



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 05:29 PM UTC

PDB ID : 2YBB / pdb_00002ybb
EMDB ID : EMD-1876
Title : Fitted model for bovine mitochondrial supercomplex I1III2IV1 by single particle cryo-EM (EMD-1876)
Authors : Althoff, T.; Mills, D.J.; Popot, J.-L.; Kuehlbrandt, W.
Deposited on : 2011-03-02
Resolution : 19.00 Å (reported)
Based on initial models : 1PP9, 3M9C, 3IAM, 1BGY, 2B4Z, 1OCC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

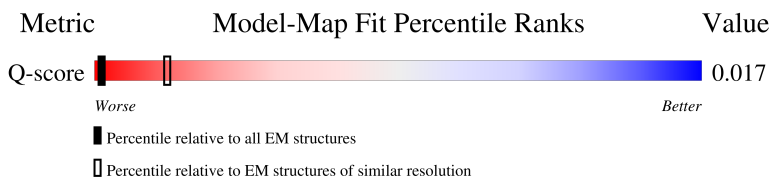
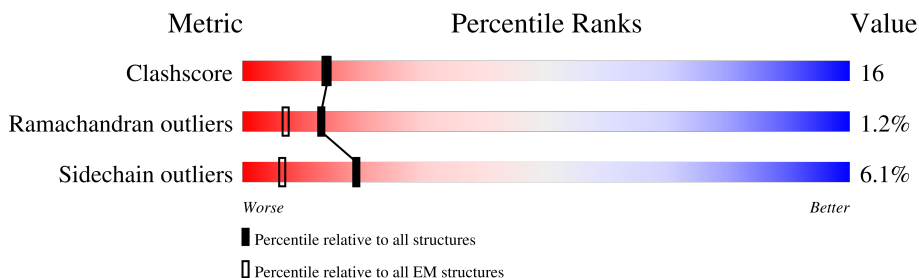
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 19.00 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.




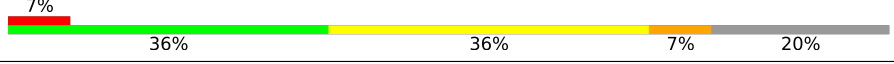
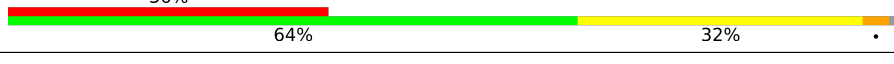
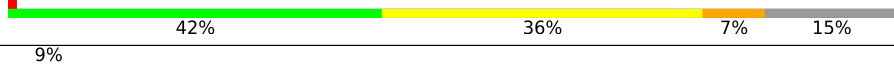

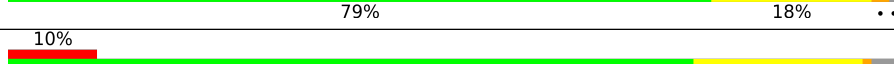
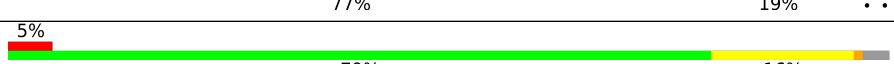
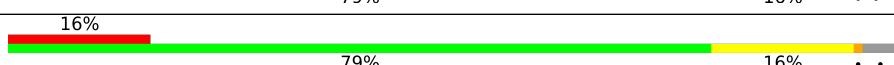
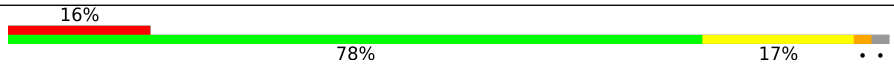


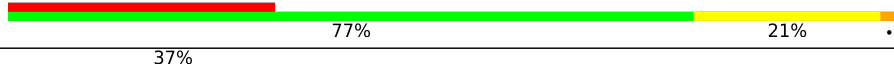
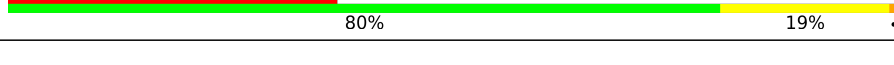

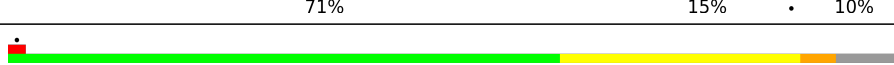



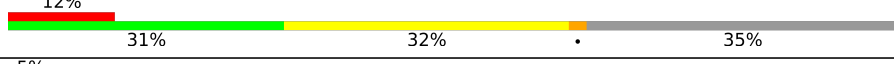
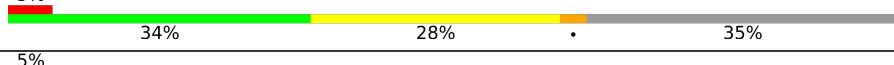





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	17 (18.70 - 19.50)

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	1	438	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">9%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 9% 53% 39% 8% </div> </div>
2	2	181	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">23%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 23% 52% 40% 7% </div> </div>
3	3	783	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">15%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 15% 48% 40% 8% </div> </div>
4	4	409	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">17%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 17% 42% 42% 9% 8% </div> </div>






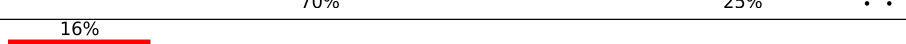




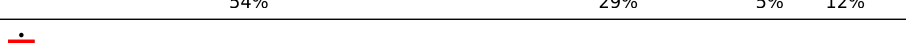



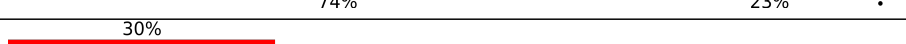


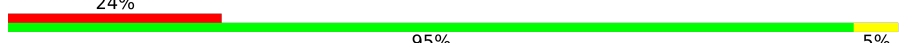
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	5	207	
6	6	181	
7	7	129	
8	8	182	
9	A	446	
9	a	446	
10	B	439	
10	b	439	
11	C	379	
11	c	379	
12	D	241	
12	d	241	
13	E	196	
13	e	196	
14	F	110	
14	f	110	
15	G	81	
15	g	81	
16	H	78	
16	h	78	
17	I	65	
17	i	65	
18	J	62	
18	j	62	
19	K	56	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
19	k	56	
20	L	514	
21	M	227	
22	N	261	
23	O	147	
24	P	109	
25	Q	98	
26	R	84	
27	S	85	
28	T	73	
29	U	59	
30	V	56	
31	W	47	
32	X	46	
33	Y	104	
34	m	474	
35	n	391	
36	o	378	
37	p	281	

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
38	SF4	8	183	-	-	X	-

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 72626 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-QUINONE OXIDOREDUCTASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	437	3417	2180	595	624	18	0	0

- Molecule 2 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	179	1410	897	239	266	8	0	0

- Molecule 3 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	754	5880	3743	1055	1051	31	0	0

- Molecule 4 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	378	3018	1946	511	550	11	0	0

- Molecule 5 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	196	1607	1043	273	288	3	0	0

- Molecule 6 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	144	1102	700	192	197	13	0	0

- Molecule 7 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	127	1031	664	183	181	3	0	0

- Molecule 8 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	154	1193	759	201	222	11	0	0

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	443	3403	2121	602	660	20	0	1
9	a	443	3403	2121	602	660	20	0	1

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	424	3177	1996	562	612	7	0	1
10	b	424	3180	1998	562	613	7	0	0

- Molecule 11 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	365	2892	1940	450	485	17	0	0
11	c	370	2931	1968	455	490	18	0	0

- Molecule 12 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	241	1919	1225	330	349	15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	d	241	1919	1225	330	349	15	0	0

- Molecule 13 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	196	1519	957	263	291	8	0	0
13	e	196	1519	957	263	291	8	0	0

- Molecule 14 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	99	861	545	155	159	2	0	0
14	f	99	861	545	155	159	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	engineered mutation	UNP P00129
f	56	ASP	ASN	engineered mutation	UNP P00129

- Molecule 15 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	75	621	406	117	97	1	0	2
15	g	76	626	409	118	98	1	0	2

- Molecule 16 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	66	539	327	98	109	5	0	0
16	h	66	539	327	98	109	5	0	0

- Molecule 17 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	42	Total	C	N	O	S	0	0
			285	174	55	55	1		
17	i	42	Total	C	N	O	S	0	0
			285	174	55	55	1		

- Molecule 18 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	J	62	Total	C	N	O	0	0
			507	333	88	86		
18	j	62	Total	C	N	O	0	0
			507	333	88	86		

- Molecule 19 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	K	22	Total	C	N	O	0	0
			159	103	29	27		
19	k	22	Total	C	N	O	0	0
			159	103	29	27		

- Molecule 20 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 22 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 23 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1,

MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	144	1195	777	196	218	4	0	0

- Molecule 24 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	109	878	558	150	168	2	0	0

- Molecule 25 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	98	748	464	134	145	5	0	0

- Molecule 26 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	84	672	431	129	111	1	0	0

- Molecule 27 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S	75	628	395	114	114	5	0	0

- Molecule 28 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	73	598	388	107	99	4	0	0

- Molecule 29 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	U	57	442	285	74	80	3	0	1

- Molecule 30 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	49	384	250	65	67	2	0	0

- Molecule 31 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	47	386	257	65	62	2	0	0

- Molecule 32 is a protein called CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	X	43	335	223	53	59	0	0

- Molecule 33 is a protein called CYTOCHROME C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y	104	875	552	155	163	5	7	0

- Molecule 34 is a protein called NADH\ : UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
34	m	474	1422	948	474	0	0

- Molecule 35 is a protein called NADH\ : UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
35	n	391	1173	782	391	0	0

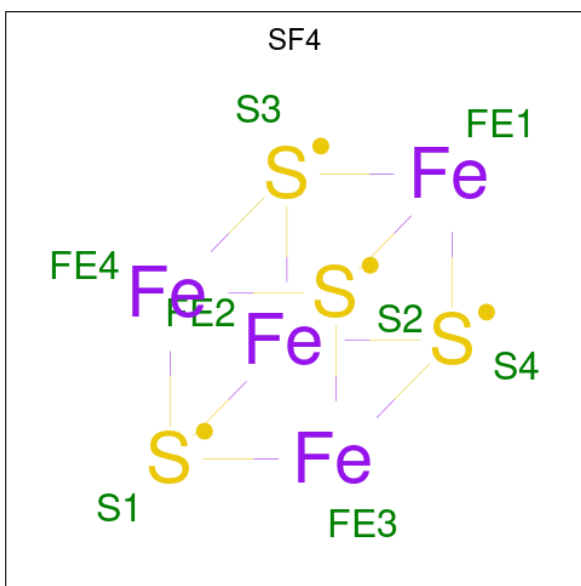
- Molecule 36 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
36	o	378	1134	756	378	0	0

- Molecule 37 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT K.

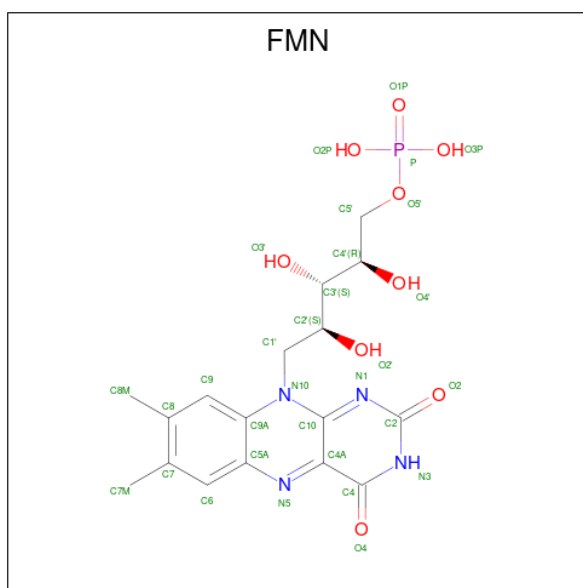
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
37	p	281	843	562	281	0	0

- Molecule 38 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



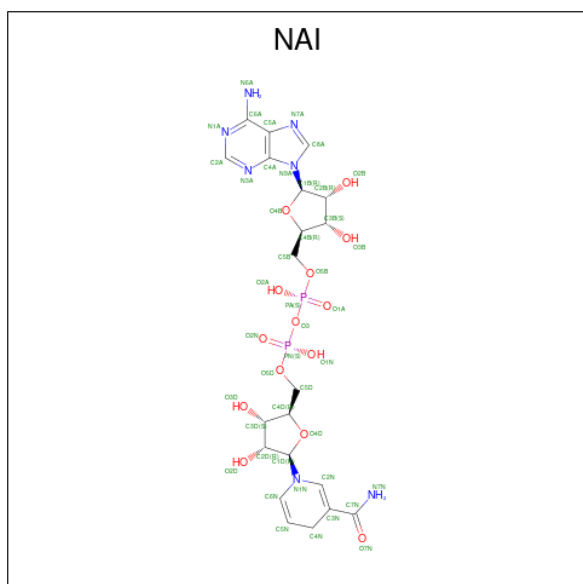
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
38	1	1	8	4	4	0
38	3	1	8	4	4	0
38	3	1	8	4	4	0
38	3	1	8	4	4	0
38	6	1	8	4	4	0
38	8	1	8	4	4	0
38	8	1	8	4	4	0

- Molecule 39 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
39	1	1	31	17	4	9	1	0

- Molecule 40 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

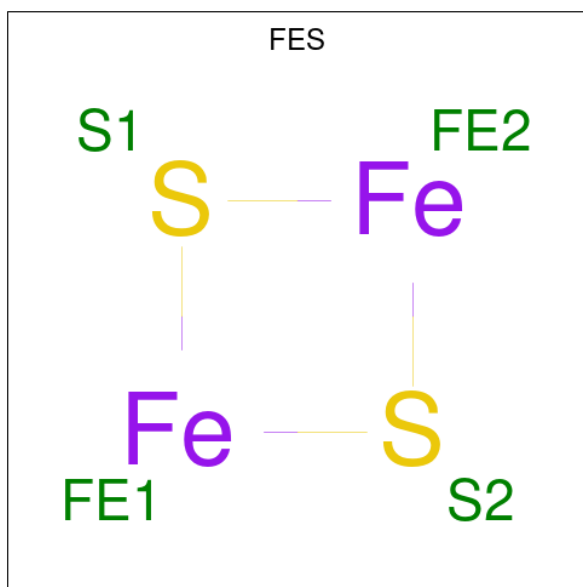


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
40	1	1	44	21	7	14	2	0

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	1	1	Total	Mg	0
			1	1	
41	2	1	Total	Mg	0
			1	1	
41	3	2	Total	Mg	0
			2	2	
41	4	1	Total	Mg	0
			1	1	
41	5	1	Total	Mg	0
			1	1	
41	L	1	Total	Mg	0
			1	1	

- Molecule 42 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

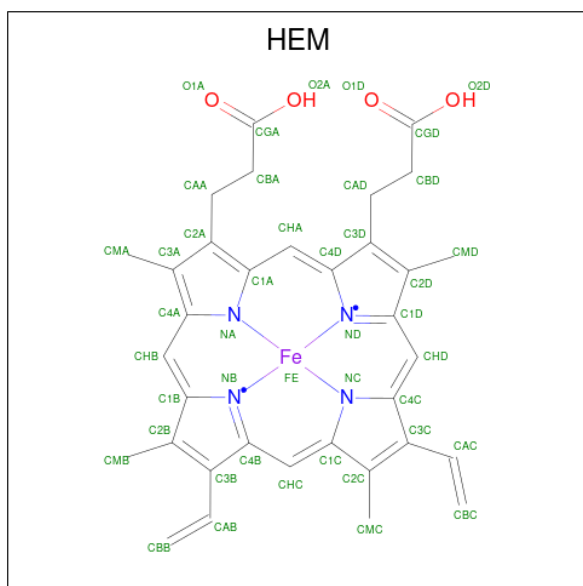


Mol	Chain	Residues	Atoms			AltConf
42	2	1	Total	Fe	S	0
			4	2	2	
42	3	1	Total	Fe	S	0
			4	2	2	
42	E	1	Total	Fe	S	0
			4	2	2	
42	e	1	Total	Fe	S	0
			4	2	2	

- Molecule 43 is CALCIUM ION (CCD ID: CA) (formula: Ca).

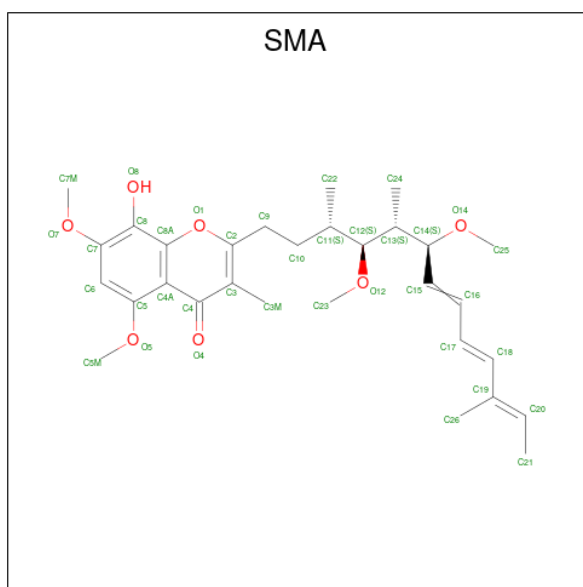
Mol	Chain	Residues	Atoms	AltConf
43	7	1	Total Ca 1 1	0

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



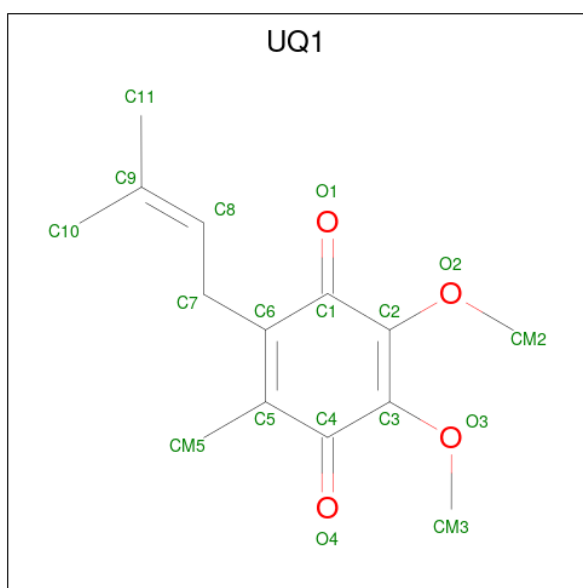
Mol	Chain	Residues	Atoms	AltConf
44	C	1	Total C Fe N O 43 34 1 4 4	0
44	C	1	Total C Fe N O 43 34 1 4 4	0
44	Y	1	Total C Fe N O 43 34 1 4 4	0
44	c	1	Total C Fe N O 43 34 1 4 4	0
44	c	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 45 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms			AltConf
45	C	1	Total	C	O	0
			37	30	7	
45	c	1	Total	C	O	0
			37	30	7	

- Molecule 46 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄).

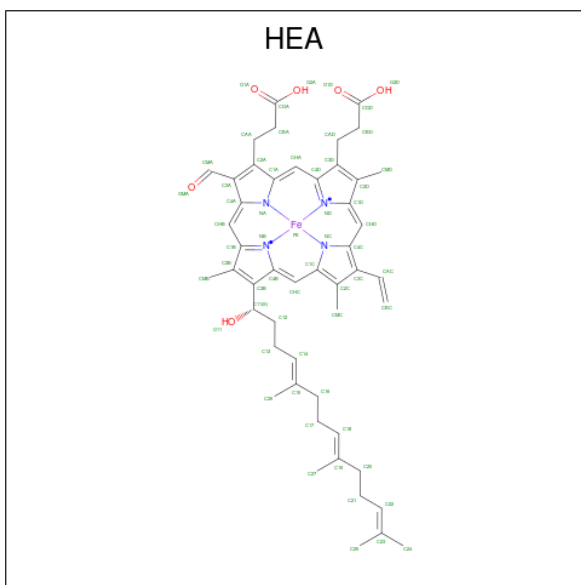


Mol	Chain	Residues	Atoms			AltConf
46	C	1	Total	C	O	0
			14	10	4	
46	c	1	Total	C	O	0
			14	10	4	

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
48	G	1	Total 44	C 25	O 17	P 2	0
48	d	1	Total 50	C 31	O 17	P 2	0
48	g	1	Total 49	C 30	O 17	P 2	0

- Molecule 49 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
49	L	1	Total 60	C 49	Fe 1	N 4	O 6	0
49	L	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 50 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
50	L	1	Total 1	Cu 1	0
50	M	2	Total 2	Cu 2	0

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	Q	1	Total 1	Zn 1	0

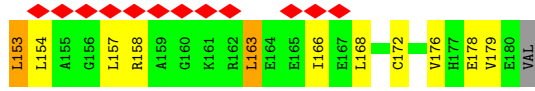
- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	187	Total 187	O 187	0
52	B	149	Total 149	O 149	0
52	C	125	Total 125	O 125	0
52	D	118	Total 118	O 118	0
52	E	54	Total 54	O 54	0
52	F	57	Total 57	O 57	0
52	G	24	Total 24	O 24	0
52	H	14	Total 14	O 14	0
52	I	16	Total 16	O 16	0
52	J	5	Total 5	O 5	0
52	Y	161	Total 161	O 161	0
52	a	134	Total 134	O 134	0
52	b	130	Total 130	O 130	0
52	c	122	Total 122	O 122	0
52	d	109	Total 109	O 109	0
52	e	64	Total 64	O 64	0
52	f	73	Total 73	O 73	0
52	g	21	Total 21	O 21	0
52	h	16	Total 16	O 16	0

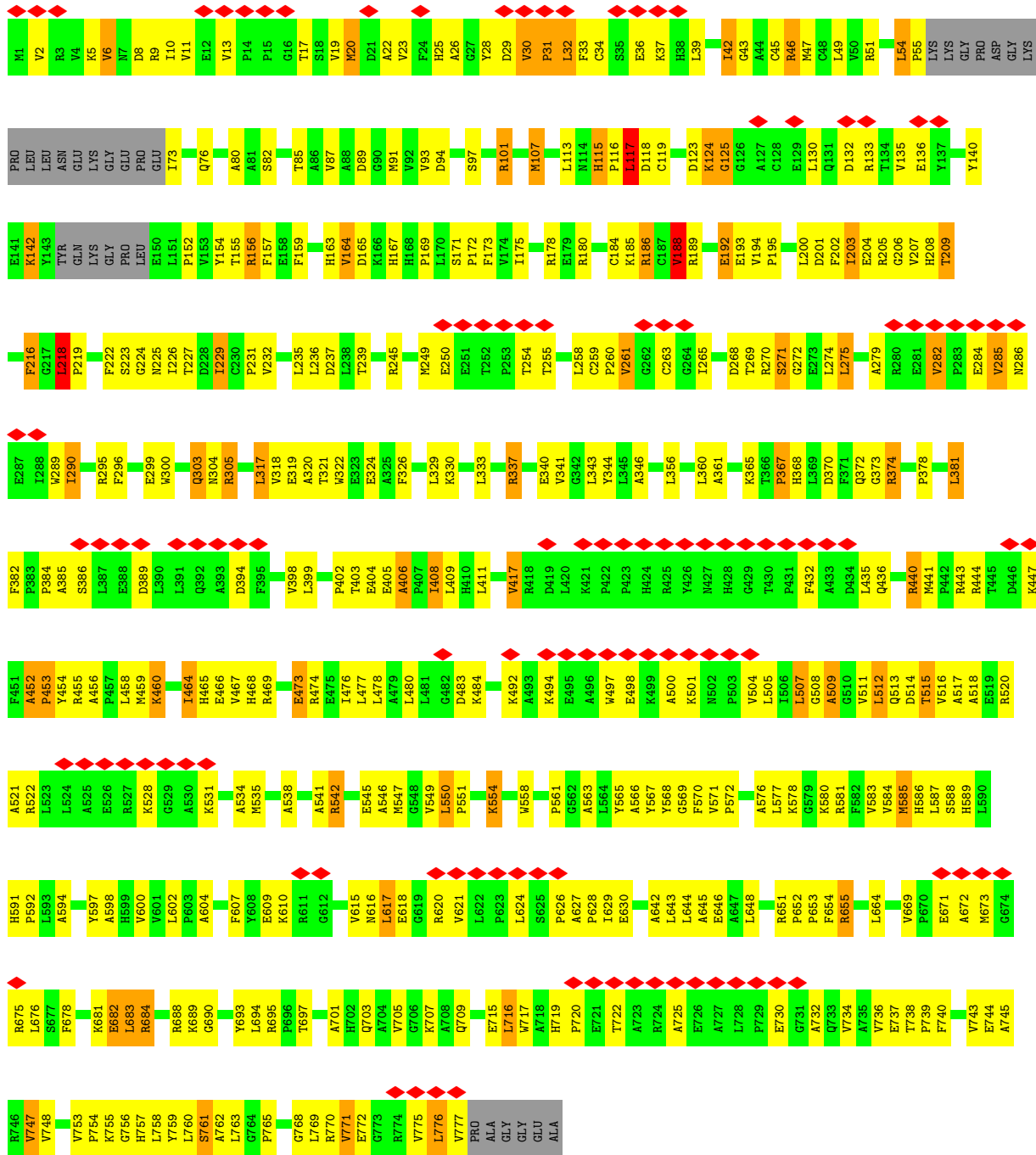
Continued on next page...

Continued from previous page...

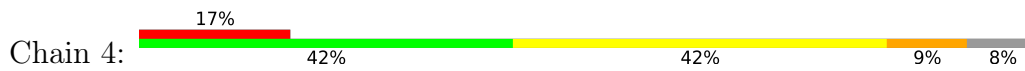
Mol	Chain	Residues	Atoms		AltConf
52	i	10	Total 10	O 10	0
52	j	9	Total 9	O 9	0

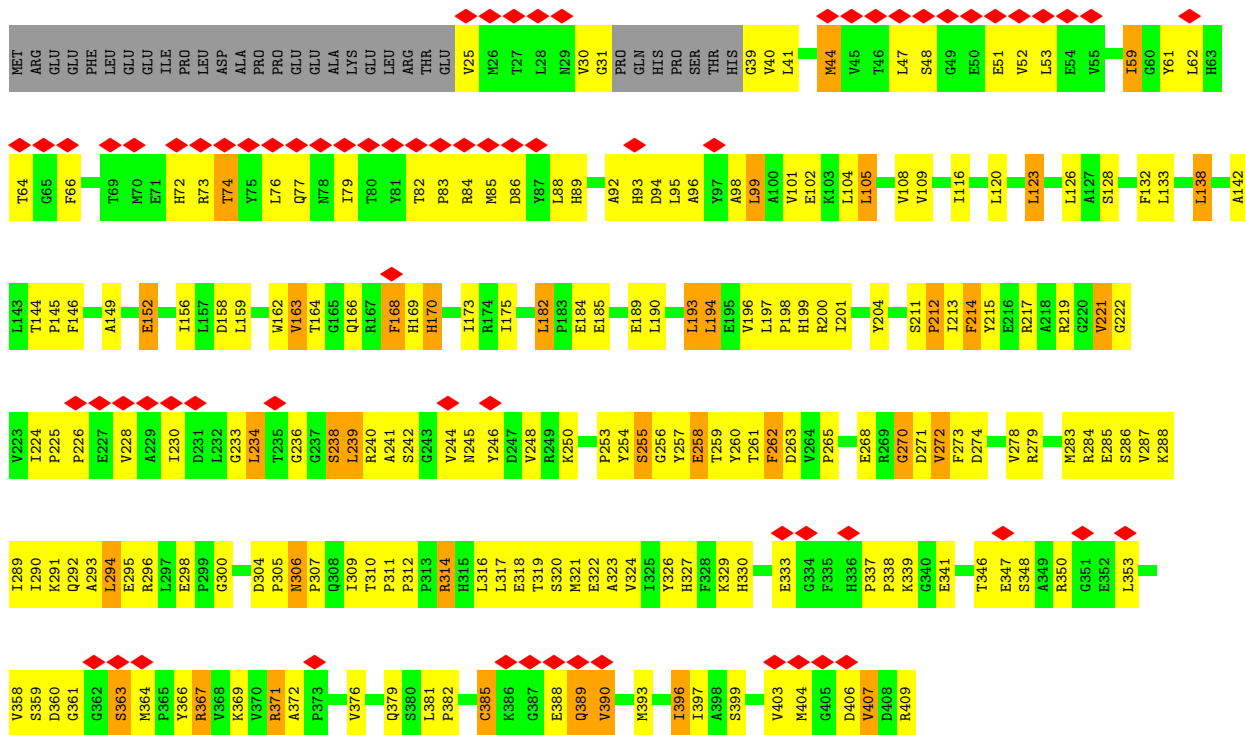


• Molecule 3: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3

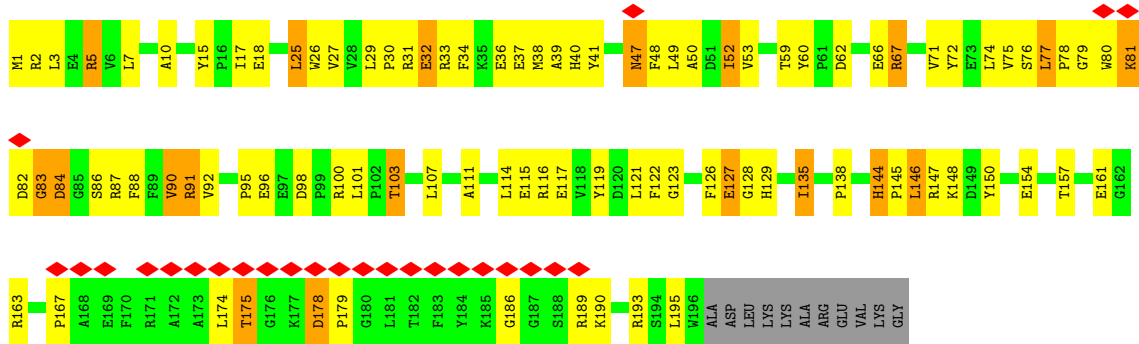


• Molecule 4: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4

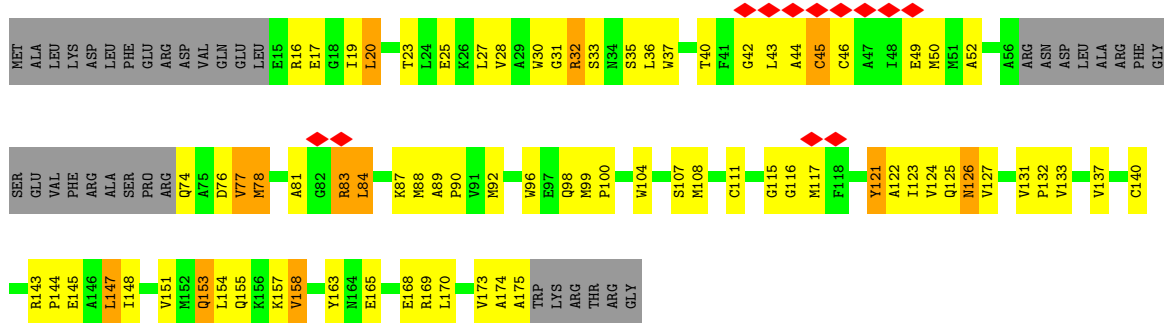




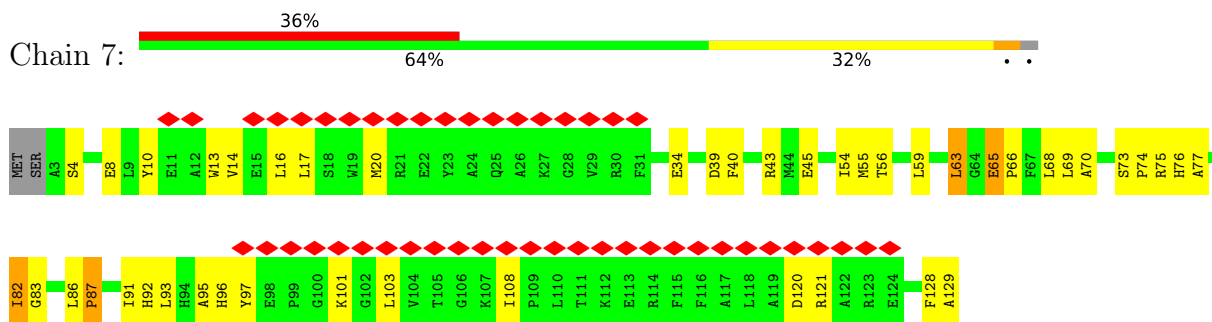
• Molecule 5: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5



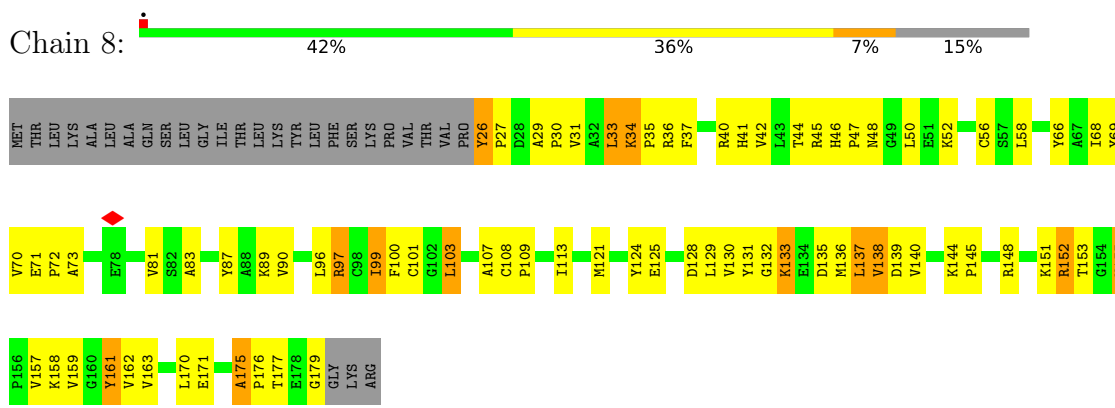
• Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6



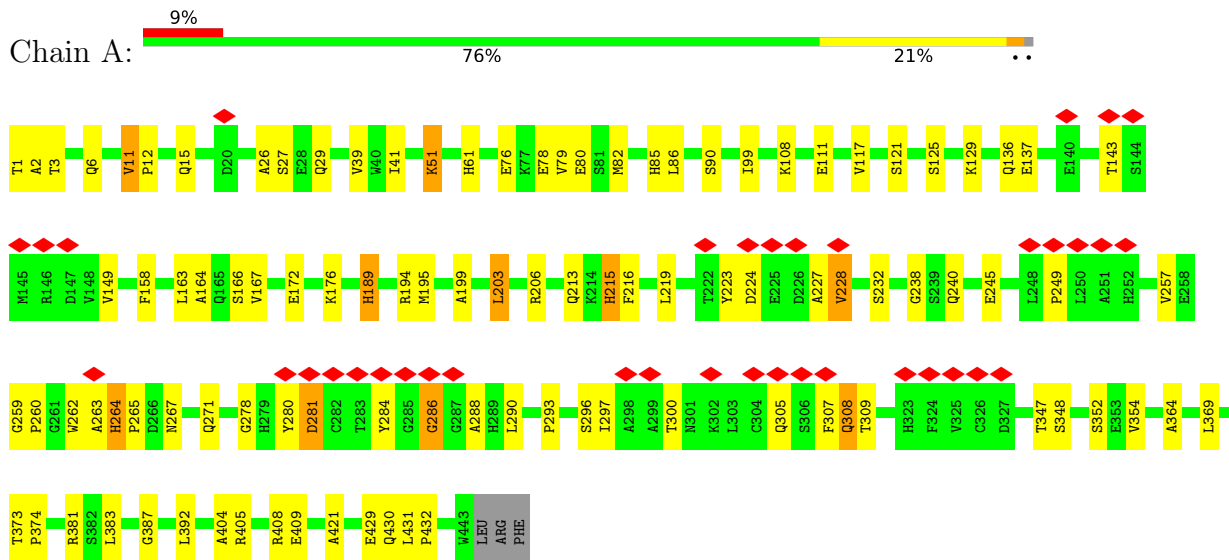
• Molecule 7: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15



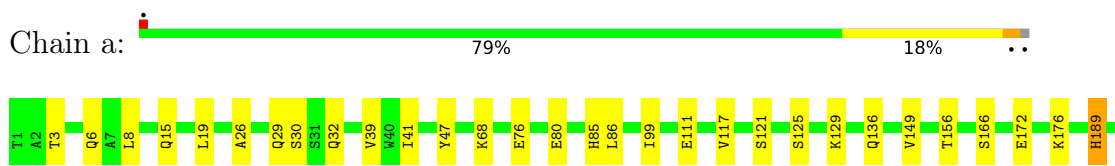
• Molecule 8: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9

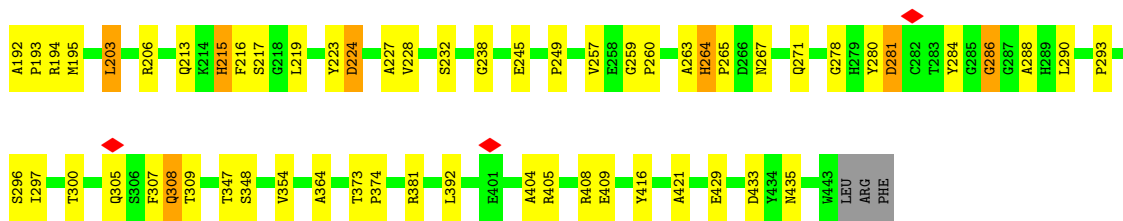


• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

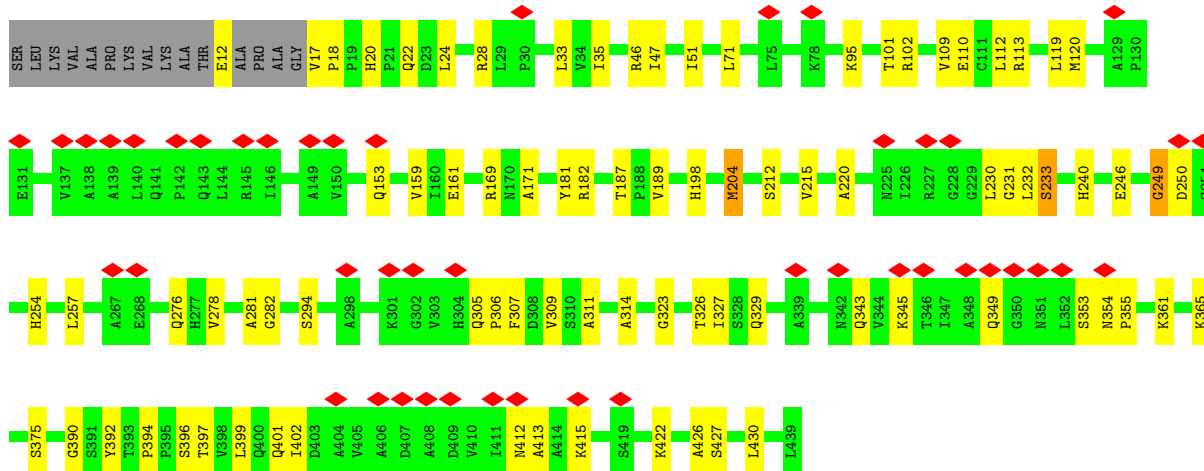
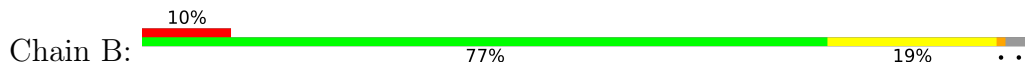


• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

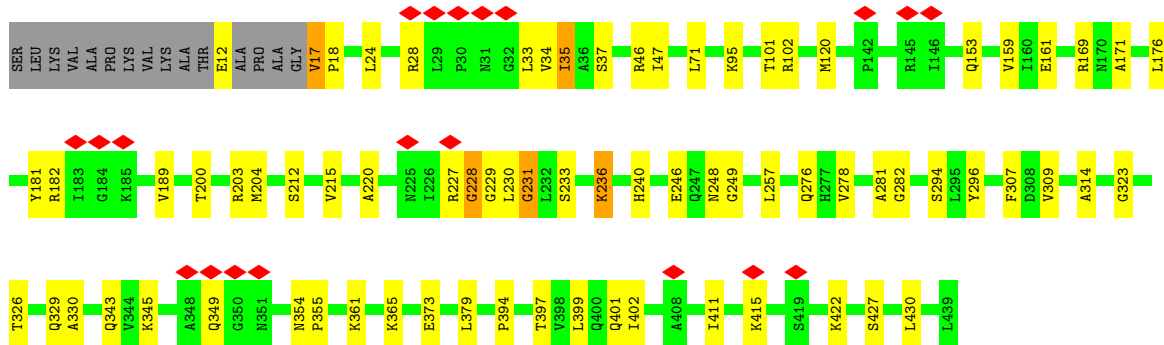
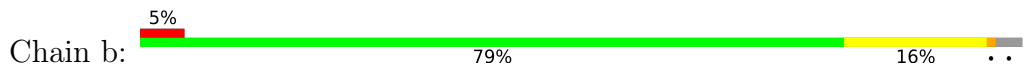




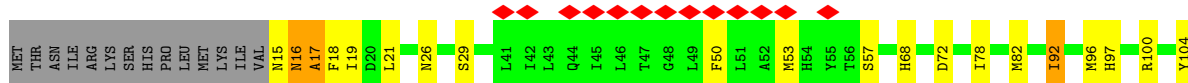
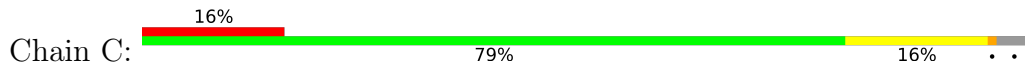
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

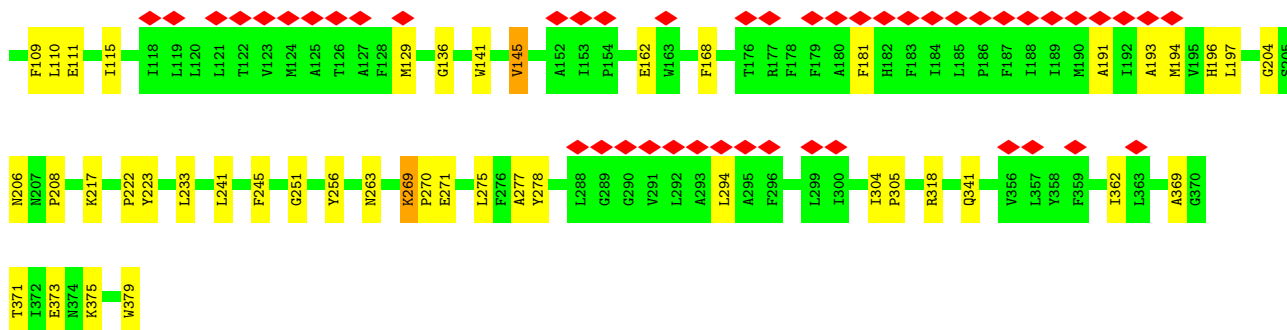


• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

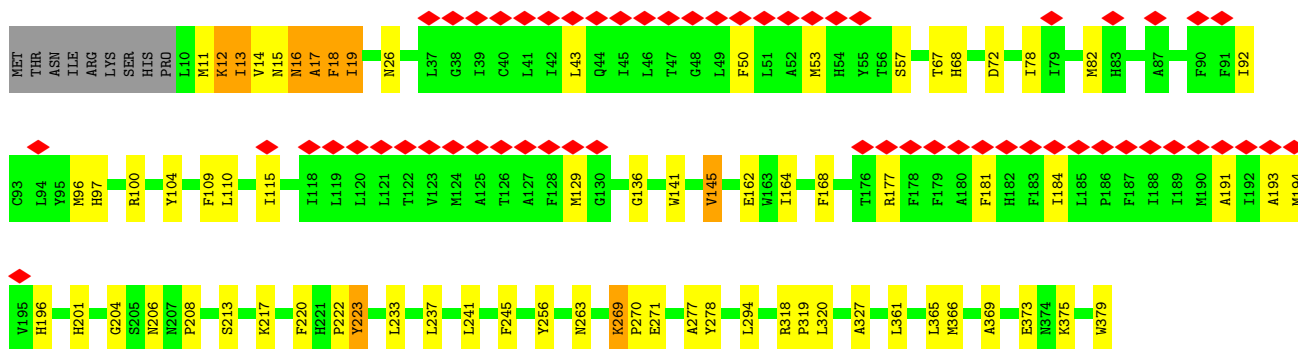
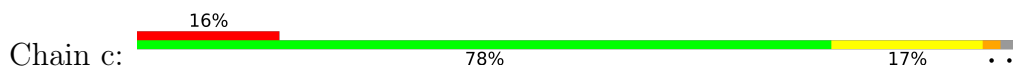


• Molecule 11: CYTOCHROME B

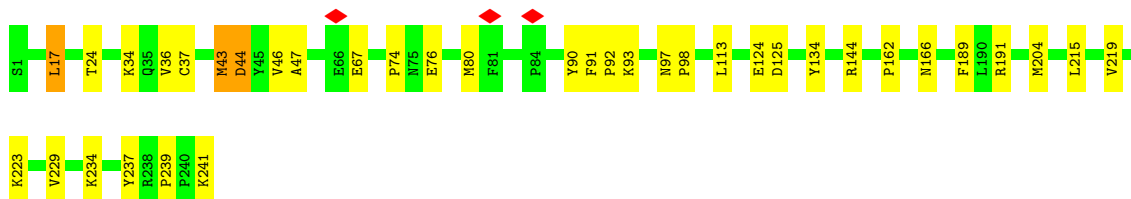
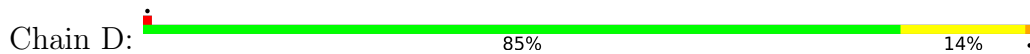




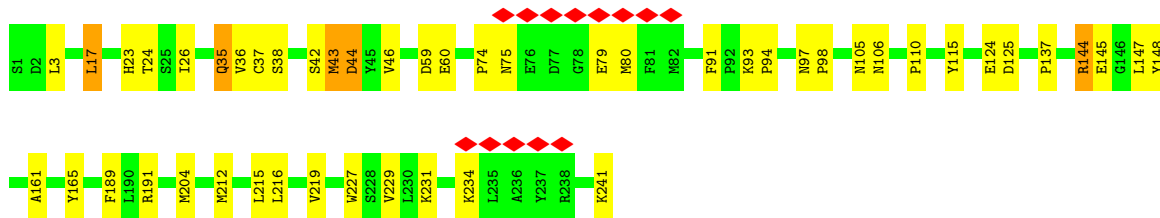
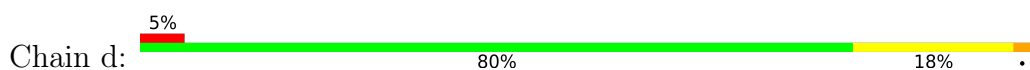
• Molecule 11: CYTOCHROME B



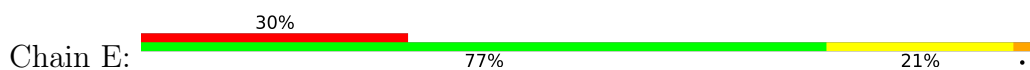
• Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



• Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



• Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



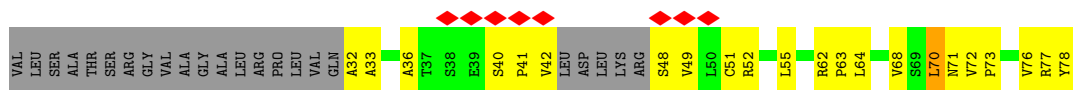
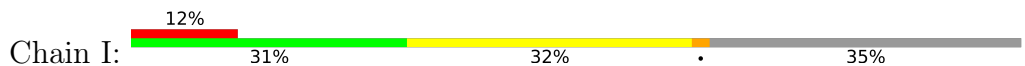
● Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



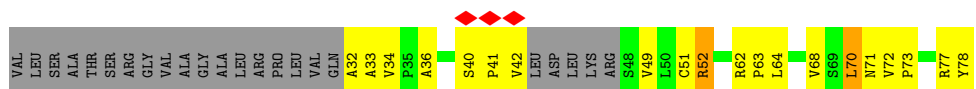
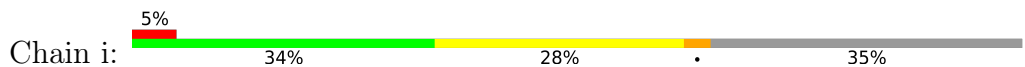
● Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



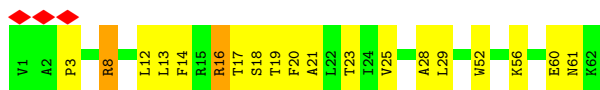
● Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



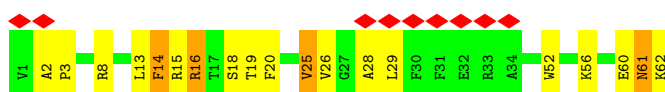
● Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



● Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

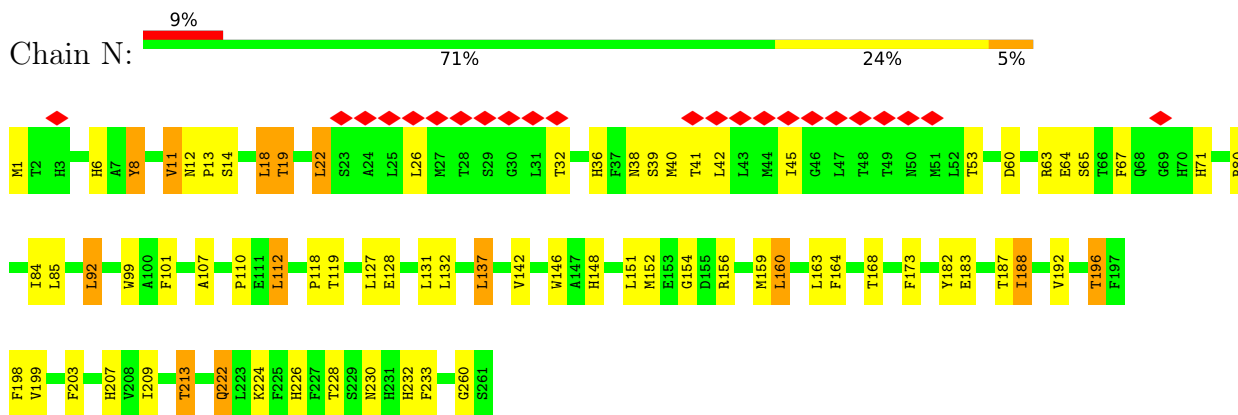


● Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

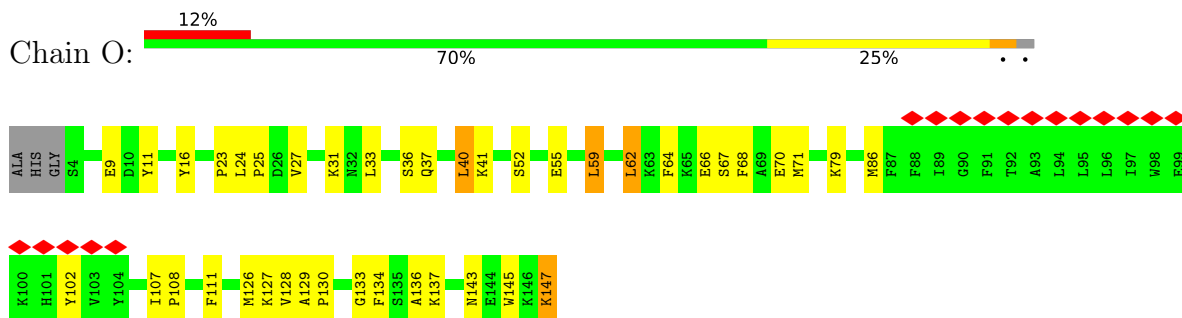


● Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

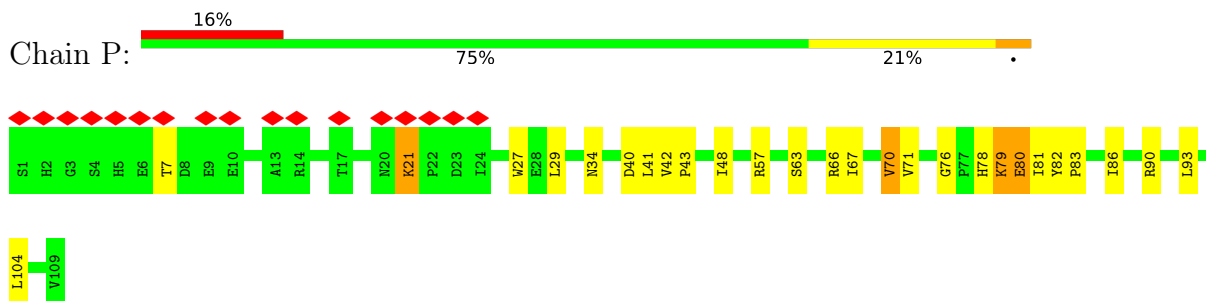




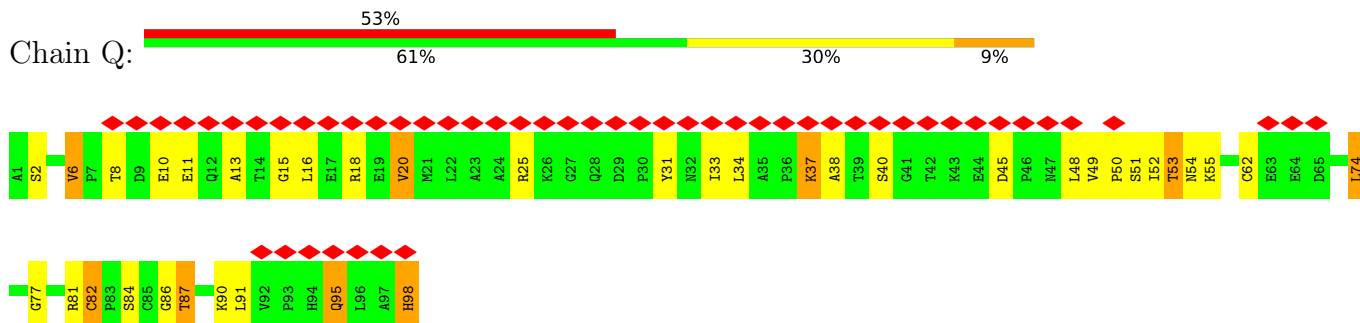
• Molecule 23: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1, MITOCHONDRIAL



• Molecule 24: CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL

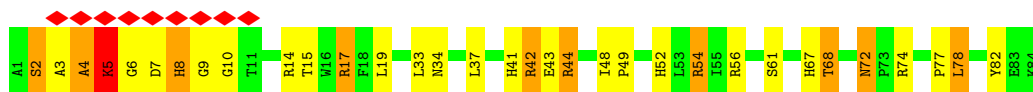


• Molecule 25: CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL

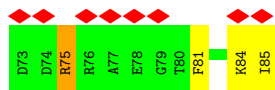
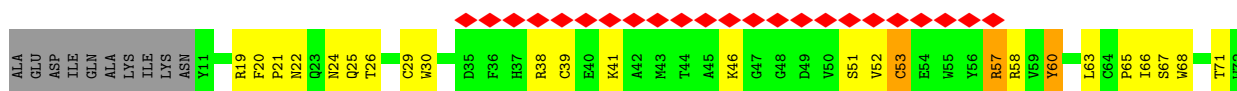


• Molecule 26: CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB





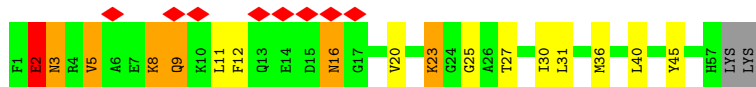
• Molecule 27: CYTOCHROME C OXIDASE SUBUNIT 6B1



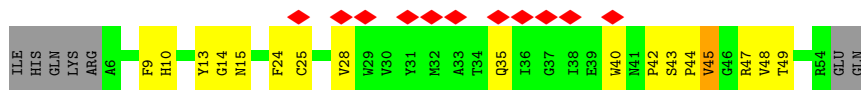
• Molecule 28: CYTOCHROME C OXIDASE SUBUNIT 6C



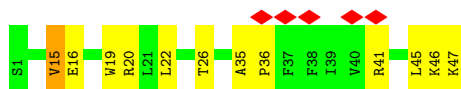
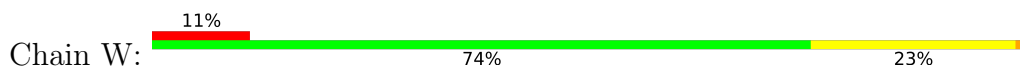
• Molecule 29: CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL



• Molecule 30: CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL

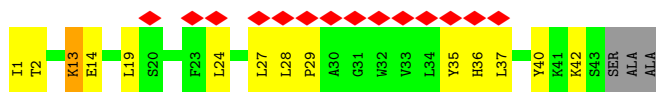


• Molecule 31: CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL

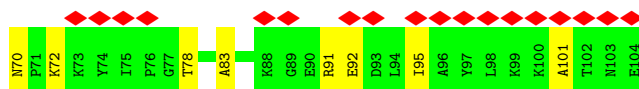
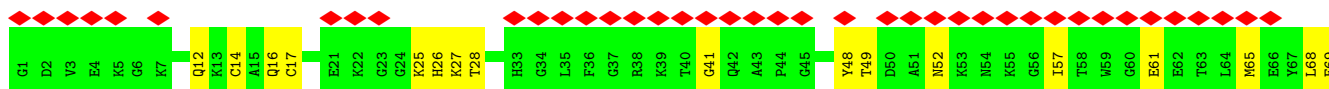
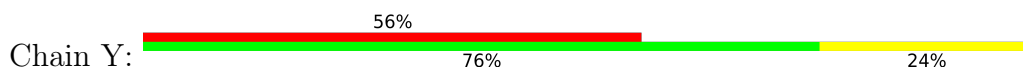


• Molecule 32: CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL

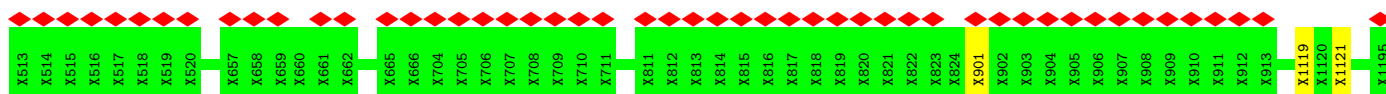
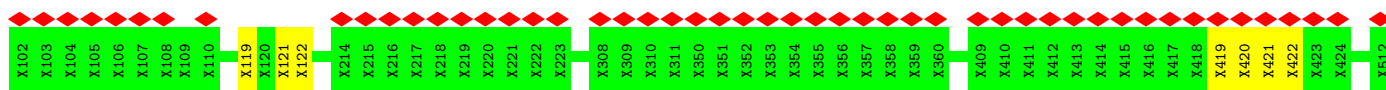




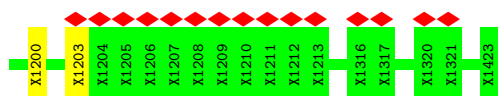
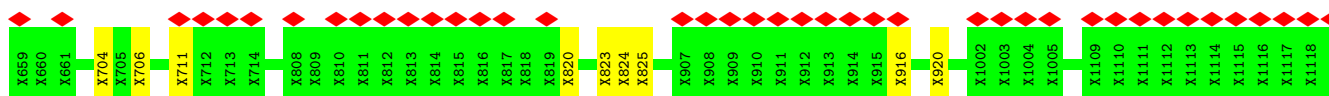
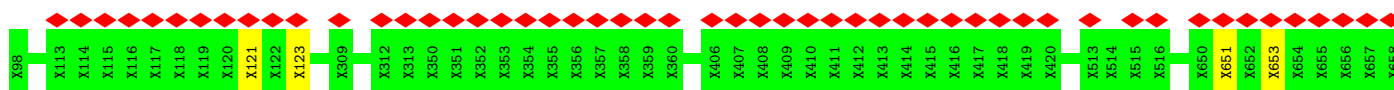
- Molecule 33: CYTOCHROME C



- Molecule 34: NADH\; UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,

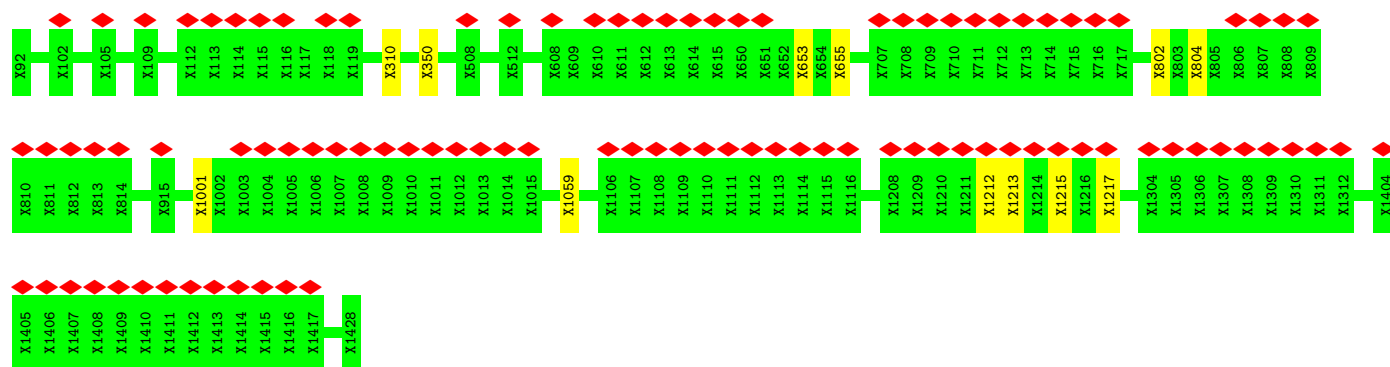


- Molecule 35: NADH\; UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,

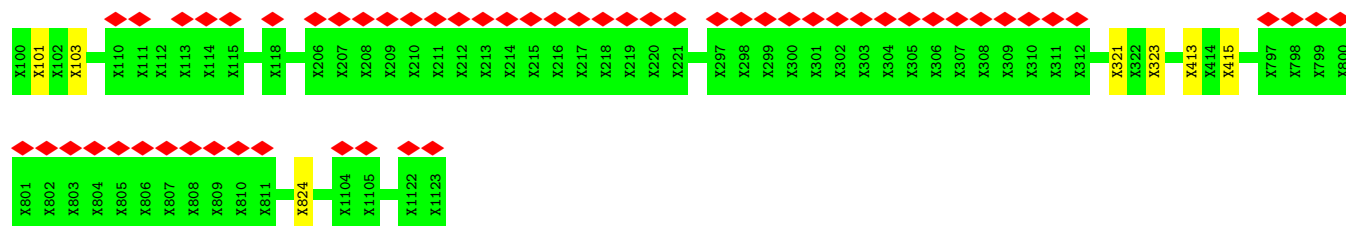


- Molecule 36: NADH-QUINONE OXIDOREDUCTASE SUBUNIT N





- Molecule 37: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10684	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE-FLIPPING ON EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	58829	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	18.839	Depositor
Minimum map value	-8.249	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.3	Depositor
Map size (\AA)	533.12, 533.12, 533.12	wwPDB
Map dimensions	112, 112, 112	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	4.76, 4.76, 4.76	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, MG, FES, CA, FMN, SMA, HEM, CU, HEC, UQ1, ZN, SF4, HEA, CDL

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	1	0.58	0/3506	1.00	17/4745 (0.4%)
2	2	0.55	0/1443	1.03	8/1958 (0.4%)
3	3	0.57	1/6019 (0.0%)	0.99	19/8163 (0.2%)
4	4	0.55	0/3096	0.93	8/4207 (0.2%)
5	5	0.57	0/1656	1.03	13/2246 (0.6%)
6	6	0.61	0/1126	1.05	5/1528 (0.3%)
7	7	0.55	0/1059	0.99	3/1429 (0.2%)
8	8	0.59	0/1224	1.10	8/1663 (0.5%)
9	A	0.43	0/3472	1.03	23/4714 (0.5%)
9	a	0.43	0/3472	1.01	21/4714 (0.4%)
10	B	0.43	0/3235	0.99	20/4387 (0.5%)
10	b	0.42	0/3239	1.01	17/4393 (0.4%)
11	C	0.49	0/2986	1.04	25/4089 (0.6%)
11	c	0.47	0/3024	1.02	23/4137 (0.6%)
12	D	0.45	0/1978	1.02	7/2684 (0.3%)
12	d	0.44	0/1978	1.04	13/2684 (0.5%)
13	E	0.41	0/1553	1.00	9/2100 (0.4%)
13	e	0.45	0/1553	1.01	11/2100 (0.5%)
14	F	0.40	0/878	0.96	5/1175 (0.4%)
14	f	0.42	0/878	0.98	6/1175 (0.5%)
15	G	0.39	0/642	1.01	7/869 (0.8%)
15	g	0.42	0/647	1.02	7/876 (0.8%)
16	H	0.40	0/544	0.93	3/729 (0.4%)
16	h	0.39	0/544	0.89	2/729 (0.3%)
17	I	0.49	0/285	1.14	3/384 (0.8%)
17	i	0.48	0/285	1.24	4/384 (1.0%)
18	J	0.41	0/520	0.94	0/699
18	j	0.43	0/520	0.94	1/699 (0.1%)
19	K	0.54	0/163	1.34	0/225
19	k	0.59	0/163	1.52	1/225 (0.4%)
20	L	0.86	7/4164 (0.2%)	1.16	35/5688 (0.6%)
21	M	0.77	0/1868	1.12	10/2544 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	N	0.74	0/2211	1.02	7/3023 (0.2%)
23	O	0.67	0/1229	0.96	3/1658 (0.2%)
24	P	0.64	0/898	1.02	6/1218 (0.5%)
25	Q	0.72	0/765	1.13	4/1038 (0.4%)
26	R	0.69	0/699	1.10	6/950 (0.6%)
27	S	0.68	0/648	1.18	5/877 (0.6%)
28	T	0.71	0/611	0.94	2/810 (0.2%)
29	U	0.70	0/451	1.04	3/610 (0.5%)
30	V	0.75	0/398	1.01	1/546 (0.2%)
31	W	0.77	0/399	0.97	2/534 (0.4%)
32	X	0.69	0/345	0.98	1/470 (0.2%)
33	Y	0.34	0/891	0.91	4/1186 (0.3%)
All	All	0.56	8/67265 (0.0%)	1.02	378/91262 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	k	0	1
34	m	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	61	HIS	CG-CD2	7.56	1.44	1.35
20	L	378	HIS	ND1-CE1	7.07	1.39	1.32
20	L	378	HIS	CE1-NE2	-6.57	1.25	1.32
20	L	69	MET	SD-CE	-6.25	1.64	1.79
20	L	61	HIS	ND1-CE1	5.68	1.38	1.32

The worst 5 of 378 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	b	228	GLY	N-CA-C	-14.09	95.71	115.30
3	3	115	HIS	CA-C-N	11.56	131.00	118.97
3	3	115	HIS	C-N-CA	11.56	131.00	118.97
3	3	218	LEU	CA-C-N	11.46	131.89	119.28
3	3	218	LEU	C-N-CA	11.46	131.89	119.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	k	24	TRP	Mainchain
34	m	1212	UNK	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3388	181	0
2	2	1410	0	1376	74	0
3	3	5880	0	5911	373	0
4	4	3018	0	3009	209	0
5	5	1607	0	1574	98	0
6	6	1102	0	1108	84	0
7	7	1031	0	1029	40	0
8	8	1193	0	1160	71	0
9	A	3403	0	3301	72	0
9	a	3403	0	3302	65	0
10	B	3177	0	3152	64	0
10	b	3180	0	3156	54	0
11	C	2892	0	2938	38	0
11	c	2931	0	2989	55	0
12	D	1919	0	1868	29	0
12	d	1919	0	1867	56	0
13	E	1519	0	1503	29	0
13	e	1519	0	1503	23	0
14	F	861	0	854	13	0
14	f	861	0	854	19	0
15	G	621	0	626	17	0
15	g	626	0	631	23	0
16	H	539	0	524	15	0
16	h	539	0	524	10	0
17	I	285	0	288	41	0
17	i	285	0	288	32	0
18	J	507	0	512	52	0
18	j	507	0	512	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	159	0	159	25	0
19	k	159	0	159	46	0
20	L	4025	0	4003	89	0
21	M	1822	0	1834	72	0
22	N	2124	0	2042	48	0
23	O	1195	0	1183	33	0
24	P	878	0	868	21	0
25	Q	748	0	728	25	0
26	R	672	0	645	30	0
27	S	628	0	582	22	0
28	T	598	0	612	14	0
29	U	442	0	439	16	0
30	V	384	0	366	11	0
31	W	386	0	388	8	0
32	X	335	0	352	13	0
33	Y	875	0	885	42	0
34	m	1422	0	52	11	0
35	n	1173	0	37	13	0
36	o	1134	0	36	10	0
37	p	843	0	24	6	0
38	1	8	0	0	0	0
38	3	24	0	0	3	0
38	6	8	0	0	1	0
38	8	16	0	0	2	0
39	1	31	0	19	7	0
40	1	44	0	27	5	0
41	1	1	0	0	0	0
41	2	1	0	0	0	0
41	3	2	0	0	0	0
41	4	1	0	0	0	0
41	5	1	0	0	0	0
41	L	1	0	0	0	0
42	2	4	0	0	0	0
42	3	4	0	0	1	0
42	E	4	0	0	0	0
42	e	4	0	0	0	0
43	7	1	0	0	0	0
44	C	86	0	60	5	0
44	Y	43	0	30	7	0
44	c	86	0	60	3	0
45	C	37	0	42	1	0
45	c	37	0	42	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	C	14	0	9	2	0
46	c	14	0	9	5	0
47	D	43	0	30	0	0
47	d	43	0	30	4	0
48	G	94	0	76	5	0
48	d	50	0	44	0	0
48	g	49	0	42	0	0
49	L	120	0	108	4	0
50	L	1	0	0	0	0
50	M	2	0	0	0	0
51	Q	1	0	0	0	0
52	A	187	0	0	11	0
52	B	149	0	0	2	0
52	C	125	0	0	4	0
52	D	118	0	0	2	0
52	E	54	0	0	2	0
52	F	57	0	0	3	0
52	G	24	0	0	1	0
52	H	14	0	0	0	0
52	I	16	0	0	2	0
52	J	5	0	0	0	0
52	Y	161	0	0	18	0
52	a	134	0	0	1	0
52	b	130	0	0	1	0
52	c	122	0	0	6	0
52	d	109	0	0	1	0
52	e	64	0	0	0	0
52	f	73	0	0	3	0
52	g	21	0	0	1	0
52	h	16	0	0	0	0
52	i	10	0	0	1	0
52	j	9	0	0	0	0
All	All	72626	0	65769	2146	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 16.

The worst 5 of 2146 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)
18:J:29:LEU:HD21	19:k:34:SER:CB	1.16	1.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:o:1001:UNK:CA	36:o:1059:UNK:C	1.85	1.52
18:J:29:LEU:CD2	19:k:34:SER:HB2	1.46	1.42
19:K:15:ARG:HG2	9:a:408:ARG:NH2	1.33	1.38
52:Y:350:HOH:O	12:d:106:ASN:HB2	1.24	1.29

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	1	435/438 (99%)	380 (87%)	48 (11%)	7 (2%)	7	38
2	2	177/181 (98%)	151 (85%)	22 (12%)	4 (2%)	5	28
3	3	748/783 (96%)	624 (83%)	101 (14%)	23 (3%)	3	22
4	4	374/409 (91%)	331 (88%)	34 (9%)	9 (2%)	4	27
5	5	194/207 (94%)	166 (86%)	24 (12%)	4 (2%)	5	30
6	6	140/181 (77%)	114 (81%)	21 (15%)	5 (4%)	2	20
7	7	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	16	54
8	8	152/182 (84%)	129 (85%)	22 (14%)	1 (1%)	18	56
9	A	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	24	63
9	a	441/446 (99%)	424 (96%)	16 (4%)	1 (0%)	43	78
10	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	43	78
10	b	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	24	63
11	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	16	54
11	c	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	9	40
12	D	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
12	d	239/241 (99%)	235 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	5	30
13	e	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	24	63
14	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
14	f	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
15	G	73/81 (90%)	72 (99%)	1 (1%)	0	100	100
15	g	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	9	40
16	H	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
16	h	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	7	38
17	I	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	4	25
17	i	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	4	25
18	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	36
18	j	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	36
19	K	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	1	16
19	k	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0	7
20	L	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
21	M	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
22	N	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
23	O	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
24	P	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
25	Q	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	17
26	R	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	13
27	S	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	40
28	T	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
29	U	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2	20
30	V	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
31	W	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
32	X	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
33	Y	109/104 (105%)	106 (97%)	3 (3%)	0	100	100
All	All	8228/8726 (94%)	7616 (93%)	511 (6%)	101 (1%)	13	44

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
2	2	108	PRO
3	3	6	VAL
3	3	117	LEU
3	3	216	PHE

5.3.2 Protein sidechains [i](#)

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	1	355/356 (100%)	316 (89%)	39 (11%)	6	20
2	2	150/152 (99%)	129 (86%)	21 (14%)	3	13
3	3	607/628 (97%)	553 (91%)	54 (9%)	9	28
4	4	326/355 (92%)	287 (88%)	39 (12%)	5	17
5	5	167/175 (95%)	151 (90%)	16 (10%)	8	25
6	6	117/149 (78%)	104 (89%)	13 (11%)	6	20
7	7	104/106 (98%)	99 (95%)	5 (5%)	23	44
8	8	126/150 (84%)	110 (87%)	16 (13%)	4	16
9	A	364/370 (98%)	358 (98%)	6 (2%)	55	70
9	a	364/370 (98%)	359 (99%)	5 (1%)	59	72
10	B	332/343 (97%)	332 (100%)	0	100	100
10	b	332/343 (97%)	330 (99%)	2 (1%)	78	83
11	C	312/327 (95%)	311 (100%)	1 (0%)	86	86
11	c	316/327 (97%)	313 (99%)	3 (1%)	70	79
12	D	206/206 (100%)	202 (98%)	4 (2%)	50	67
12	d	206/206 (100%)	202 (98%)	4 (2%)	50	67
13	E	168/168 (100%)	166 (99%)	2 (1%)	63	75
13	e	168/168 (100%)	164 (98%)	4 (2%)	43	64
14	F	90/98 (92%)	87 (97%)	3 (3%)	33	55
14	f	90/98 (92%)	87 (97%)	3 (3%)	33	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	G	66/71 (93%)	65 (98%)	1 (2%)	57	72
15	g	66/71 (93%)	64 (97%)	2 (3%)	36	57
16	H	63/74 (85%)	61 (97%)	2 (3%)	34	56
16	h	63/74 (85%)	62 (98%)	1 (2%)	55	70
17	I	28/51 (55%)	26 (93%)	2 (7%)	13	35
17	i	28/51 (55%)	25 (89%)	3 (11%)	6	21
18	J	51/52 (98%)	49 (96%)	2 (4%)	28	49
18	j	51/52 (98%)	49 (96%)	2 (4%)	28	49
19	K	15/46 (33%)	11 (73%)	4 (27%)	0	3
19	k	15/46 (33%)	10 (67%)	5 (33%)	0	2
20	L	427/427 (100%)	387 (91%)	40 (9%)	8	26
21	M	211/211 (100%)	191 (90%)	20 (10%)	8	25
22	N	226/226 (100%)	199 (88%)	27 (12%)	5	18
23	O	128/129 (99%)	118 (92%)	10 (8%)	11	32
24	P	95/95 (100%)	89 (94%)	6 (6%)	16	37
25	Q	81/81 (100%)	73 (90%)	8 (10%)	7	24
26	R	68/68 (100%)	52 (76%)	16 (24%)	1	5
27	S	67/75 (89%)	58 (87%)	9 (13%)	4	14
28	T	58/58 (100%)	51 (88%)	7 (12%)	5	17
29	U	47/50 (94%)	41 (87%)	6 (13%)	4	15
30	V	39/46 (85%)	36 (92%)	3 (8%)	12	32
31	W	40/40 (100%)	37 (92%)	3 (8%)	12	33
32	X	37/38 (97%)	34 (92%)	3 (8%)	11	31
33	Y	91/84 (108%)	91 (100%)	0	100	100
All	All	6961/7311 (95%)	6539 (94%)	422 (6%)	19	38

5 of 422 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	L	35	LEU
21	M	171	LYS
12	d	35	GLN
20	L	150	LEU
20	L	383	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
20	L	512	ASN
11	c	159	ASN
22	N	222	GLN
11	c	68	HIS
17	i	71	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 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	$\# Z > 2$
47	HEC	d	501	12	46,50,50	1.58	6 (13%)	58,82,82	1.86	4 (6%)
44	HEM	Y	500	33	50,50,50	1.68	12 (24%)	67,82,82	1.53	10 (14%)
48	CDL	d	3003	-	49,49,99	1.10	3 (6%)	55,61,111	1.17	4 (7%)
38	SF4	8	183	8	0,12,12	-	-	-	-	-
38	SF4	3	786	3	0,12,12	-	-	-	-	-
39	FMN	1	440	-	33,33,33	1.22	2 (6%)	48,50,50	1.88	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	HEA	L	515	20	67,67,67	1.21	4 (5%)	81,103,103	1.35	10 (12%)
38	SF4	1	439	1	0,12,12	-	-	-		
38	SF4	8	184	8	0,12,12	-	-	-		
44	HEM	C	502	11	50,50,50	1.62	8 (16%)	67,82,82	1.67	13 (19%)
44	HEM	c	502	11	50,50,50	1.83	12 (24%)	67,82,82	1.38	10 (14%)
42	FES	3	787	3	0,4,4	-	-	-		
48	CDL	G	2003	-	49,49,99	1.11	2 (4%)	55,61,111	1.11	4 (7%)
44	HEM	c	501	11	50,50,50	1.65	6 (12%)	67,82,82	1.22	7 (10%)
45	SMA	C	2001	-	38,38,38	1.44	7 (18%)	47,52,52	1.08	3 (6%)
42	FES	e	501	13	0,4,4	-	-	-		
42	FES	2	182	2	0,4,4	-	-	-		
48	CDL	g	3004	-	48,48,99	1.15	4 (8%)	54,60,111	1.13	2 (3%)
38	SF4	3	784	3	0,12,12	-	-	-		
44	HEM	C	501	11	50,50,50	1.77	8 (16%)	67,82,82	1.71	18 (26%)
48	CDL	G	2004	-	43,43,99	1.14	2 (4%)	49,55,111	1.23	4 (8%)
42	FES	E	501	13	0,4,4	-	-	-		
38	SF4	3	785	3	0,12,12	-	-	-		
46	UQ1	C	2002	-	14,14,18	2.31	8 (57%)	20,20,25	0.54	0
47	HEC	D	501	12	46,50,50	1.51	4 (8%)	58,82,82	2.02	4 (6%)
38	SF4	6	182	6	0,12,12	-	-	-		
45	SMA	c	3001	-	38,38,38	1.59	10 (26%)	47,52,52	1.12	4 (8%)
46	UQ1	c	3002	-	14,14,18	2.11	8 (57%)	20,20,25	0.42	0
49	HEA	L	516	20	67,67,67	1.19	7 (10%)	81,103,103	1.33	13 (16%)
40	NAI	1	441	-	47,48,48	4.06	33 (70%)	64,73,73	1.71	14 (21%)

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
47	HEC	d	501	12	-	8/14/54/54	-
44	HEM	Y	500	33	-	4/14/54/54	-
48	CDL	d	3003	-	-	37/58/58/110	-
38	SF4	8	183	8	-	-	0/6/5/5
38	SF4	3	786	3	-	-	0/6/5/5
39	FMN	1	440	-	-	6/18/18/18	0/3/3/3
49	HEA	L	515	20	-	6/36/76/76	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SF4	1	439	1	-	-	0/6/5/5
38	SF4	8	184	8	-	-	0/6/5/5
44	HEM	C	502	11	-	4/14/54/54	-
44	HEM	c	502	11	-	4/14/54/54	-
42	FES	3	787	3	-	-	0/1/1/1
48	CDL	G	2003	-	-	26/58/58/110	-
44	HEM	c	501	11	-	4/14/54/54	-
48	CDL	g	3004	-	-	20/57/57/110	-
45	SMA	C	2001	-	-	2/34/34/34	0/2/2/2
42	FES	2	182	2	-	-	0/1/1/1
42	FES	e	501	13	-	-	0/1/1/1
44	HEM	C	501	11	-	4/14/54/54	-
48	CDL	G	2004	-	-	35/52/52/110	-
38	SF4	3	784	3	-	-	0/6/5/5
42	FES	E	501	13	-	-	0/1/1/1
46	UQ1	C	2002	-	-	0/4/28/33	0/1/1/1
38	SF4	3	785	3	-	-	0/6/5/5
47	HEC	D	501	12	-	8/14/54/54	-
45	SMA	c	3001	-	-	2/34/34/34	0/2/2/2
49	HEA	L	516	20	-	7/36/76/76	-
46	UQ1	c	3002	-	-	2/4/28/33	0/1/1/1
38	SF4	6	182	6	-	-	0/6/5/5
40	NAI	1	441	-	-	8/29/72/72	0/5/5/5

The worst 5 of 146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	C2A-N1A	11.94	1.55	1.33
40	1	441	NAI	PA-O3	7.65	1.67	1.59
40	1	441	NAI	C5A-N7A	7.42	1.52	1.39
40	1	441	NAI	C8A-N9A	7.35	1.50	1.37
40	1	441	NAI	PN-O3	6.34	1.66	1.59

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	D	501	HEC	CBB-CAB-C3B	-9.78	107.89	127.43
47	d	501	HEC	CBB-CAB-C3B	-9.61	108.22	127.43
47	D	501	HEC	CBC-CAC-C3C	-8.83	109.79	127.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	C	502	HEM	C3B-C4B-NB	6.75	114.32	109.47
47	d	501	HEC	CBC-CAC-C3C	-6.33	114.79	127.43

There are no chirality outliers.

5 of 187 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	1	440	FMN	N10-C1'-C2'-O2'
39	1	440	FMN	N10-C1'-C2'-C3'
39	1	440	FMN	C1'-C2'-C3'-O3'
39	1	440	FMN	C1'-C2'-C3'-C4'
40	1	441	NAI	O4B-C4B-C5B-O5B

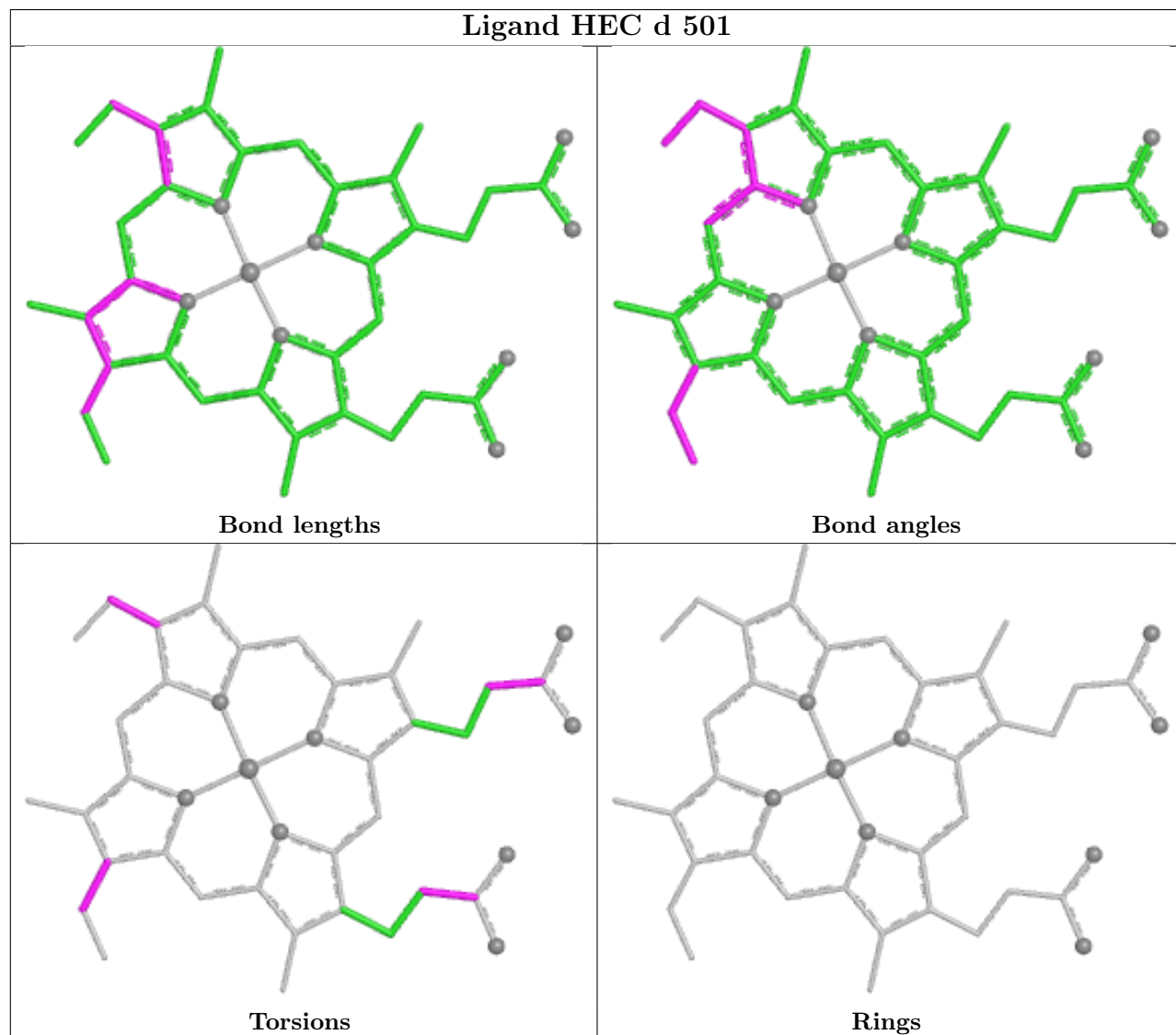
There are no ring outliers.

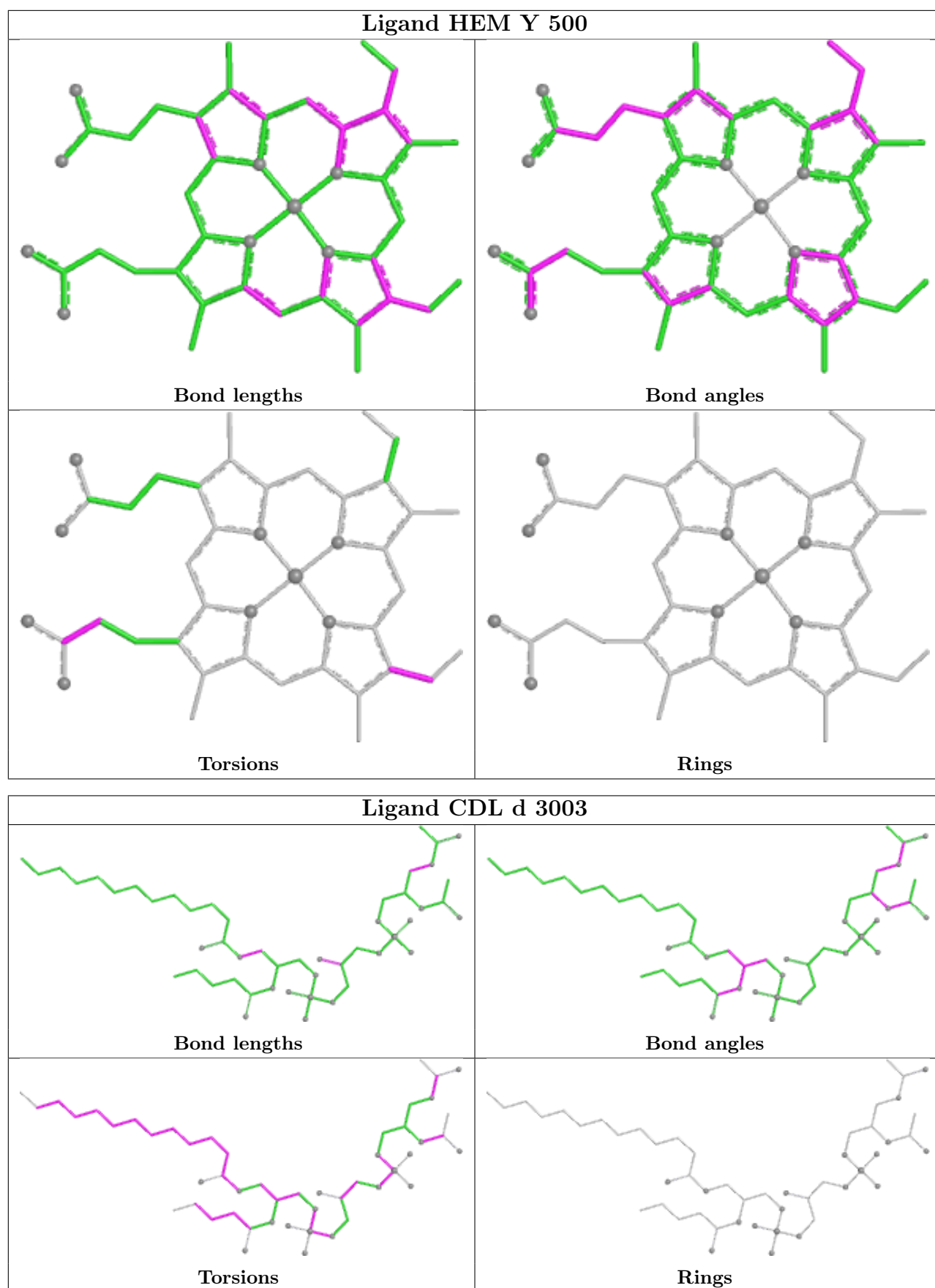
21 monomers are involved in 54 short contacts:

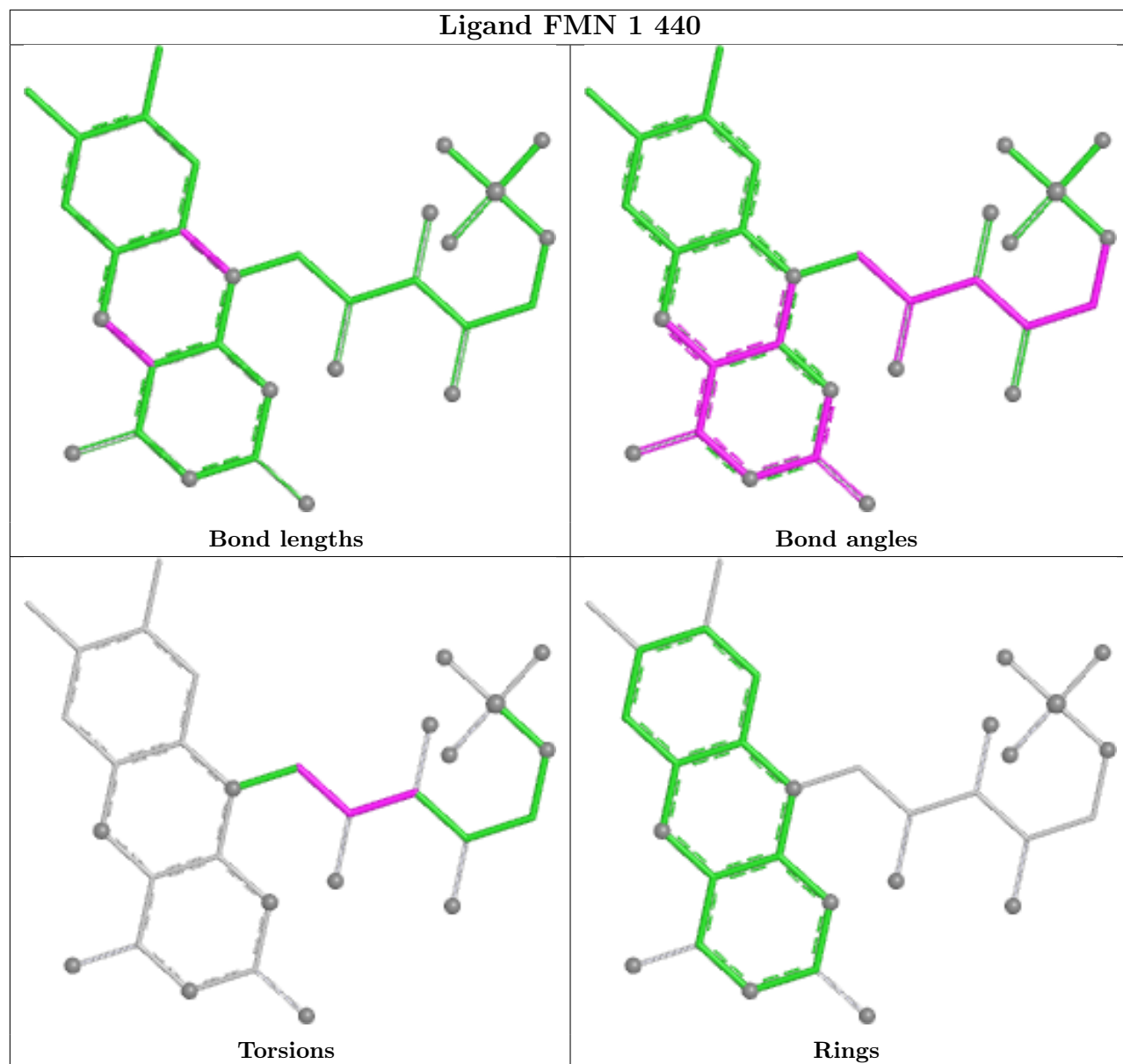
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	d	501	HEC	4	0
44	Y	500	HEM	7	0
38	8	183	SF4	2	0
38	3	786	SF4	1	0
39	1	440	FMN	7	0
49	L	515	HEA	1	0
44	C	502	HEM	3	0
44	c	502	HEM	2	0
42	3	787	FES	1	0
44	c	501	HEM	1	0
45	C	2001	SMA	1	0
38	3	784	SF4	1	0
44	C	501	HEM	2	0
48	G	2004	CDL	5	0
38	3	785	SF4	1	0
46	C	2002	UQ1	2	0
38	6	182	SF4	1	0
45	c	3001	SMA	1	0
46	c	3002	UQ1	5	0
49	L	516	HEA	3	0
40	1	441	NAI	5	0

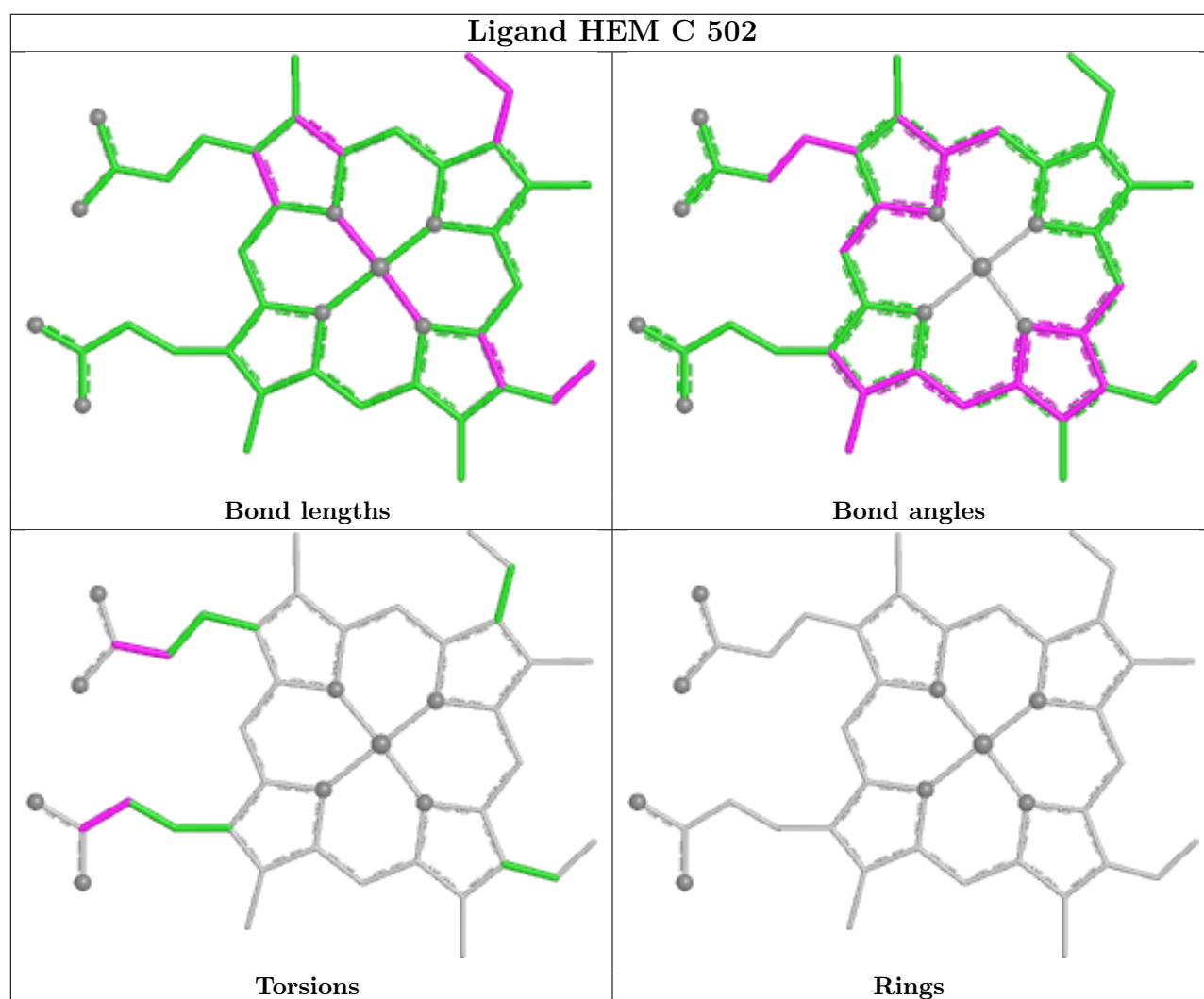
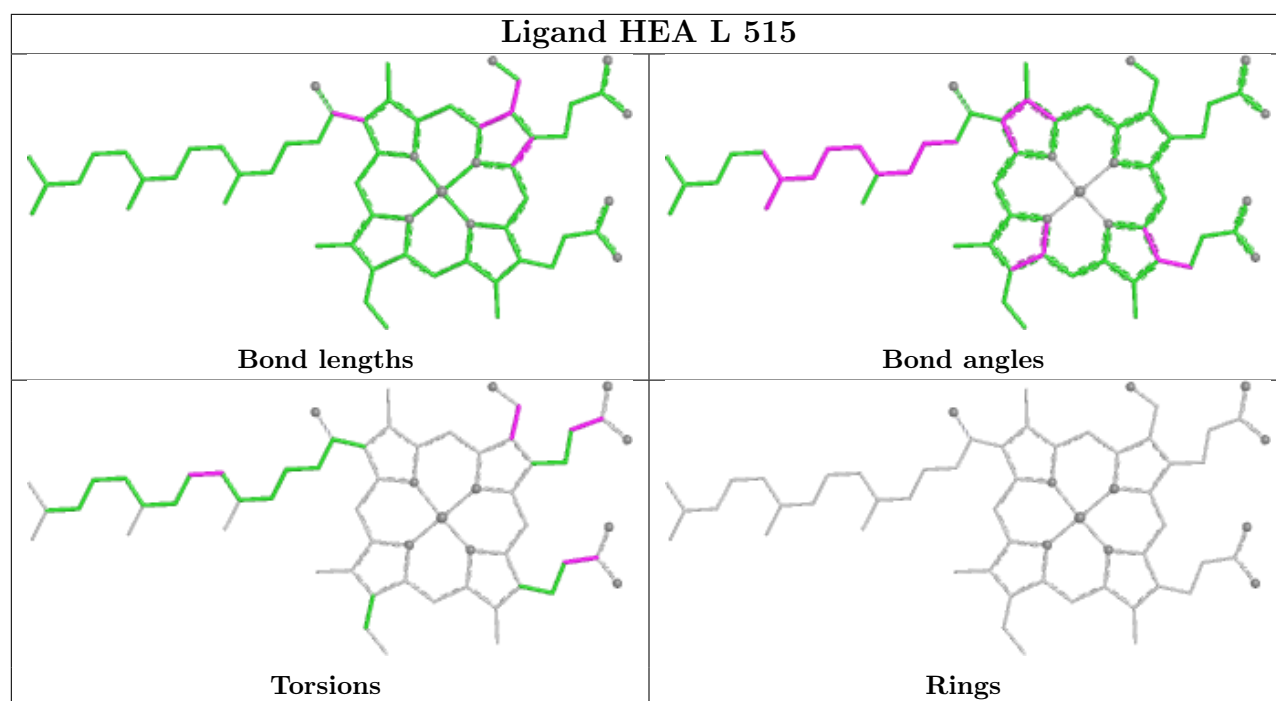
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

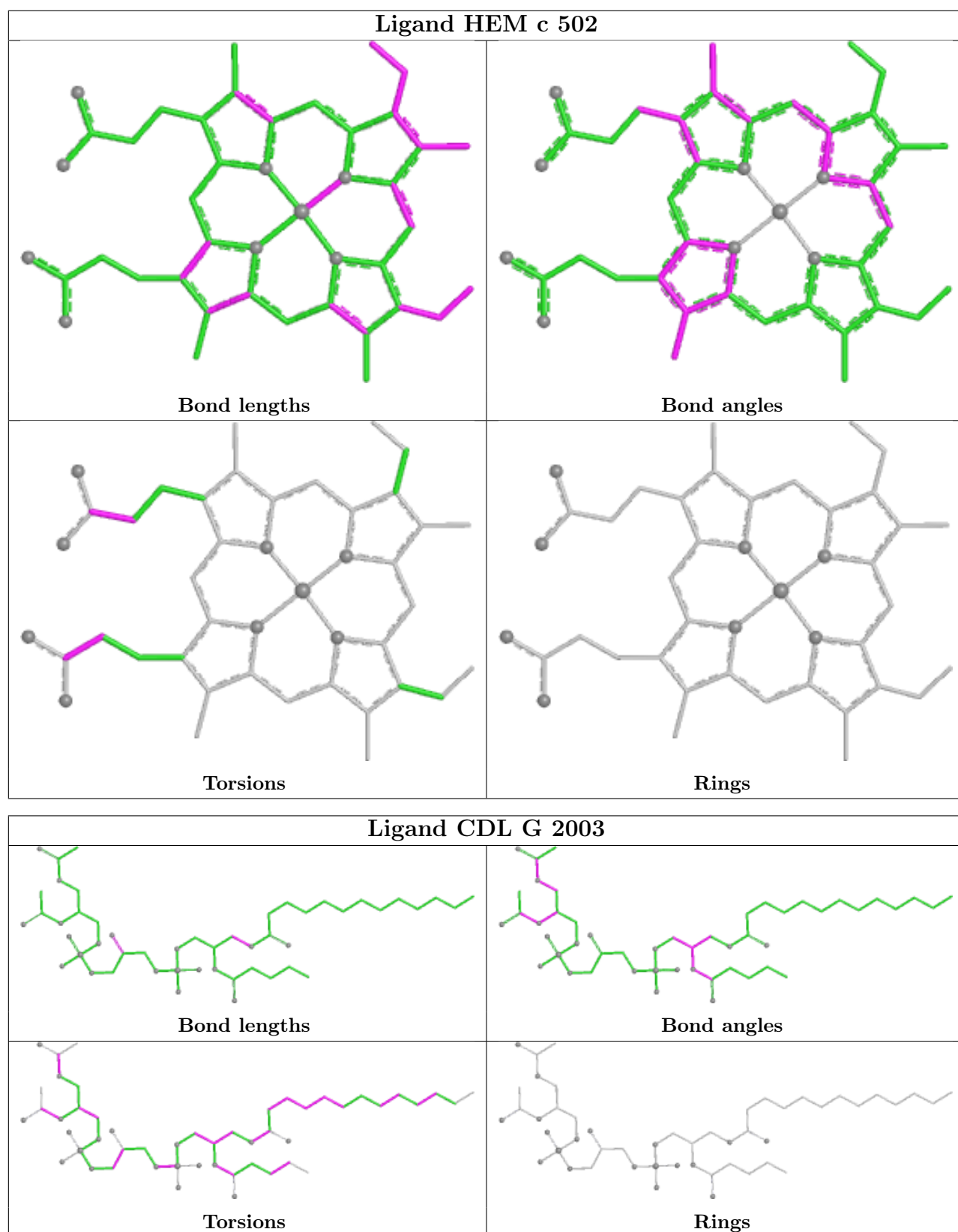
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

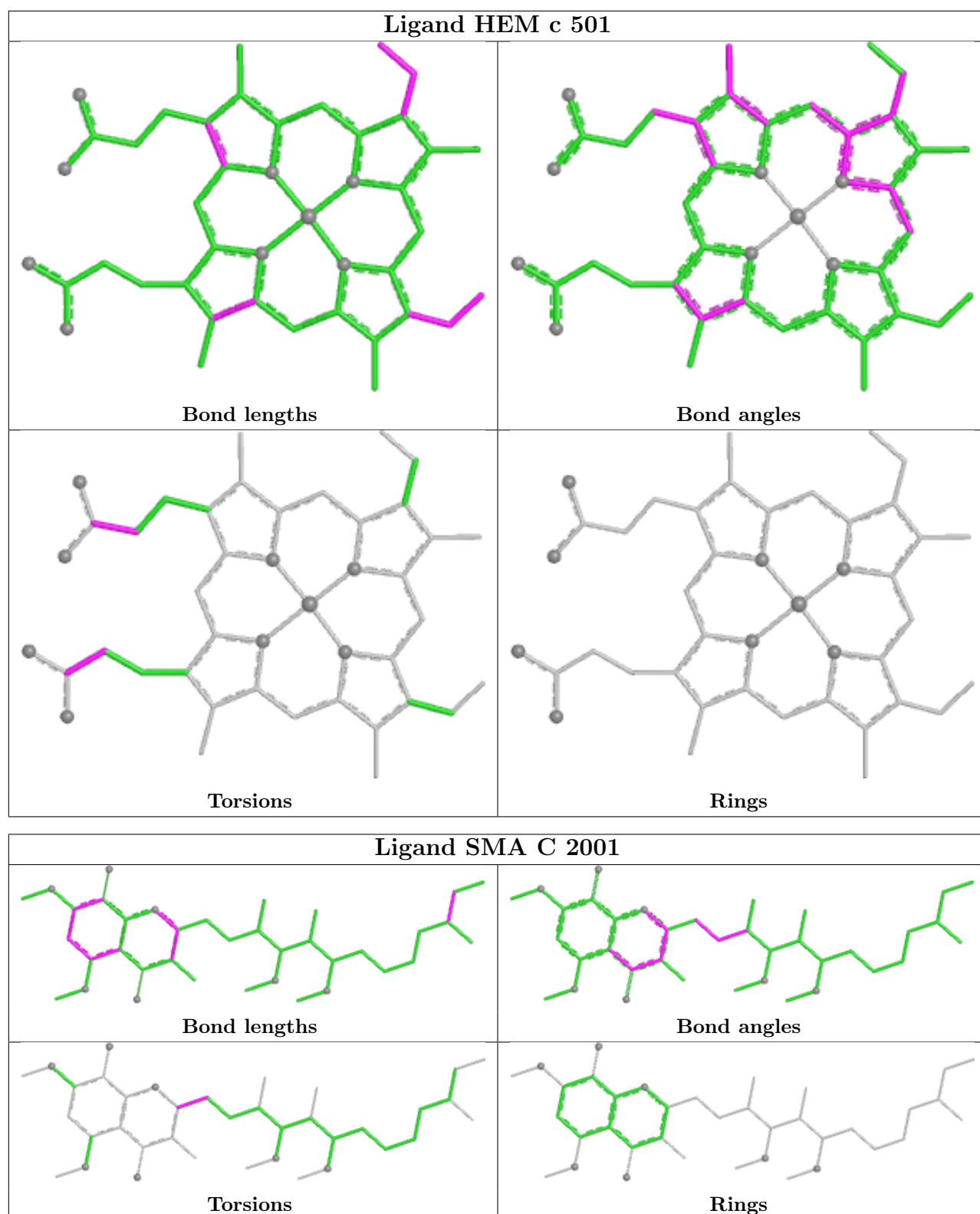


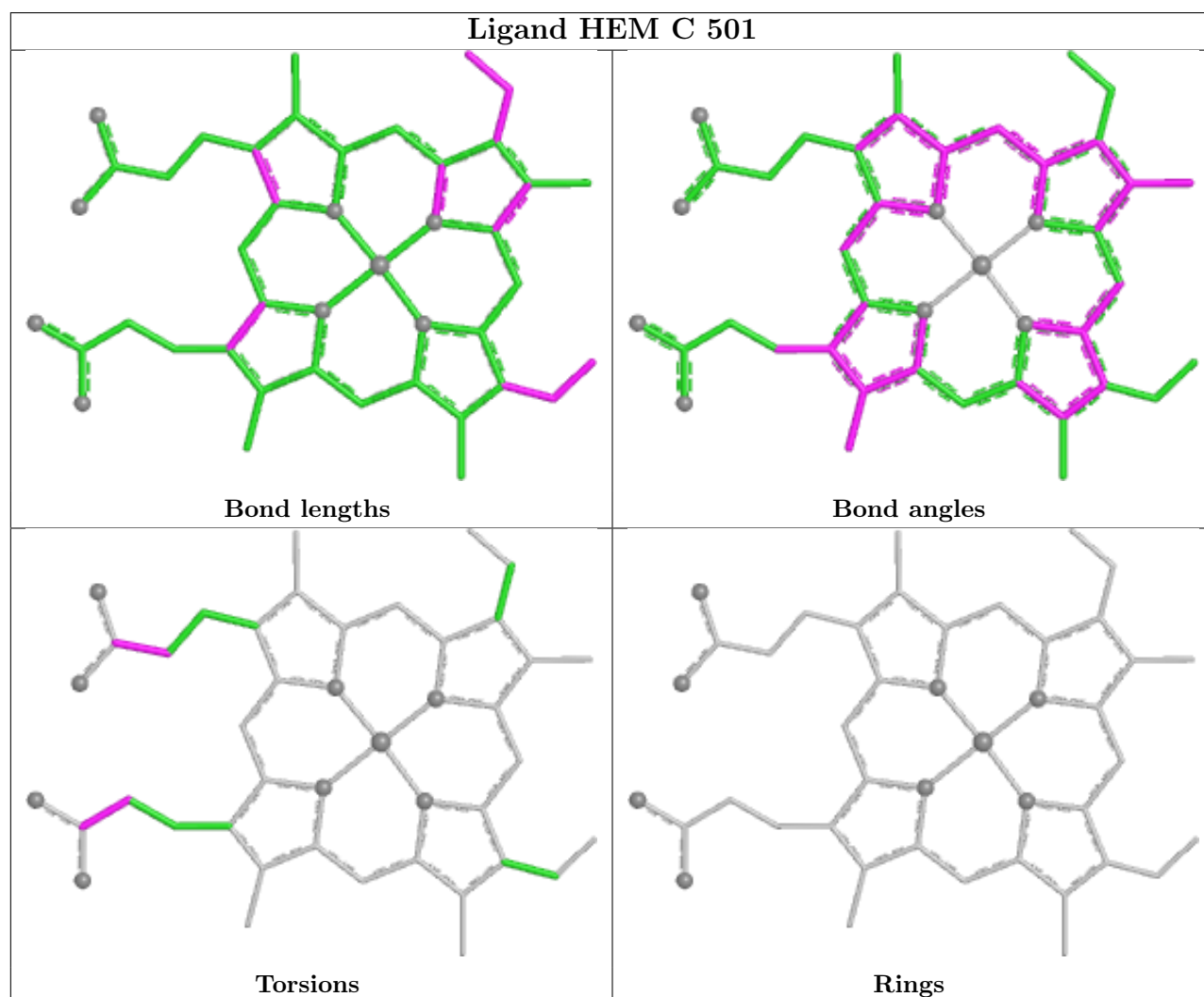
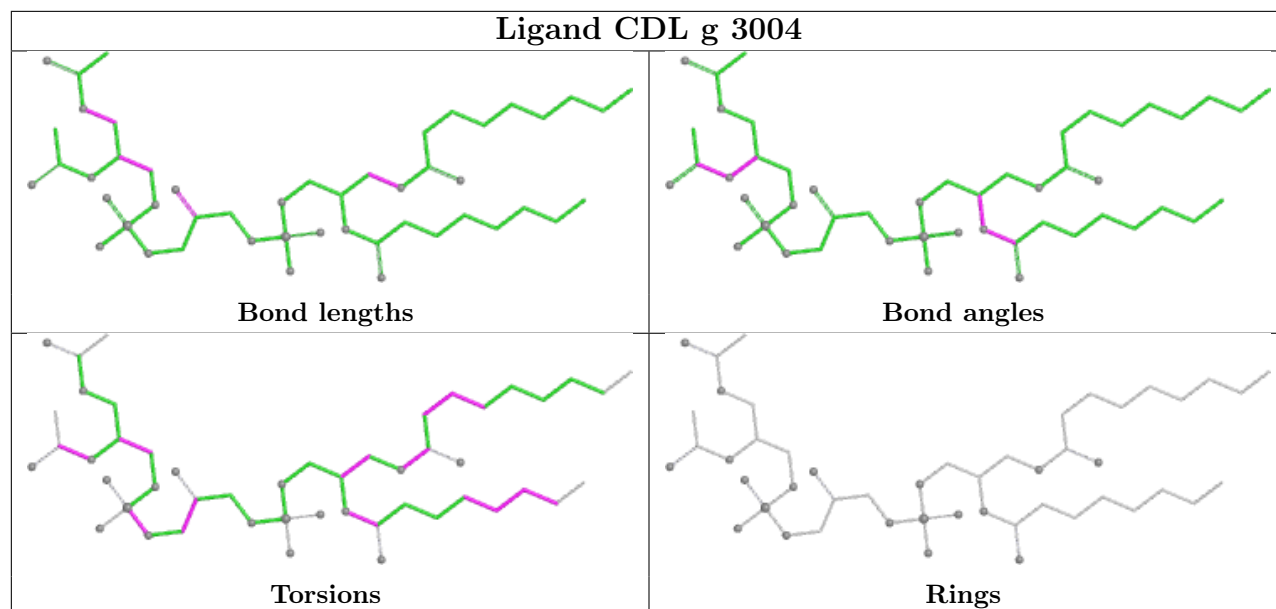


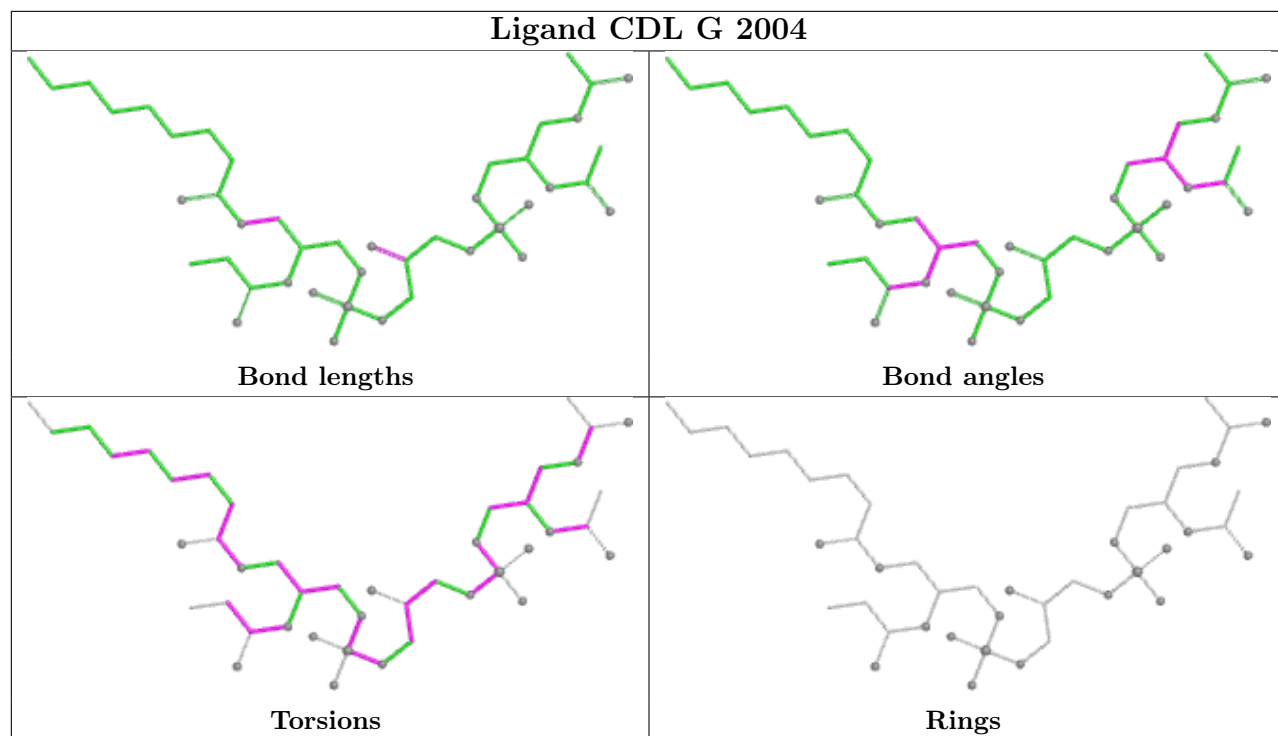


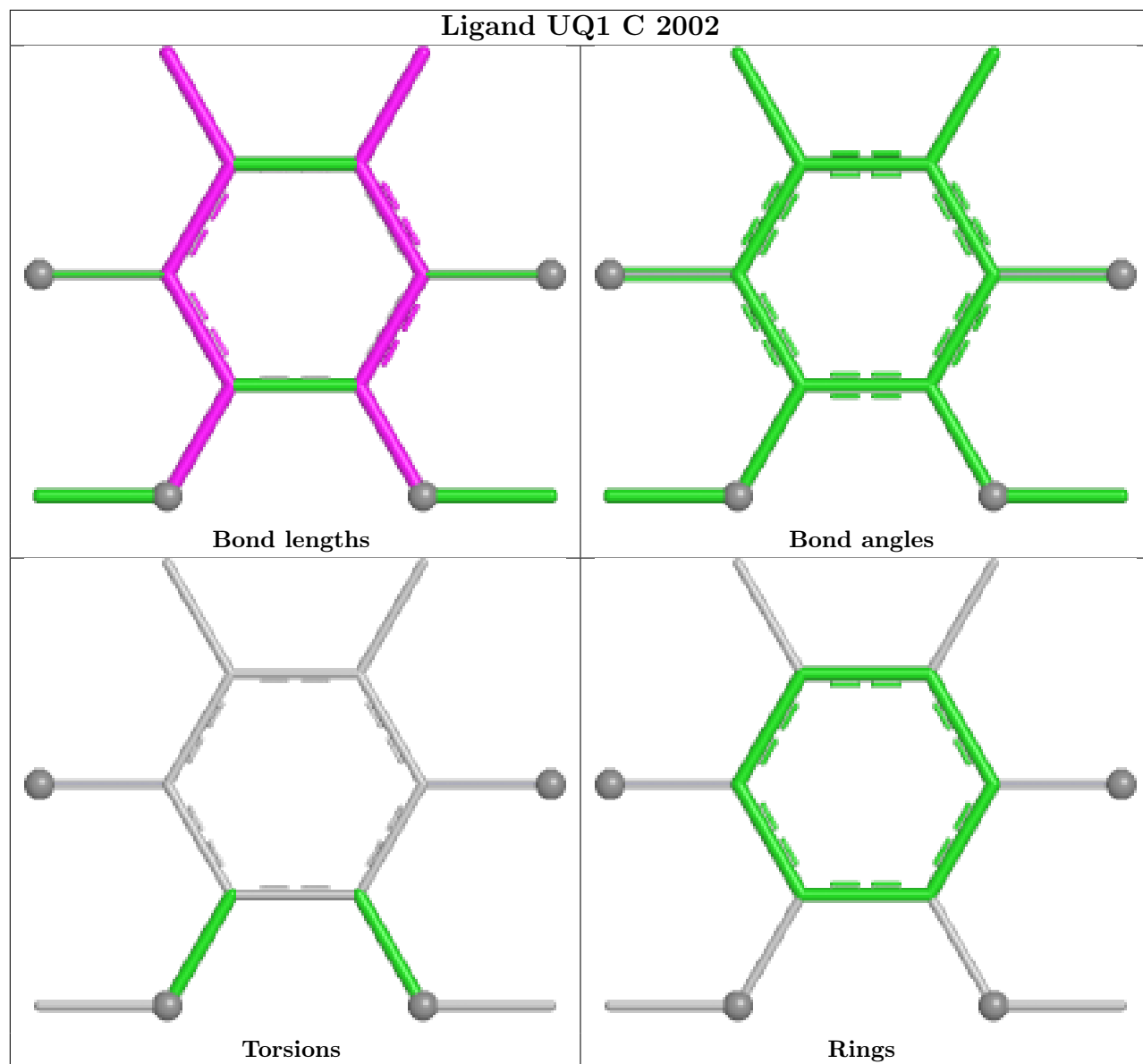


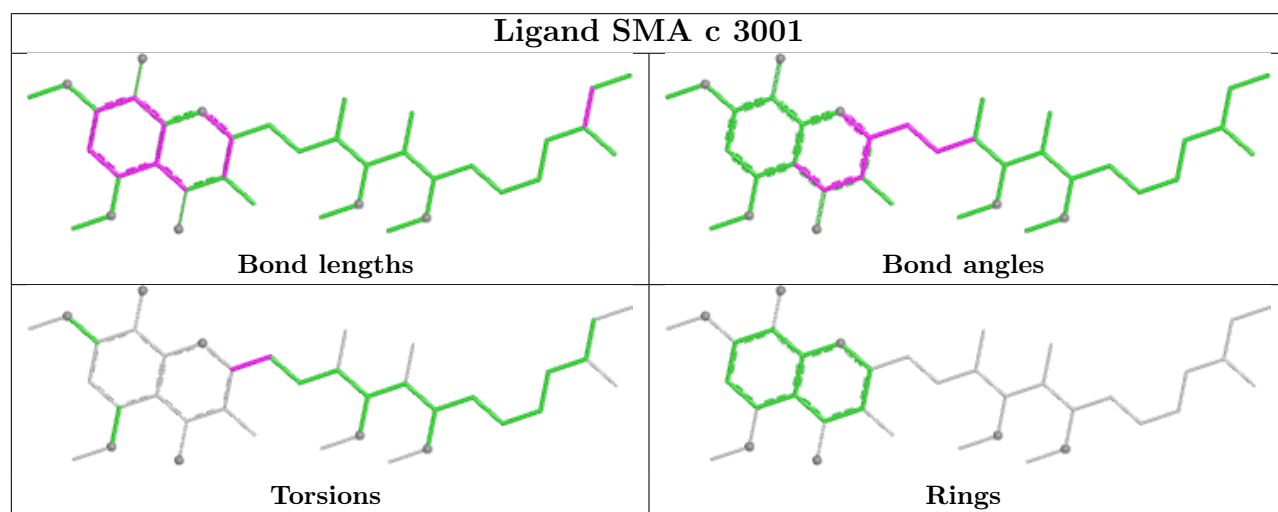
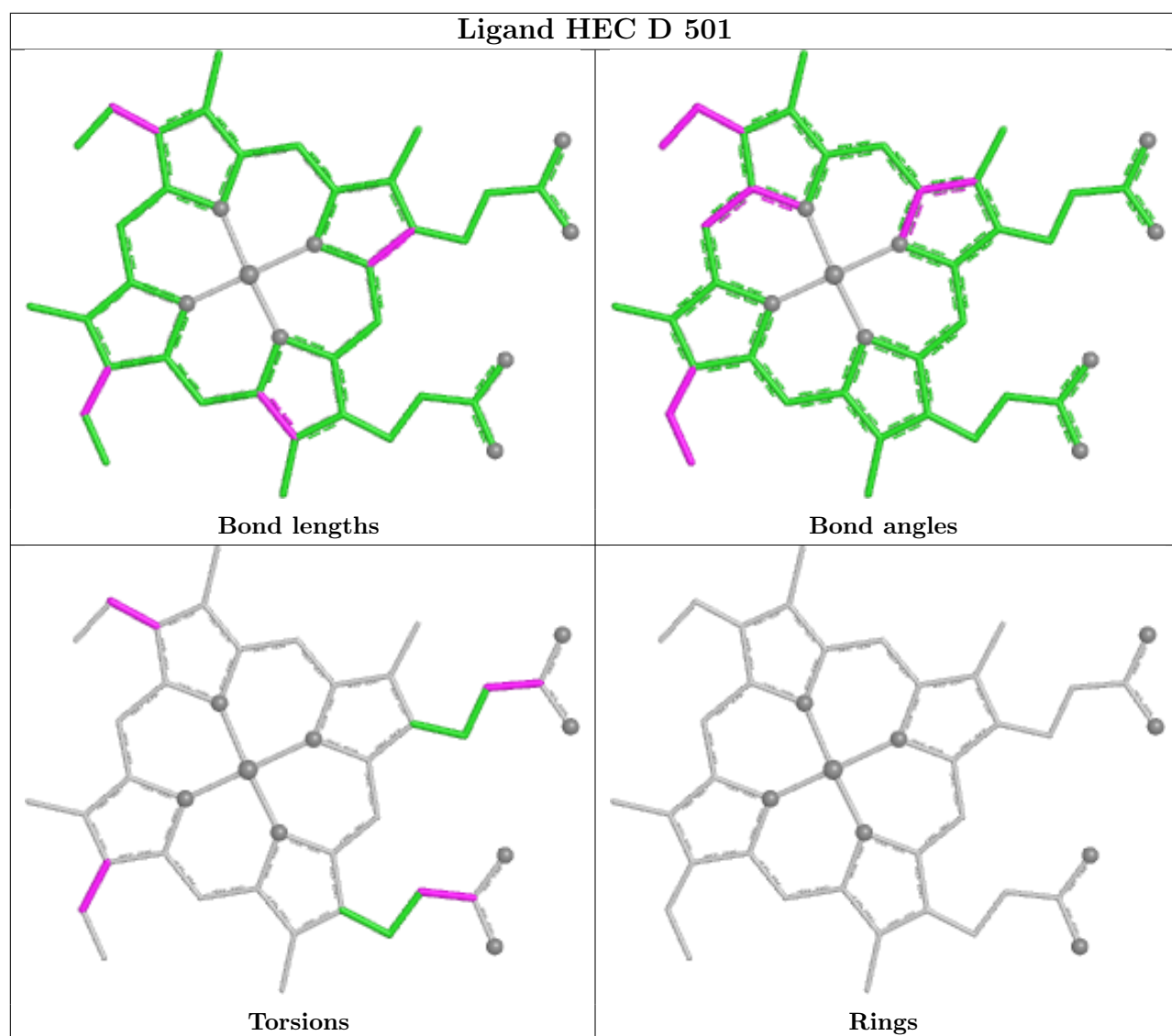


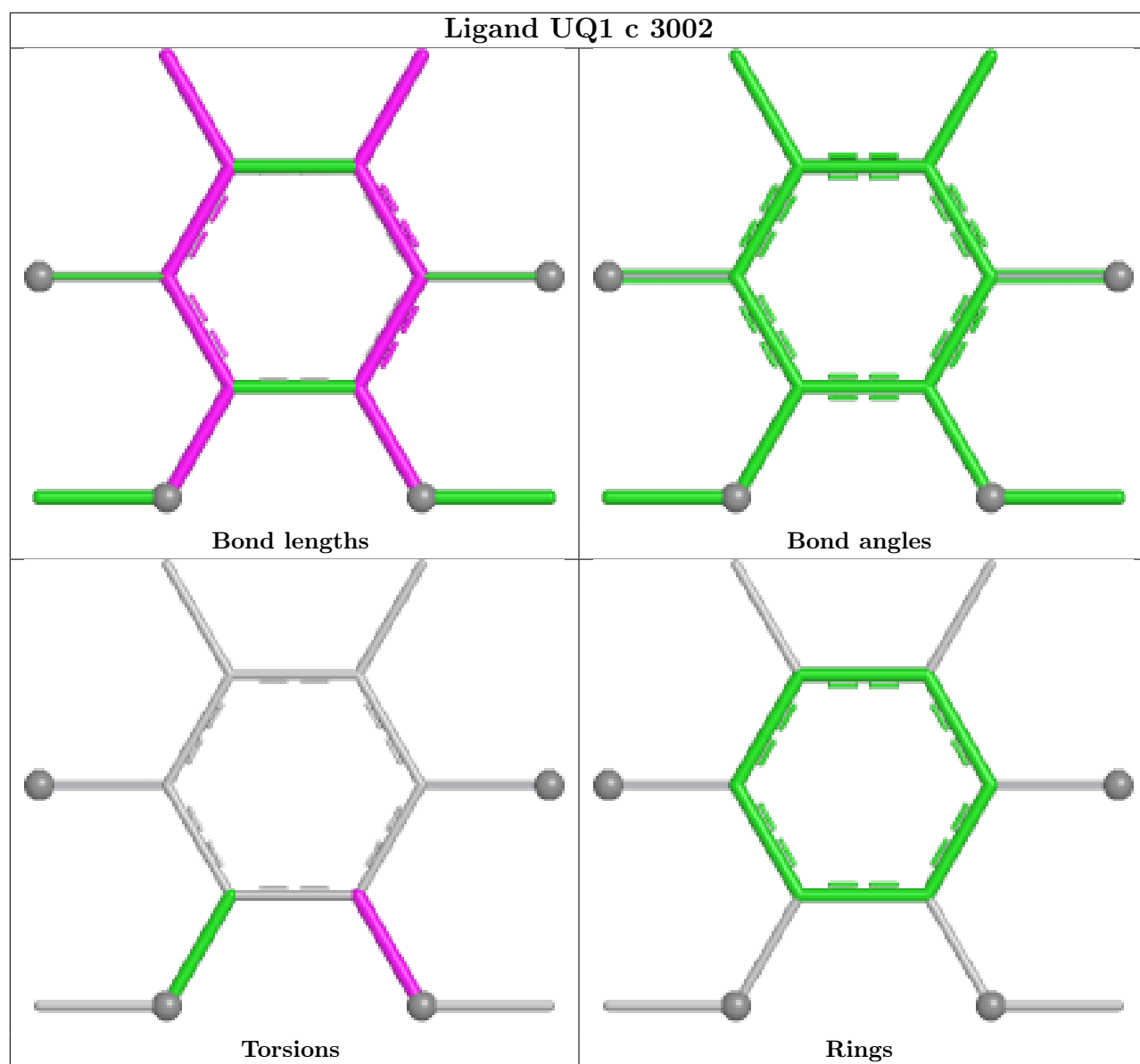


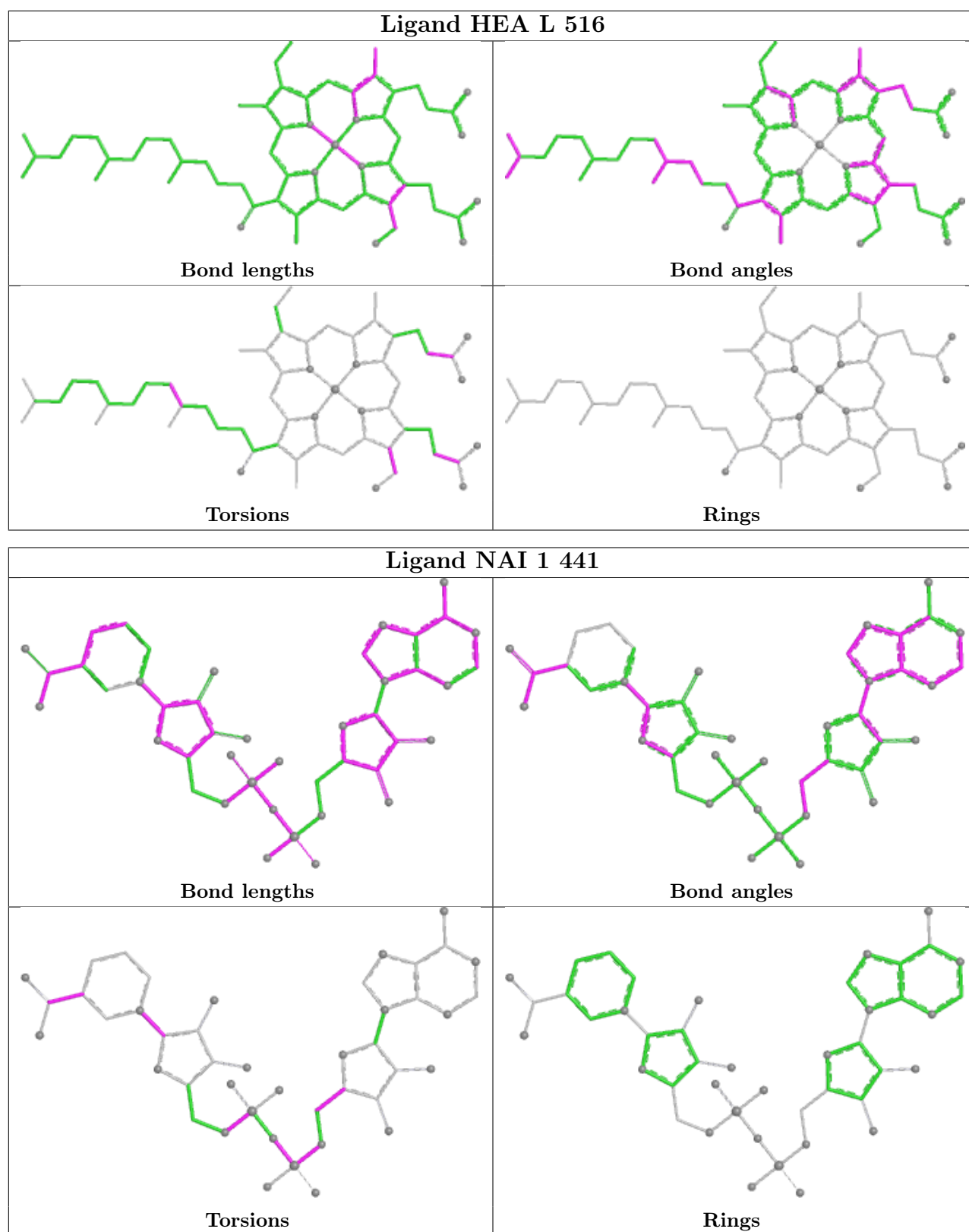












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	m	20
35	n	16
36	o	16
37	p	10
29	U	1

The worst 5 of 63 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m	428:UNK	C	495:UNK	N	56.90
1	n	1024:UNK	C	1050:UNK	N	55.04
1	o	366:UNK	C	395:UNK	N	50.88
1	m	1417:UNK	C	1501:UNK	N	47.70
1	o	665:UNK	C	700:UNK	N	47.65

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1876. 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

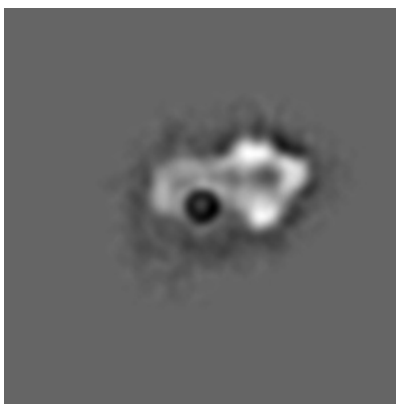
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 56



Y Index: 56



Z Index: 56

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: 67



Y Index: 37



Z Index: 45

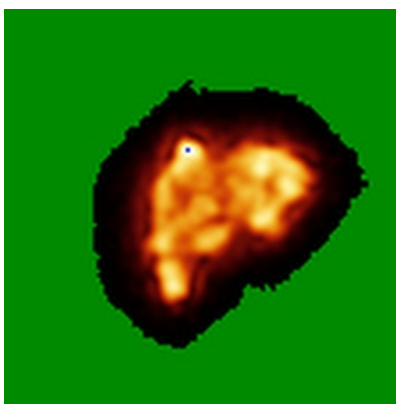
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

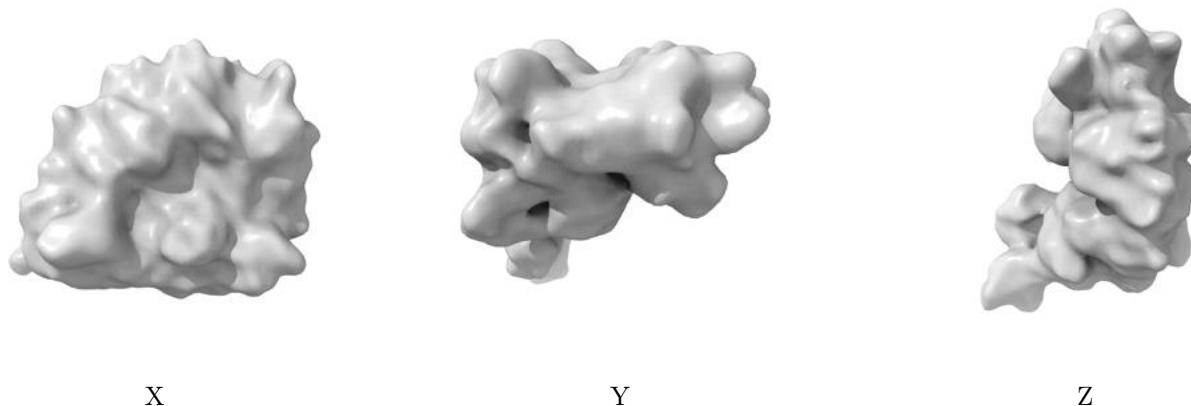


Z

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

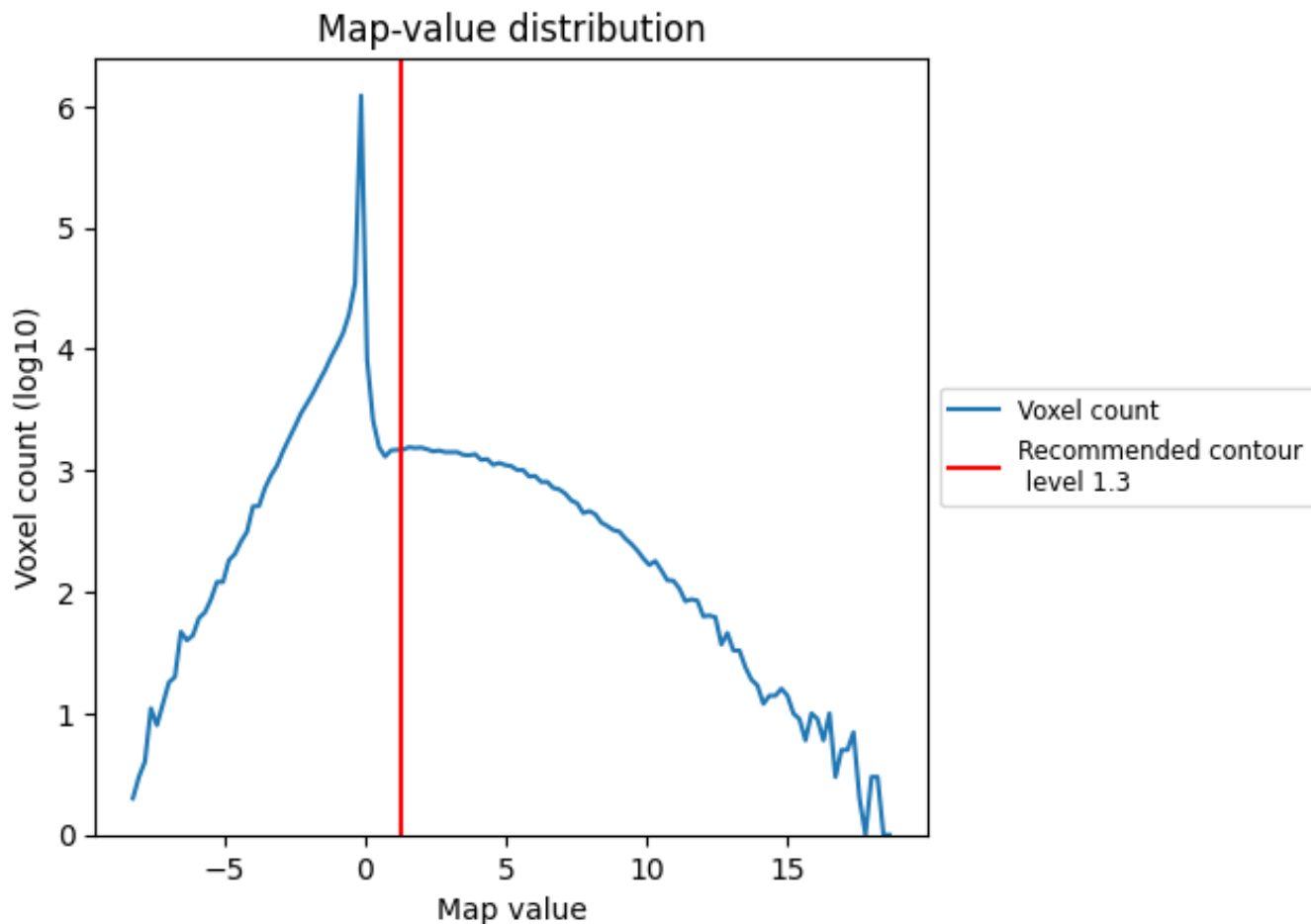
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

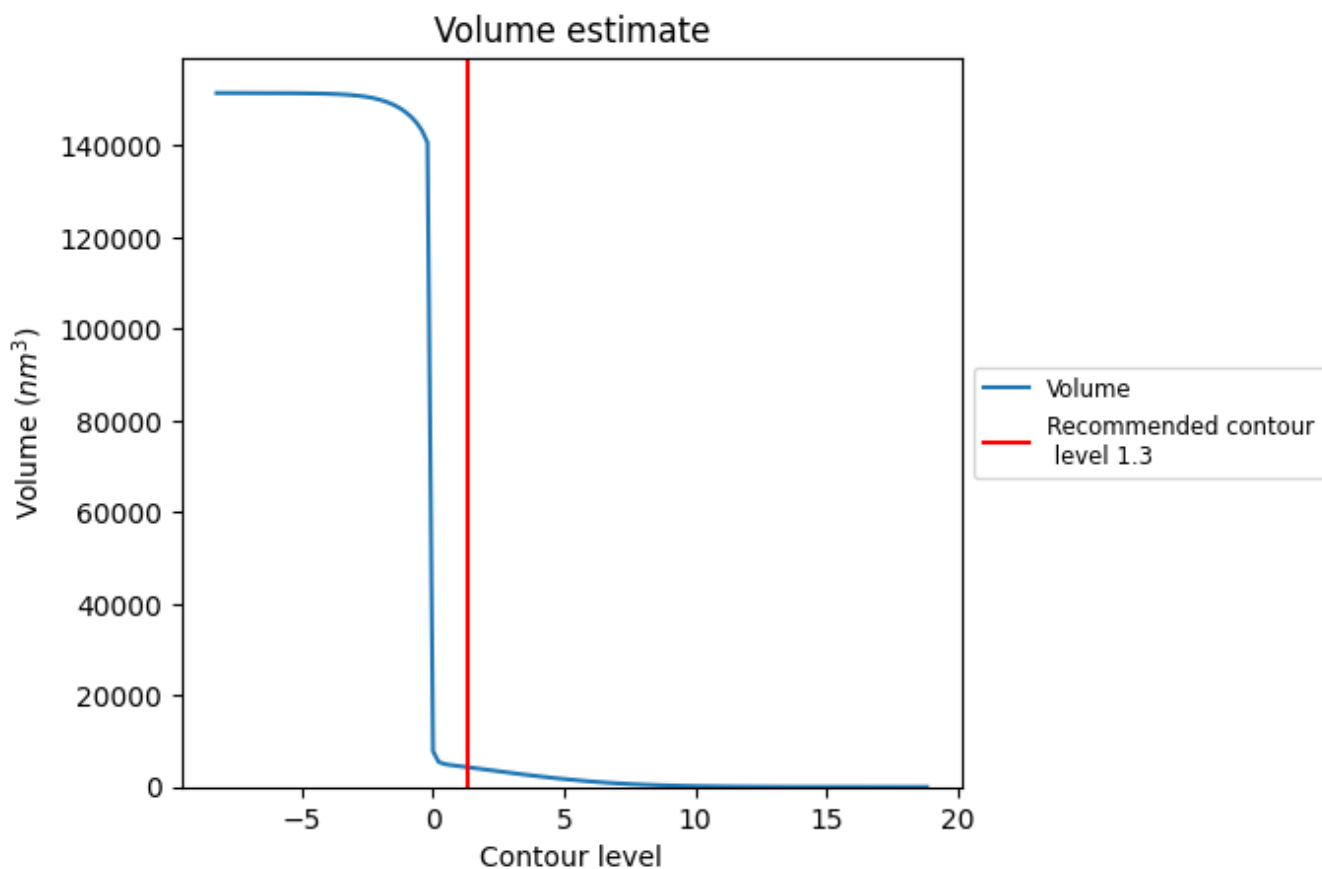
This section contains the results of statistical analysis of the map.

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.

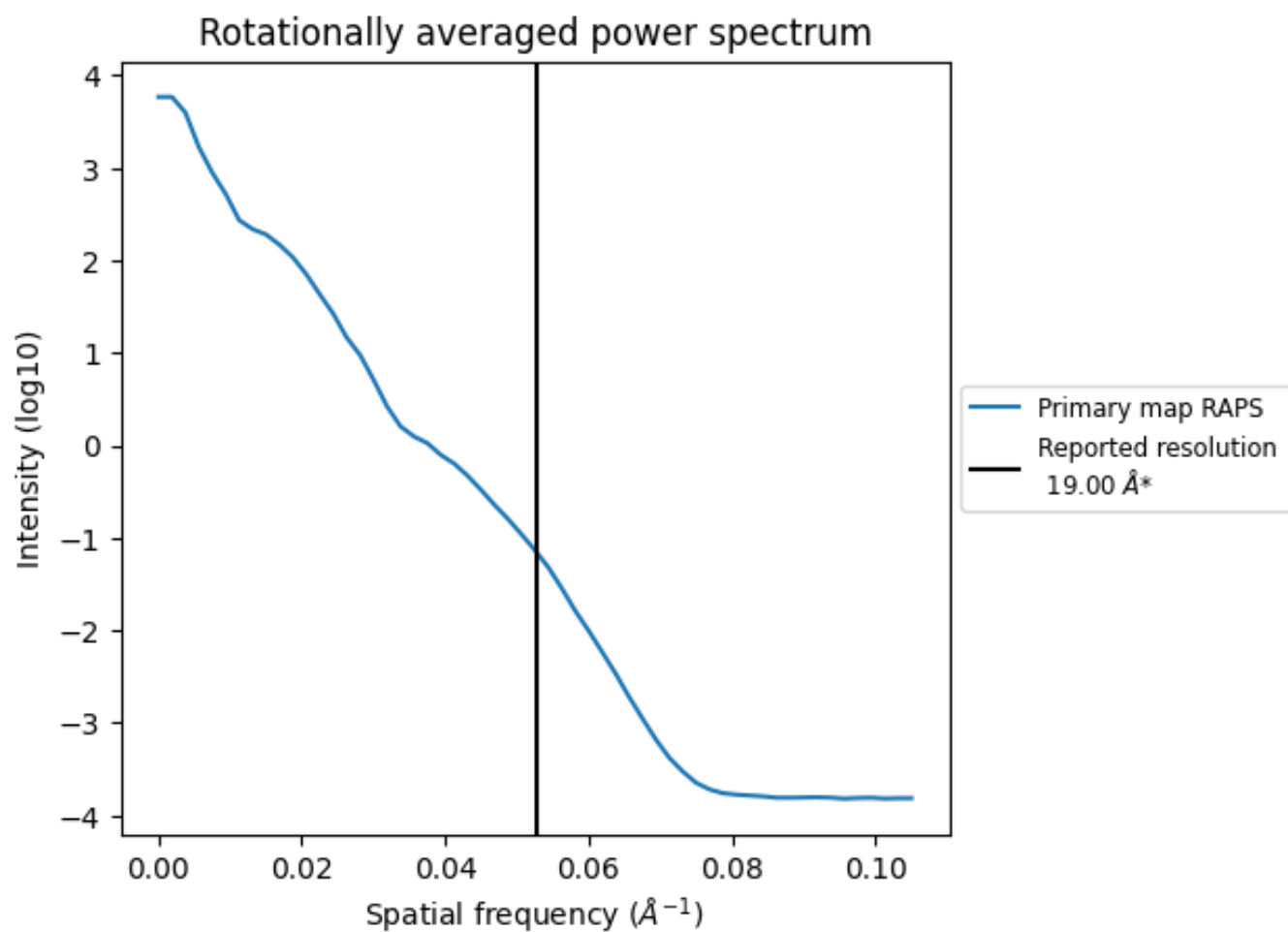
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 4344 nm^3 ; this corresponds to an approximate mass of 3924 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.053 Å⁻¹

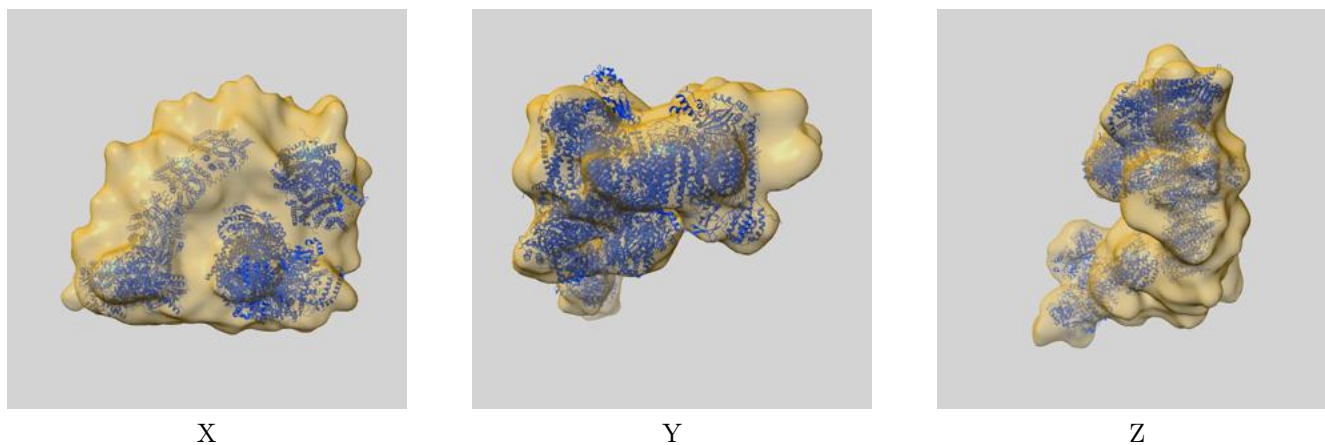
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

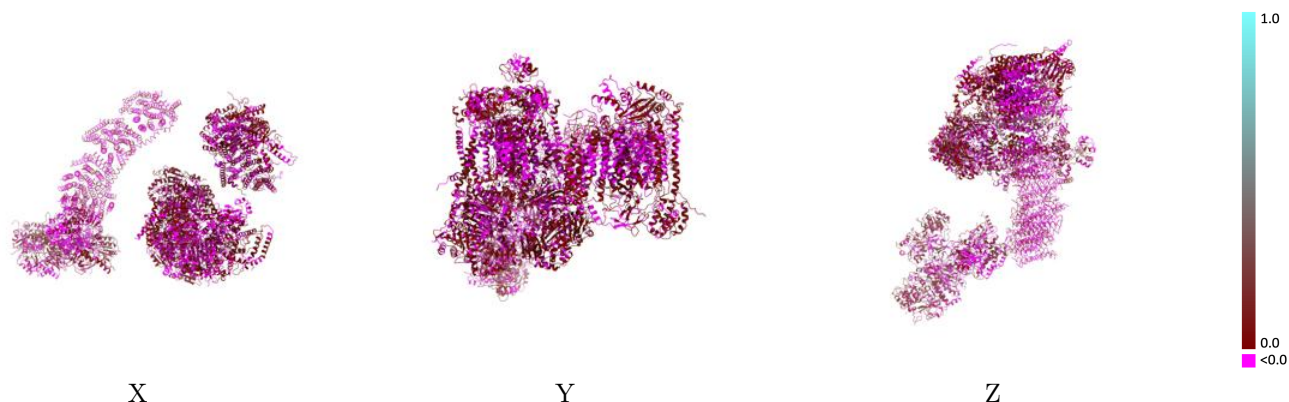
This section contains information regarding the fit between EMDB map EMD-1876 and PDB model 2YBB. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



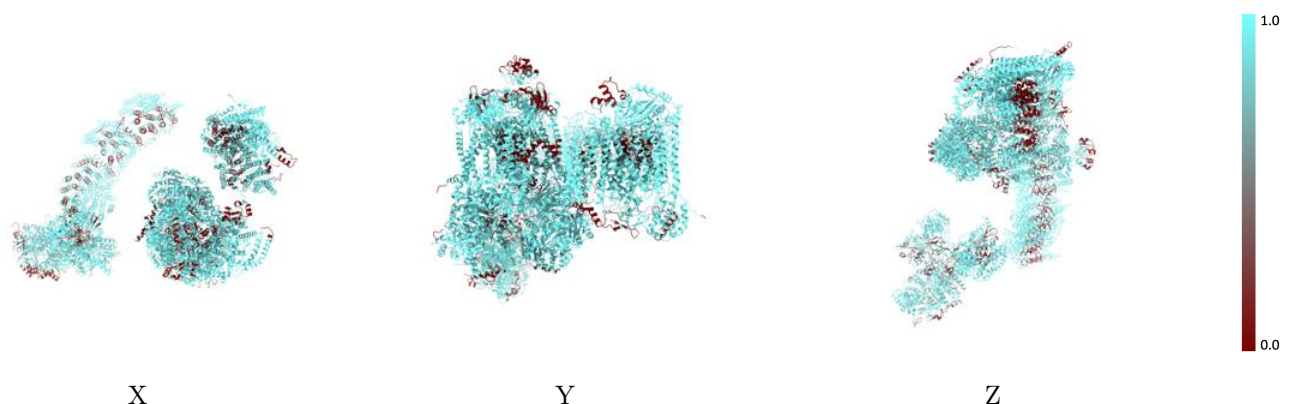
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



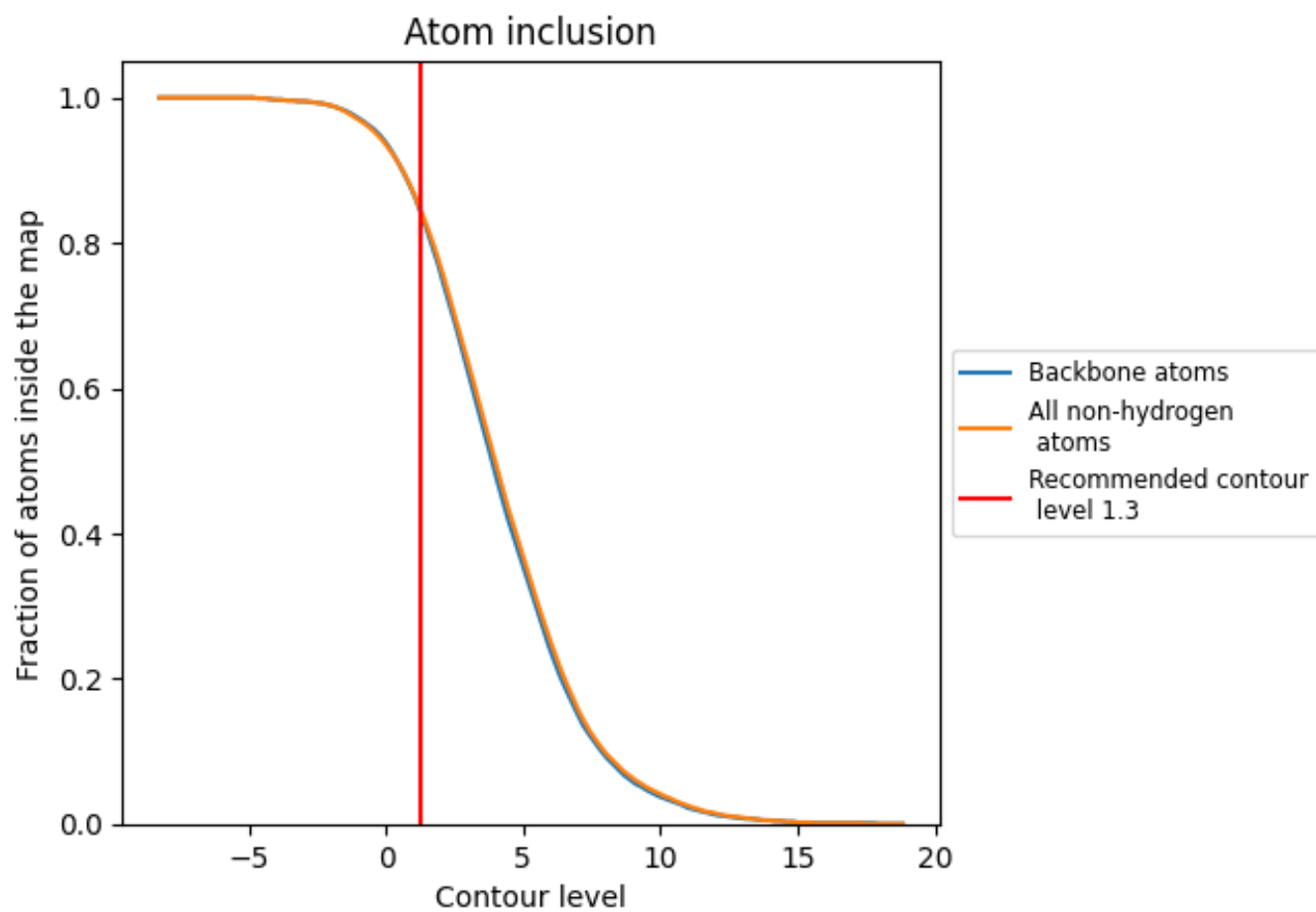
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.0170
1	 0.8930	 0.0350
2	 0.7620	 0.0130
3	 0.8340	 0.0270
4	 0.7930	 -0.0220
5	 0.8620	 -0.0010
6	 0.9050	 0.0170
7	 0.6070	 -0.0040
8	 0.9860	 0.0240
A	 0.9030	 0.0290
B	 0.8770	 0.0320
C	 0.8100	 0.0030
D	 0.9790	 0.0410
E	 0.6420	 -0.0200
F	 0.9990	 0.0630
G	 0.9840	 0.0320
H	 0.8670	 0.0440
I	 0.8380	 0.0050
J	 0.9430	 0.0100
K	 0.6000	 -0.0350
L	 0.7930	 -0.0120
M	 1.0000	 0.0490
N	 0.9200	 0.0280
O	 0.8660	 0.0450
P	 0.8330	 0.0410
Q	 0.4720	 -0.0070
R	 0.8910	 0.0240
S	 0.5920	 -0.0160
T	 0.9810	 0.0360
U	 0.8390	 0.0360
V	 0.7330	 0.0010
W	 0.8630	 0.0270
X	 0.6390	 -0.0240
Y	 0.4550	 0.0100
a	 0.9850	 0.0300



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9430	 0.0450
c	 0.8190	 -0.0010
d	 0.9330	 0.0440
e	 0.6120	 -0.0070
f	 0.6280	 0.0300
g	 0.8820	 0.0310
h	 0.9720	 0.0510
i	 0.9350	 -0.0200
j	 0.8400	 0.0400
k	 1.0000	 0.1370
m	 0.7620	 -0.0210
n	 0.7310	 -0.0200
o	 0.7370	 -0.0140
p	 0.8050	 0.0010