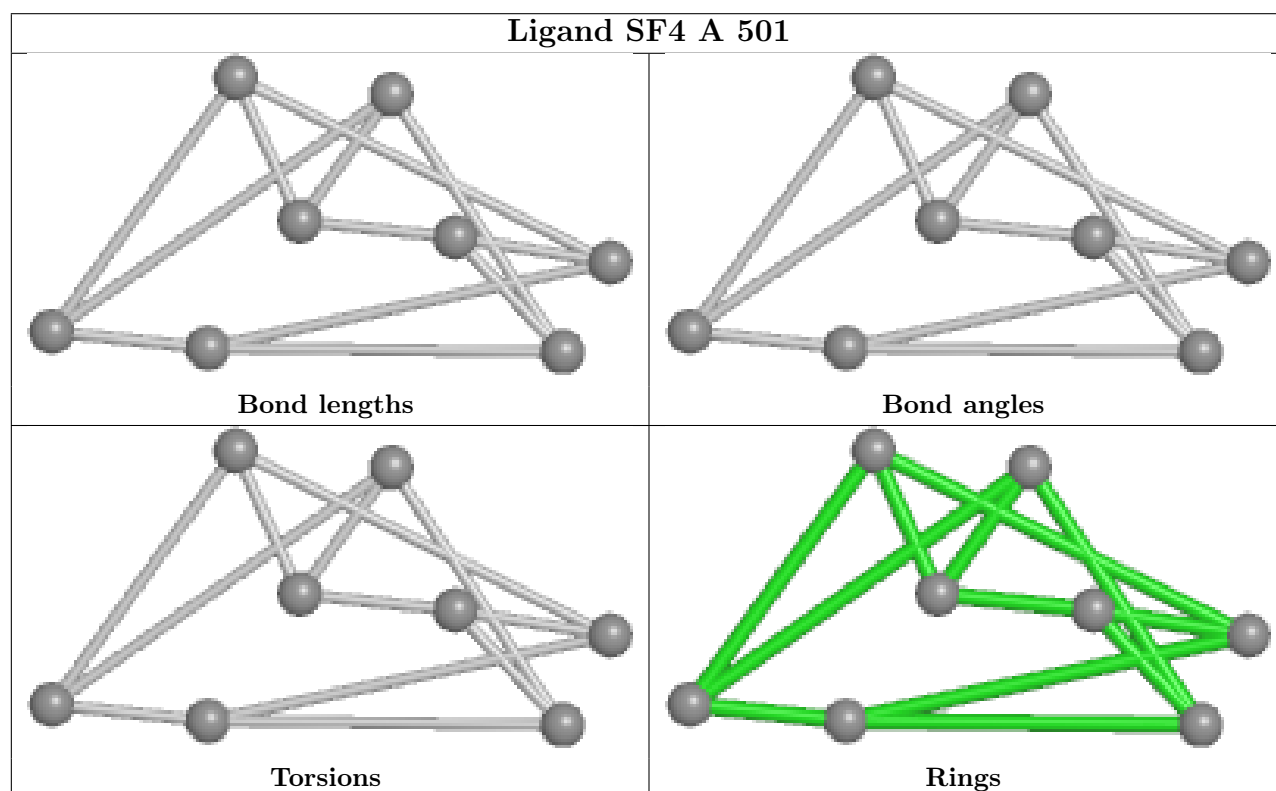
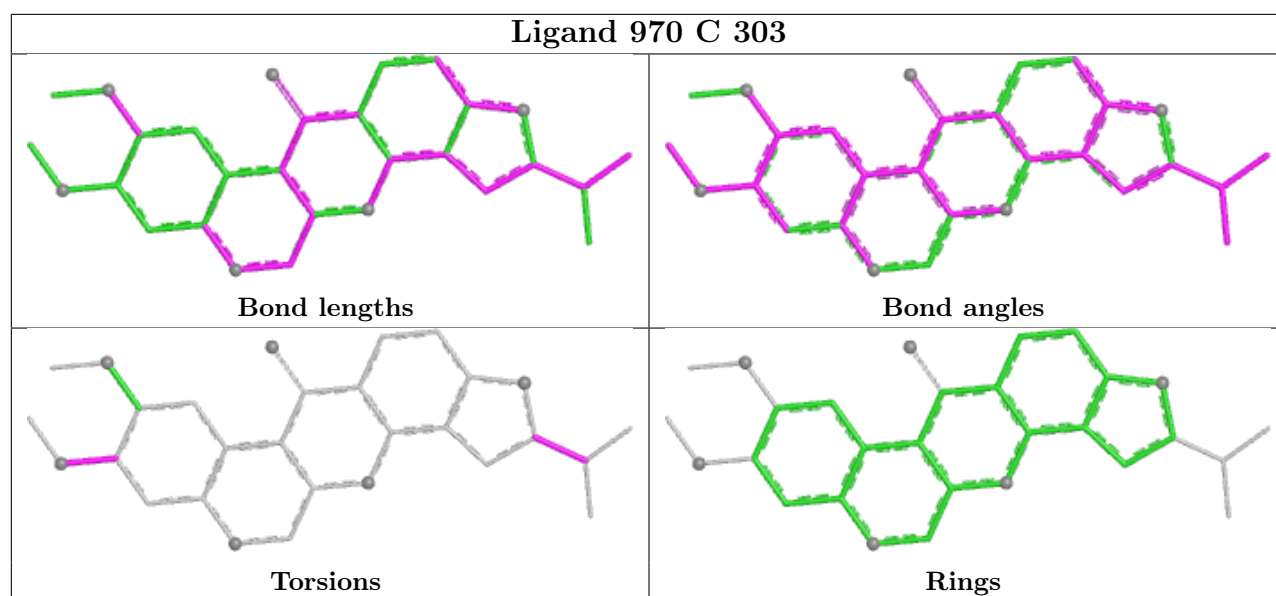


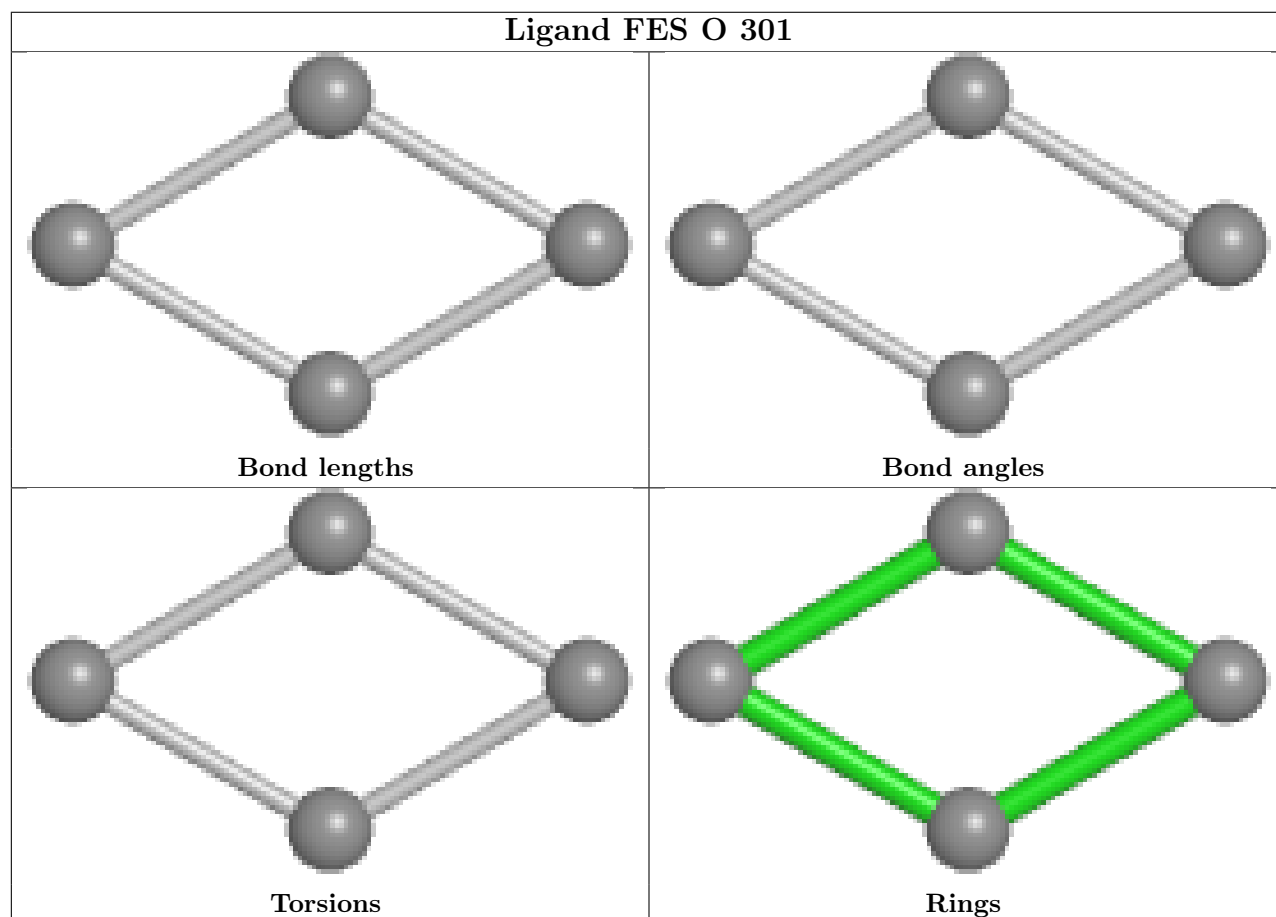
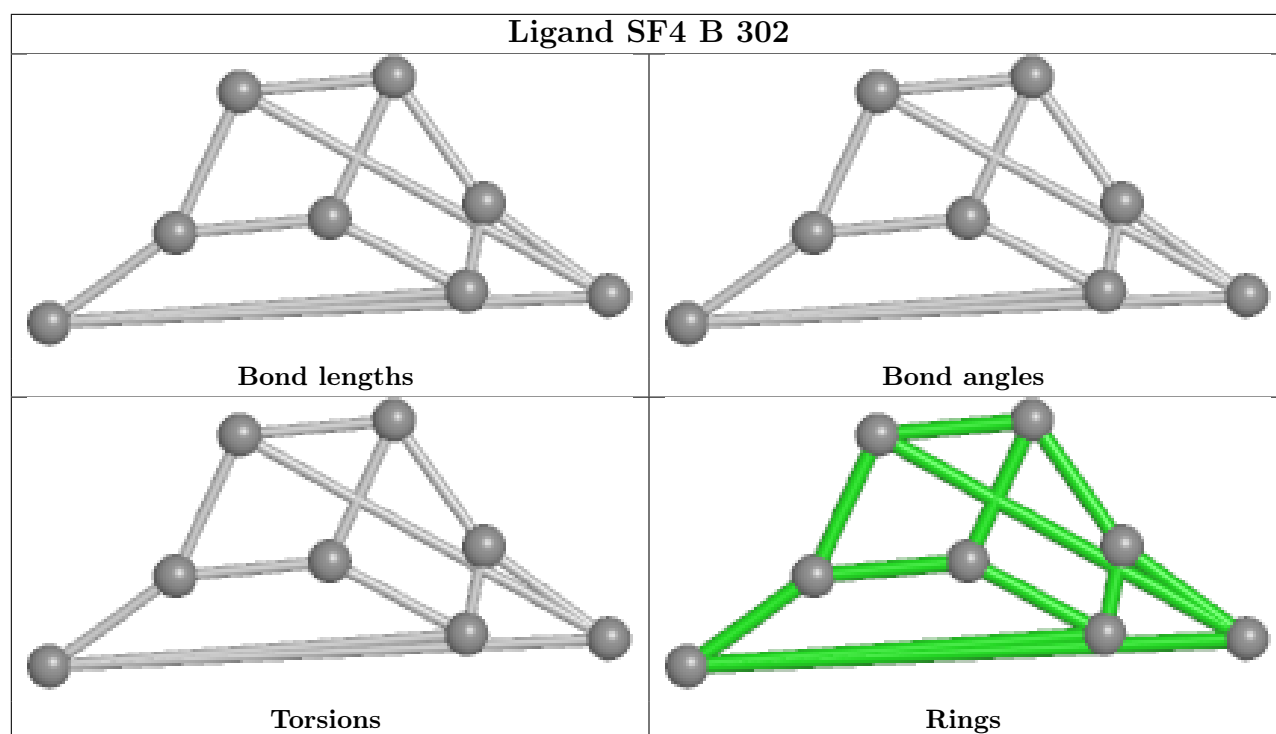


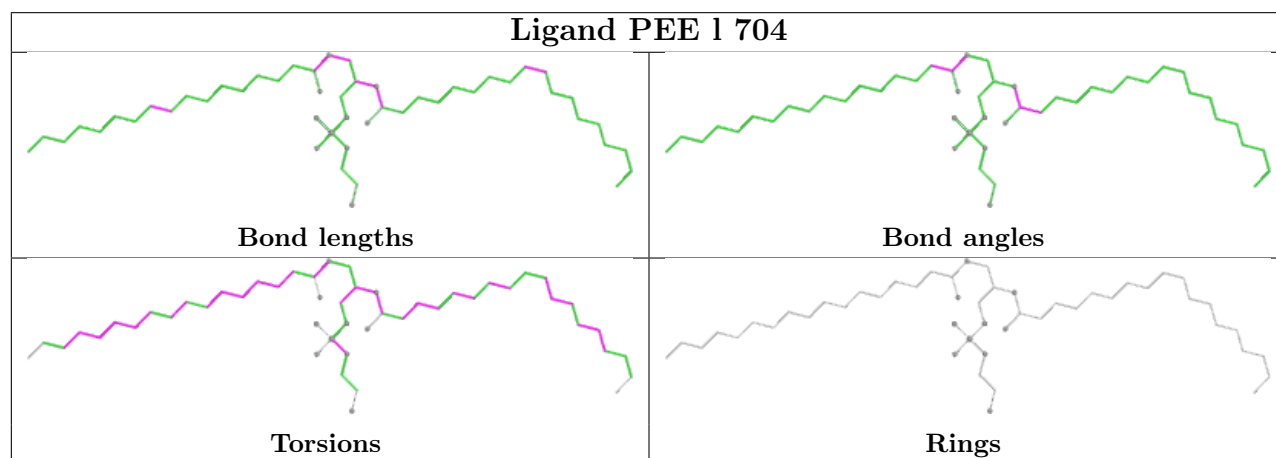
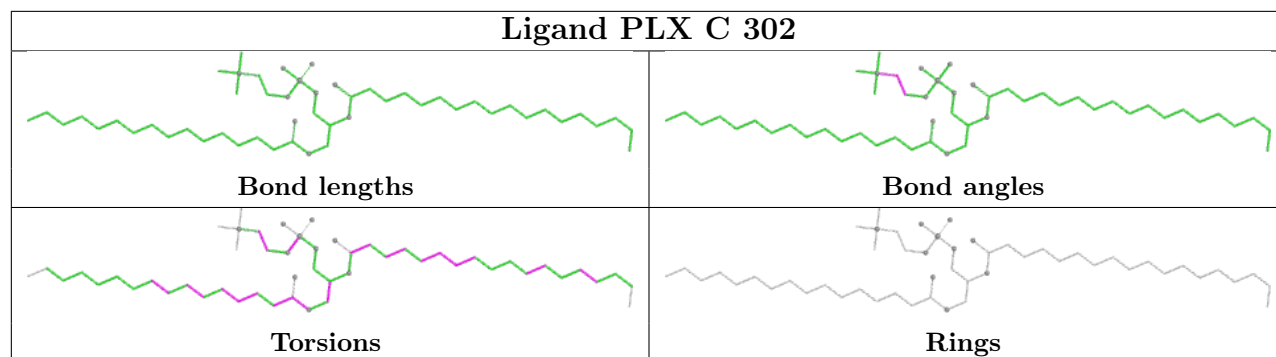


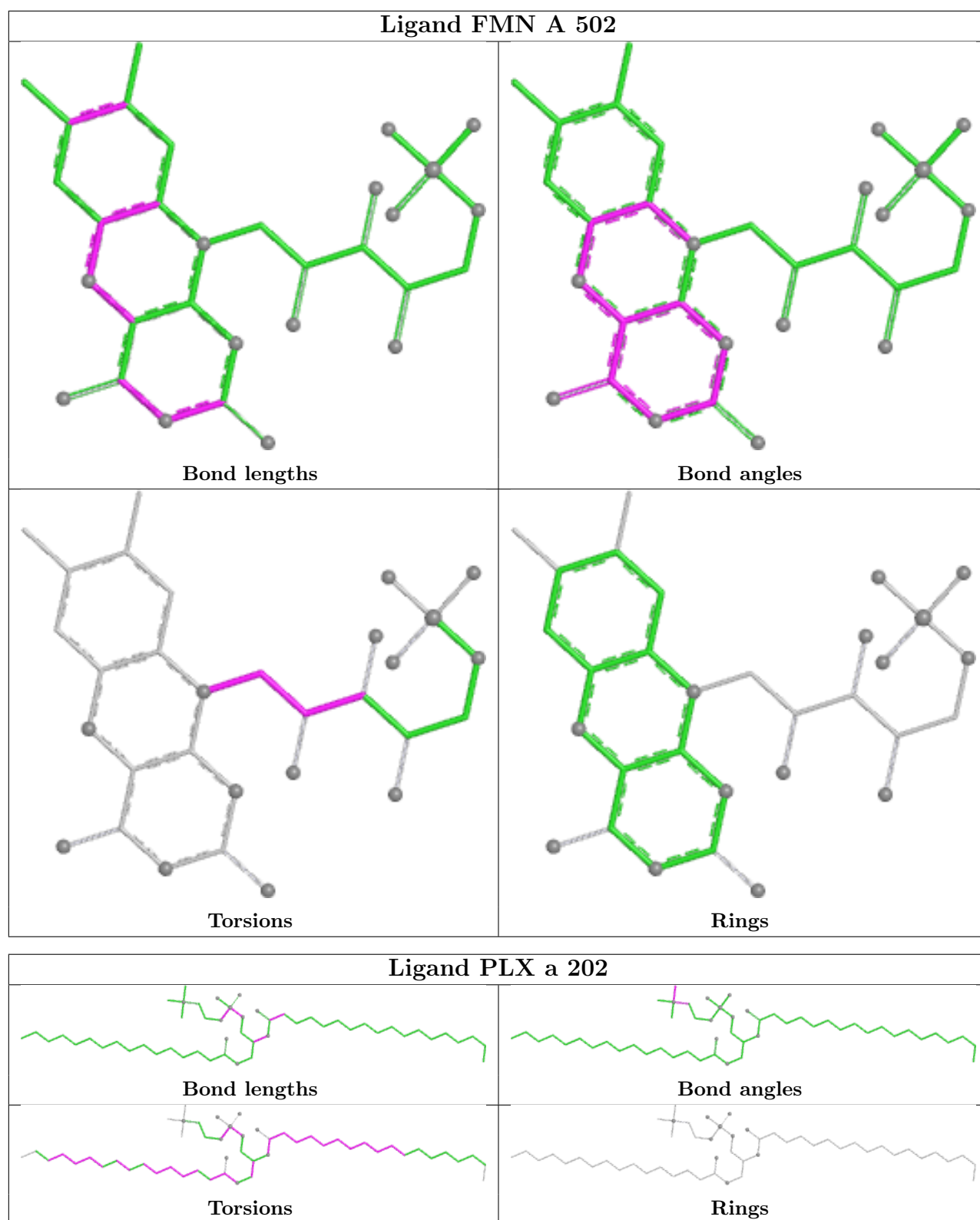


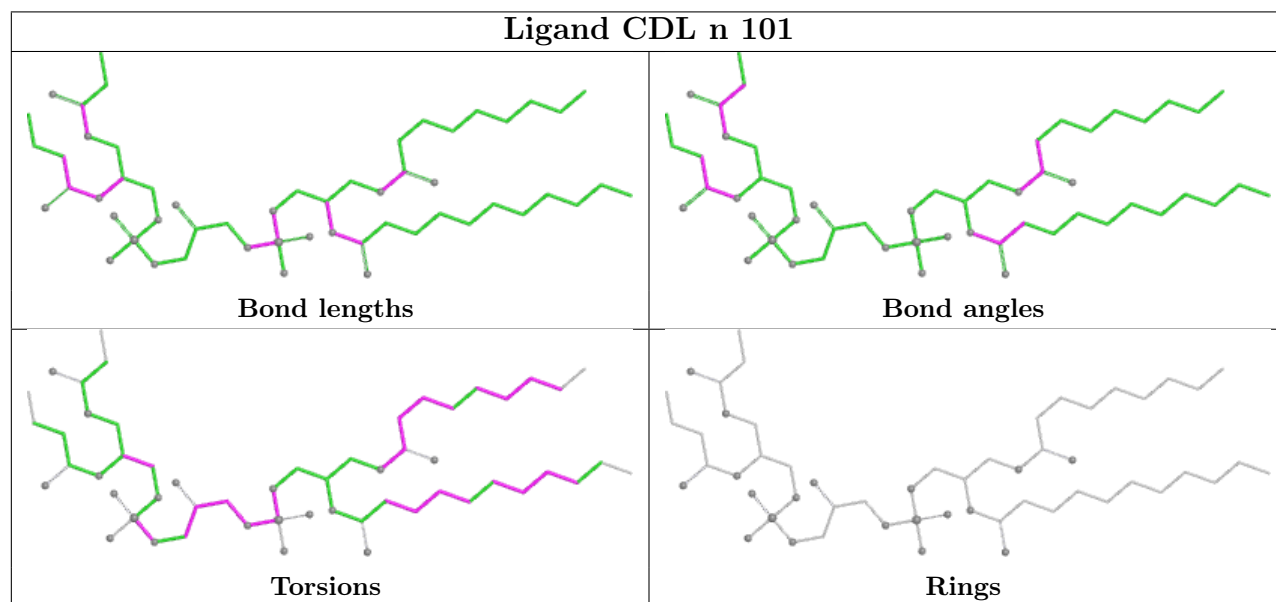
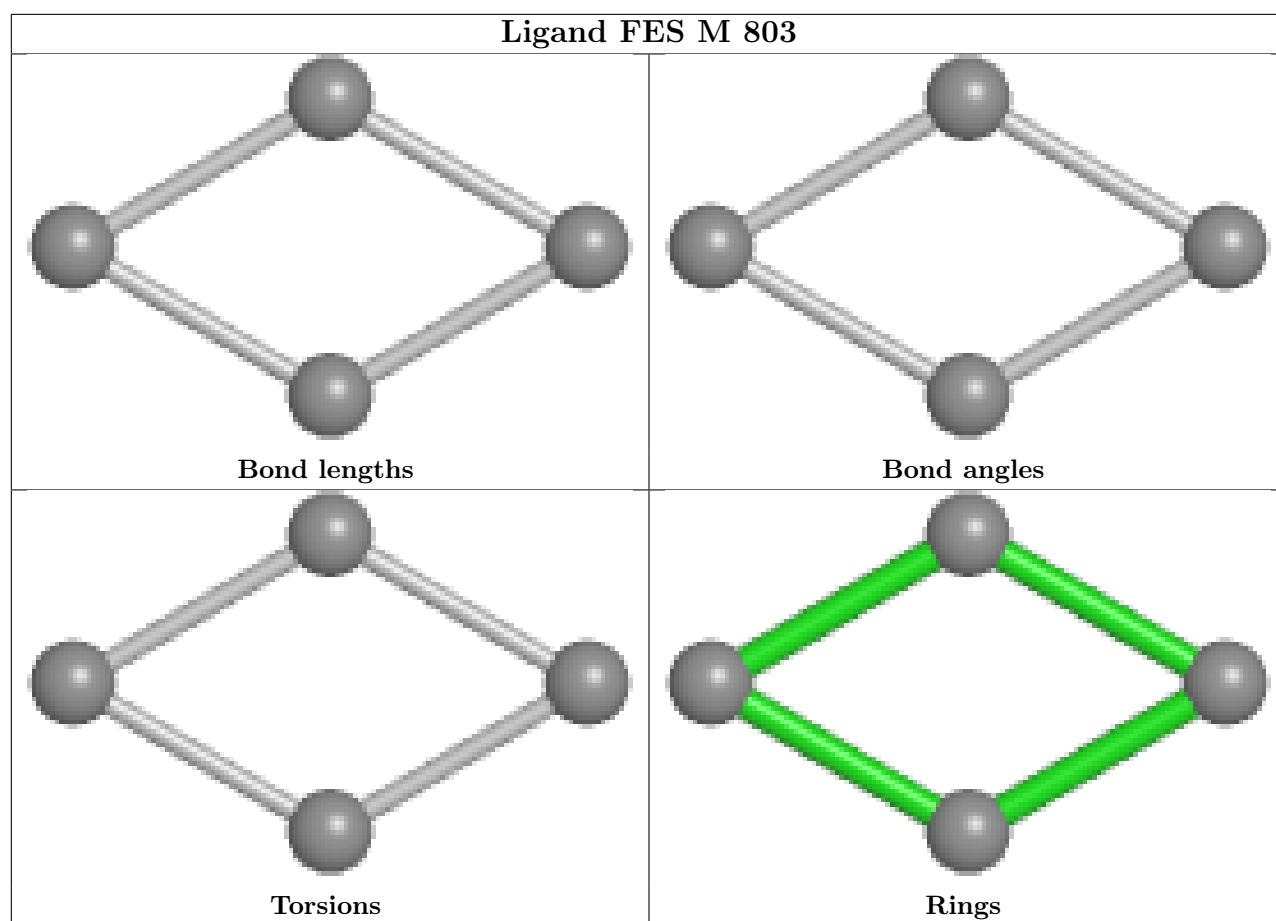


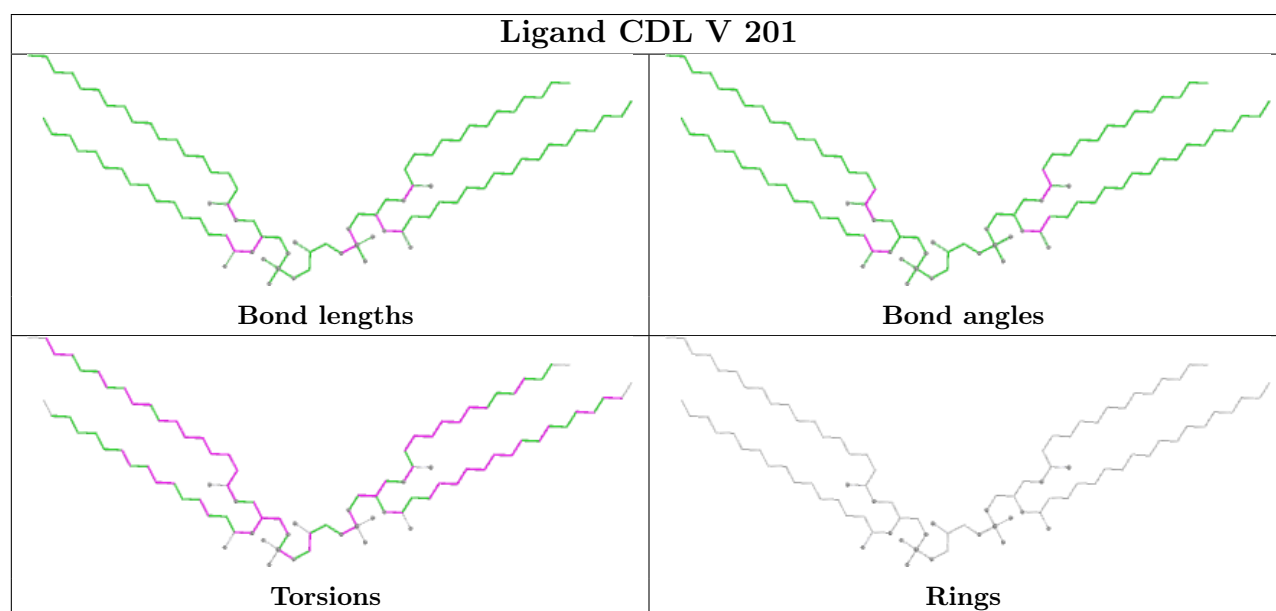
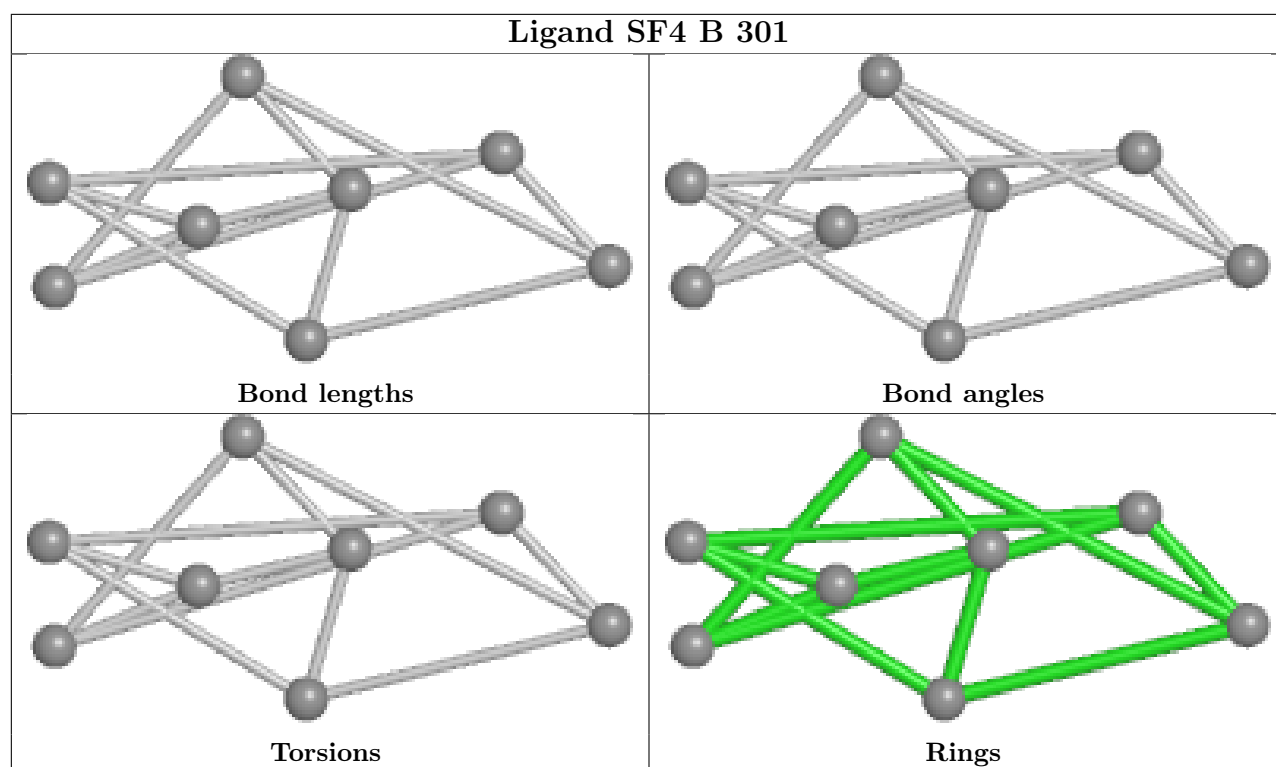


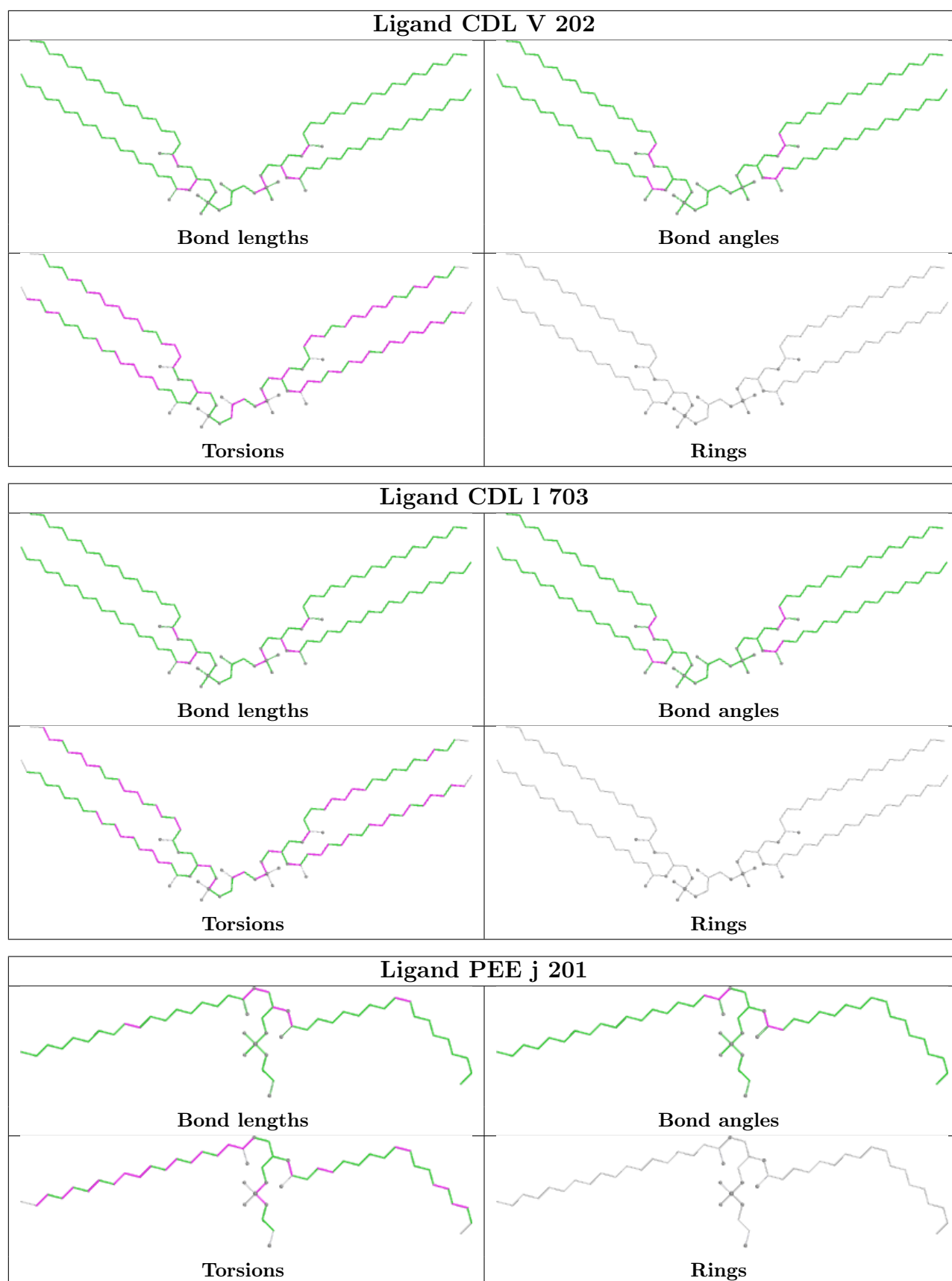


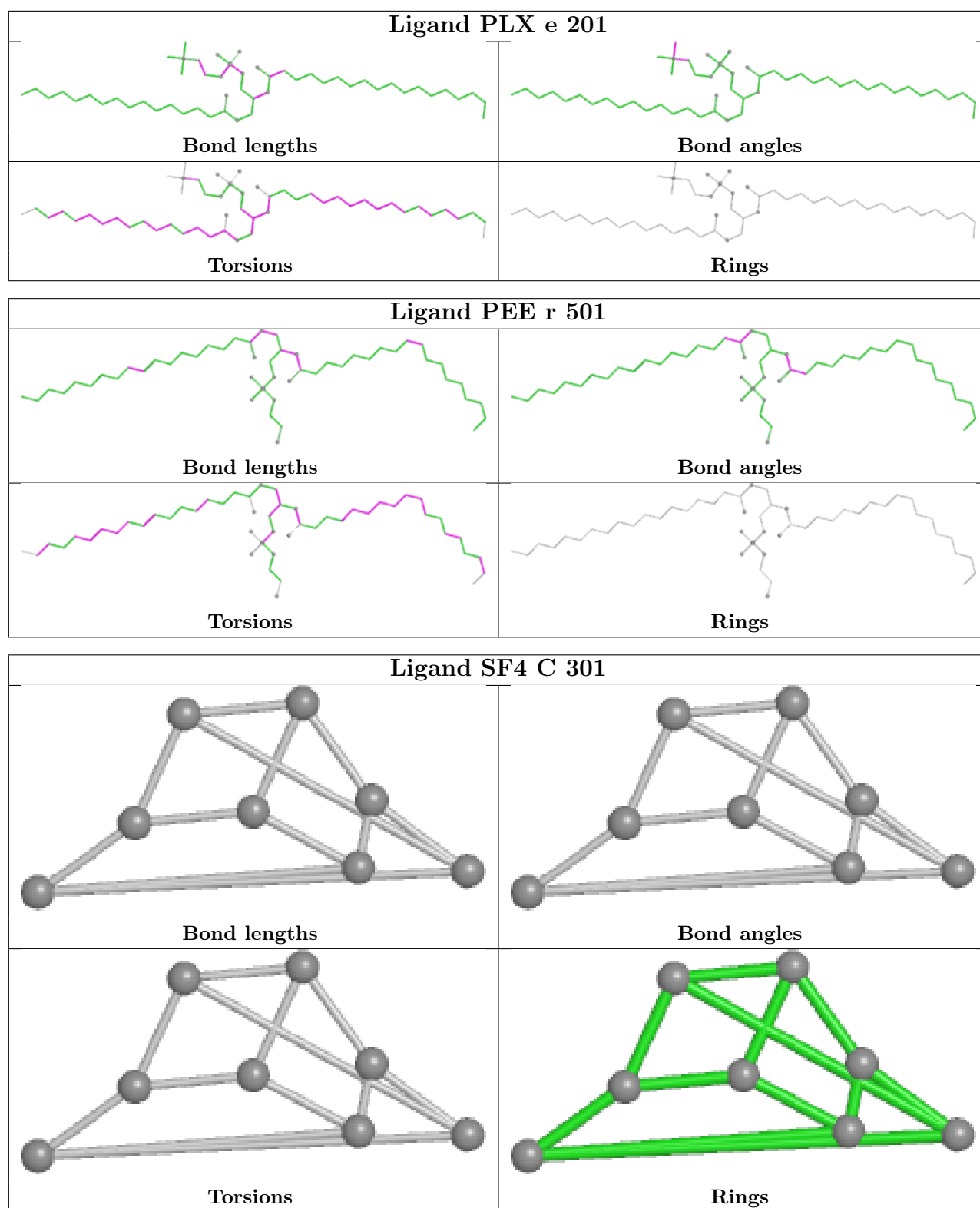


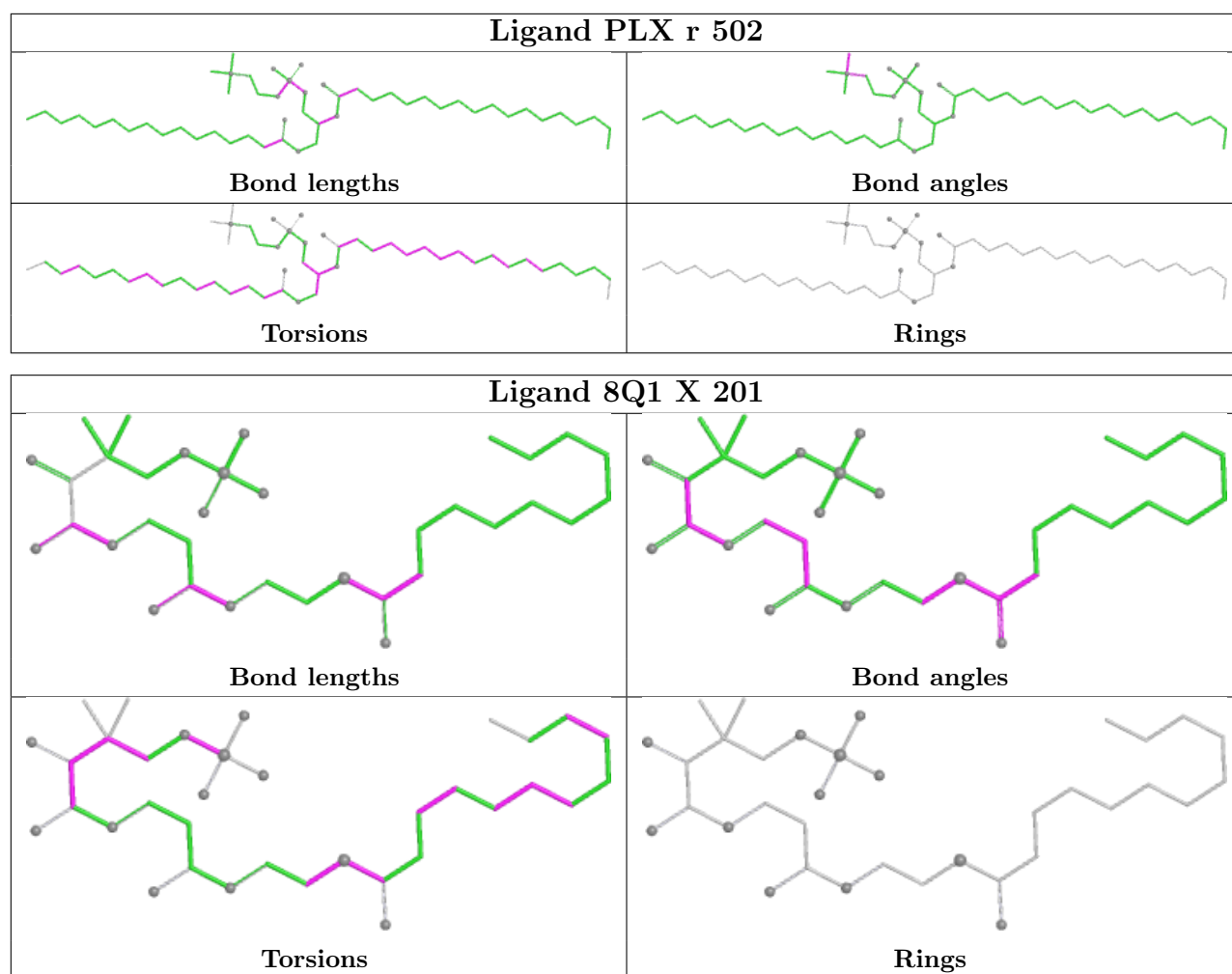


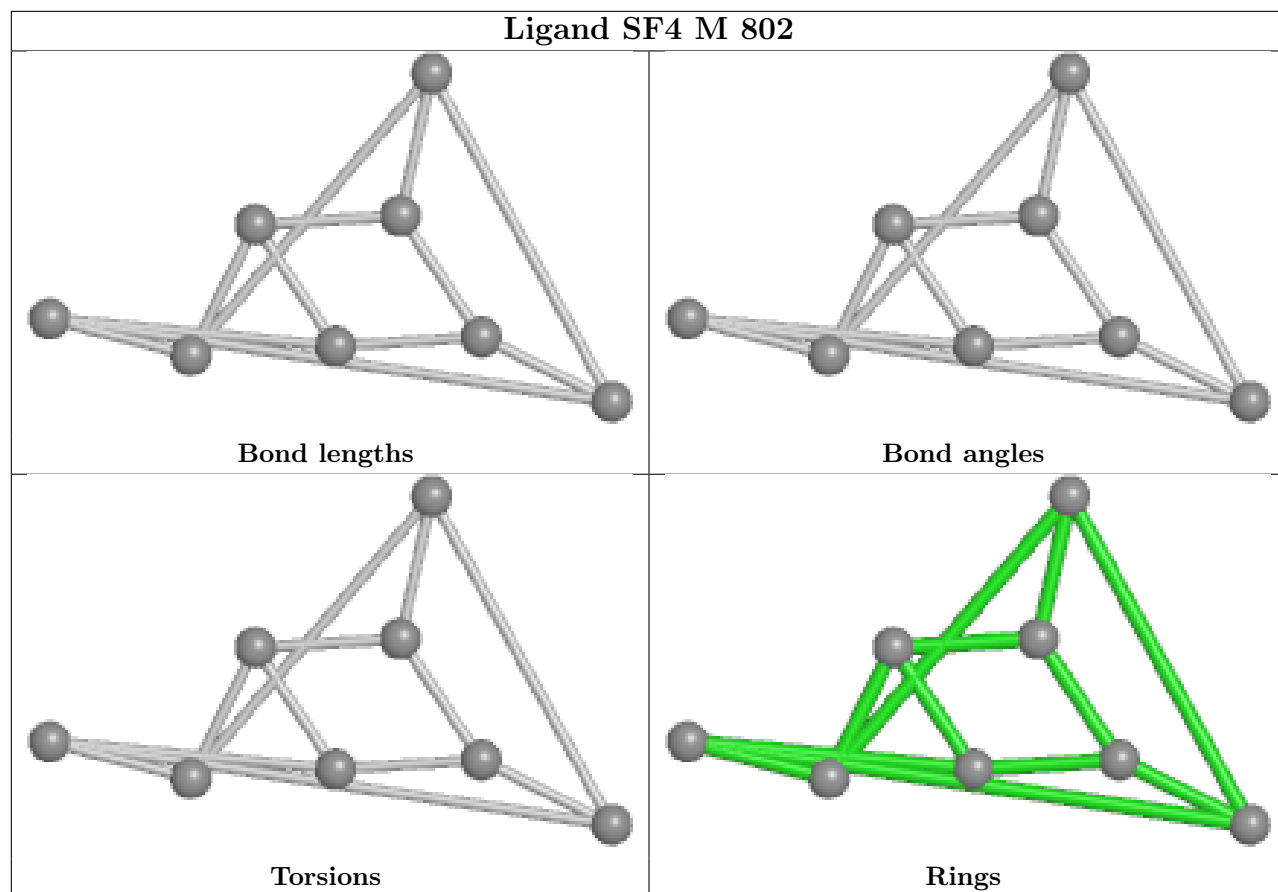




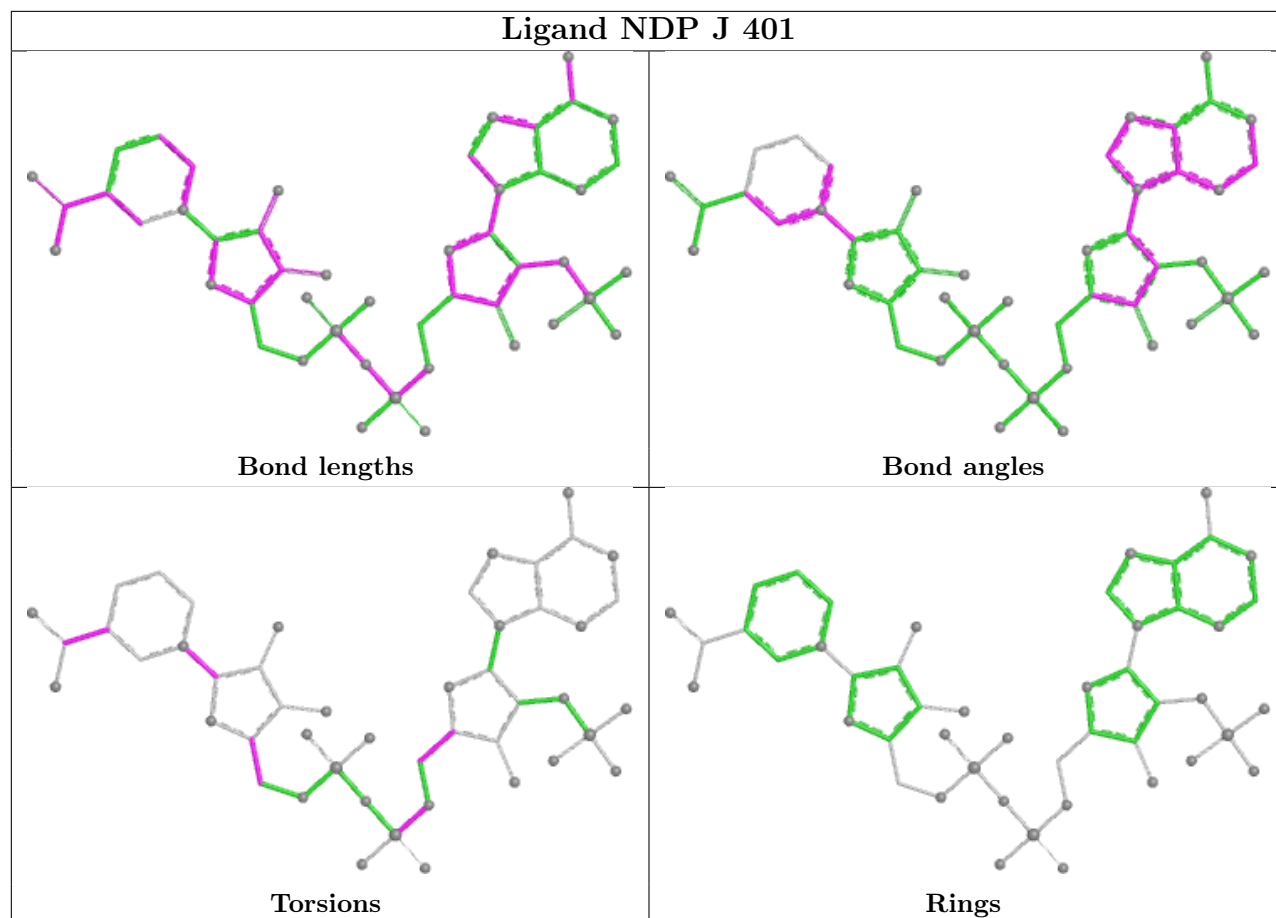




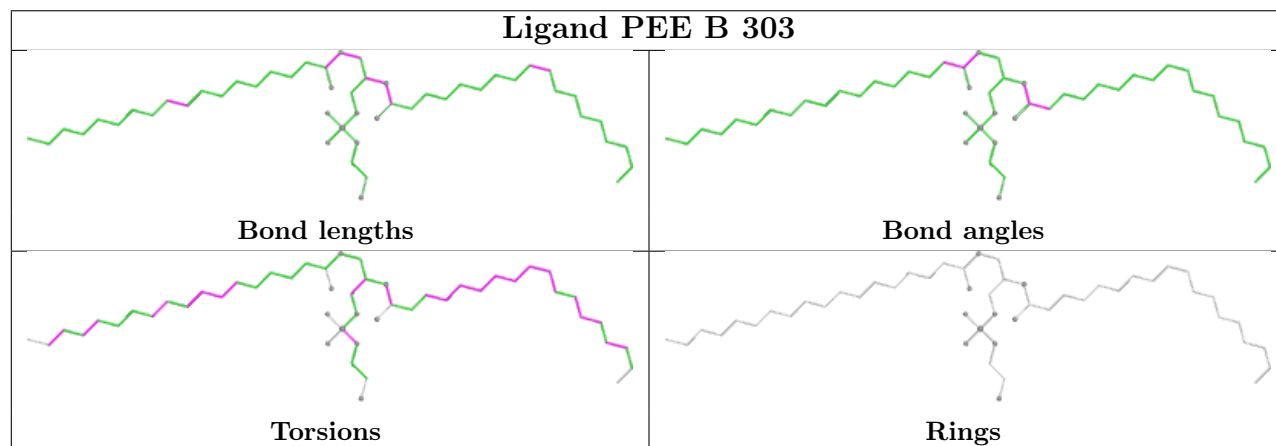


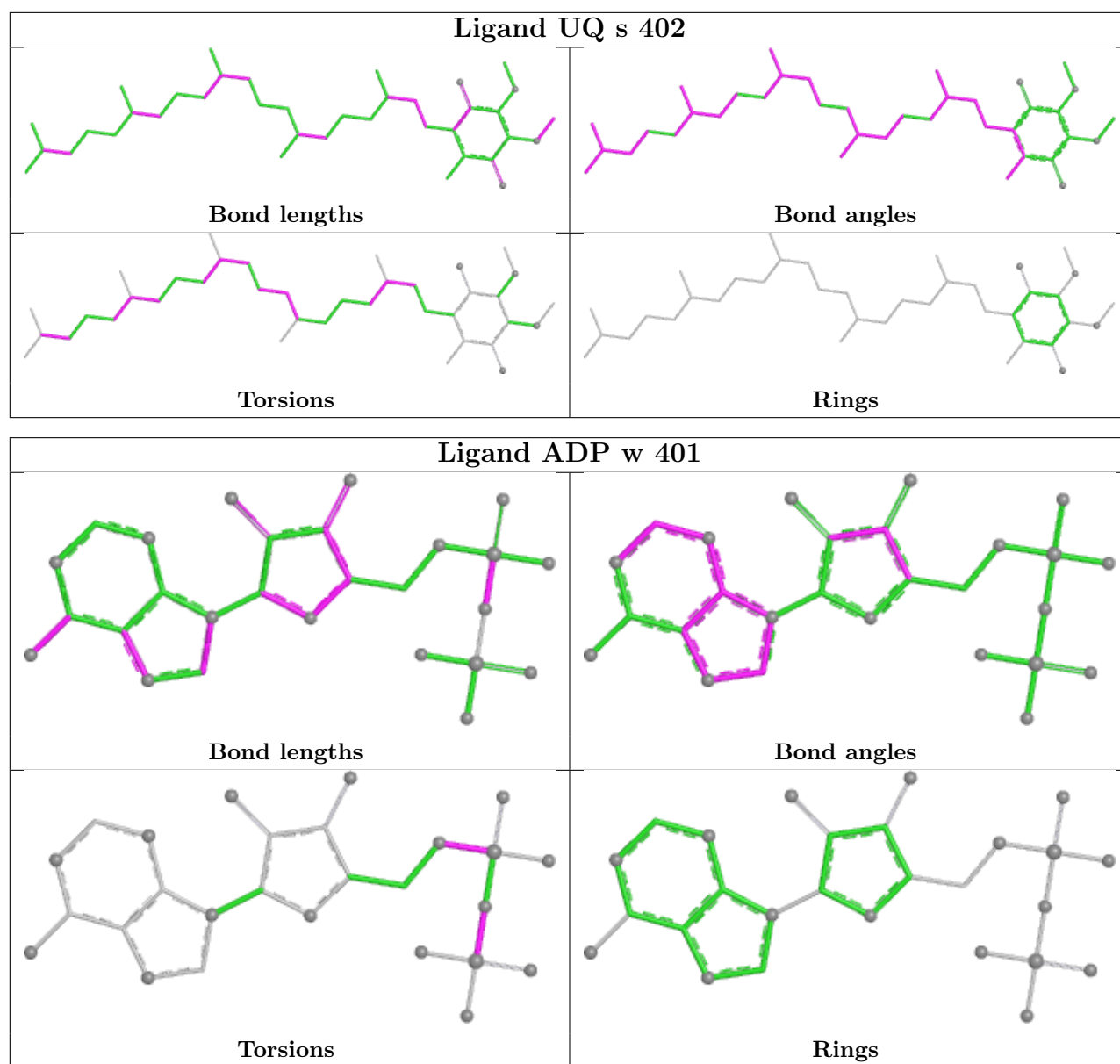


Ligand NDP J 401



Ligand PEE B 303





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.

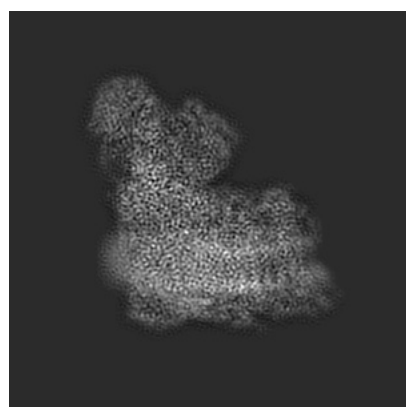
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32256. These allow visual inspection of the internal detail of the map and identification of artifacts.

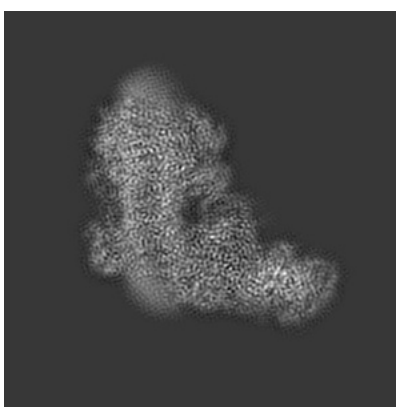
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

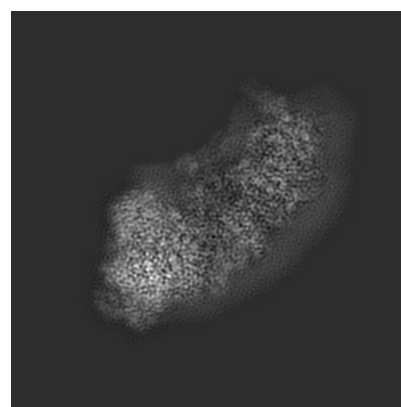
6.1.1 Primary map



X



Y

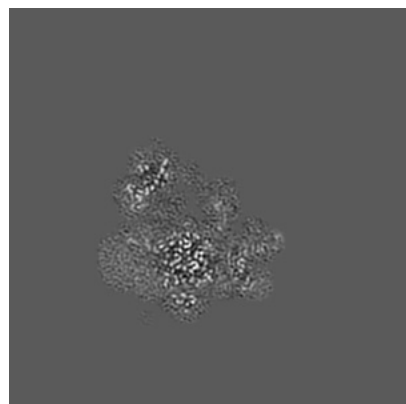


Z

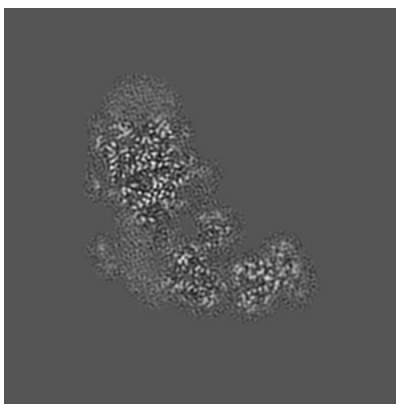
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

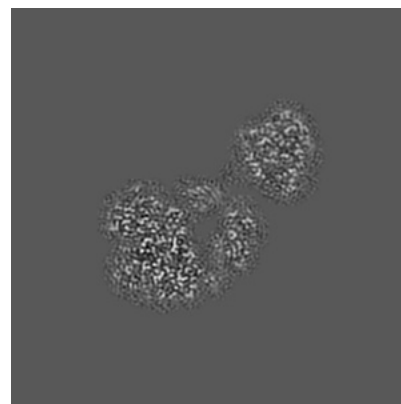
6.2.1 Primary map



X Index: 155



Y Index: 155



Z Index: 155

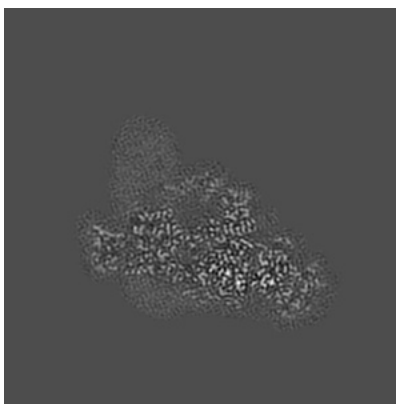
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

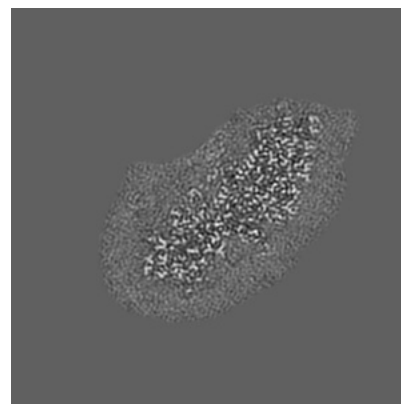
6.3.1 Primary map



X Index: 105



Y Index: 112

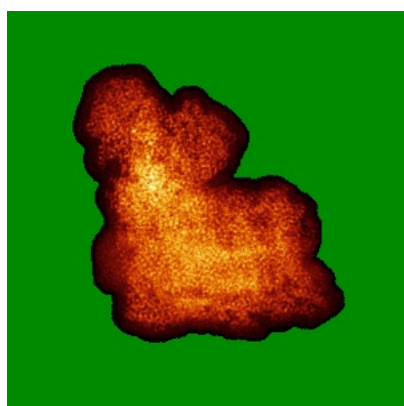


Z Index: 123

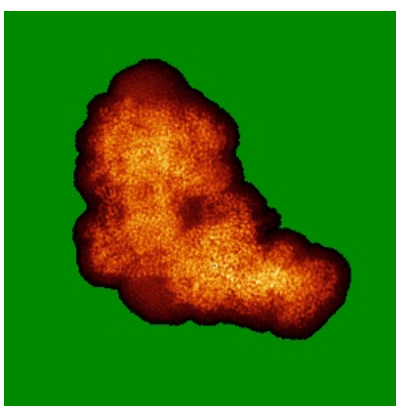
The images above show the largest variance slices of the map in three orthogonal directions.

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

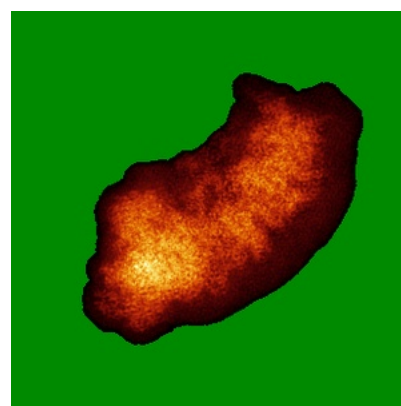
6.4.1 Primary map



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

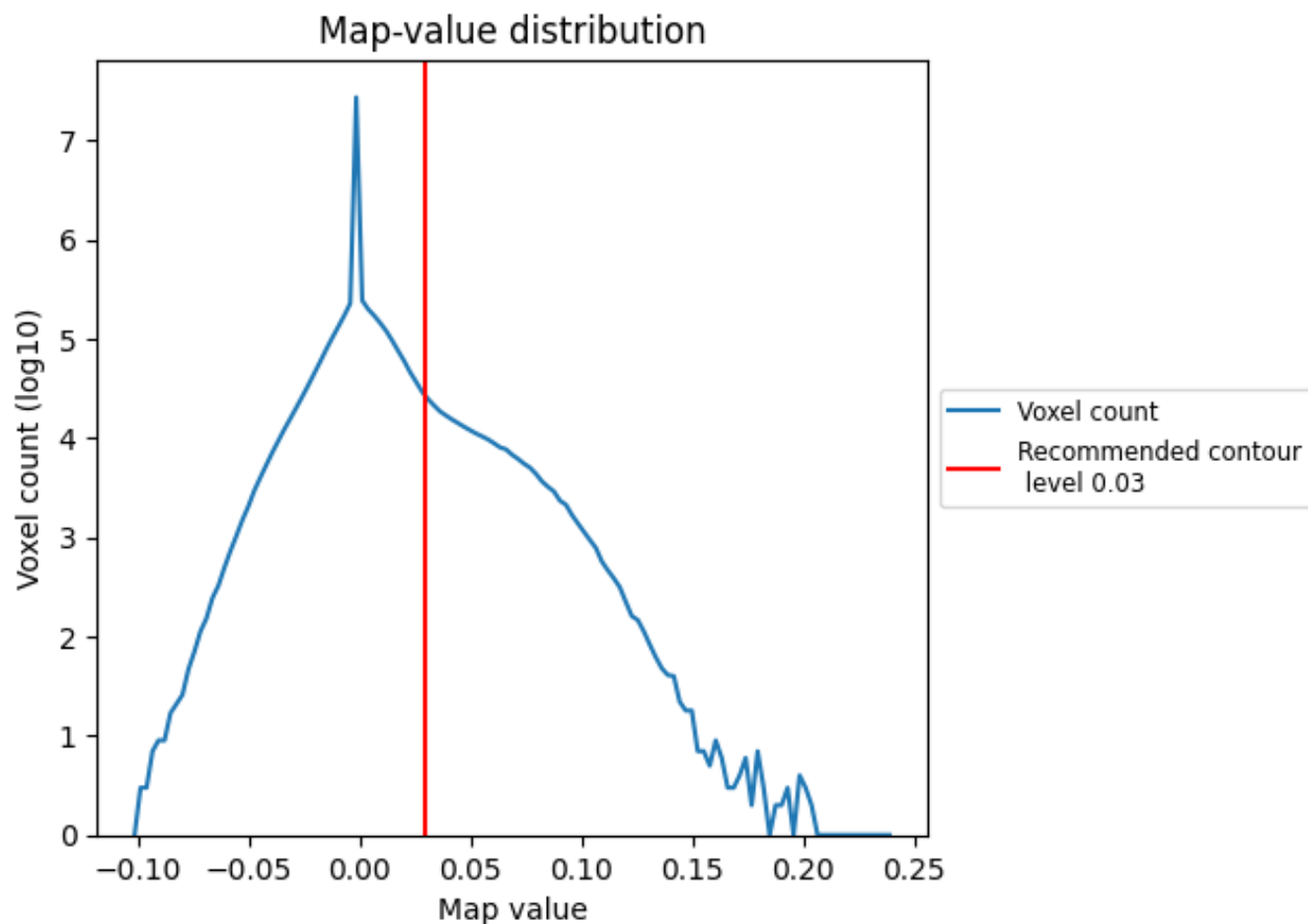
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

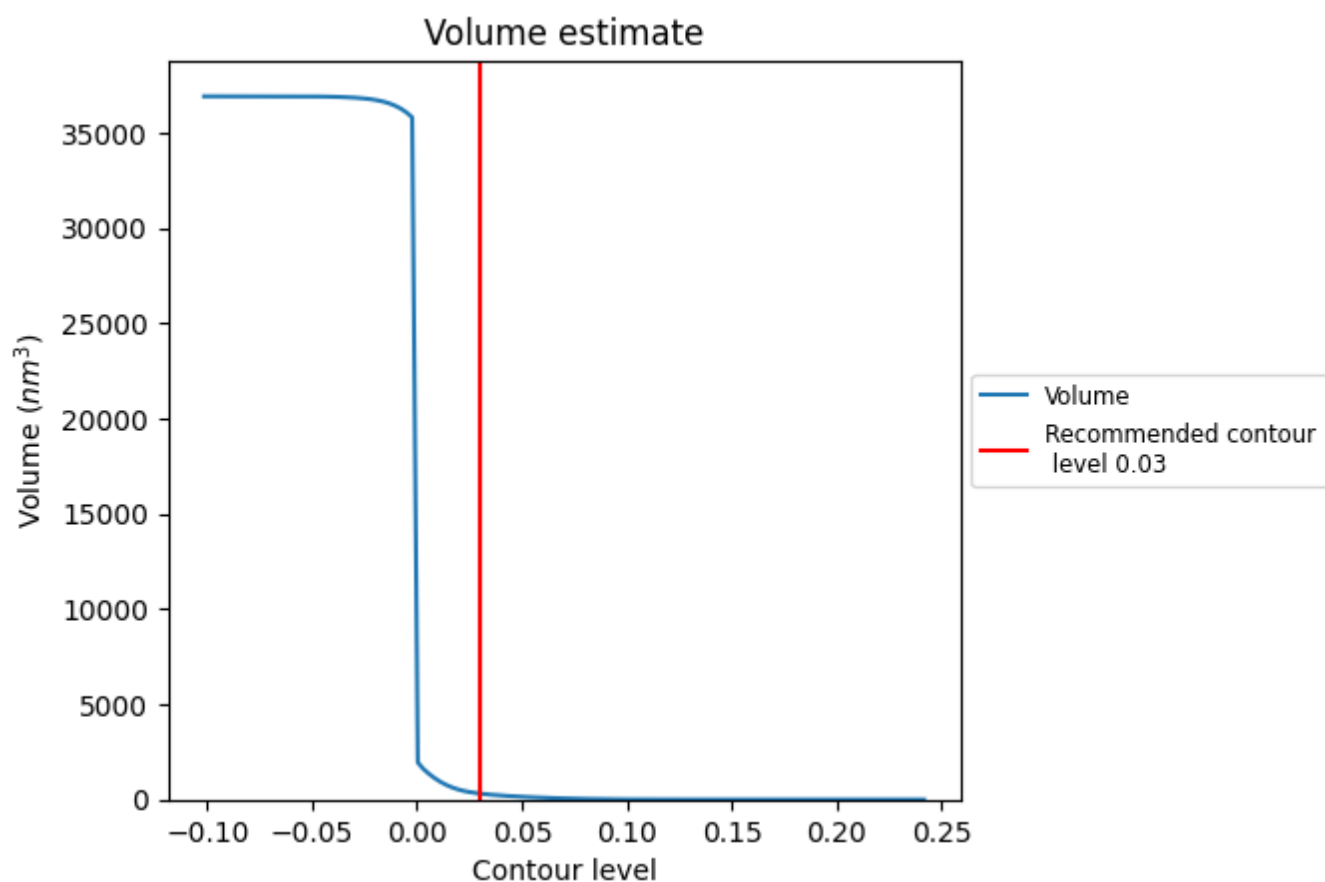
This section contains the results of statistical analysis of the map.

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.

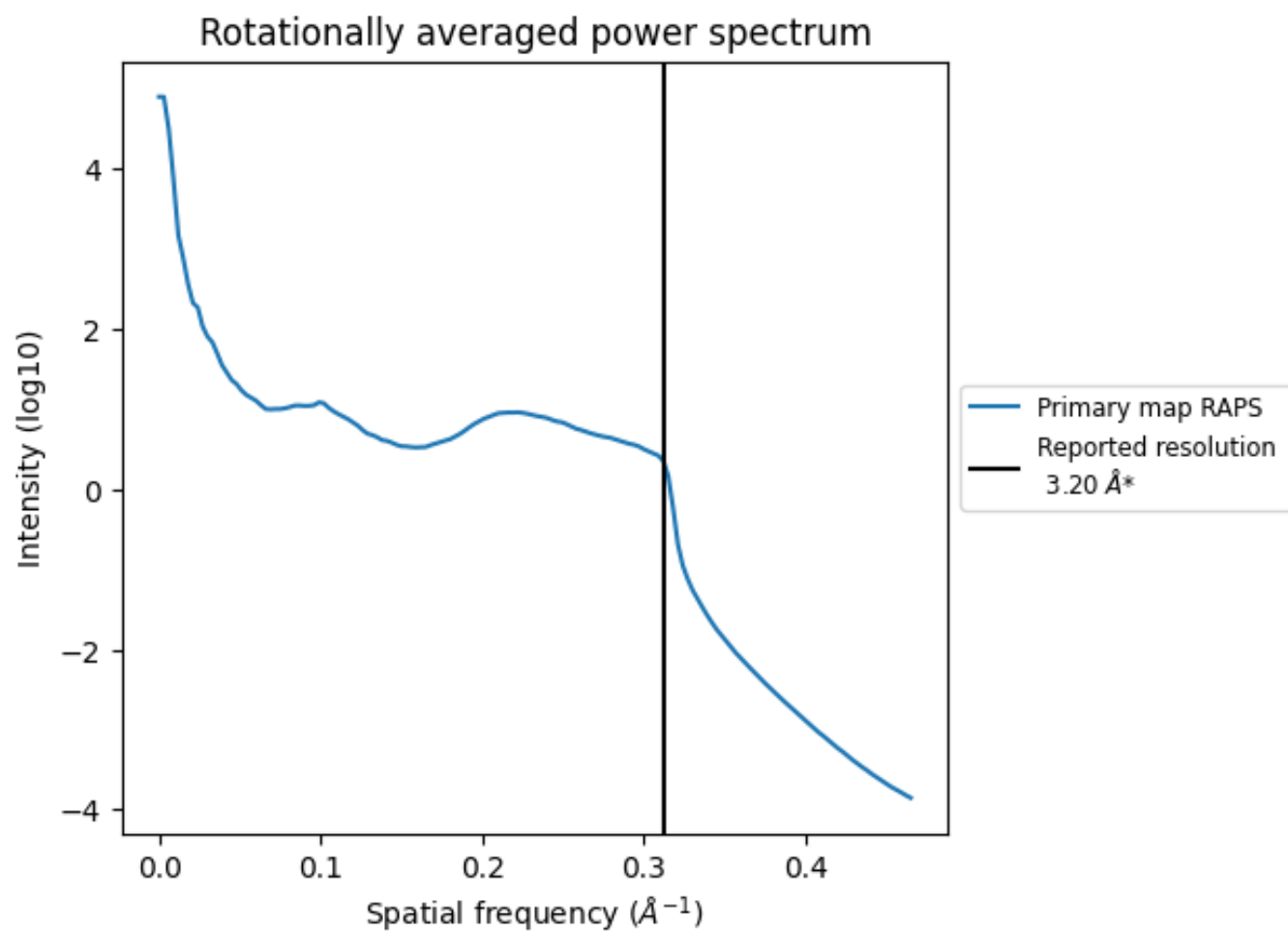
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 314 nm^3 ; this corresponds to an approximate mass of 283 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 0.312 Å⁻¹

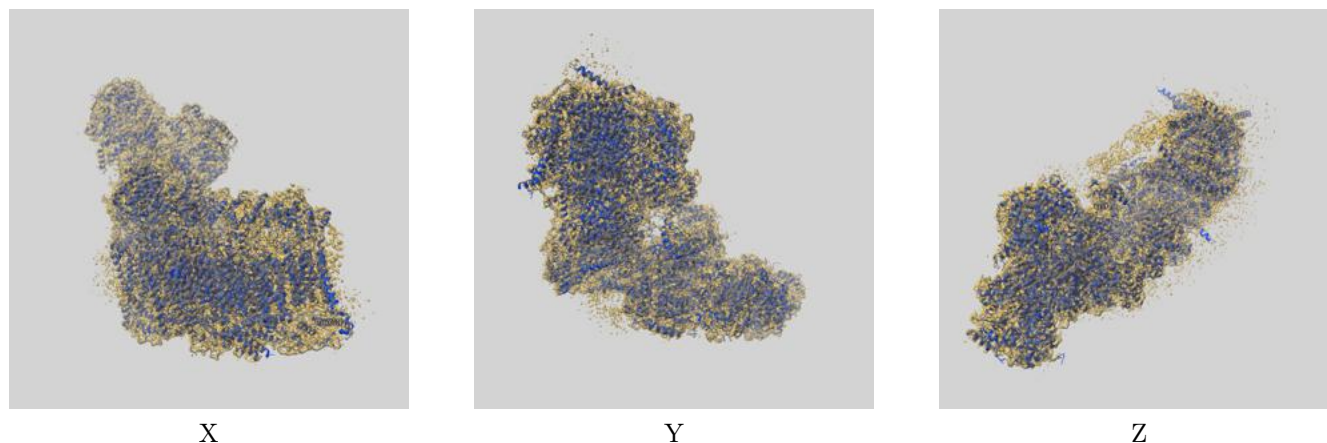
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

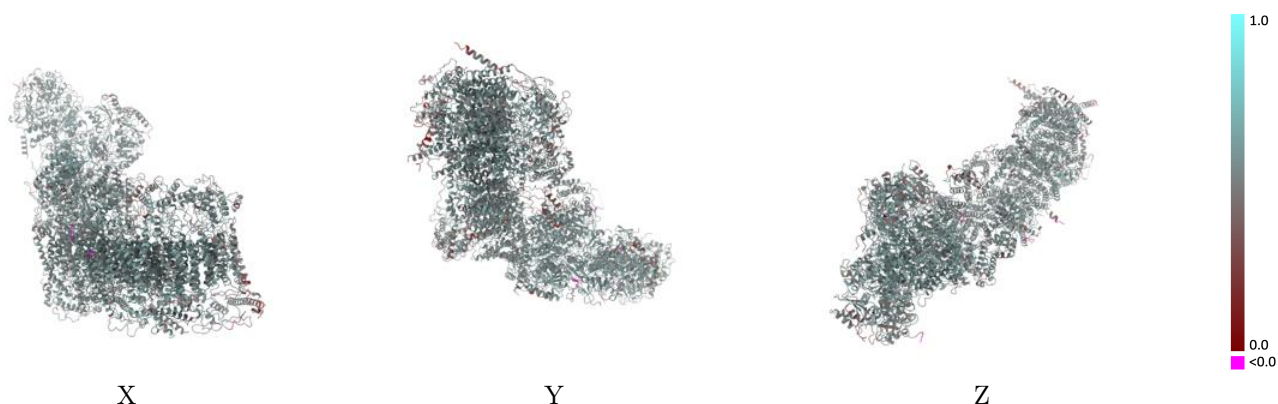
This section contains information regarding the fit between EMDB map EMD-32256 and PDB model 7W1U. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)

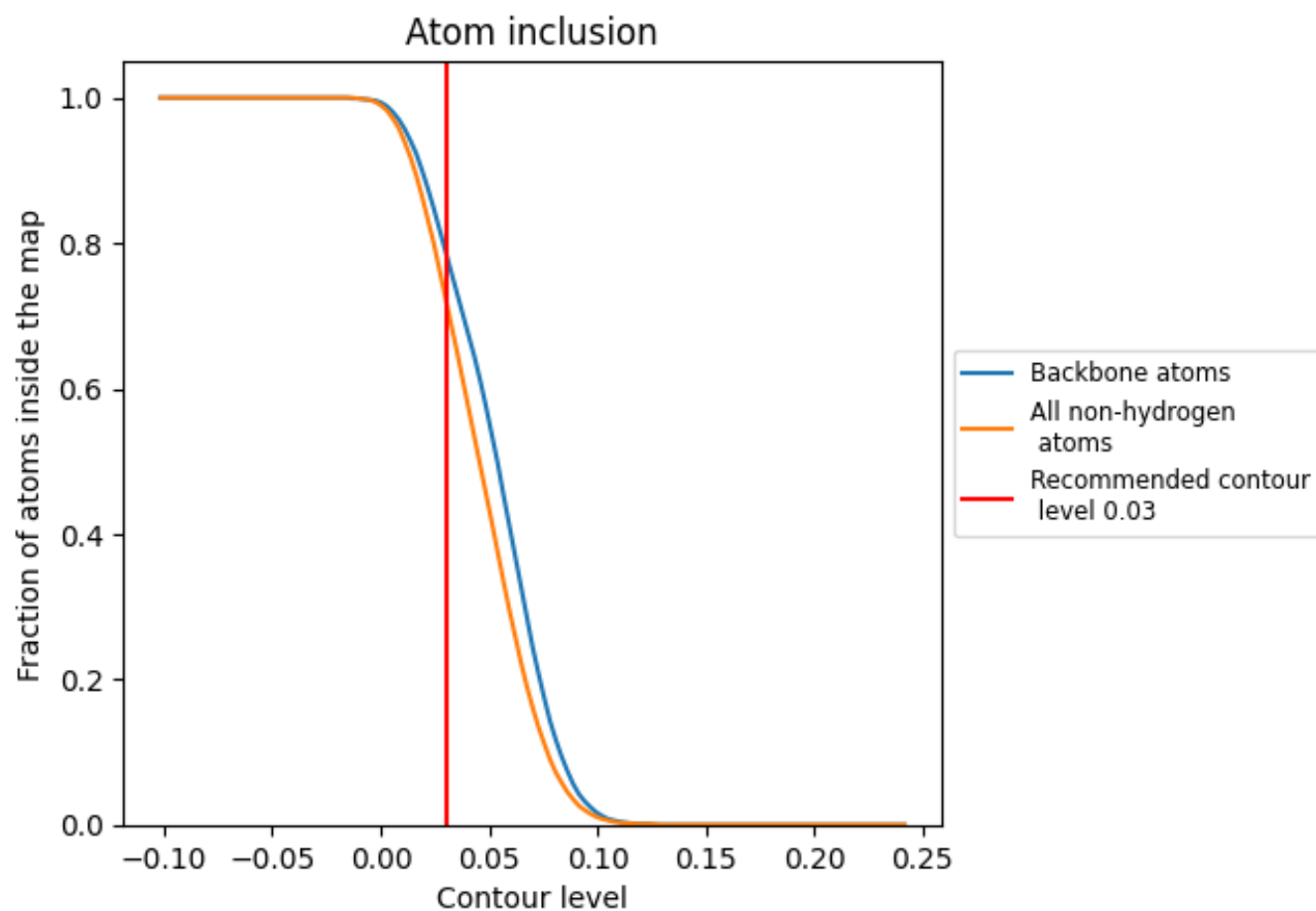


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 79% of all backbone atoms, 72% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.5370
A	 0.7170	 0.5350
B	 0.8380	 0.5850
C	 0.8330	 0.5880
E	 0.7470	 0.5460
F	 0.6260	 0.4730
G	 0.5050	 0.4210
H	 0.7230	 0.5270
I	 0.6570	 0.5150
J	 0.7410	 0.5400
K	 0.5130	 0.4610
L	 0.7480	 0.5540
M	 0.7600	 0.5530
N	 0.6330	 0.5220
O	 0.6700	 0.5110
P	 0.8330	 0.5890
Q	 0.8200	 0.5800
S	 0.7200	 0.5270
T	 0.6010	 0.5060
U	 0.6740	 0.5100
V	 0.6180	 0.5150
W	 0.7070	 0.5300
X	 0.6650	 0.5090
Y	 0.6200	 0.4710
Z	 0.5740	 0.4500
a	 0.7220	 0.5510
b	 0.6650	 0.4900
c	 0.7240	 0.5260
d	 0.6990	 0.5190
e	 0.6560	 0.5150
f	 0.5310	 0.4430
g	 0.7500	 0.5440
h	 0.6940	 0.5170
i	 0.8020	 0.5740
j	 0.7120	 0.5490



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Chain	Atom inclusion	Q-score
k	 0.7830	 0.5650
l	 0.7380	 0.5450
m	 0.6520	 0.5050
n	 0.5530	 0.4720
o	 0.7020	 0.5260
p	 0.7310	 0.5310
r	 0.7810	 0.5710
s	 0.7580	 0.5380
u	 0.7260	 0.5340
v	 0.6150	 0.4700
w	 0.6890	 0.5220