wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 07:15 PM JST

PDB ID	:	8IB9 / pdb_00008ib9
EMDB ID	:	EMD-35336
Title	:	Respiratory complex CI:CIII2, type IB, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-10
Resolution	:	4.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

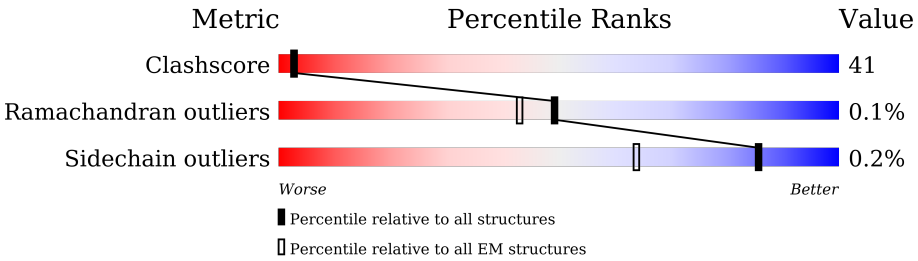
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

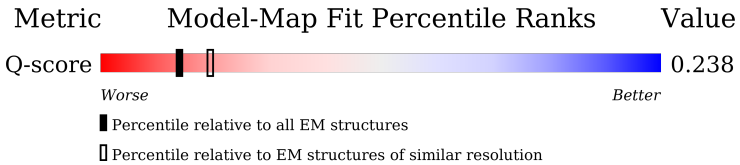
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	115	8% 25% 53% • 19%
2	B	224	• 28% 36% 5% 30%
3	C	263	10% 38% 33% • 25%
4	D	463	8% 37% 50% 5% 8%

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Mol	Chain	Length	Quality of chain
5	E	248	46% 27% 54% • 15%
6	F	464	47% 31% 54% 6% 8%
7	G	727	36% 38% 50% 7% 6%
8	H	318	6% 31% 57% 11% •
9	I	212	• 37% 40% 6% 18%
10	J	172	12% 32% 54% 5% • 9%
11	K	98	• 39% 58% • •
12	L	607	• 32% 57% 10%
13	M	459	• 29% 59% 13%
14	N	345	34% 57% 8%
15	O	355	15% 35% 51% • 10%
16	P	377	44% 32% 53% 5% 10%
17	Q	175	28% 35% 29% • 33%
18	R	116	47% 24% 38% 9% 28%
19	S	99	46% 31% 46% 6% 16%
20	T	156	31% 13% 29% 6% 52%
20	U	156	• 21% 30% • • 44%
21	V	116	16% 47% 44% 6% •
22	W	131	24% 42% 42% • 13%
23	X	172	• 38% 55% 5% •
24	Y	143	8% 49% 48% • •
25	Z	144	• 36% 56% 5% •
26	a	70	• 34% 57% • •
27	b	84	• 32% 61% • 6%
28	c	76	7% 22% 34% 5% 38%

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Mol	Chain	Length	Quality of chain
29	d	120	7% 39% 58%
30	e	106	40% 57%
31	f	57	5% 42% 37% 12% 9%
32	g	151	35% 25% 7% 34%
33	h	189	33% 39% 27%
34	i	128	30% 35% 7% 28%
35	j	105	30% 32% 5% 33%
36	k	104	31% 28% 11% 31%
37	l	186	45% 33% 6% 16%
38	m	129	50% 41% 6%
39	n	179	40% 53% 6%
40	o	137	12% 34% 50% 13%
41	p	176	45% 47%
42	q	145	67% 32% 43% 8% 17%
43	r	113	27% 22% 17% 5% 56%
44	s	104	23% 12% 12% 75%
45	AA	480	54% 46% 36% 17%
45	Aa	480	20% 52% 30% 16%
46	AB	453	64% 62% 29% 9%
46	Ab	453	37% 60% 30% 9%
47	AC	381	72% 68% 30%
47	Ac	381	46% 58% 38%
48	AD	325	46% 30% 43% 27%
48	Ad	325	39% 30% 42% 27%
49	AE	274	65% 20% 47% 32%

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Mol	Chain	Length	Quality of chain
49	AI	274	17% 9% 9% 81%
49	Ae	274	61% 16% 49% 31%
50	AF	111	50% 61% 27% 12%
50	Af	111	33% 41% 47% 12%
51	AG	82	72% 46% 46% 7%
51	Ag	82	35% 41% 51% 7%
52	AH	89	47% 19% 49% 28%
52	Ah	89	39% 20% 54% 26%
53	AJ	64	59% 30% 30% 41%
53	Aj	64	61% 36% 38% 25%
54	AK	56	55% 20% 41% 39%
54	Ak	56	75% 36% 39% 21%

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
55	SF4	B	301	-	-	X	-
55	SF4	F	502	-	-	X	-
55	SF4	G	802	-	-	X	-
55	SF4	I	303	-	-	X	-
55	SF4	I	304	-	-	X	-
56	UQ1	B	302	-	-	X	-
58	3PE	M	503	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
70	HEC	AD	401	X	-	-	-
70	HEC	Ad	401	X	-	-	-

2 Entry composition (i)

There are 70 unique types of molecules in this entry. The entry contains 97317 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	93	762	528	108	120	6	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	796	223	214	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	198	1641	1060	279	299	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	425	3423	2188	588	623	24	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1635	1039	275	310	11	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	426	3288	2073	588	605	22	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	687	5287	3316	918	1012	41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	316	2525	1698	382	423	22	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	174	1398	880	240	266	12	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	157	1193	806	169	203	15	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	97	729	473	111	135	10	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	606	4798	3181	746	826	45	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3630	2407	567	616	40	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	344	2694	1790	416	451	37	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	319	2599	1668	430	491	10	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	340	2730	1765	479	479	7	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	118	957	608	165	180	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	83	660	411	120	126	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	83	667	419	126	119	3	0	0

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	75	604	388	89	122	5	0	0
			Total	C	N	O	S		
20	U	87	700	450	103	142	5	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	112	915	596	152	164	3	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	114	970	619	180	165	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	169	1385	882	248	245	10	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	139	1030	657	174	191	8	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	139	1152	741	204	199	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	67	548	356	97	91	4	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	79	620	408	98	110	4	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	47	389	255	67	66	1	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	120	996	651	171	165	9	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	103	859	544	157	150	8	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	52	447	290	80	75	2	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	100	842	545	135	158	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	138	1162	762	194	203	3	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	92	773	506	132	132	3	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	70	587	383	98	105	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	72	578	381	101	94	2	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	156	1312	846	219	236	11	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	m	125	1044	673	188	183	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	177	1534	981	275	267	11	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	119	1019	642	191	178	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	170	1438	904	258	268	8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	120	1004	645	178	177	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	50	413	263	77	72	1	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	s	26	226	147	38	41	0	0

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	AA	399	3117	1943	554	604	16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Aa	401	3131	1955	555	605	16	0	0

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	AB	414	3107	1954	546	598	9	0	0
			Total	C	N	O	S		
46	Ab	413	3101	1948	543	601	9	0	0

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	AC	373	2988	2018	461	489	20	0	0
			Total	C	N	O	S		
47	Ac	373	2988	2018	461	489	20	0	0

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	AD	238	1896	1211	326	345	14	0	0
			Total	C	N	O	S		
48	Ad	238	1895	1211	325	345	14	0	0

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	AE	185	1427	902	250	268	7	0	0
			Total	C	N	O			
49	AI	51	347	221	65	61		0	0
			Total	C	N	O	S		
49	Ae	188	1451	916	254	274	7	0	0

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	AF	98	864	552	154	155	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Af	98	864	552	154	155	3	0	0

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	AG	76	643	418	116	108	1	0	0
			Total	C	N	O	S		
51	Ag	76	643	418	116	108	1	0	0

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	AH	64	527	321	98	103	5	0	0
			Total	C	N	O	S		
52	Ah	66	544	333	101	105	5	0	0

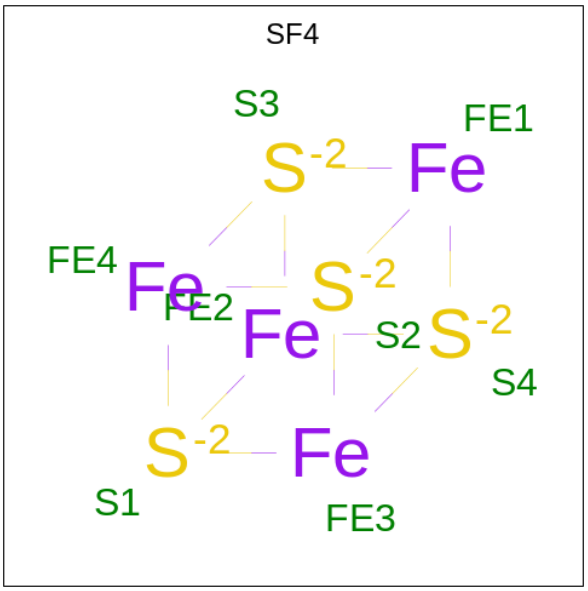
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	AJ	38	307	201	51	55	0	0
			Total	C	N	O		
53	Aj	48	392	257	67	68	0	0

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

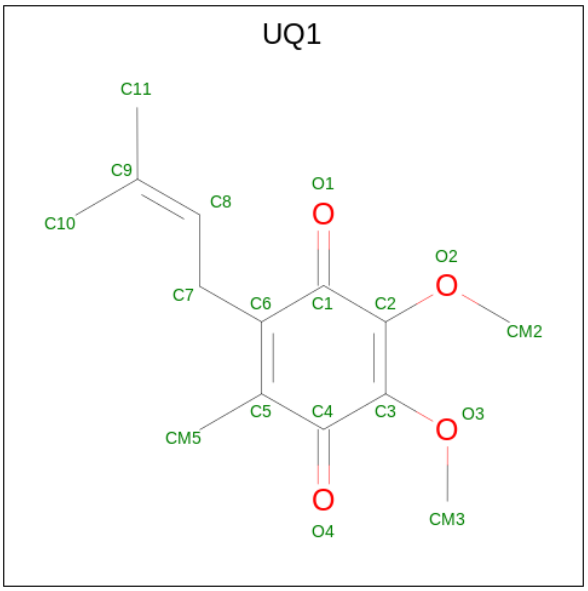
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	AK	34	278	183	51	43	1	0	0
			Total	C	N	O	S		
54	Ak	44	357	236	63	57	1	0	0

- Molecule 55 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



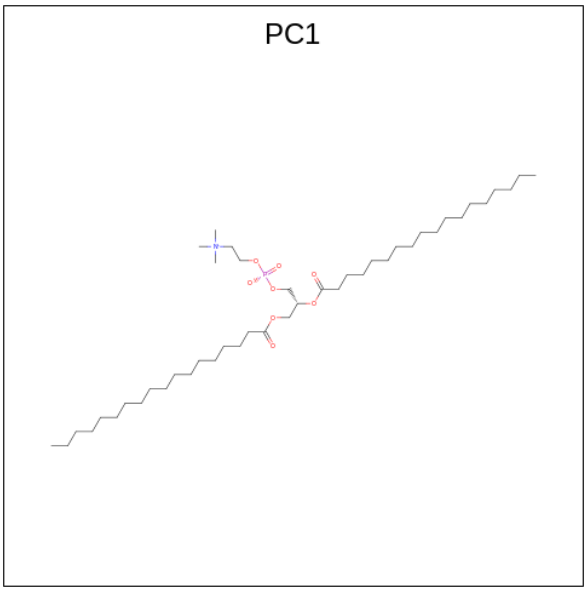
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
55	B	1	8	4	4	0
55	F	1	8	4	4	0
55	G	1	8	4	4	0
55	G	1	8	4	4	0
55	I	1	8	4	4	0
55	I	1	8	4	4	0

- Molecule 56 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
56	B	1	18	14	4	0

- Molecule 57 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	B	1	35	25	1	8	1	0
			Total	C	N	O	P	
57	I	1	47	37	1	8	1	0

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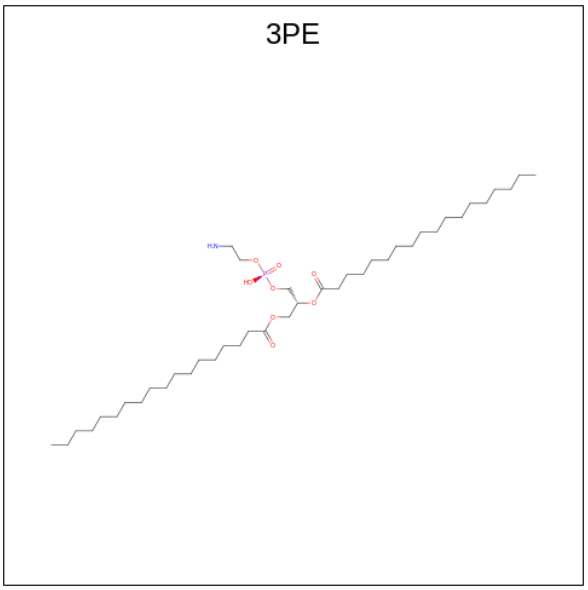
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	L	1	50	40	1	8	1	0

- Molecule 58 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	D	1	38	28	1	8	1	0
			Total	C	N	O	P	
58	I	1	46	36	1	8	1	0
			Total	C	N	O	P	
58	J	1	46	36	1	8	1	0
			Total	C	N	O	P	
58	K	1	46	36	1	8	1	0
			Total	C	N	O	P	
58	L	1	49	39	1	8	1	0
			Total	C	N	O	P	
58	L	1	39	29	1	8	1	0
			Total	C	N	O	P	
58	L	1	47	37	1	8	1	0
			Total	C	N	O	P	
58	M	1	37	27	1	8	1	0
			Total	C	N	O	P	
58	M	1	51	41	1	8	1	0
			Total	C	N	O	P	
58	M	1	51	41	1	8	1	0

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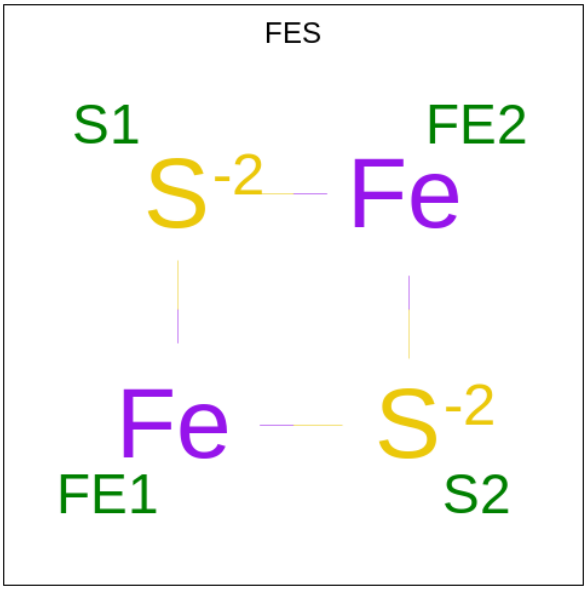
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	O	1	44	34	1	8	1	0
58	b	1	46	36	1	8	1	0
58	i	1	40	30	1	8	1	0
58	j	1	40	30	1	8	1	0
58	m	1	51	41	1	8	1	0
58	m	1	41	31	1	8	1	0
58	AC	1	25	15	1	8	1	0
58	Ac	1	35	25	1	8	1	0

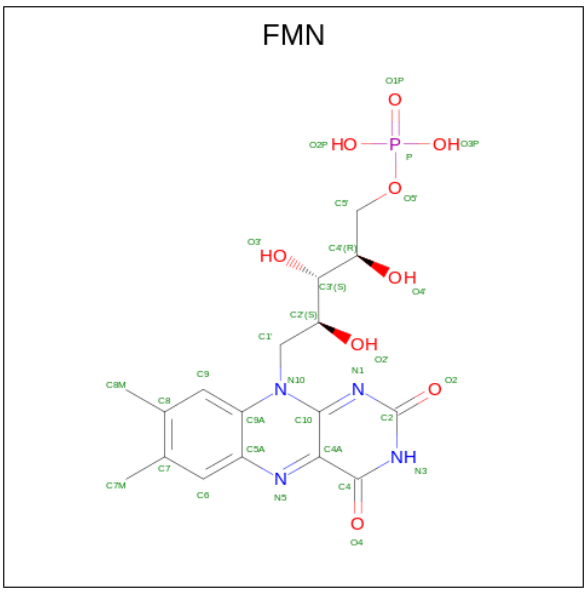
- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	E	1	4	2	2	0
59	G	1	4	2	2	0

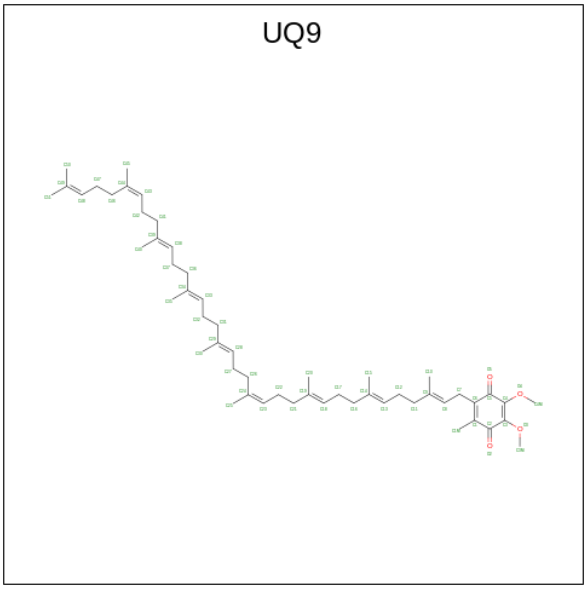
- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$)

(labeled as "Ligand of Interest" by depositor).



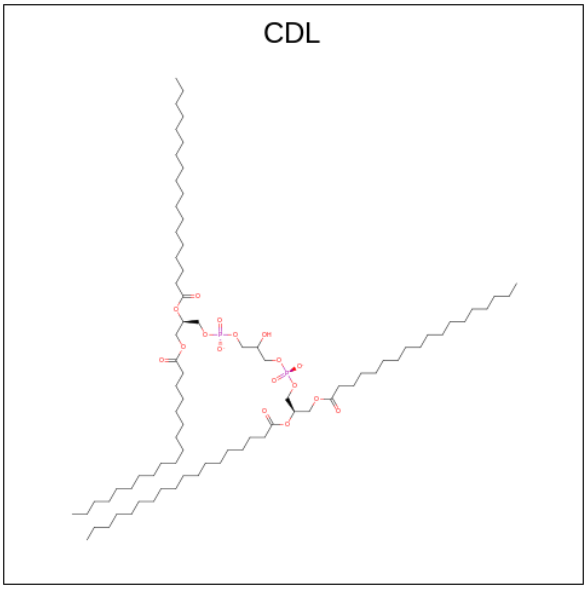
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	F	1	31	17	4	9	1	0

- Molecule 61 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



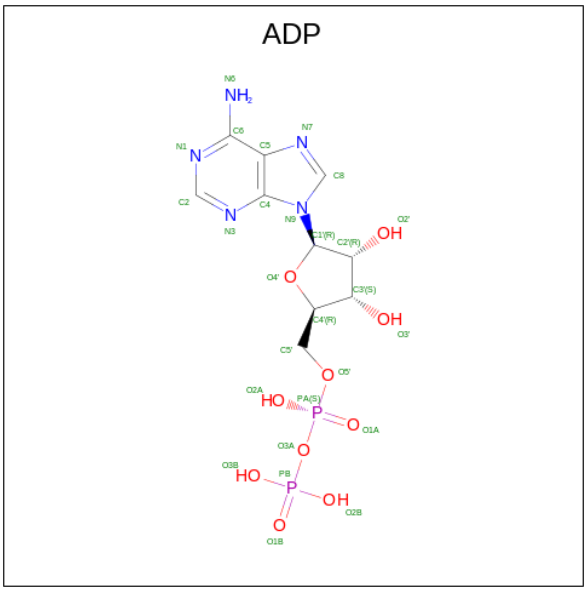
Mol	Chain	Residues	Atoms					AltConf
			Total	C	O			
61	H	1	35	31	4			0

- Molecule 62 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



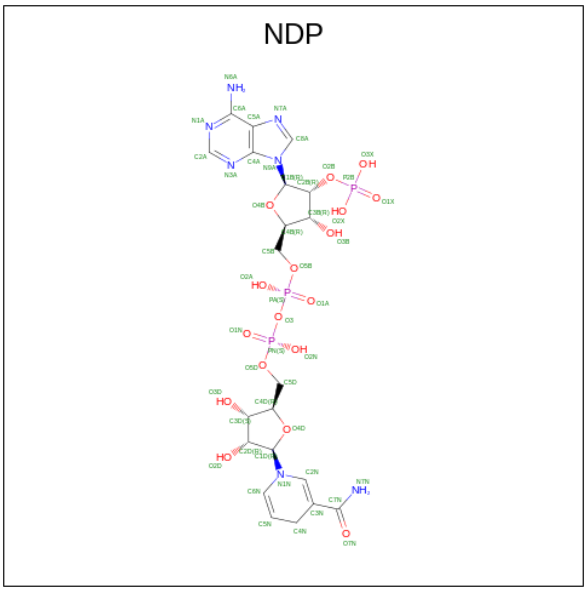
Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			77	58	17	2	
62	L	1	Total	C	O	P	0
			81	62	17	2	
62	a	1	Total	C	O	P	0
			57	38	17	2	
62	d	1	Total	C	O	P	0
			67	48	17	2	
62	h	1	Total	C	O	P	0
			70	51	17	2	
62	Aa	1	Total	C	O	P	0
			46	27	17	2	
62	Ac	1	Total	C	O	P	0
			42	23	17	2	
62	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 63 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	
63	O	1	27	10	5	10	2	0

- Molecule 64 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



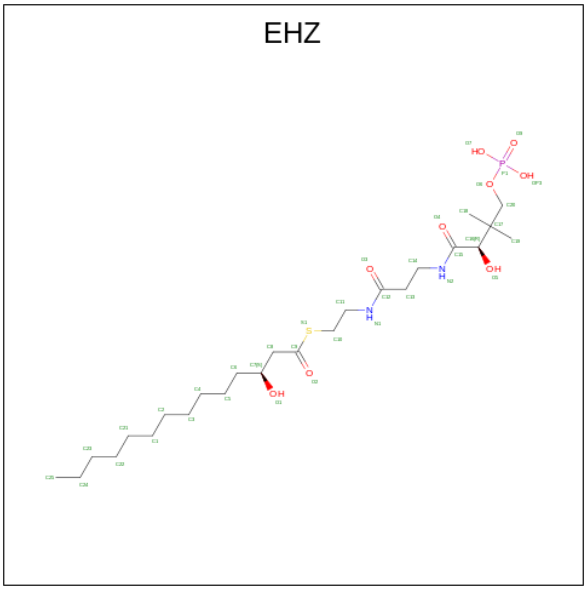
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	P	1	48	21	7	17	3	0

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

depositor).

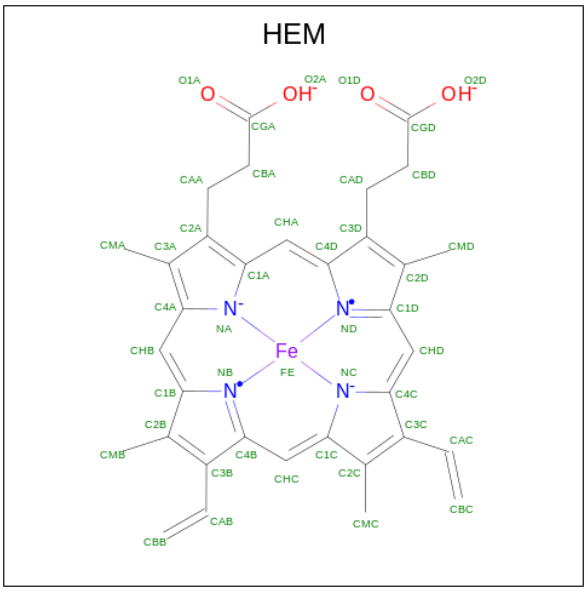
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
65	R	1	1	1	0

- Molecule 66 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



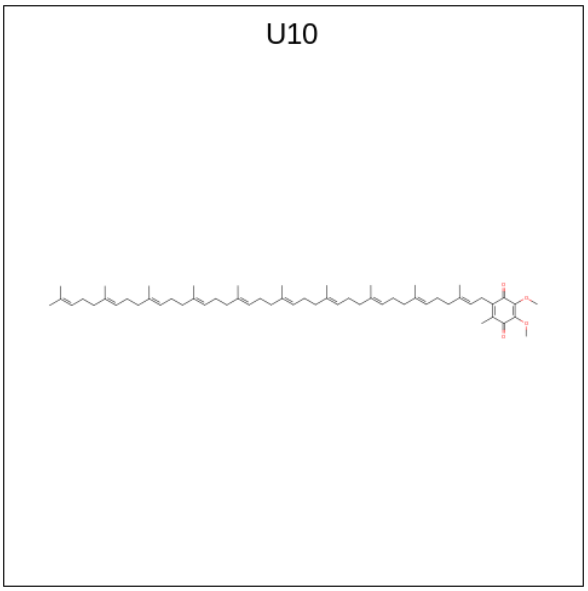
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
66	W	1	32	19	2	9	1	1	0
			Total	C	N	O	P	S	
66	n	1	32	19	2	9	1	1	0

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



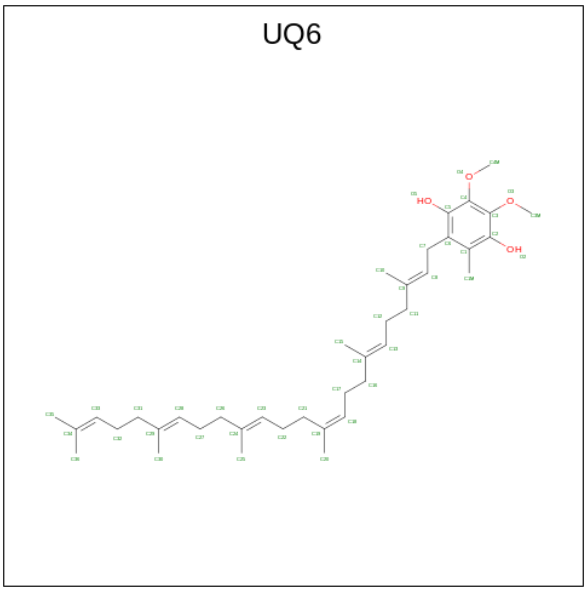
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
67	AC	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
67	AC	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
67	Ac	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
67	Ac	1	43	34	1	4	4	0

- Molecule 68 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



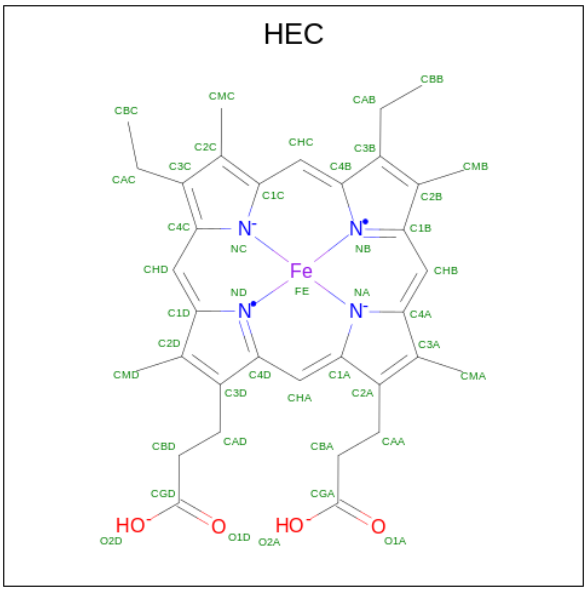
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
68	AC	1	23	19	4	0
68	Ac	1	23	19	4	0

- Molecule 69 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
69	AC	1	28	24	4	0
69	Ac	1	28	24	4	0

- Molecule 70 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



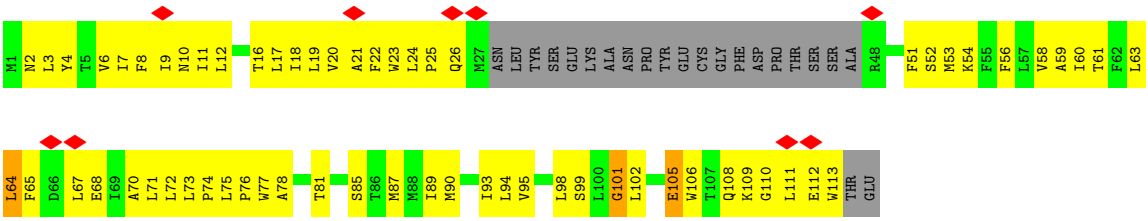
Mol	Chain	Residues	Atoms					AltConf
70	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots (i)

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

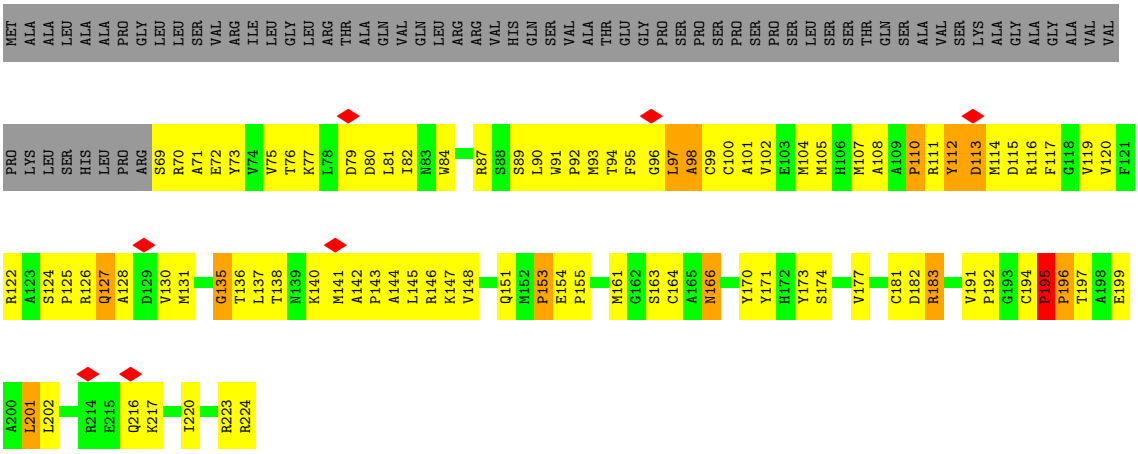
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 8% 25% 53% • 19%



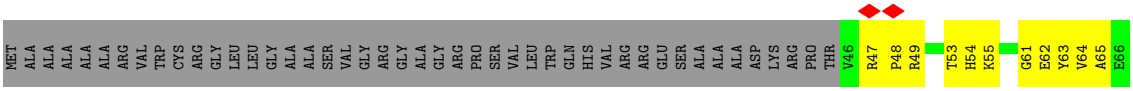
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

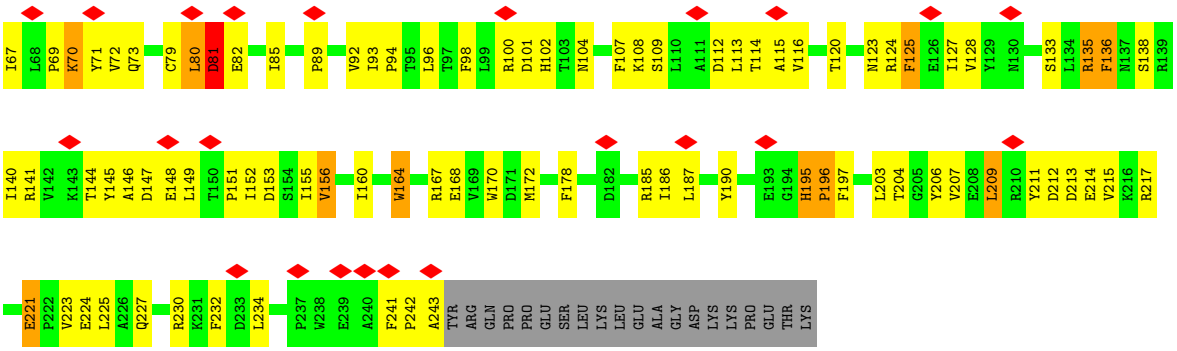
Chain B: • 28% 36% 5% 30%



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

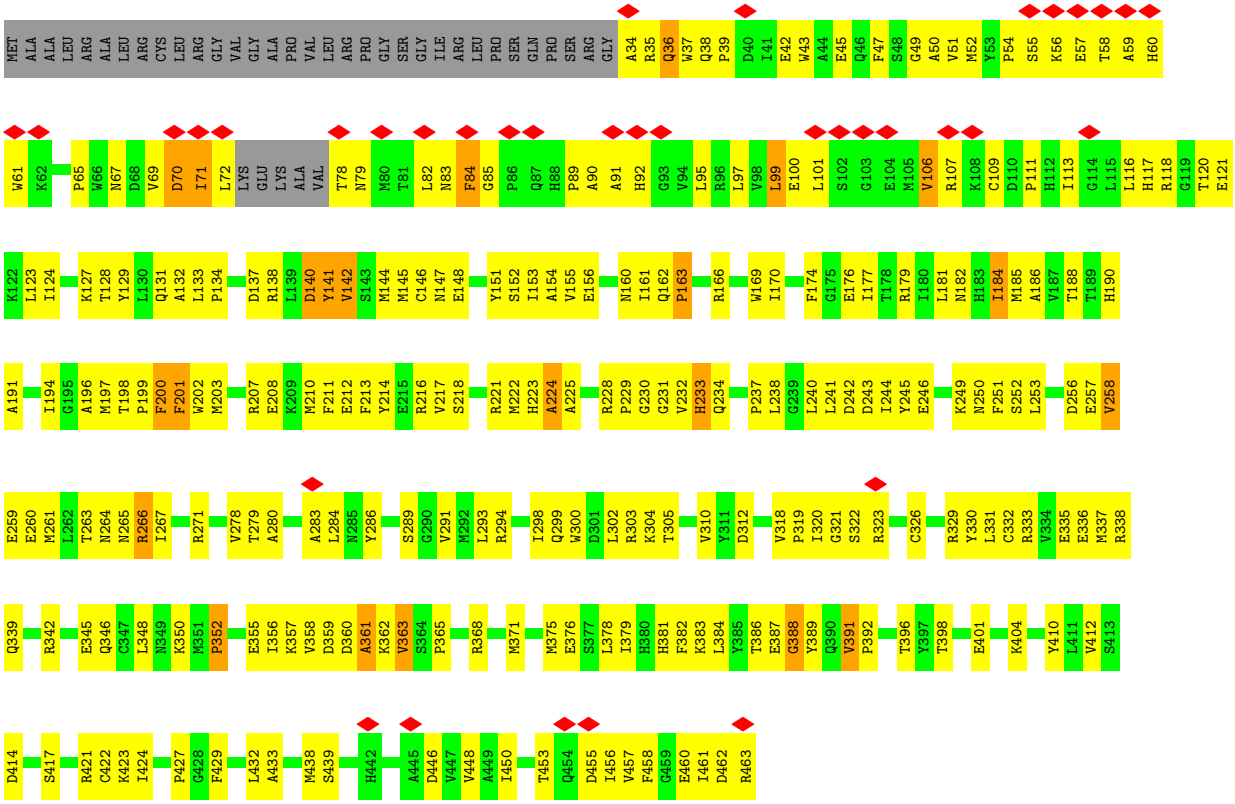
Chain C: 10% 38% 33% • 25%





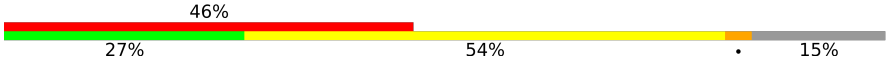
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

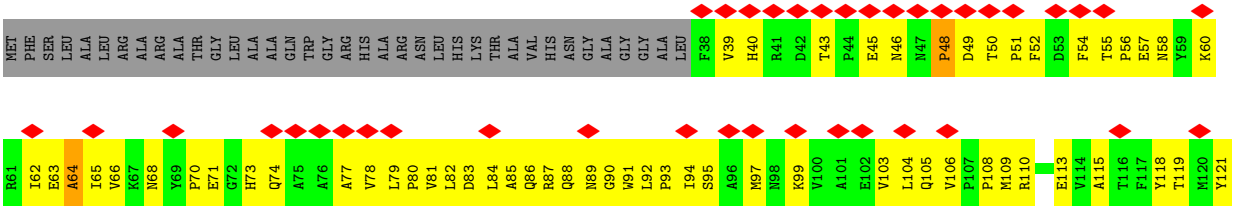
Chain D:

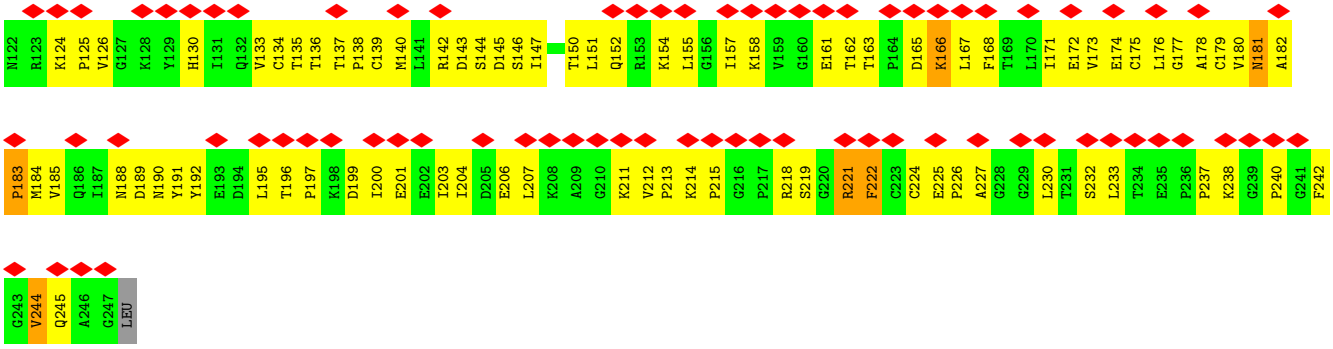


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

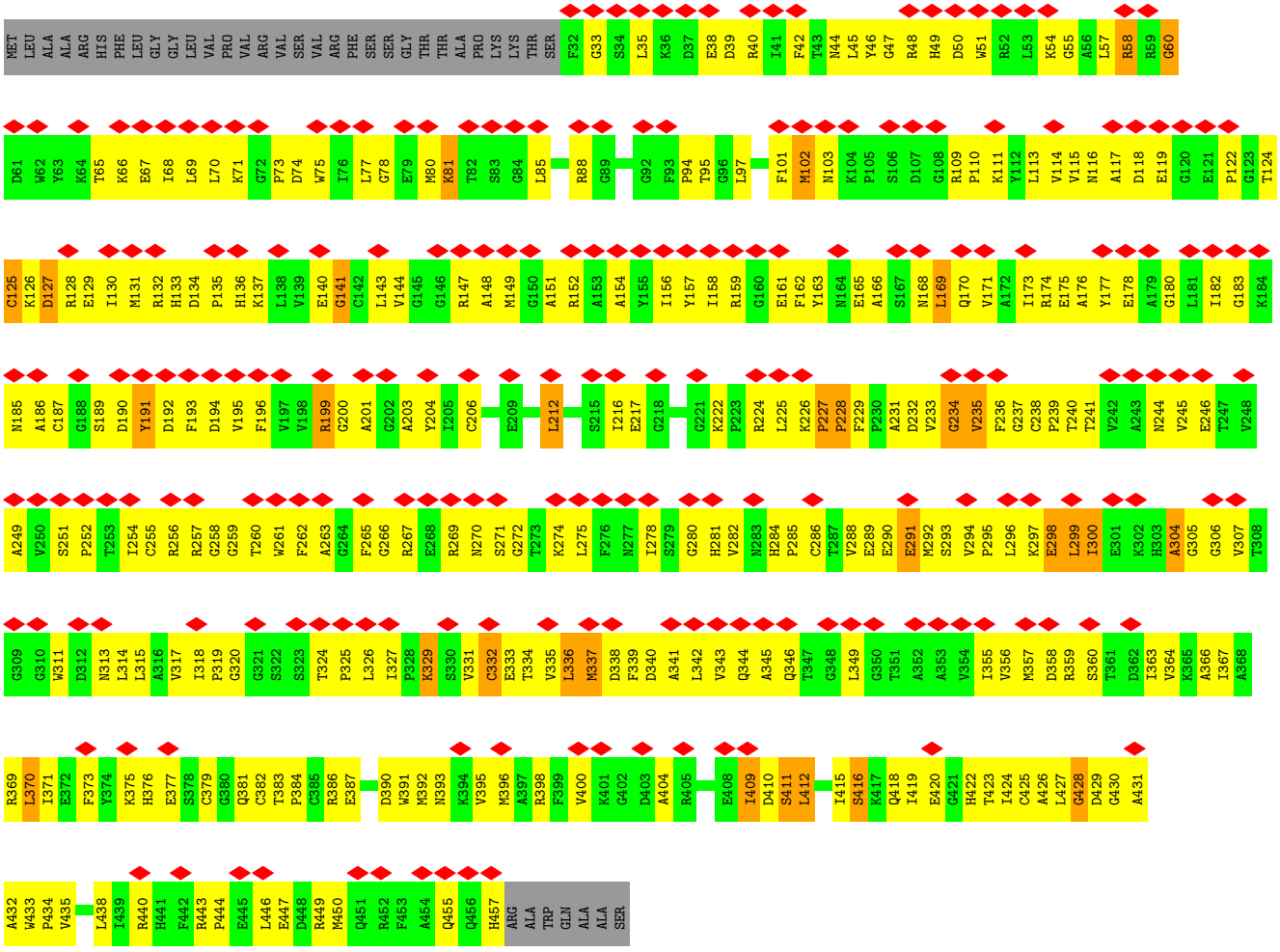






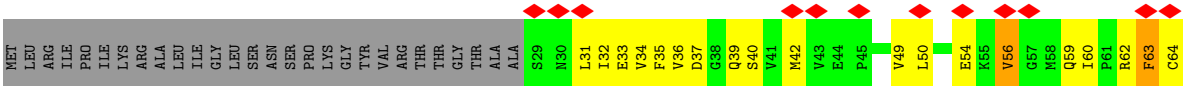
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

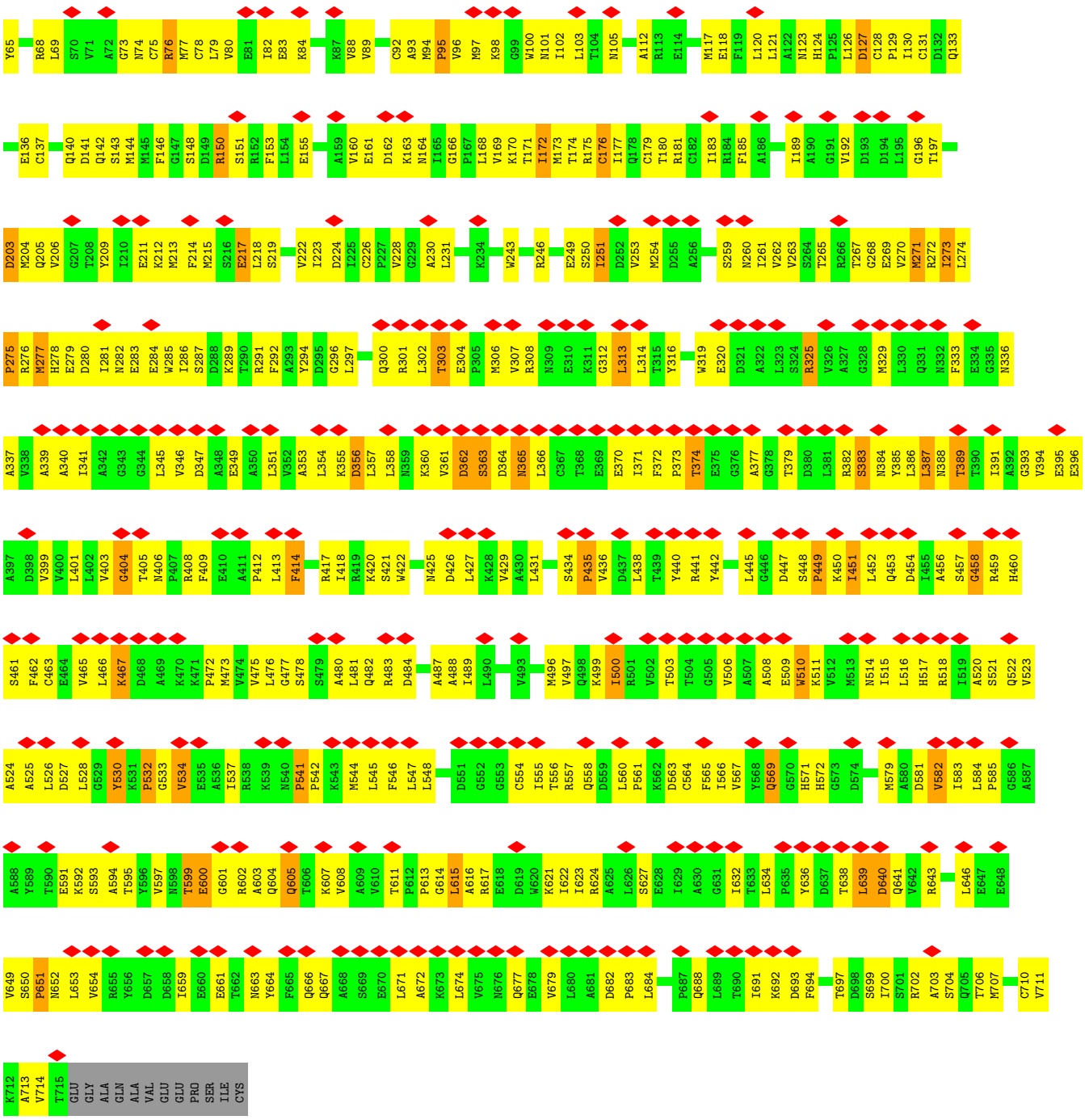
Chain F: 47% 31% 54% 6% 8%



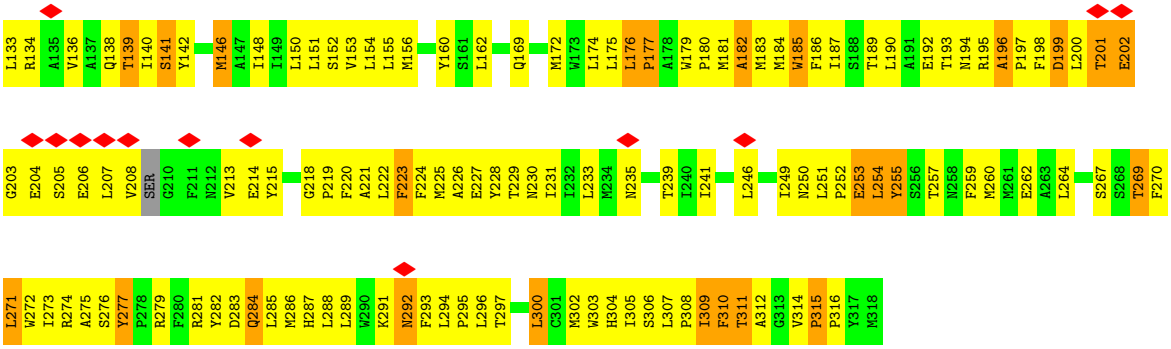
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 36% 38% 50% 7% 6%



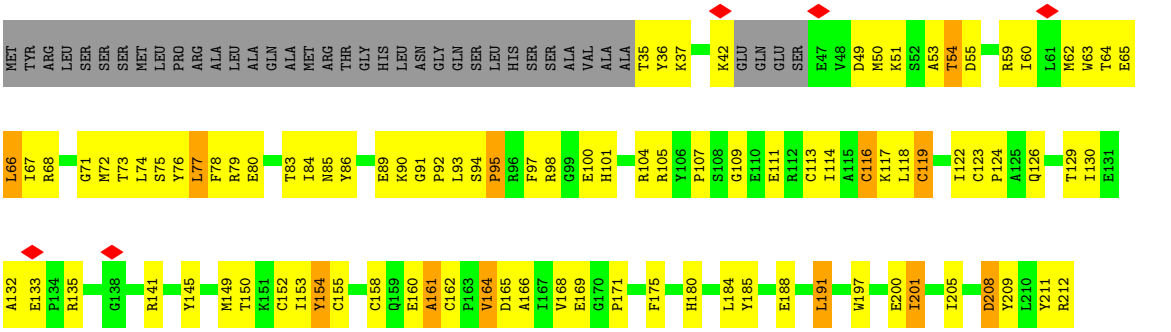


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



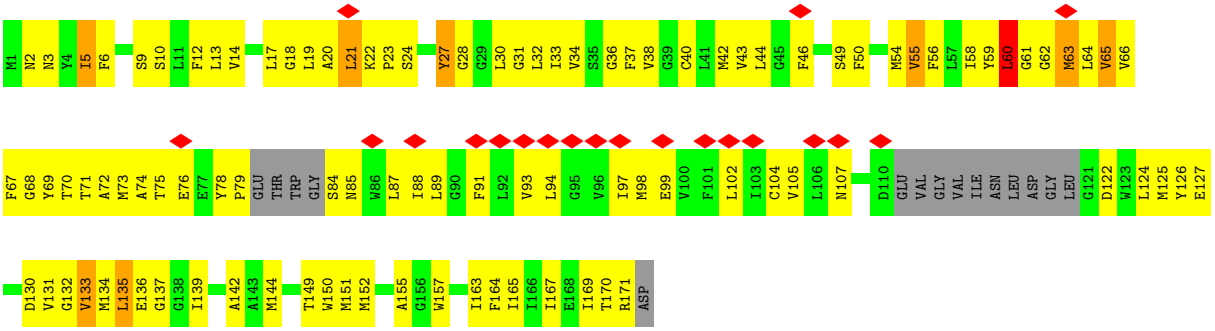
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

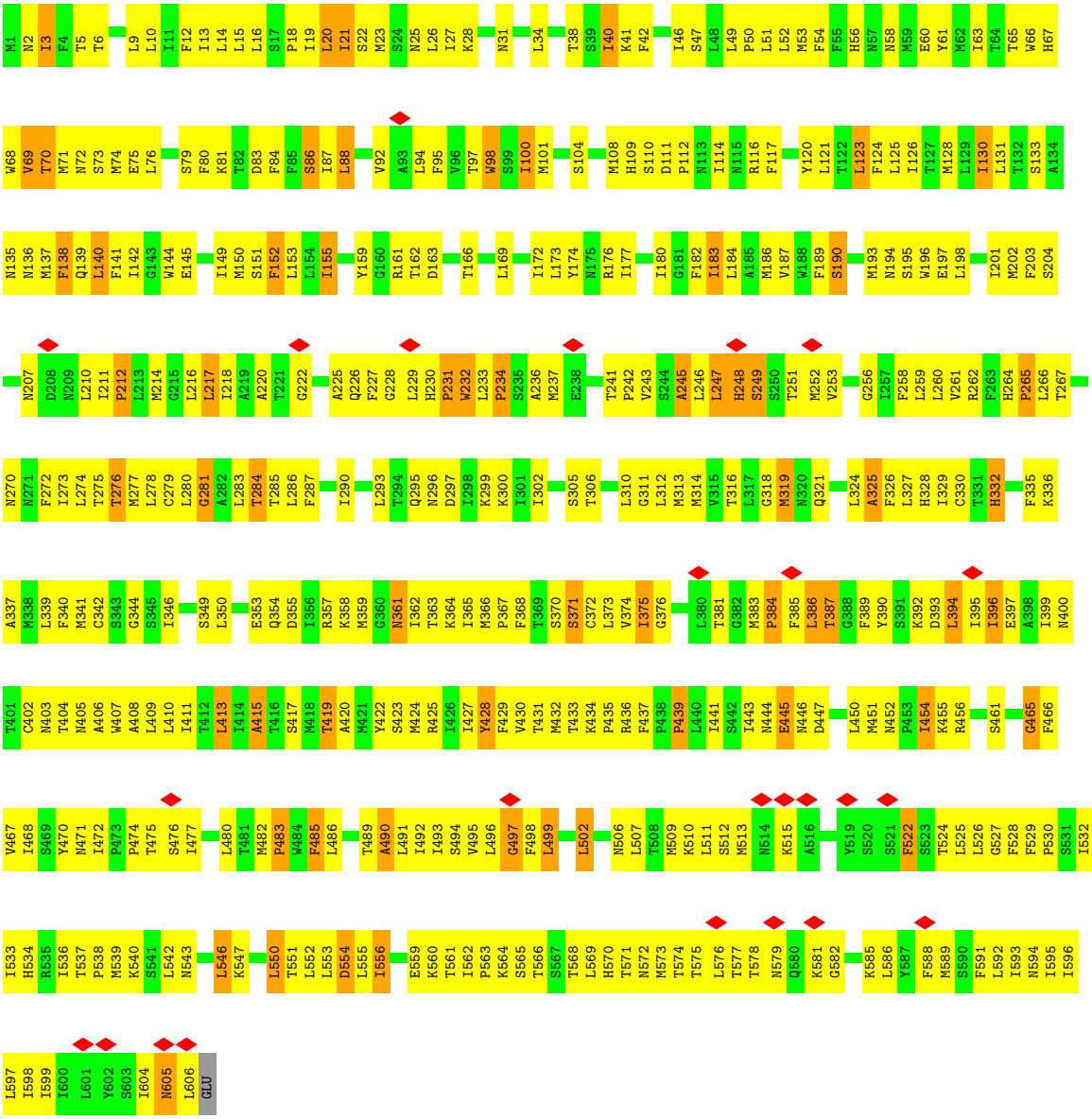


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

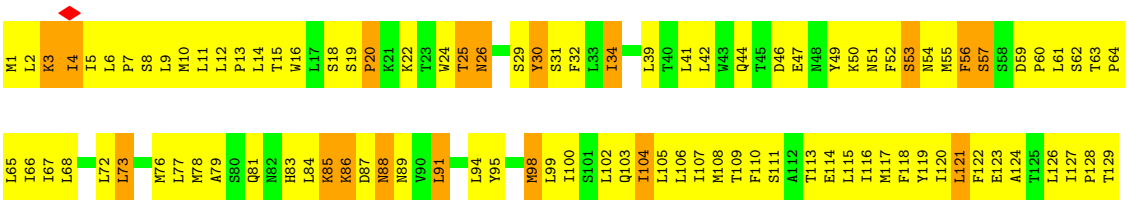
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

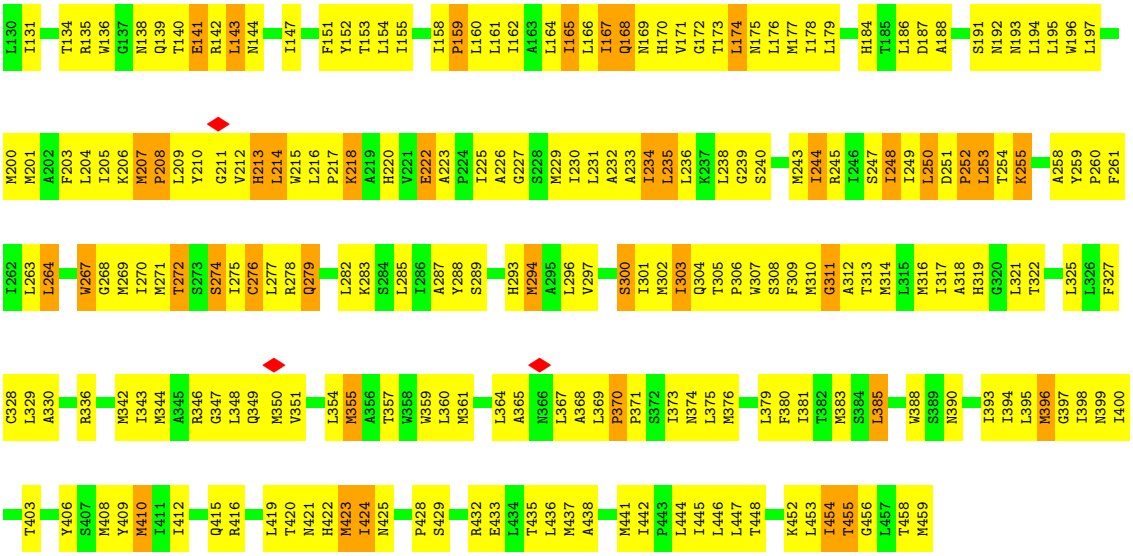
Chain L: 32% 57% 10%



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

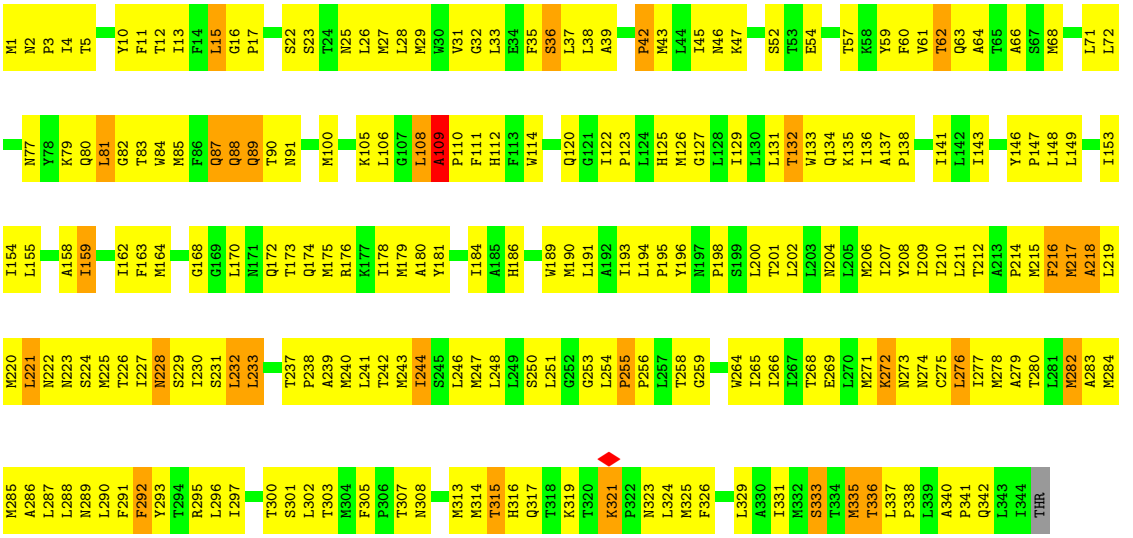
Chain M: 29% 59% 13%





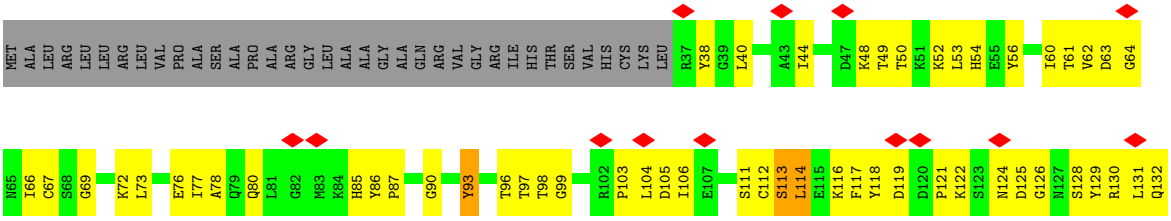
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

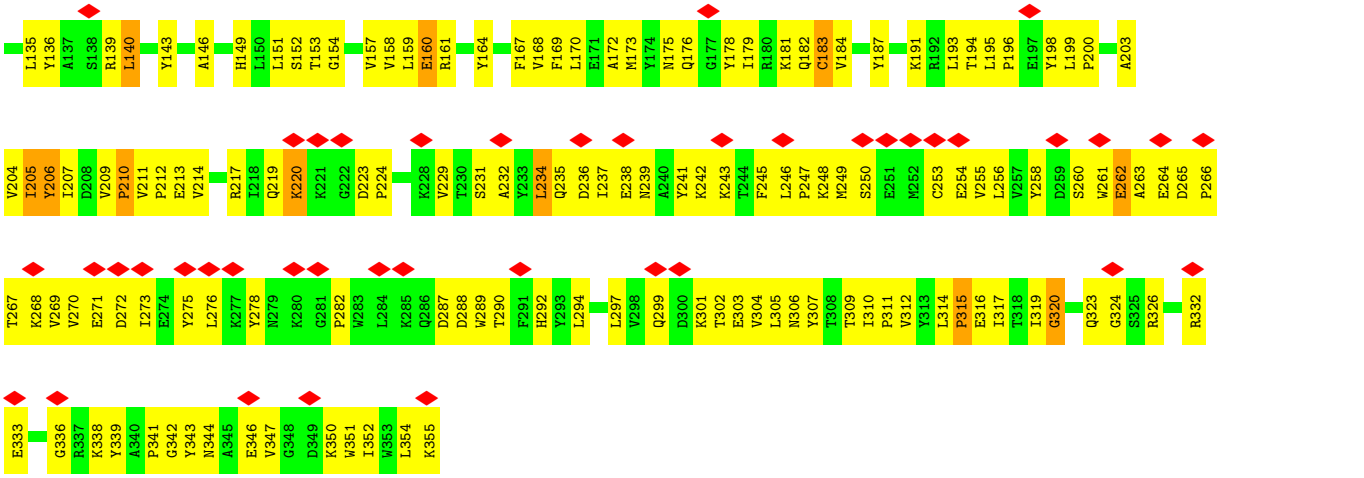
Chain N:



• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

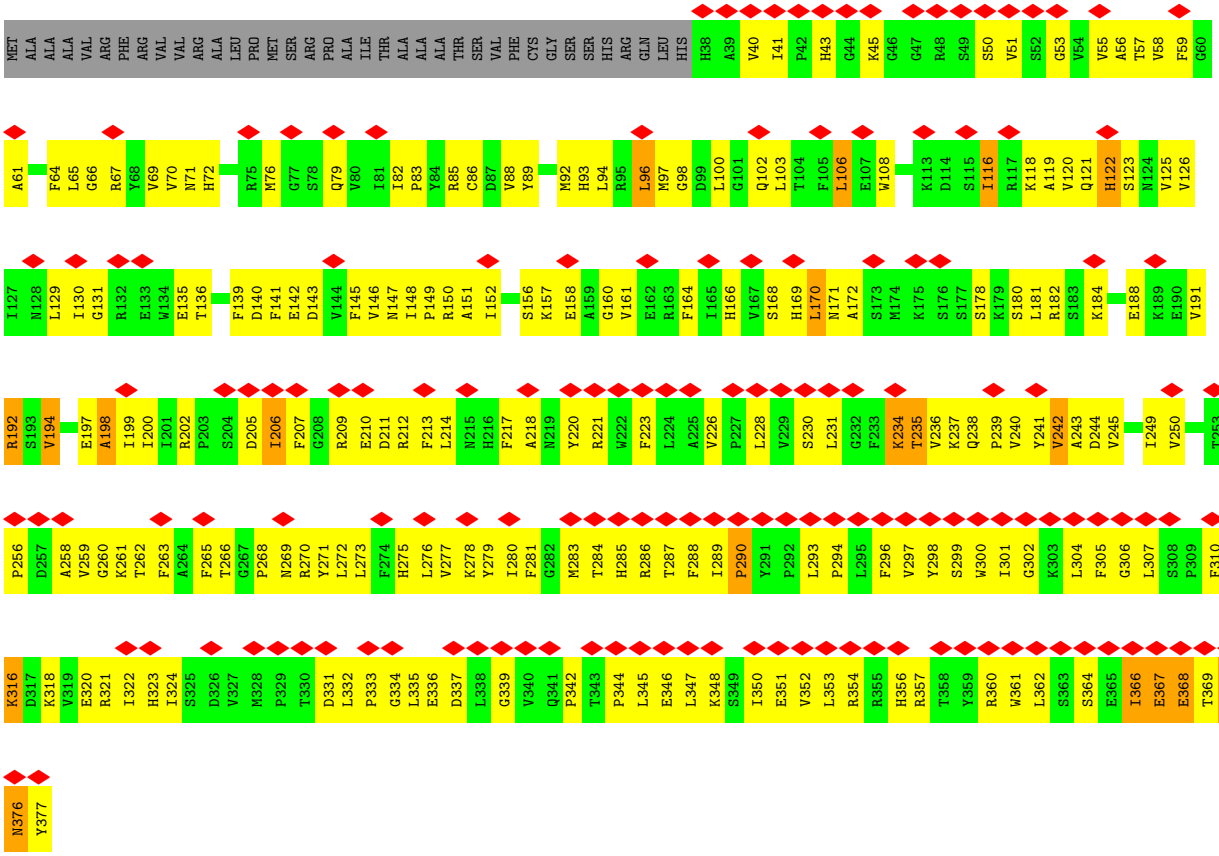
Chain O:





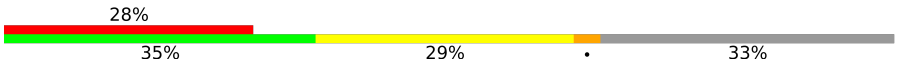
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

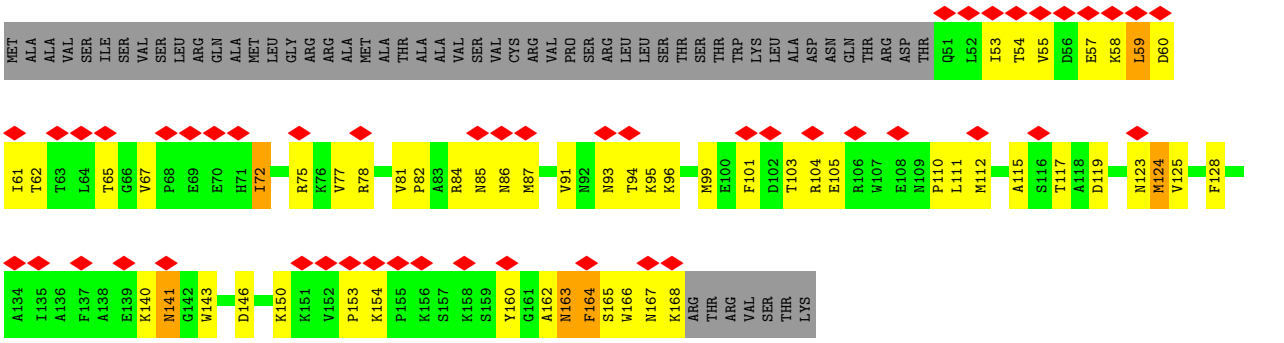
Chain P:



• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

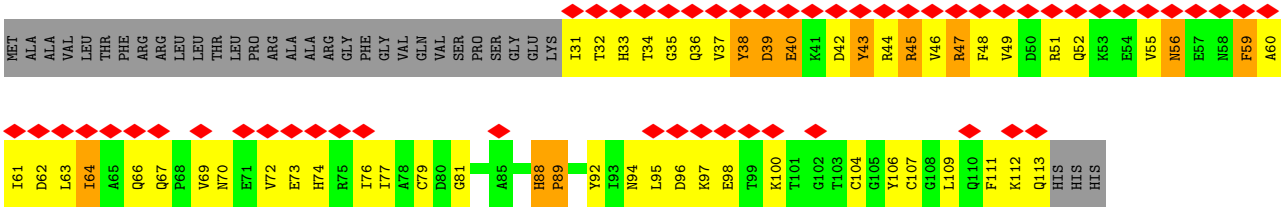
Chain Q:





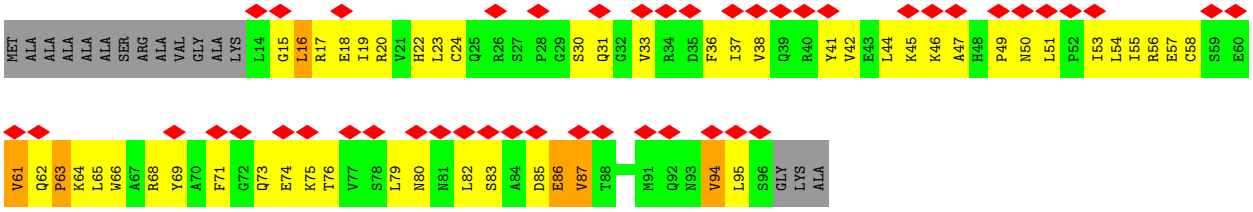
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



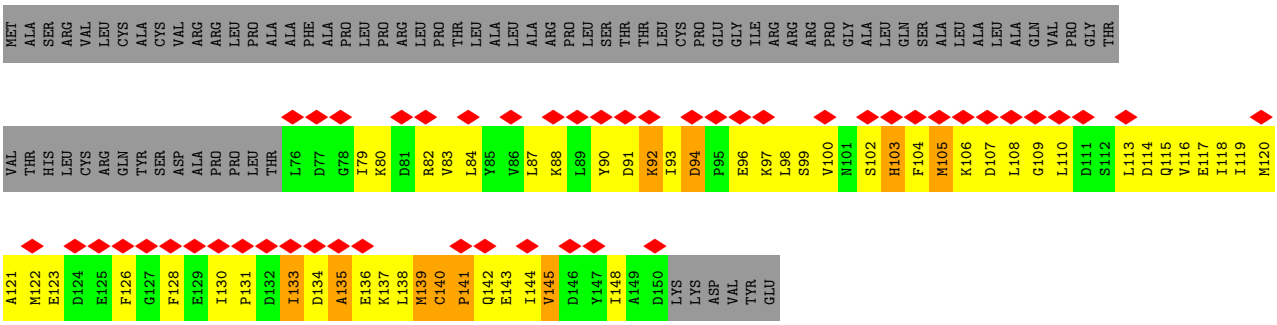
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



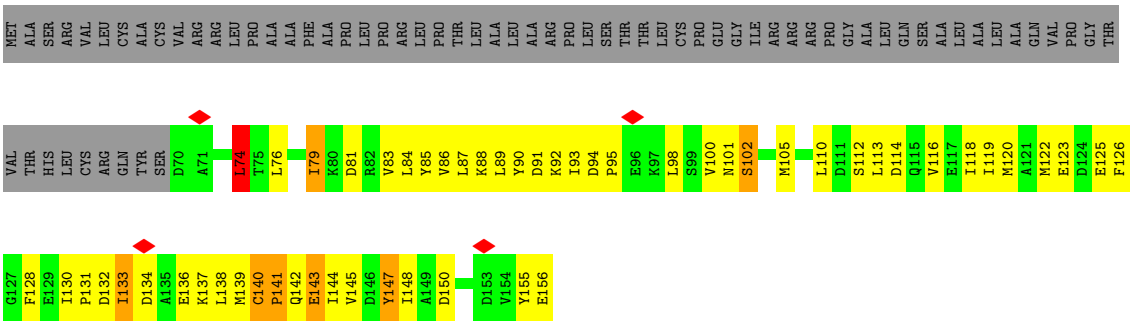
- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



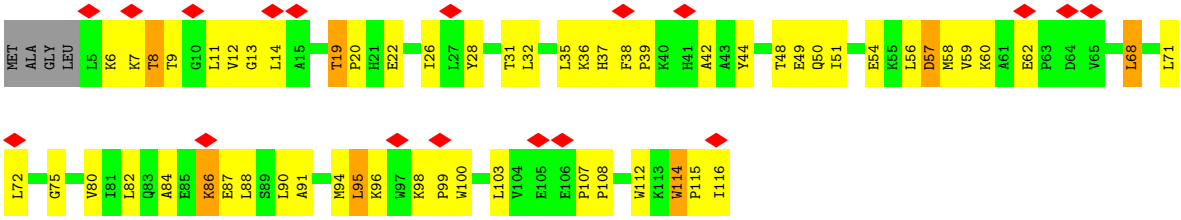
- Molecule 20: Acyl carrier protein, mitochondrial

Chain U:



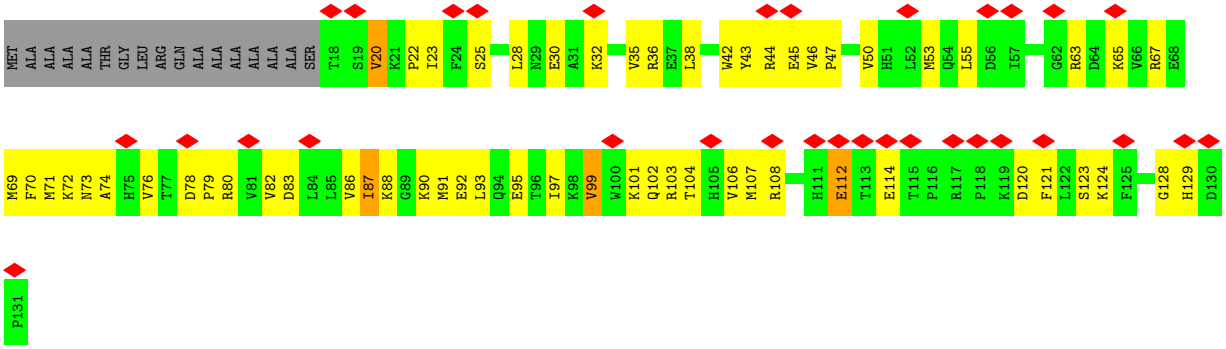
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:

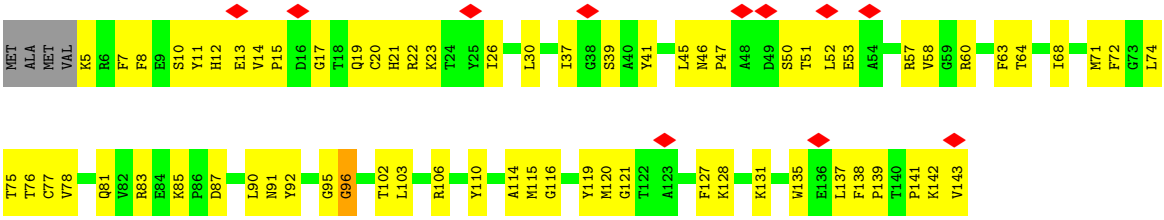


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:

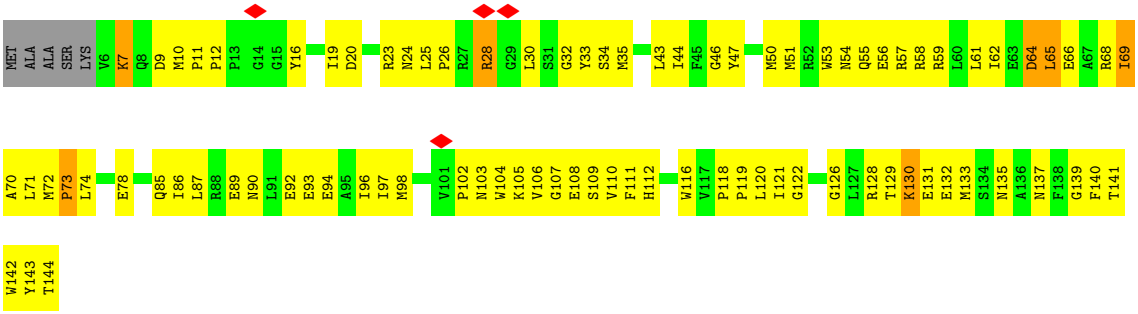
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:



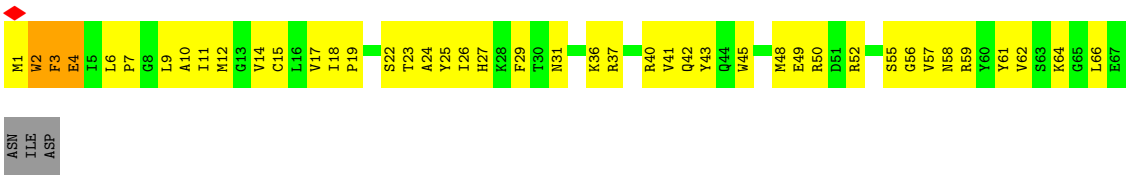
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



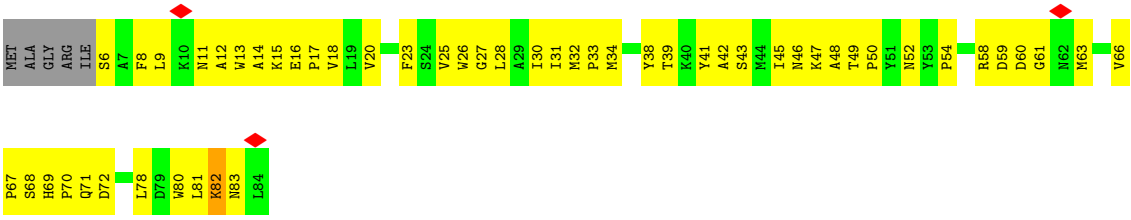
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



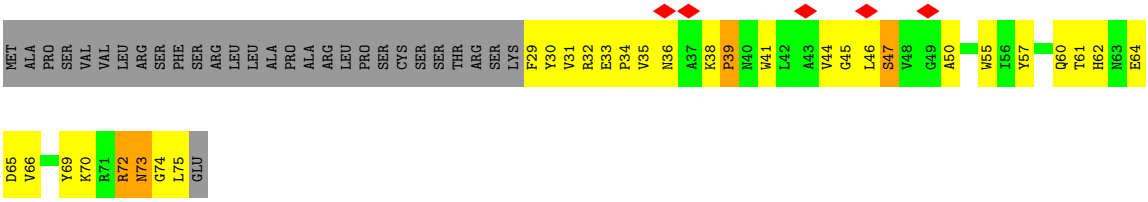
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:

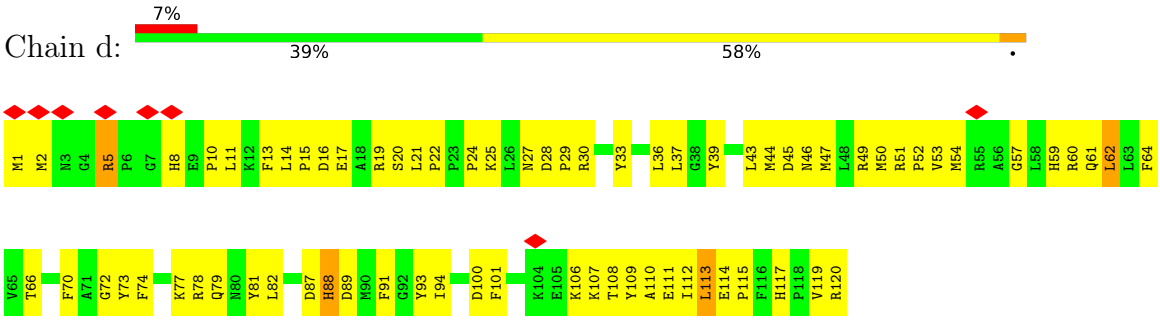


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

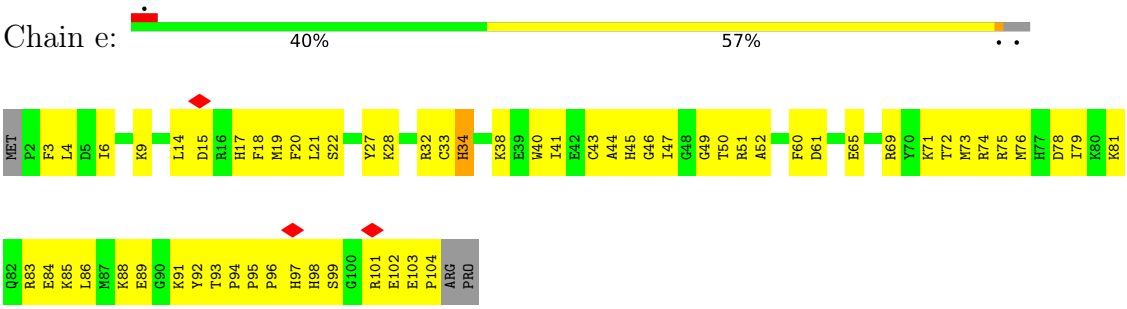
Chain c:



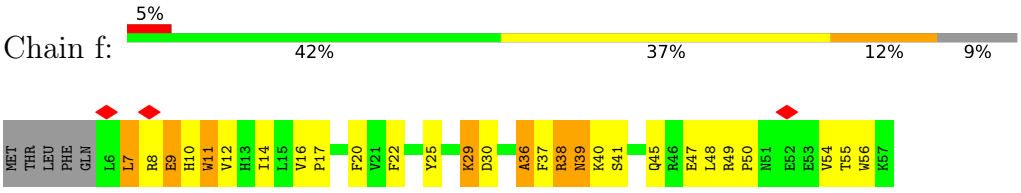
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



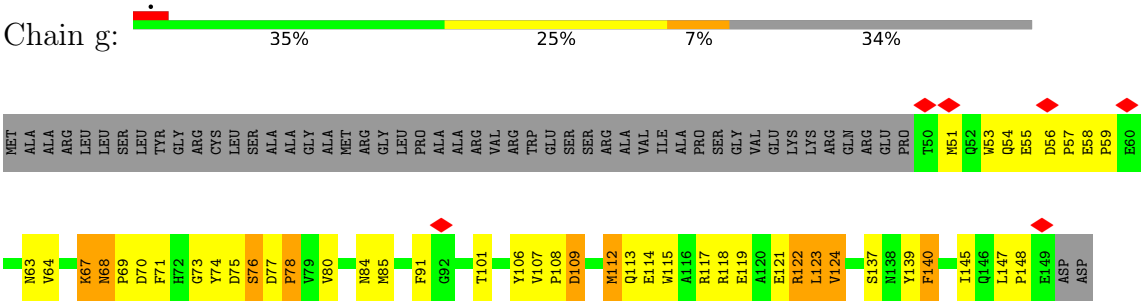
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

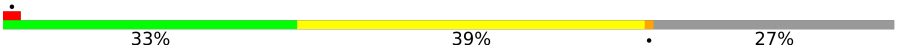


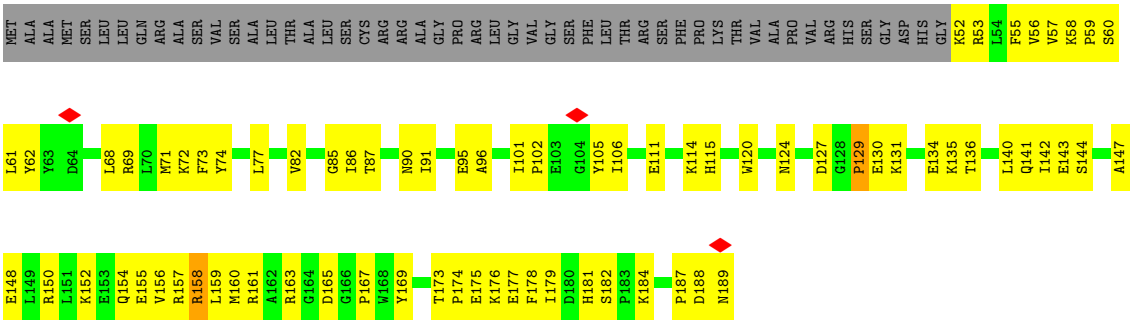
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

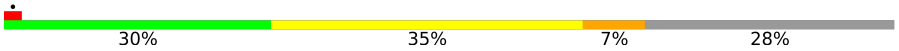
Chain h:

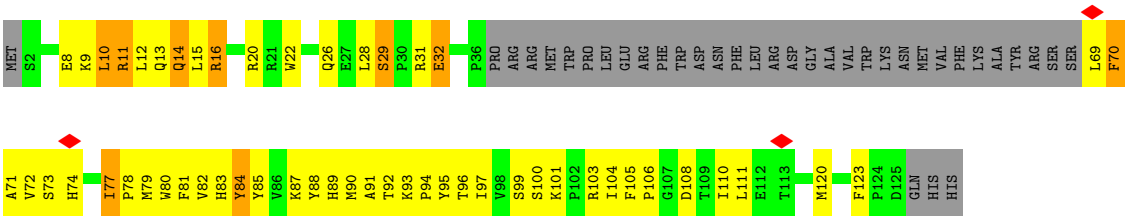




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

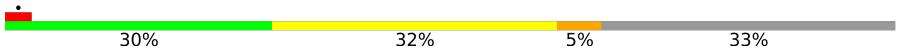
Chain i:

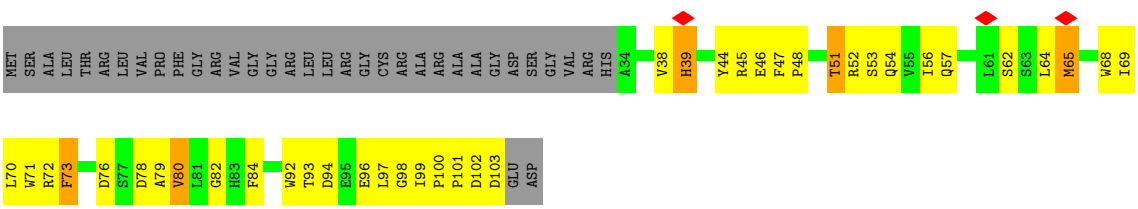




• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

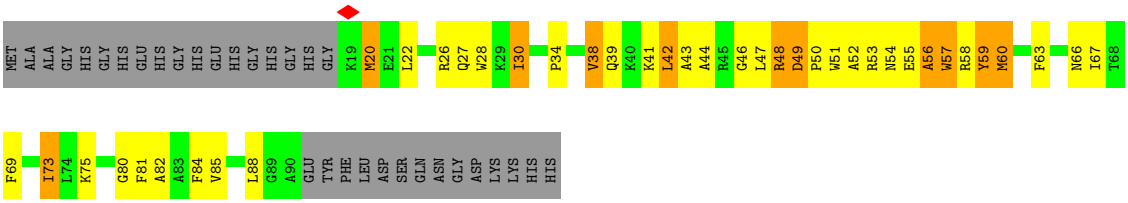
Chain j:





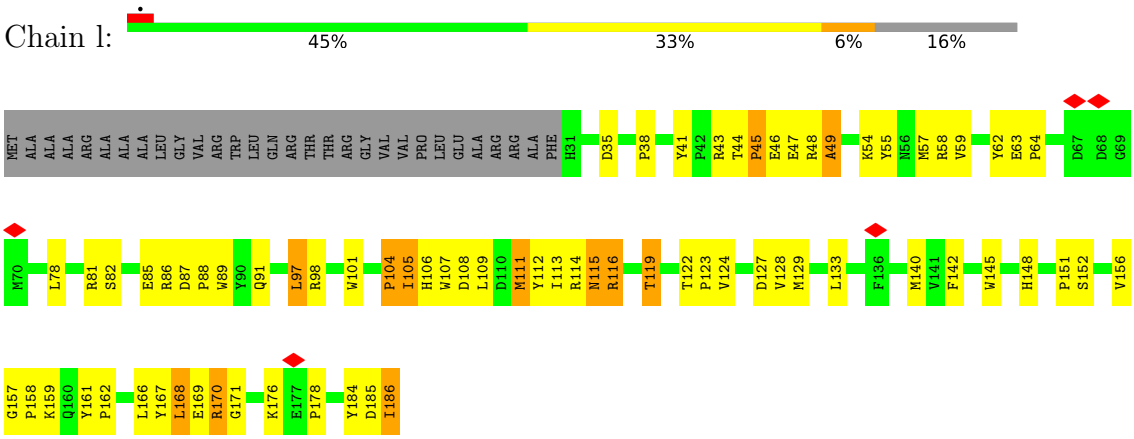
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



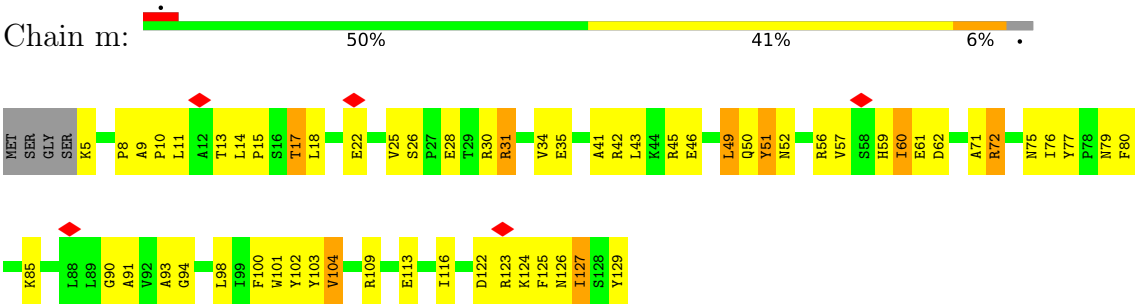
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



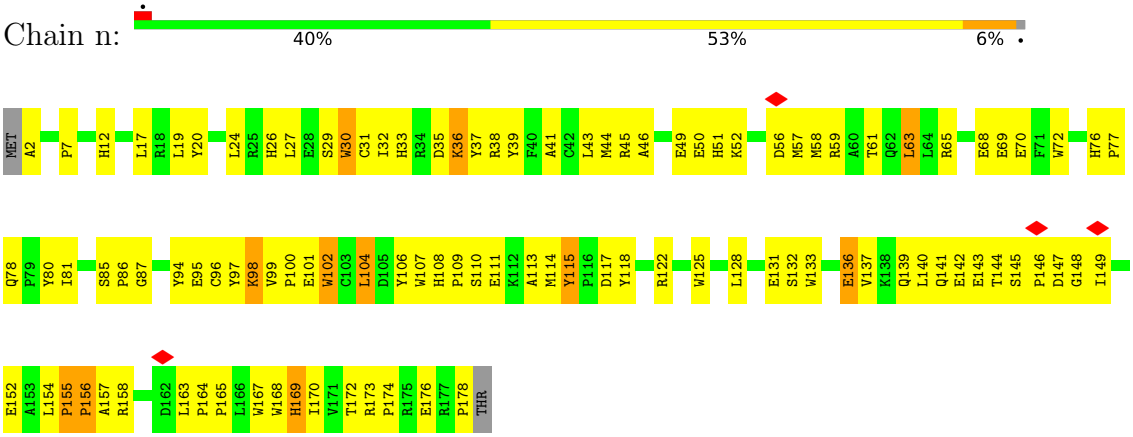
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



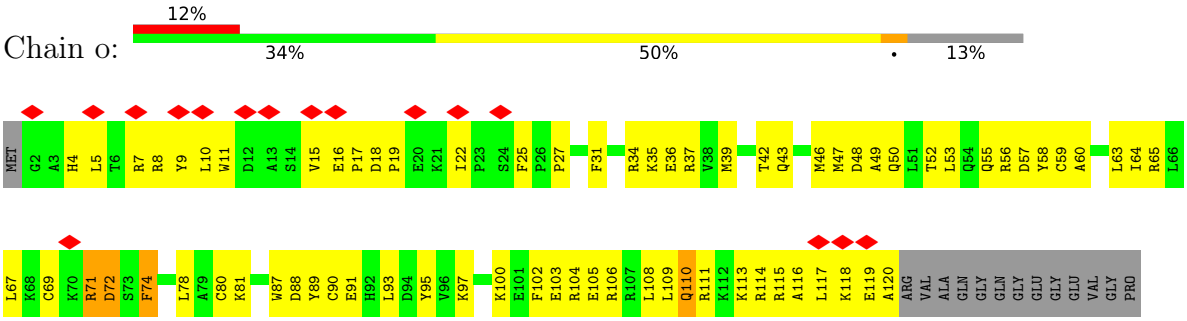
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



GLU VAL ALA LEU

• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p: 45% 47%

MET PRO ASP SER W5 D6 K7 D8 V9 Y10 P11 E12 P13 R16 T17 P18 A19 P20 T24 S25 L26 P29 I30 T31 Y32 L33 T34 K35 A36 Y37 D38 L39 V40 V41 D42 W43 P44 V45 T46 L47 V48 R49 E50 F51 I52 E53 R54 Q55 H56 Y63 Y64 H65 R66 Q67 Y68 R69

R70 V71 P72 D73 I74 T75 E79 V82 L83 C84 I85 Q91 R94 V98 D99 Q100 E101 I102 M103 Q107 E108 R109 L110 K111 A112 C113 Q114 Q115 R116 E117 G118 E119 N120 Y121 Q122 Q123 K127 E128 Q131 F132 T133 K134 V135 T136 Q140 D141 R142 Y143 L144 D145 L146

G147 A148 A152 L156 K160 M163 L164 E165 E166 R167 K168 Q172 E173 A174 ALA ALA

• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 67% 32% 43% 8% 17%

MET E2 L3 V4 E5 V6 L7 K8 R9 G10 V11 Q12 Q13 V14 T15 G16 H17 G18 G19 L20 R21 G22 L23 L24 R25 V26 F27 F28 R29 A30 N31 D32 I33 R34 I35 G36 T37 L38 V39 G40 E41 D42 K43 Y44 G45 N46 K47 Y48 Y49 E50 D51 N52 K53 Q54 F55 F56 G57 R58 H59 R60

W61 V62 I63 Y64 T65 T66 E67 M68 N69 G70 K71 N72 T73 F74 W75 D76 V77 D78 G79 S80 M81 V82 P83 P84 E85 W86 H87 R88 W89 L90 H91 C92 M93 T94 D95 D96 P97 P98 T99 THR ASN PRO PRO THR ALA ARG LYS PHE ILE TRP THR ASN HIS LYS PHE ASN VAL SER ALA THR

PRO GLU Q123 Y124 V125 P126 Y127 S128 T129 T130 R131 K132 K133 I134 H135 E136 W137 V138 P139 P140 S141 T142 P143 Y144 LYS

• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r: 27% 22% 17% 5% 56%

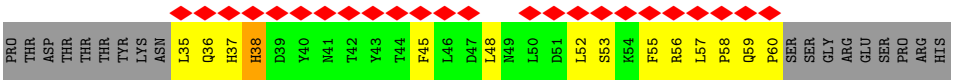
MET ALA S3 A4 T5 R6 V7 I8 Q9 K10 L11 R12 N13 W14 A15 S16 G17 Q18 D19 L20 Q21 A22 K23 L24 Q25 L26 R27 Y28 Q29 GLU ILE ALA LYS ARG THR GLN PRO PRO PRO LYS LEU PRO VAL GLY PRO SER HIS LYS LEU SER ASN ASN TYR TYR CYS THR ARG ASP GLY ARG

ARG GLU VAL VAL PRO PRO SER ILE ILE MET SER SER GLN LYS ALA LEU VAL SER GLY LYS ALA ALA GLU SER SER ALA MET ALA ALA THR E91 K92 K93 A94 V96 T96 P97 R103 W104 S107 K108 D109 Q110 P111 Y112 L113

• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

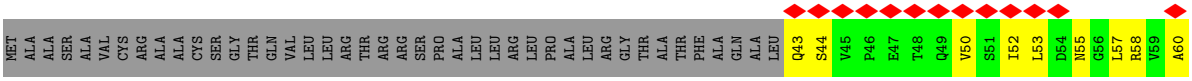
Chain s: 23% 12% 12% 75%

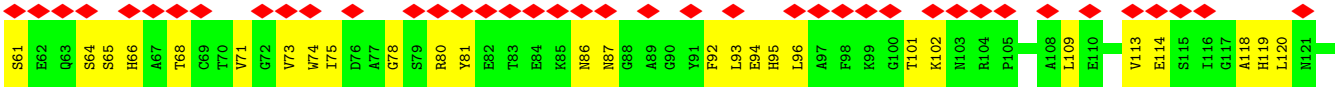
MET ALA VAL SER LEU LEU LEU ARG GLY GLY ARG ILE ARG ALA LEU LYS ALA VAL LEU LEU GLU ALA ARG VAL PHE PRO GLY GLU LEU VAL SER VAL VAL ARG LEU SER THR GLU SER GLU LYS SER ALA LYS GLU LYS GLU LEU HIS PRO LYS THR GLN SER VAL LEU LYS GLU PRO GLU

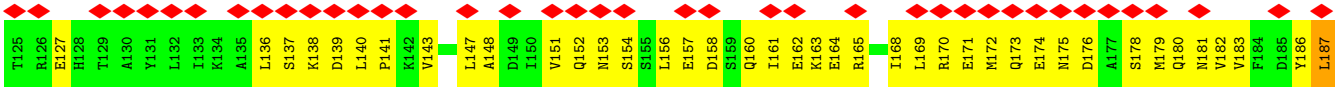


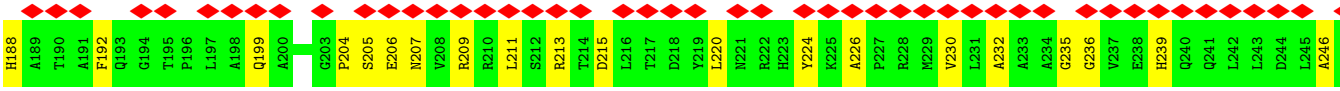
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

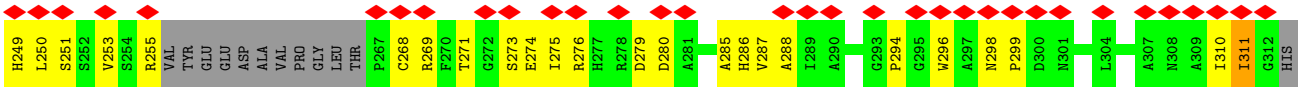
Chain AA:

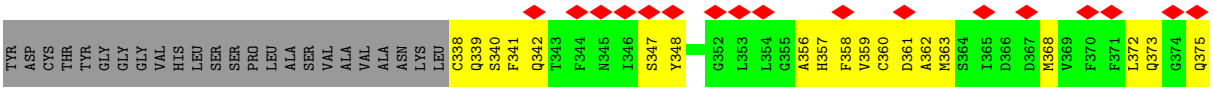


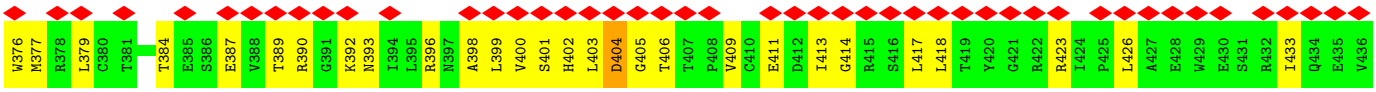


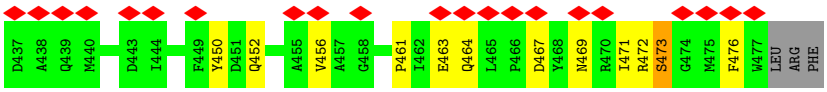






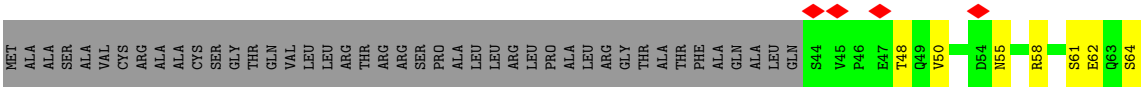


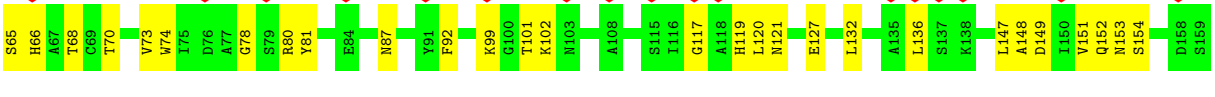


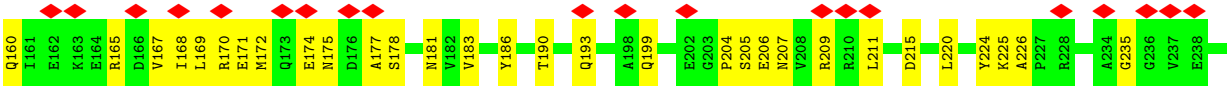


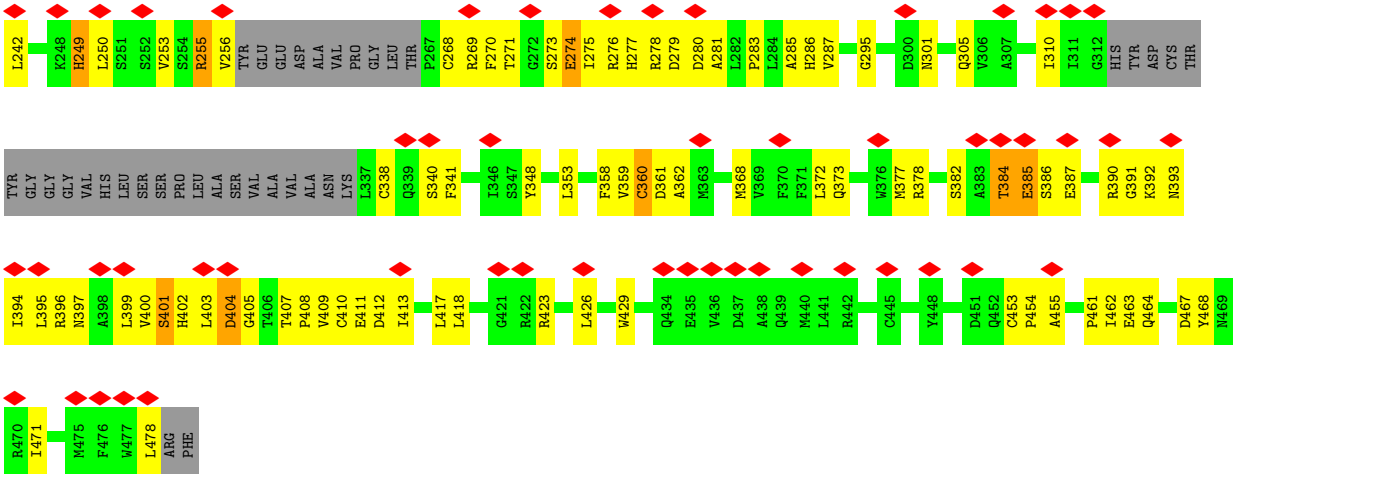
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Aa:



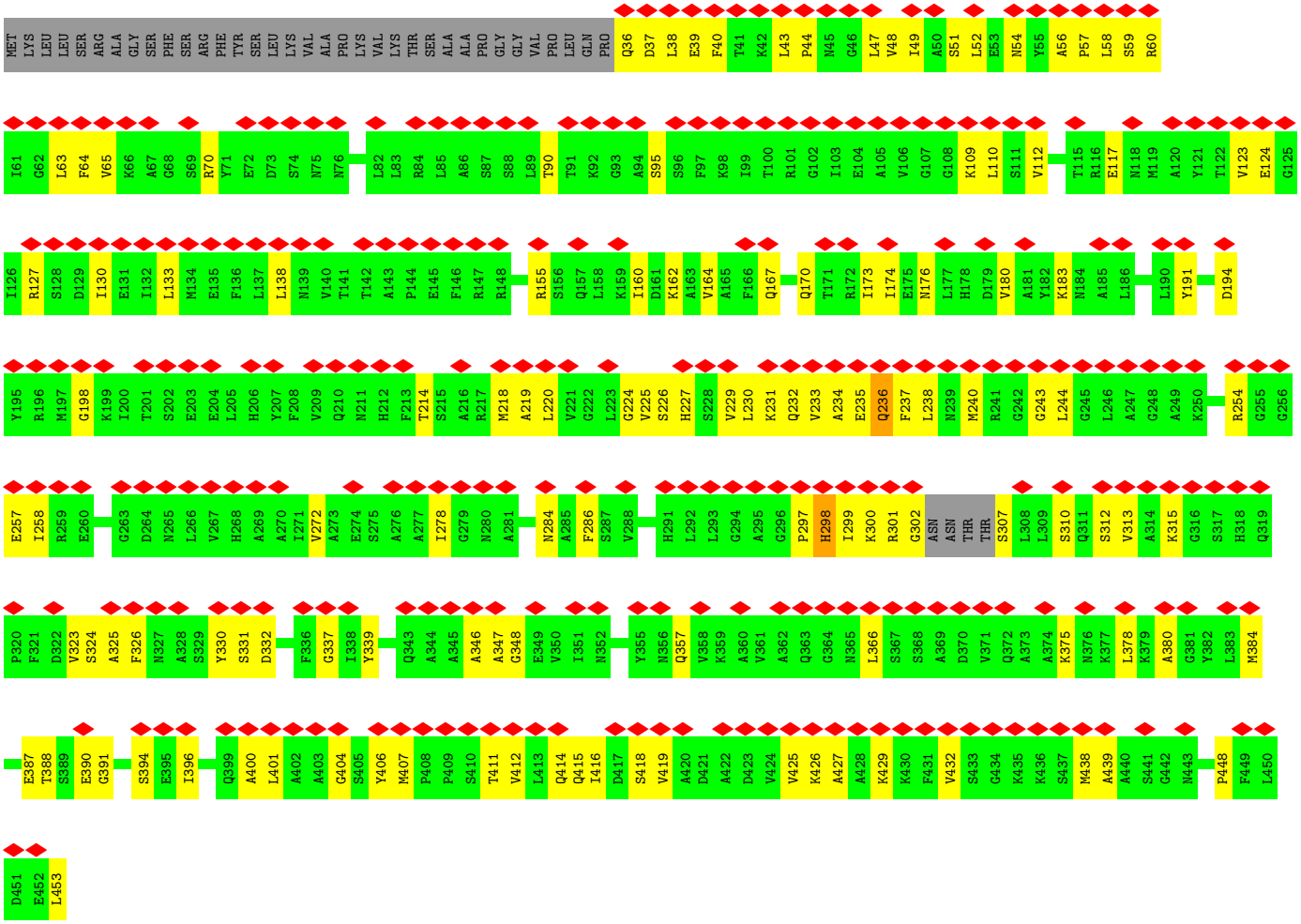






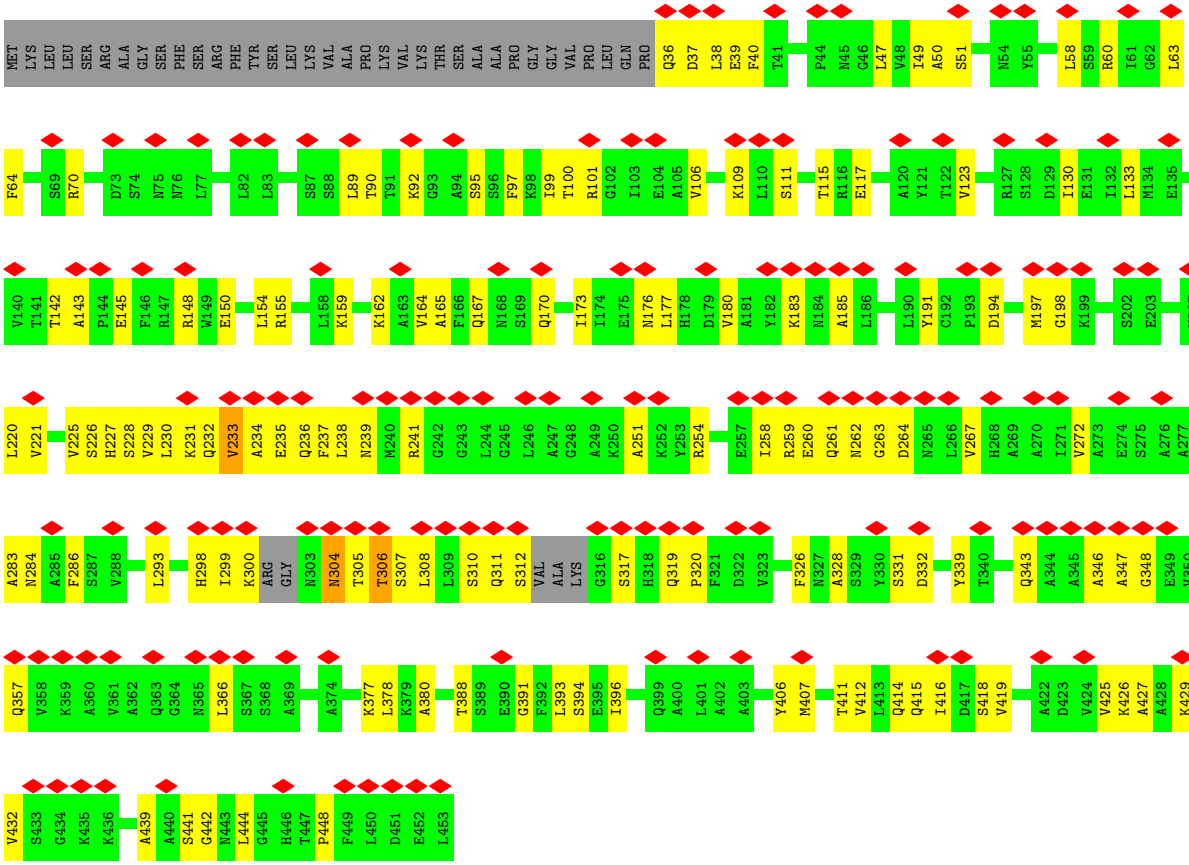
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AB:



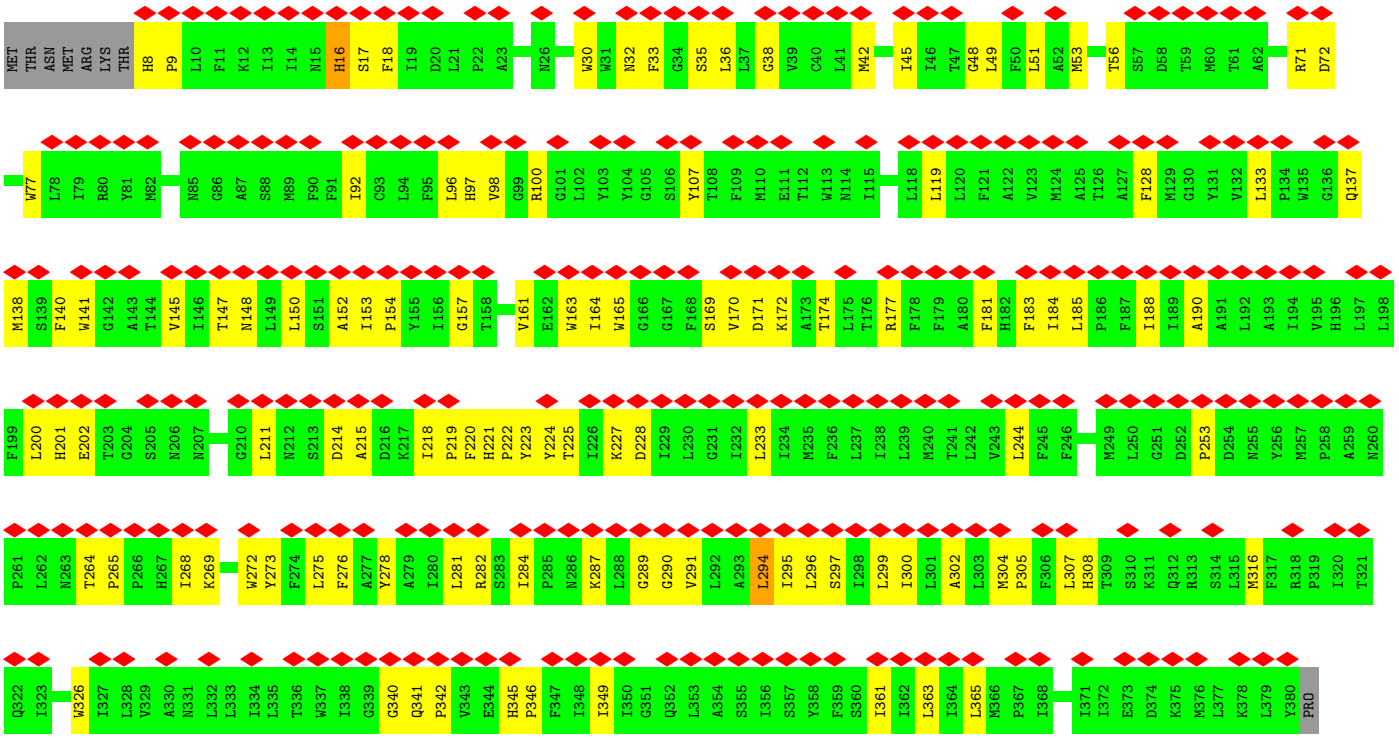
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Ab:



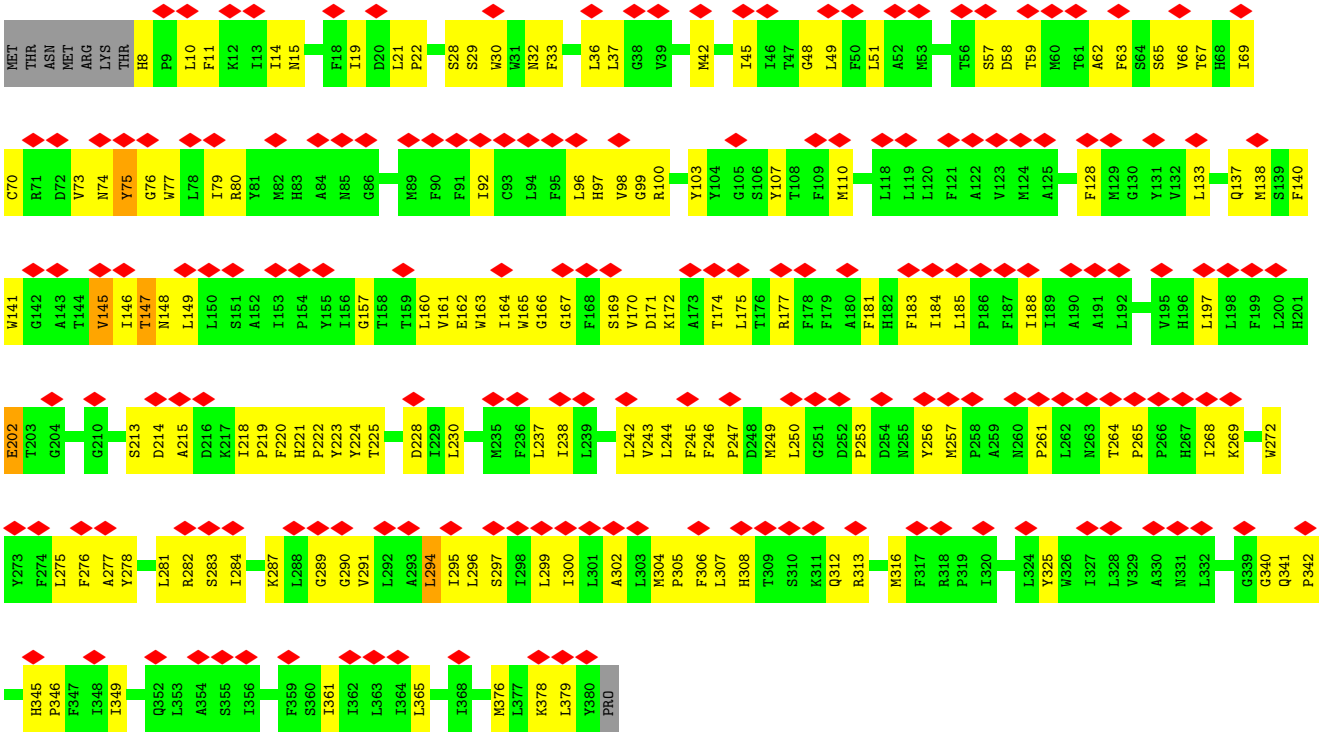
- Molecule 47: Cytochrome b

Chain AC:



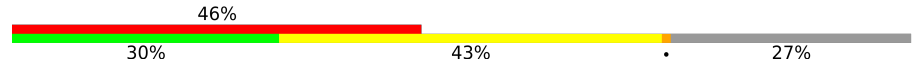
- Molecule 47: Cytochrome b

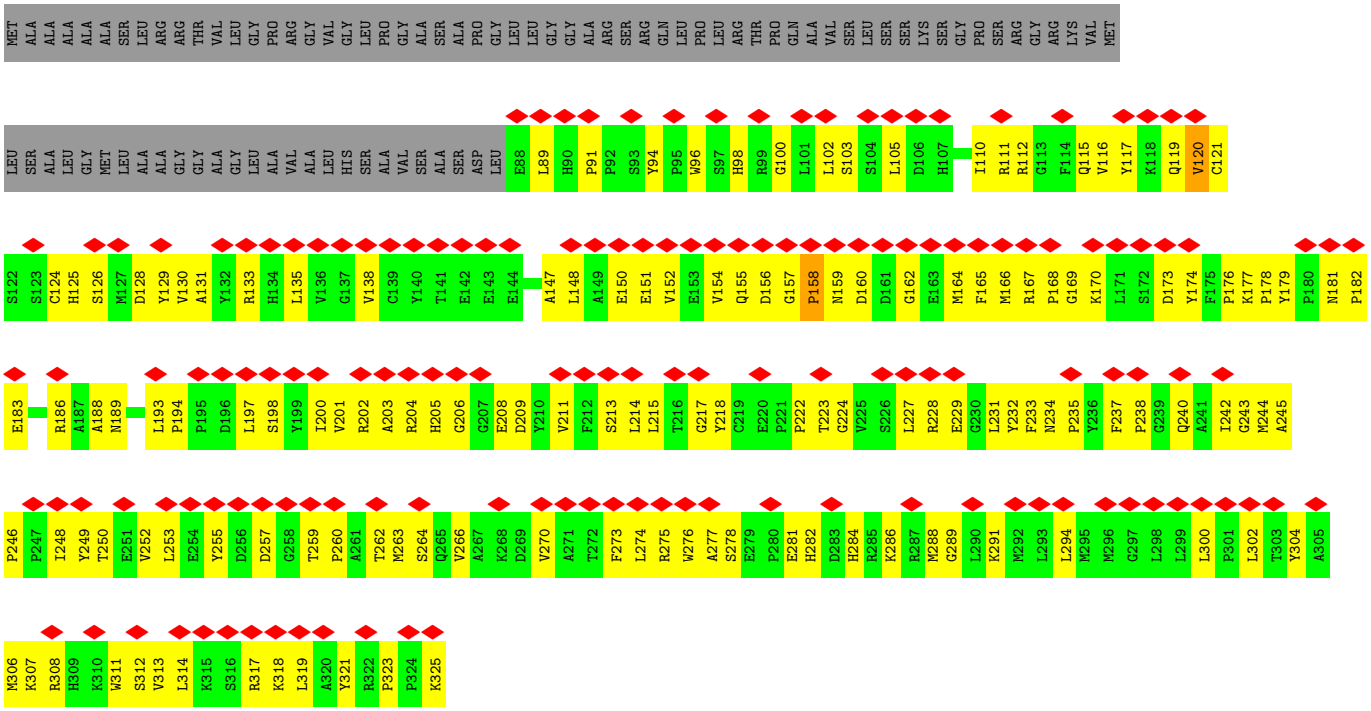
Chain Ac:



- Molecule 48: Cytochrome c1, heme protein, mitochondrial

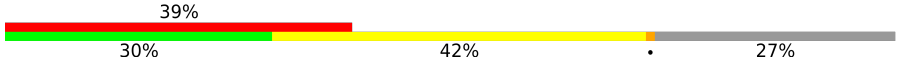
Chain AD:

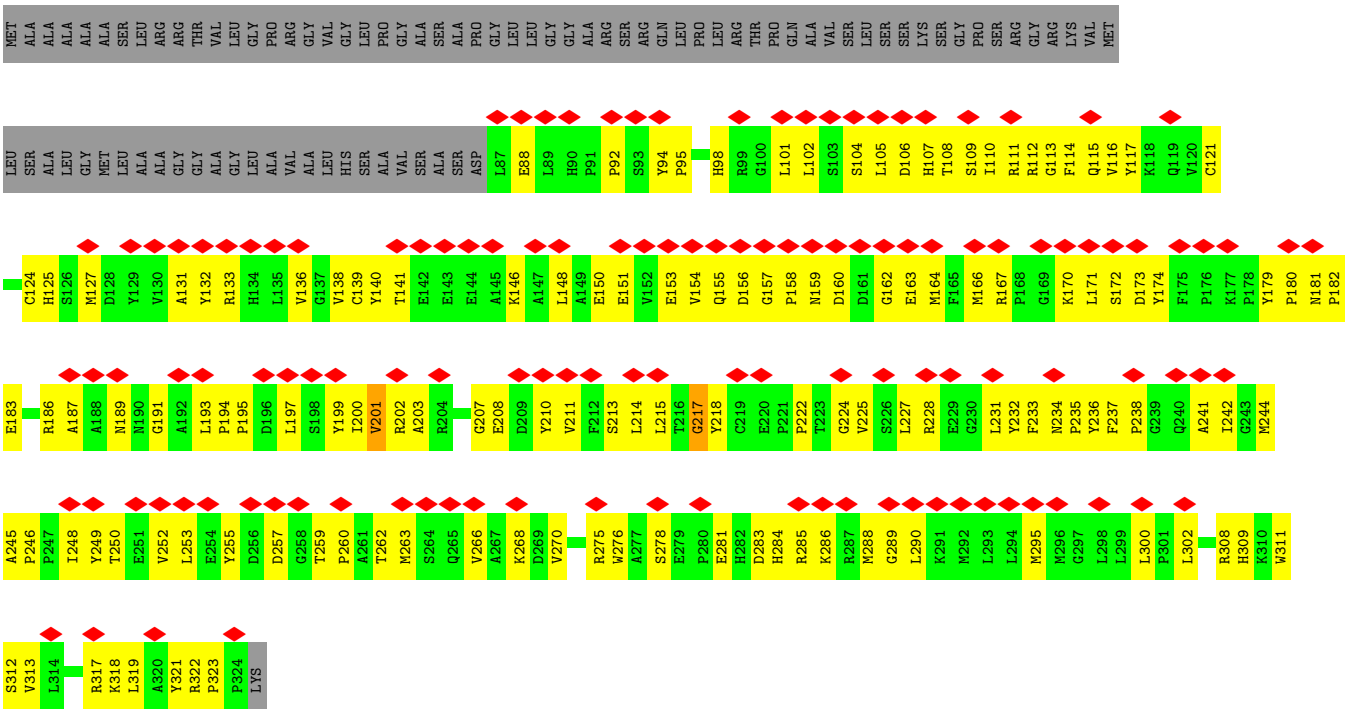




- Molecule 48: Cytochrome c1, heme protein, mitochondrial

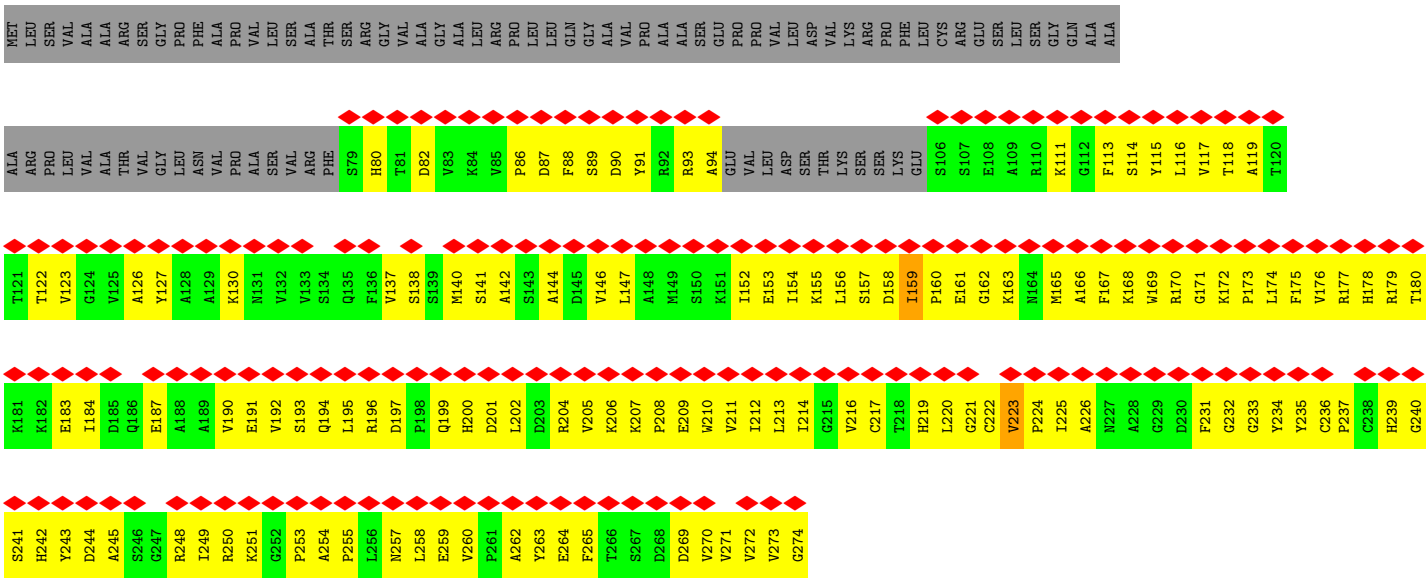
Chain Ad:





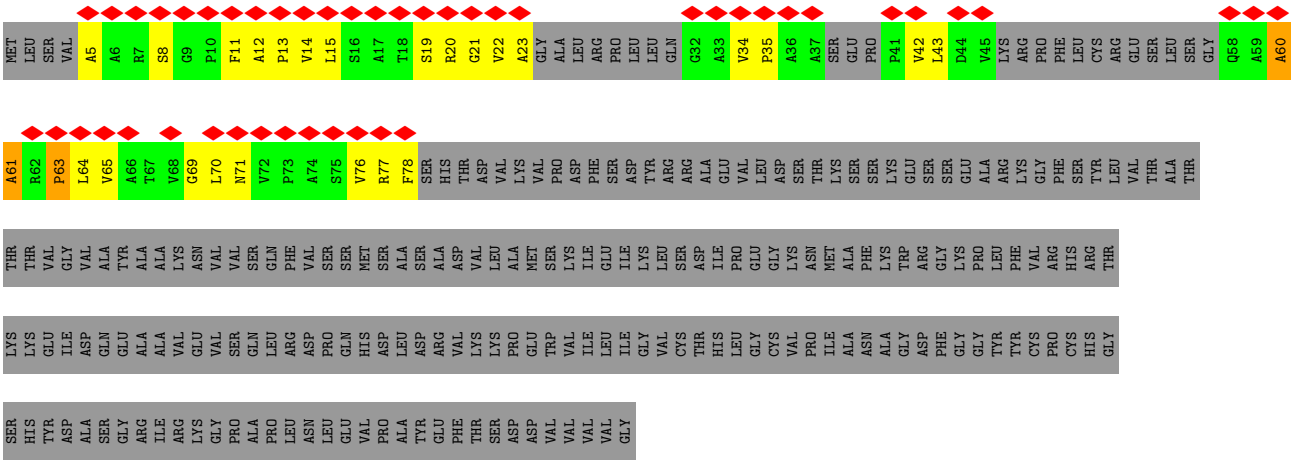
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE:



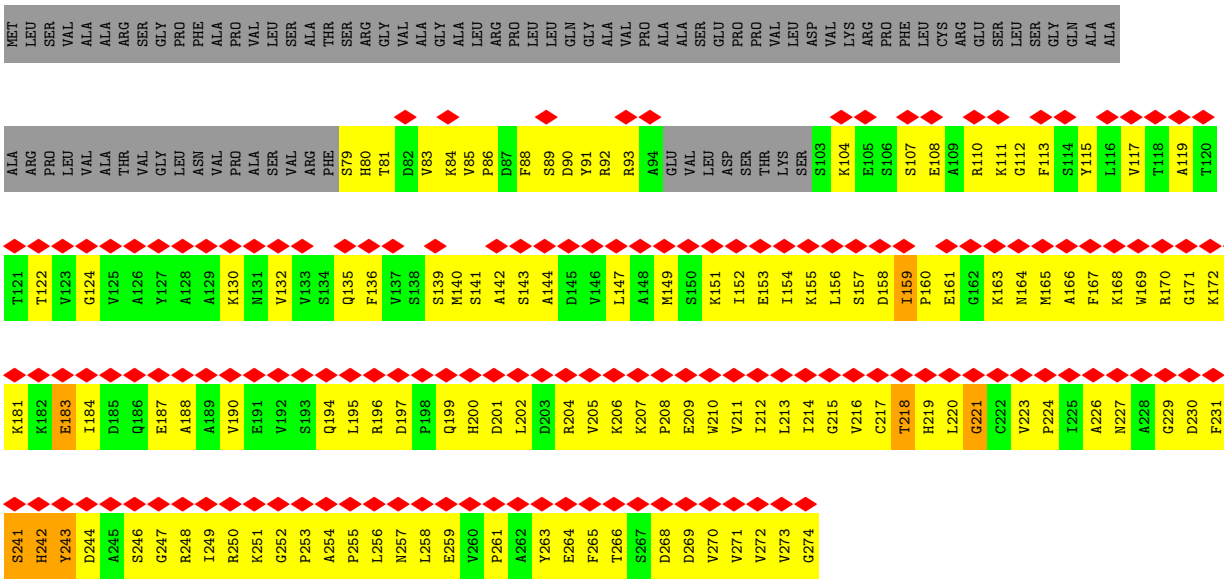
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:



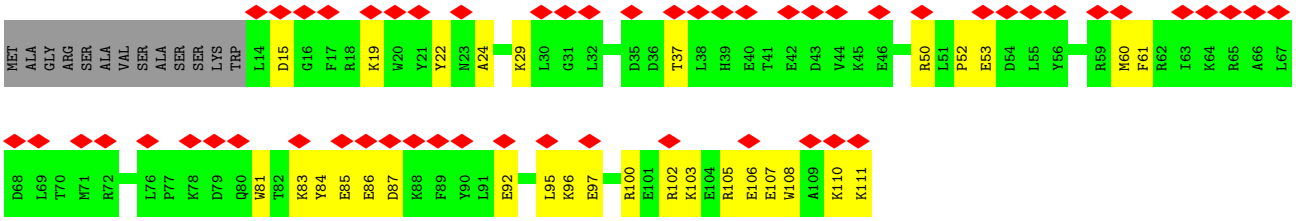
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ae:



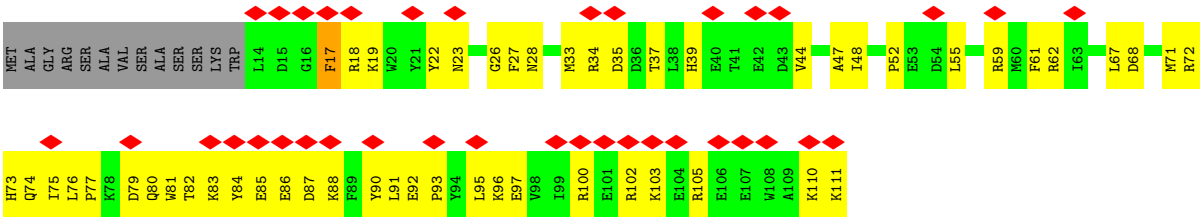
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain AF:



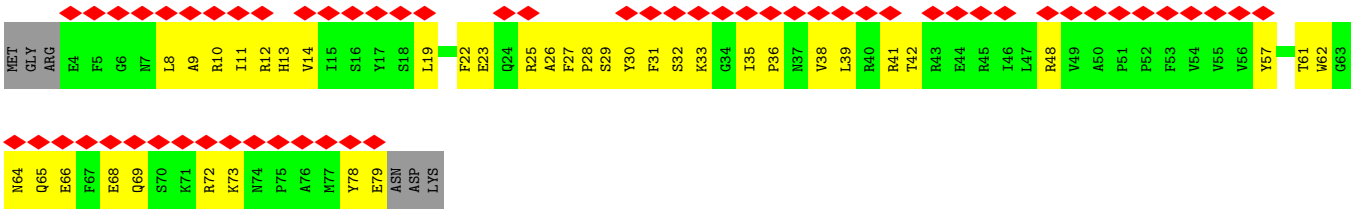
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain Af:



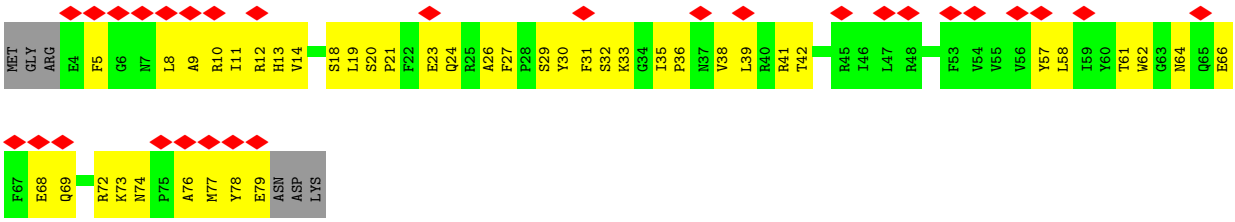
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain AG:



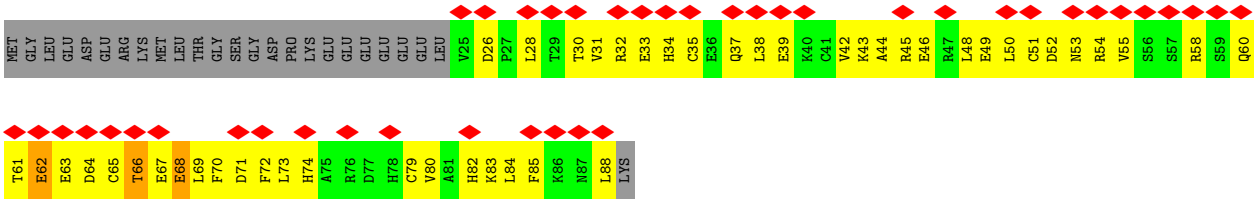
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain Ag:



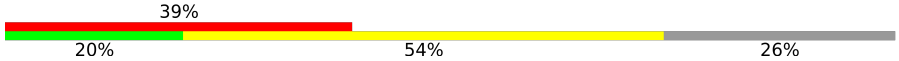
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

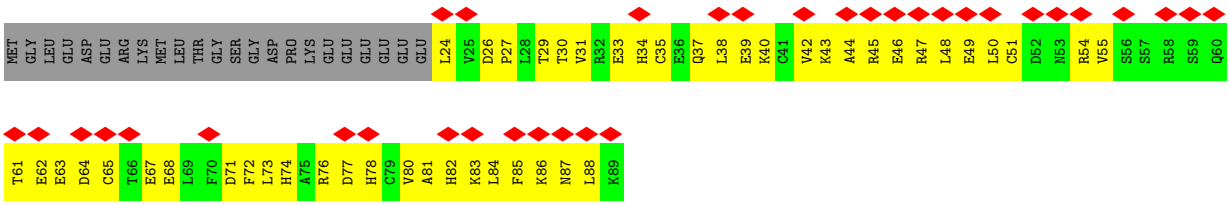
Chain AH:



- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

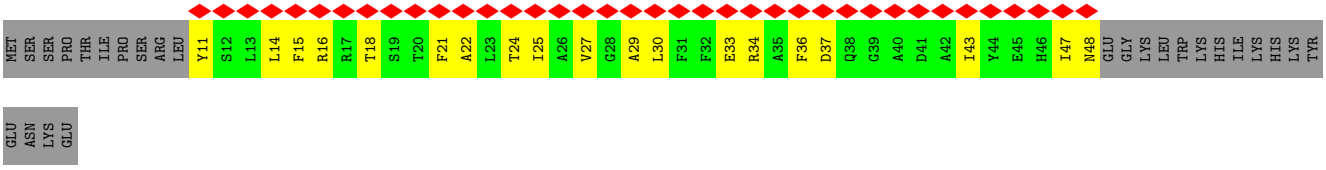
Chain Ah:





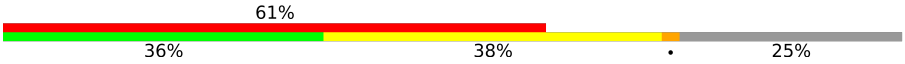
• Molecule 53: Cytochrome b-c1 complex subunit 9

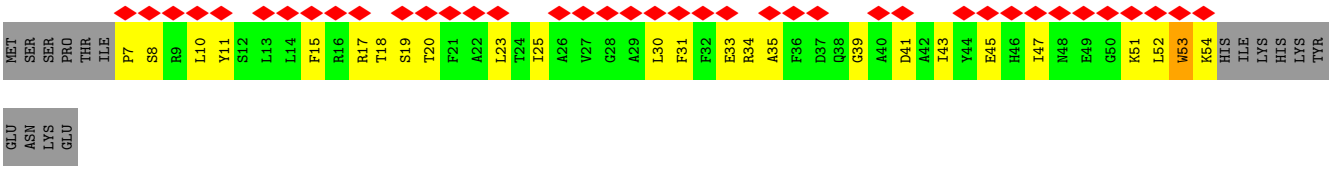
Chain AJ:



• Molecule 53: Cytochrome b-c1 complex subunit 9

Chain Aj:



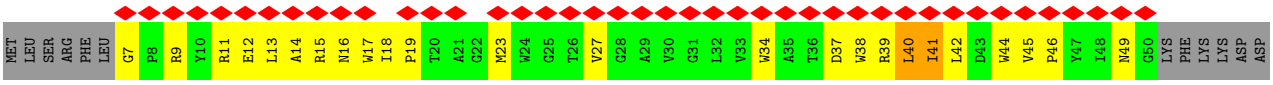


• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain AK:

• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain Ak:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, FMN, HEM, SF4, HEC, FES, NDP, ADP, EHZ, 3PE, UQ1, UQ6, CDL, U10, ZN, UQ9

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	0.81	0/782	1.19	6/1066 (0.6%)
2	B	0.97	1/1278 (0.1%)	1.37	13/1730 (0.8%)
3	C	0.94	2/1687 (0.1%)	1.33	14/2297 (0.6%)
4	D	0.94	7/3512 (0.2%)	1.39	35/4758 (0.7%)
5	E	0.82	2/1675 (0.1%)	1.31	22/2282 (1.0%)
6	F	0.96	6/3363 (0.2%)	1.53	63/4543 (1.4%)
7	G	0.93	10/5374 (0.2%)	1.59	107/7281 (1.5%)
8	H	0.96	3/2600 (0.1%)	1.49	54/3550 (1.5%)
9	I	0.93	1/1427 (0.1%)	1.52	19/1927 (1.0%)
10	J	0.80	0/1221	1.34	16/1656 (1.0%)
11	K	0.91	0/740	1.50	14/1005 (1.4%)
12	L	0.98	5/4921 (0.1%)	1.57	109/6696 (1.6%)
13	M	1.01	7/3717 (0.2%)	1.57	87/5062 (1.7%)
14	N	1.00	4/2756 (0.1%)	1.43	50/3751 (1.3%)
15	O	0.87	6/2666 (0.2%)	1.22	27/3615 (0.7%)
16	P	0.83	3/2804 (0.1%)	1.23	29/3802 (0.8%)
17	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
18	R	1.04	4/671 (0.6%)	1.38	13/903 (1.4%)
19	S	0.90	1/678 (0.1%)	1.47	11/915 (1.2%)
20	T	1.04	1/613 (0.2%)	1.56	12/826 (1.5%)
20	U	1.02	1/712 (0.1%)	1.42	17/962 (1.8%)
21	V	0.86	0/937	1.46	14/1270 (1.1%)
22	W	0.82	1/993 (0.1%)	1.00	3/1335 (0.2%)
23	X	0.79	0/1422	1.31	19/1921 (1.0%)
24	Y	0.87	0/1054	0.97	3/1429 (0.2%)
25	Z	0.82	1/1183 (0.1%)	1.22	12/1597 (0.8%)
26	a	0.88	0/561	1.38	8/755 (1.1%)
27	b	0.74	0/643	0.95	1/884 (0.1%)
28	c	0.96	1/400 (0.2%)	1.34	11/544 (2.0%)
29	d	1.02	2/1028 (0.2%)	1.16	11/1387 (0.8%)
30	e	0.74	1/881 (0.1%)	1.00	2/1173 (0.2%)
31	f	0.90	1/459 (0.2%)	1.32	11/618 (1.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.88	3/870 (0.3%)	1.36	19/1185 (1.6%)
33	h	0.75	0/1197	1.22	6/1621 (0.4%)
34	i	0.85	0/798	1.38	17/1085 (1.6%)
35	j	0.87	2/612 (0.3%)	1.28	10/837 (1.2%)
36	k	1.12	2/596 (0.3%)	1.55	20/805 (2.5%)
37	l	1.02	4/1367 (0.3%)	1.27	10/1866 (0.5%)
38	m	0.85	1/1073 (0.1%)	1.20	15/1455 (1.0%)
39	n	0.95	1/1589 (0.1%)	1.26	17/2152 (0.8%)
40	o	0.82	0/1044	1.14	7/1401 (0.5%)
41	p	0.73	1/1471 (0.1%)	1.01	13/1988 (0.7%)
42	q	0.98	2/1037 (0.2%)	1.41	17/1408 (1.2%)
43	r	0.94	2/421 (0.5%)	1.37	8/566 (1.4%)
44	s	0.43	0/233	0.75	1/317 (0.3%)
45	AA	0.57	1/3176 (0.0%)	0.85	7/4305 (0.2%)
45	Aa	0.45	0/3190	0.78	9/4325 (0.2%)
46	AB	0.44	1/3156 (0.0%)	0.62	3/4263 (0.1%)
46	Ab	0.44	0/3149	0.69	5/4255 (0.1%)
47	AC	0.41	0/3089	0.72	6/4221 (0.1%)
47	Ac	0.48	0/3089	0.79	5/4221 (0.1%)
48	AD	0.54	0/1955	0.81	1/2655 (0.0%)
48	Ad	0.65	2/1954 (0.1%)	0.86	4/2655 (0.2%)
49	AE	0.50	0/1459	0.94	4/1976 (0.2%)
49	AI	0.96	1/351 (0.3%)	1.34	5/478 (1.0%)
49	Ae	0.56	0/1483	1.04	8/2007 (0.4%)
50	AF	0.38	0/884	0.52	0/1184
50	Af	0.72	1/884 (0.1%)	0.82	0/1184
51	AG	0.50	0/662	0.87	1/895 (0.1%)
51	Ag	0.54	0/662	0.94	2/895 (0.2%)
52	AH	0.54	0/534	0.95	4/717 (0.6%)
52	Ah	0.65	0/551	0.82	0/739
53	AJ	0.46	0/314	0.60	0/424
53	Aj	0.62	0/402	0.80	1/541 (0.2%)
54	AK	0.49	0/287	0.84	1/393 (0.3%)
54	Ak	0.53	0/371	0.82	2/511 (0.4%)
All	All	0.81	96/97648 (0.1%)	1.22	1053/132394 (0.8%)

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	89	PRO	N-CD	-15.12	1.26	1.47
29	d	115	PRO	N-CD	-14.11	1.28	1.47
12	L	265	PRO	N-CD	13.82	1.67	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	50	PRO	N-CD	-13.63	1.28	1.47
14	N	255	PRO	N-CD	-13.58	1.28	1.47

The worst 5 of 1053 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	142	VAL	N-CA-CB	19.28	132.44	110.65
4	D	142	VAL	N-CA-C	-19.03	92.53	110.42
7	G	174	THR	N-CA-C	-16.87	89.00	114.64
6	F	125	CYS	N-CA-C	-15.62	93.48	113.17
6	F	332	CYS	N-CA-C	15.55	129.99	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	762	0	823	117	0
2	B	1247	0	1258	156	0
3	C	1641	0	1596	135	0
4	D	3423	0	3364	356	0
5	E	1635	0	1626	166	0
6	F	3288	0	3243	356	0
7	G	5287	0	5323	554	0
8	H	2525	0	2613	380	0
9	I	1398	0	1359	166	0
10	J	1193	0	1215	203	0
11	K	729	0	764	111	0
12	L	4798	0	4986	622	0
13	M	3630	0	3854	550	0
14	N	2694	0	2896	348	0
15	O	2599	0	2552	264	0
16	P	2730	0	2747	226	0
17	Q	957	0	949	70	0
18	R	660	0	639	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	667	0	683	71	0
20	T	604	0	596	93	0
20	U	700	0	691	74	0
21	V	915	0	954	80	0
22	W	970	0	991	80	0
23	X	1385	0	1370	137	0
24	Y	1030	0	1015	96	0
25	Z	1152	0	1148	142	0
26	a	548	0	562	56	0
27	b	620	0	617	90	0
28	c	389	0	385	38	0
29	d	996	0	1001	91	0
30	e	859	0	849	105	0
31	f	447	0	444	31	0
32	g	842	0	779	69	0
33	h	1162	0	1163	126	0
34	i	773	0	780	71	0
35	j	587	0	533	71	0
36	k	578	0	581	55	0
37	l	1312	0	1204	100	0
38	m	1044	0	1056	112	0
39	n	1534	0	1463	159	0
40	o	1019	0	1006	108	0
41	p	1438	0	1404	122	0
42	q	1004	0	962	90	0
43	r	413	0	429	45	0
44	s	226	0	214	14	0
45	AA	3117	0	3032	188	0
45	Aa	3131	0	3055	165	0
46	AB	3107	0	3116	148	0
46	Ab	3101	0	3098	134	0
47	AC	2988	0	3045	144	0
47	Ac	2988	0	3045	187	0
48	AD	1896	0	1846	188	0
48	Ad	1895	0	1844	173	0
49	AE	1427	0	1407	230	0
49	AI	347	0	363	46	0
49	Ae	1451	0	1433	250	0
50	AF	864	0	854	27	0
50	Af	864	0	854	56	0
51	AG	643	0	643	64	0
51	Ag	643	0	643	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AH	527	0	507	73	0
52	Ah	544	0	529	56	0
53	AJ	307	0	295	34	0
53	Aj	392	0	388	30	0
54	AK	278	0	278	37	0
54	Ak	357	0	347	25	0
55	B	8	0	0	5	0
55	F	8	0	0	10	0
55	G	16	0	0	5	0
55	I	16	0	0	16	0
56	B	18	0	18	12	0
57	B	35	0	44	3	0
57	I	47	0	71	7	0
57	L	50	0	74	17	0
58	AC	25	0	24	4	0
58	Ac	35	0	44	4	0
58	D	38	0	50	13	0
58	I	46	0	69	10	0
58	J	46	0	69	18	0
58	K	46	0	66	6	0
58	L	135	0	198	35	0
58	M	139	0	212	40	0
58	O	44	0	65	7	0
58	b	46	0	69	11	0
58	i	40	0	54	11	0
58	j	40	0	54	9	0
58	m	92	0	138	16	0
59	E	4	0	0	4	0
59	G	4	0	0	4	0
60	F	31	0	19	3	0
61	H	35	0	43	16	0
62	Aa	46	0	36	3	0
62	Ac	42	0	28	5	0
62	Ag	56	0	56	6	0
62	L	158	0	204	31	0
62	a	57	0	58	15	0
62	d	67	0	81	5	0
62	h	70	0	87	13	0
63	O	27	0	12	6	0
64	P	48	0	26	4	0
65	R	1	0	0	0	0
66	W	32	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	n	32	0	0	0	0
67	AC	86	0	60	8	0
67	Ac	86	0	60	6	0
68	AC	23	0	23	9	0
68	Ac	23	0	23	12	0
69	AC	28	0	31	7	0
69	Ac	28	0	31	8	0
70	AD	43	0	32	5	0
70	Ad	43	0	32	18	0
All	All	97317	0	97570	7945	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 41.

The worst 5 of 7945 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)
12:L:302:ILE:HG22	12:L:340:PHE:CZ	1.64	1.31
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.17	1.28
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
62:L:705:CDL:H111	24:Y:115:MET:SD	1.75	1.27
58:M:503:3PE:HN3	15:O:338:LYS:CE	1.50	1.23

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	89/115 (77%)	82 (92%)	7 (8%)	0	100 100
2	B	154/224 (69%)	142 (92%)	10 (6%)	2 (1%)	9 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	196/263 (74%)	186 (95%)	8 (4%)	2 (1%)	12	47
4	D	421/463 (91%)	392 (93%)	29 (7%)	0	100	100
5	E	208/248 (84%)	191 (92%)	17 (8%)	0	100	100
6	F	424/464 (91%)	406 (96%)	18 (4%)	0	100	100
7	G	685/727 (94%)	631 (92%)	54 (8%)	0	100	100
8	H	310/318 (98%)	291 (94%)	18 (6%)	1 (0%)	36	71
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	J	151/172 (88%)	140 (93%)	11 (7%)	0	100	100
11	K	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
12	L	604/607 (100%)	572 (95%)	32 (5%)	0	100	100
13	M	457/459 (100%)	438 (96%)	19 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	71
15	O	317/355 (89%)	306 (96%)	11 (4%)	0	100	100
16	P	338/377 (90%)	312 (92%)	26 (8%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	75 (93%)	6 (7%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	110 (98%)	1 (1%)	1 (1%)	14	49
23	X	167/172 (97%)	155 (93%)	12 (7%)	0	100	100
24	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
25	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
26	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
27	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
28	c	45/76 (59%)	45 (100%)	0	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
31	f	50/57 (88%)	48 (96%)	2 (4%)	0	100	100
32	g	98/151 (65%)	92 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	88/128 (69%)	79 (90%)	9 (10%)	0	100	100
35	j	68/105 (65%)	64 (94%)	4 (6%)	0	100	100
36	k	70/104 (67%)	67 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	m	123/129 (95%)	114 (93%)	9 (7%)	0	100	100
39	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	21	58
40	o	117/137 (85%)	113 (97%)	4 (3%)	0	100	100
41	p	168/176 (96%)	150 (89%)	18 (11%)	0	100	100
42	q	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
43	r	46/113 (41%)	44 (96%)	2 (4%)	0	100	100
44	s	24/104 (23%)	24 (100%)	0	0	100	100
45	AA	393/480 (82%)	378 (96%)	15 (4%)	0	100	100
45	Aa	395/480 (82%)	384 (97%)	11 (3%)	0	100	100
46	AB	410/453 (90%)	400 (98%)	10 (2%)	0	100	100
46	Ab	407/453 (90%)	397 (98%)	10 (2%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	362 (98%)	8 (2%)	1 (0%)	36	71
48	AD	236/325 (73%)	229 (97%)	6 (2%)	1 (0%)	30	66
48	Ad	236/325 (73%)	224 (95%)	12 (5%)	0	100	100
49	AE	181/274 (66%)	168 (93%)	13 (7%)	0	100	100
49	AI	43/274 (16%)	41 (95%)	2 (5%)	0	100	100
49	Ae	184/274 (67%)	171 (93%)	12 (6%)	1 (0%)	24	62
50	AF	96/111 (86%)	96 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	74 (100%)	0	0	100	100
51	Ag	74/82 (90%)	73 (99%)	1 (1%)	0	100	100
52	AH	62/89 (70%)	62 (100%)	0	0	100	100
52	Ah	64/89 (72%)	63 (98%)	1 (2%)	0	100	100
53	AJ	36/64 (56%)	36 (100%)	0	0	100	100
53	Aj	46/64 (72%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	AK	32/56 (57%)	31 (97%)	1 (3%)	0	100	100
54	Ak	42/56 (75%)	41 (98%)	1 (2%)	0	100	100
All	All	11748/14118 (83%)	11208 (95%)	529 (4%)	11 (0%)	49	83

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	GLN
3	C	135	ARG
8	H	92	PRO
14	N	109	ALA
3	C	81	ASP

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	A	85/104 (82%)	85 (100%)	0	100	100
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	367/395 (93%)	367 (100%)	0	100	100
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	81
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	278/280 (99%)	278 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	J	126/138 (91%)	123 (98%)	3 (2%)	43	63
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	82
13	M	415/415 (100%)	414 (100%)	1 (0%)	87	85
14	N	307/308 (100%)	306 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	297/325 (91%)	295 (99%)	2 (1%)	76	79
17	Q	105/153 (69%)	104 (99%)	1 (1%)	68	76
18	R	70/96 (73%)	69 (99%)	1 (1%)	59	71
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
20	T	69/135 (51%)	68 (99%)	1 (1%)	59	71
20	U	80/135 (59%)	79 (99%)	1 (1%)	61	72
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	152/154 (99%)	152 (100%)	0	100	100
24	Y	104/107 (97%)	104 (100%)	0	100	100
25	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	70/73 (96%)	70 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	48/53 (91%)	48 (100%)	0	100	100
32	g	91/129 (70%)	91 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	87/120 (72%)	86 (99%)	1 (1%)	65	74
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	55/78 (70%)	55 (100%)	0	100	100
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	111/114 (97%)	111 (100%)	0	100	100
39	n	162/164 (99%)	161 (99%)	1 (1%)	78	80
40	o	109/121 (90%)	109 (100%)	0	100	100
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	108/131 (82%)	108 (100%)	0	100	100
43	r	44/96 (46%)	44 (100%)	0	100	100
44	s	26/95 (27%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	AA	337/398 (85%)	337 (100%)	0	100	100
45	Aa	339/398 (85%)	338 (100%)	1 (0%)	86	84
46	AB	324/356 (91%)	324 (100%)	0	100	100
46	Ab	325/356 (91%)	324 (100%)	1 (0%)	86	84
47	AC	325/333 (98%)	324 (100%)	1 (0%)	86	84
47	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
48	AD	203/260 (78%)	203 (100%)	0	100	100
48	Ad	203/260 (78%)	202 (100%)	1 (0%)	81	81
49	AE	155/224 (69%)	154 (99%)	1 (1%)	78	80
49	AI	34/224 (15%)	34 (100%)	0	100	100
49	Ae	158/224 (70%)	158 (100%)	0	100	100
50	AF	90/99 (91%)	90 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	69/74 (93%)	69 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	61/83 (74%)	61 (100%)	0	100	100
52	Ah	63/83 (76%)	63 (100%)	0	100	100
53	AJ	30/55 (54%)	30 (100%)	0	100	100
53	Aj	39/55 (71%)	39 (100%)	0	100	100
54	AK	26/46 (56%)	26 (100%)	0	100	100
54	Ak	34/46 (74%)	34 (100%)	0	100	100
All	All	10324/12037 (86%)	10299 (100%)	25 (0%)	85	85

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	103	HIS
34	i	72	VAL
48	Ad	201	VAL
25	Z	7	LYS
39	n	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 234 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	275	HIS
47	Ac	32	ASN
34	i	83	HIS
46	Ab	415	GLN
51	AG	69	GLN

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 55 ligands modelled in this entry, 1 is monoatomic - leaving 54 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	$\#\|Z\| > 2$
67	HEM	Ac	401	47	50,50,50	1.59	10 (20%)	66,82,82	1.78	16 (24%)
62	CDL	L	704	-	76,76,99	1.03	4 (5%)	82,88,111	1.17	5 (6%)
58	3PE	L	703	-	46,46,50	0.95	2 (4%)	49,51,55	1.03	3 (6%)
58	3PE	j	700	-	39,39,50	1.02	2 (5%)	42,44,55	1.23	4 (9%)
67	HEM	AC	402	47	50,50,50	1.59	9 (18%)	66,82,82	1.85	16 (24%)
68	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.09	7 (25%)
55	SF4	G	801	7	0,12,12	-	-	-		
62	CDL	Ag	101	62	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.20	3 (8%)
57	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.13	2 (5%)
63	ADP	O	402	-	27,29,29	1.32	4 (14%)	42,45,45	2.01	11 (26%)
69	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
58	3PE	K	101	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
57	PC1	L	706	-	49,49,53	0.97	2 (4%)	55,57,61	1.09	3 (5%)
62	CDL	Ac	406	62	41,41,99	1.39	4 (9%)	47,53,111	1.45	7 (14%)
58	3PE	AC	403	-	24,24,50	1.30	2 (8%)	27,29,55	1.17	2 (7%)
60	FMN	F	501	-	33,33,33	1.38	4 (12%)	48,50,50	1.21	6 (12%)
59	FES	E	301	5	0,4,4	-	-	-		
59	FES	G	803	7	0,4,4	-	-	-		
67	HEM	AC	401	47	50,50,50	1.59	8 (16%)	66,82,82	1.85	13 (19%)
55	SF4	F	502	6	0,12,12	-	-	-		
58	3PE	M	503	-	50,50,50	0.90	2 (4%)	53,55,55	1.05	4 (7%)
55	SF4	G	802	7	0,12,12	-	-	-		
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
62	CDL	L	705	-	80,80,99	1.01	4 (5%)	86,92,111	1.12	7 (8%)
66	EHZ	W	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.86	11 (29%)
58	3PE	m	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.06	4 (7%)
68	U10	AC	404	-	23,23,63	1.75	2 (8%)	28,31,79	1.70	7 (25%)
58	3PE	b	201	-	45,45,50	1.11	5 (11%)	48,50,55	1.23	3 (6%)
66	EHZ	n	201	-	27,31,37	1.85	7 (25%)	37,41,47	1.99	11 (29%)
67	HEM	Ac	402	47	50,50,50	1.56	8 (16%)	66,82,82	1.82	14 (21%)
55	SF4	B	301	2	0,12,12	-	-	-		
57	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.03	3 (5%)
58	3PE	i	201	-	39,39,50	1.04	2 (5%)	42,44,55	1.06	2 (4%)
58	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.07	3 (5%)
58	3PE	D	501	-	37,37,50	1.05	2 (5%)	40,42,55	1.16	3 (7%)
58	3PE	O	401	-	43,43,50	0.99	2 (4%)	46,48,55	1.04	3 (6%)
70	HEC	Ad	401	48	50,50,50	2.78	25 (50%)	68,82,82	2.48	26 (38%)
58	3PE	L	702	-	38,38,50	1.06	2 (5%)	41,43,55	1.15	2 (4%)
58	3PE	m	202	-	40,40,50	1.00	2 (5%)	43,45,55	1.12	3 (6%)
64	NDP	P	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.66	11 (16%)
70	HEC	AD	401	48	50,50,50	2.82	27 (54%)	68,82,82	2.42	27 (39%)
55	SF4	I	303	9	0,12,12	-	-	-		
69	UQ6	AC	405	-	28,28,43	2.44	6 (21%)	33,37,55	1.65	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	3PE	M	501	-	36,36,50	1.07	2 (5%)	39,41,55	1.21	3 (7%)
56	UQ1	B	302	-	18,18,18	1.94	2 (11%)	22,25,25	1.35	3 (13%)
55	SF4	I	304	9	0,12,12	-	-	-		
58	3PE	J	401	-	45,45,50	1.12	5 (11%)	48,50,55	1.19	3 (6%)
61	UQ9	H	400	-	35,35,58	0.83	2 (5%)	42,45,73	0.52	0
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
62	CDL	d	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.29	7 (9%)
62	CDL	Aa	501	-	45,45,99	1.34	4 (8%)	51,57,111	1.32	6 (11%)
58	3PE	L	701	-	48,48,50	0.91	2 (4%)	51,53,55	1.13	4 (7%)
58	3PE	I	301	-	45,45,50	0.98	2 (4%)	48,50,55	1.08	3 (6%)

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
67	HEM	Ac	401	47	-	9/14/54/54	-
62	CDL	L	704	-	-	27/87/87/110	-
58	3PE	L	703	-	-	10/50/50/54	-
58	3PE	j	700	-	-	6/43/43/54	-
67	HEM	AC	402	47	-	9/14/54/54	-
68	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
55	SF4	G	801	7	-	-	0/6/5/5
62	CDL	Ag	101	62	-	22/66/66/110	-
58	3PE	Ac	403	-	-	3/38/38/54	-
57	PC1	B	303	-	-	8/38/38/57	-
63	ADP	O	402	-	-	1/16/32/32	0/3/3/3
69	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
58	3PE	K	101	-	-	14/49/49/54	-
57	PC1	L	706	-	-	10/53/53/57	-
62	CDL	Ac	406	62	-	18/52/52/110	-
58	3PE	AC	403	-	-	7/28/28/54	-
60	FMN	F	501	-	-	3/18/18/18	0/3/3/3
59	FES	E	301	5	-	-	0/1/1/1
59	FES	G	803	7	-	-	0/1/1/1
67	HEM	AC	401	47	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	SF4	F	502	6	-	-	0/6/5/5
58	3PE	M	503	-	-	8/54/54/54	-
55	SF4	G	802	7	-	-	0/6/5/5
62	CDL	h	201	-	-	23/80/80/110	-
62	CDL	L	705	-	-	21/91/91/110	-
66	EHZ	W	201	-	-	21/39/39/45	-
58	3PE	m	201	-	-	13/54/54/54	-
68	U10	AC	404	-	-	5/15/39/87	0/1/1/1
58	3PE	b	201	-	-	19/49/49/54	-
66	EHZ	n	201	-	-	14/39/39/45	-
67	HEM	Ac	402	47	-	8/14/54/54	-
55	SF4	B	301	2	-	-	0/6/5/5
57	PC1	I	302	-	-	10/50/50/57	-
58	3PE	i	201	-	-	12/43/43/54	-
58	3PE	M	502	-	-	16/54/54/54	-
58	3PE	D	501	-	-	10/41/41/54	-
58	3PE	O	401	-	-	9/47/47/54	-
70	HEC	Ad	401	48	1/1/3/7	8/14/54/54	-
58	3PE	L	702	-	-	16/42/42/54	-
58	3PE	m	202	-	-	7/44/44/54	-
64	NDP	P	401	-	-	3/34/77/77	0/5/5/5
70	HEC	AD	401	48	1/1/3/7	7/14/54/54	-
69	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
55	SF4	I	303	9	-	-	0/6/5/5
58	3PE	M	501	-	-	8/40/40/54	-
56	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
55	SF4	I	304	9	-	-	0/6/5/5
58	3PE	J	401	-	-	18/49/49/54	-
61	UQ9	H	400	-	-	14/30/54/81	0/1/1/1
62	CDL	a	101	-	-	18/67/67/110	-
62	CDL	d	201	-	-	27/77/77/110	-
62	CDL	Aa	501	-	-	12/56/56/110	-
58	3PE	L	701	-	-	13/52/52/54	-
58	3PE	I	301	-	-	12/49/49/54	-

The worst 5 of 210 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	B	302	UQ1	C6-C5	7.36	1.48	1.35
68	AC	404	U10	C6-C1	7.36	1.48	1.35
69	AC	405	UQ6	C2-C3	5.91	1.49	1.39
69	AC	405	UQ6	C5-C4	5.85	1.48	1.39
69	AC	405	UQ6	C5-C6	5.74	1.48	1.40

The worst 5 of 300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	Ac	404	U10	C6-C1-C2	7.85	125.39	119.18
66	W	201	EHZ	C8-C9-S1	6.35	121.48	113.63
70	Ad	401	HEC	C2B-C1B-NB	6.18	117.29	109.88
64	P	401	NDP	C5A-C4A-N3A	-6.07	118.83	126.75
67	AC	401	HEM	CHC-C4B-NB	6.04	130.98	124.42

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
70	AD	401	HEC	NA
70	Ad	401	HEC	NA

5 of 529 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	I	302	PC1	C11-O13-P-O14
57	L	706	PC1	C1-O11-P-O14
57	L	706	PC1	C22-C21-O21-C2
57	L	706	PC1	O32-C31-O31-C3
57	L	706	PC1	C32-C31-O31-C3

There are no ring outliers.

52 monomers are involved in 442 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	Ac	401	HEM	3	0
62	L	704	CDL	16	0
58	L	703	3PE	20	0
58	j	700	3PE	9	0
67	AC	402	HEM	5	0
68	Ac	404	U10	12	0
62	Ag	101	CDL	6	0
58	Ac	403	3PE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	B	303	PC1	3	0
63	O	402	ADP	6	0
69	Ac	405	UQ6	8	0
58	K	101	3PE	6	0
57	L	706	PC1	17	0
62	Ac	406	CDL	5	0
58	AC	403	3PE	4	0
60	F	501	FMN	3	0
59	E	301	FES	4	0
59	G	803	FES	4	0
67	AC	401	HEM	3	0
55	F	502	SF4	10	0
58	M	503	3PE	27	0
55	G	802	SF4	5	0
62	h	201	CDL	13	0
62	L	705	CDL	15	0
66	W	201	EHZ	7	0
58	m	201	3PE	12	0
68	AC	404	U10	9	0
58	b	201	3PE	11	0
67	Ac	402	HEM	3	0
55	B	301	SF4	5	0
57	I	302	PC1	7	0
58	i	201	3PE	11	0
58	M	502	3PE	4	0
58	D	501	3PE	13	0
58	O	401	3PE	7	0
70	Ad	401	HEC	18	0
58	L	702	3PE	6	0
58	m	202	3PE	4	0
64	P	401	NDP	4	0
70	AD	401	HEC	5	0
55	I	303	SF4	11	0
69	AC	405	UQ6	7	0
58	M	501	3PE	9	0
56	B	302	UQ1	12	0
55	I	304	SF4	5	0
58	J	401	3PE	18	0
61	H	400	UQ9	16	0
62	a	101	CDL	15	0
62	d	201	CDL	5	0
62	Aa	501	CDL	3	0

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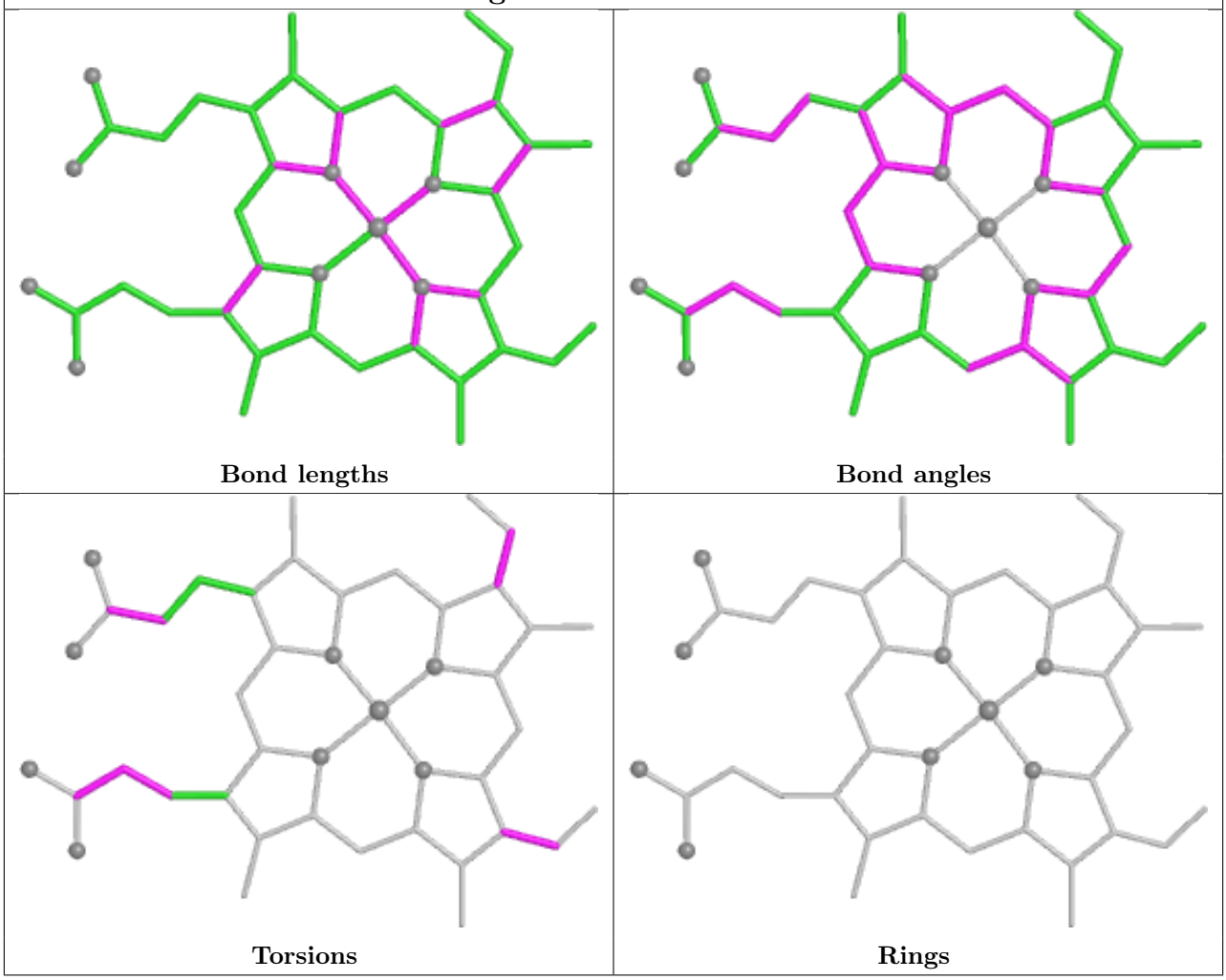
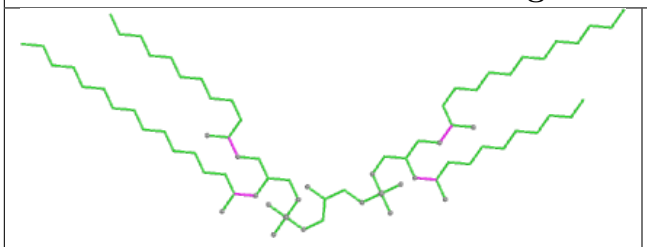
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	L	701	3PE	9	0
58	I	301	3PE	10	0

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 then 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 HEM Ac 401



Ligand CDL L 704



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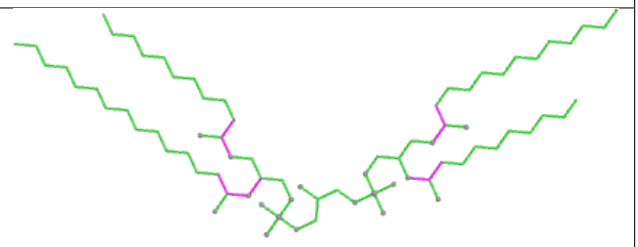
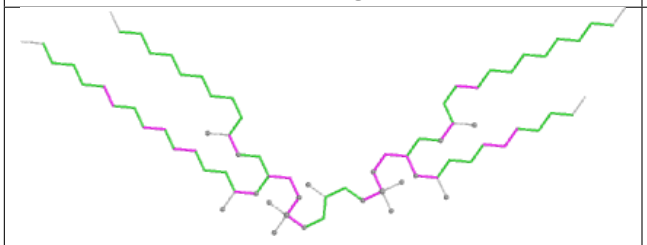
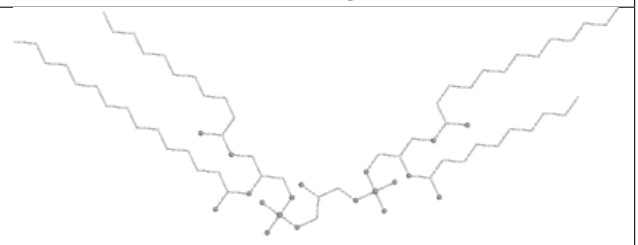


Bond angles

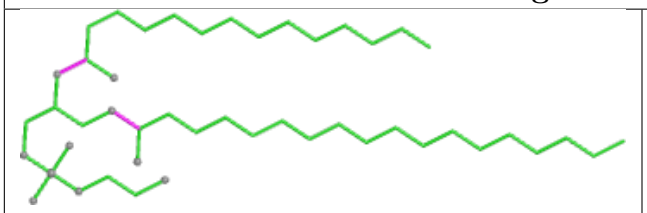


Torsions



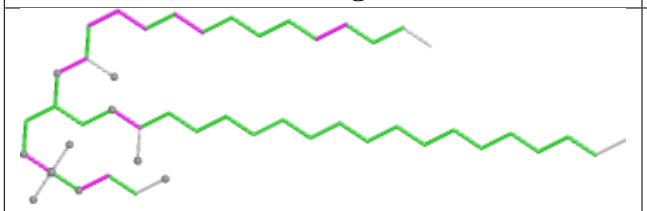
Rings

Ligand 3PE L 703



Bond lengths

Bond angles



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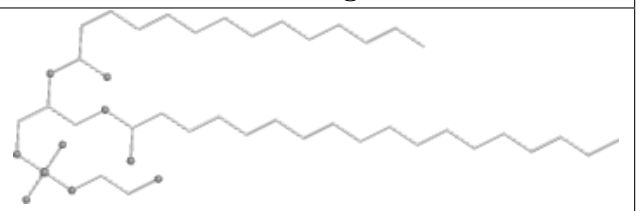
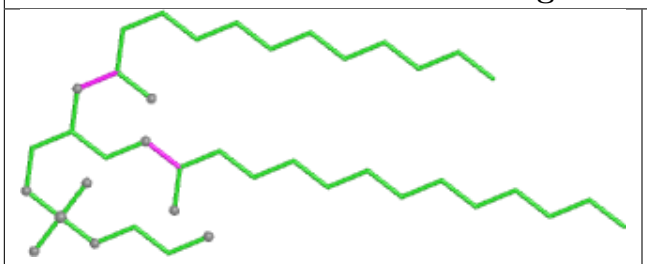


Rings

Ligand 3PE j 700



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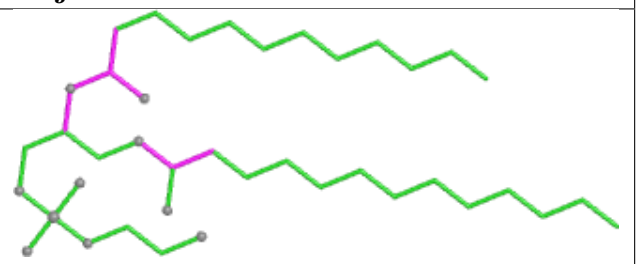

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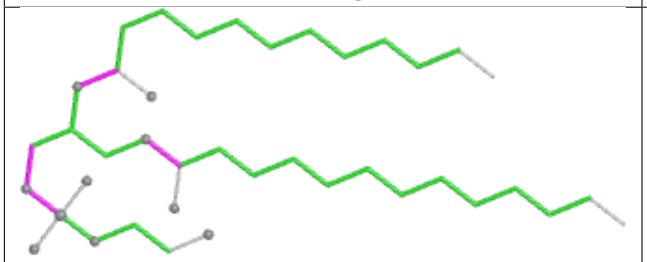

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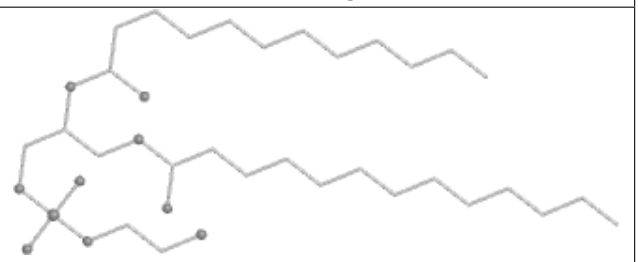
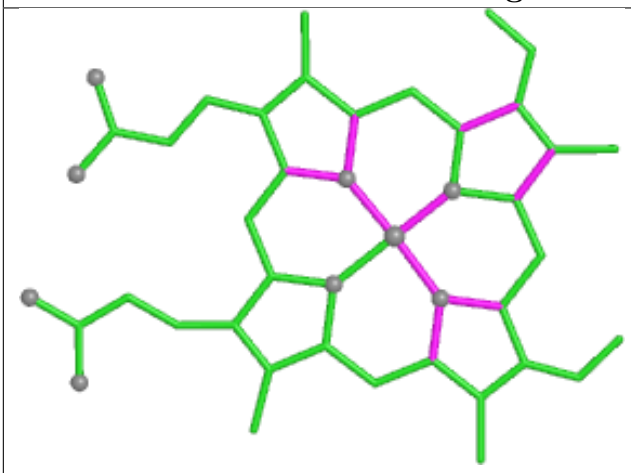


Rings

Ligand HEM AC 402



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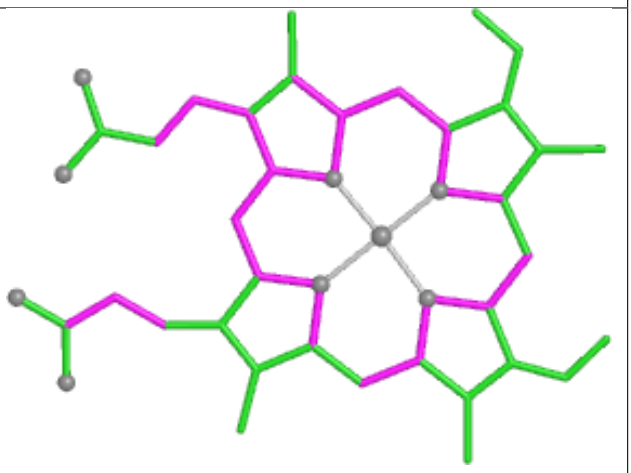

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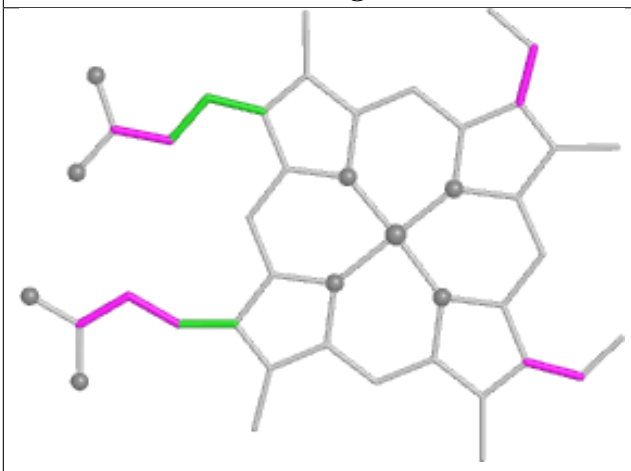

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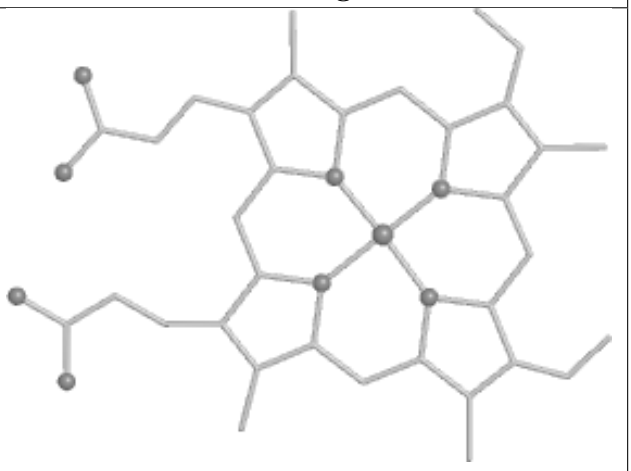
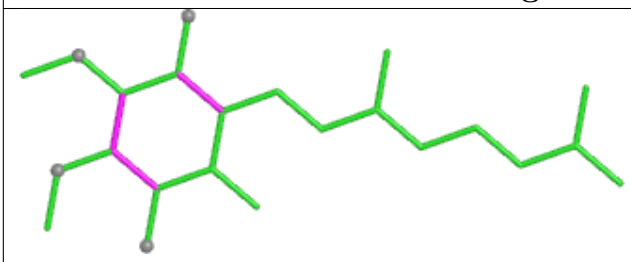


Rings

Ligand U10 Ac 404



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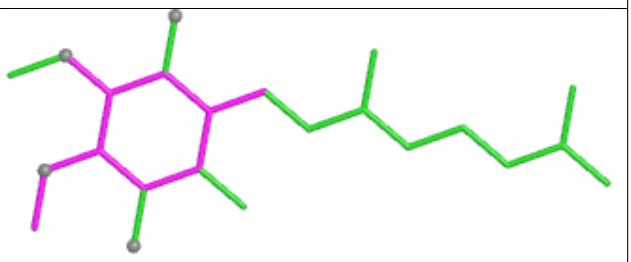

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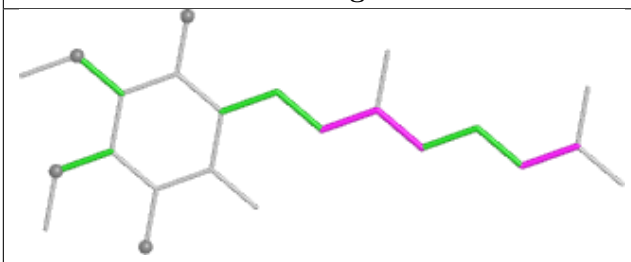

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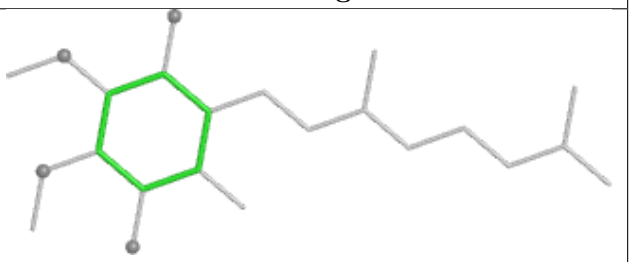
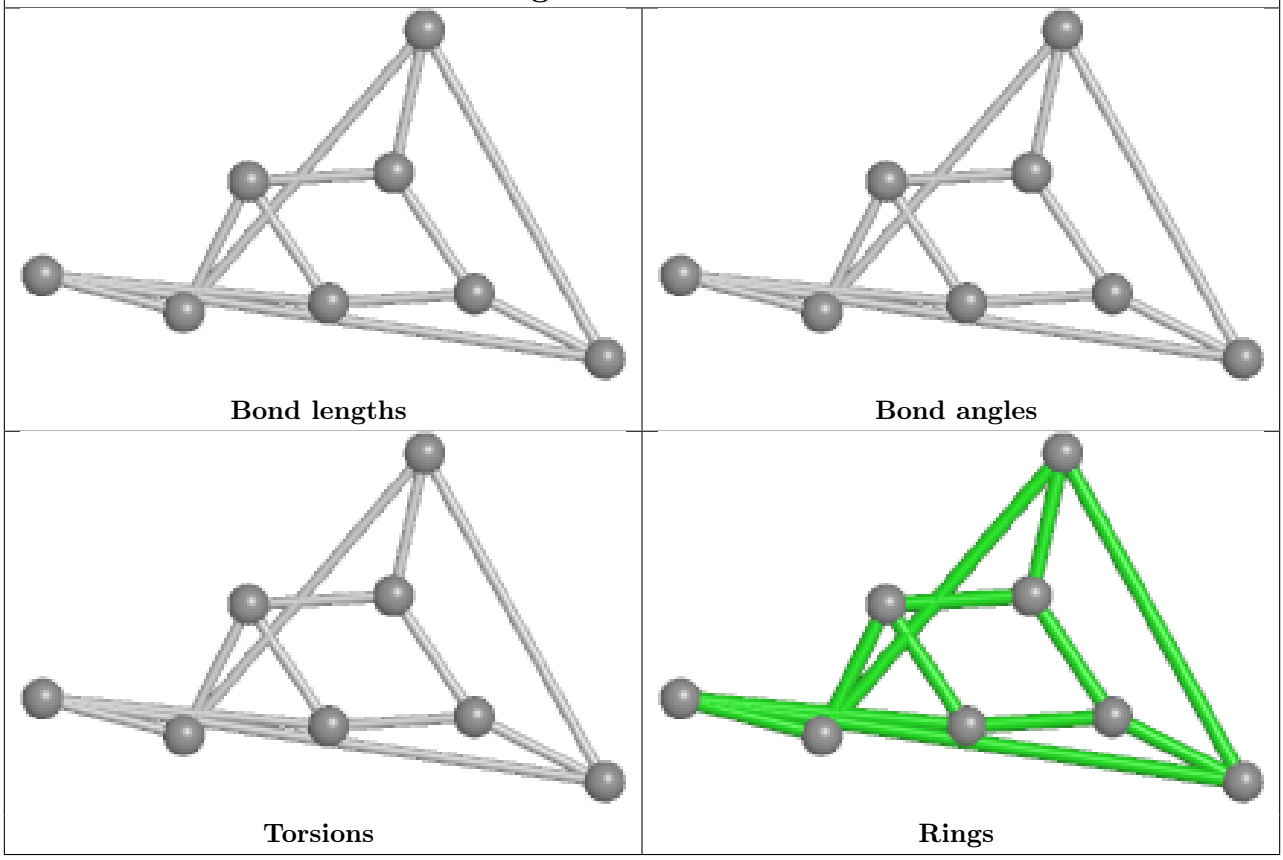
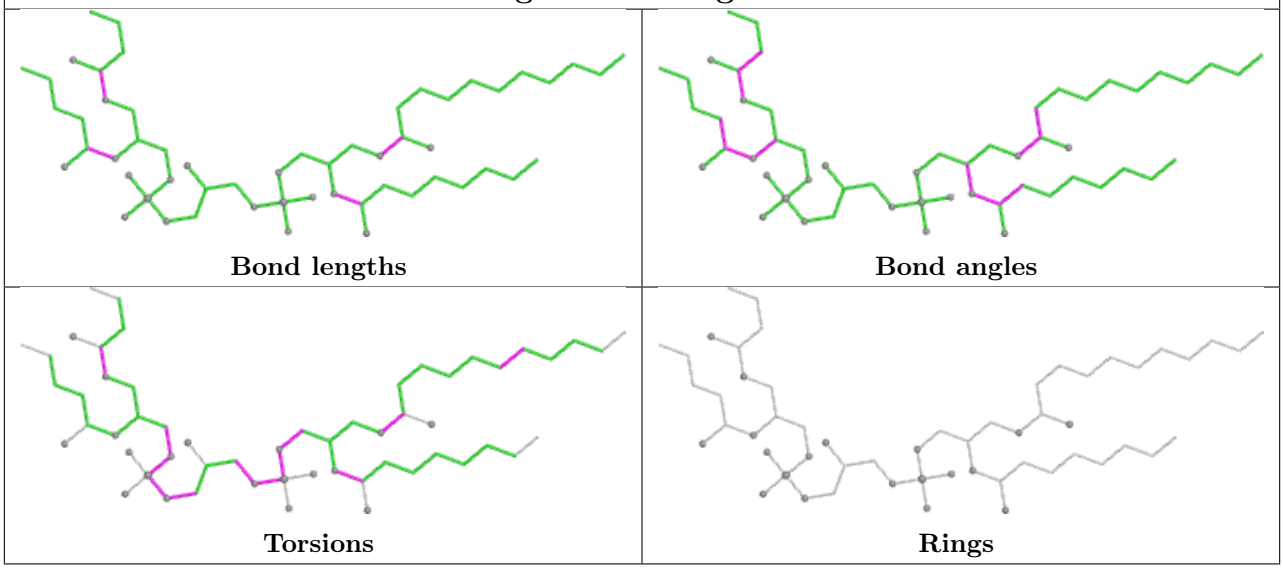


Rings

Ligand SF4 G 801



Ligand CDL Ag 101



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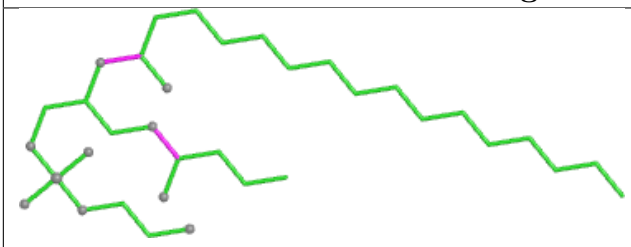
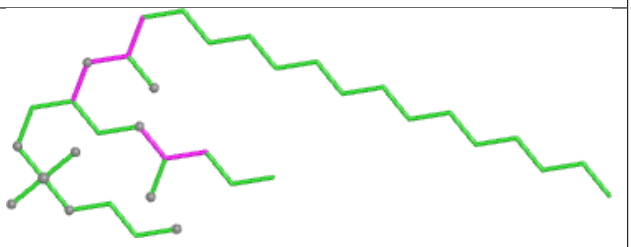
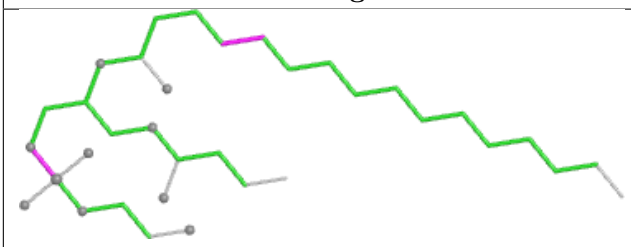
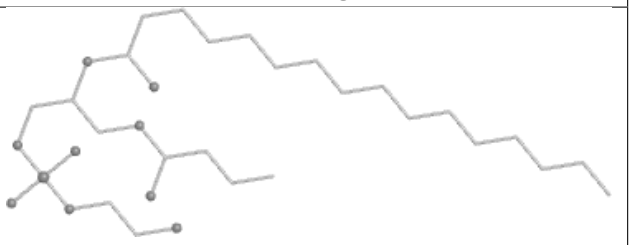
 Bond lengths	 Bond angles
 Torsions	 Rings

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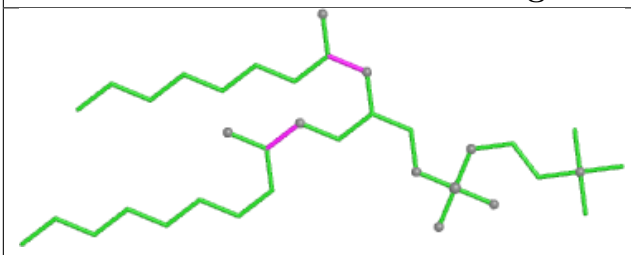
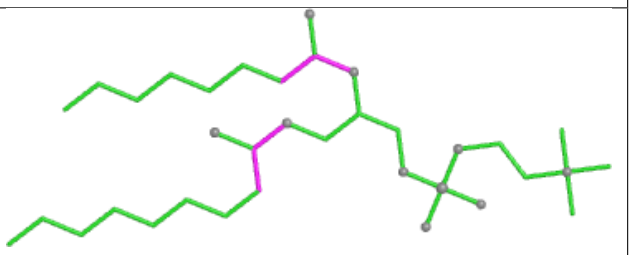
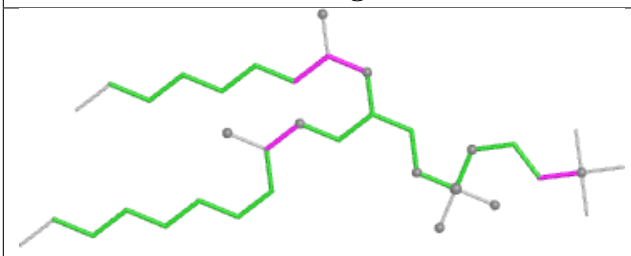
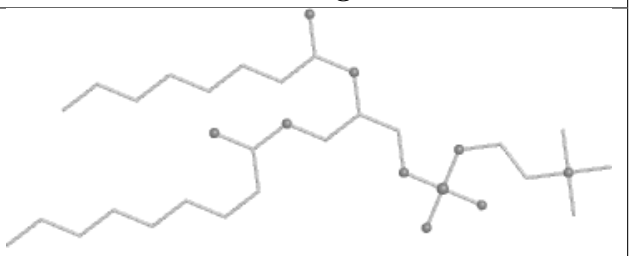
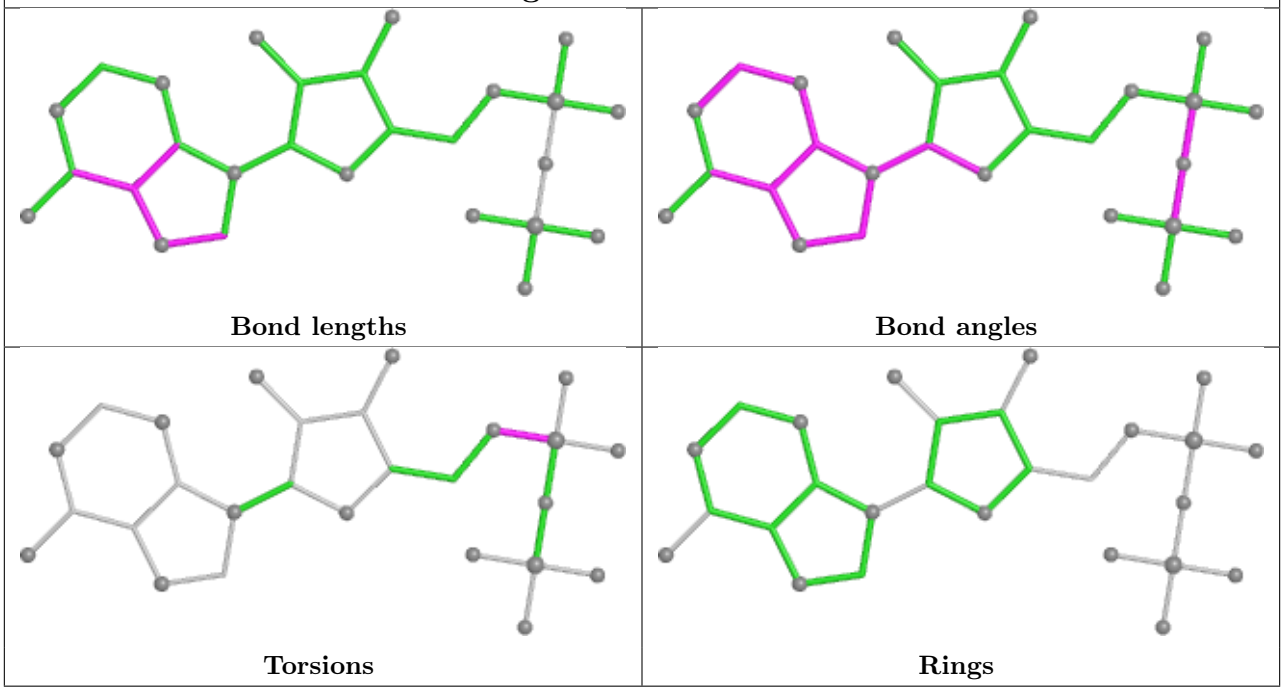
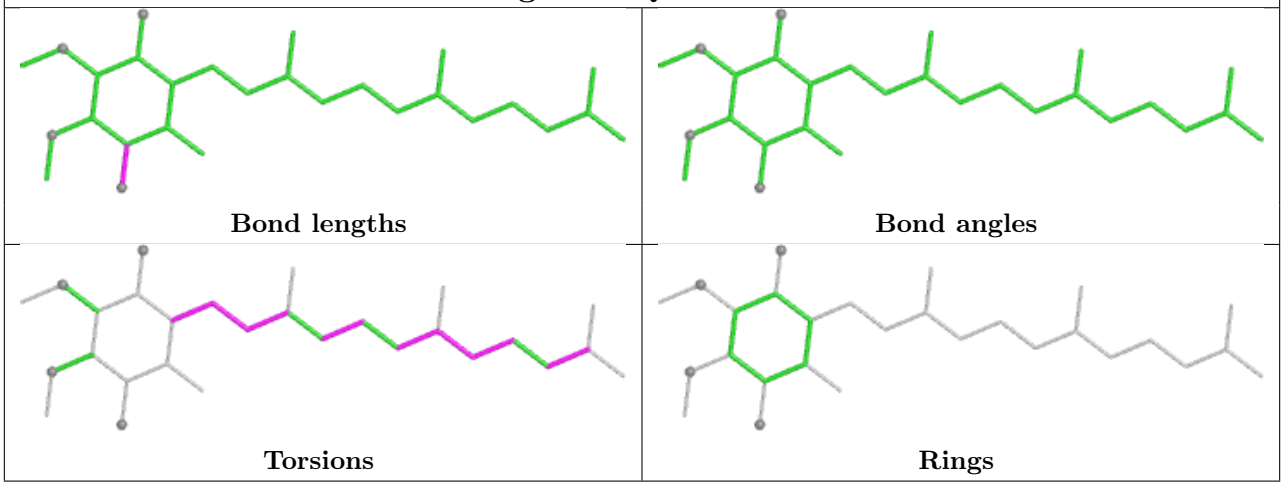
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP O 402



Ligand UQ6 Ac 405



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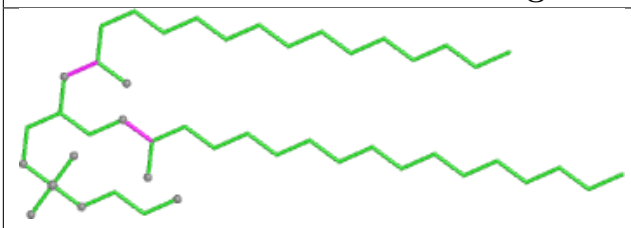
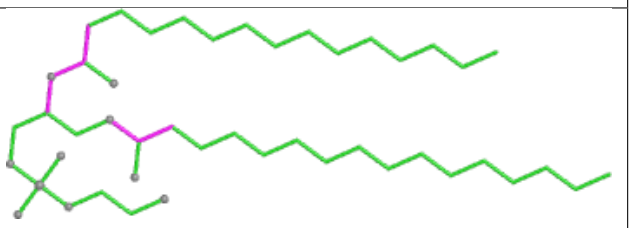
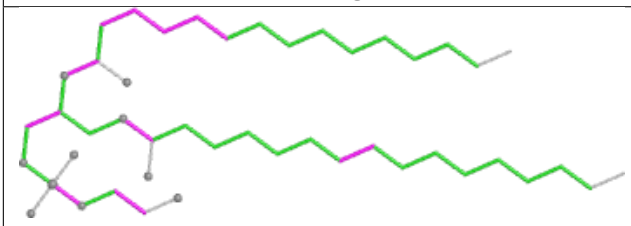
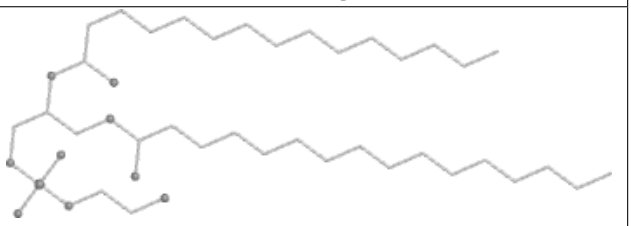
 Bond lengths	 Bond angles
 Torsions	 Rings

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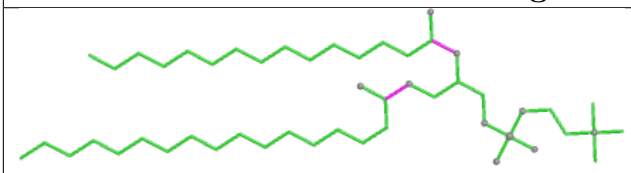
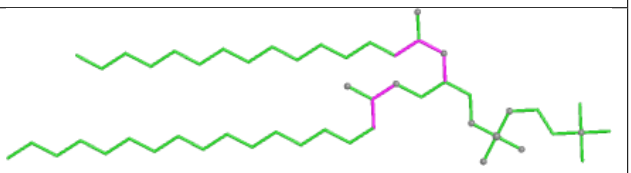
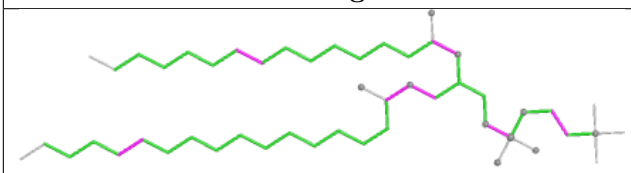
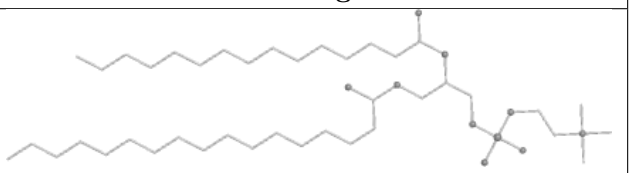
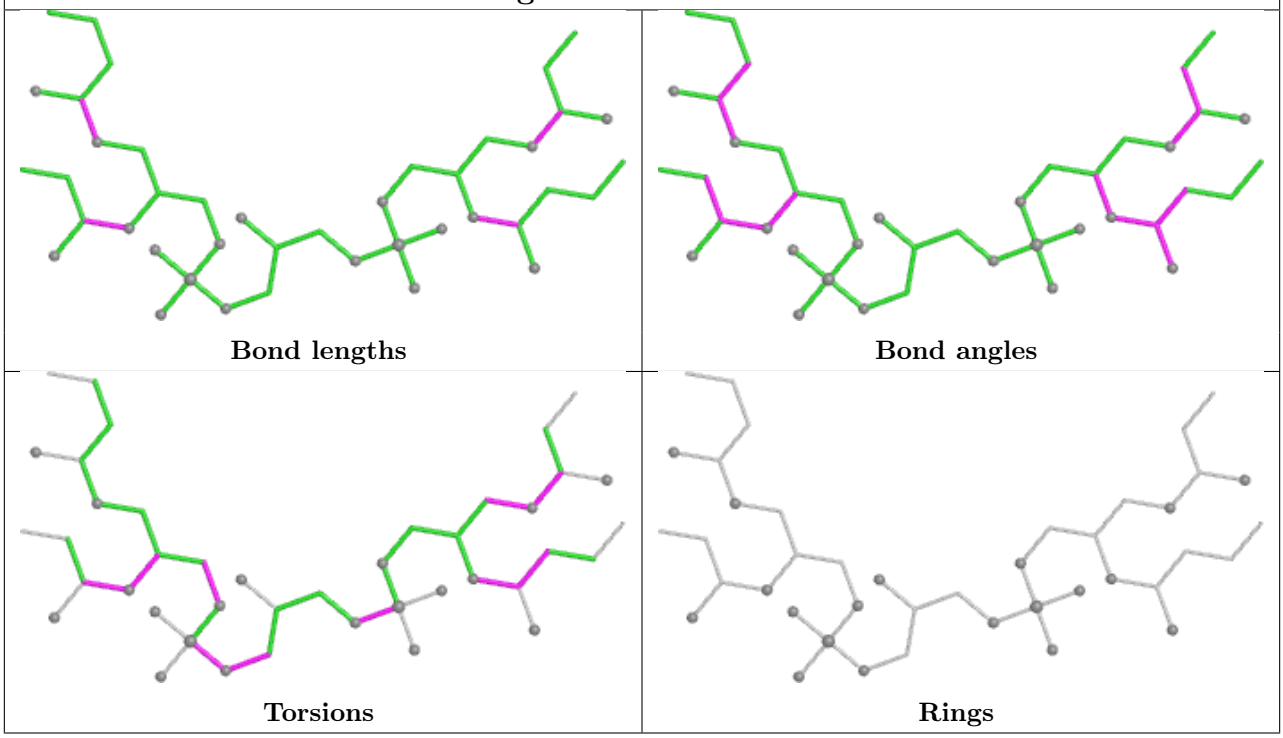
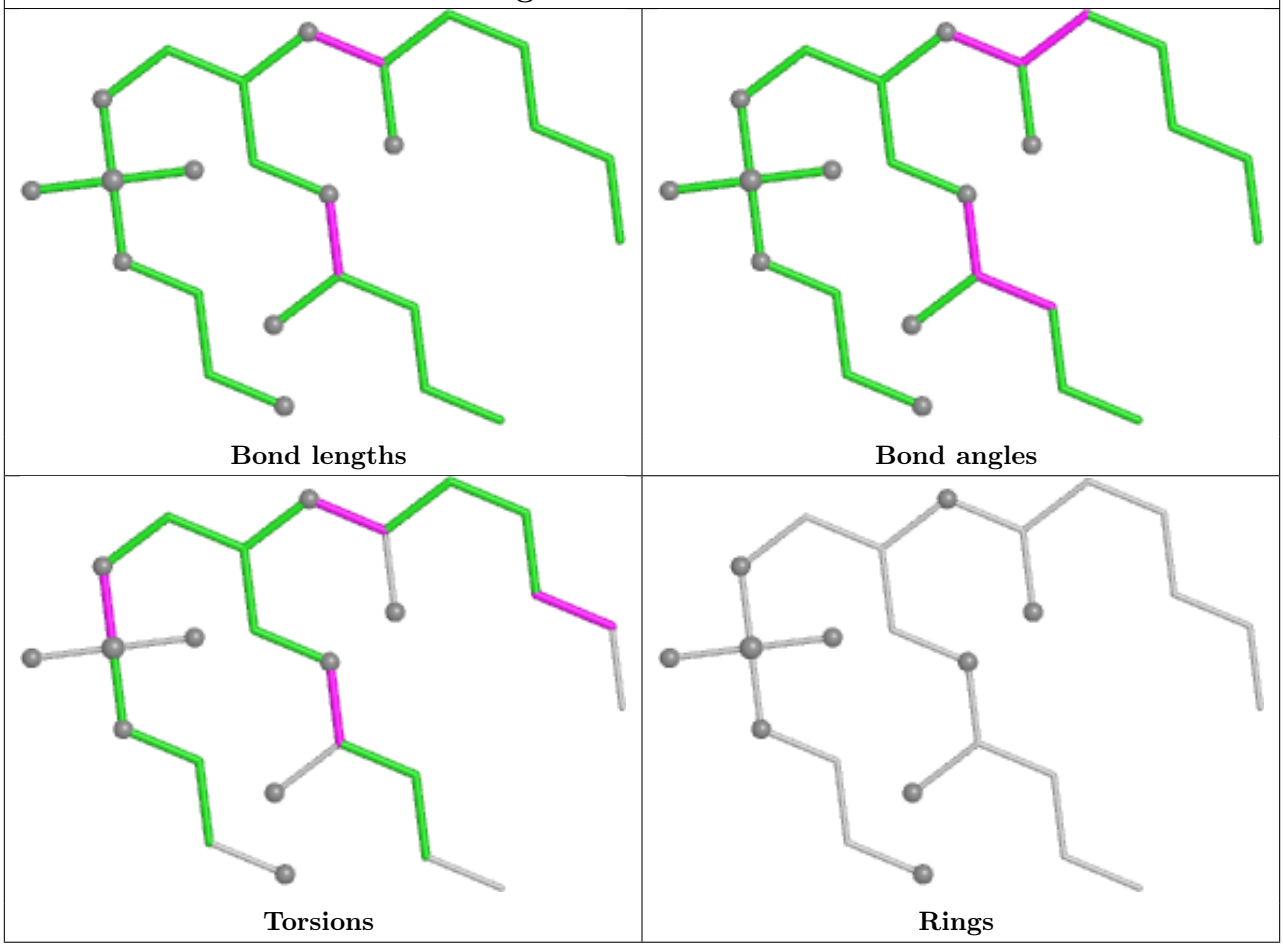
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Ac 406



Ligand 3PE AC 403



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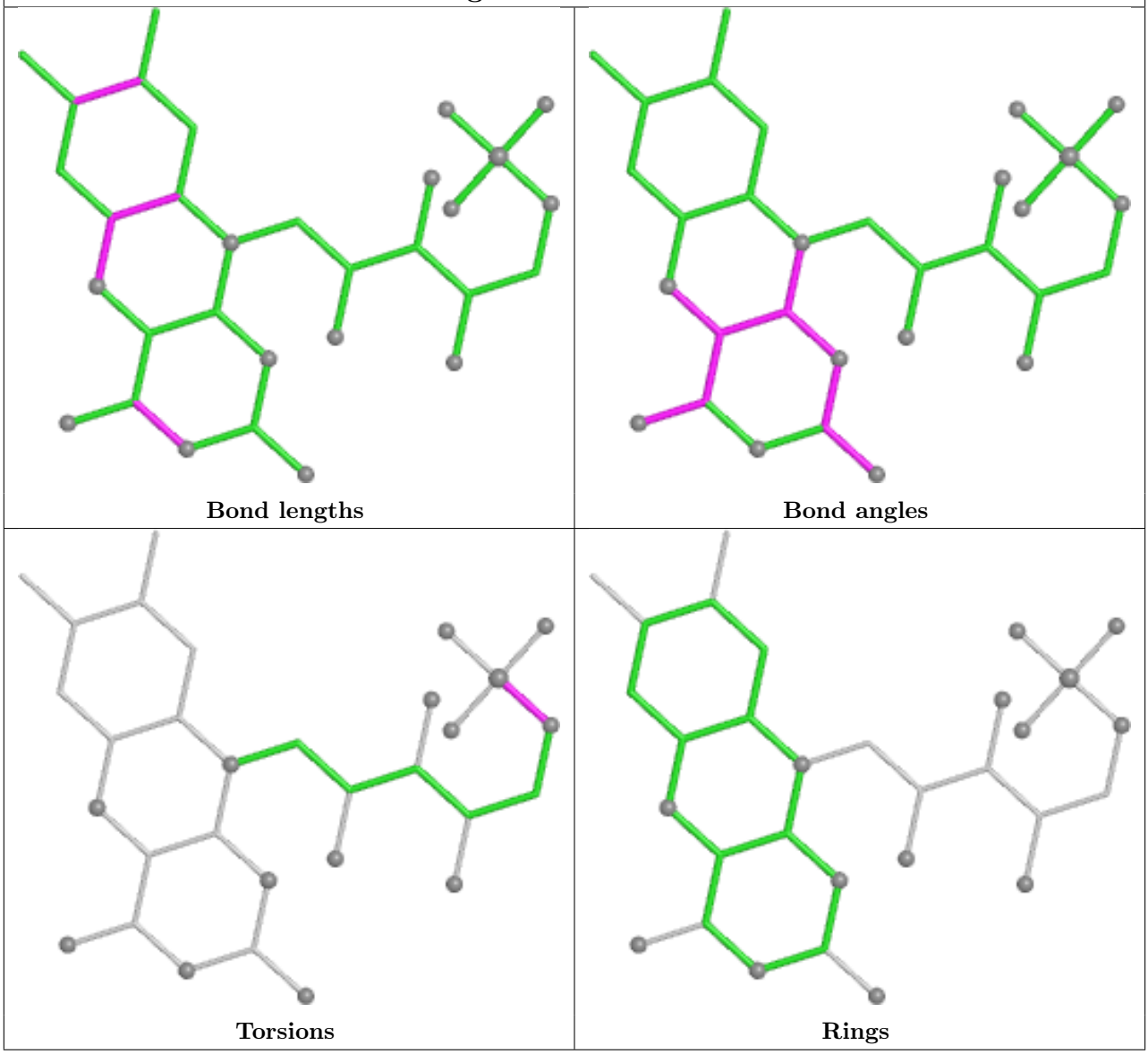

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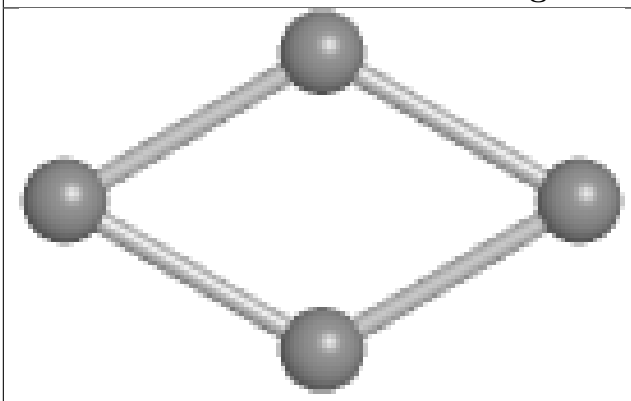
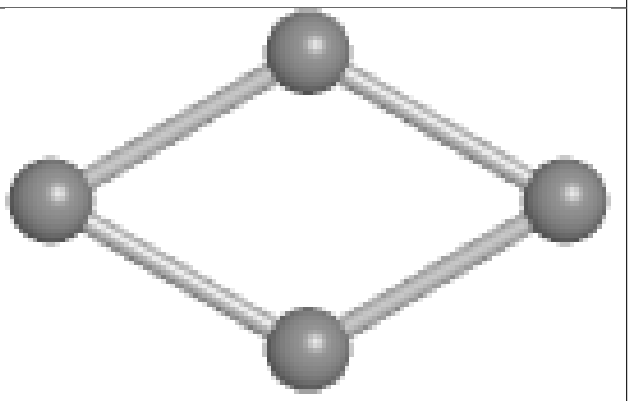
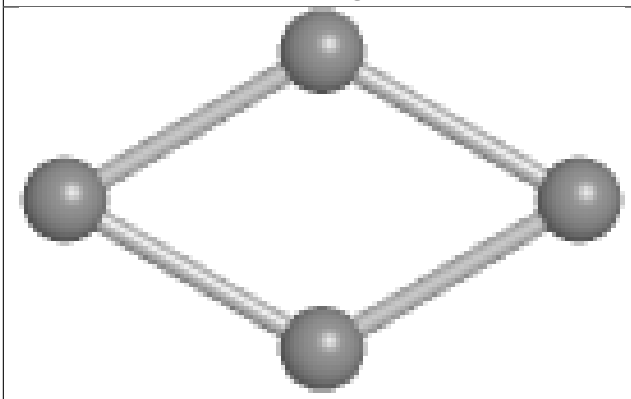
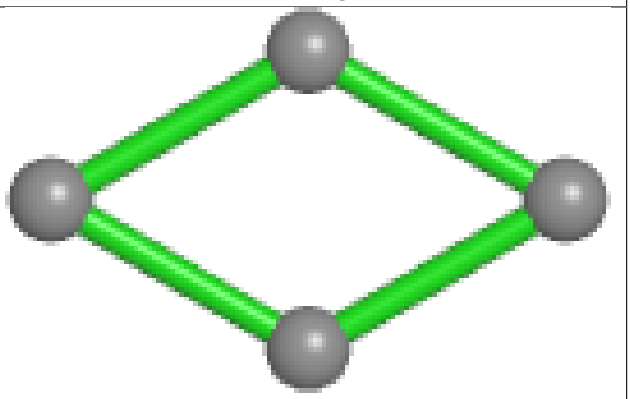
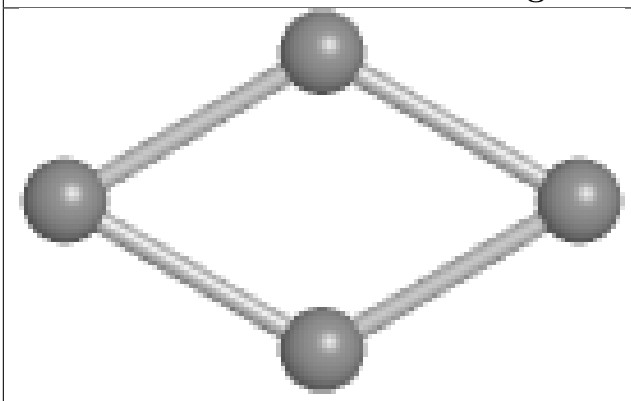
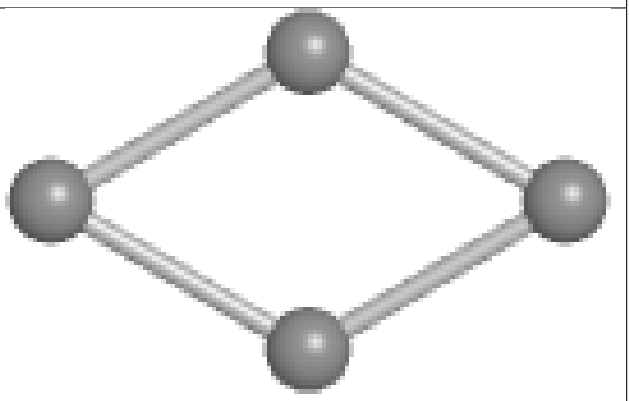
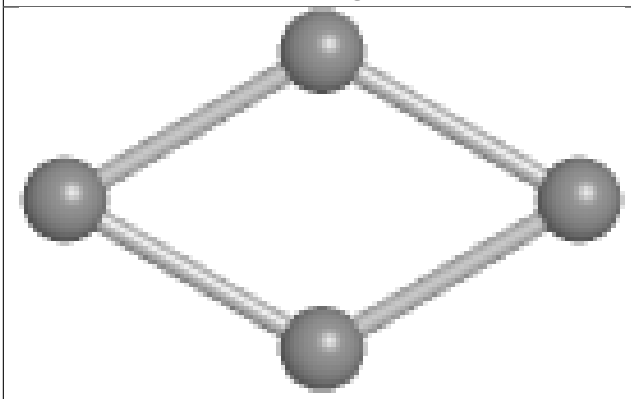
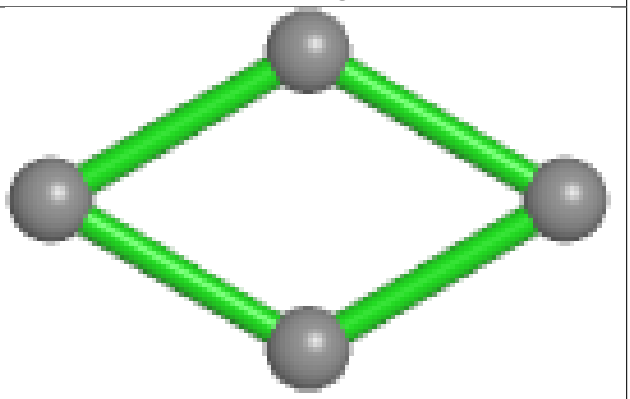
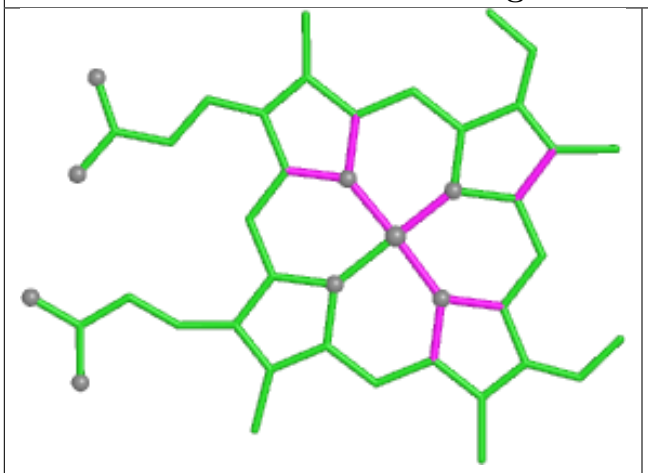
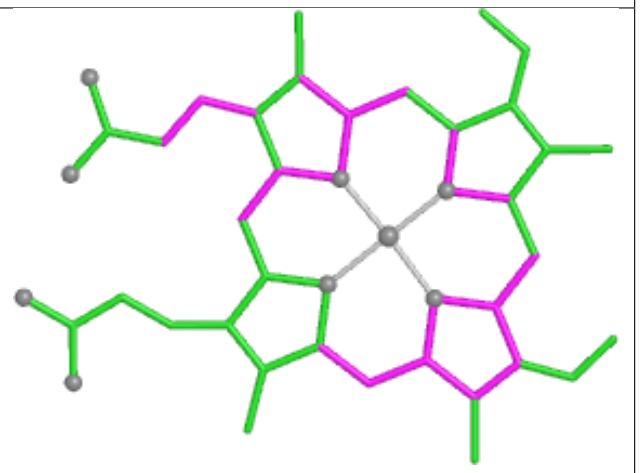
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES G 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

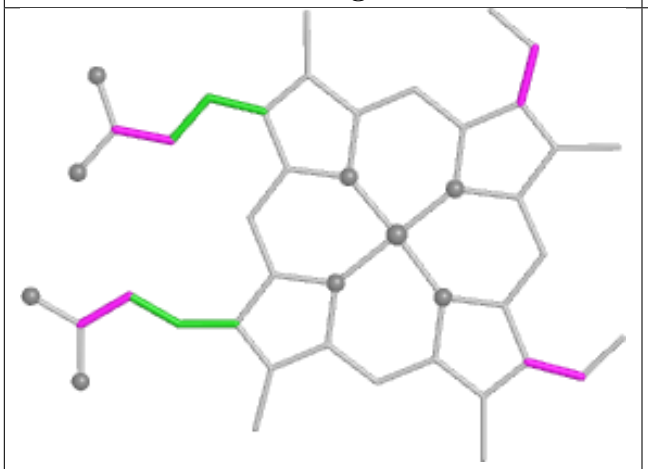
Ligand HEM AC 401



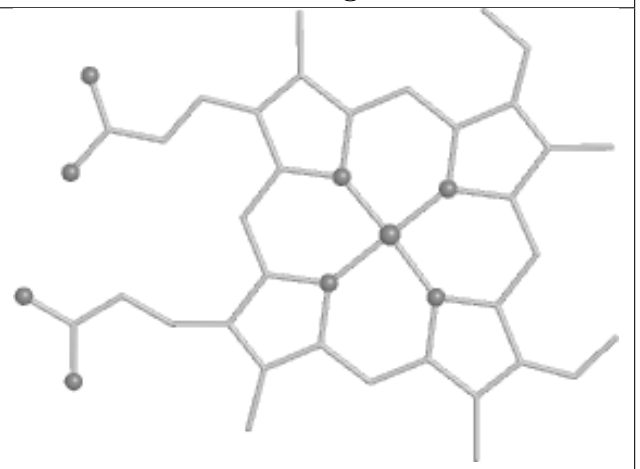
Bond lengths



Bond angles

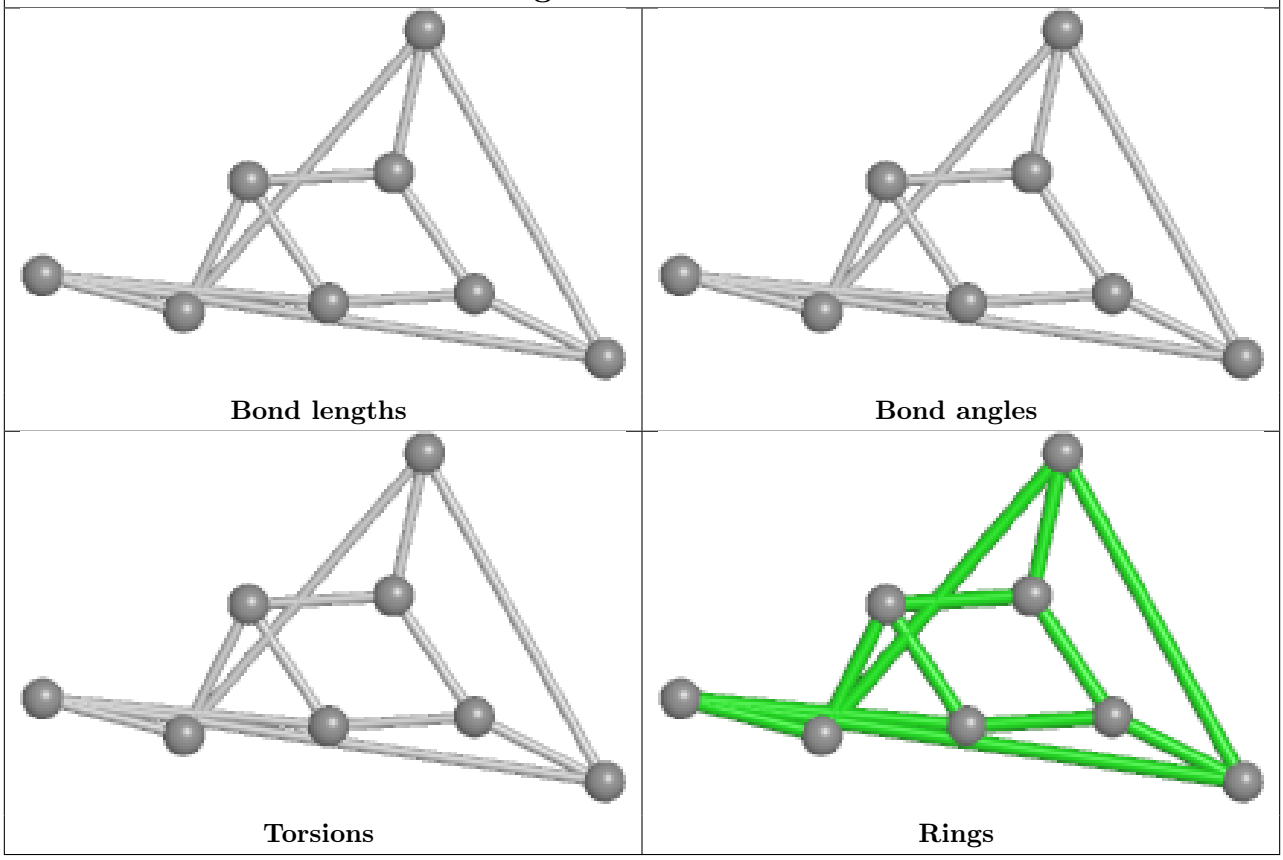


Torsions

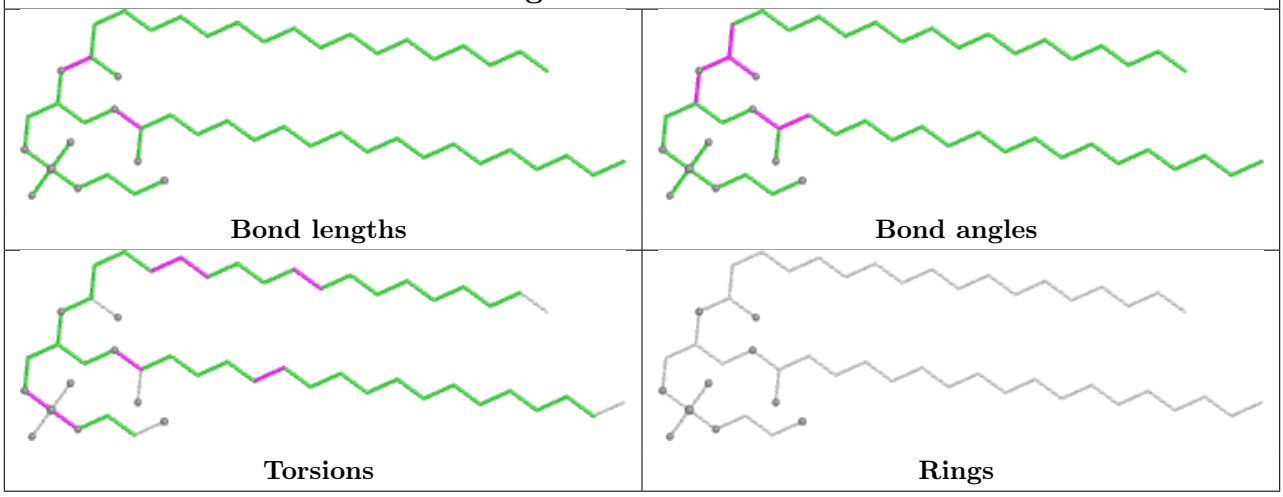


Rings

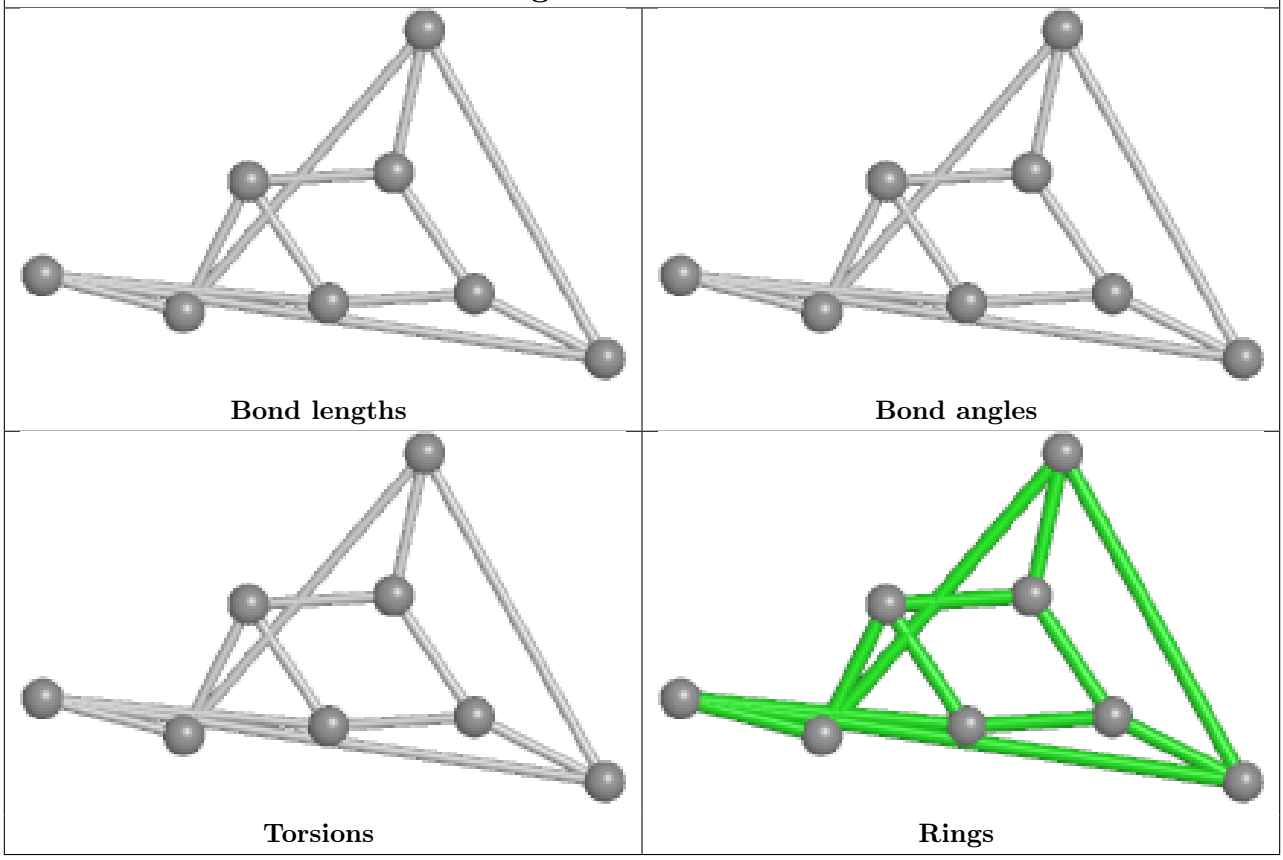
Ligand SF4 F 502



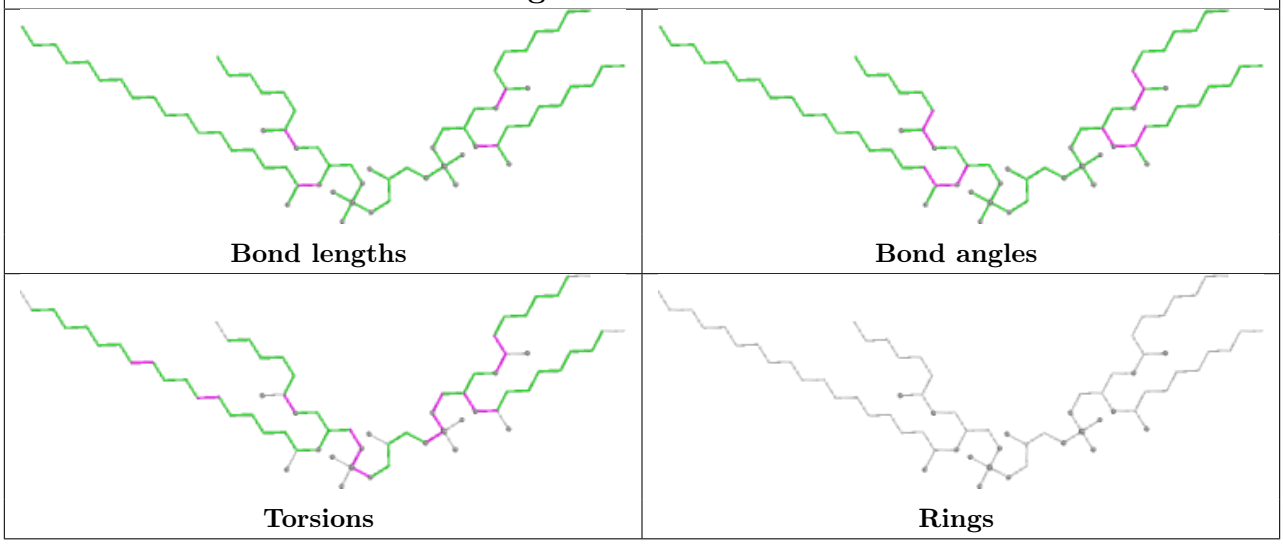
Ligand 3PE M 503



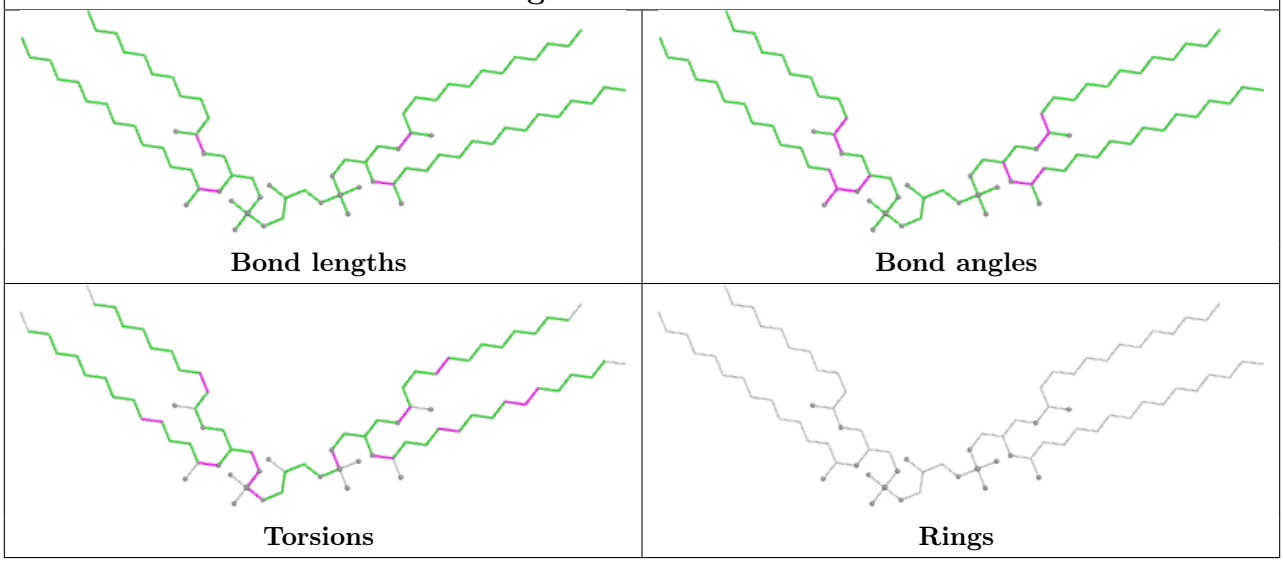
Ligand SF4 G 802



Ligand CDL h 201



Ligand CDL L 705



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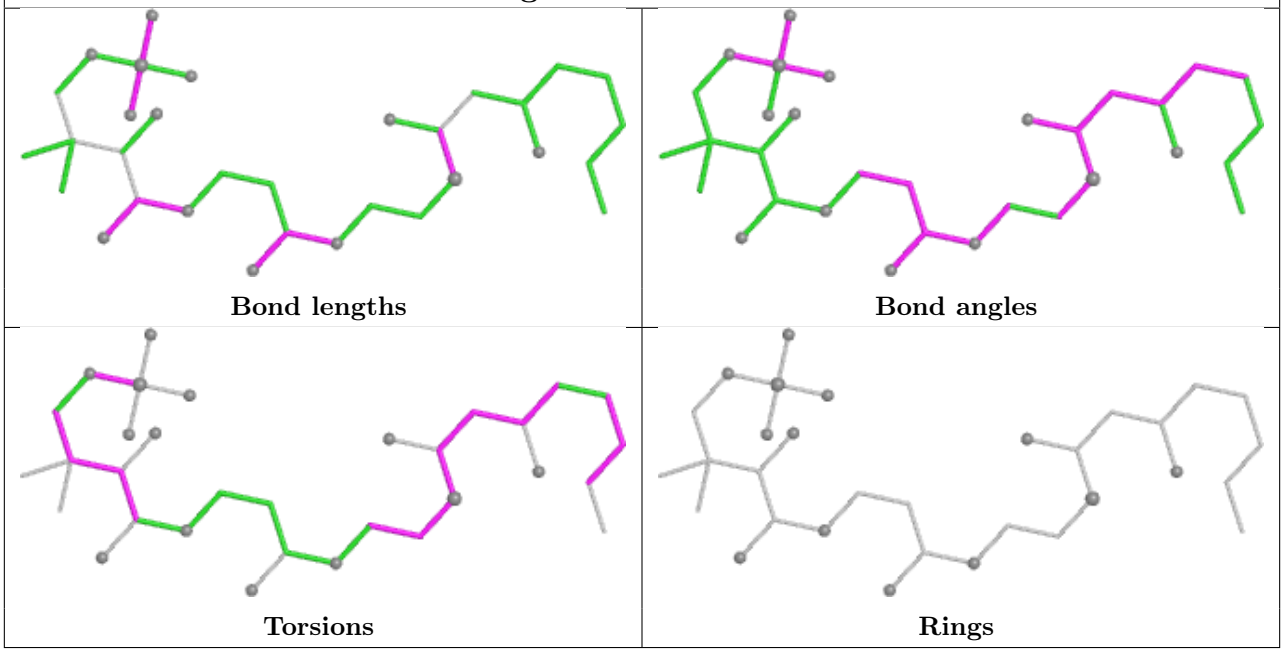

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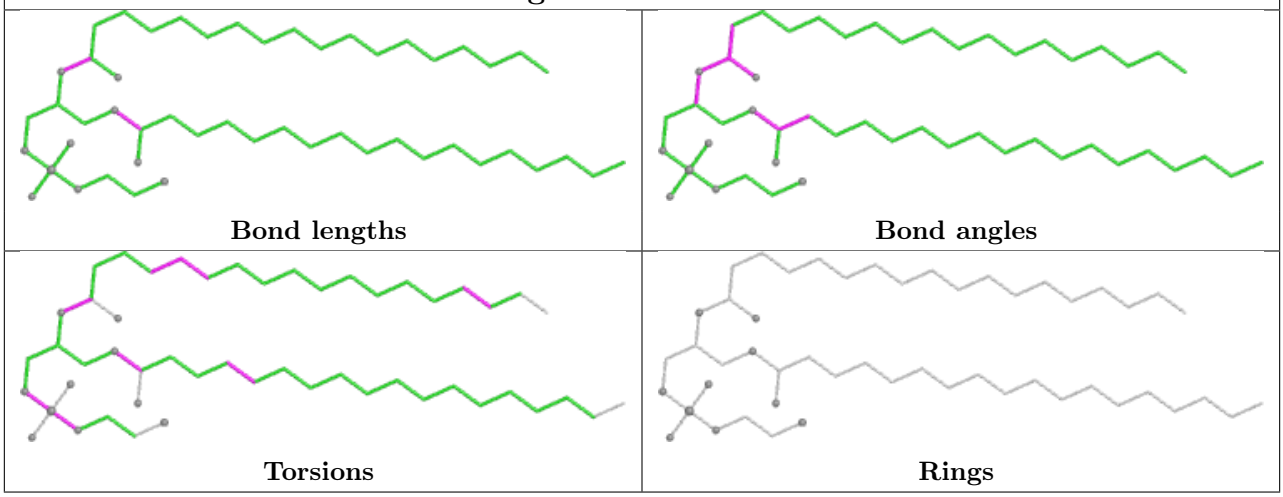
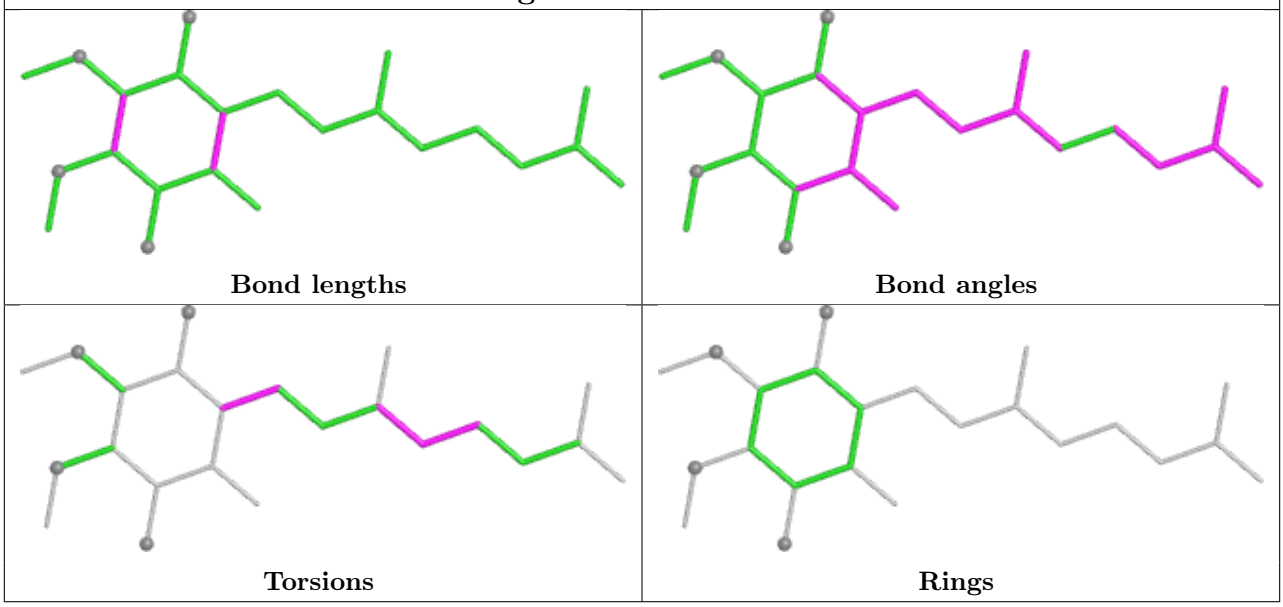


Ligand U10 AC 404



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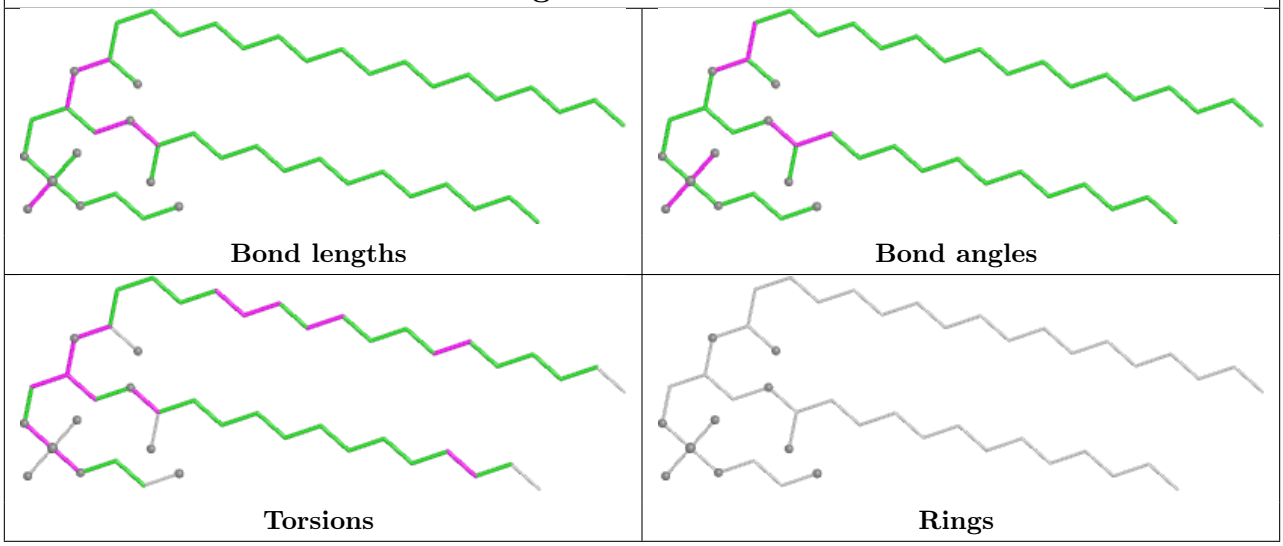

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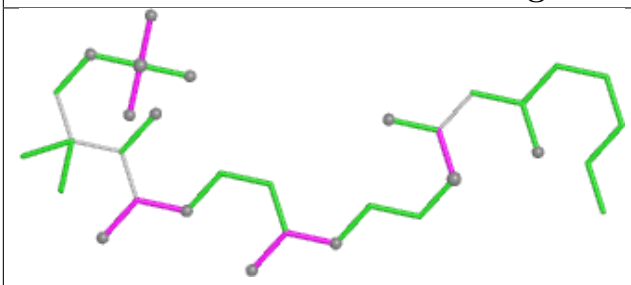
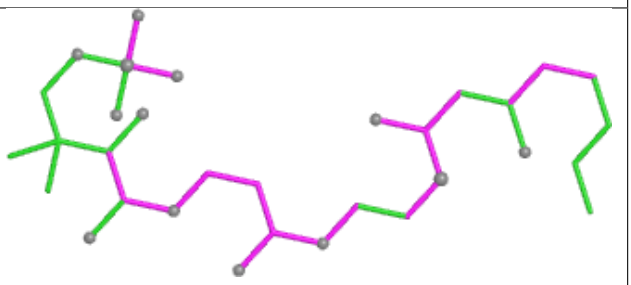
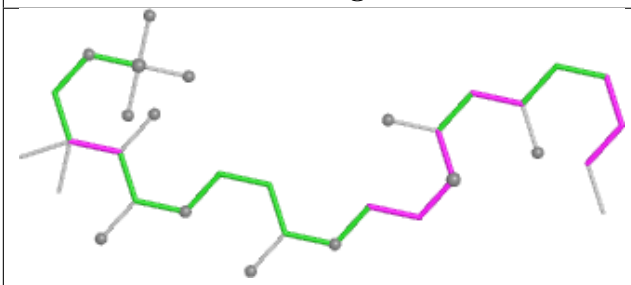


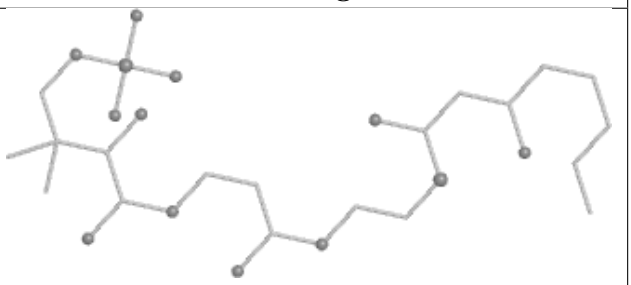
Bond lengths



Bond angles

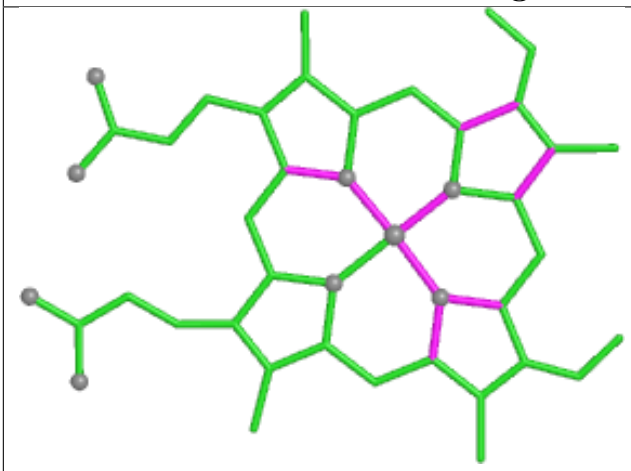


Torsions



Rings

Ligand HEM Ac 402



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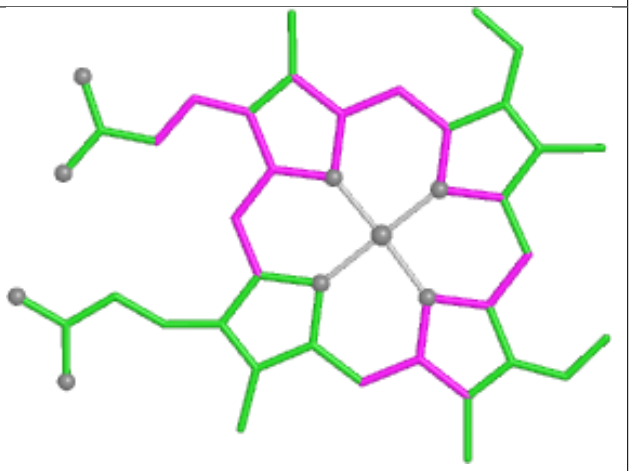
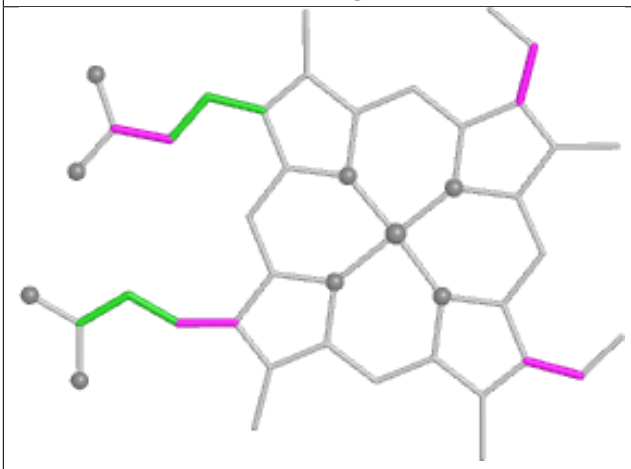


Bond angles



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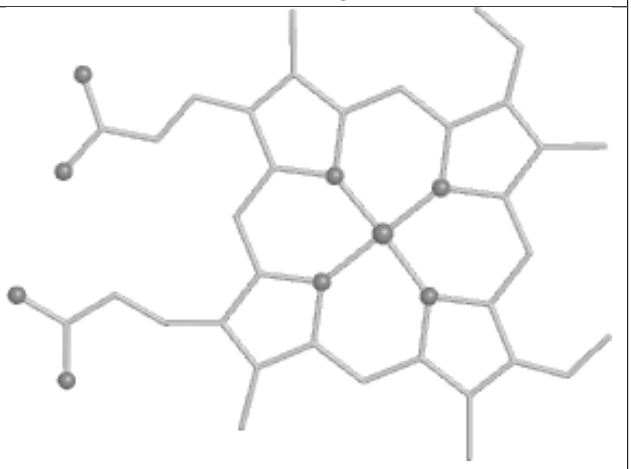
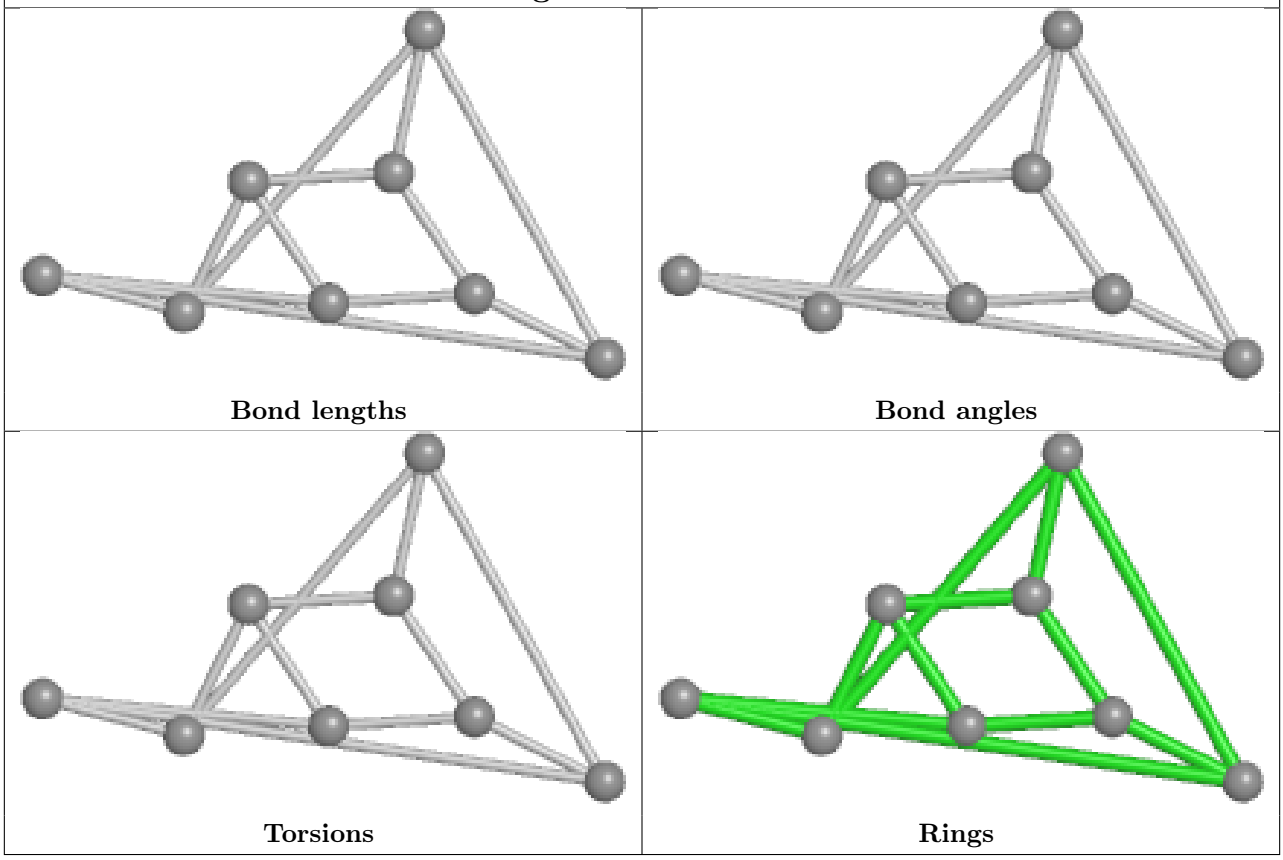


Rings

Ligand SF4 B 301



Ligand PC1 I 302

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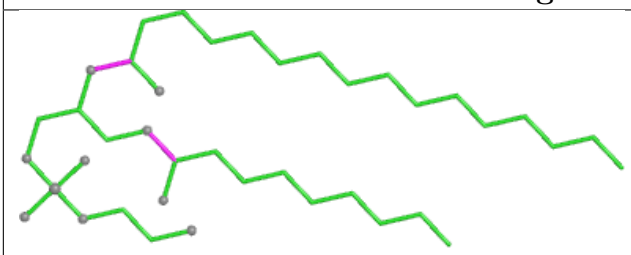
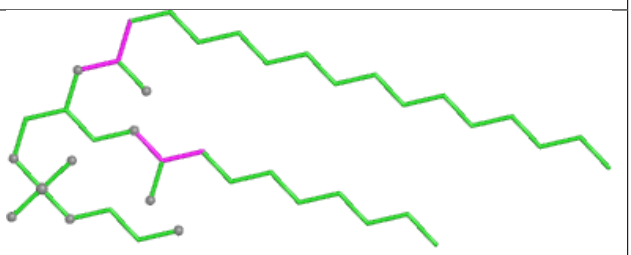
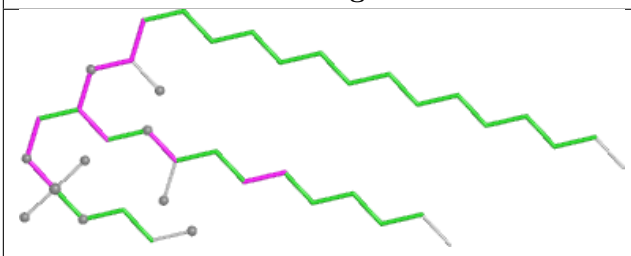
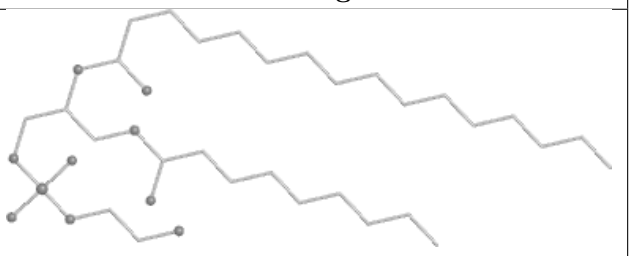
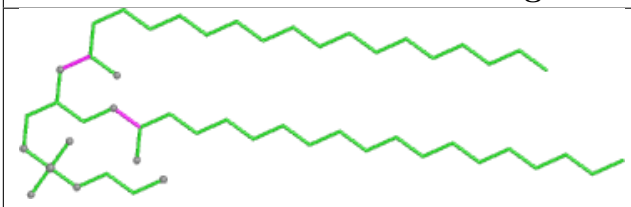
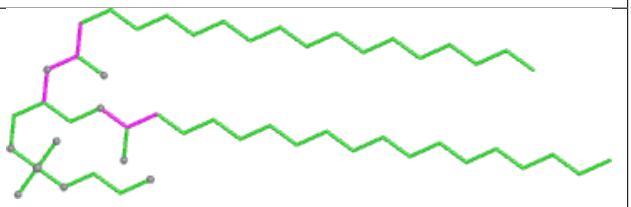
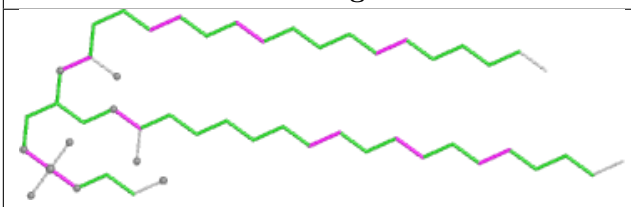
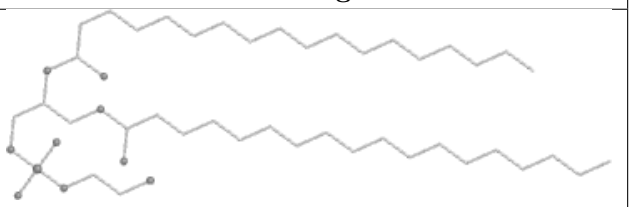
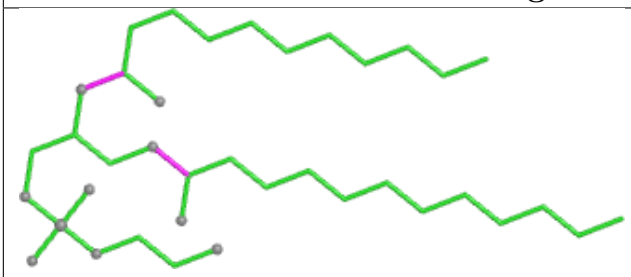
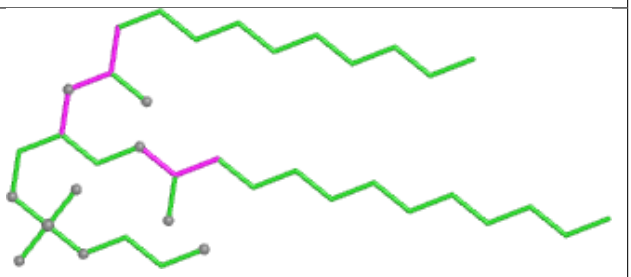
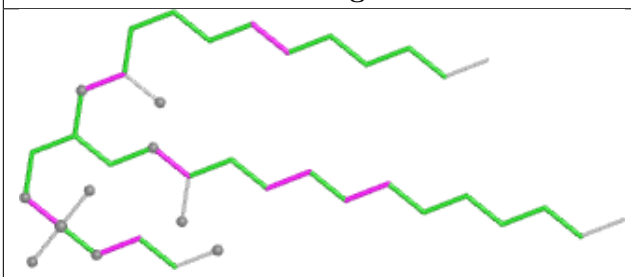
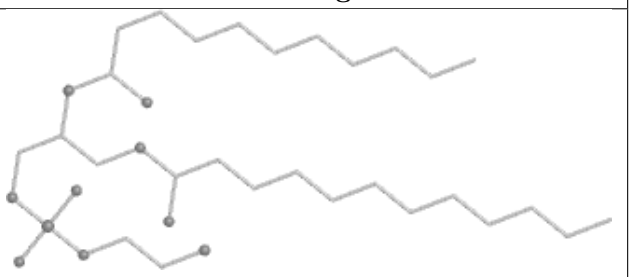
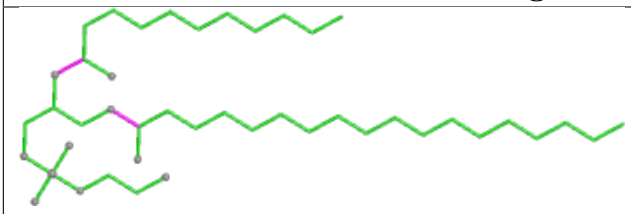
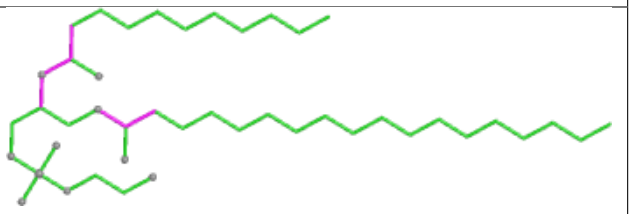
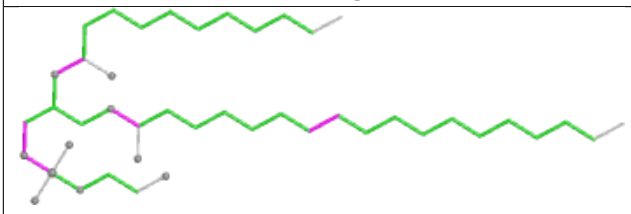
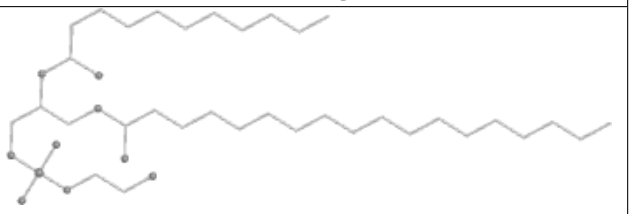
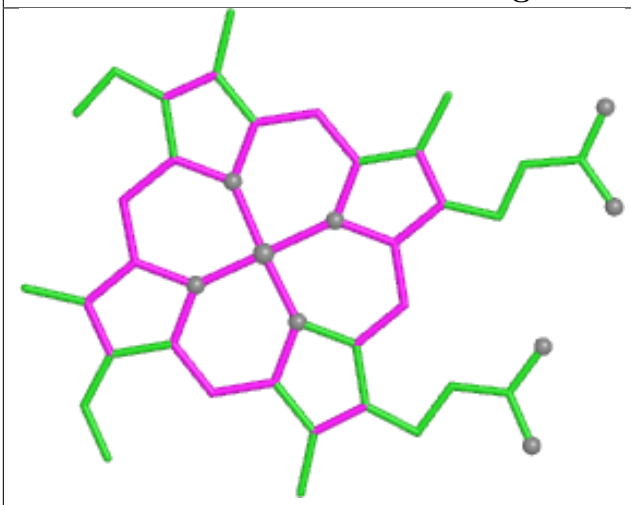
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE M 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

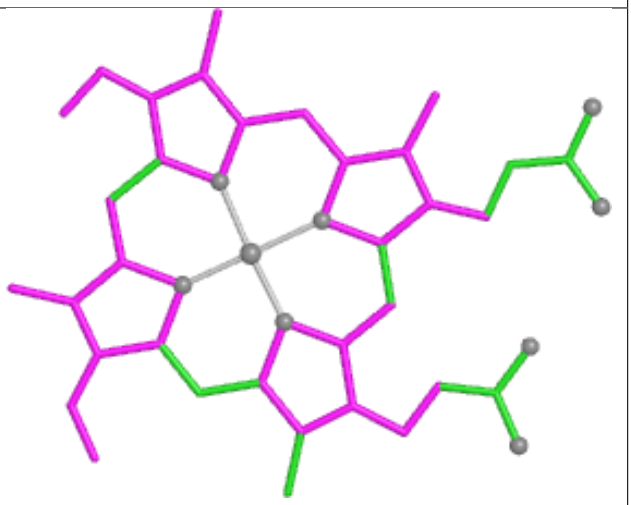
Ligand 3PE D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE O 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

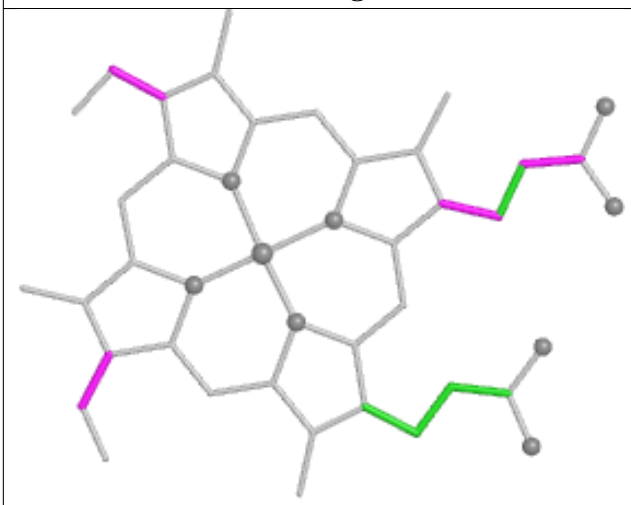
Ligand HEC Ad 401



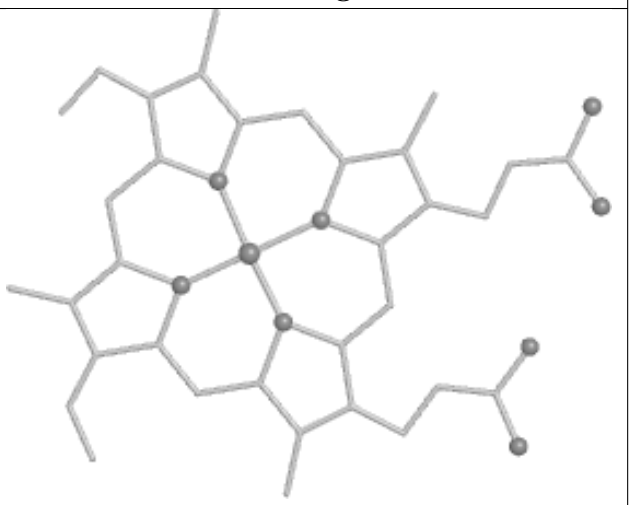
Bond lengths



Bond angles

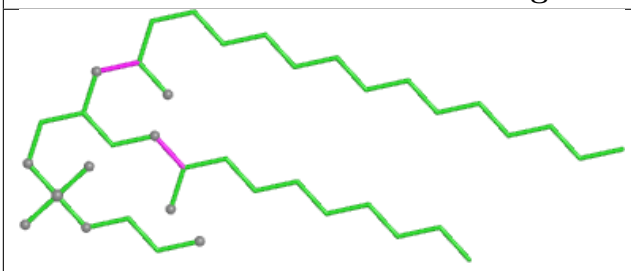


Torsions

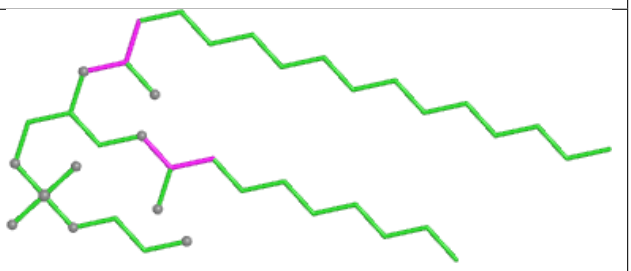


Rings

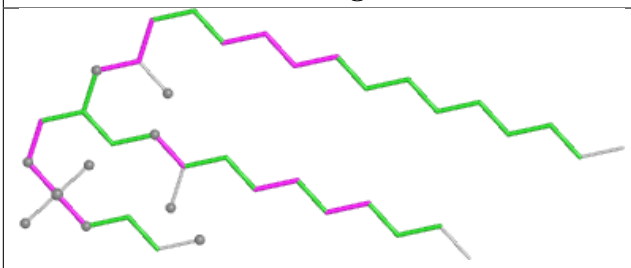
Ligand 3PE L 702



Bond lengths



Bond angles



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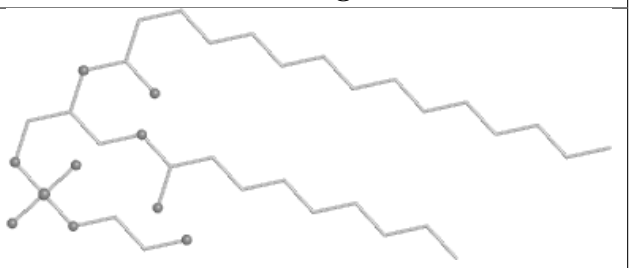
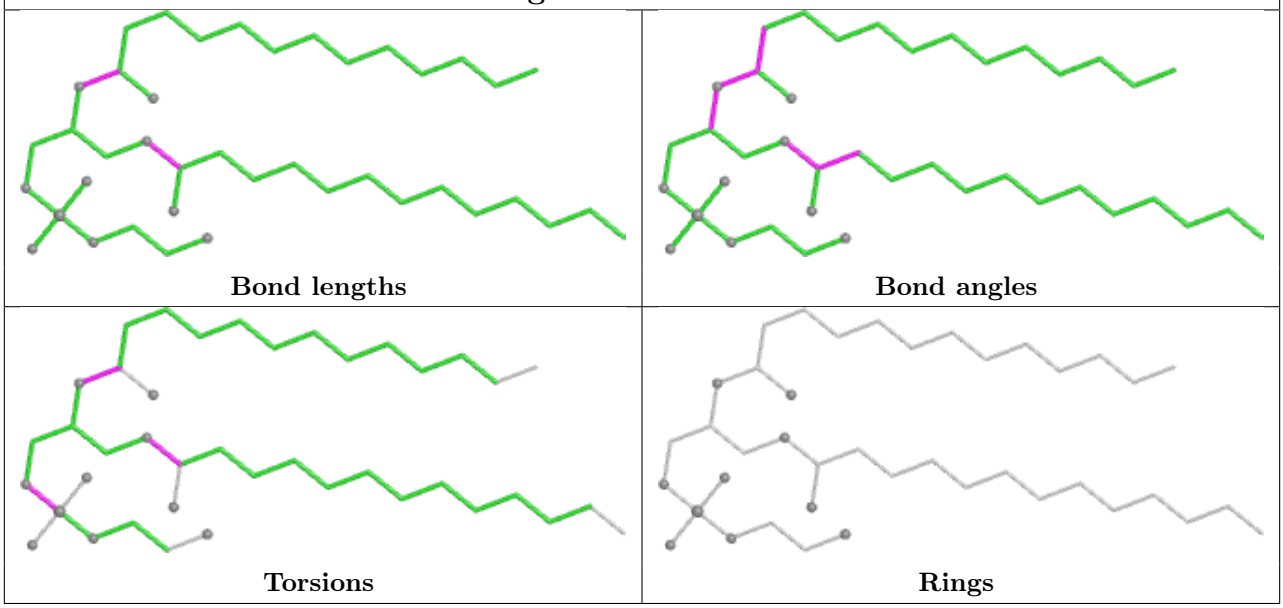
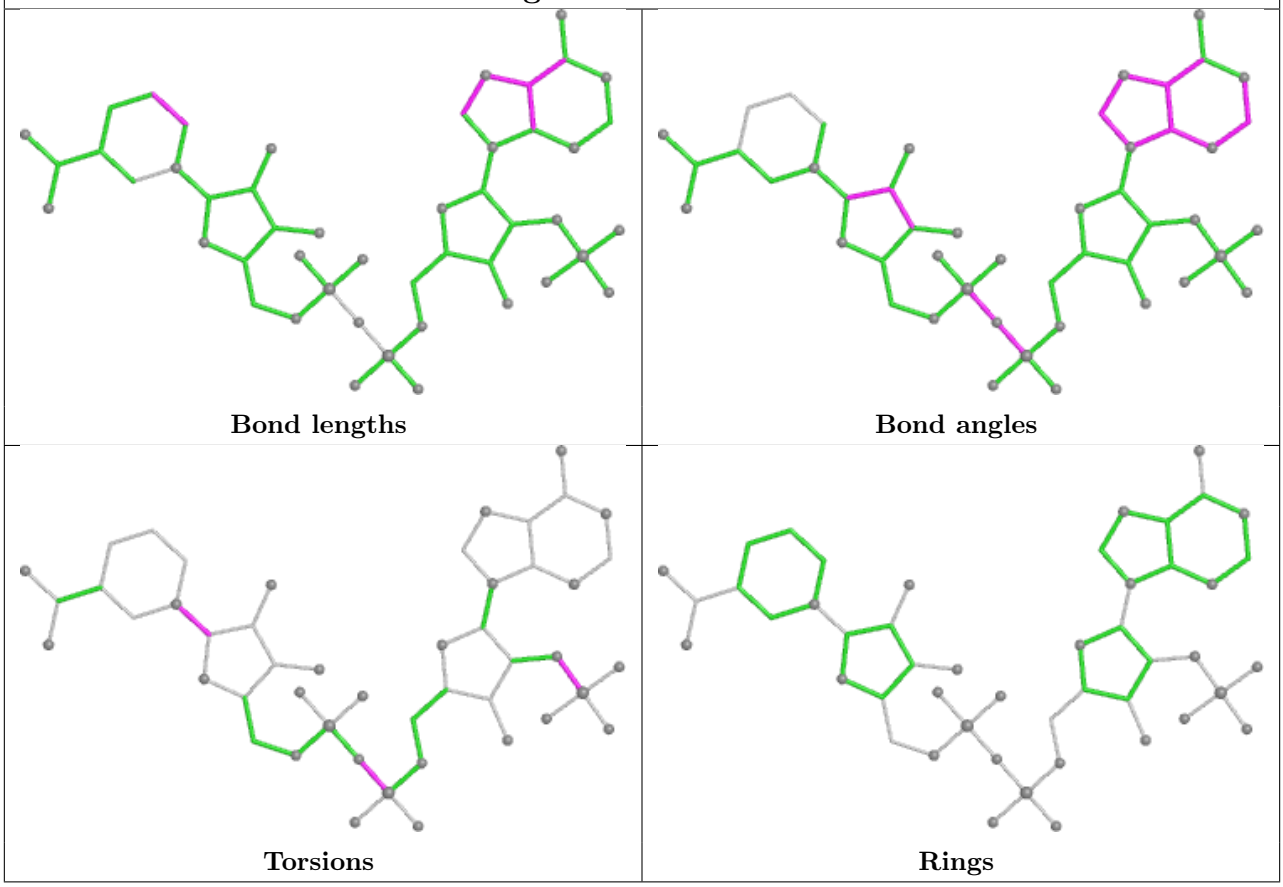


Rings

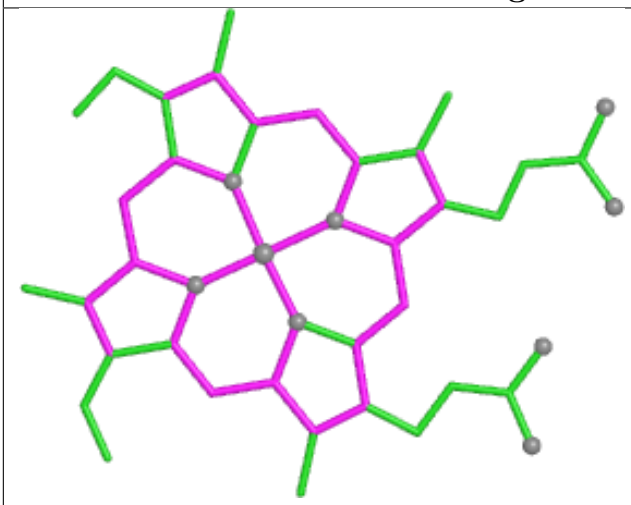
Ligand 3PE m 202



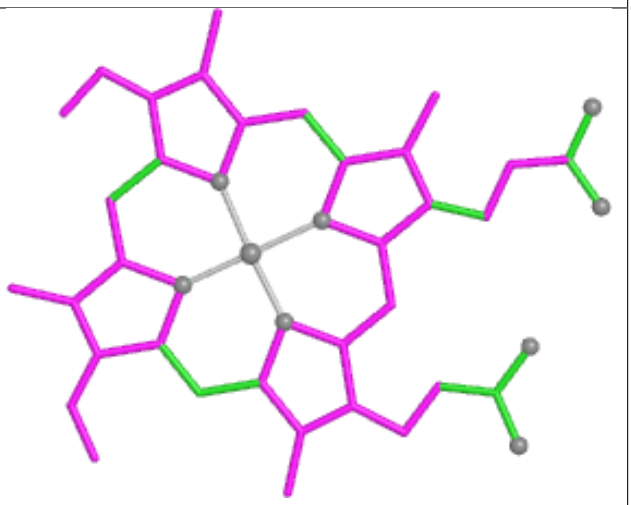
Ligand NDP P 401



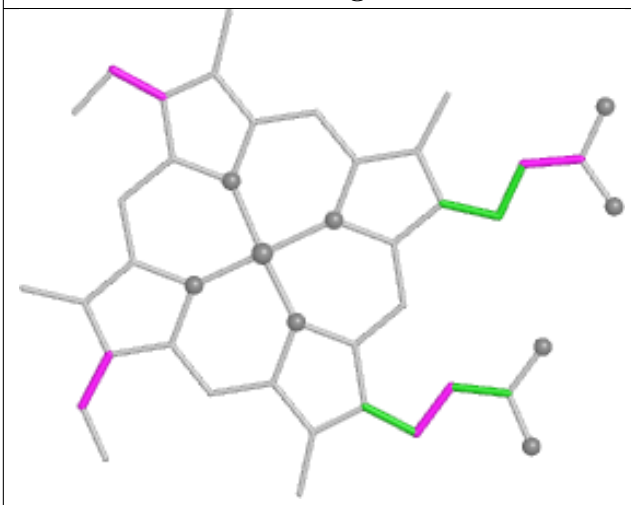
Ligand HEC AD 401



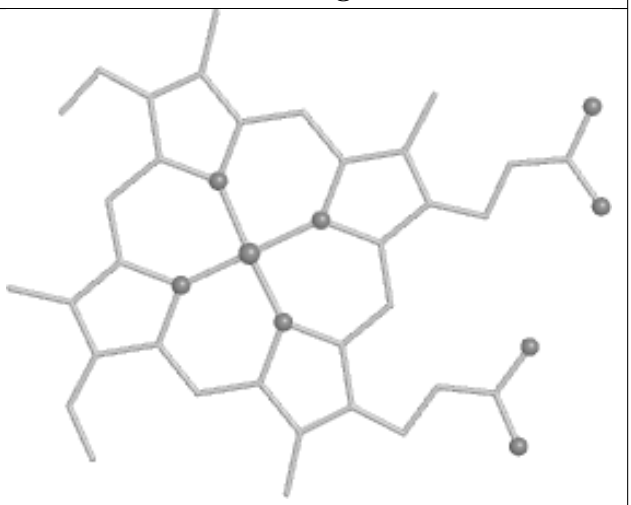
Bond lengths



Bond angles

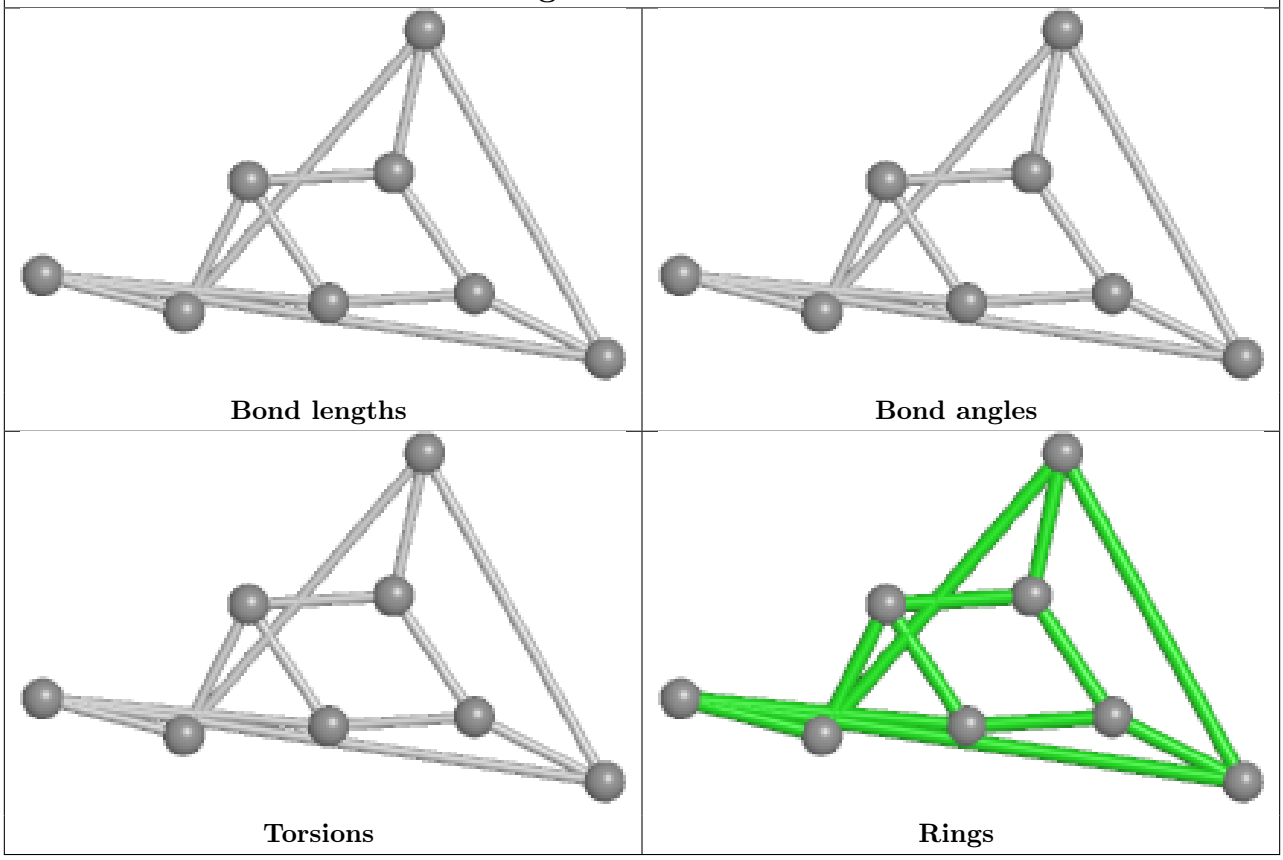


Torsions

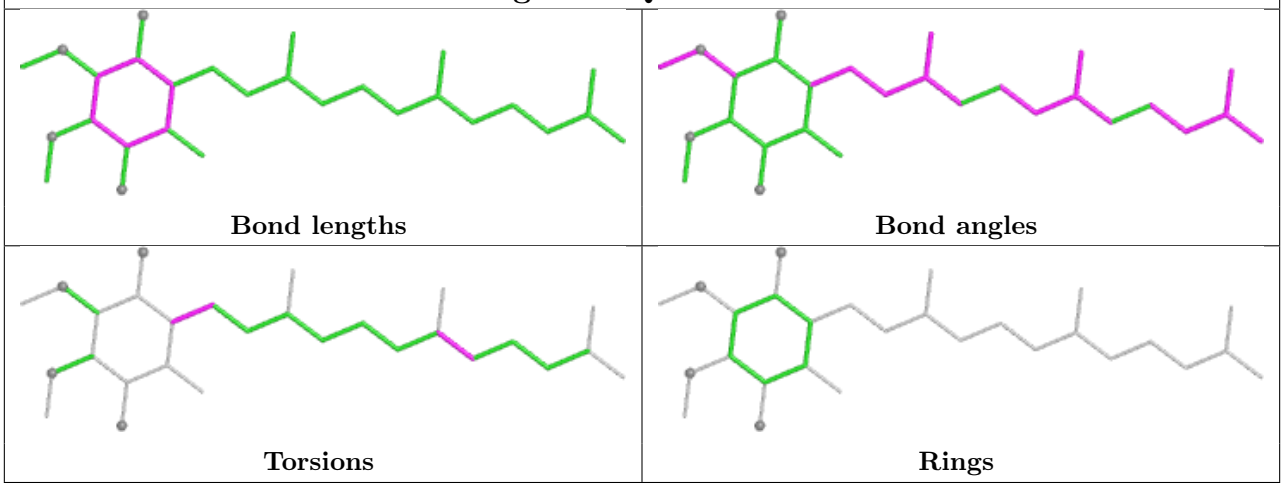


Rings

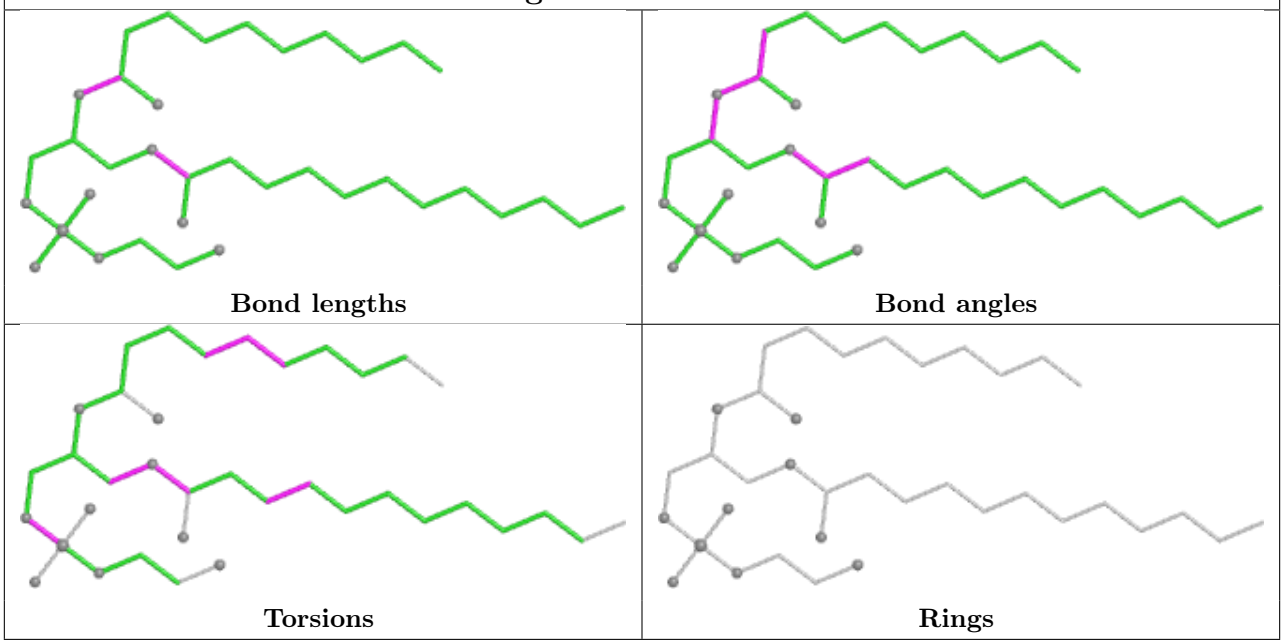
Ligand SF4 I 303



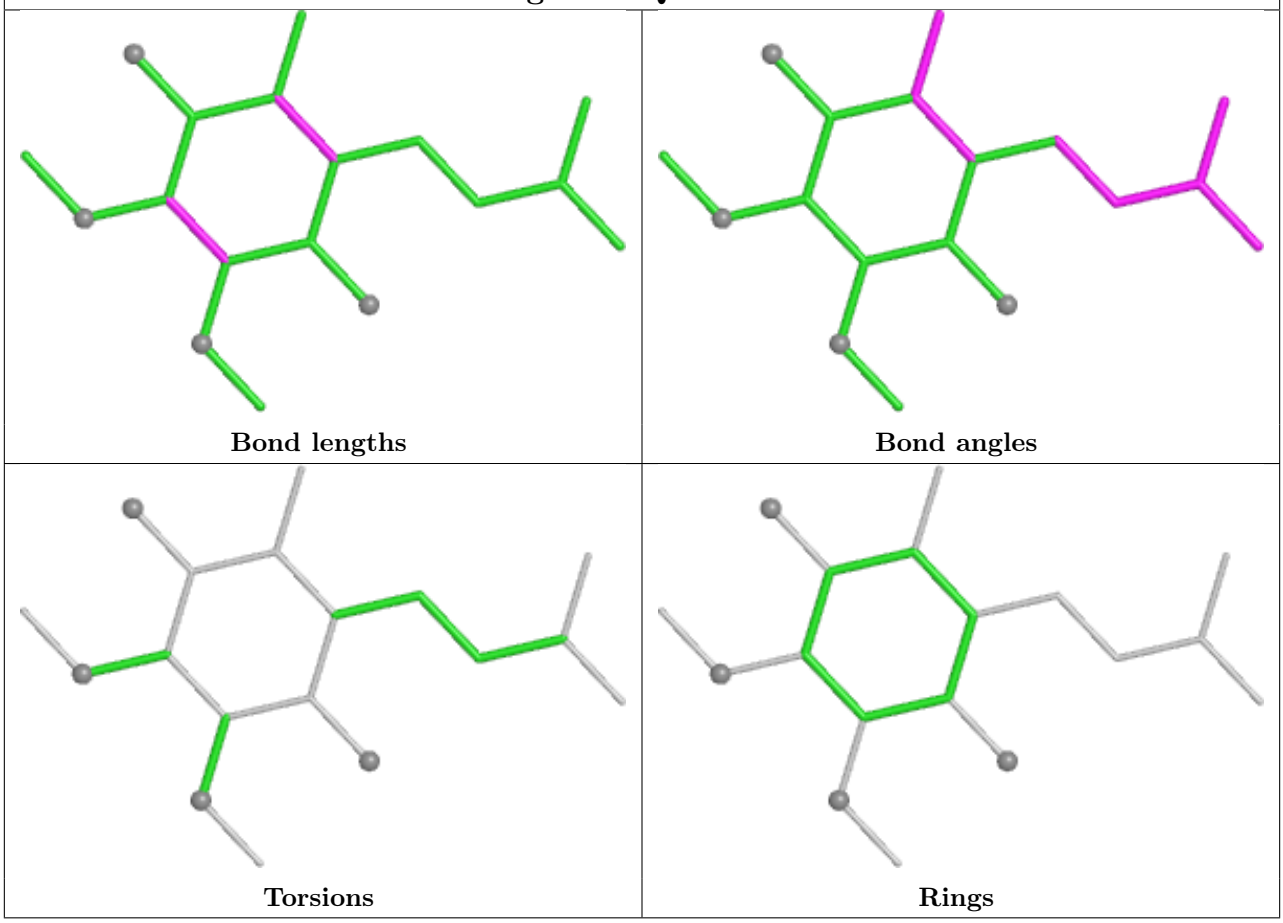
Ligand UQ6 AC 405



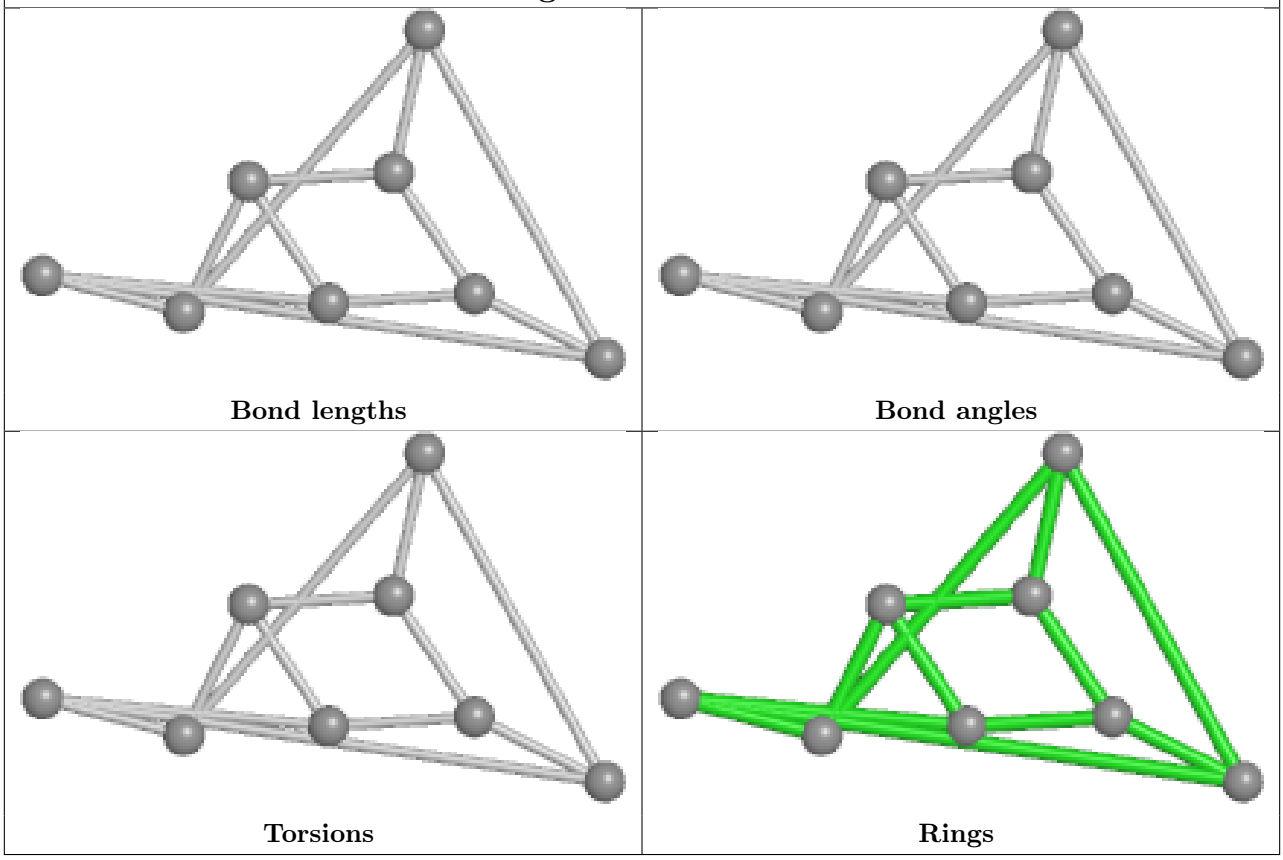
Ligand 3PE M 501



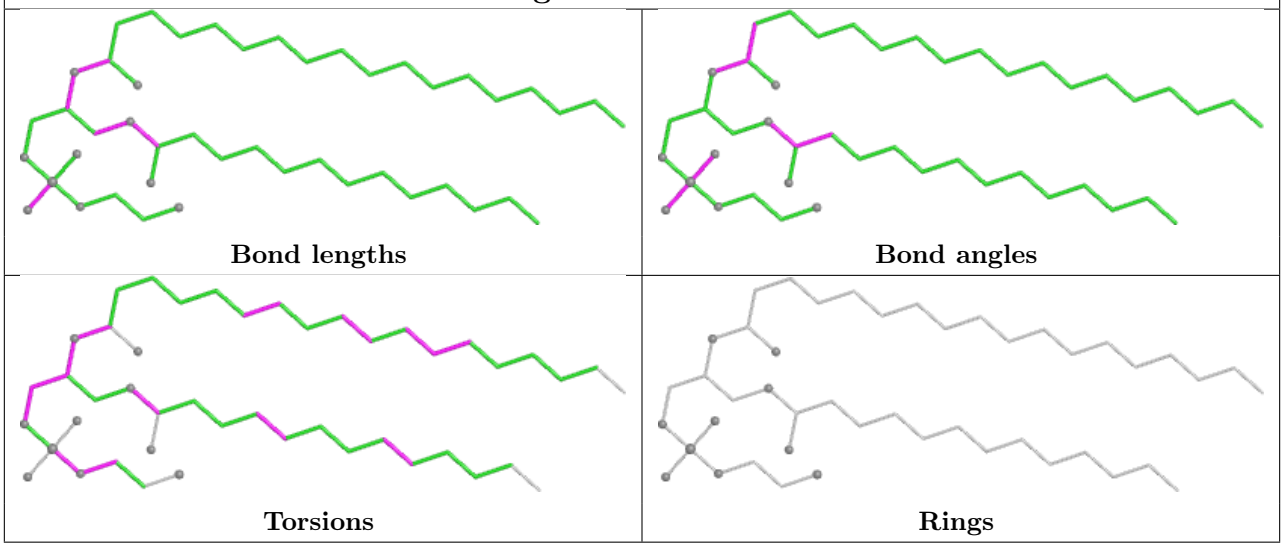
Ligand UQ1 B 302



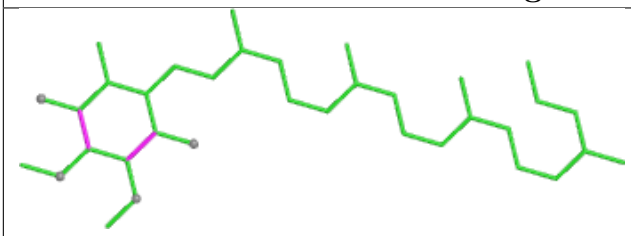
Ligand SF4 I 304



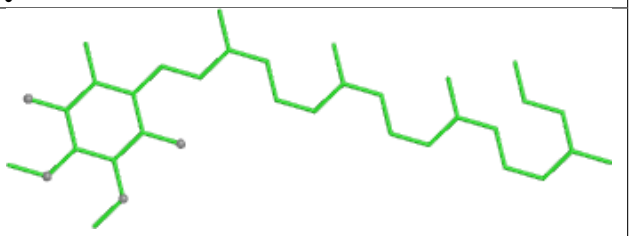
Ligand 3PE J 401



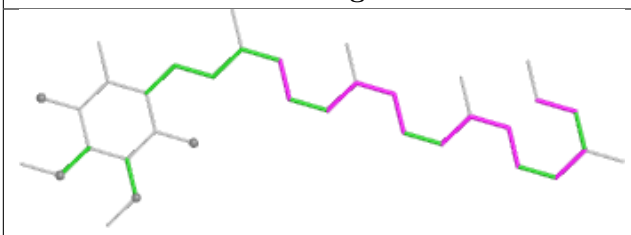
Ligand UQ9 H 400



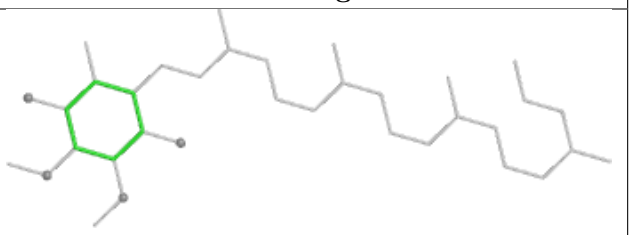
Bond lengths



Bond angles

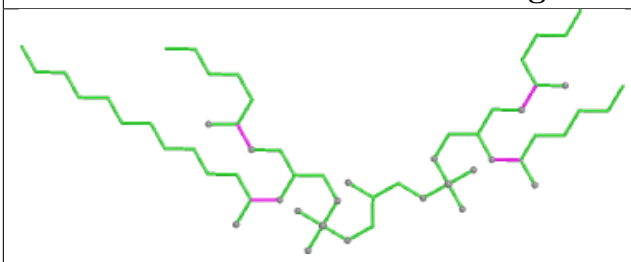


Torsions

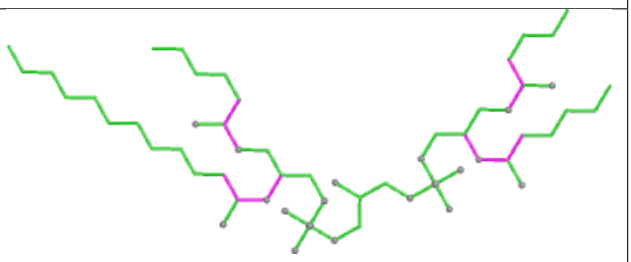


Rings

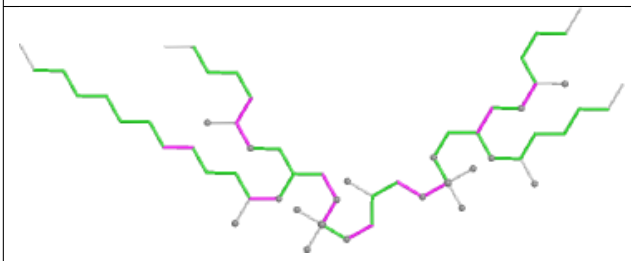
Ligand CDL a 101



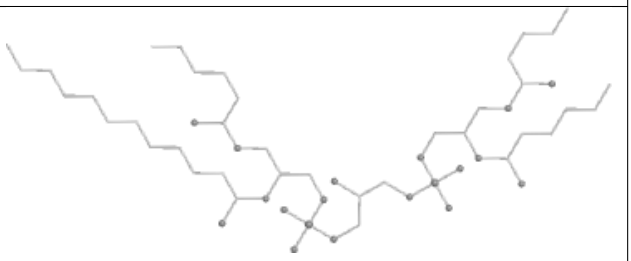
Bond lengths



Bond angles

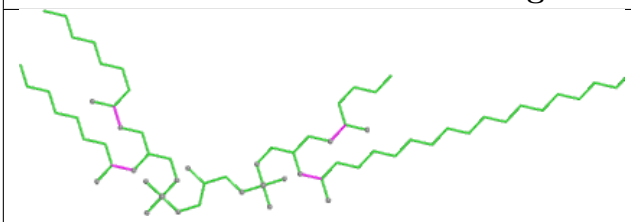


Torsions

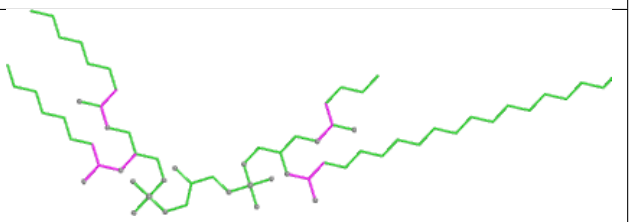


Rings

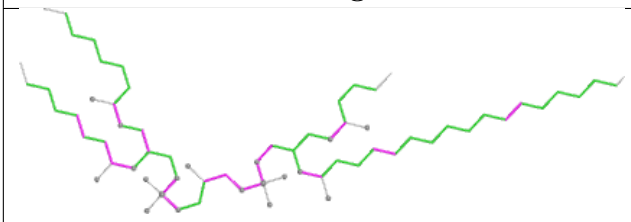
Ligand CDL d 201



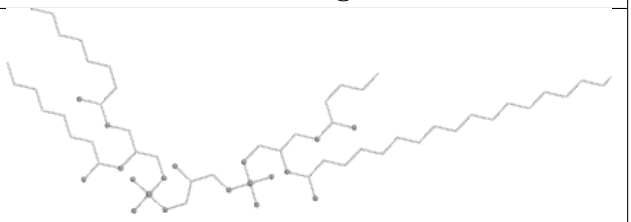
Bond lengths



Bond angles

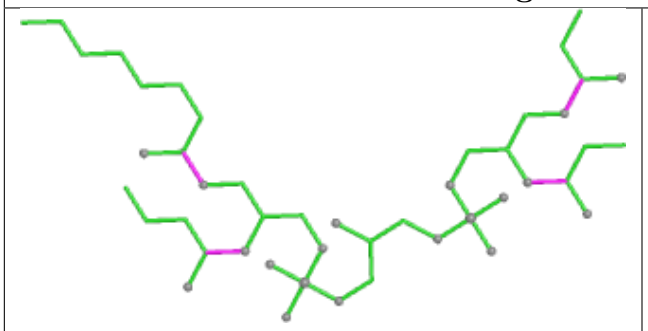


Torsions

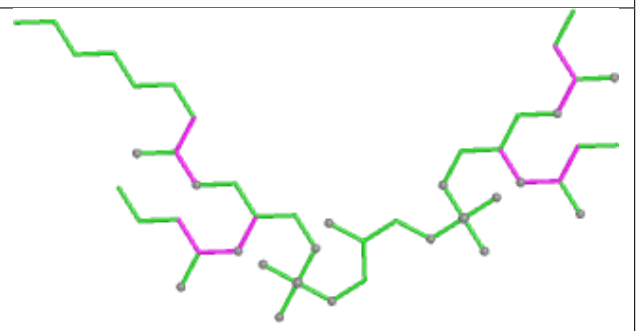


Rings

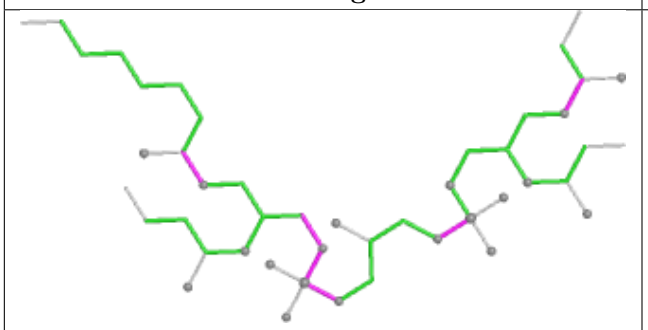
Ligand CDL Aa 501



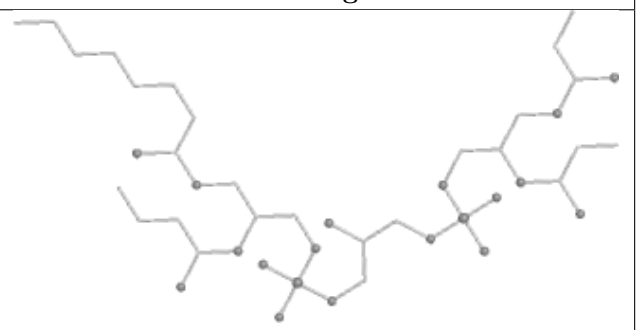
Bond lengths



Bond angles

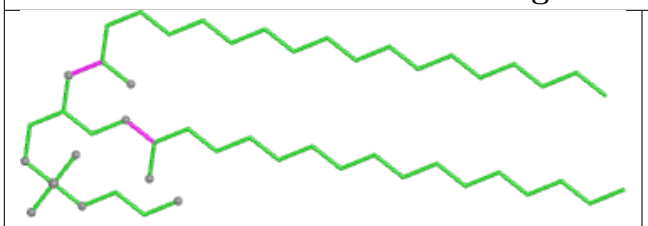


Torsions

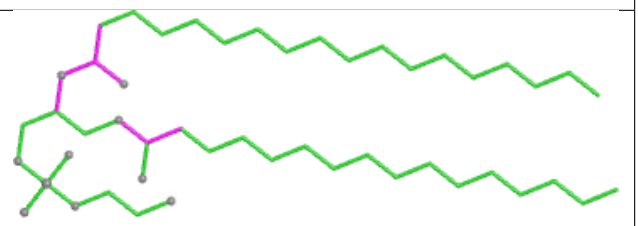


Rings

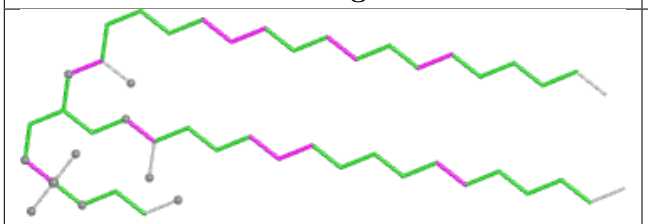
Ligand 3PE L 701



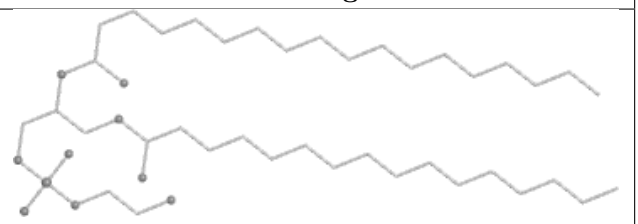
Bond lengths



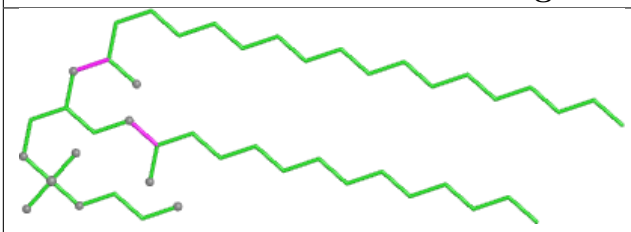
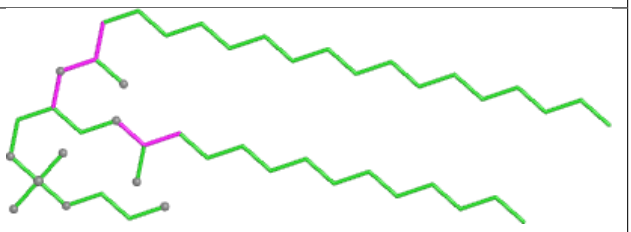
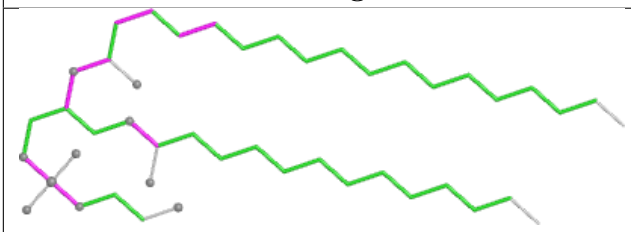
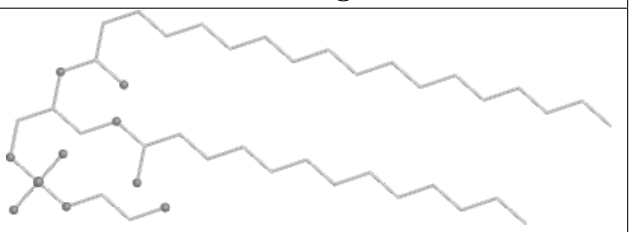
Bond angles



Torsions



Rings

Ligand 3PE I 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

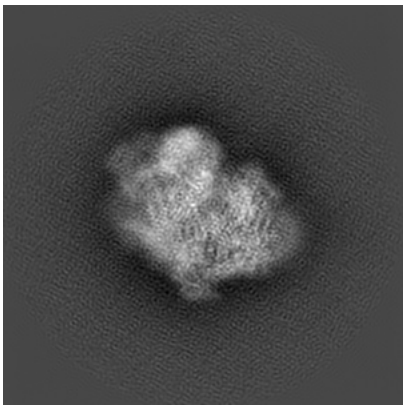
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35336. These allow visual inspection of the internal detail of the map and identification of artifacts.

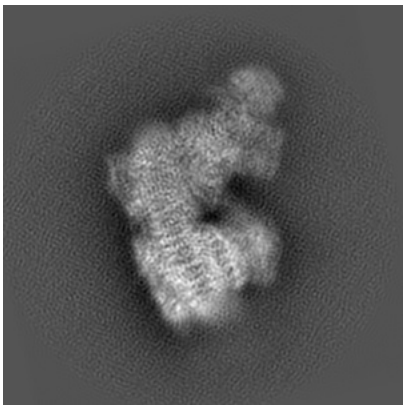
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

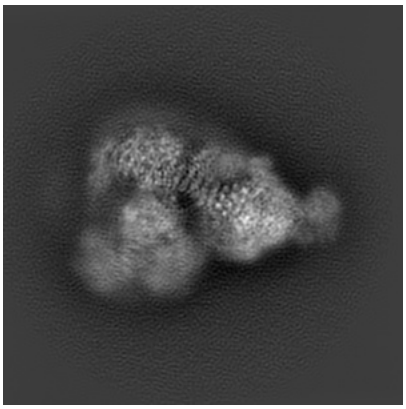
6.1.1 Primary map



X

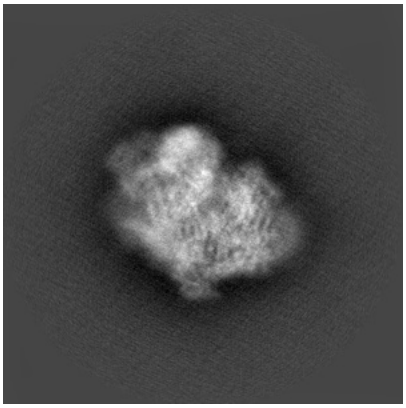


Y

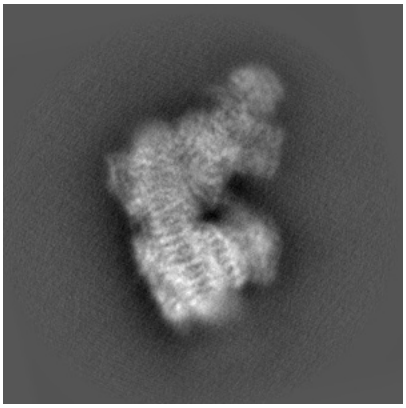


Z

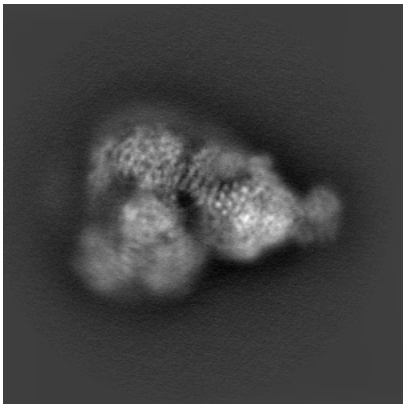
6.1.2 Raw map



X



Y

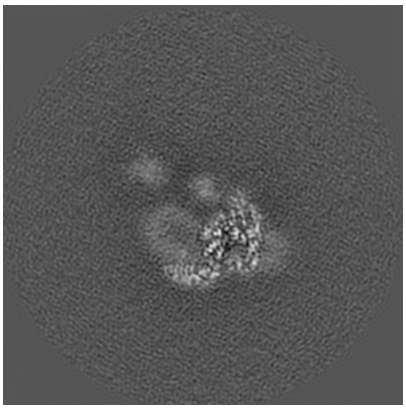


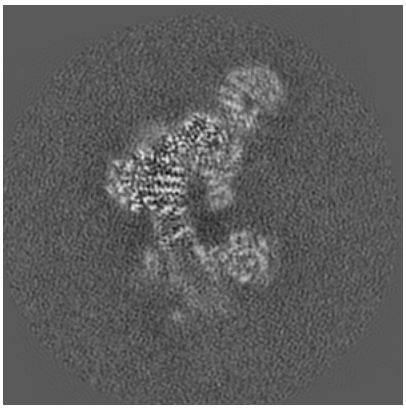
Z

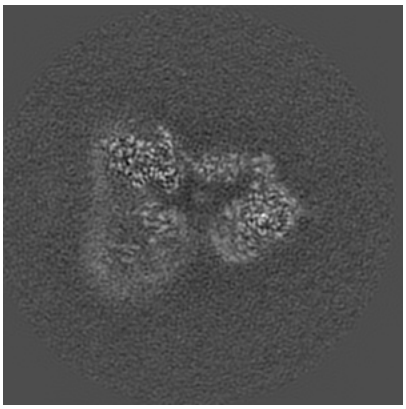
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

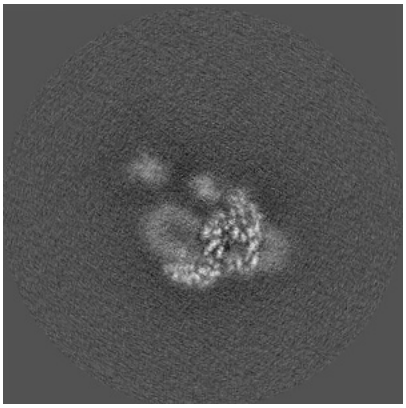
6.2.1 Primary map

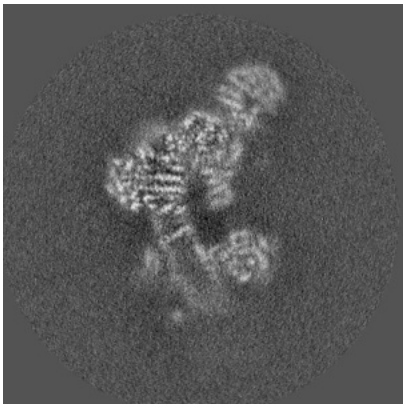

X Index: 192

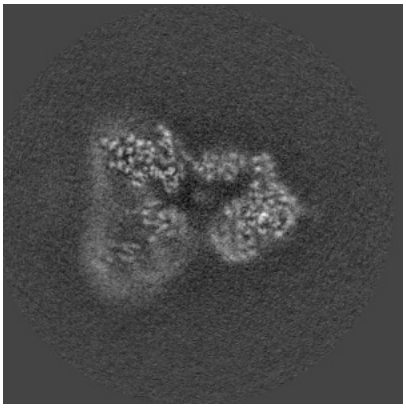

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

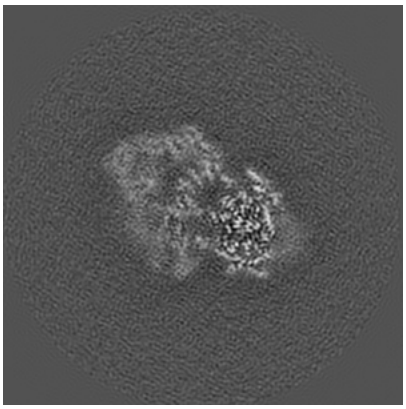

Y Index: 192

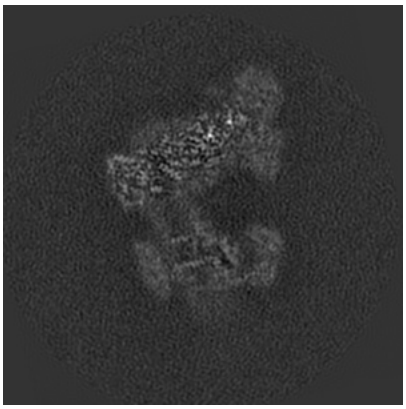

Z Index: 192

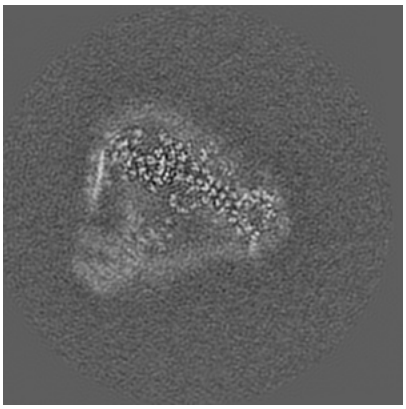
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

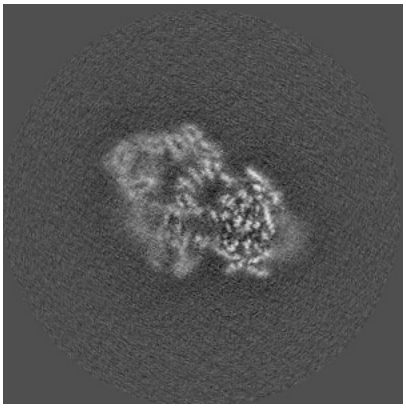
6.3.1 Primary map

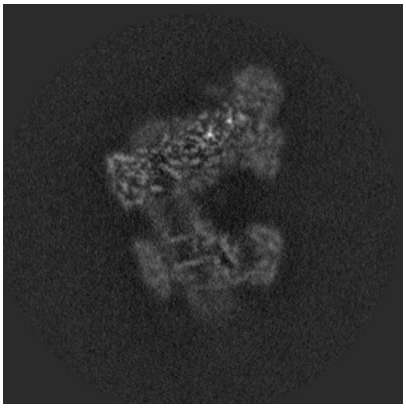

X Index: 154

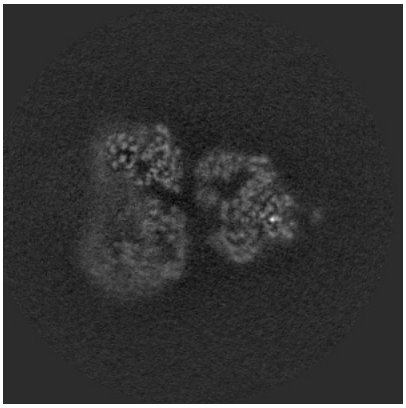

Y Index: 177


Z Index: 167

6.3.2 Raw map


X Index: 154

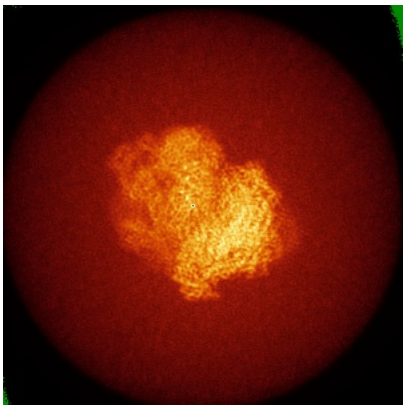

Y Index: 177

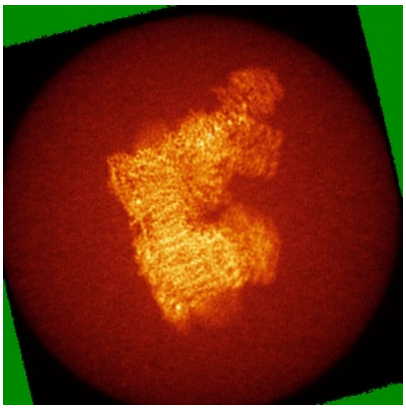

Z Index: 198

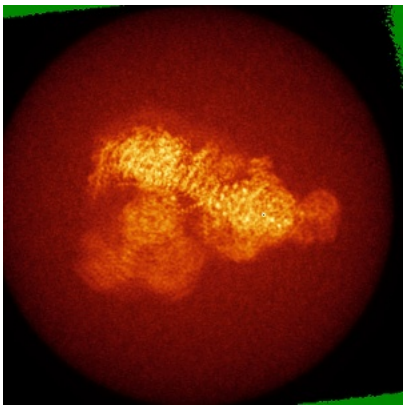
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

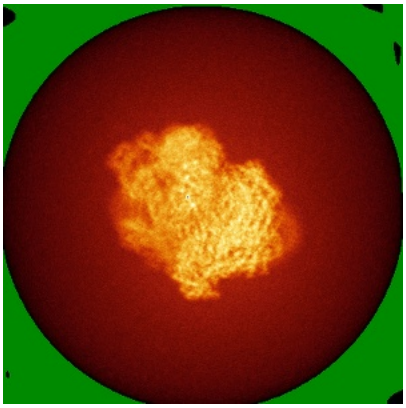
6.4.1 Primary map

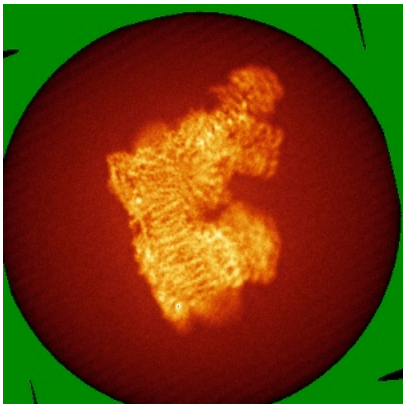

X

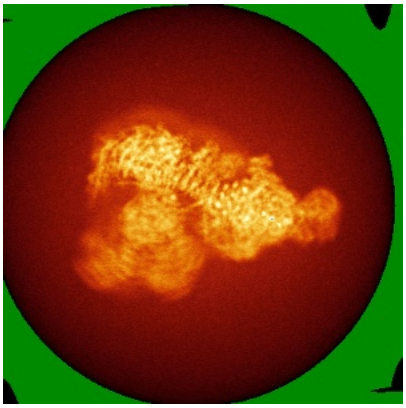

Y


Z

6.4.2 Raw map


X


Y


Z

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

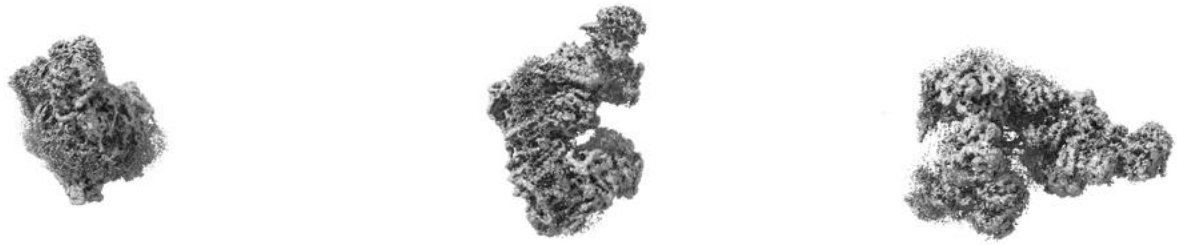
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

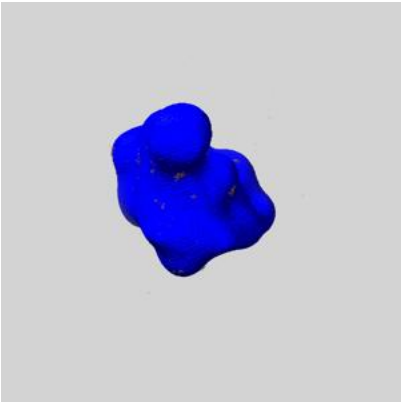
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

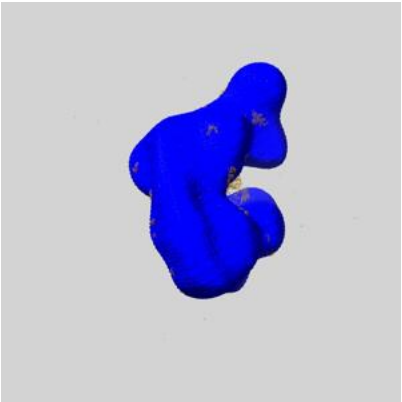
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

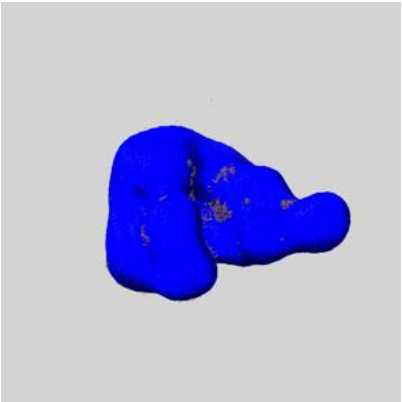
6.6.1 emd_35336_msk_1.map (i)



X



Y

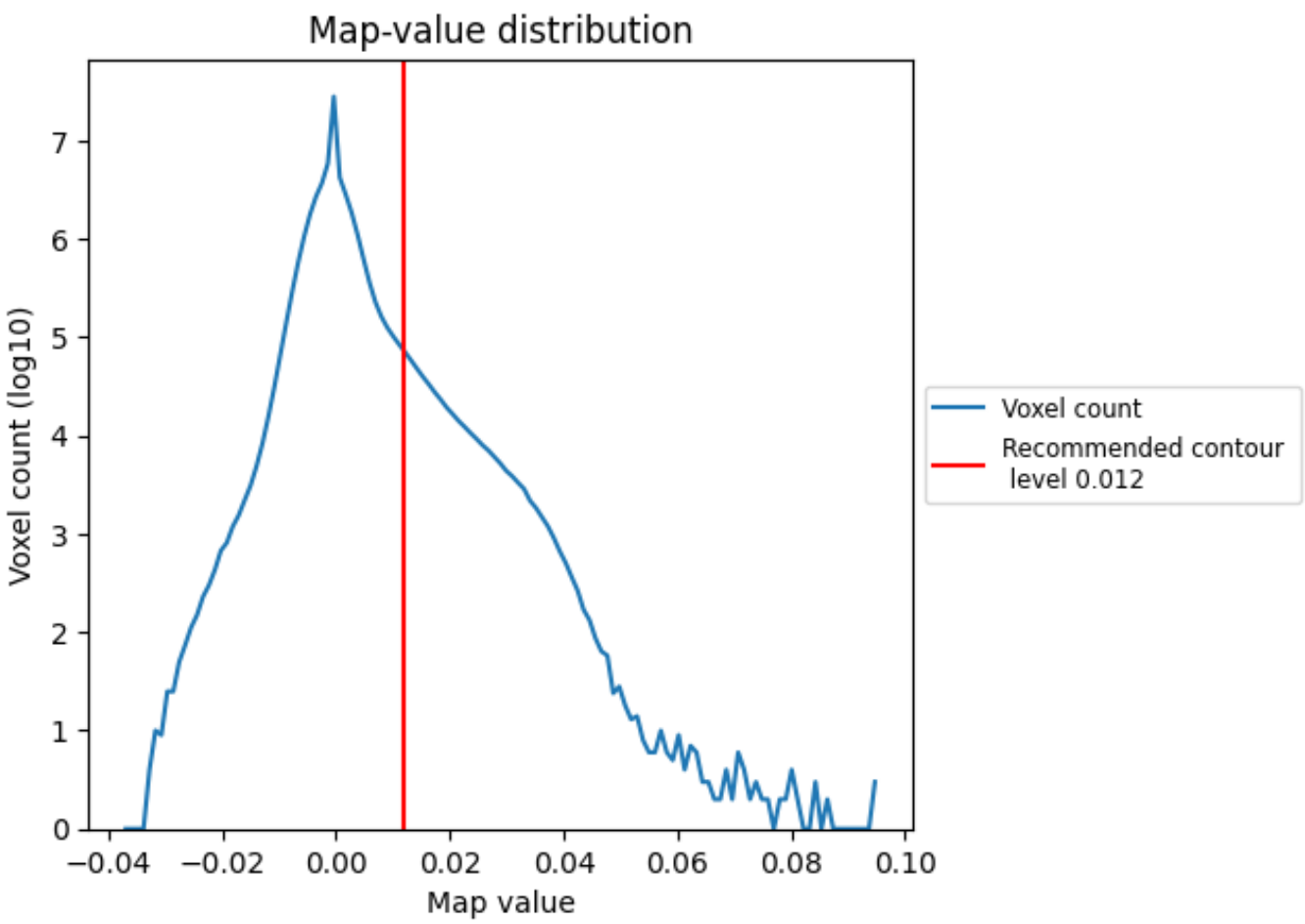


Z

7 Map analysis (i)

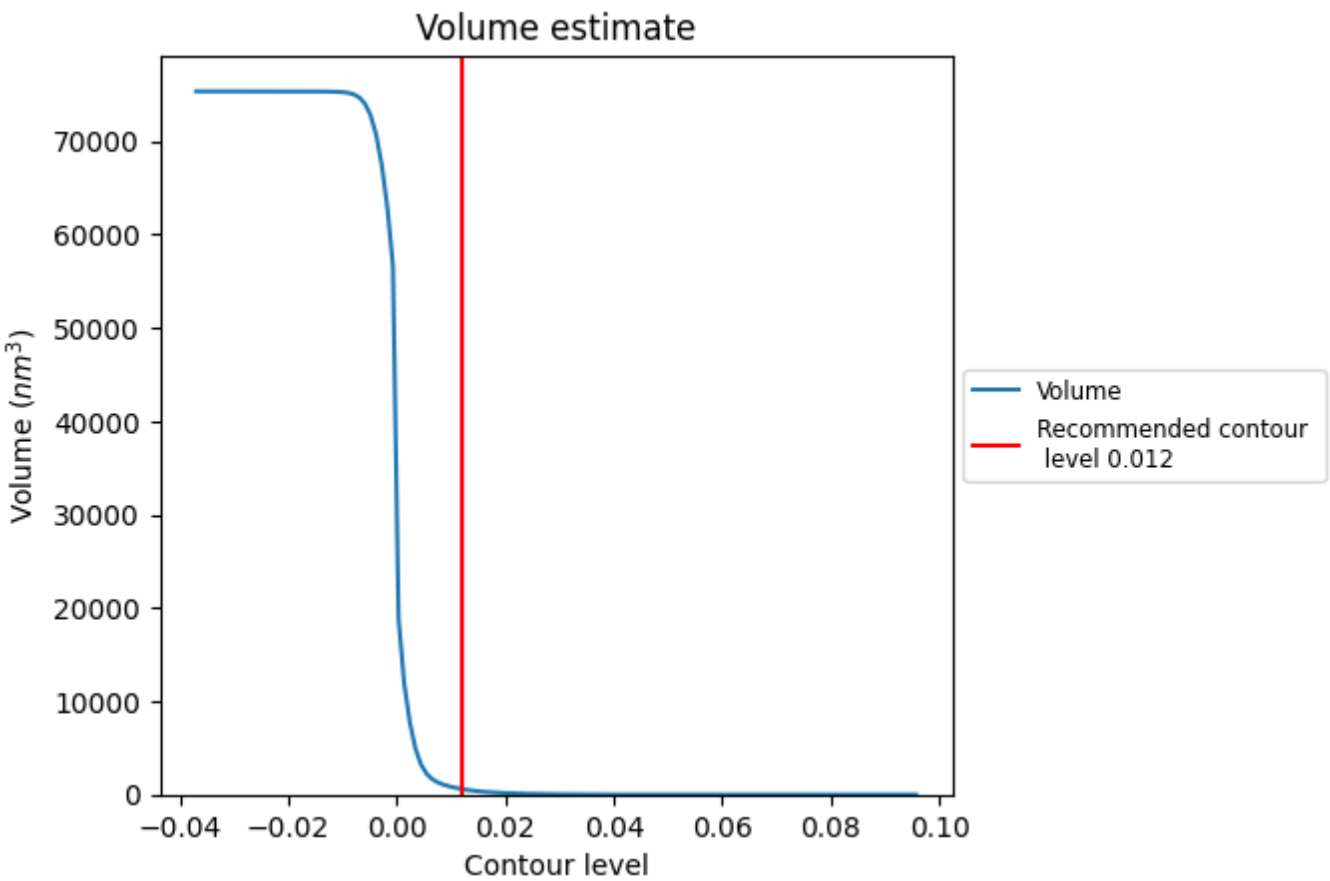
This section contains the results of statistical analysis of the map.

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.

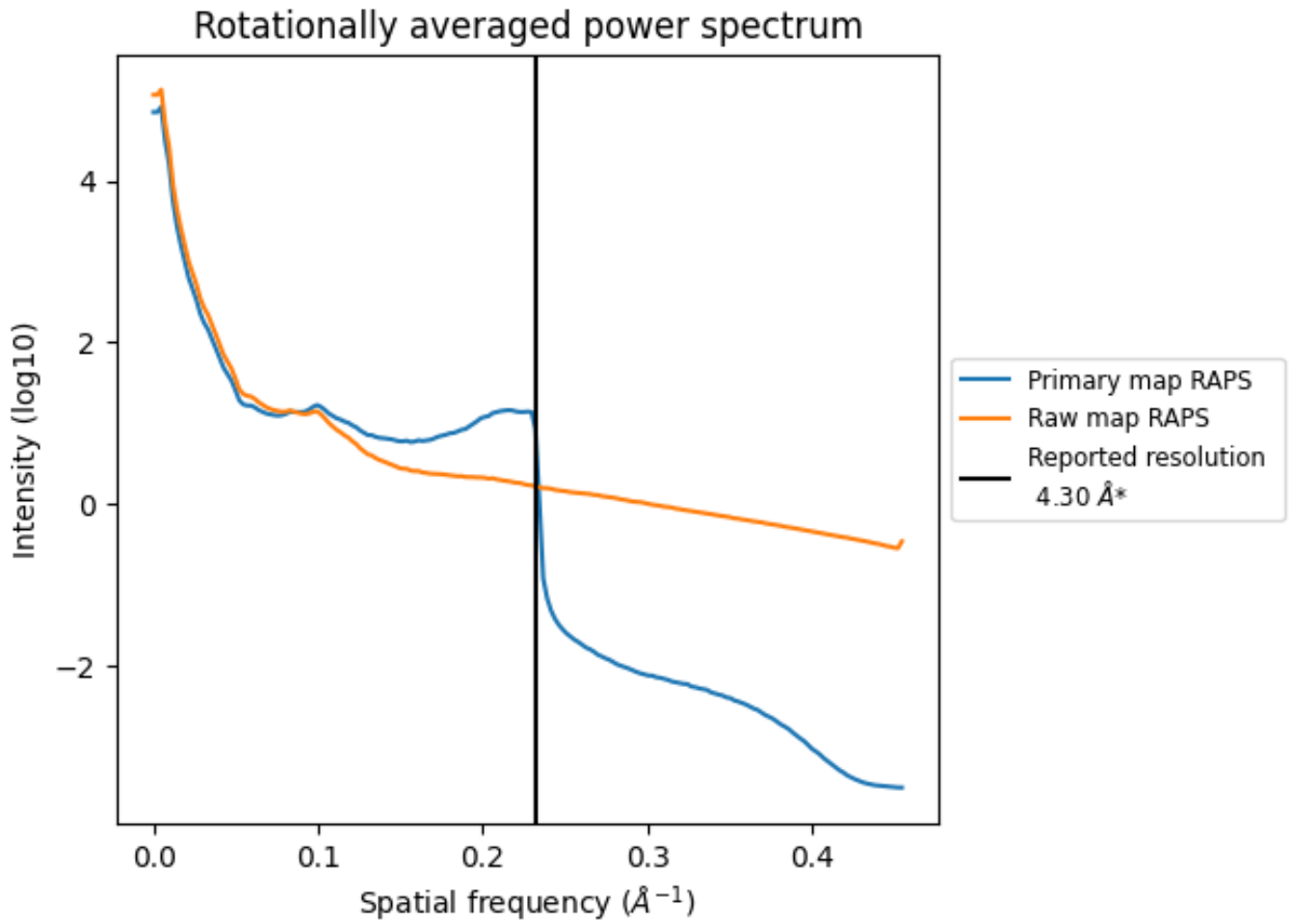
7.2 Volume estimate (i)



The volume at the recommended contour level is 593 nm^3; this corresponds to an approximate mass of 535 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)

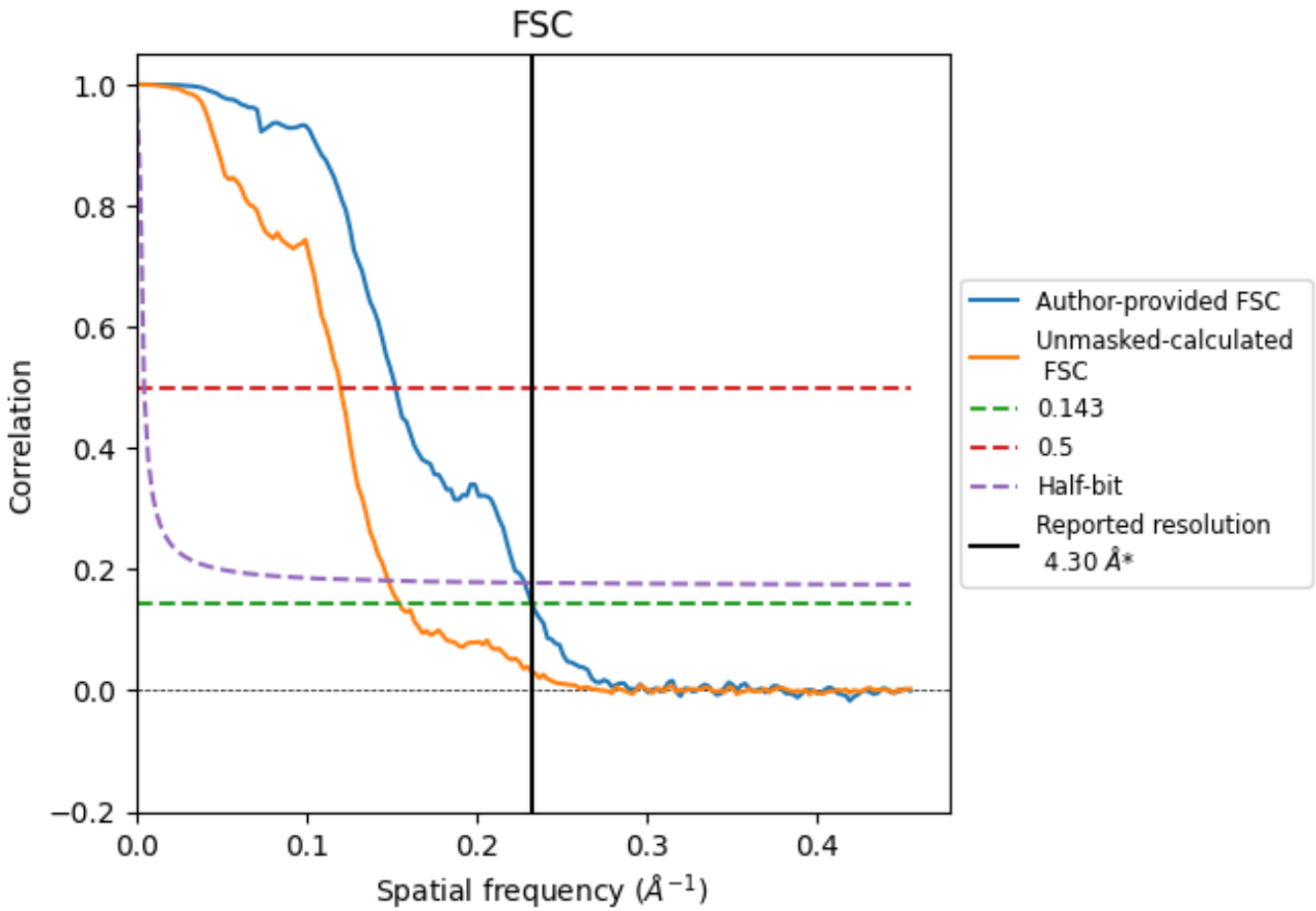


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

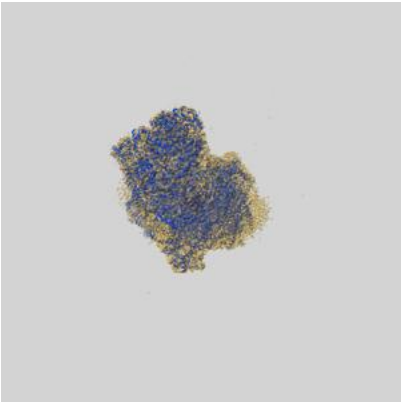
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.30	6.57	4.39
Unmasked-calculated*	6.47	8.34	6.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.47 differs from the reported value 4.3 by more than 10 %

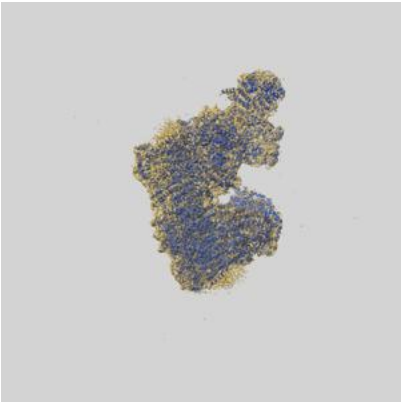
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35336 and PDB model 8IB9. Per-residue inclusion information can be found in section 3 on page 26.

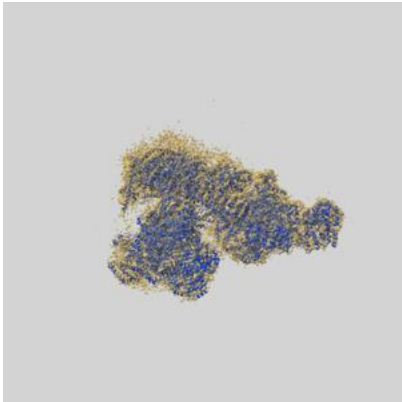
9.1 Map-model overlay (i)



X



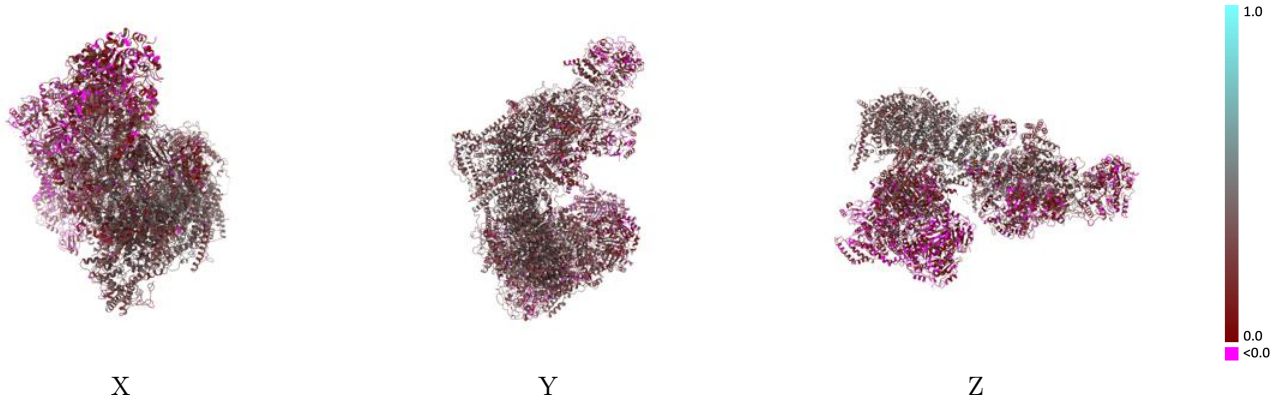
Y



Z

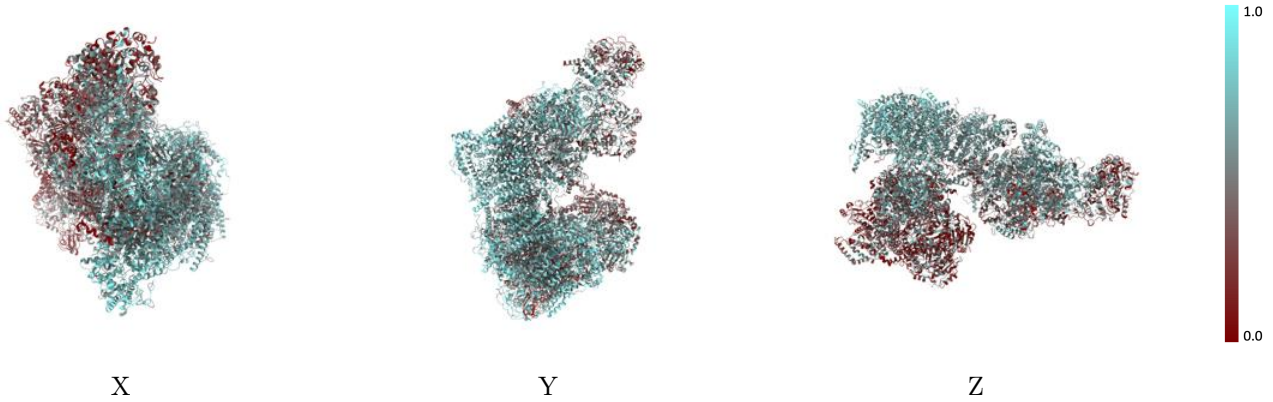
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



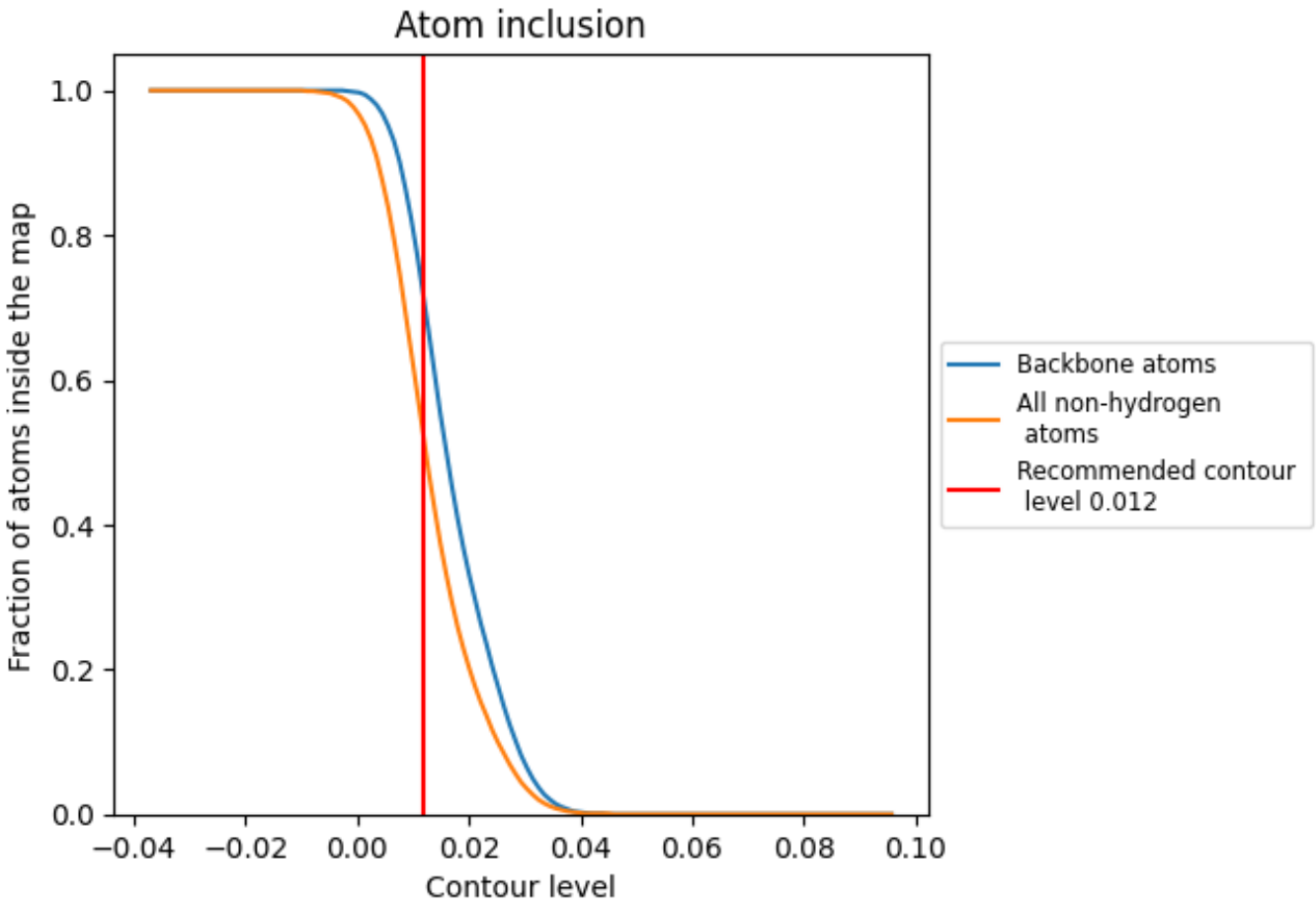
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5140	0.2380
A	0.5960	0.3270
AA	0.3290	0.1030
AB	0.2800	0.0900
AC	0.2780	0.1230
AD	0.3430	0.0940
AE	0.0840	0.0530
AF	0.3680	0.1070
AG	0.2370	0.0720
AH	0.3380	0.0940
AI	0.1240	0.0610
AJ	0.0640	0.0090
AK	0.1170	0.0500
Aa	0.5520	0.2310
Ab	0.4690	0.1540
Ac	0.4130	0.2080
Ad	0.4000	0.1620
Ae	0.1310	0.0920
Af	0.4420	0.2140
Ag	0.4580	0.2400
Ah	0.4290	0.1560
Aj	0.2020	0.1590
Ak	0.1080	0.0950
B	0.6790	0.3330
C	0.6230	0.2680
D	0.6690	0.3310
E	0.3600	0.1540
F	0.4060	0.1480
G	0.4830	0.1870
H	0.6610	0.3420
I	0.6850	0.3280
J	0.5890	0.3280
K	0.6280	0.3540
L	0.6350	0.3430
M	0.6780	0.3790

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Chain	Atom inclusion	Q-score
N	0.6860	0.3750
O	0.5860	0.2720
P	0.4300	0.1700
Q	0.4520	0.2360
R	0.2640	0.1660
S	0.3870	0.0920
T	0.3070	0.1080
U	0.7020	0.3260
V	0.5970	0.2090
W	0.5010	0.1940
X	0.7410	0.3300
Y	0.6210	0.3320
Z	0.7270	0.3200
a	0.6720	0.3210
b	0.6520	0.2910
c	0.6350	0.2860
d	0.6950	0.3610
e	0.7320	0.3330
f	0.6430	0.2960
g	0.6770	0.3440
h	0.6950	0.3330
i	0.6980	0.3340
j	0.6830	0.3100
k	0.7330	0.3390
l	0.7130	0.3600
m	0.6280	0.3340
n	0.7510	0.3480
o	0.6680	0.2740
p	0.7220	0.3290
q	0.2190	0.2020
r	0.3220	0.1890
s	0.1130	0.0810