



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 09:14 AM JST

PDB ID : 7W1V / pdb_00007w1v
EMDB ID : EMD-32257
Title : Active state CI from Rotenone-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-20
Resolution : 3.00 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

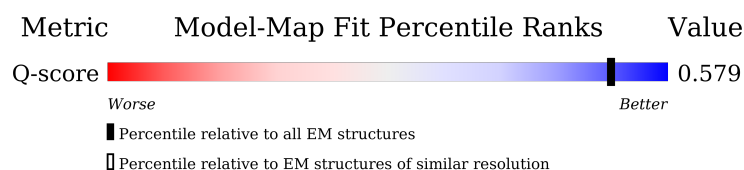
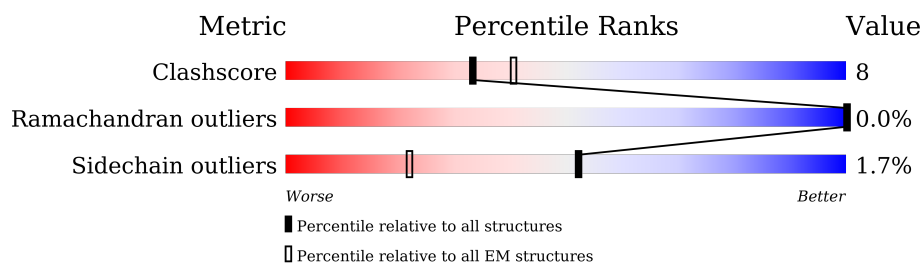
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	 8% 73% 26%
2	B	176	 82% 18%
3	C	156	 80% 18%
4	E	115	 8% 84% 16%

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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	122	
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	124	
44	w	320	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68209 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
			3330	2103	593	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
			1411	887	243	268	13		

- 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
			1248	794	227	213	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
			684	431	129	122	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
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			693	448	103	137	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
			5284	3314	923	1008	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
			1200	767	217	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
			1667	1062	280	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
			3459	2212	594	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
			643	417	110	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
			1161	749	197	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
			856	548	142	162	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	122	Total	C	N	O	S	0	0
			1005	653	174	172	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
			4797	3181	743	822	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
			1276	850	187	226	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
			1530	979	278	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
			3624	2406	572	608	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
			2508	1678	385	424	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		

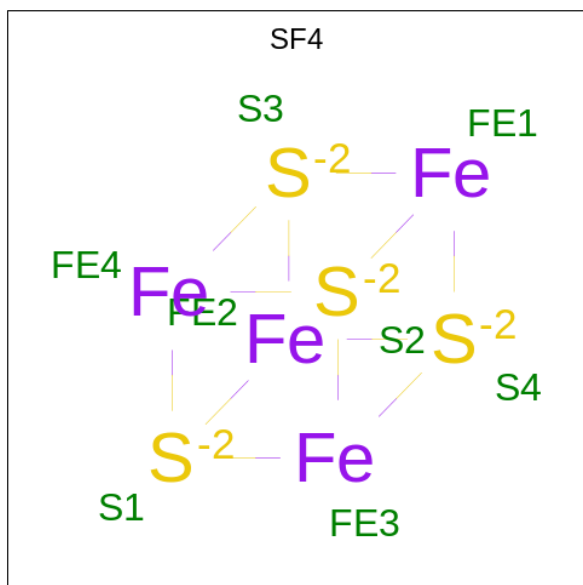
- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1036	646	196	185	9		

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

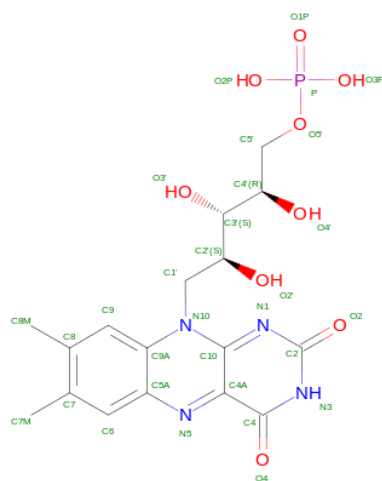
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

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



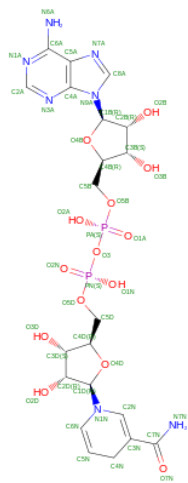
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



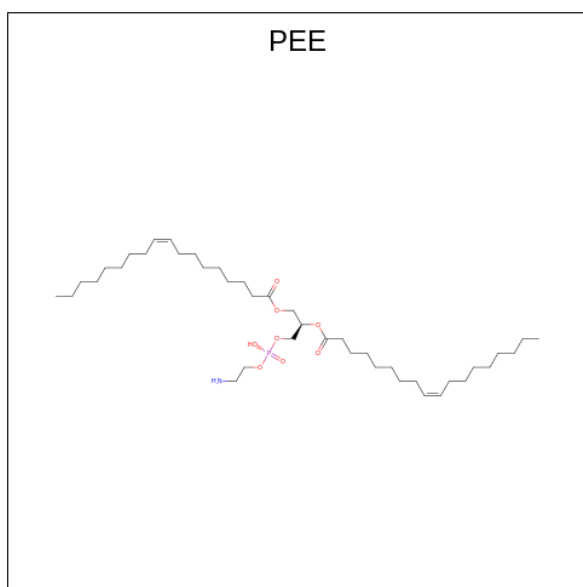
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



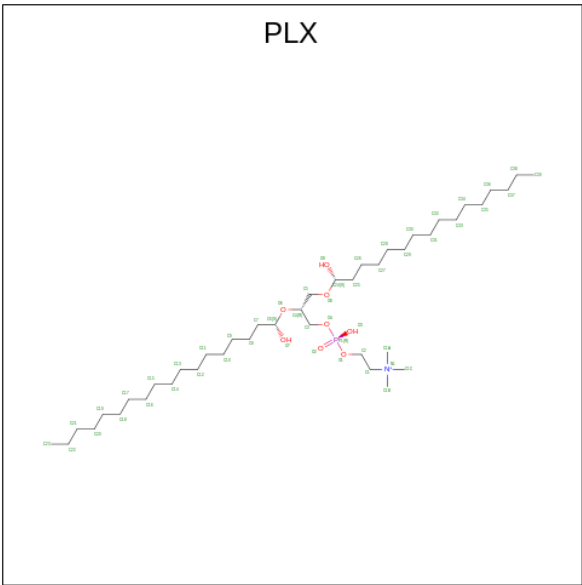
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total 44	C 21	N 7	O 14	P 2	0

- Molecule 48 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).



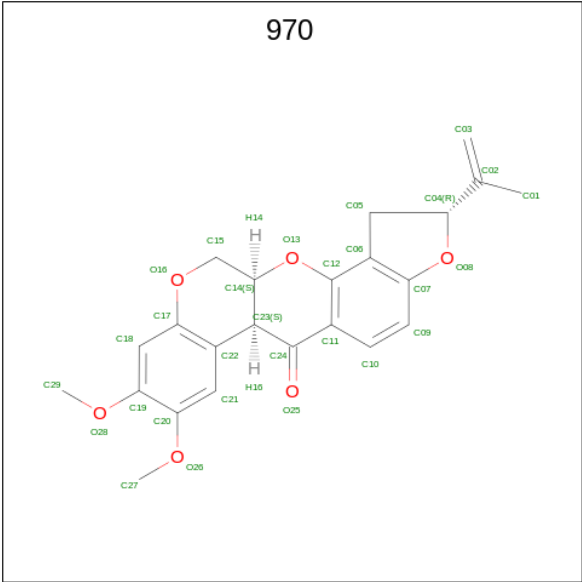
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 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).



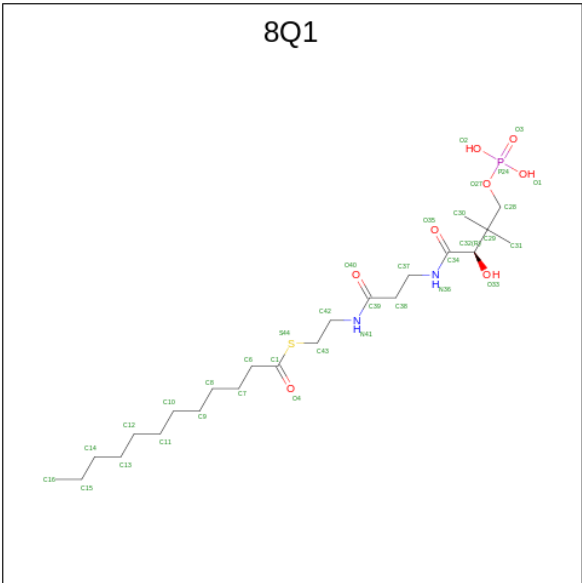
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 50 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).



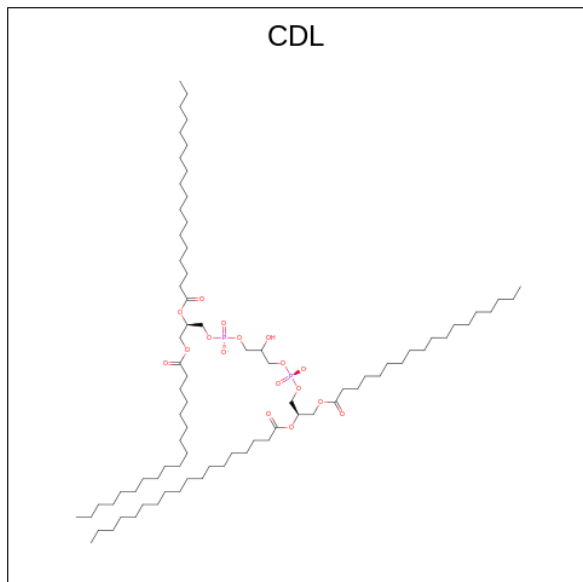
Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			29	23	6	

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

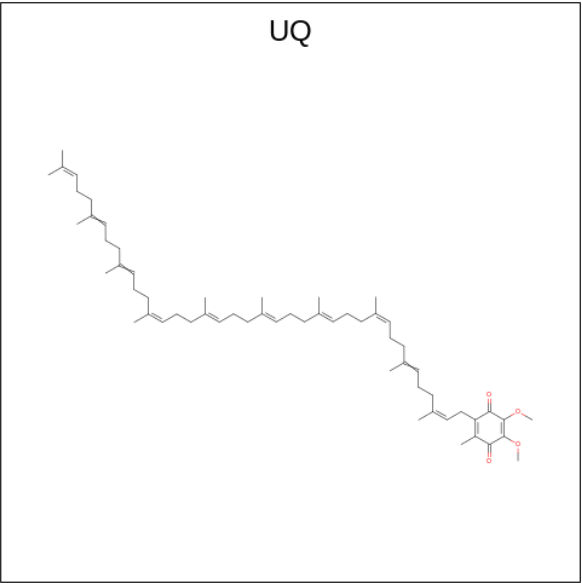


Mol	Chain	Residues	Atoms				AltConf
52	I	1	Total	C	O	P	0
			51	32	17	2	
52	V	1	Total	C	O	P	0
			94	75	17	2	
52	V	1	Total	C	O	P	0
			78	59	17	2	
52	a	1	Total	C	O	P	0
			100	81	17	2	
52	g	1	Total	C	O	P	0
			55	36	17	2	
52	i	1	Total	C	O	P	0
			100	81	17	2	
52	i	1	Total	C	O	P	0
			99	80	17	2	
52	l	1	Total	C	O	P	0
			99	80	17	2	
52	l	1	Total	C	O	P	0
			100	81	17	2	
52	o	1	Total	C	O	P	0
			100	81	17	2	
52	s	1	Total	C	O	P	0
			89	70	17	2	

- Molecule 53 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"

NDP

- Molecule 54 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).

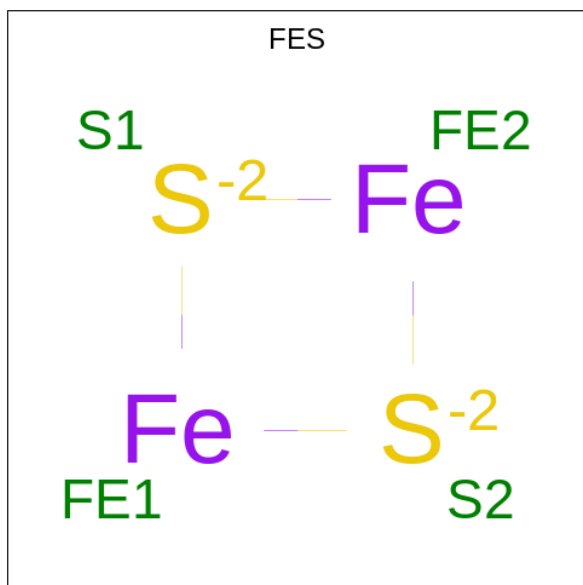


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Mol	Chain	Residues	Atoms			AltConf
54	s	1	Total	C	O	0
			38	34	4	

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

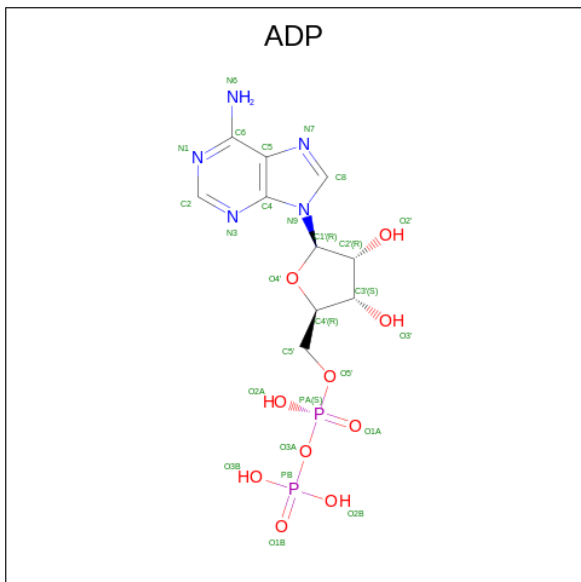
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

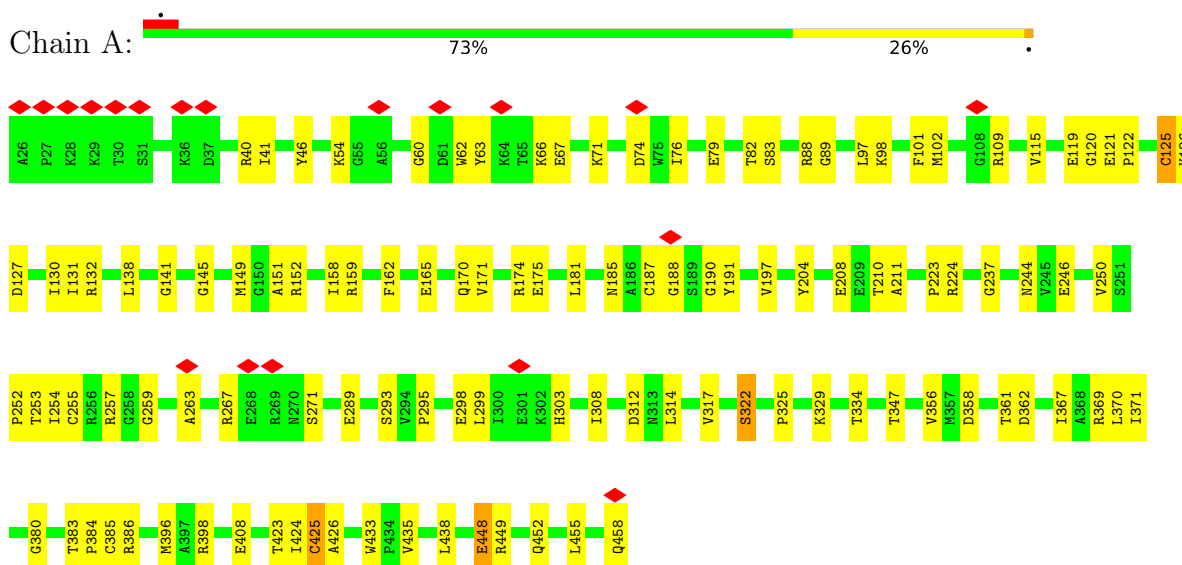


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	27	10	5	10	2	0

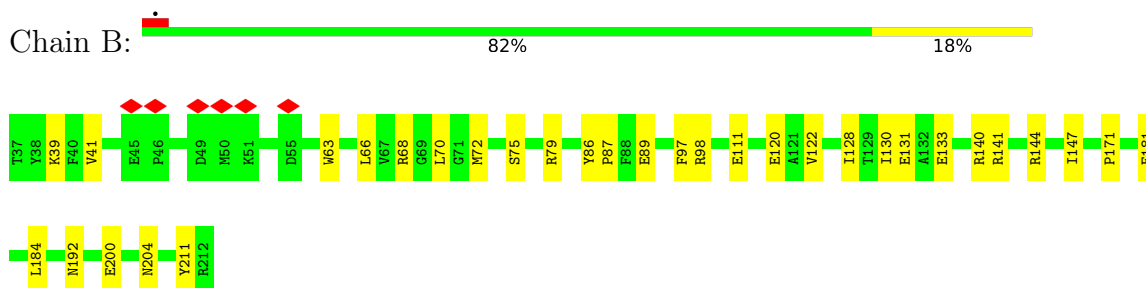
3 Residue-property plots

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

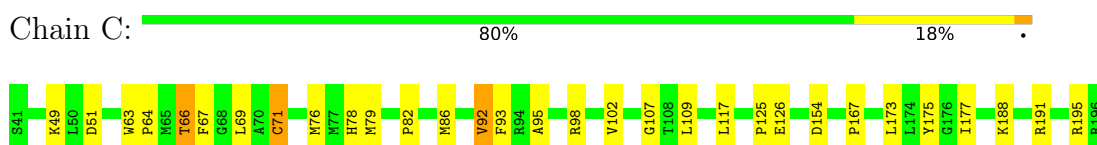
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



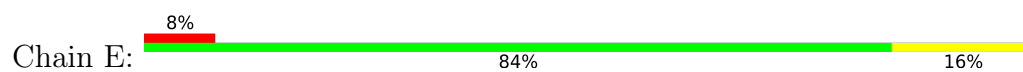
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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



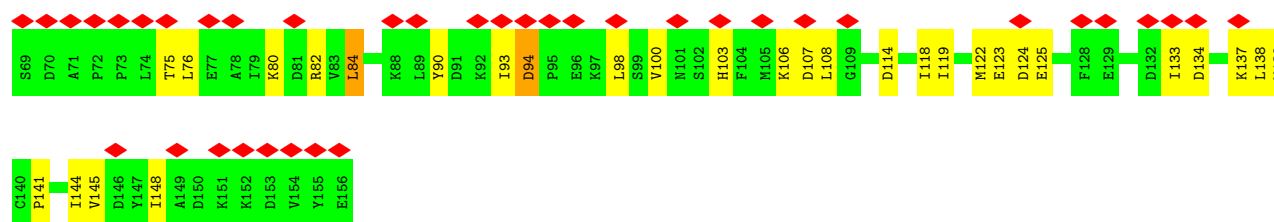
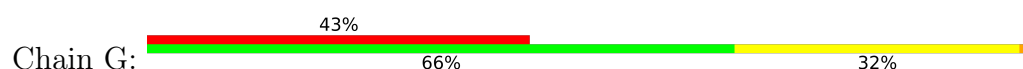
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



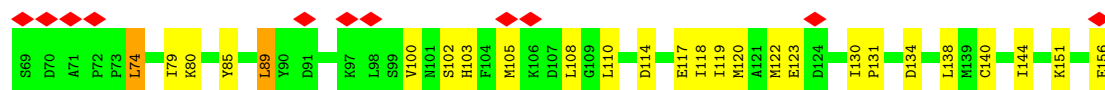
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



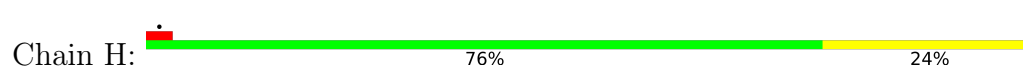
- Molecule 6: Acyl carrier protein



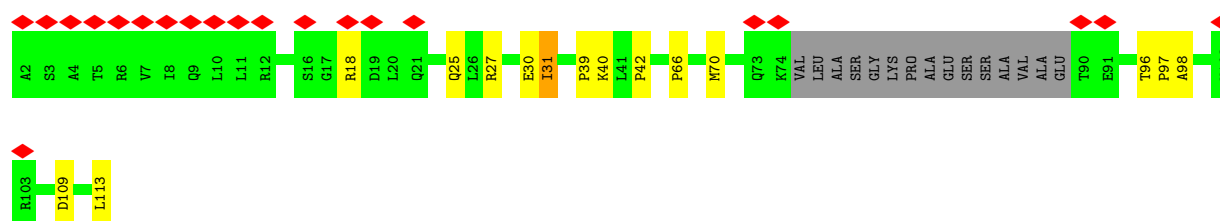
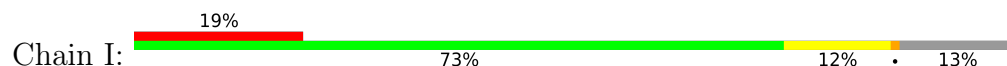
- Molecule 6: Acyl carrier protein



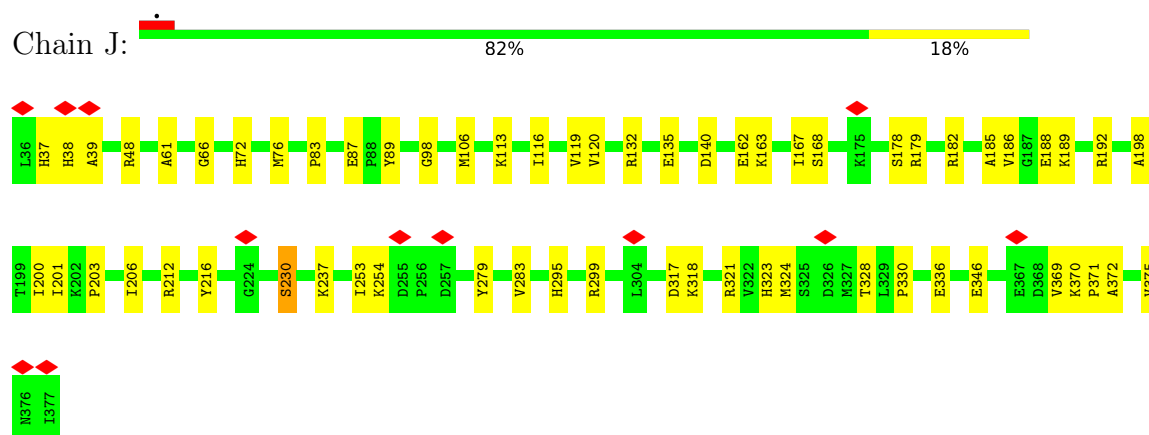
- Molecule 7: Complex I subunit B13



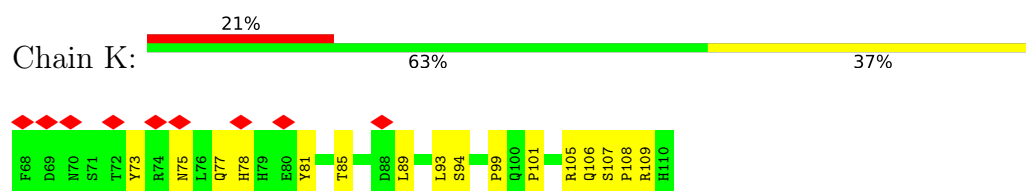
- Molecule 8: Complex I-B14.5a



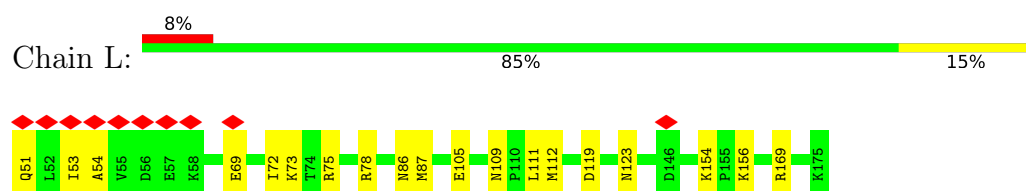
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



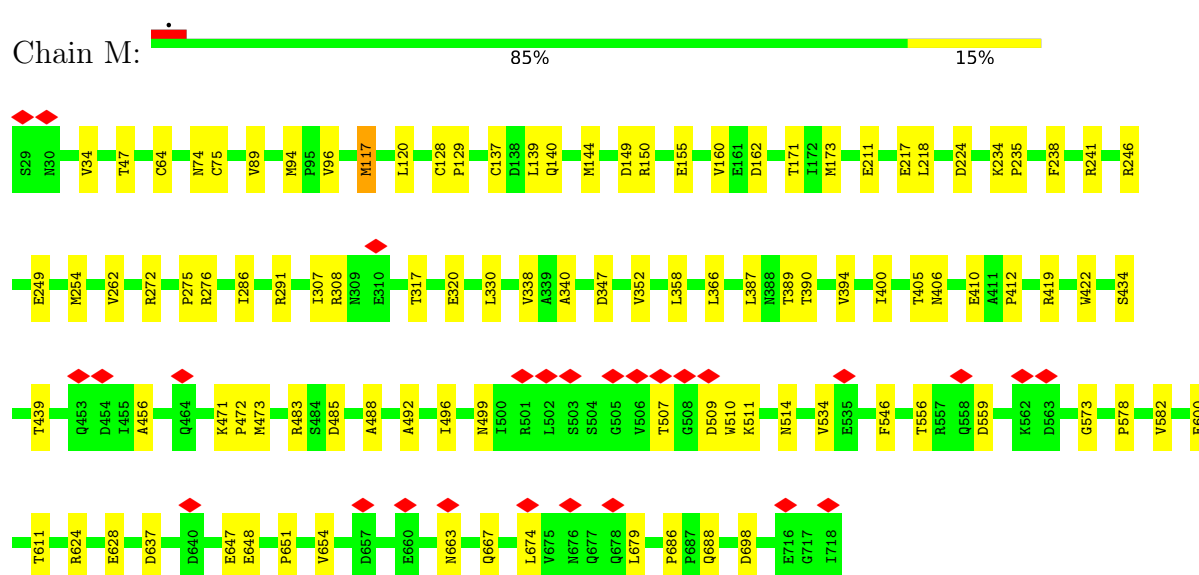
- Molecule 10: Complex I-9kD



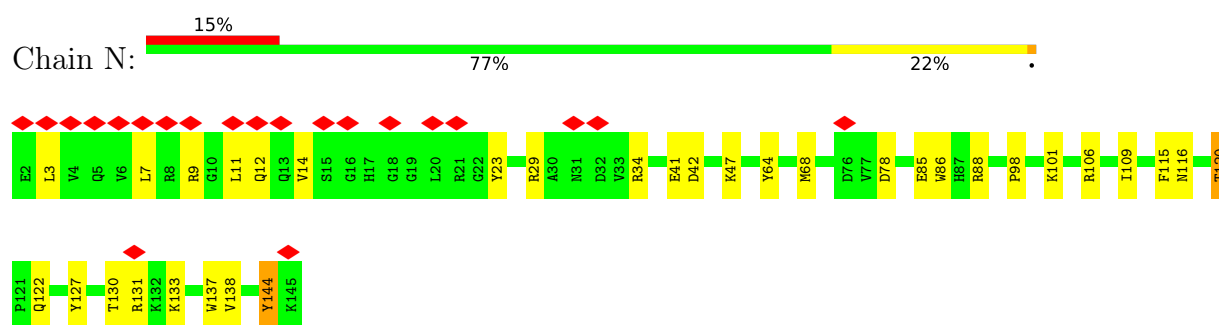
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



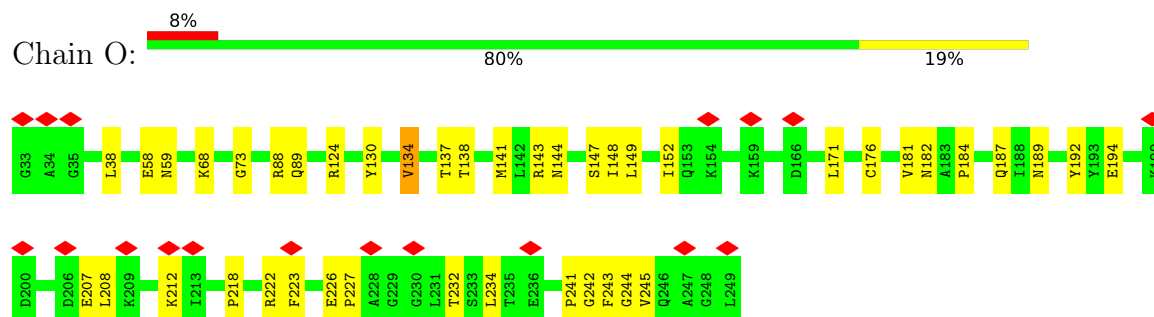
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



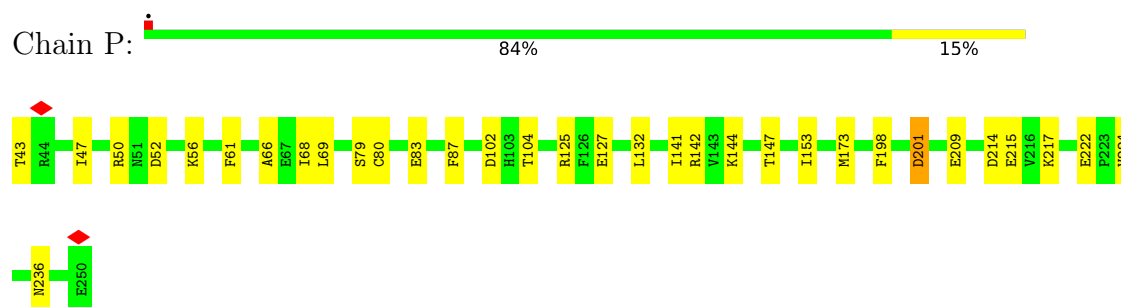
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



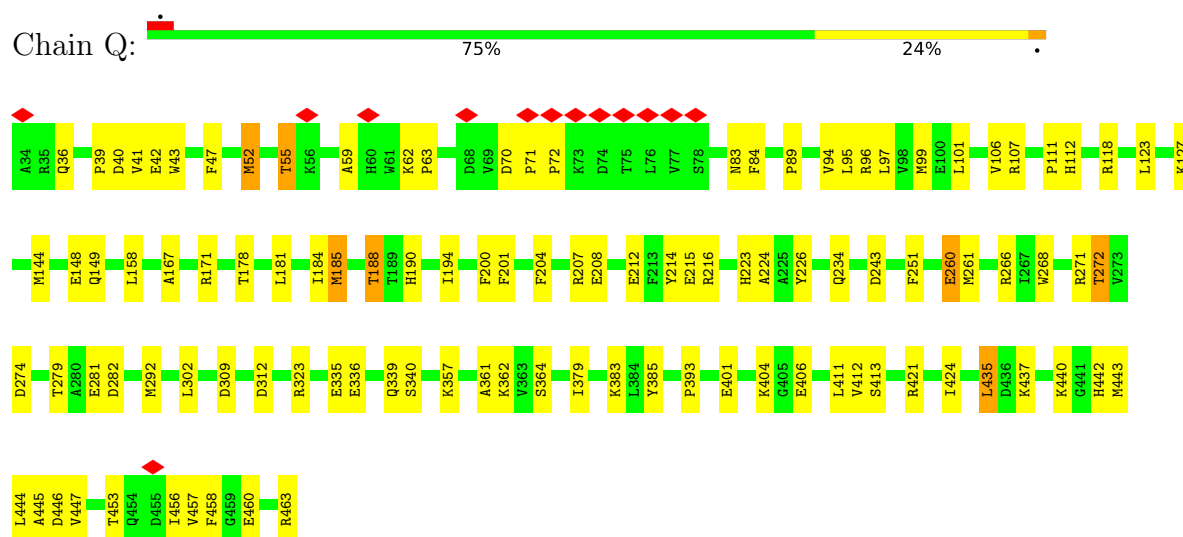
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



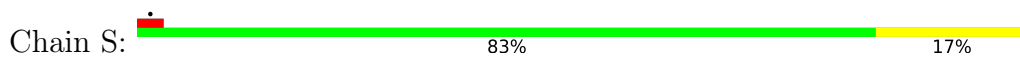
- Molecule 15: Complex I-30kD



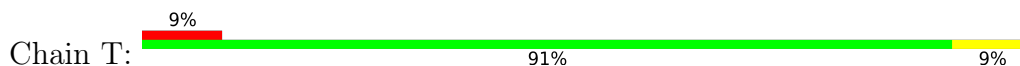
- Molecule 16: Complex I-49kD



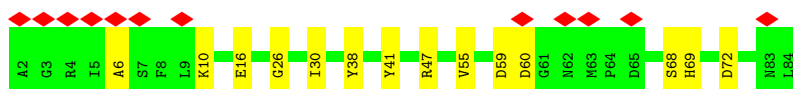
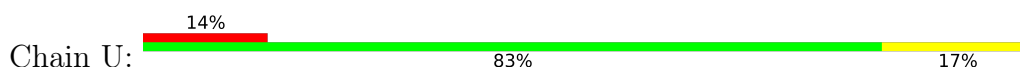
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



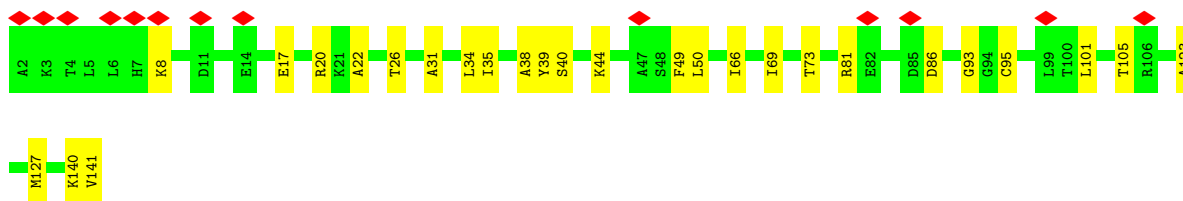
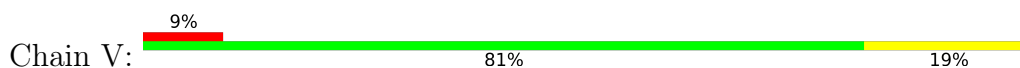
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



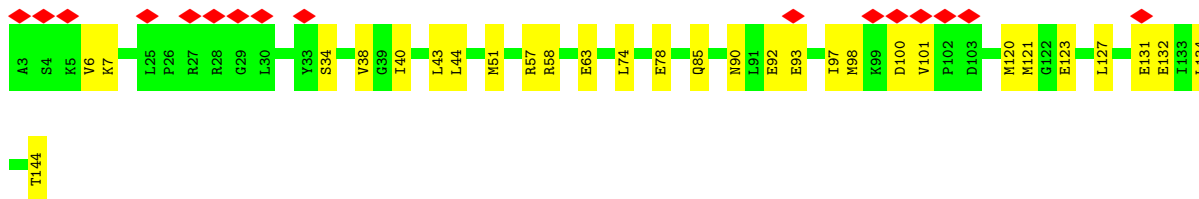
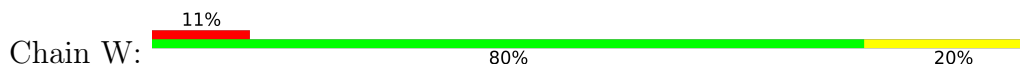
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



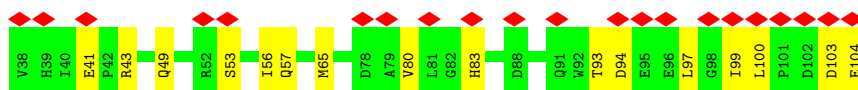
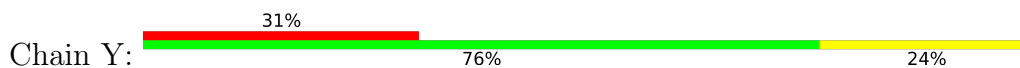
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



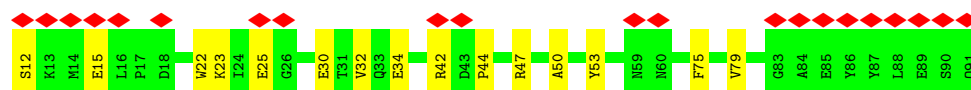
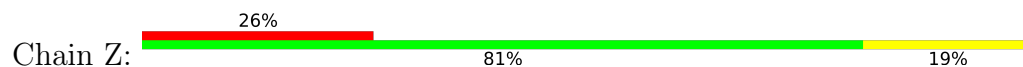
- Molecule 21: Complex I-B16.6



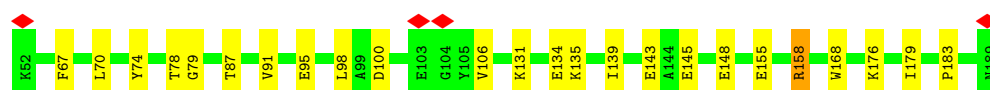
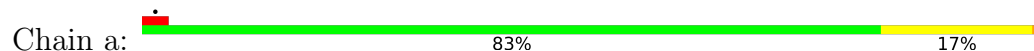
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



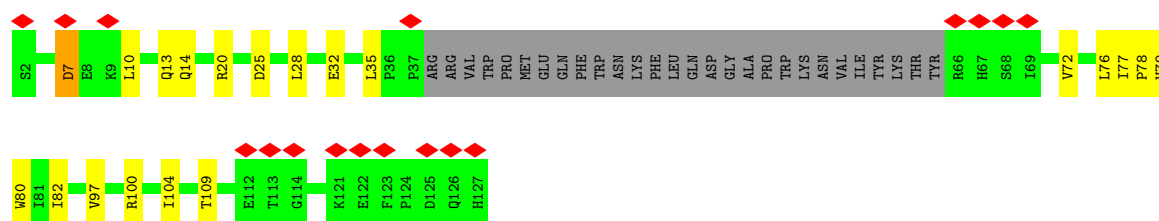
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



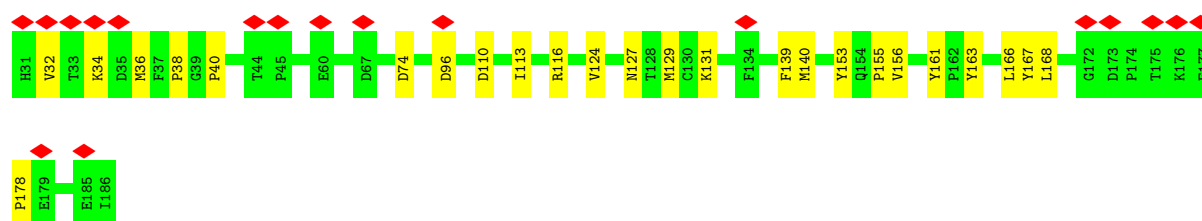
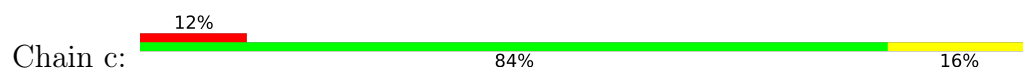
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



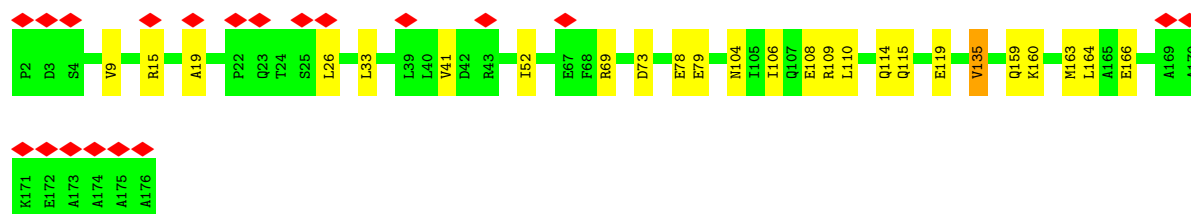
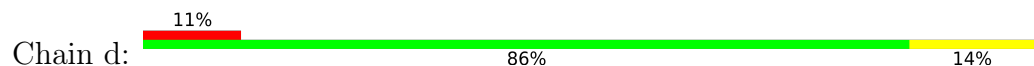
- Molecule 25: Complex I-B17



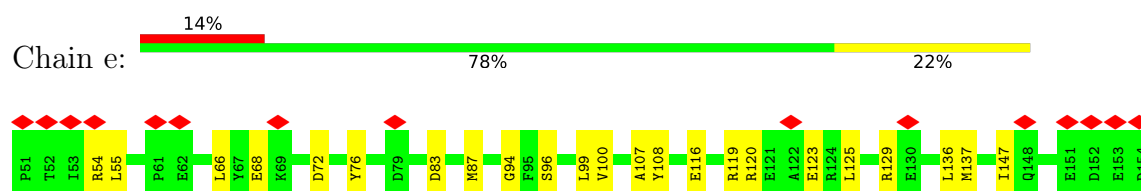
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



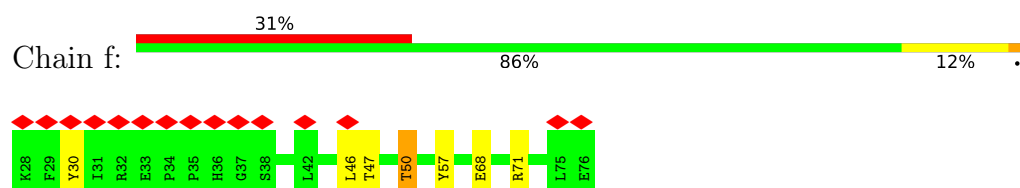
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



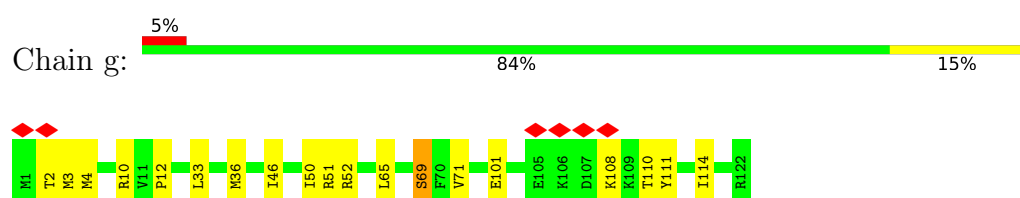
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



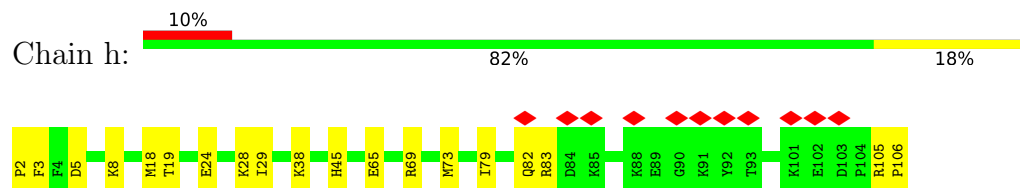
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



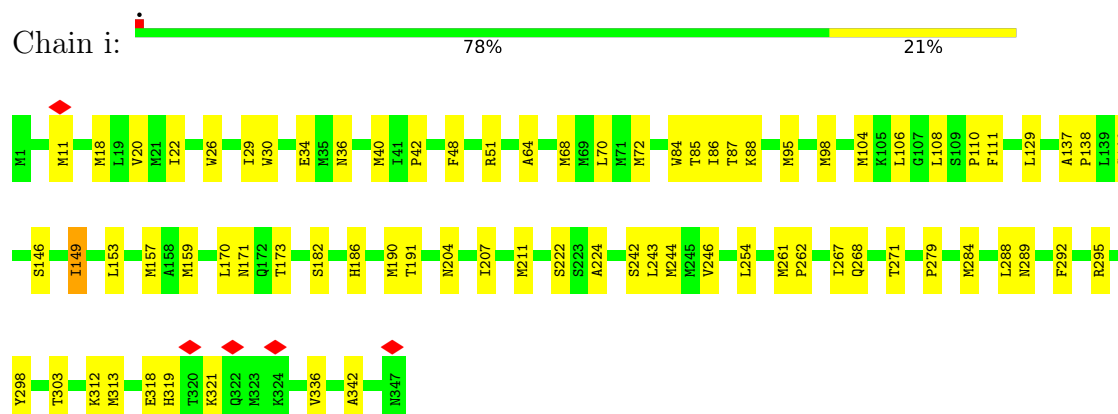
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



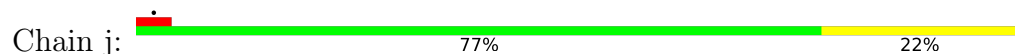
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

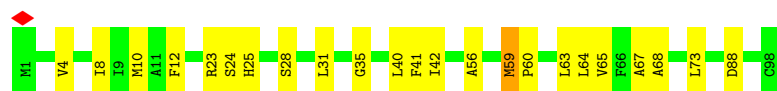
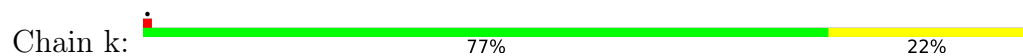


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

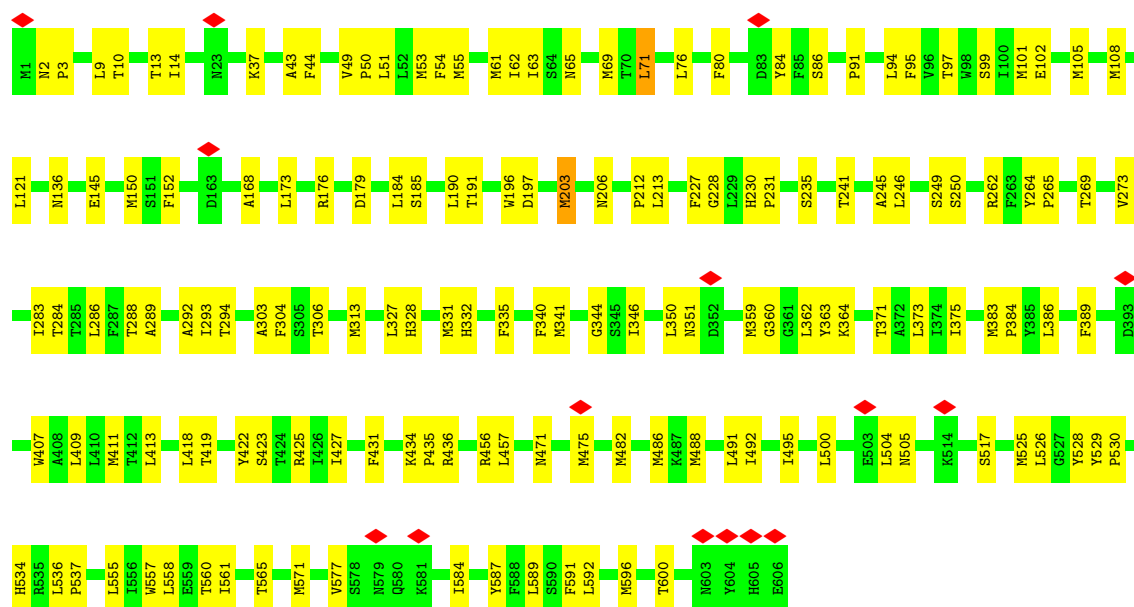




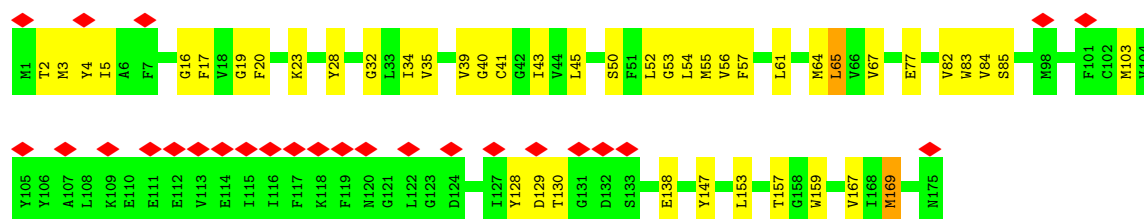
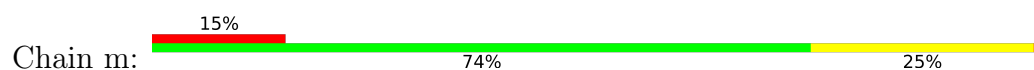
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



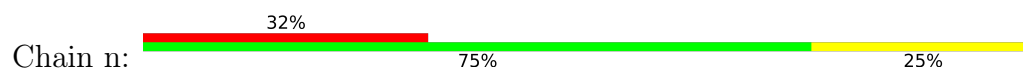
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

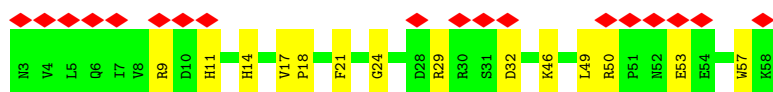


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

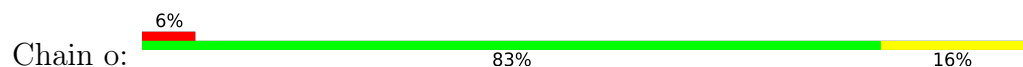


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

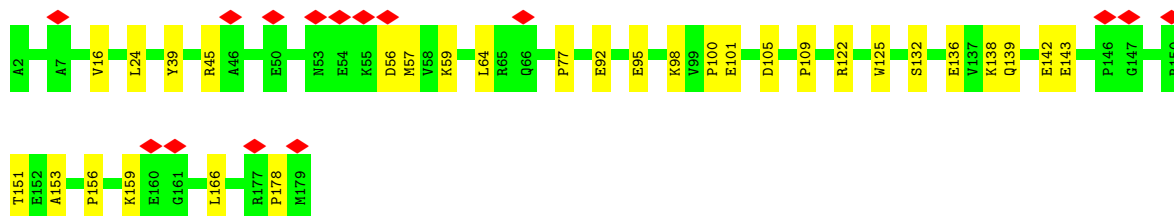
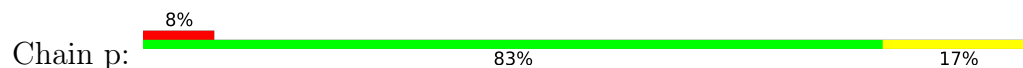




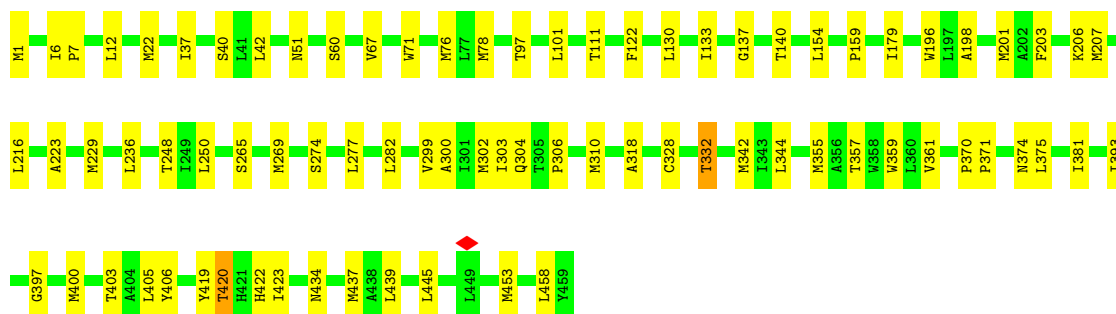
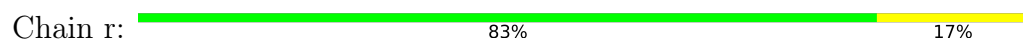
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



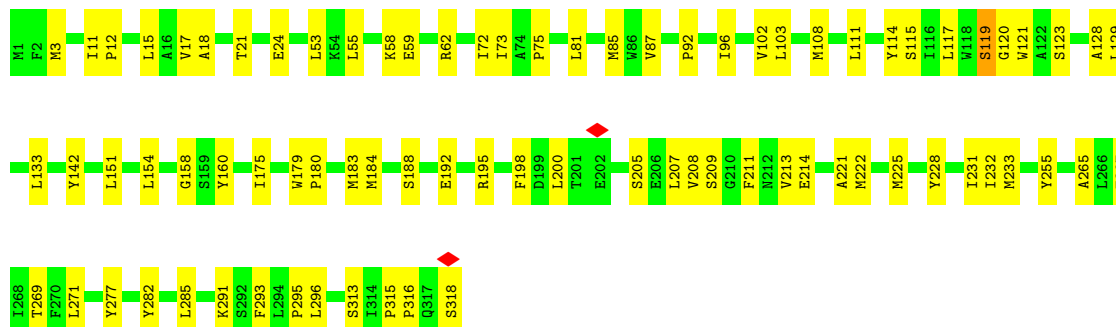
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



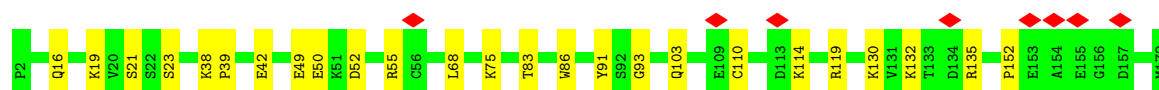
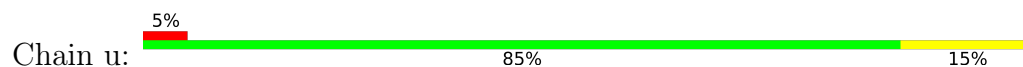
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



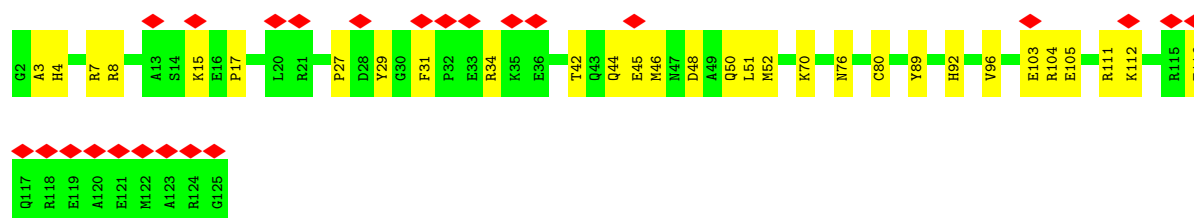
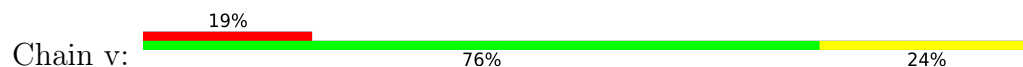
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



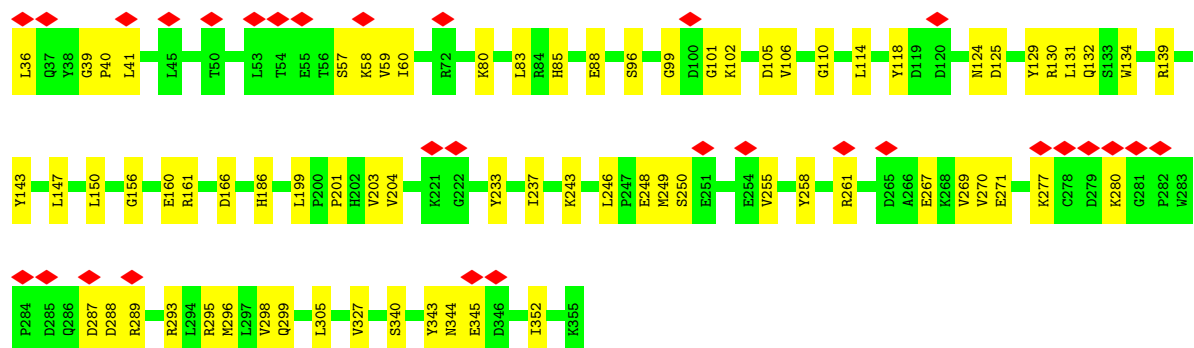
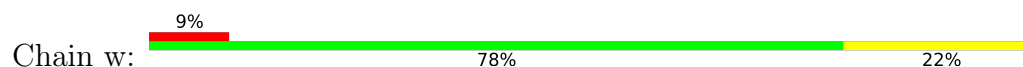
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: Complex I-B18



- 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	63357	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	0.204	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0336	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ZN, SF4, PEE, PLX, FMN, MG, 8Q1, 970, FES, NDP, UQ, ADP, 2MR, CDL, NAI

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	0.13	0/3406	0.34	0/4603
2	B	0.11	0/1442	0.29	0/1951
3	C	0.12	0/1279	0.32	0/1730
4	E	0.12	0/995	0.28	0/1340
5	F	0.16	0/695	0.44	0/936
6	G	0.14	0/705	0.38	0/956
6	X	0.14	0/705	0.39	0/955
7	H	0.12	0/929	0.33	0/1258
8	I	0.14	0/798	0.38	0/1079
9	J	0.11	0/2828	0.30	0/3834
10	K	0.18	0/377	0.42	0/509
11	L	0.11	0/1039	0.30	0/1403
12	M	0.11	0/5372	0.31	0/7279
13	N	0.14	0/1241	0.43	2/1690 (0.1%)
14	O	0.13	0/1707	0.35	0/2324
15	P	0.12	0/1789	0.31	0/2436
16	Q	0.15	0/3538	0.34	0/4796
17	S	0.13	0/581	0.35	0/781
18	T	0.10	0/755	0.28	0/1018
19	U	0.11	0/664	0.30	0/912
20	V	0.11	0/1042	0.26	0/1411
21	W	0.15	0/1192	0.35	0/1610
22	Y	0.12	0/610	0.31	0/836
23	Z	0.14	0/660	0.37	0/892
24	a	0.12	0/1184	0.29	0/1603
25	b	0.14	0/844	0.38	0/1149
26	c	0.15	0/1371	0.38	0/1875
27	d	0.11	0/1494	0.29	0/2015
28	e	0.14	0/880	0.38	0/1196
29	f	0.10	0/385	0.27	0/522
30	g	0.11	0/1036	0.26	0/1401
31	h	0.11	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.16	0/2773	0.39	1/3768 (0.0%)
33	j	0.12	0/938	0.31	0/1281
34	k	0.13	0/759	0.34	0/1029
35	l	0.14	0/4926	0.35	0/6700
36	m	0.21	0/1307	0.46	0/1777
37	n	0.13	0/491	0.29	0/663
38	o	0.12	0/1092	0.28	0/1481
39	p	0.12	0/1586	0.31	1/2151 (0.0%)
40	r	0.12	0/3715	0.29	0/5067
41	s	0.16	0/2581	0.37	0/3529
42	u	0.14	0/1436	0.35	0/1938
43	v	0.15	0/1060	0.35	0/1421
44	w	0.10	0/2646	0.30	0/3584
All	All	0.13	0/67742	0.34	4/91879 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	138	VAL	CA-C-N	7.18	124.83	119.66
13	N	138	VAL	C-N-CA	7.18	124.83	119.66
39	p	109	PRO	CA-N-CD	-5.89	103.75	112.00
32	i	48	PHE	N-CA-C	5.02	116.91	108.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	87	0
2	B	1411	0	1360	25	0
3	C	1248	0	1254	25	0
4	E	971	0	975	14	0
5	F	684	0	698	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	693	0	671	20	0
6	X	693	0	678	19	0
7	H	910	0	950	17	0
8	I	780	0	808	15	0
9	J	2751	0	2773	40	0
10	K	366	0	338	12	0
11	L	1016	0	1016	16	0
12	M	5284	0	5311	68	0
13	N	1200	0	1151	24	0
14	O	1667	0	1662	33	0
15	P	1738	0	1693	23	0
16	Q	3459	0	3396	80	0
17	S	566	0	561	9	0
18	T	741	0	702	6	0
19	U	643	0	642	14	0
20	V	1021	0	1025	18	0
21	W	1161	0	1144	25	0
22	Y	584	0	529	11	0
23	Z	641	0	620	12	0
24	a	1151	0	1164	22	0
25	b	819	0	835	14	0
26	c	1315	0	1208	18	0
27	d	1461	0	1429	21	0
28	e	856	0	807	16	0
29	f	377	0	353	5	0
30	g	1005	0	999	15	0
31	h	867	0	871	17	0
32	i	2710	0	2874	62	0
33	j	914	0	951	27	0
34	k	748	0	799	20	0
35	l	4797	0	4935	113	0
36	m	1276	0	1243	47	0
37	n	479	0	486	13	0
38	o	1062	0	1072	14	0
39	p	1530	0	1459	21	0
40	r	3624	0	3832	56	0
41	s	2508	0	2607	64	0
42	u	1398	0	1374	20	0
43	v	1036	0	992	22	0
44	w	2586	0	2542	49	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	4	0
47	A	44	0	27	4	0
48	B	51	0	82	4	0
48	C	47	0	71	3	0
48	U	51	0	82	4	0
48	W	41	0	59	1	0
48	i	47	0	71	0	0
48	j	41	0	59	3	0
48	l	96	0	146	7	0
48	r	51	0	82	6	0
49	C	52	0	88	2	0
49	J	52	0	88	5	0
49	a	52	0	88	1	0
49	g	52	0	88	3	0
49	j	52	0	88	3	0
49	r	104	0	176	10	0
50	C	29	0	0	0	0
51	G	35	0	0	0	0
51	X	35	0	0	0	0
52	I	51	0	46	1	0
52	V	172	0	244	11	0
52	a	100	0	156	8	0
52	g	55	0	54	1	0
52	i	199	0	307	14	0
52	l	199	0	307	17	0
52	o	100	0	156	8	0
52	s	89	0	125	12	0
53	J	48	0	25	3	0
54	J	33	0	39	3	0
54	s	38	0	47	3	0
55	M	4	0	0	0	0
55	O	4	0	0	0	0
56	M	1	0	0	0	0
57	T	1	0	0	0	0
58	w	27	0	11	3	0
All	All	68209	0	68912	1138	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 1138 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)
53:J:401:NDP:O4D	53:J:401:NDP:C4D	1.68	1.20
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.17
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.02	1.14
36:m:64:MET:HE2	36:m:64:MET:HA	1.32	1.10
1:A:89:GLY:HA2	1:A:244:ASN:ND2	1.67	1.07

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%)	418 (97%)	13 (3%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	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%)	104 (94%)	5 (4%)	1 (1%)	14	48
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	340/342 (99%)	330 (97%)	9 (3%)	1 (0%)	36	70
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	672 (98%)	16 (2%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	427/430 (99%)	411 (96%)	16 (4%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	94 (100%)	0	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	89 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	604/606 (100%)	588 (97%)	16 (3%)	0	100	100
36	m	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	454 (99%)	3 (1%)	0	100	100
41	s	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	36	70
42	u	169/171 (99%)	166 (98%)	2 (1%)	1 (1%)	21	56
43	v	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8175/8313 (98%)	7919 (97%)	252 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
7	H	77	ILE
41	s	208	VAL
42	u	152	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	340 (98%)	6 (2%)	53	78
2	B	150/151 (99%)	148 (99%)	2 (1%)	61	81
3	C	132/132 (100%)	128 (97%)	4 (3%)	36	69
4	E	107/107 (100%)	105 (98%)	2 (2%)	50	76
5	F	74/76 (97%)	74 (100%)	0	100	100
6	G	76/81 (94%)	73 (96%)	3 (4%)	28	62
6	X	76/81 (94%)	71 (93%)	5 (7%)	15	46
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	84
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	83
9	J	296/296 (100%)	294 (99%)	2 (1%)	76	86
10	K	42/42 (100%)	39 (93%)	3 (7%)	13	43
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	85
12	M	576/580 (99%)	568 (99%)	8 (1%)	59	80
13	N	129/130 (99%)	125 (97%)	4 (3%)	35	68
14	O	182/183 (100%)	179 (98%)	3 (2%)	55	79
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	89
16	Q	370/370 (100%)	360 (97%)	10 (3%)	39	71
17	S	57/58 (98%)	56 (98%)	1 (2%)	51	77
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	81
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	98 (97%)	3 (3%)	36	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	W	121/123 (98%)	120 (99%)	1 (1%)	73	86
22	Y	62/62 (100%)	61 (98%)	1 (2%)	55	79
23	Z	62/62 (100%)	61 (98%)	1 (2%)	55	79
24	a	121/121 (100%)	119 (98%)	2 (2%)	53	78
25	b	90/119 (76%)	86 (96%)	4 (4%)	25	60
26	c	141/141 (100%)	138 (98%)	3 (2%)	47	75
27	d	155/155 (100%)	153 (99%)	2 (1%)	61	81
28	e	93/96 (97%)	91 (98%)	2 (2%)	45	74
29	f	35/45 (78%)	34 (97%)	1 (3%)	37	70
30	g	108/109 (99%)	105 (97%)	3 (3%)	38	70
31	h	93/93 (100%)	92 (99%)	1 (1%)	65	83
32	i	311/311 (100%)	307 (99%)	4 (1%)	61	81
33	j	100/100 (100%)	97 (97%)	3 (3%)	36	69
34	k	85/85 (100%)	83 (98%)	2 (2%)	43	73
35	l	536/540 (99%)	529 (99%)	7 (1%)	61	81
36	m	127/141 (90%)	124 (98%)	3 (2%)	43	73
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	110 (97%)	3 (3%)	39	71
39	p	158/159 (99%)	157 (99%)	1 (1%)	78	88
40	r	409/410 (100%)	400 (98%)	9 (2%)	45	74
41	s	275/275 (100%)	272 (99%)	3 (1%)	65	83
42	u	153/153 (100%)	150 (98%)	3 (2%)	48	76
43	v	106/111 (96%)	106 (100%)	0	100	100
44	w	282/283 (100%)	281 (100%)	1 (0%)	84	90
All	All	7140/7241 (99%)	7019 (98%)	121 (2%)	52	78

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	X	74	LEU
40	r	274	SER
26	c	113	ILE
40	r	248	THR
42	u	42	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
42	u	65	GLN
42	u	163	HIS
22	Y	83	HIS
22	Y	46	GLN
43	v	85	HIS

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	1.99	1 (10%)	5,13,15	5.82	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	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.75	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	11.89	130.38	119.48
16	Q	118	2MR	CD-NE-CZ	4.07	131.03	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.20	130.94	123.86

There are no chirality outliers.

All (2) 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

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 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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	$\# Z > 2$
52	CDL	s	401	-	88,88,99	1.14	9 (10%)	94,100,111	0.91	4 (4%)
52	CDL	o	201	-	99,99,99	1.09	9 (9%)	105,111,111	0.87	4 (3%)
47	NAI	A	503	-	45,48,48	3.91	20 (44%)	60,73,73	1.77	12 (20%)
53	NDP	J	401	-	49,52,52	4.39	23 (46%)	66,80,80	2.24	14 (21%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
55	FES	O	301	14	0,4,4	-	-	-	-	-
49	PLX	J	403	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
54	UQ	s	402	-	38,38,63	3.54	9 (23%)	46,49,79	2.85	16 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
48	PEE	B	303	-	50,50,50	1.17	6 (12%)	53,55,55	0.97	2 (3%)
55	FES	M	803	12	0,4,4	-	-	-		
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.97	2 (4%)
48	PEE	j	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
48	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	0.97	2 (4%)
48	PEE	i	402	-	46,46,50	1.21	6 (13%)	49,51,55	0.97	2 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
52	CDL	V	201	-	93,93,99	1.12	9 (9%)	99,105,111	0.85	4 (4%)
48	PEE	l	703	-	49,49,50	1.17	6 (12%)	52,54,55	0.95	2 (3%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
52	CDL	i	401	-	99,99,99	1.10	9 (9%)	105,111,111	0.84	4 (3%)
52	CDL	I	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.12	4 (7%)
58	ADP	w	401	-	27,29,29	2.97	8 (29%)	42,45,45	2.02	10 (23%)
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.22	7 (14%)
54	UQ	J	402	-	33,33,63	3.47	8 (24%)	40,43,79	2.70	14 (35%)
52	CDL	V	202	-	77,77,99	1.20	7 (9%)	83,89,111	0.97	4 (4%)
48	PEE	U	101	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
45	SF4	A	501	1	0,12,12	-	-	-		
51	8Q1	X	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.52	4 (10%)
49	PLX	r	502	-	51,51,51	1.16	5 (9%)	55,59,59	0.59	1 (1%)
52	CDL	i	403	-	98,98,99	1.10	9 (9%)	104,110,111	0.86	4 (3%)
52	CDL	l	702	-	99,99,99	1.09	9 (9%)	105,111,111	0.89	4 (3%)
45	SF4	M	802	12	0,12,12	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
51	8Q1	G	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.55	6 (15%)
52	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.84	4 (3%)
52	CDL	g	202	-	54,54,99	1.37	8 (14%)	60,66,111	1.13	4 (6%)
52	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
49	PLX	r	503	-	51,51,51	1.15	4 (7%)	55,59,59	0.55	1 (1%)
49	PLX	g	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
50	970	C	304	-	33,33,33	4.92	16 (48%)	48,50,50	2.53	18 (37%)
49	PLX	C	303	-	51,51,51	1.16	4 (7%)	55,59,59	0.60	1 (1%)

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
52	CDL	s	401	-	-	50/99/99/110	-
52	CDL	o	201	-	-	56/110/110/110	-
47	NAI	A	503	-	-	10/29/72/72	0/5/5/5
53	NDP	J	401	-	-	9/34/77/77	0/4/5/5
48	PEE	l	704	-	-	20/49/49/54	-
55	FES	O	301	14	-	-	0/1/1/1
49	PLX	J	403	-	-	29/55/55/55	-
54	UQ	s	402	-	-	12/33/57/87	0/1/1/1
49	PLX	a	202	-	-	32/55/55/55	-
48	PEE	B	303	-	-	26/54/54/54	-
55	FES	M	803	12	-	-	0/1/1/1
48	PEE	C	302	-	-	29/50/50/54	-
48	PEE	j	201	-	-	24/44/44/54	-
48	PEE	W	201	-	-	20/44/44/54	-
48	PEE	i	402	-	-	29/50/50/54	-
45	SF4	B	302	2	-	-	0/6/5/5
52	CDL	V	201	-	-	55/104/104/110	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	l	703	-	-	27/53/53/54	-
48	PEE	r	501	-	-	32/54/54/54	-
52	CDL	i	401	-	-	56/110/110/110	-
52	CDL	I	201	-	-	32/61/61/110	-
58	ADP	w	401	-	-	3/16/32/32	0/3/3/3
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
54	UQ	J	402	-	-	10/27/51/87	0/1/1/1
52	CDL	V	202	-	-	51/88/88/110	-
48	PEE	U	101	-	-	22/54/54/54	-
45	SF4	A	501	1	-	-	0/6/5/5
51	8Q1	X	201	-	-	16/41/41/41	-
49	PLX	r	502	-	-	32/55/55/55	-
52	CDL	i	403	-	-	62/109/109/110	-
52	CDL	l	702	-	-	54/110/110/110	-
45	SF4	M	802	12	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	C	301	3	-	-	0/6/5/5
51	8Q1	G	201	6	-	16/41/41/41	-
52	CDL	a	201	-	-	64/110/110/110	-
52	CDL	g	202	-	-	34/65/65/110	-
45	SF4	M	801	12	-	-	0/6/5/5
52	CDL	l	701	-	-	52/109/109/110	-
49	PLX	j	202	-	-	31/55/55/55	-
49	PLX	r	503	-	-	34/55/55/55	-
49	PLX	g	201	-	-	37/55/55/55	-
50	970	C	304	-	-	2/8/41/41	0/5/5/5
49	PLX	C	303	-	-	23/55/55/55	-

The worst 5 of 272 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	304	970	O16-C17	17.90	1.57	1.37
53	J	401	NDP	C3B-C2B	-12.77	1.24	1.52
53	J	401	NDP	C6N-C5N	12.48	1.55	1.33
50	C	304	970	O25-C24	11.10	1.37	1.22
53	J	401	NDP	O4D-C4D	10.66	1.68	1.45

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	401	NDP	C3N-C2N-N1N	-8.97	110.30	123.10
54	s	402	UQ	C7-C8-C9	-8.13	113.26	126.79
50	C	304	970	O25-C24-C11	-7.98	109.19	121.98
54	J	402	UQ	C7-C8-C9	-7.12	114.94	126.79
50	C	304	970	O08-C07-C06	-6.85	108.82	113.00

There are no chirality outliers.

5 of 1097 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'
47	A	503	NAI	C5B-O5B-PA-O3
48	B	303	PEE	C11-C10-O2-C2
48	B	303	PEE	O4-C10-O2-C2

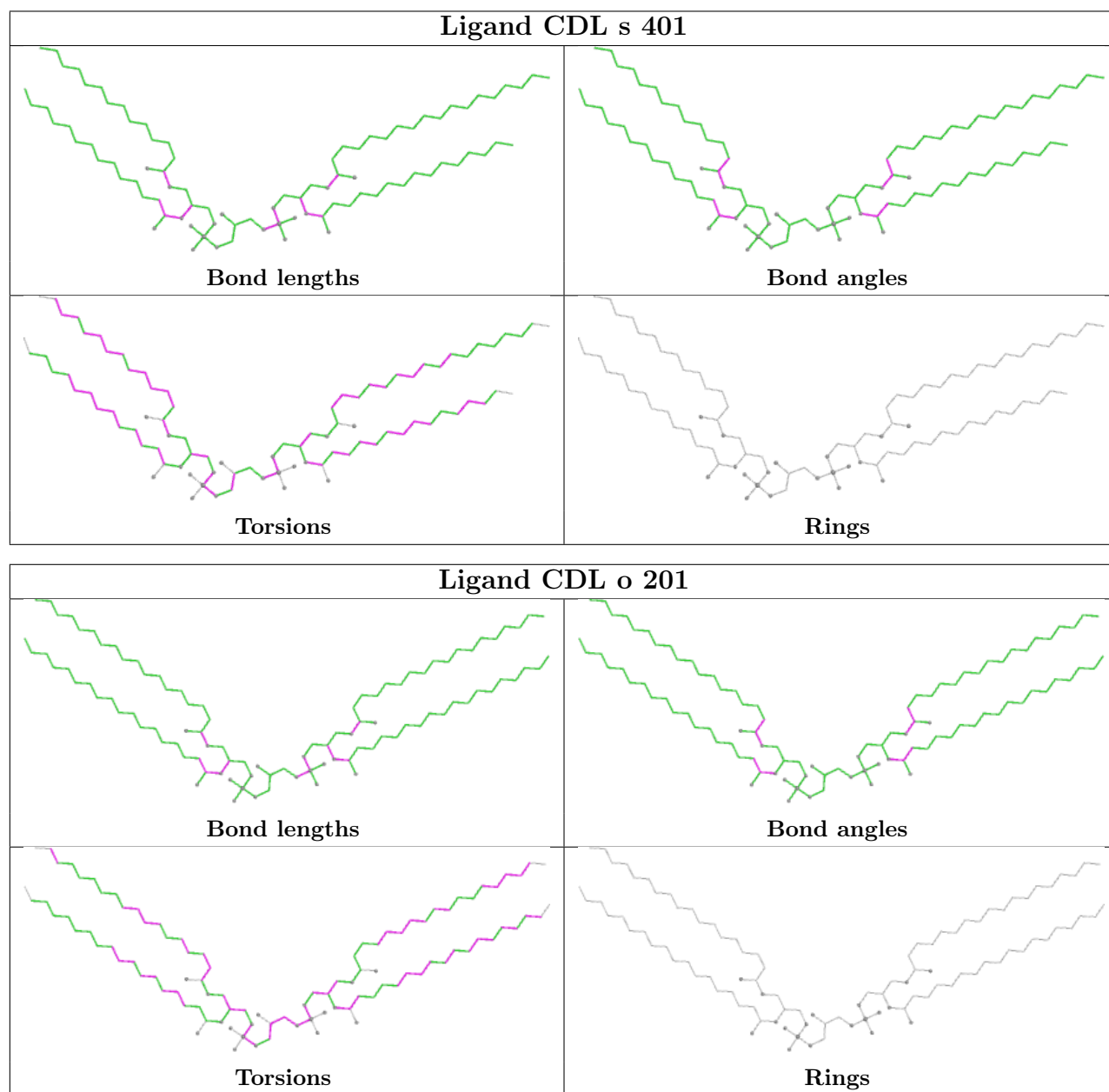
There are no ring outliers.

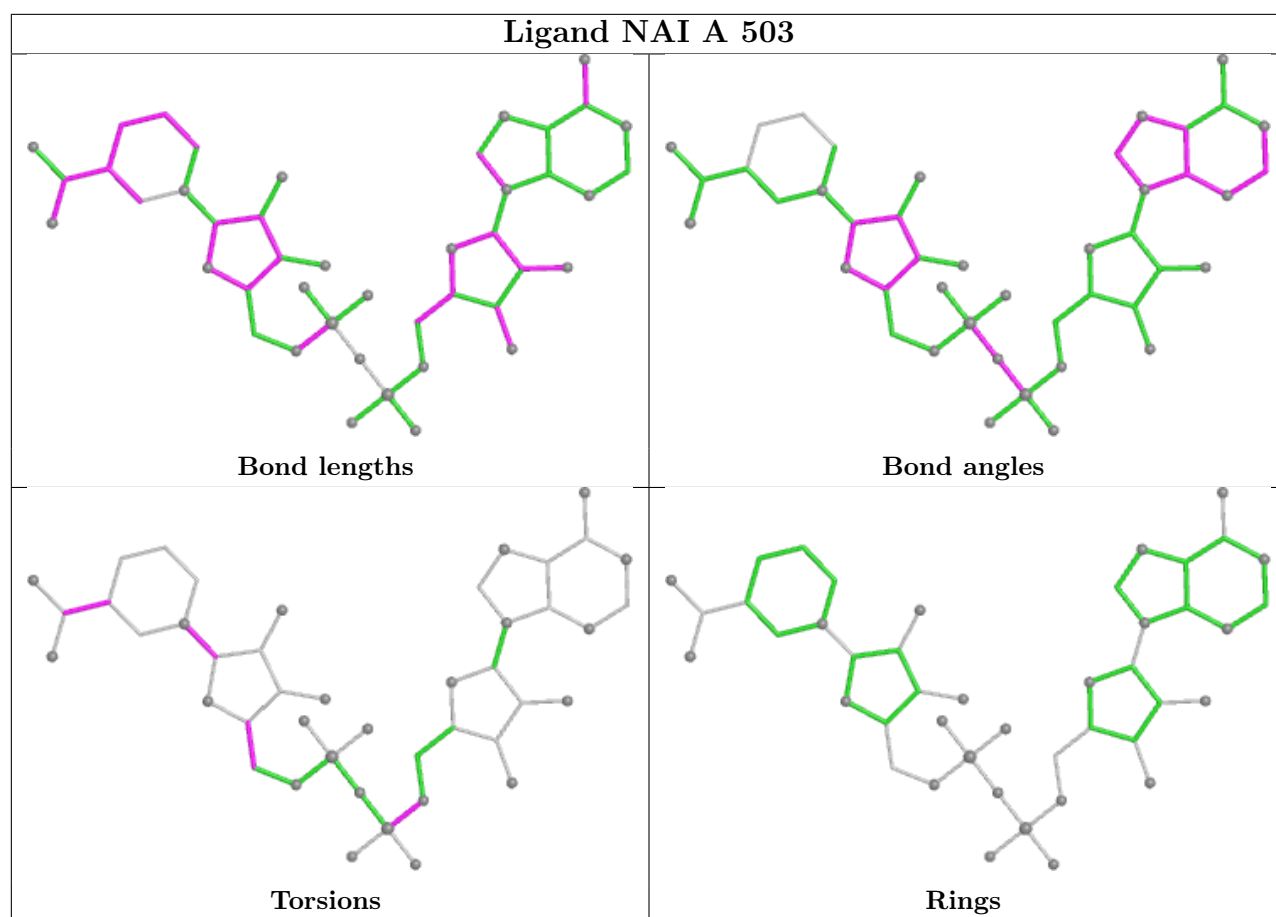
34 monomers are involved in 138 short contacts:

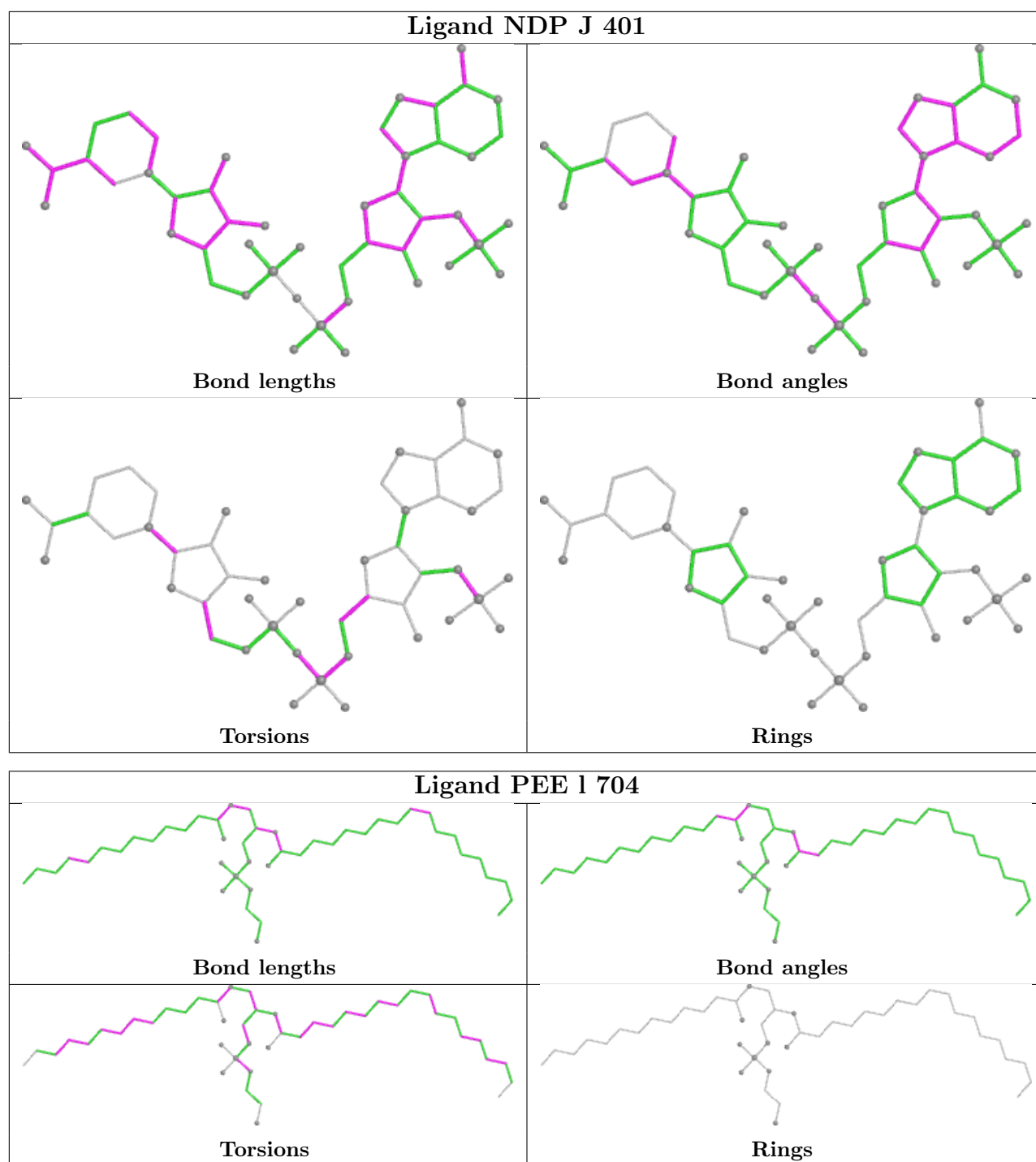
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	s	401	CDL	12	0
52	o	201	CDL	8	0
47	A	503	NAI	4	0
53	J	401	NDP	3	0
48	l	704	PEE	4	0
49	J	403	PLX	5	0
54	s	402	UQ	3	0
49	a	202	PLX	1	0
48	B	303	PEE	4	0
48	C	302	PEE	3	0
48	j	201	PEE	3	0
48	W	201	PEE	1	0
52	V	201	CDL	5	0
48	l	703	PEE	3	0
48	r	501	PEE	6	0
52	i	401	CDL	6	0
52	I	201	CDL	1	0
58	w	401	ADP	3	0
46	A	502	FMN	4	0
54	J	402	UQ	3	0
52	V	202	CDL	6	0
48	U	101	PEE	4	0
45	A	501	SF4	1	0
49	r	502	PLX	6	0
52	i	403	CDL	8	0
52	l	702	CDL	7	0
45	C	301	SF4	1	0
52	a	201	CDL	8	0
52	g	202	CDL	1	0
52	l	701	CDL	10	0
49	j	202	PLX	3	0
49	r	503	PLX	4	0
49	g	201	PLX	3	0
49	C	303	PLX	2	0

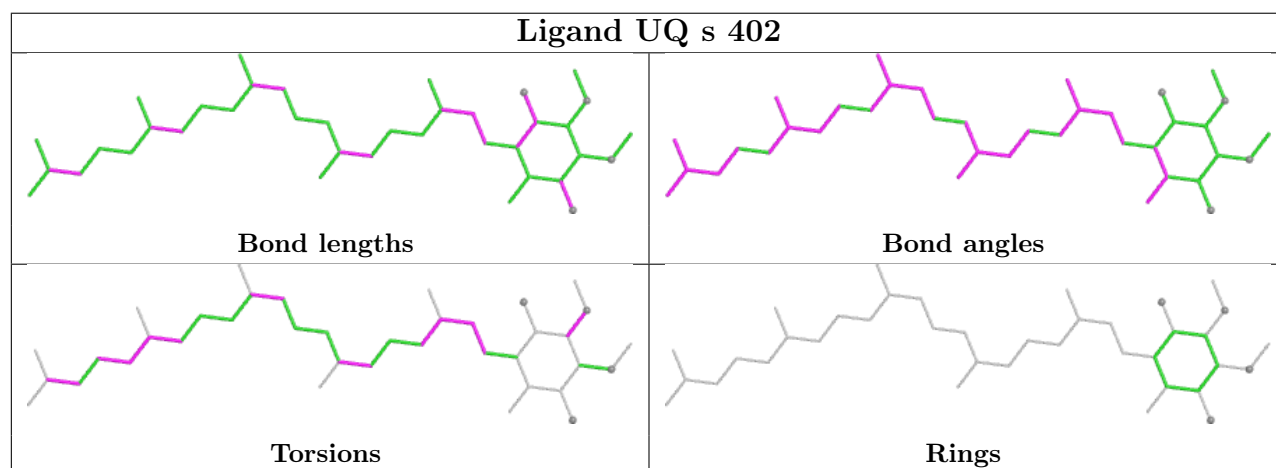
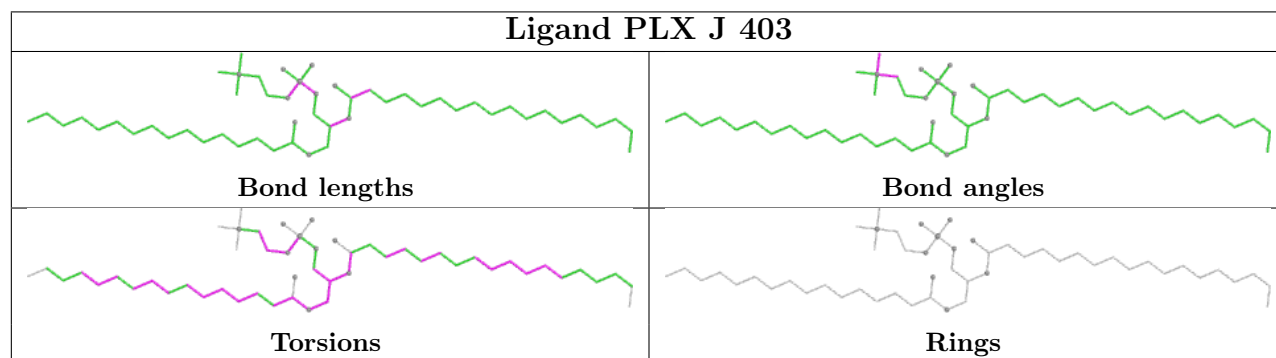
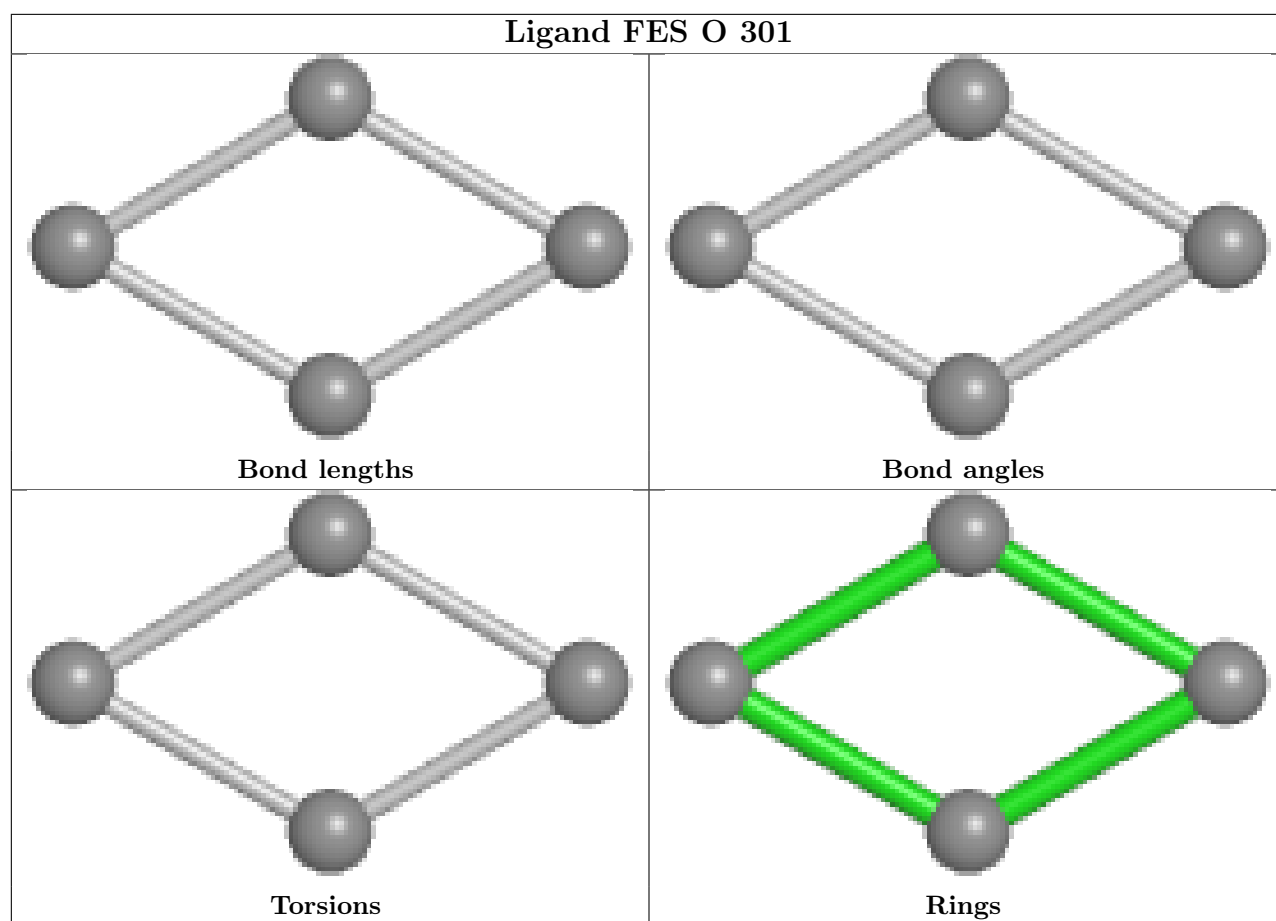
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

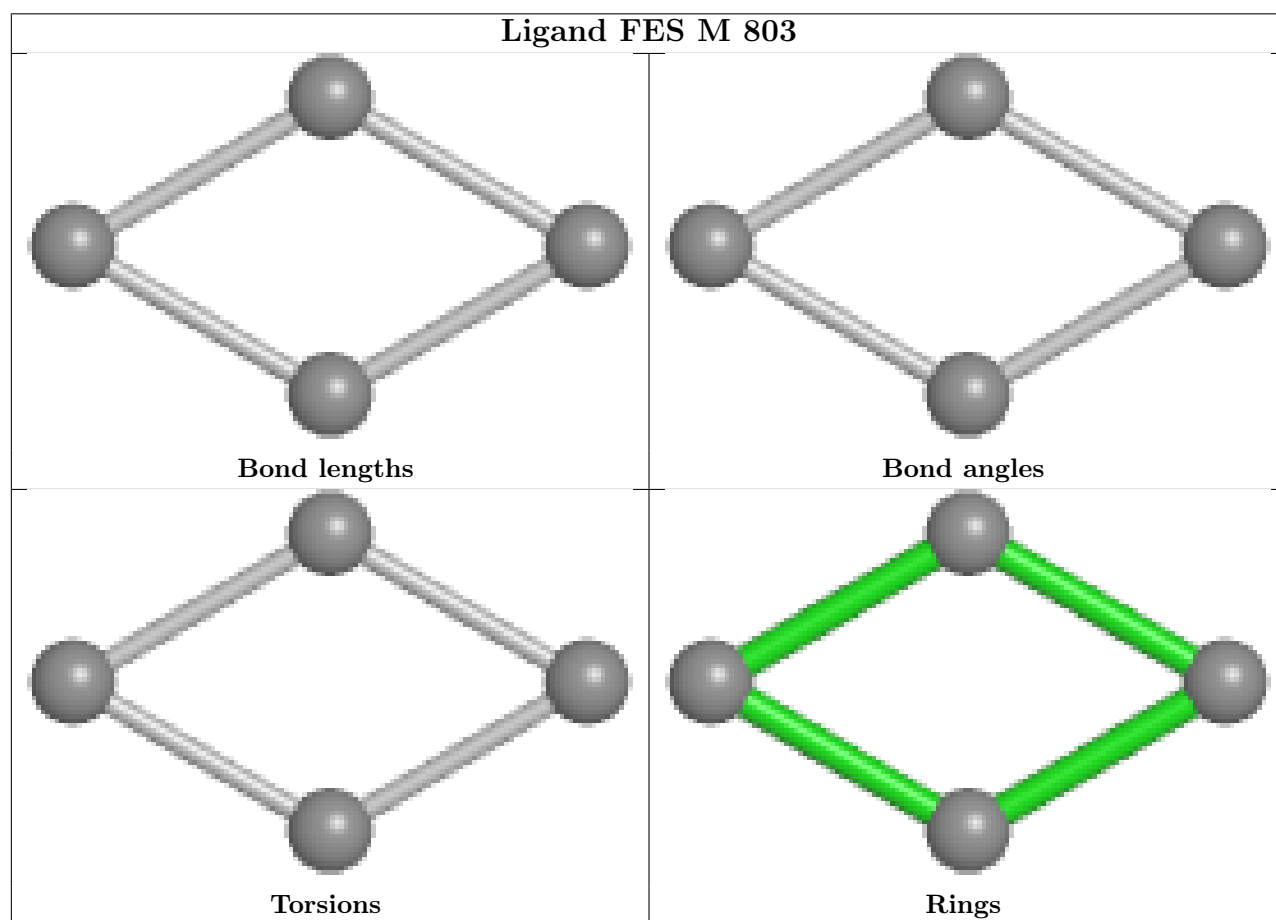
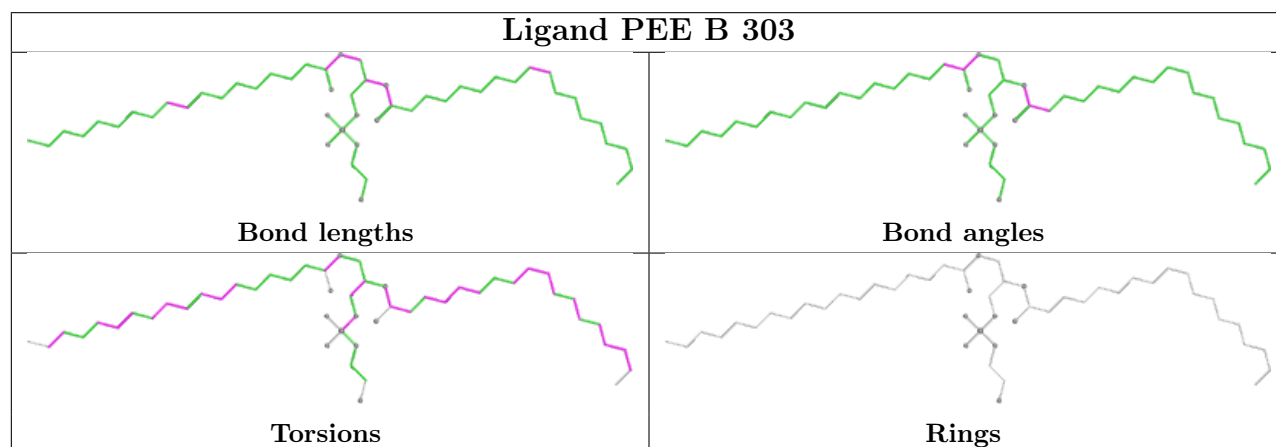
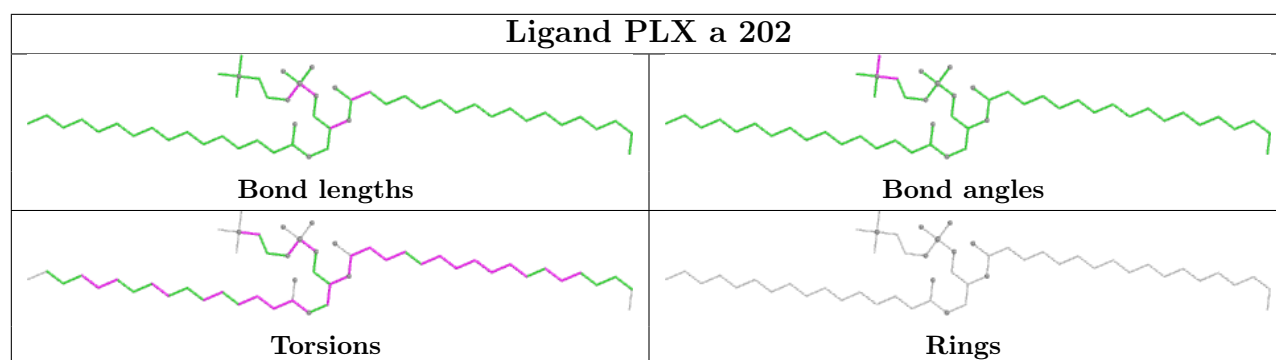
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

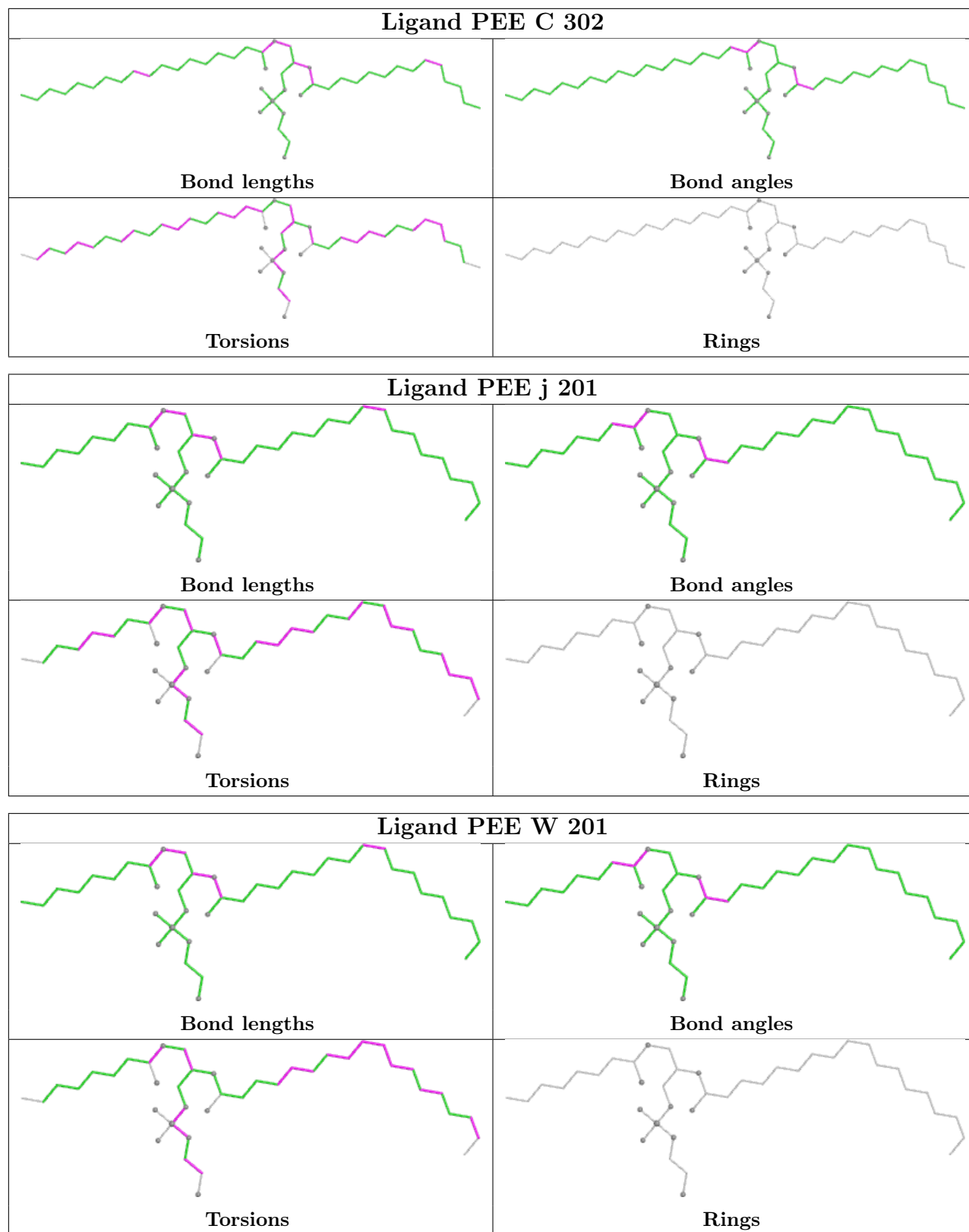


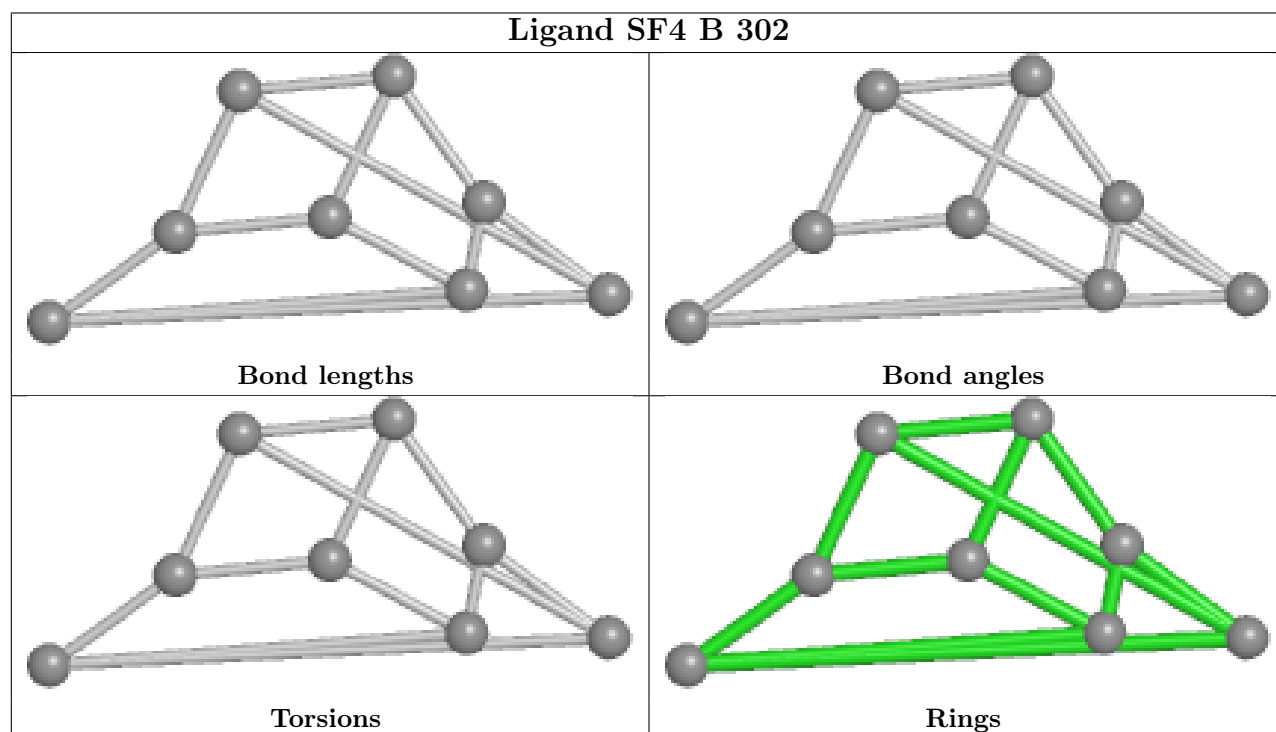
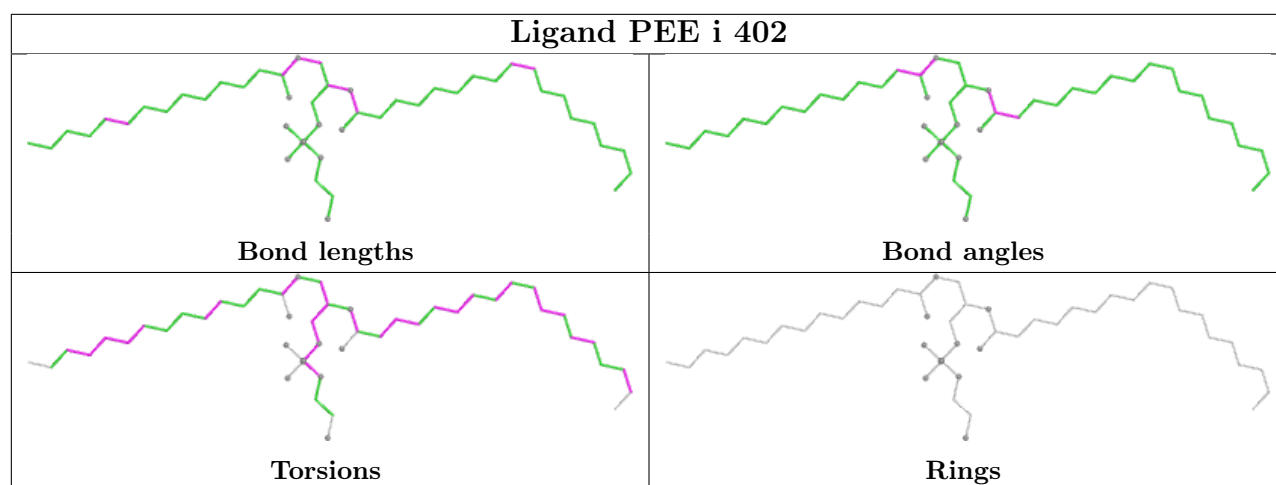


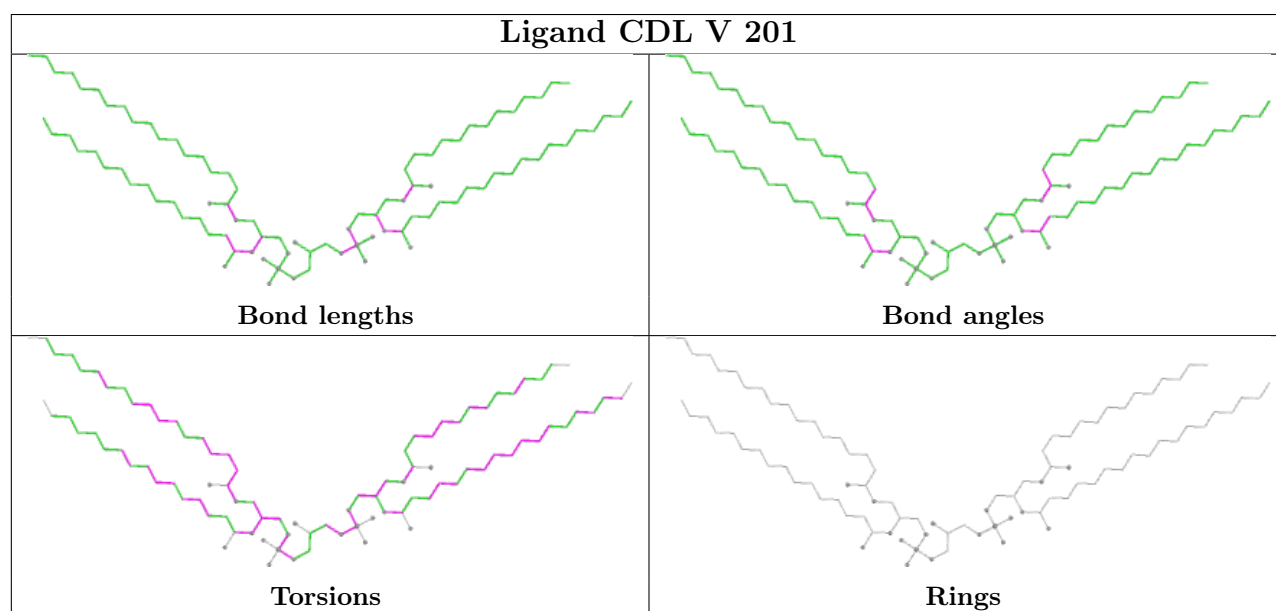
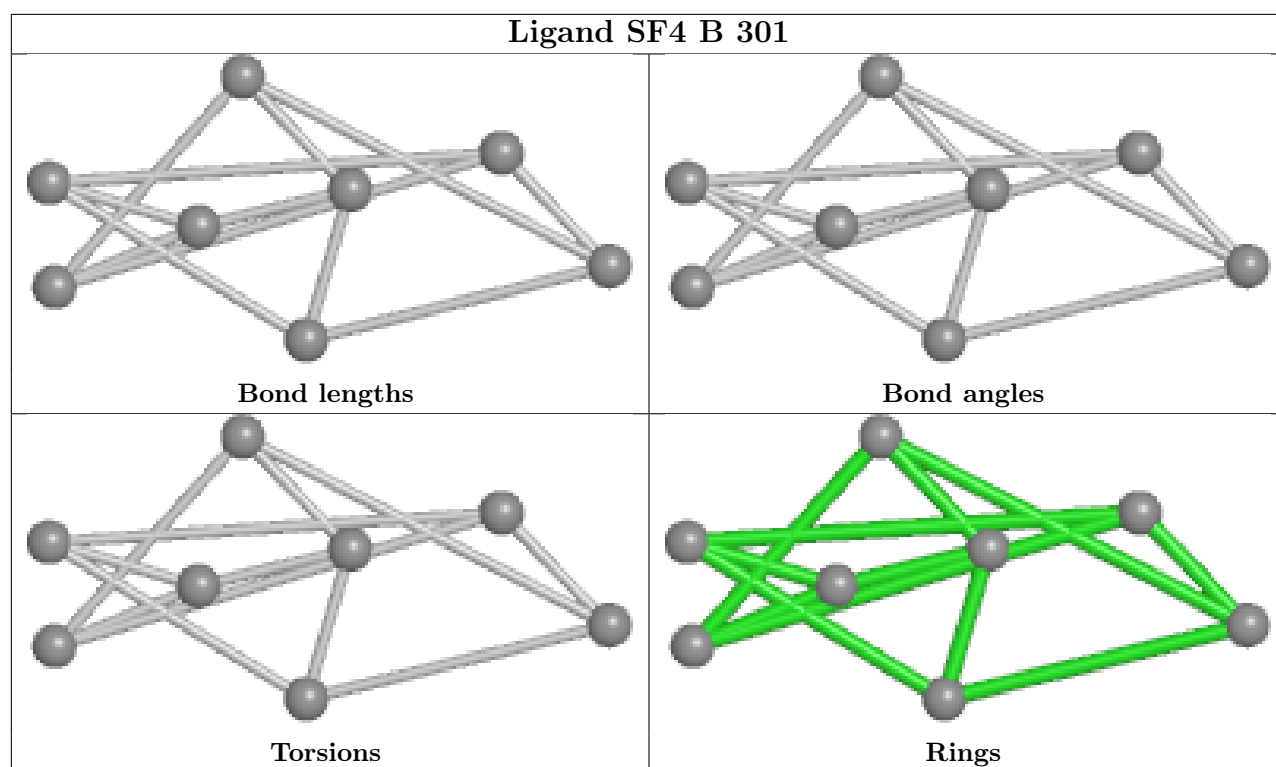


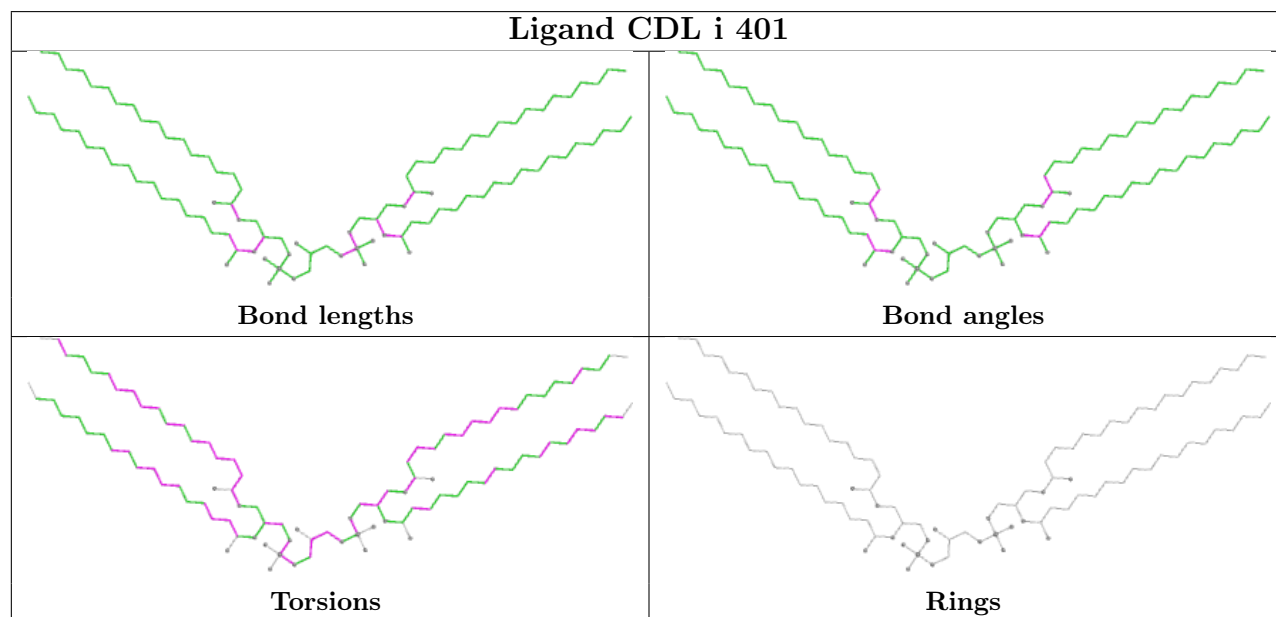
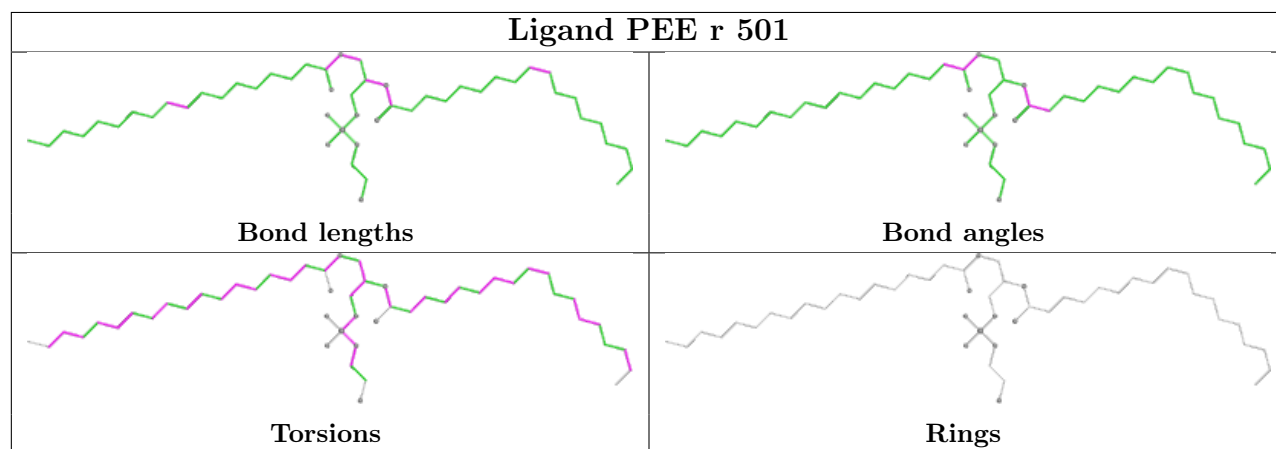
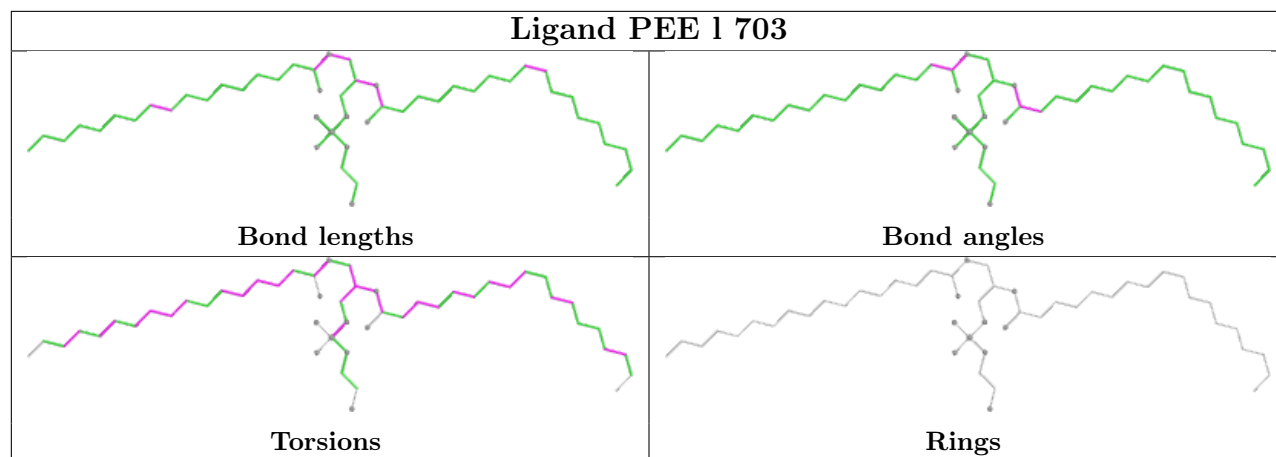


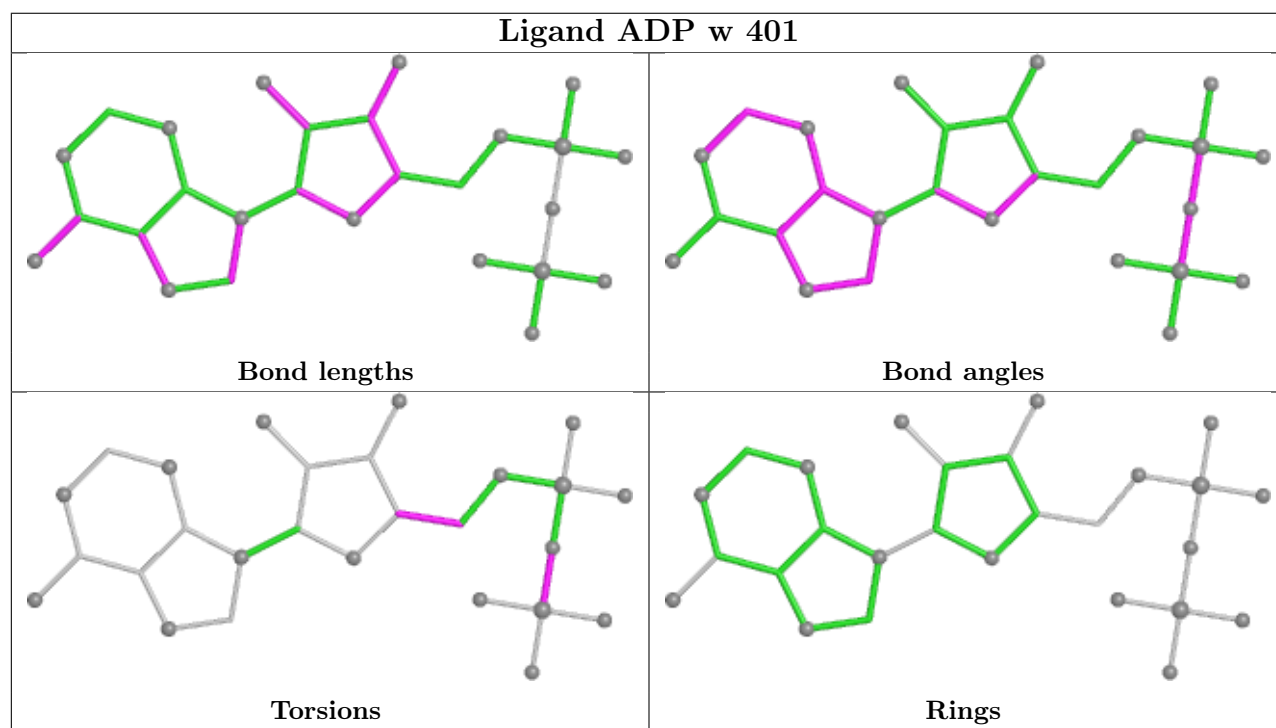
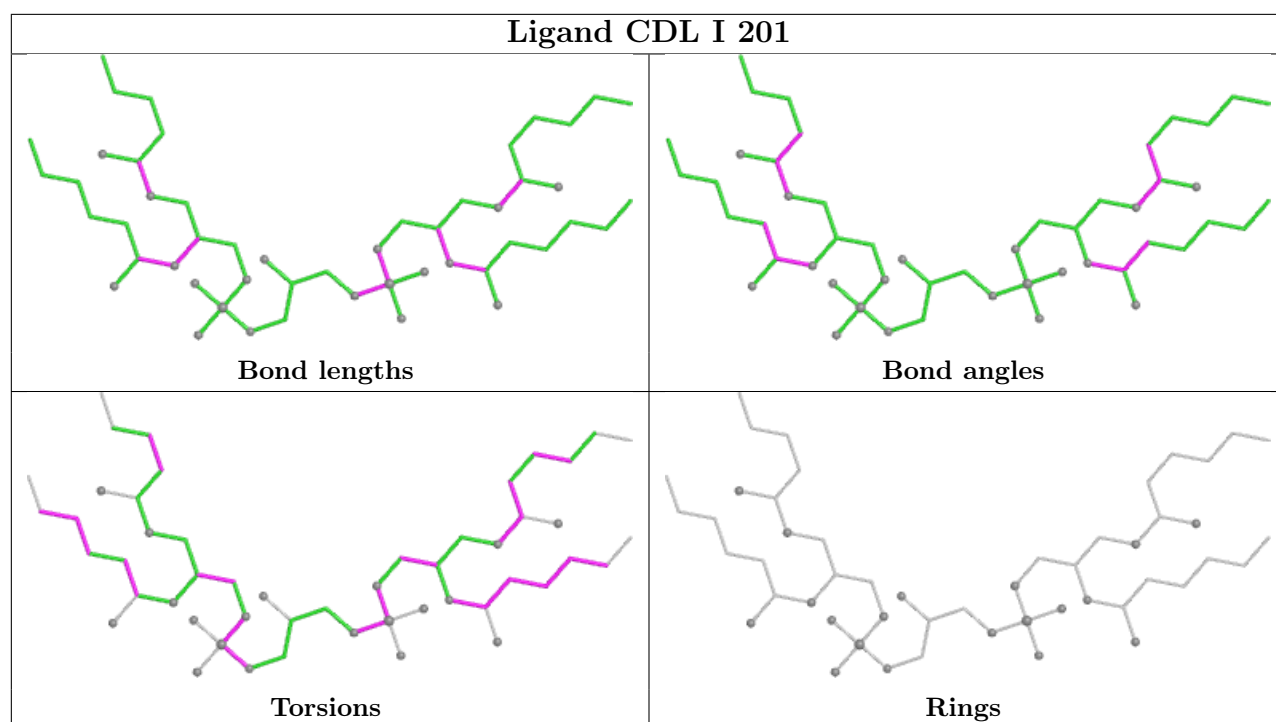


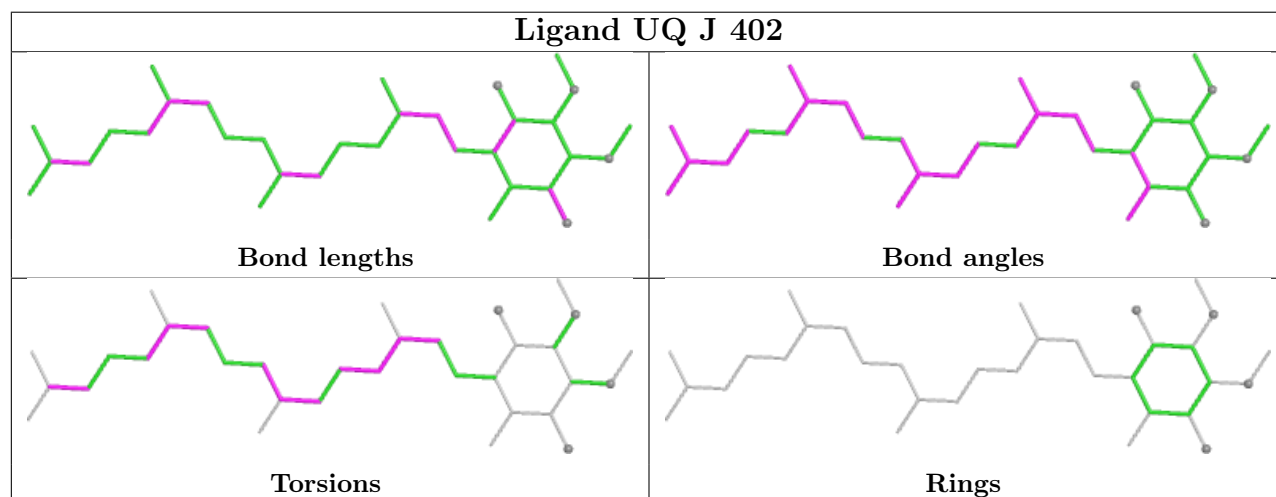
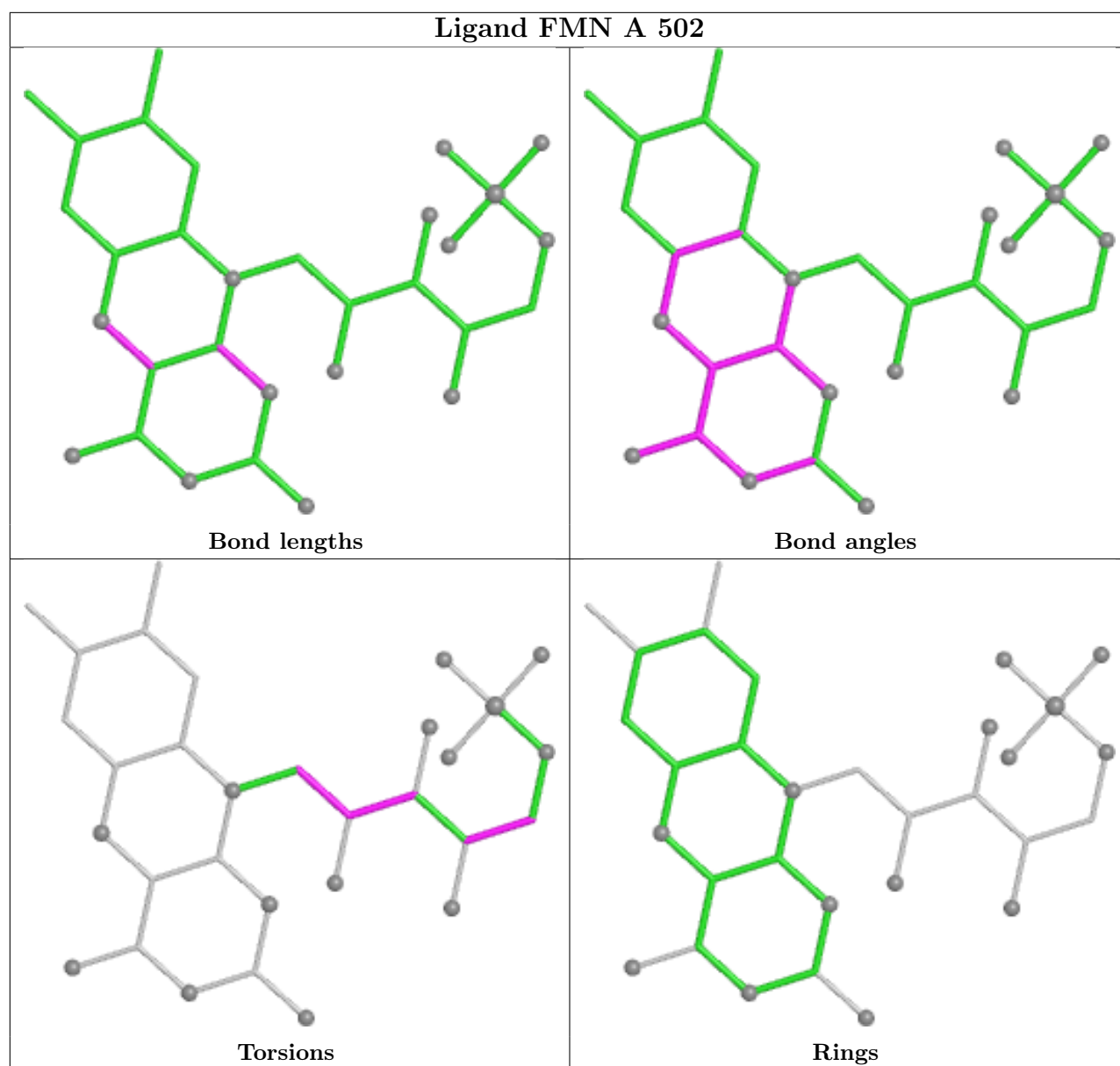


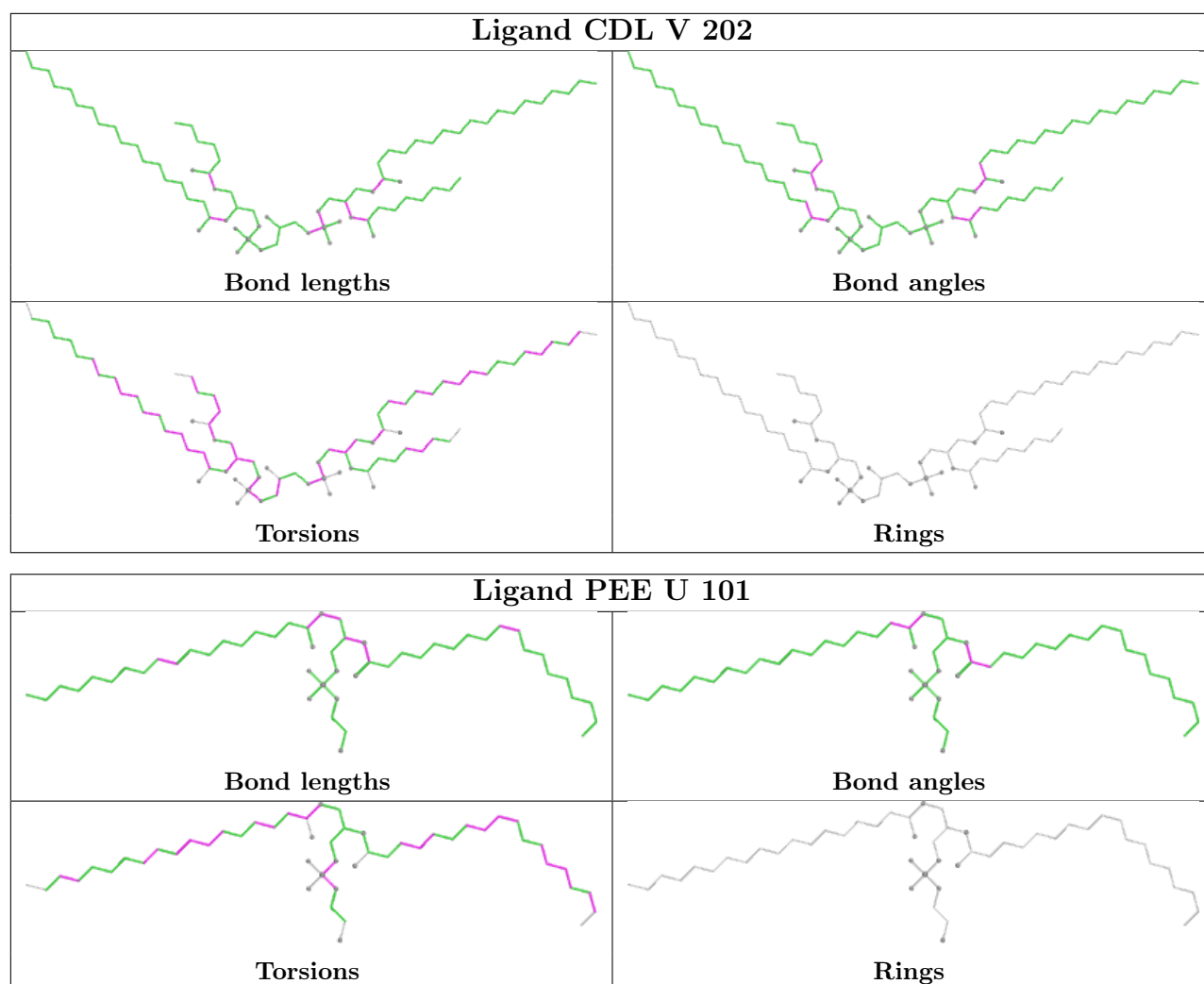


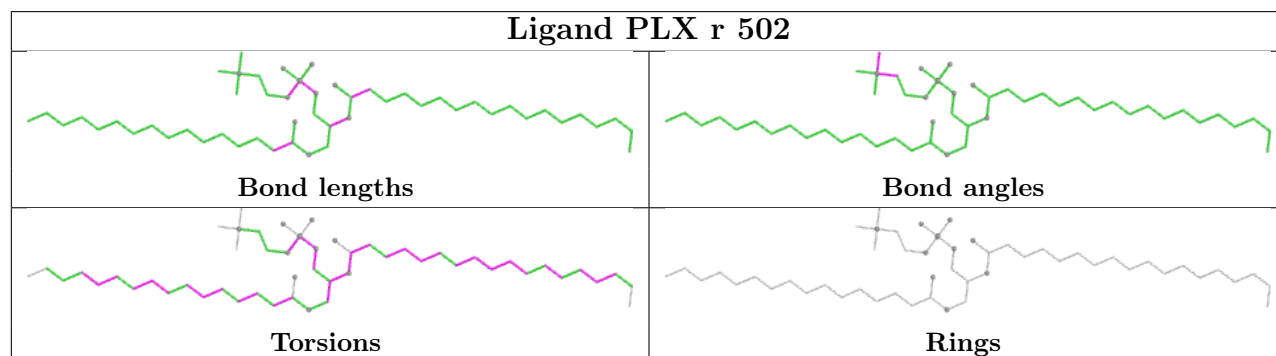
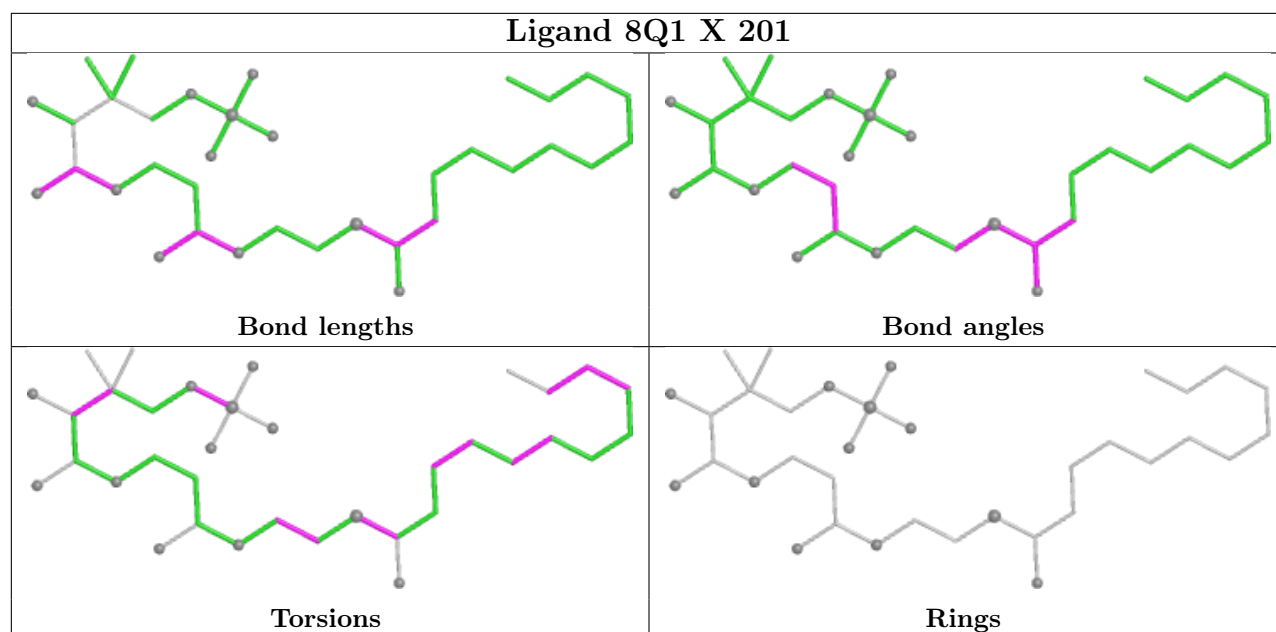
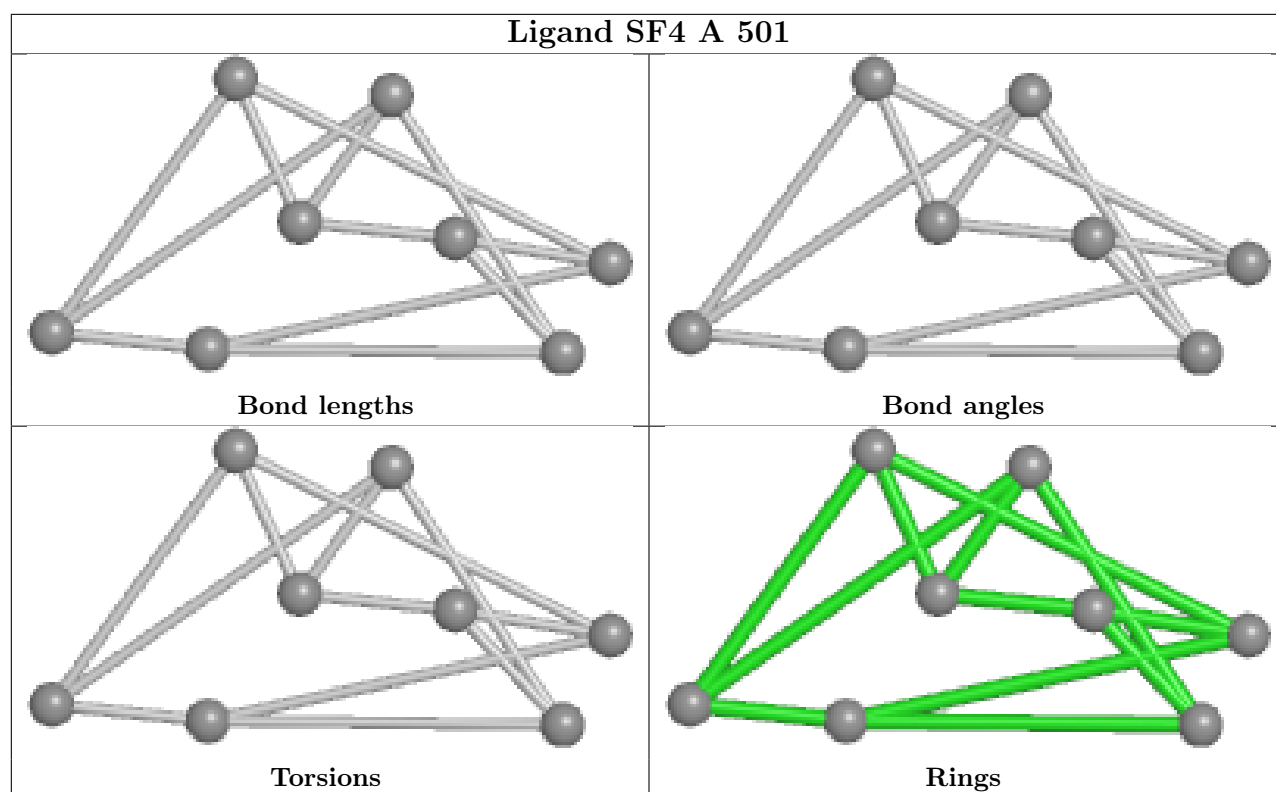


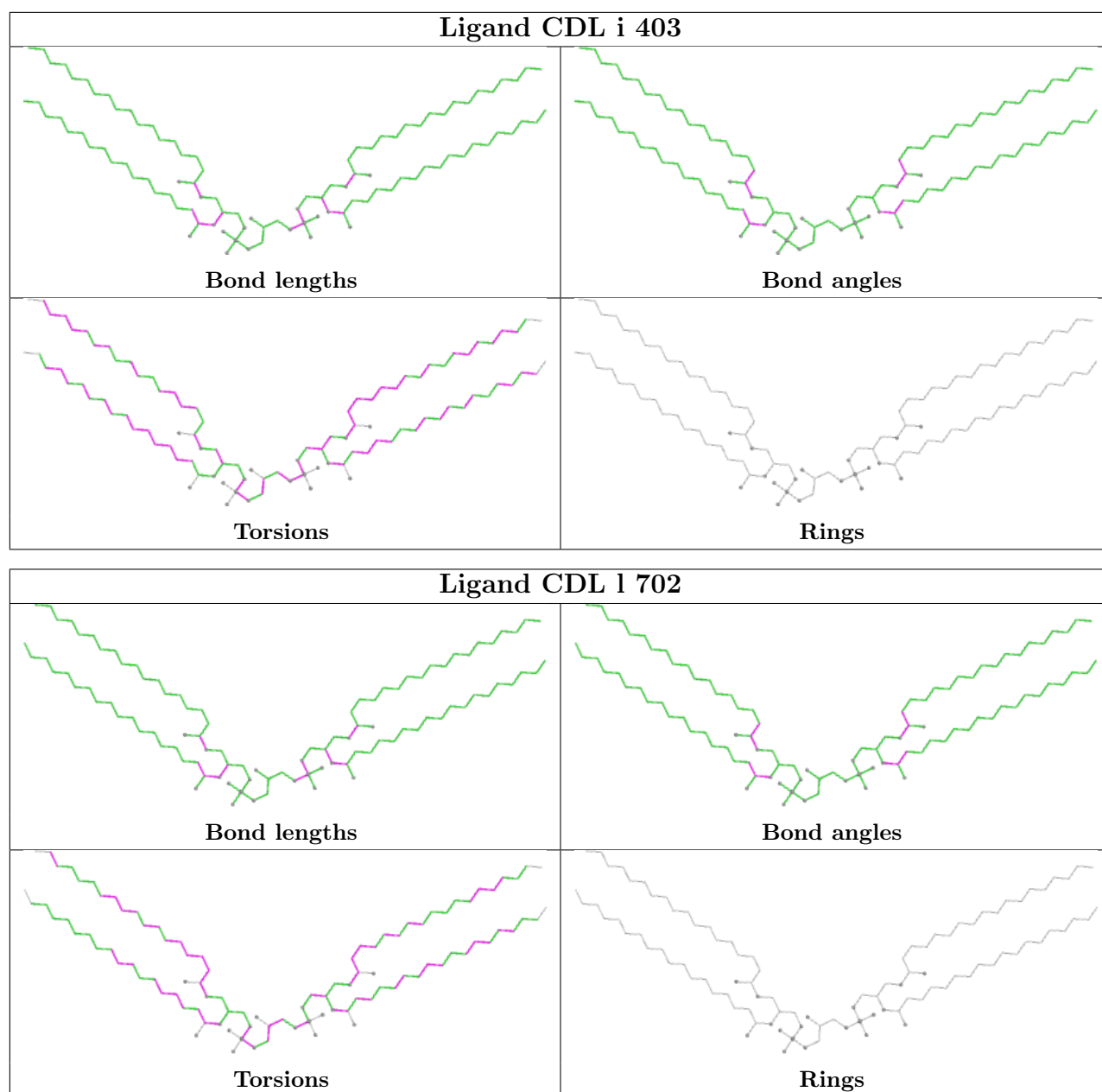




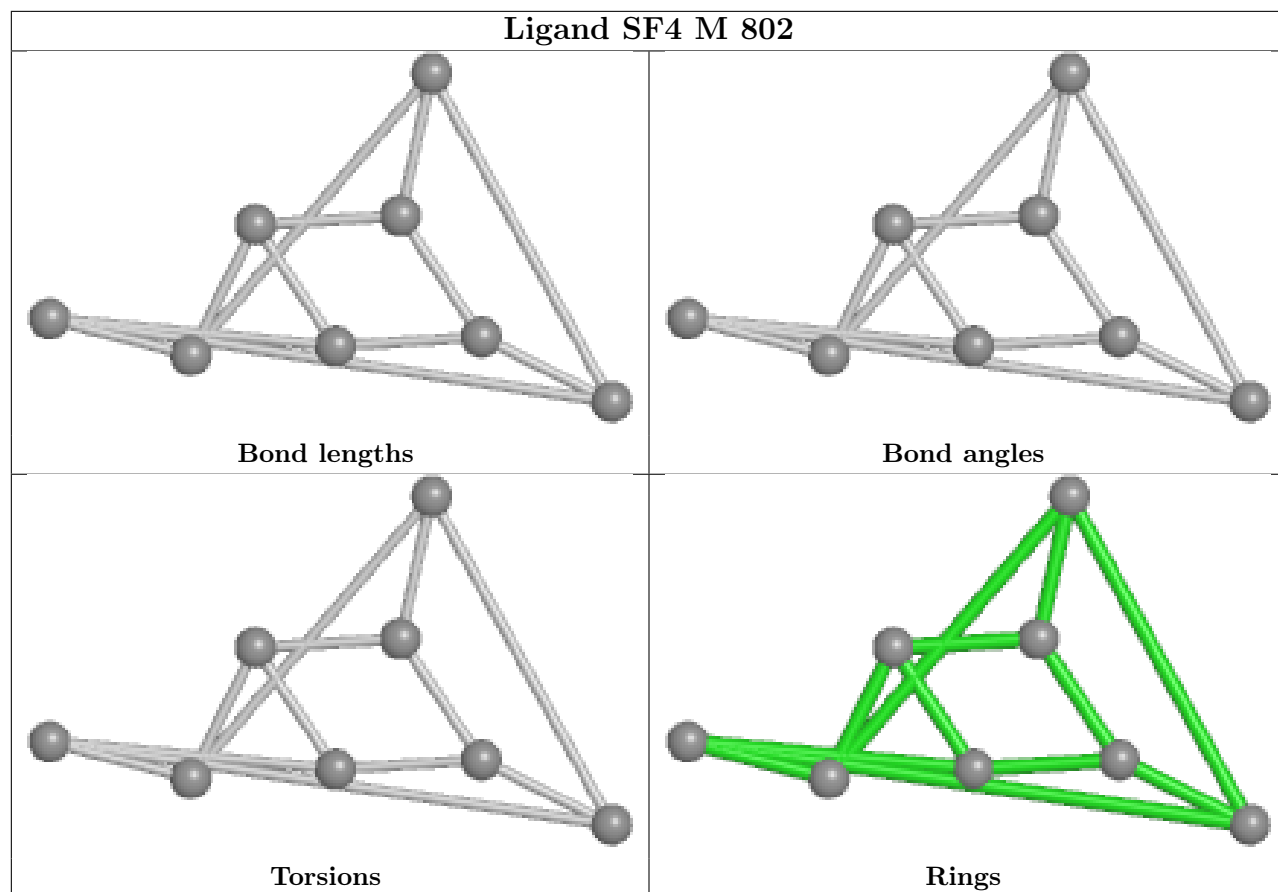




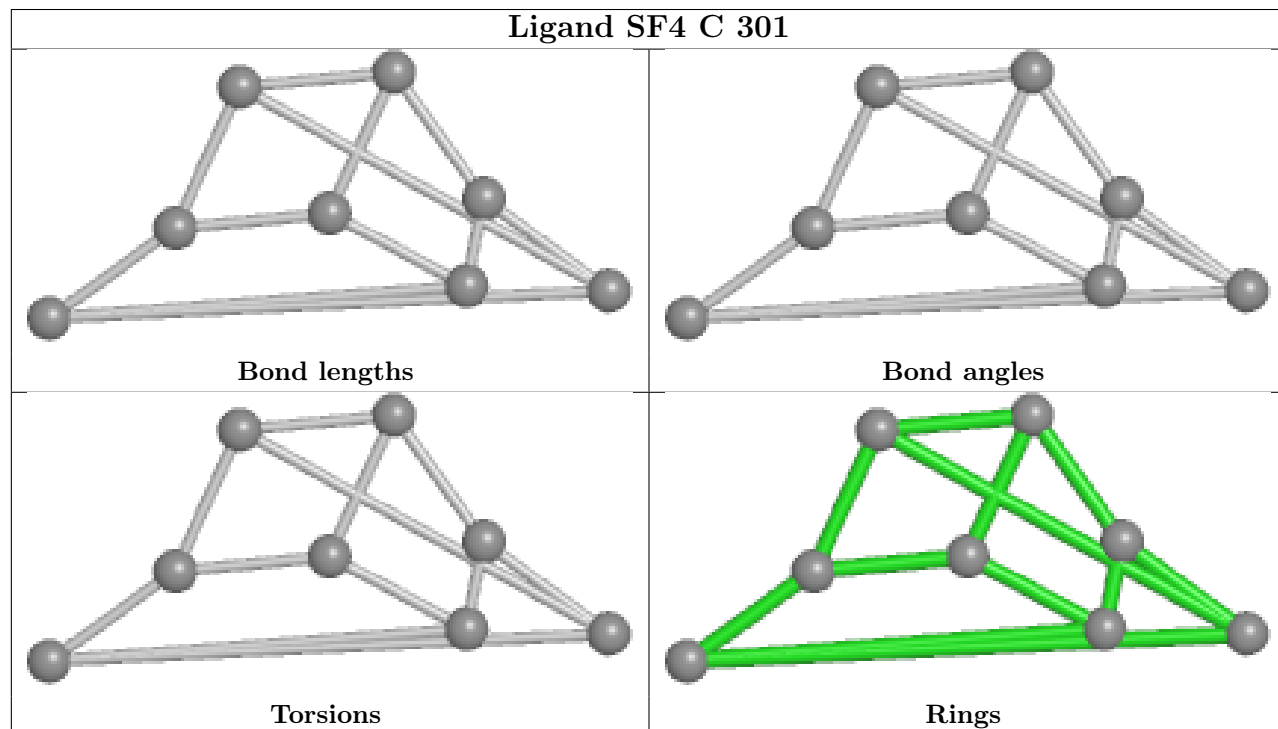


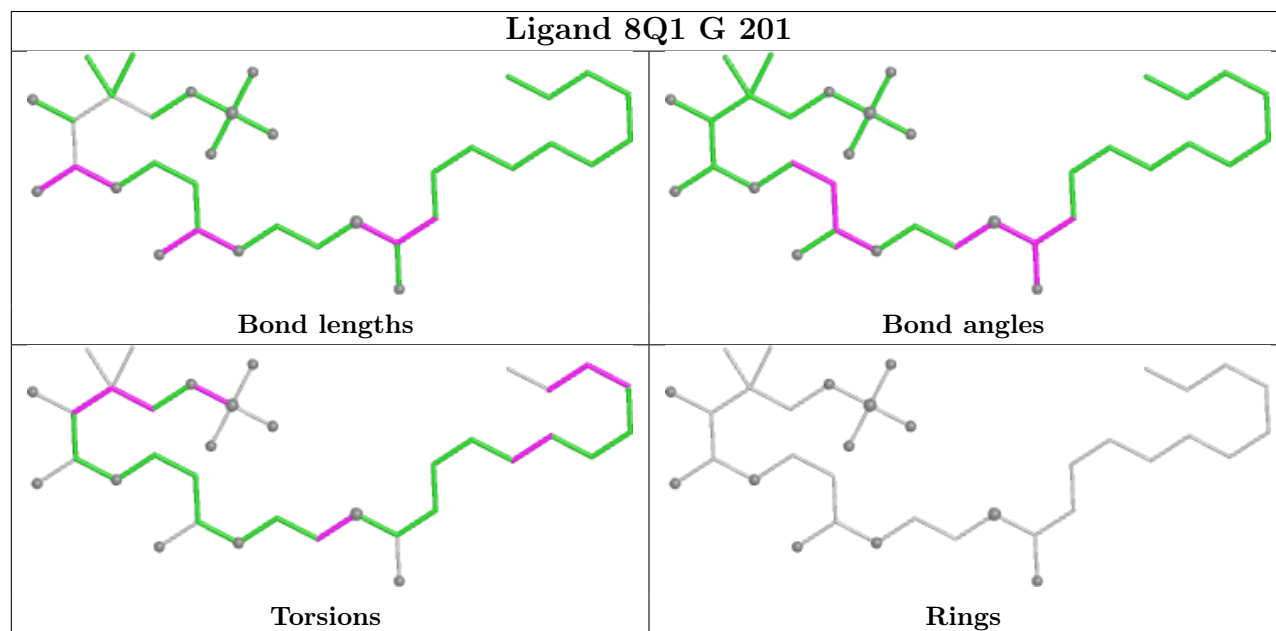
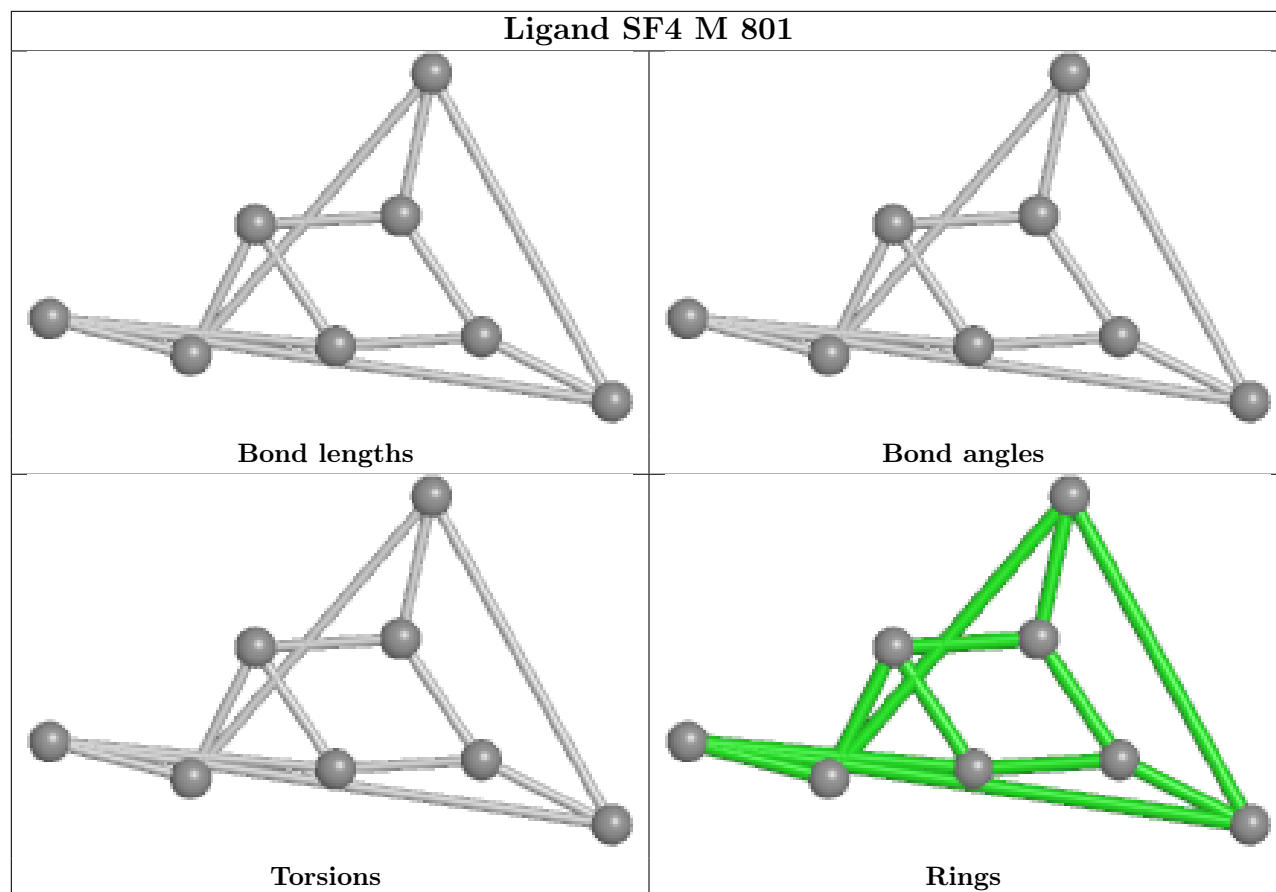


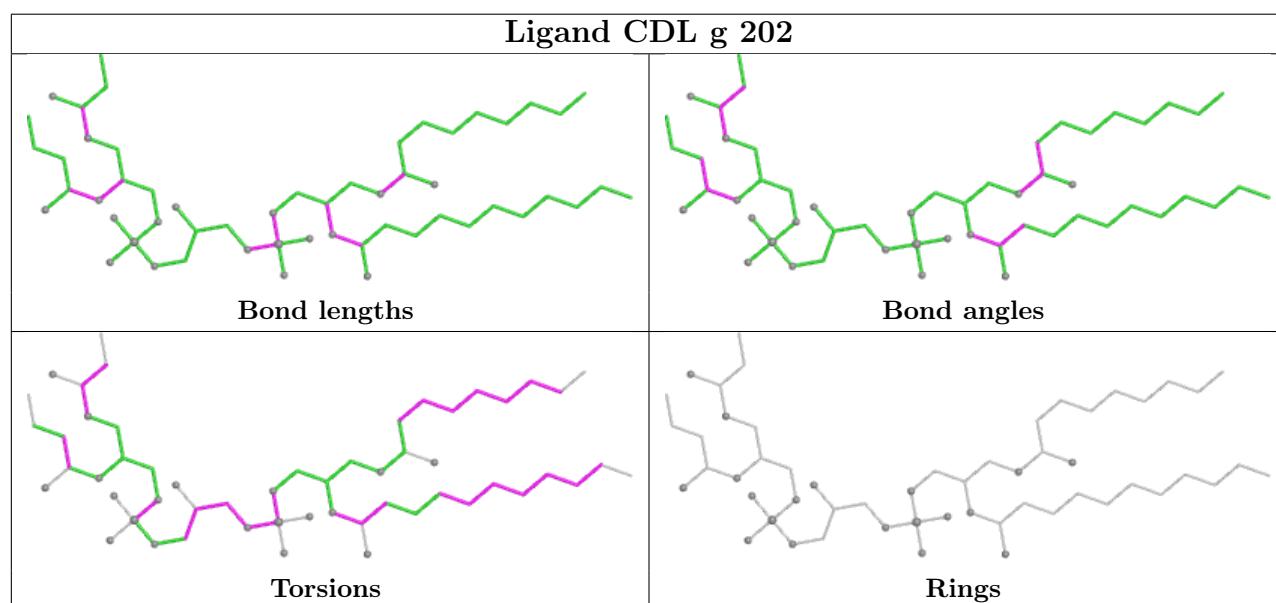
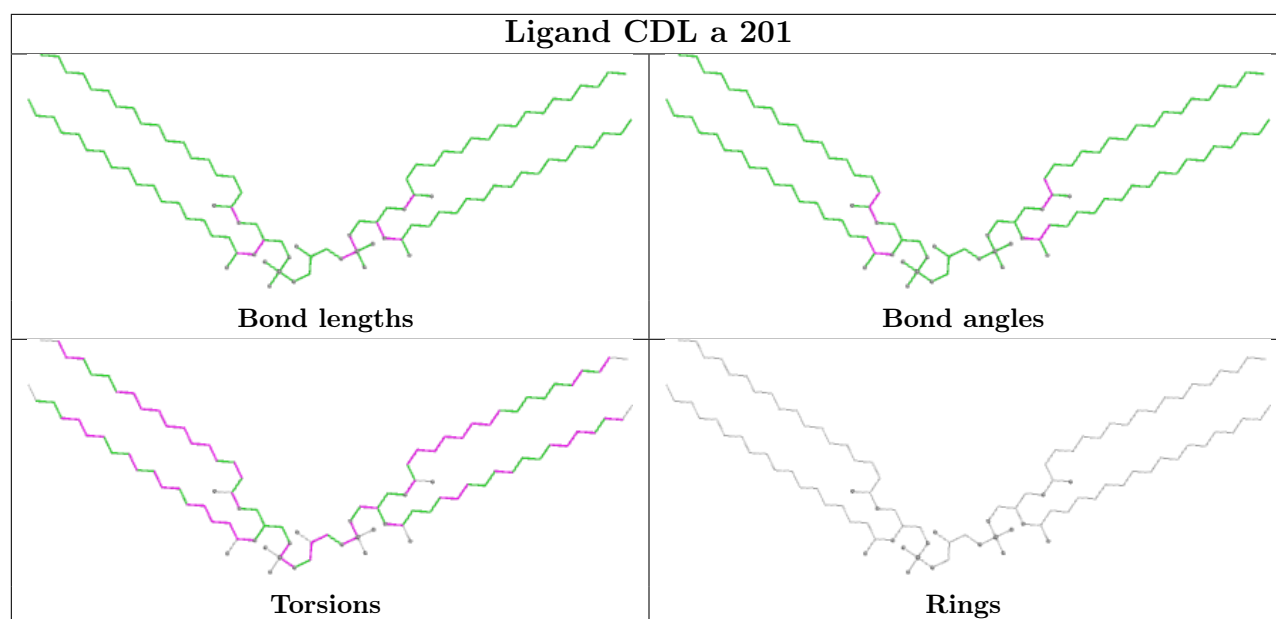
Ligand SF4 M 802

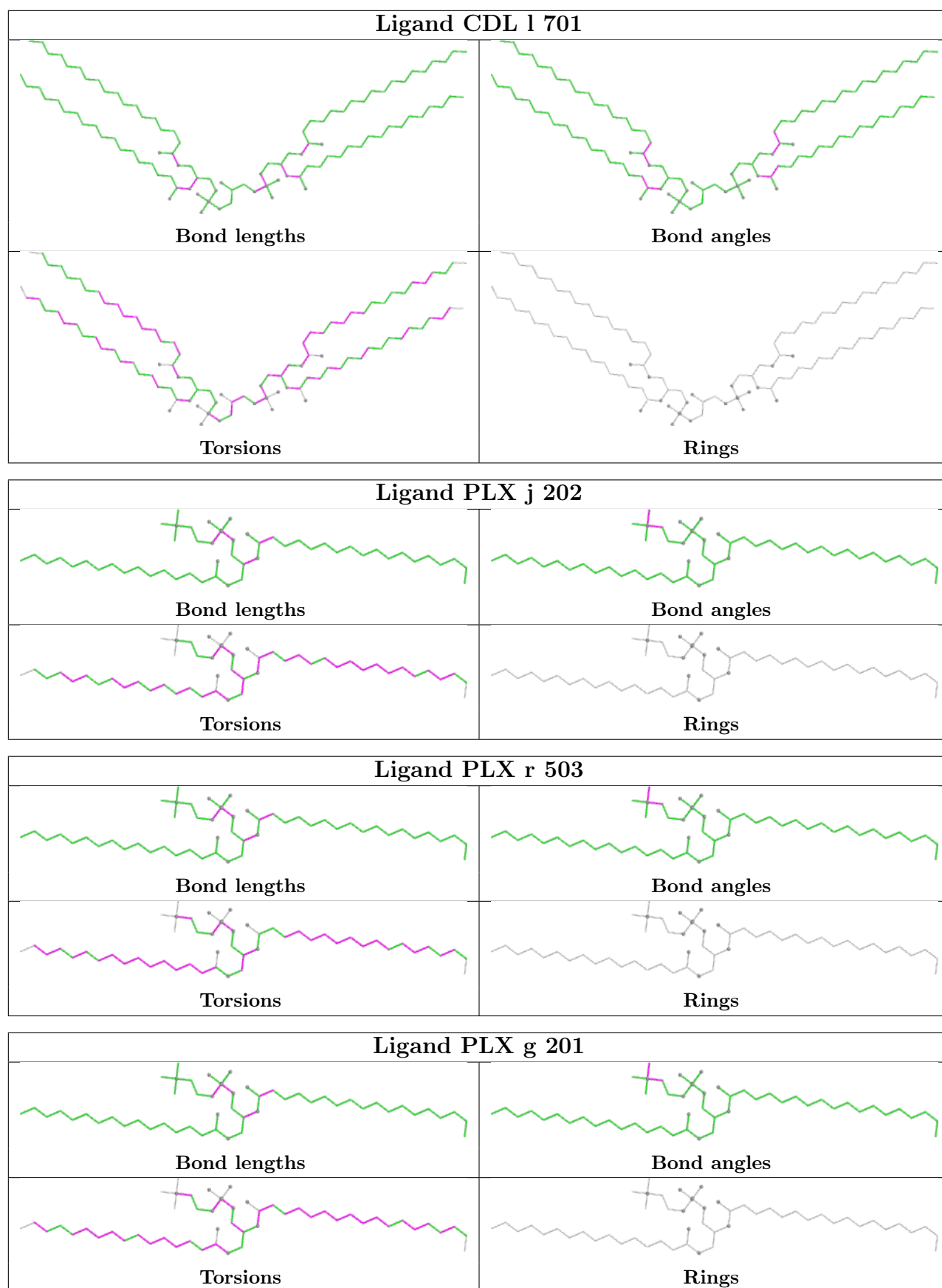


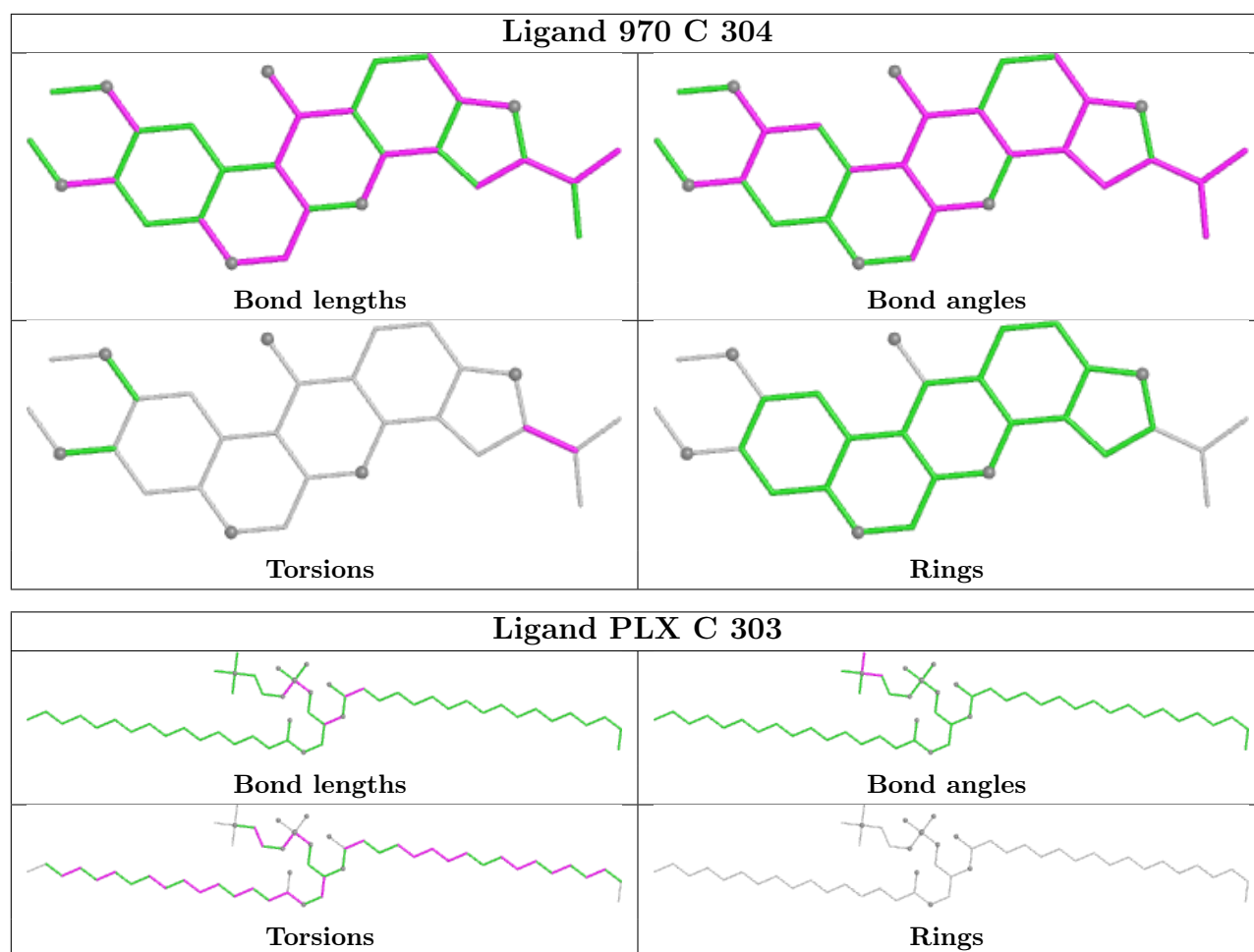
Ligand SF4 C 301











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.

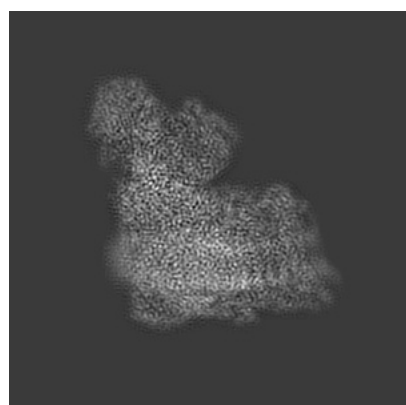
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32257. These allow visual inspection of the internal detail of the map and identification of artifacts.

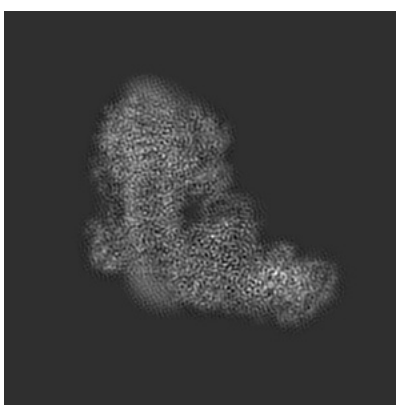
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

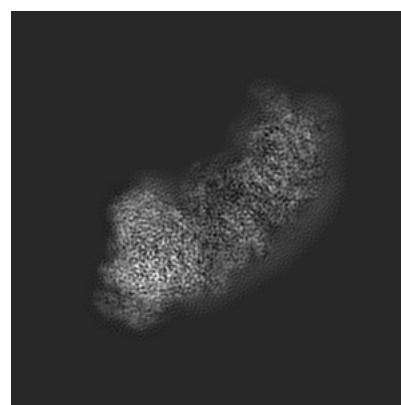
6.1.1 Primary map



X



Y

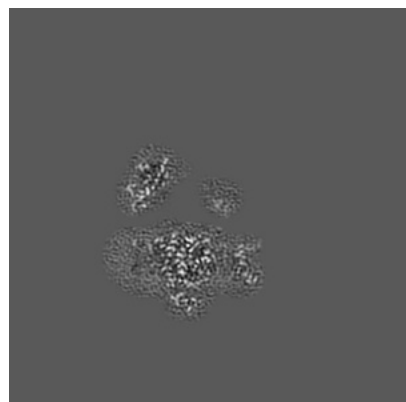


Z

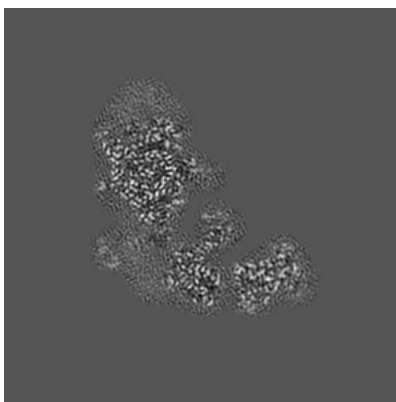
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

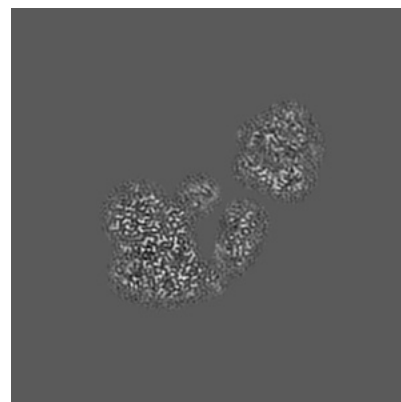
6.2.1 Primary map



X Index: 155



Y Index: 155

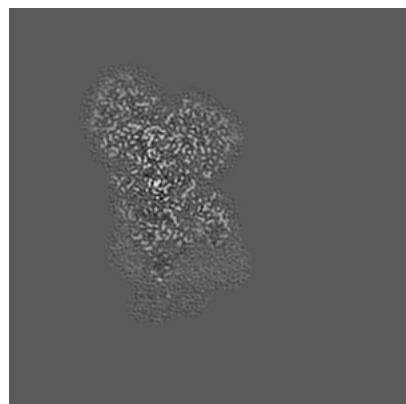


Z Index: 155

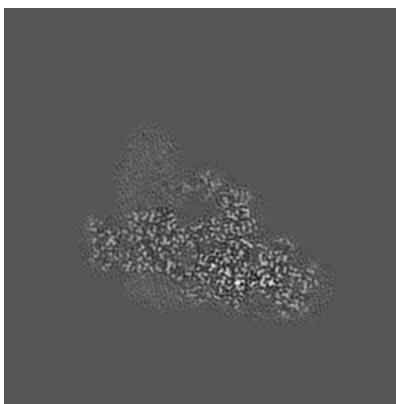
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

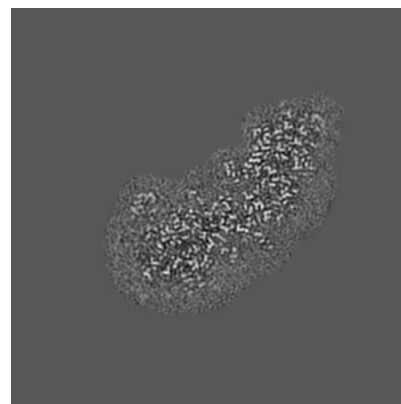
6.3.1 Primary map



X Index: 105



Y Index: 112

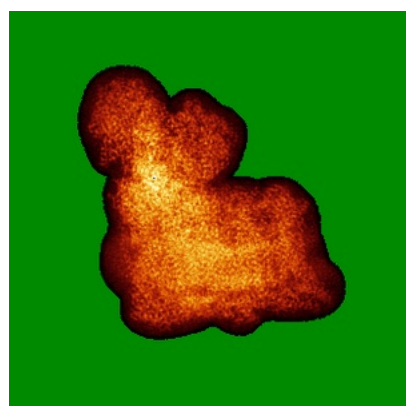


Z Index: 128

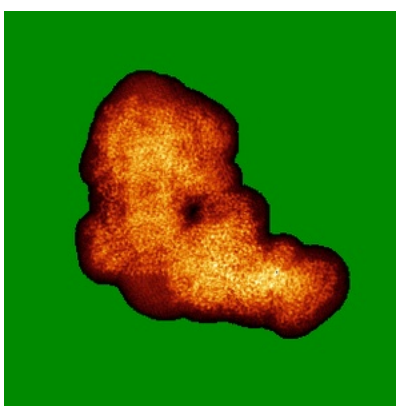
The images above show the largest variance slices of the map in three orthogonal directions.

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

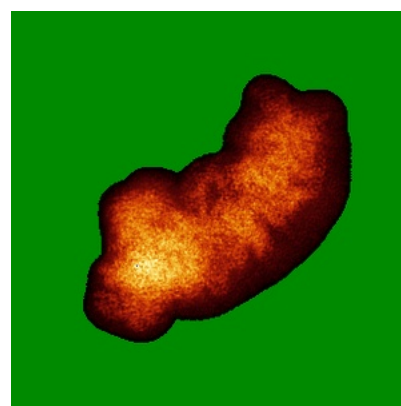
6.4.1 Primary map



X



Y

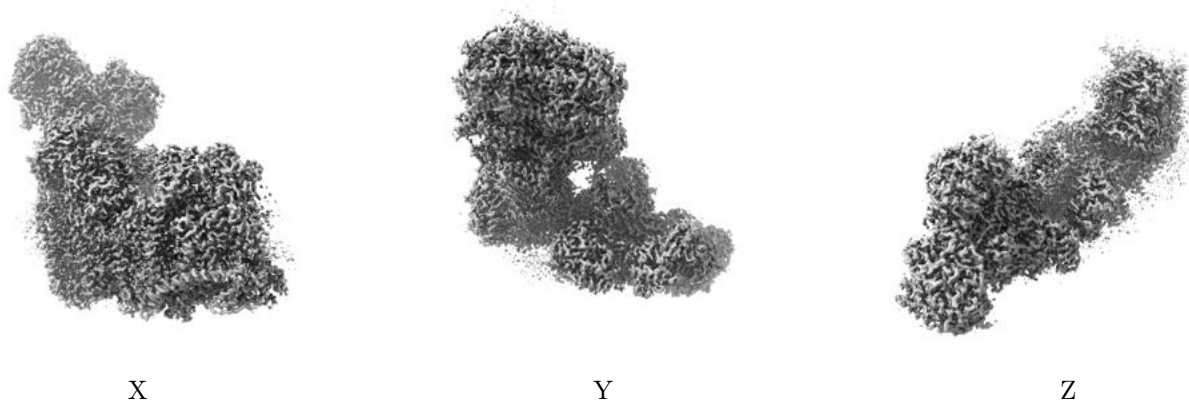


Z

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 0.0336. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

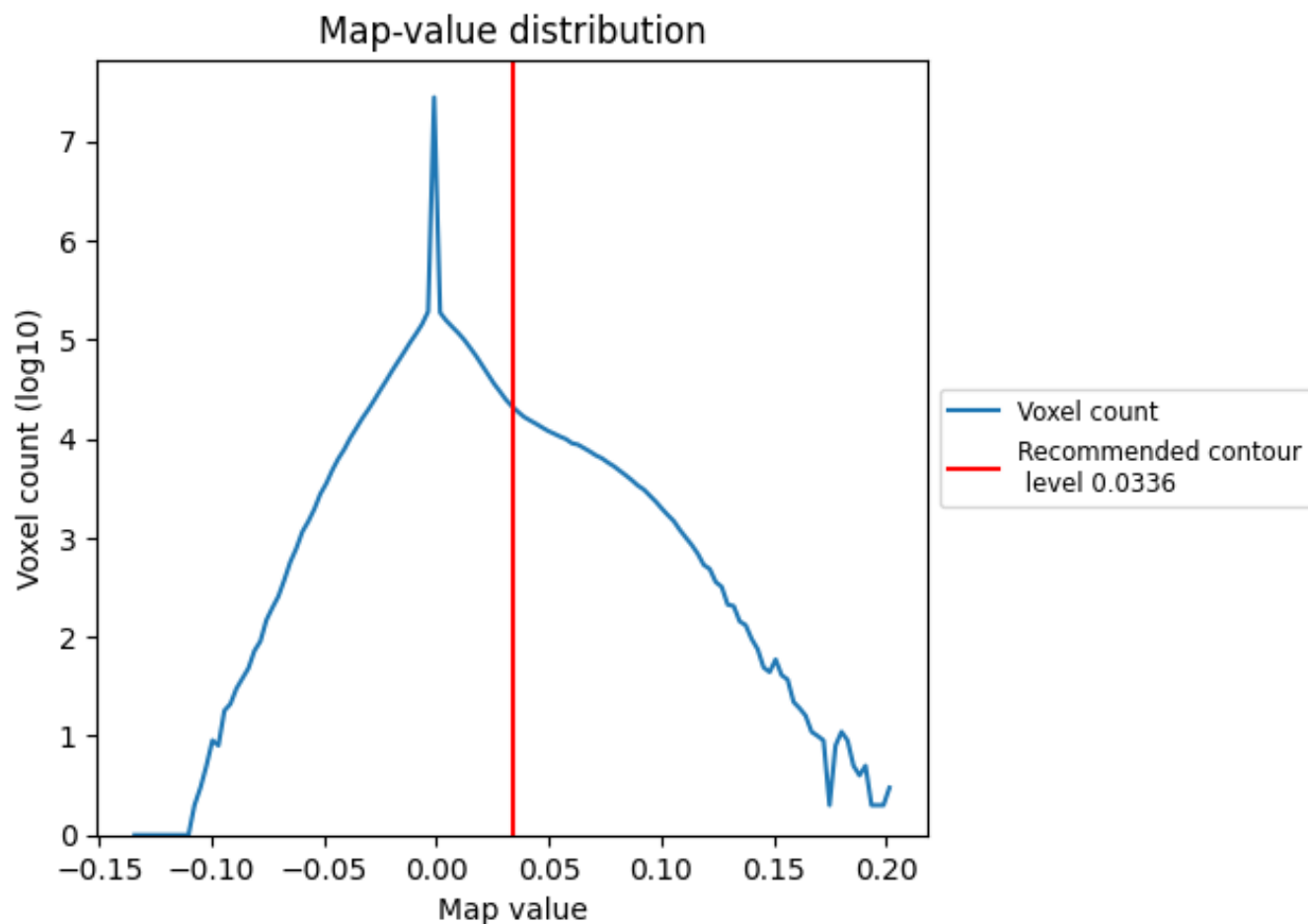
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

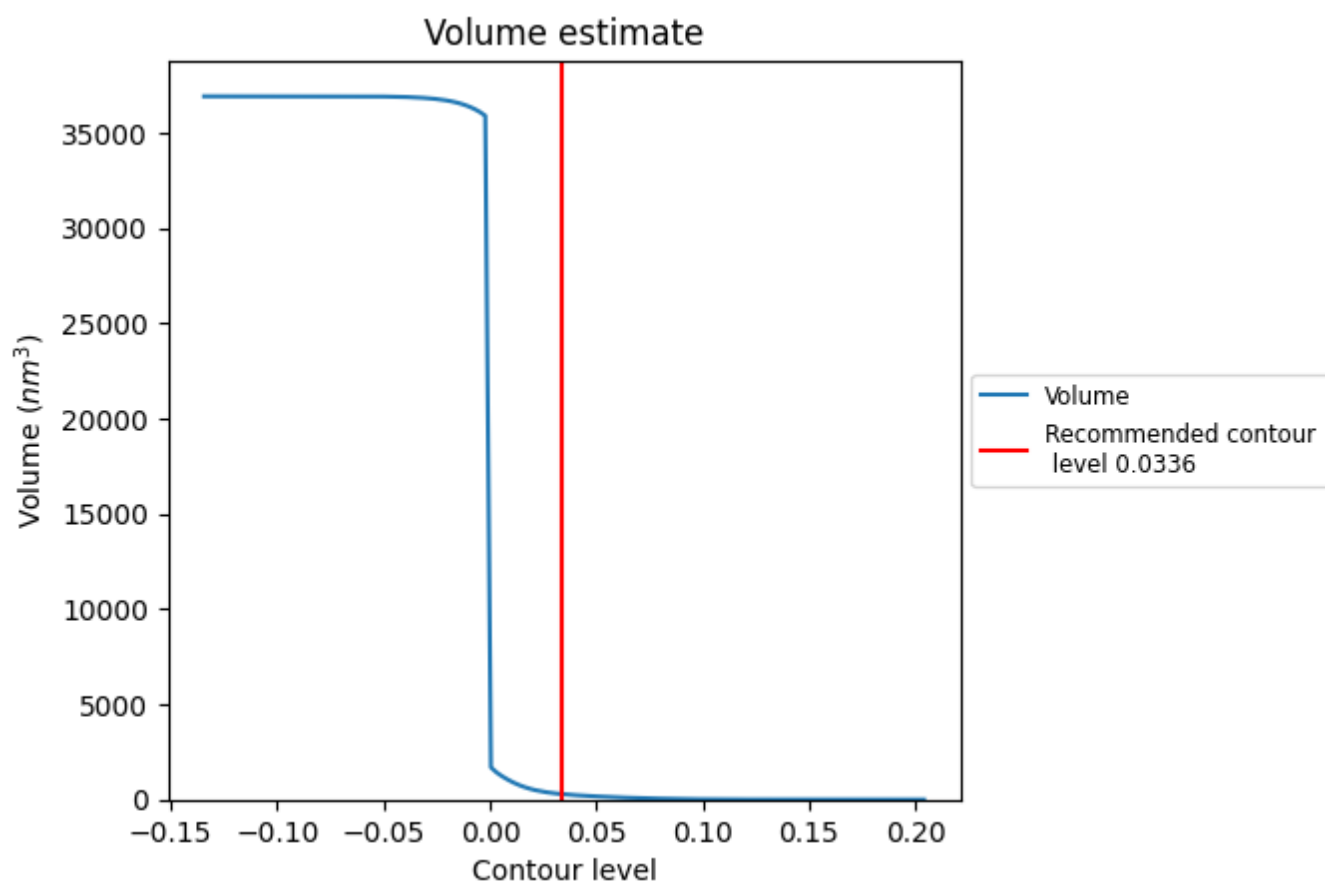
This section contains the results of statistical analysis of the map.

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.

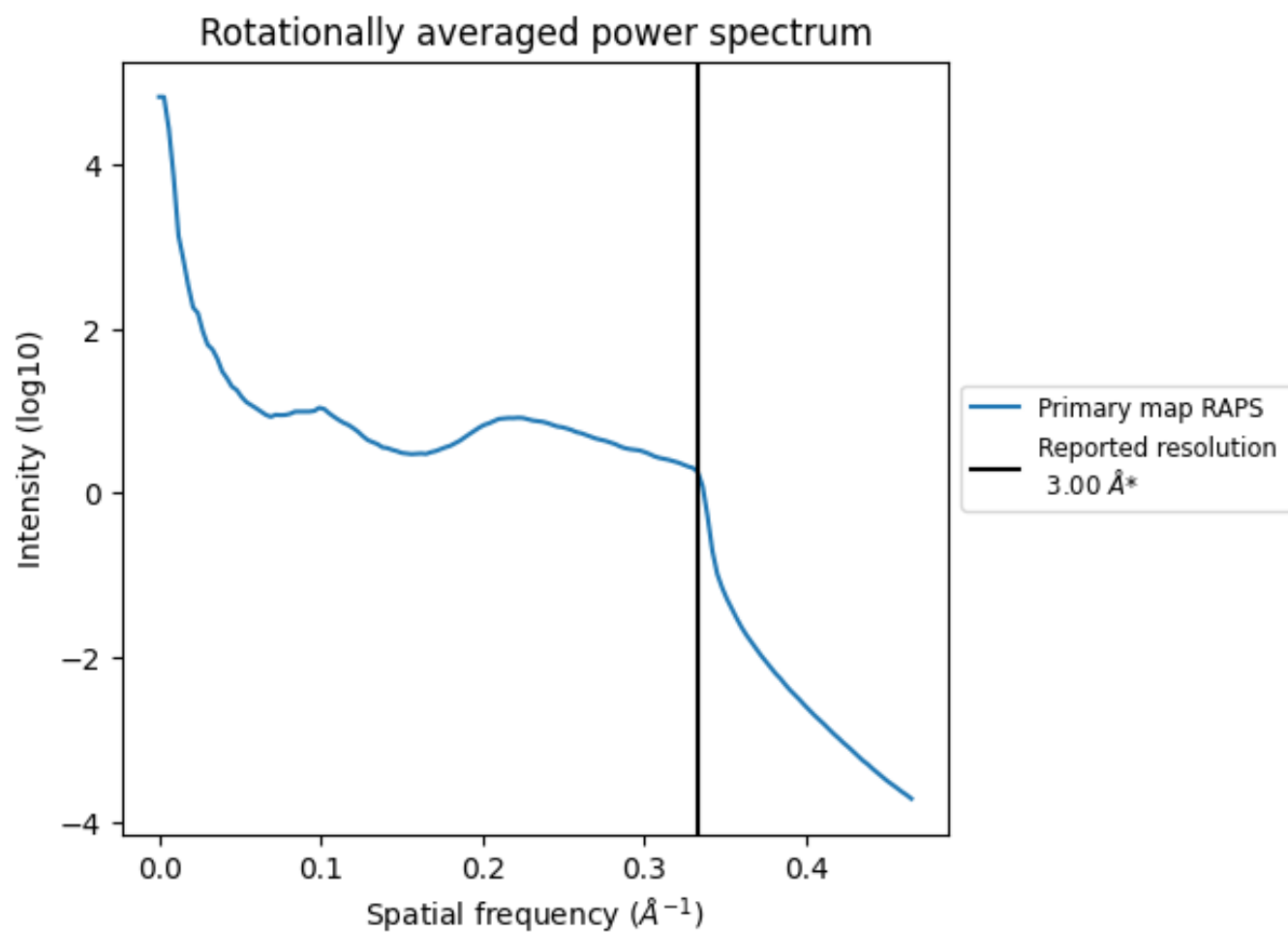
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 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 0.333 Å⁻¹

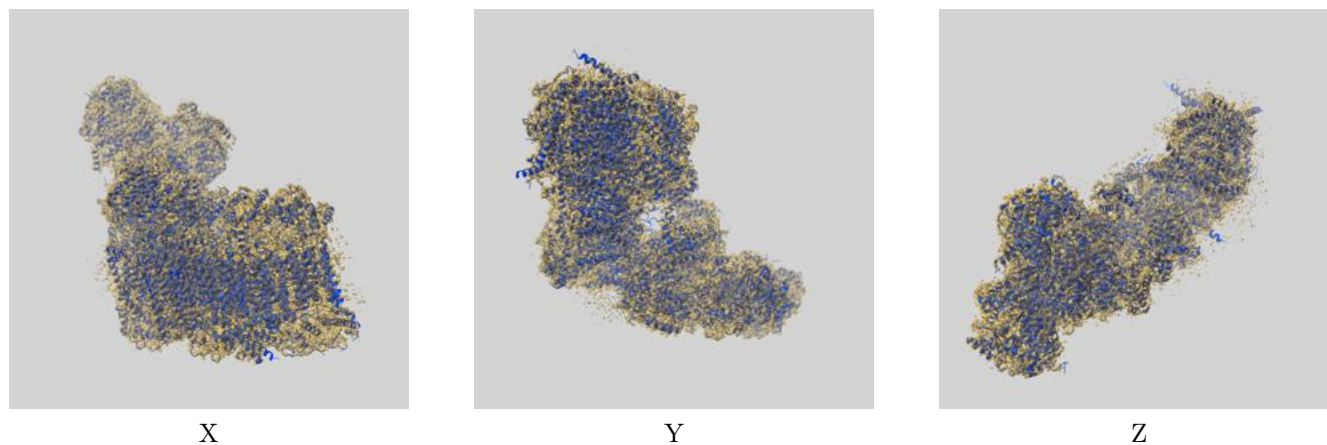
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

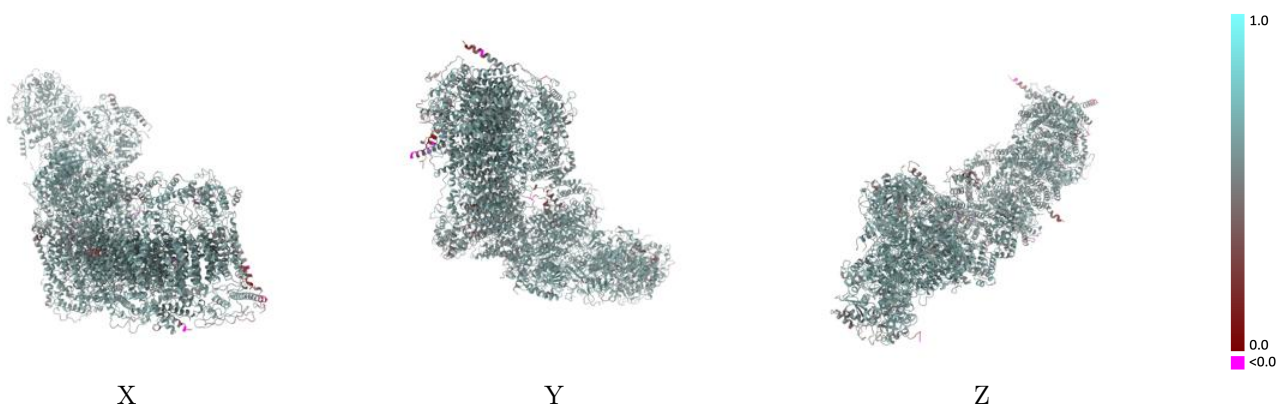
This section contains information regarding the fit between EMDB map EMD-32257 and PDB model 7W1V. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



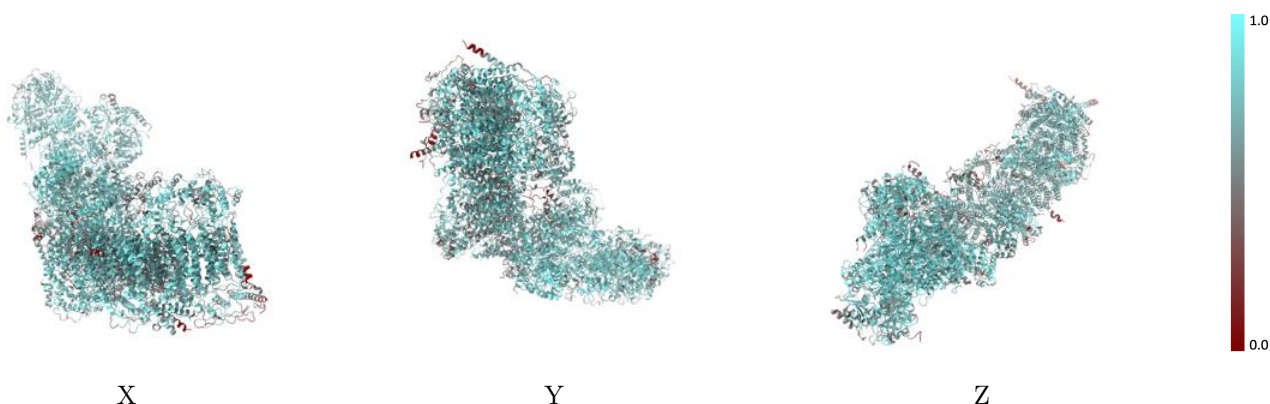
The images above show the 3D surface view of the map at the recommended contour level 0.0336 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



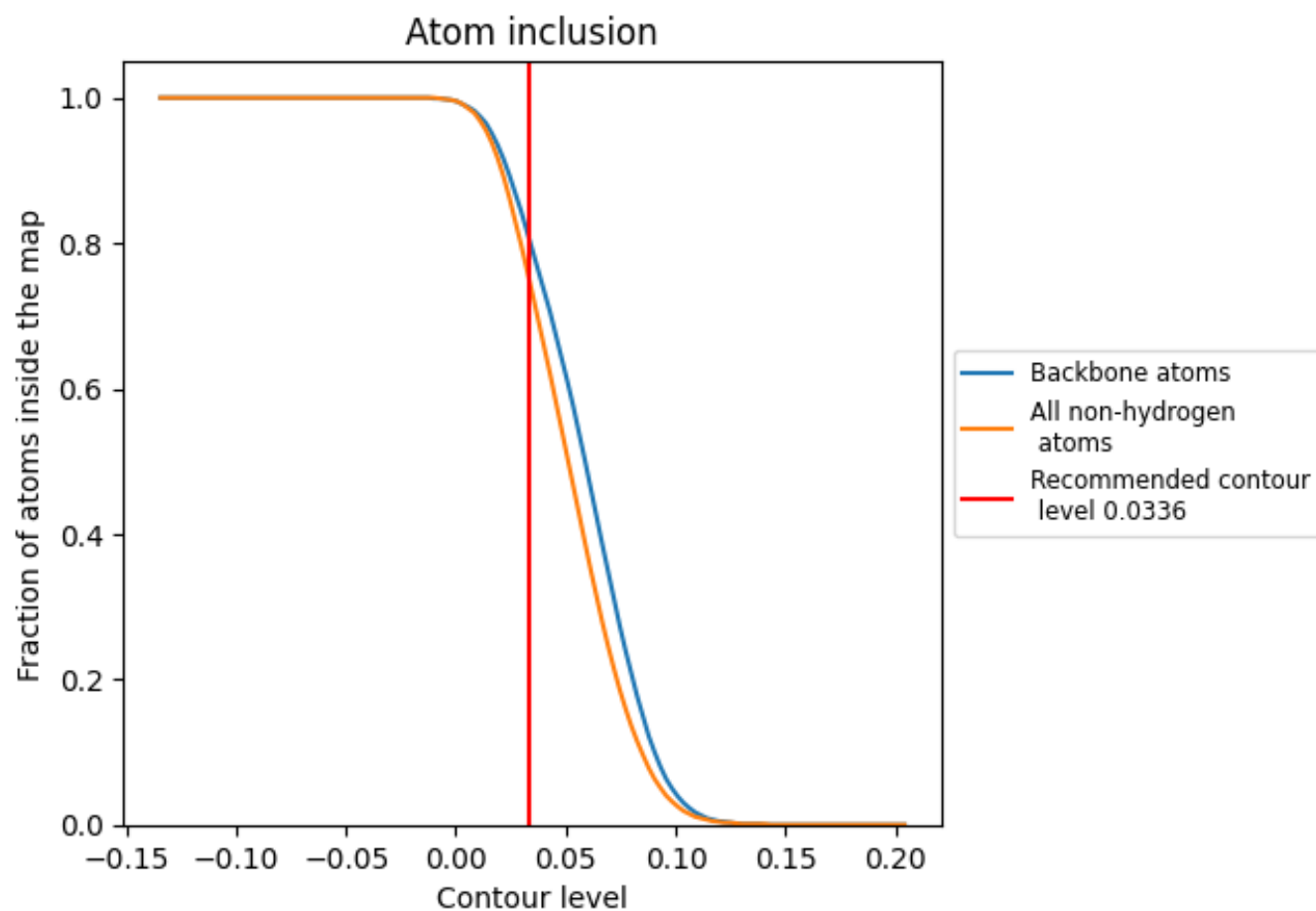
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0336).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.0336) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.5790
A	 0.7400	 0.5720
B	 0.8570	 0.6170
C	 0.8590	 0.6170
E	 0.7860	 0.5940
F	 0.6410	 0.5260
G	 0.4720	 0.4590
H	 0.7530	 0.5850
I	 0.6170	 0.5480
J	 0.7820	 0.5930
K	 0.6390	 0.5370
L	 0.7900	 0.5950
M	 0.7980	 0.5910
N	 0.6980	 0.5790
O	 0.7230	 0.5570
P	 0.8710	 0.6220
Q	 0.8480	 0.6150
S	 0.7930	 0.5980
T	 0.7420	 0.5850
U	 0.6680	 0.5410
V	 0.6160	 0.5560
W	 0.7110	 0.5670
X	 0.6580	 0.5520
Y	 0.6130	 0.5150
Z	 0.5650	 0.4840
a	 0.7240	 0.5920
b	 0.6670	 0.5420
c	 0.7220	 0.5760
d	 0.6820	 0.5500
e	 0.6730	 0.5570
f	 0.5370	 0.4900
g	 0.7290	 0.5780
h	 0.7150	 0.5650
i	 0.7950	 0.5970
j	 0.7190	 0.5810



Continued on next page...

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Chain	Atom inclusion	Q-score
k	 0.8280	 0.6060
l	 0.7590	 0.5880
m	 0.6870	 0.5510
n	 0.5500	 0.5050
o	 0.6760	 0.5720
p	 0.7230	 0.5730
r	 0.8080	 0.6010
s	 0.8010	 0.5970
u	 0.7350	 0.5760
v	 0.6000	 0.5160
w	 0.7230	 0.5710