wwPDB EM Validation Summary Report ⓘ

Nov 24, 2024 – 03:29 AM JST

PDB ID	:	8IB4
EMDB ID	:	EMD-35331
Title	:	Respiratory complex CI:CIII2, type IA, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-09
Resolution	:	4.30 Å(reported)

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

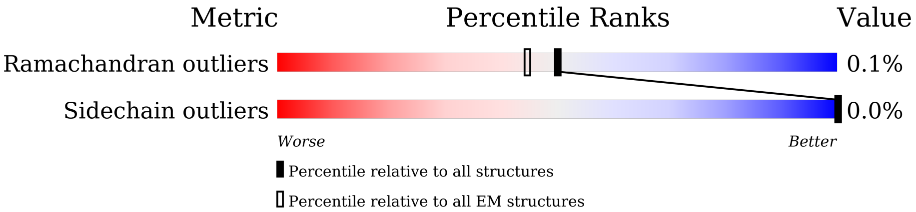
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

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

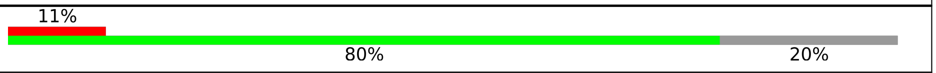
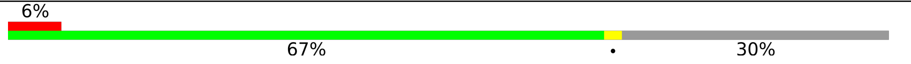
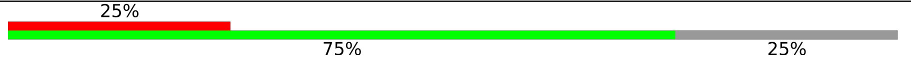
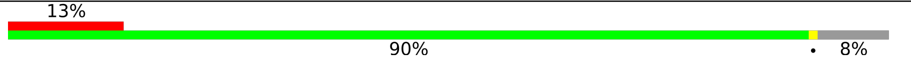
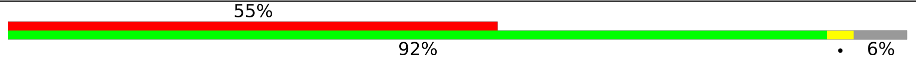
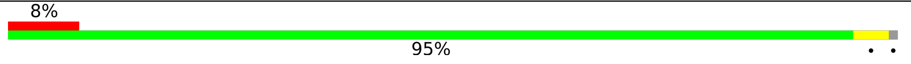
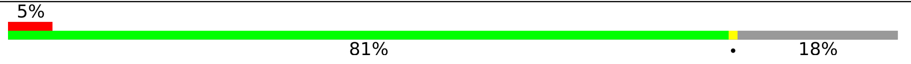
The reported resolution of this entry is 4.30 Å.

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
2	B	224	
3	C	263	
4	D	463	
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	

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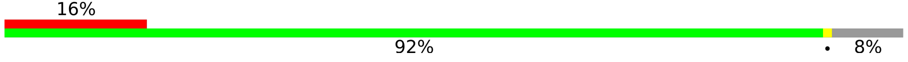
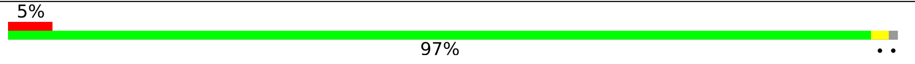
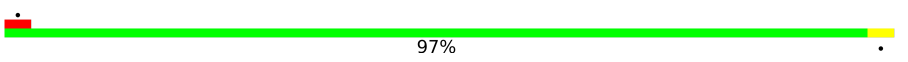
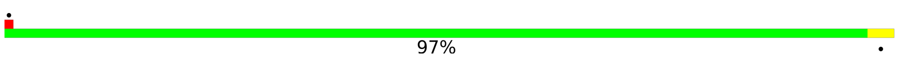
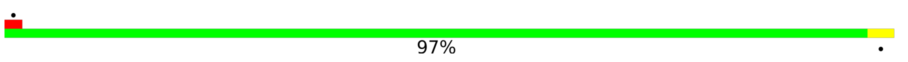
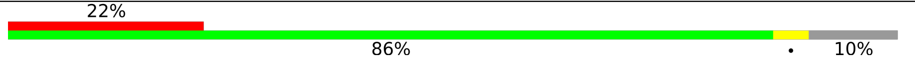
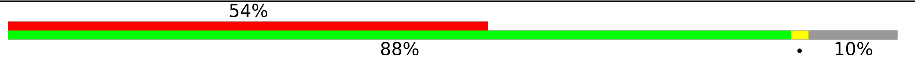
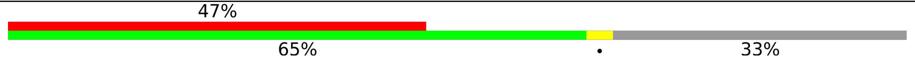
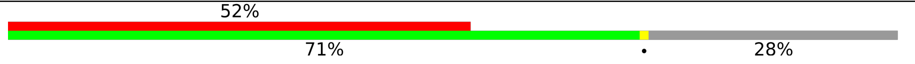
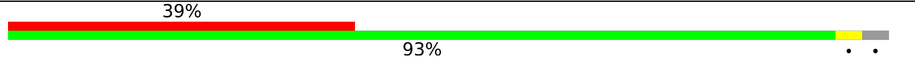
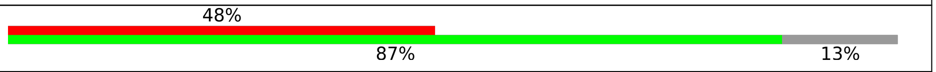
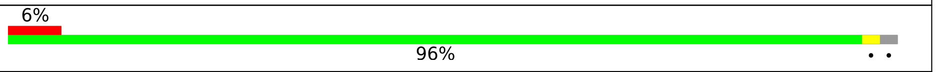
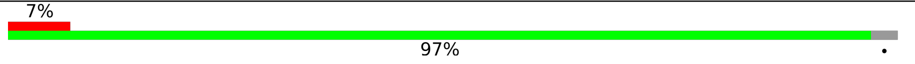
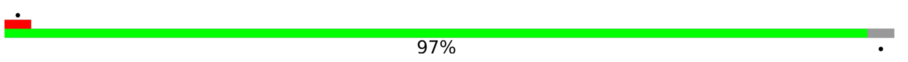
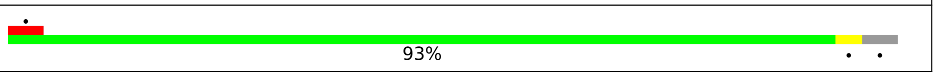
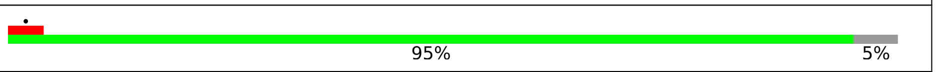
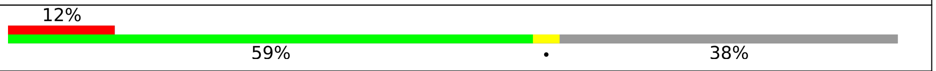
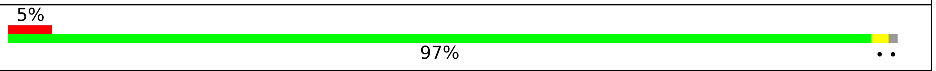
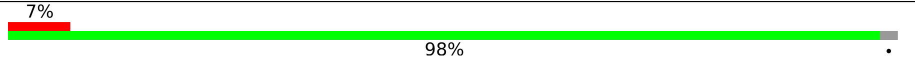
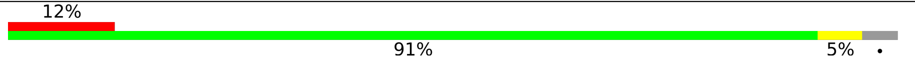
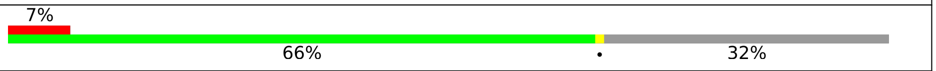
Mol	Chain	Length	Quality of chain
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	

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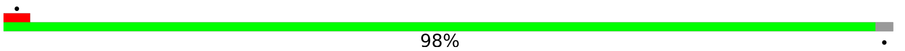
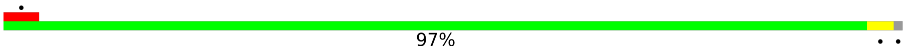
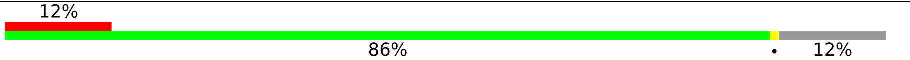
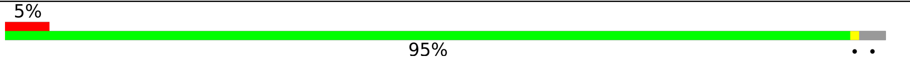
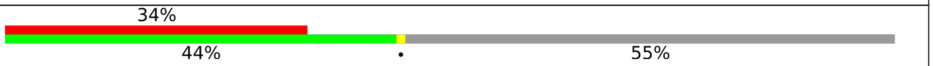
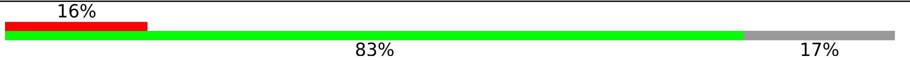
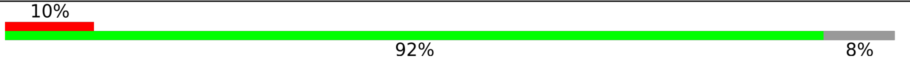
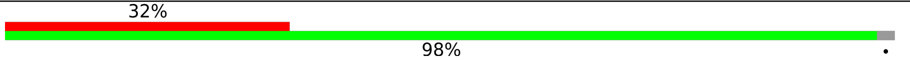
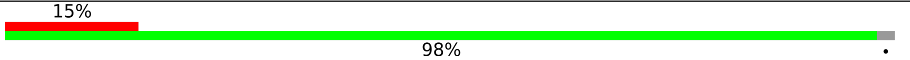
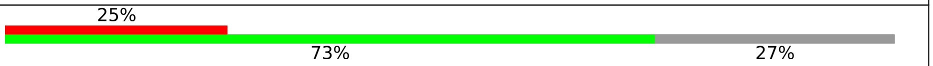
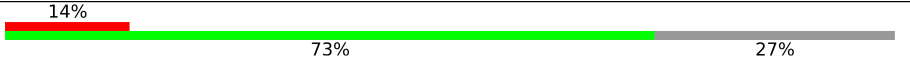
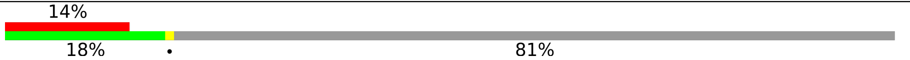
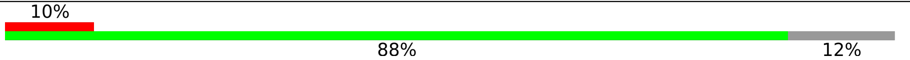
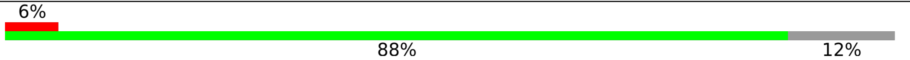
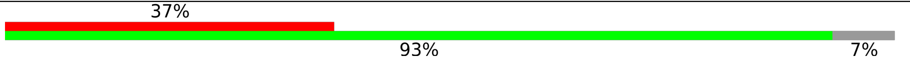
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	
49	AI	274	
49	Ae	274	
50	AF	111	
50	Af	111	
51	AG	82	

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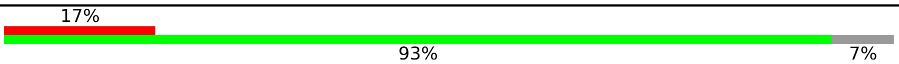
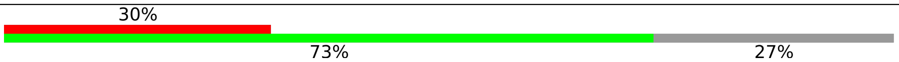
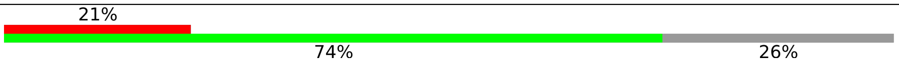
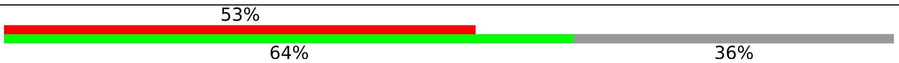
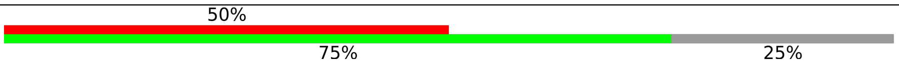
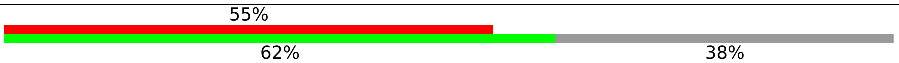
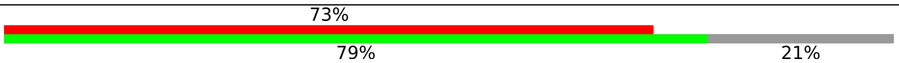
Mol	Chain	Length	Quality of chain
51	Ag	82	
52	AH	89	
52	Ah	89	
53	AJ	64	
53	Aj	64	
54	AK	56	
54	Ak	56	

2 Entry composition

There are 71 unique types of molecules in this entry. The entry contains 97639 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
1	A	92	Total	C	N	O	S	0	0
			754	523	107	119	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	424	Total	C	N	O	S	0	0
			3415	2182	587	622	24		

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

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

- 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	314	2510	1687	380	421	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	159	1205	814	171	205	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	458	3622	2402	566	615	39	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	84	678	438	100	135	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	80	628	414	99	111	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	119	988	646	170	164	8	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	104	863	546	158	151	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	55	475	310	84	79	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	102	858	553	137	164	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	136	1146	754	191	198	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	94	796	520	139	134	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	65	563	369	93	100	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	71	569	375	99	93	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	158	1328	858	221	238	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	127	1054	678	190	186	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	178	1541	985	276	269	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	120	1027	647	192	179	9	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	51	418	266	78	73	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	14	115	75	17	23	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	400	3128	1952	557	603	16	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
45	Aa	412	Total C N O S 3225 2016 569 624 16	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
46	AB	418	Total C N O S 3137 1970 552 606 9	0	0
46	Ab	418	Total C N O S 3137 1970 552 606 9	0	0

- Molecule 47 is a protein called Cytochrome b.

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

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

Mol	Chain	Residues	Atoms	AltConf	Trace
48	AD	238	Total C N O S 1896 1211 326 345 14	0	0
48	Ad	238	Total C N O S 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
49	AE	185	Total C N O S 1427 902 250 268 7	0	0
49	AI	51	Total C N O 345 221 64 60	0	0
49	Ae	185	Total C N O S 1432 905 250 270 7	0	0

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AH	65	Total 535	C 327	N 99	O 104	S 5	0	0
52	Ah	66	Total 544	C 333	N 101	O 105	S 5	0	0

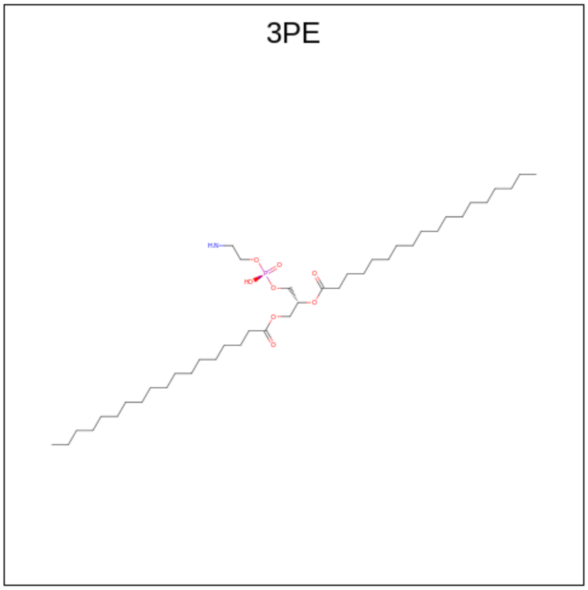
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	41	Total 332	C 216	N 57	O 59	0	0
53	Aj	48	Total 392	C 257	N 67	O 68	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	35	Total 281	C 184	N 52	O 44	S 1	0	0
54	Ak	44	Total 357	C 236	N 63	O 57	S 1	0	0

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
55	A	1	Total C N O P 46 36 1 8 1	0
55	I	1	Total C N O P 51 41 1 8 1	0
55	J	1	Total C N O P 46 36 1 8 1	0
55	L	1	Total C N O P 42 32 1 8 1	0
55	L	1	Total C N O P 40 30 1 8 1	0
55	L	1	Total C N O P 51 41 1 8 1	0
55	L	1	Total C N O P 47 37 1 8 1	0
55	L	1	Total C N O P 45 35 1 8 1	0
55	M	1	Total C N O P 51 41 1 8 1	0
55	M	1	Total C N O P 51 41 1 8 1	0
55	M	1	Total C N O P 51 41 1 8 1	0
55	N	1	Total C N O P 37 27 1 8 1	0
55	O	1	Total C N O P 31 21 1 8 1	0
55	Y	1	Total C N O P 40 30 1 8 1	0

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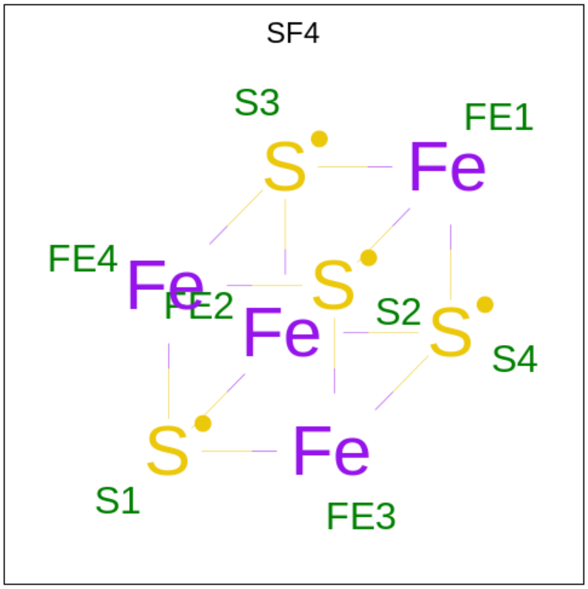
Mol	Chain	Residues	Atoms	AltConf
55	b	1	Total C N O P 46 36 1 8 1	0
55	AC	1	Total C N O P 35 25 1 8 1	0
55	AF	1	Total C N O P 42 32 1 8 1	0
55	Ac	1	Total C N O P 23 13 1 8 1	0
55	Ac	1	Total C N O P 35 25 1 8 1	0
55	Ag	1	Total C N O P 39 29 1 8 1	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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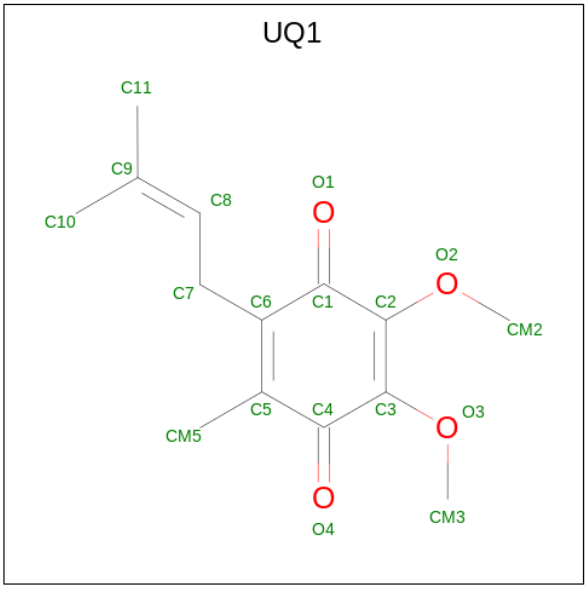
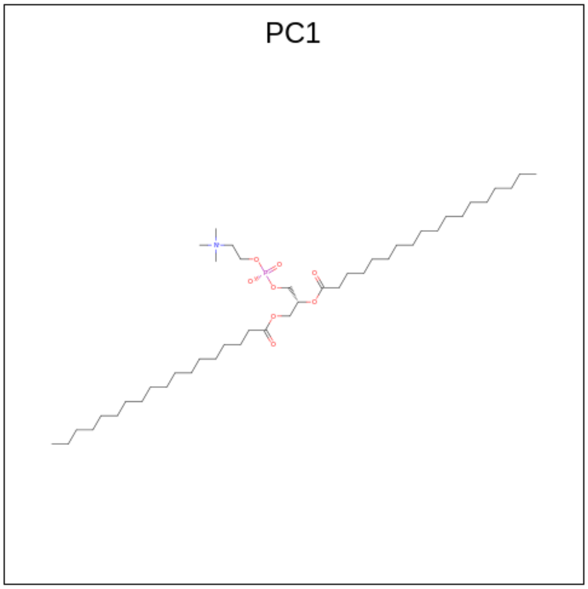
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
56	I	1	8	4	4	0

- Molecule 57 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



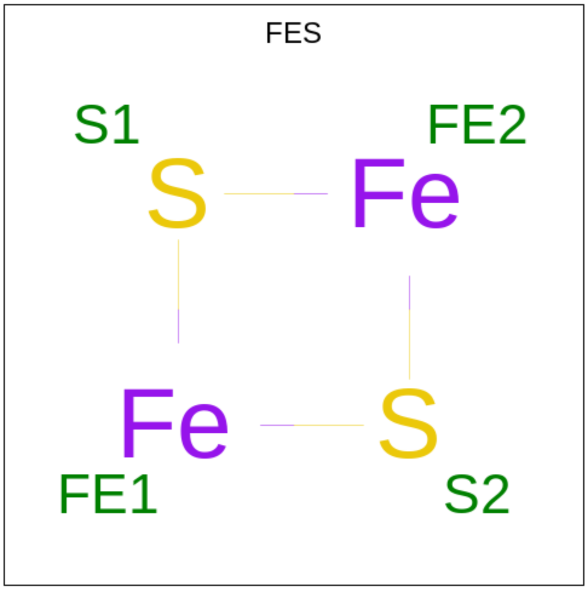
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
57	B	1	18	14	4	0

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



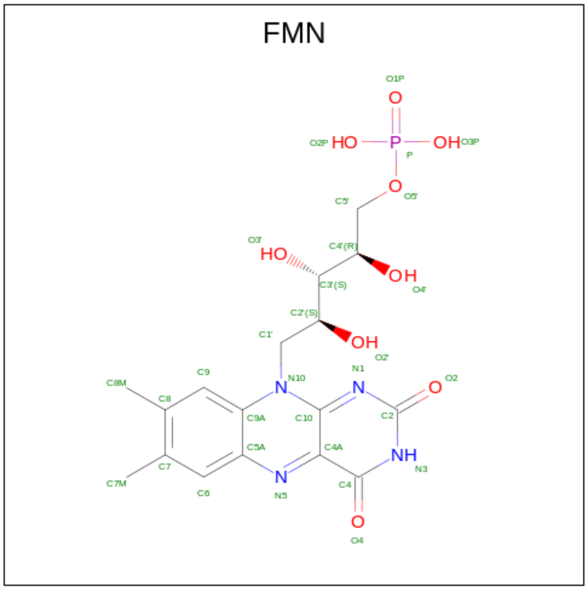
Mol	Chain	Residues	Atoms	AltConf
58	B	1	Total C N O P 35 25 1 8 1	0
58	I	1	Total C N O P 47 37 1 8 1	0
58	J	1	Total C N O P 42 32 1 8 1	0

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



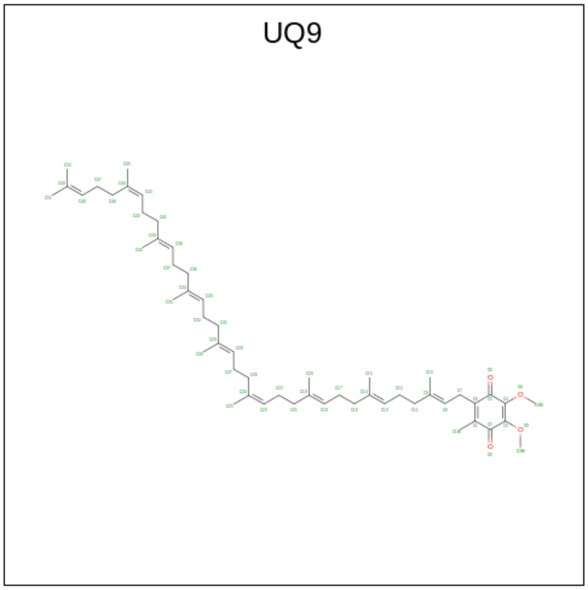
Mol	Chain	Residues	Atoms	AltConf
59	E	1	Total Fe S 4 2 2	0
59	G	1	Total Fe S 4 2 2	0

- Molecule 60 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



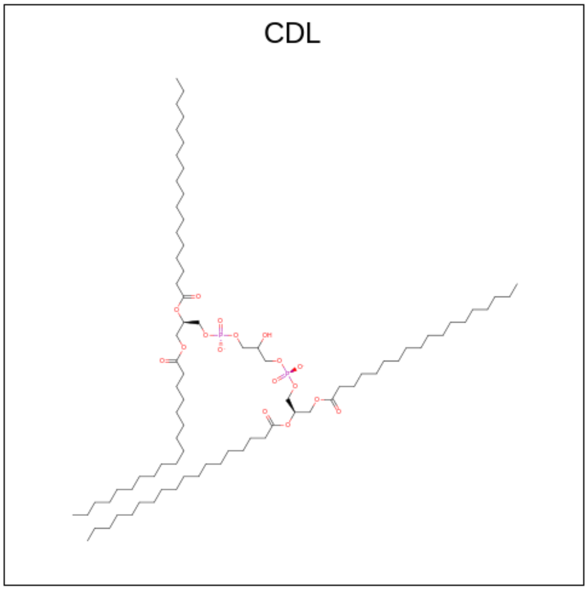
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	F	1	31	17	4	9	1	0

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



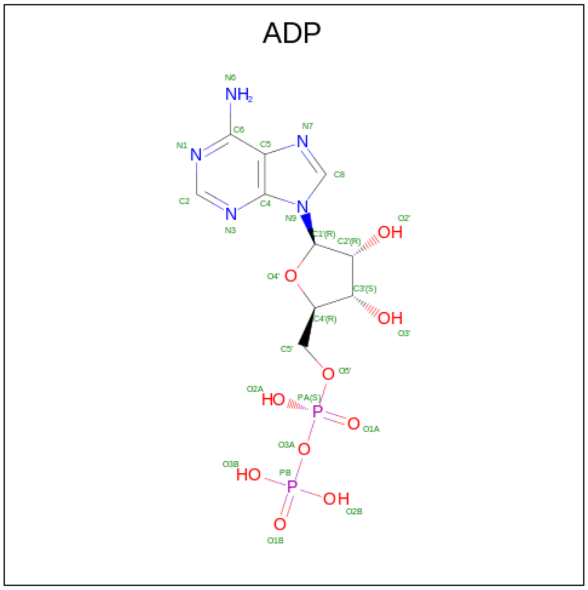
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
61	H	1	35	31	4	0

- Molecule 62 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



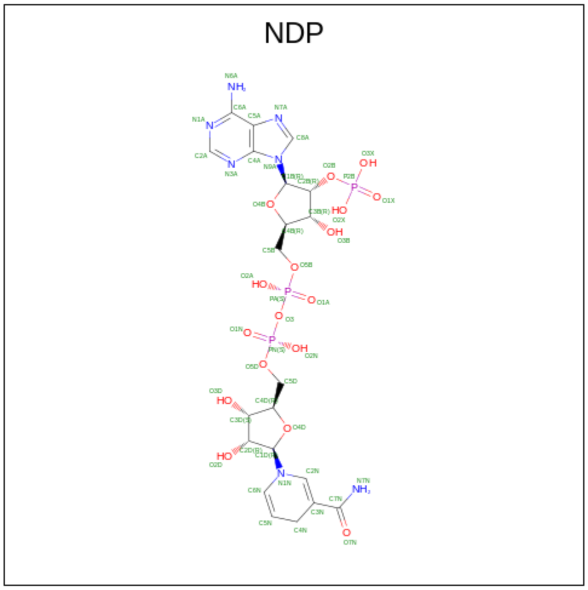
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
62	L	1	77	58	17	2	0
62	L	1	86	67	17	2	0
62	X	1	67	48	17	2	0
62	a	1	57	38	17	2	0
62	h	1	70	51	17	2	0
62	AC	1	56	37	17	2	0
62	Aa	1	46	27	17	2	0
62	Ac	1	42	23	17	2	0
62	Ag	1	56	37	17	2	0

- Molecule 63 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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 (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

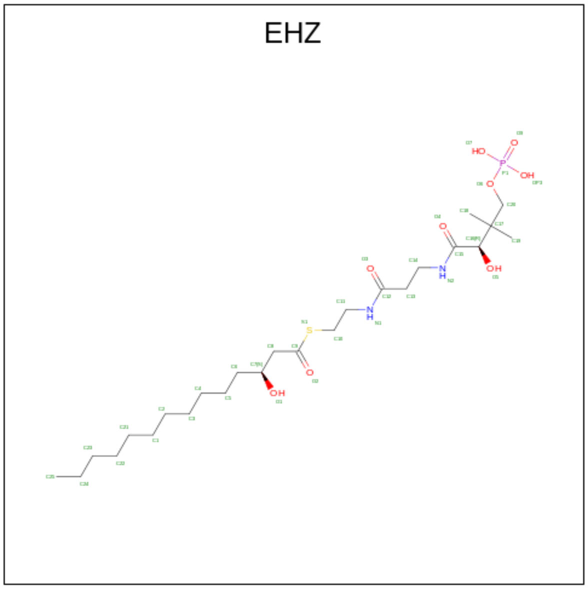


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	P	1	48	21	7	17	3	0

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

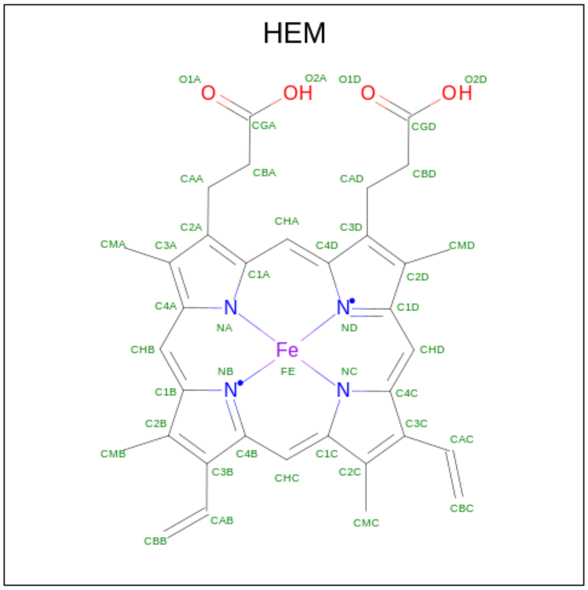
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
65	R	1	1	1	0

- Molecule 66 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



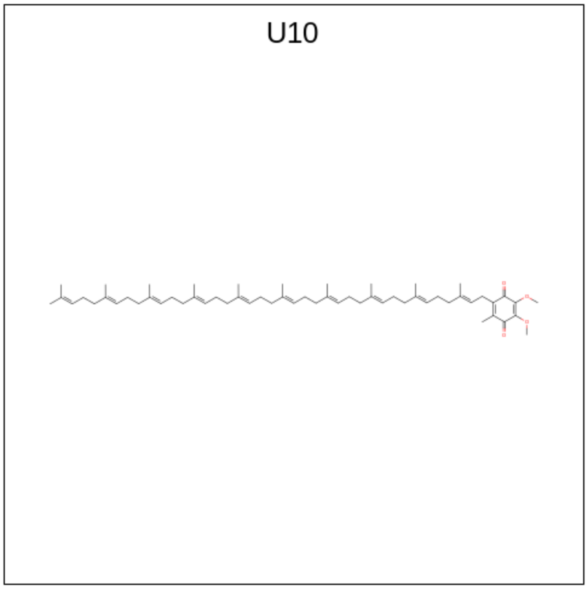
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
66	W	1	32	19	2	9	1	1	0
			Total	C	N	O	P	S	
66	n	1	32	19	2	9	1	1	0

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



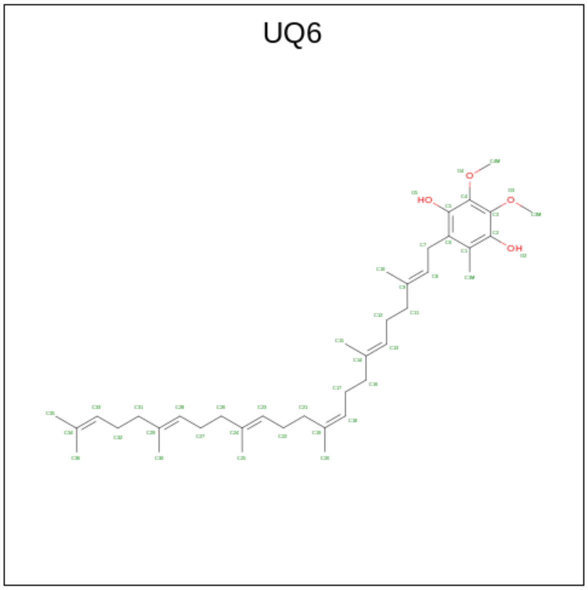
Mol	Chain	Residues	Atoms	AltConf
67	AC	1	Total C Fe N O 43 34 1 4 4	0
67	AC	1	Total C Fe N O 43 34 1 4 4	0
67	Ac	1	Total C Fe N O 43 34 1 4 4	0
67	Ac	1	Total C Fe N O 43 34 1 4 4	0

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



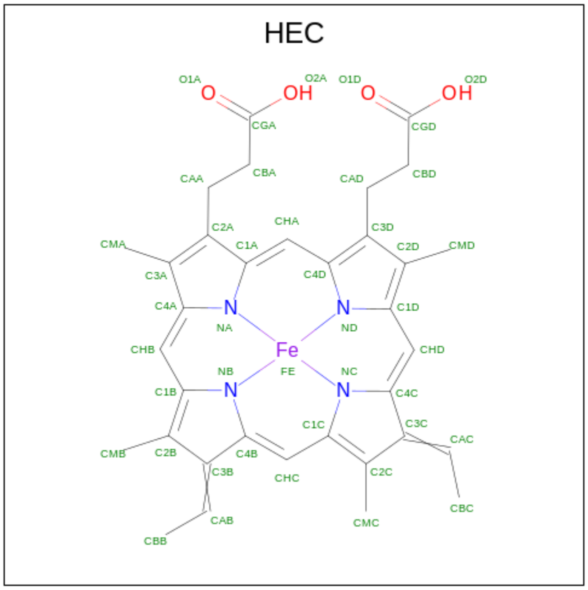
Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			23	19	4	
68	Ac	1	Total	C	O	0
			38	34	4	

- 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 (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



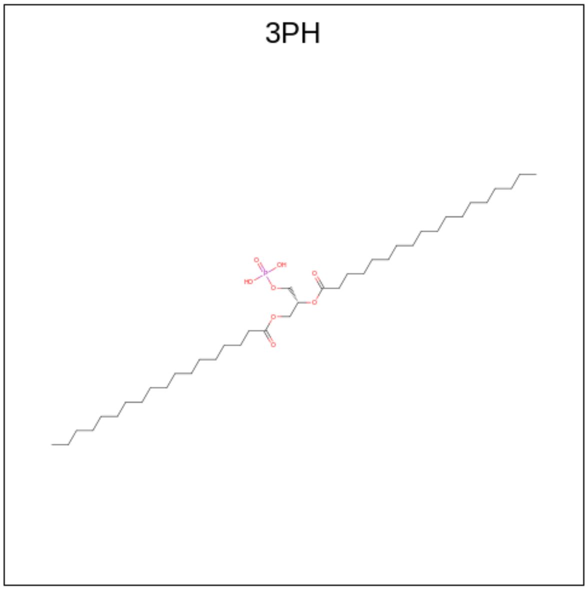
Mol	Chain	Residues	Atoms			AltConf
69	AC	1	Total	C	O	0
			28	24	4	
69	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 70 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 71 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms	AltConf
71	AD	1	Total C O P 36 27 8 1	0

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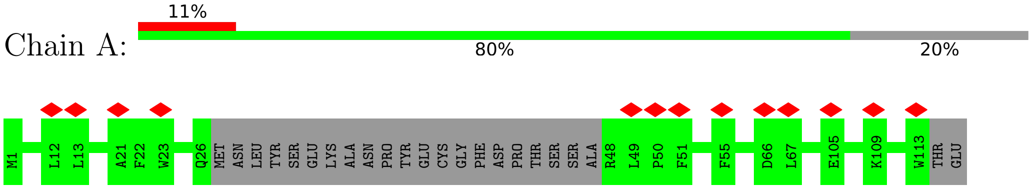
Mol	Chain	Residues	Atoms	AltConf
71	Ad	1	Total C O P 36 27 8 1	0

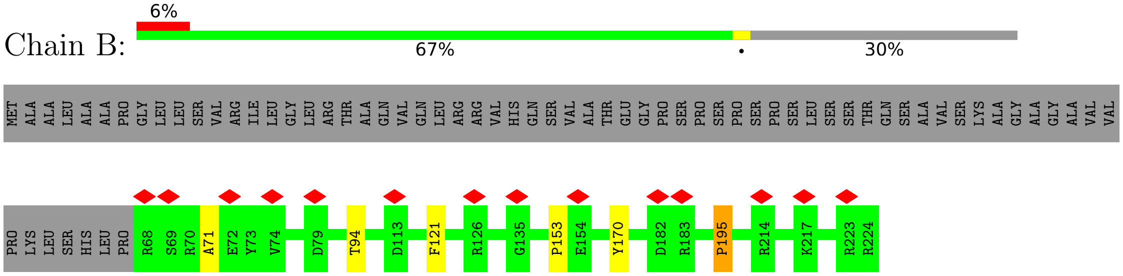
3 Residue-property plots ⓘ

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

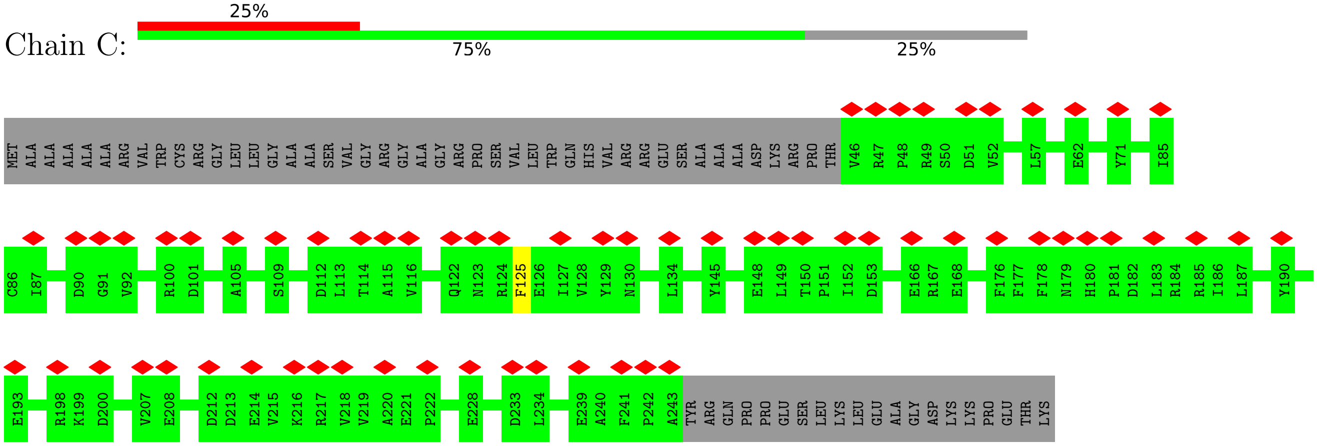
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



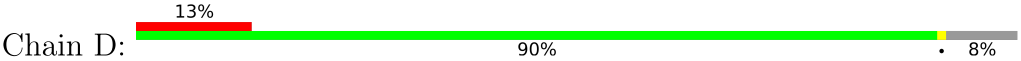
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

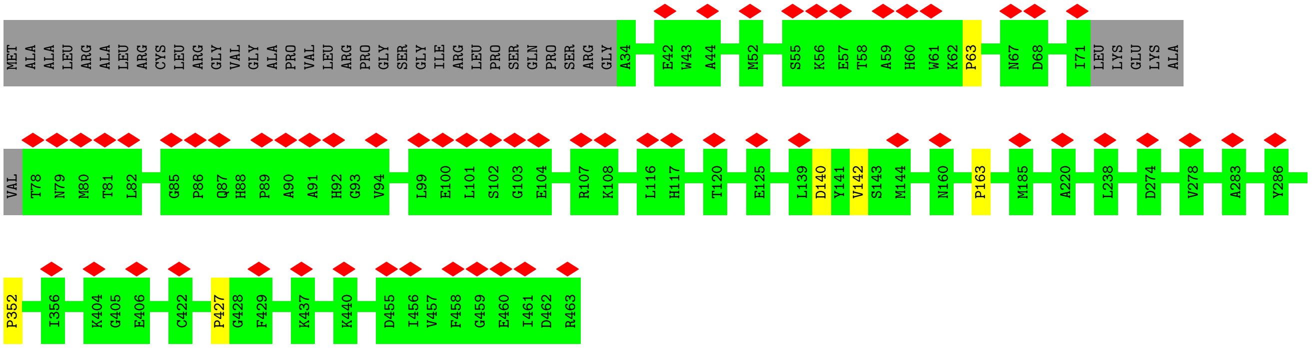


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



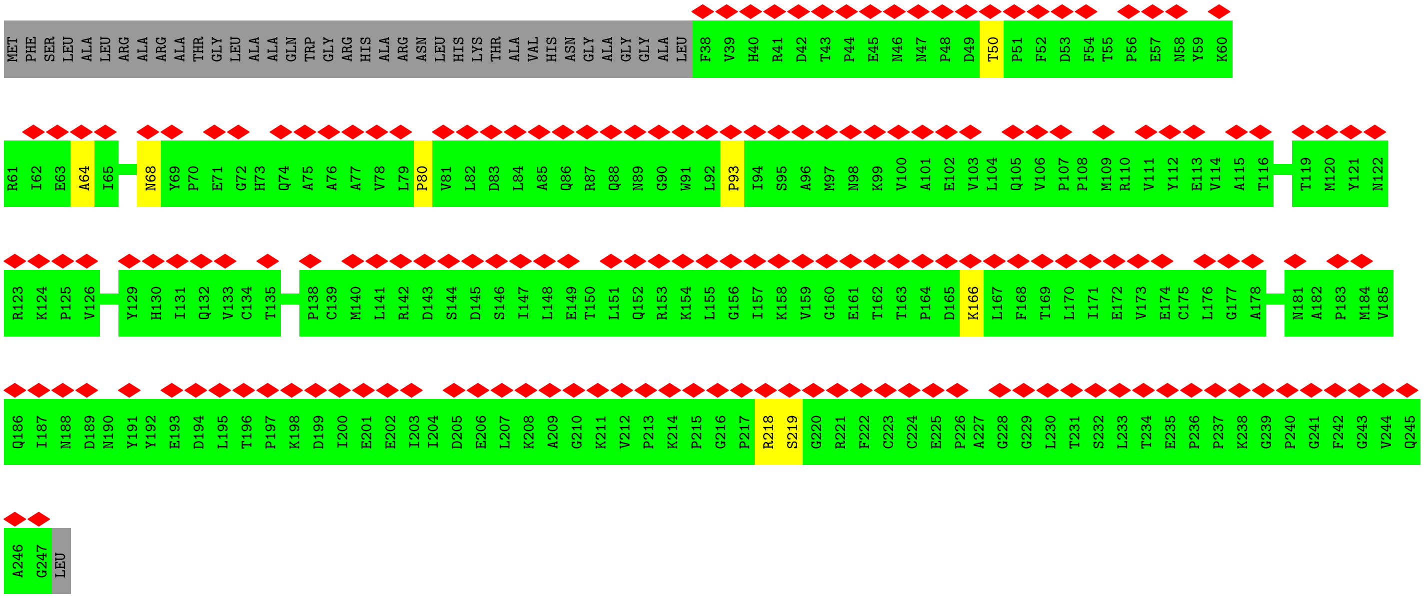
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





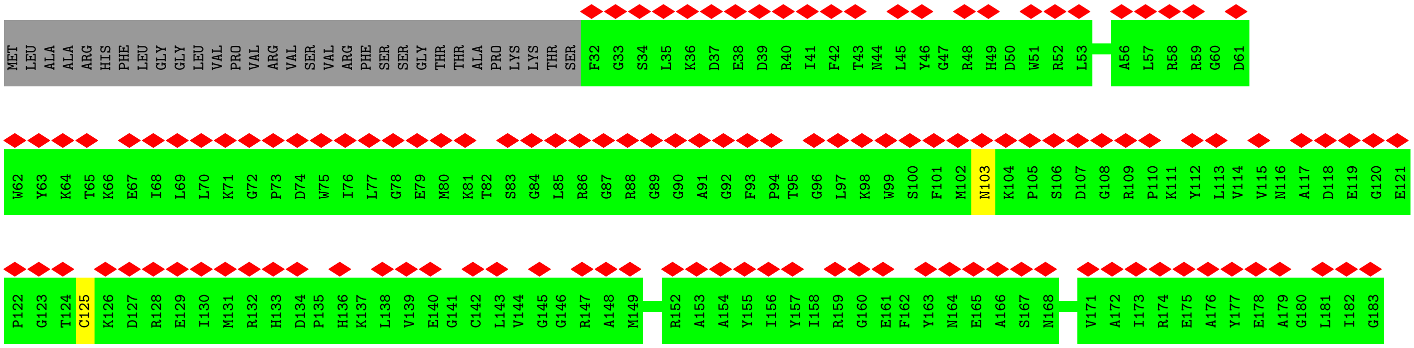
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

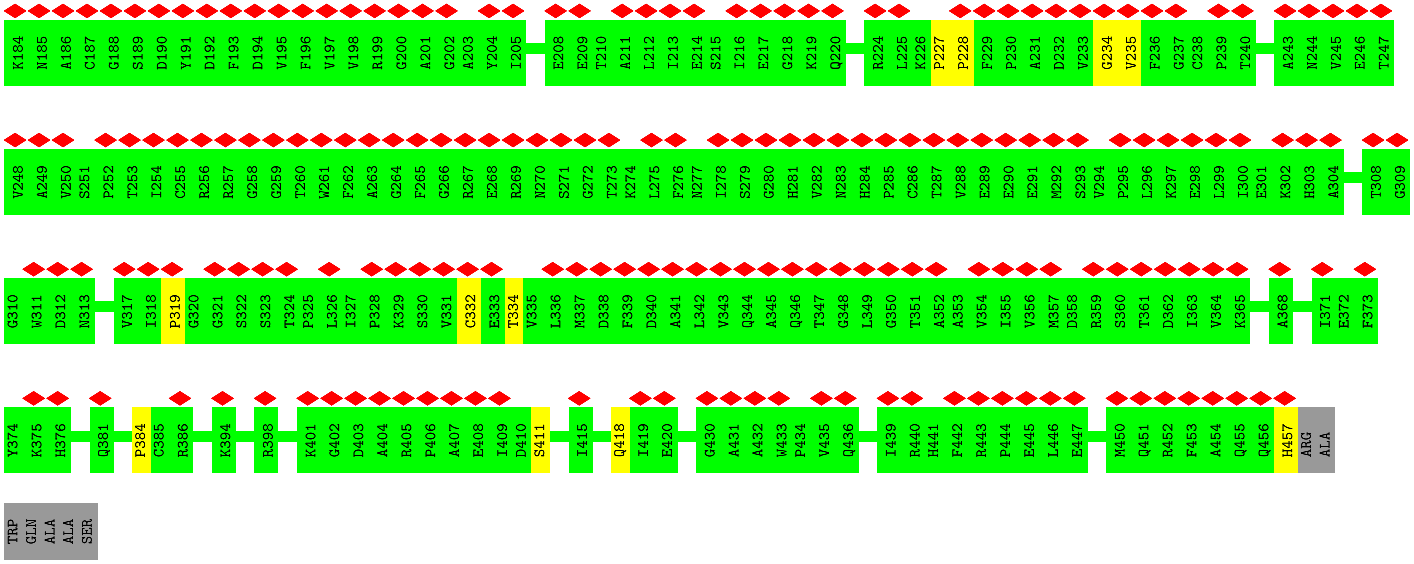
Chain E:



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

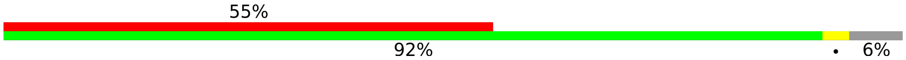
Chain F:

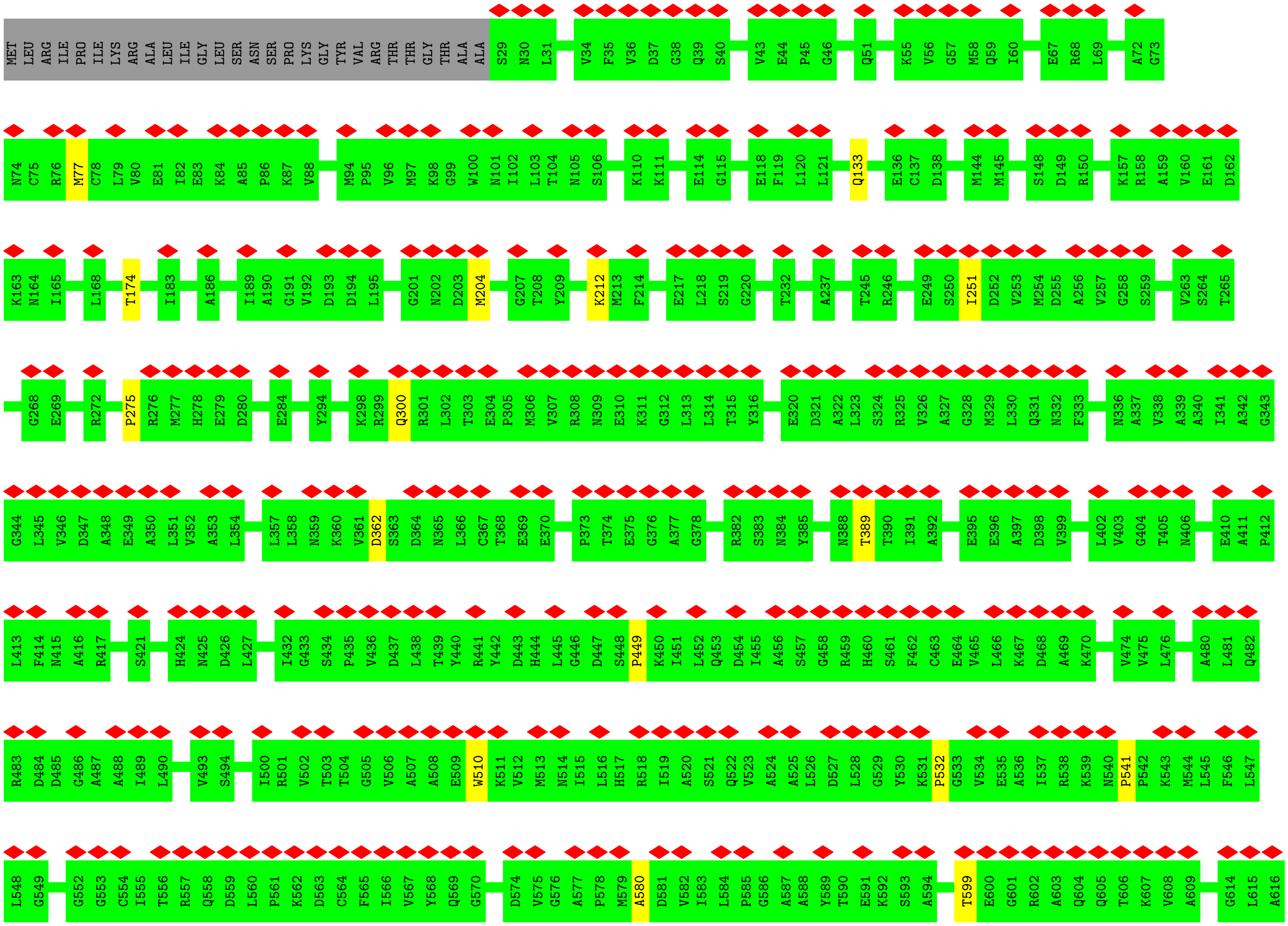


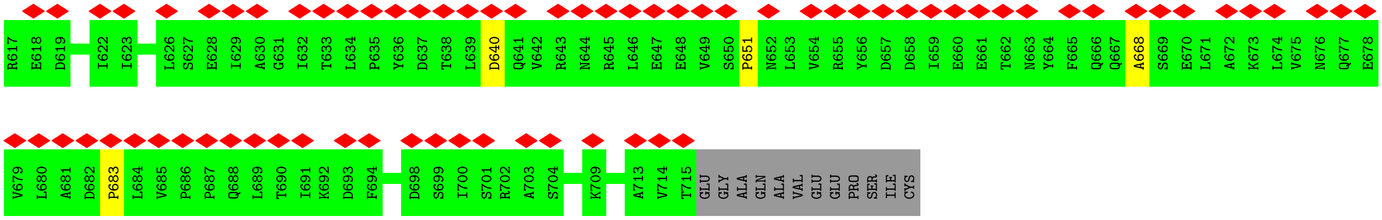


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:

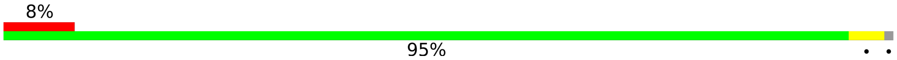


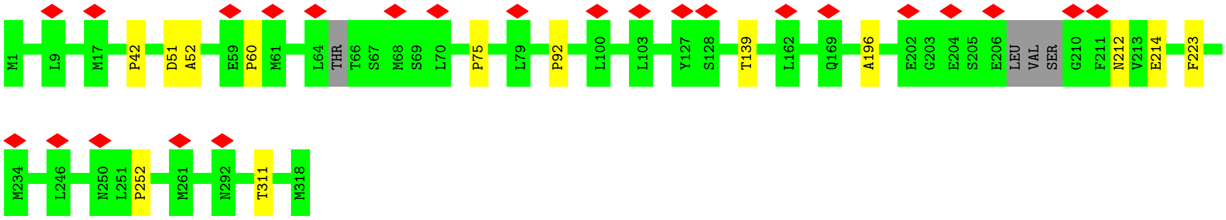




- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

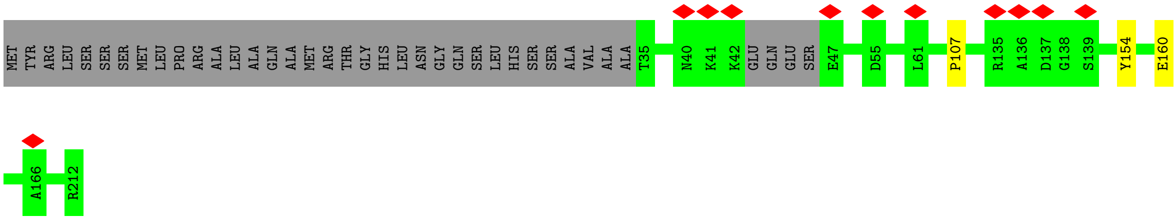
Chain H:





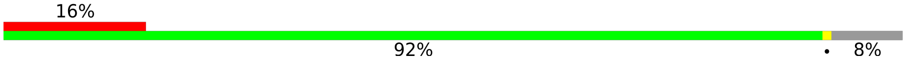
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

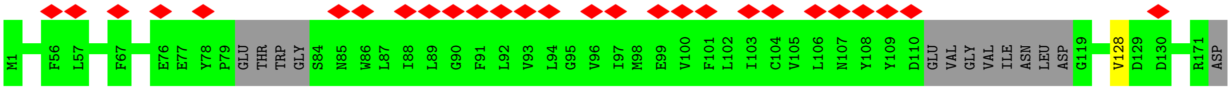
Chain I:



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

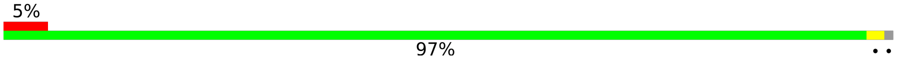
Chain J:

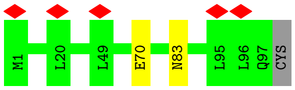




- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

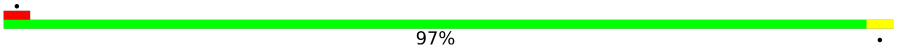
Chain K:

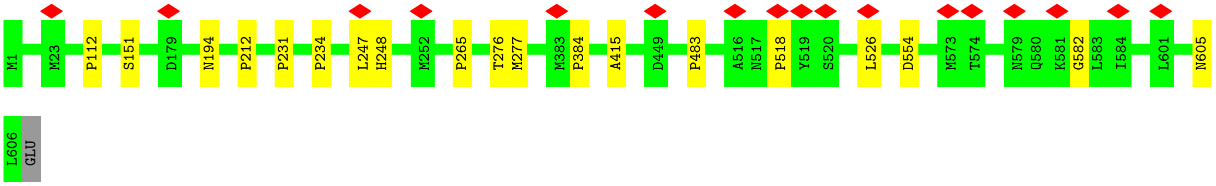




- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

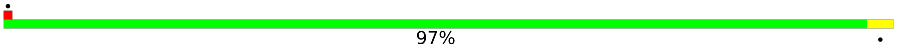
Chain L:

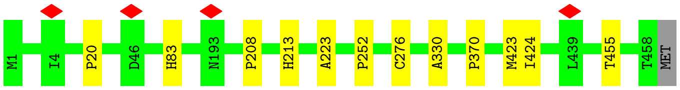




- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

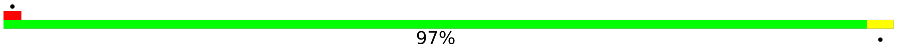
Chain M:

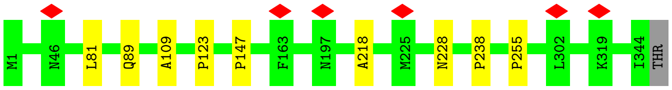




- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

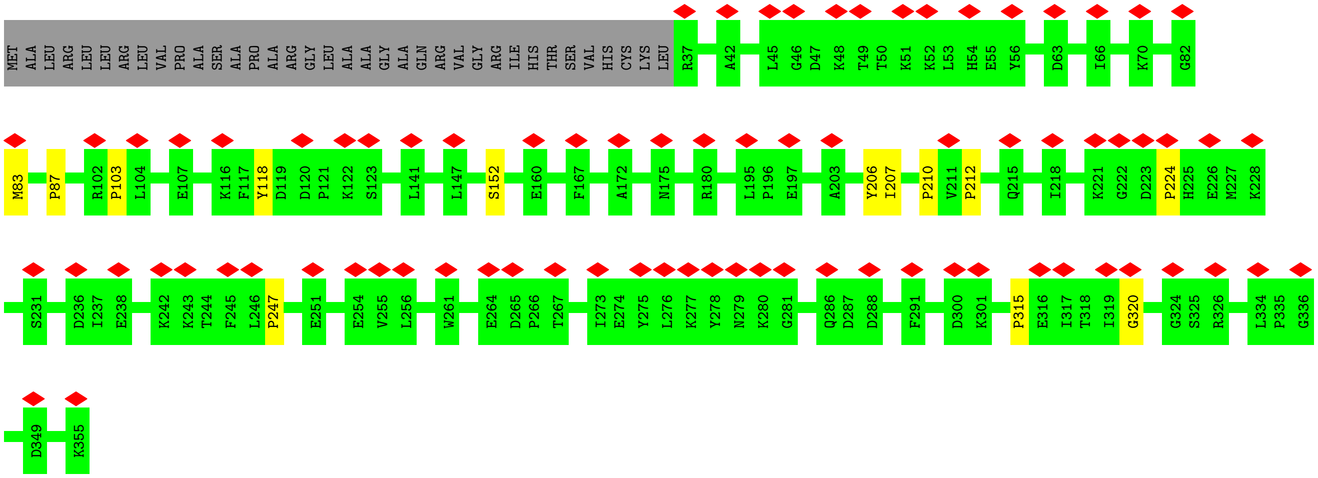
Chain N:





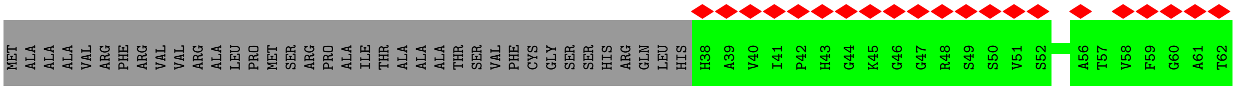
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

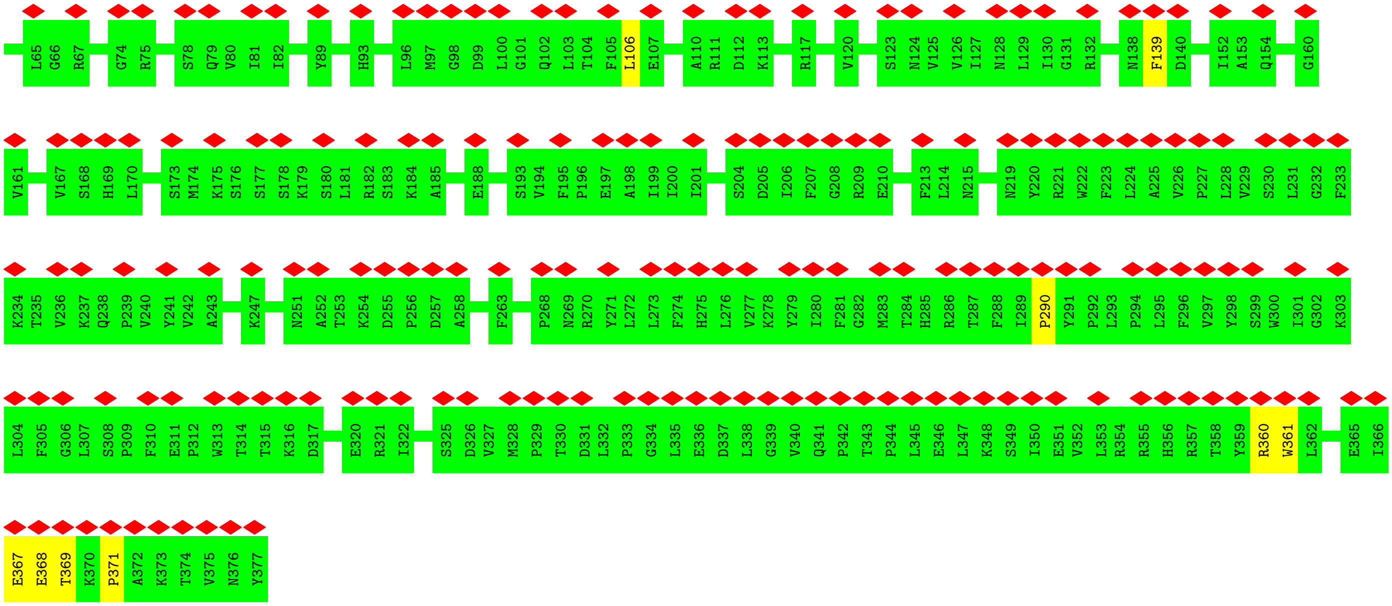
Chain O:



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

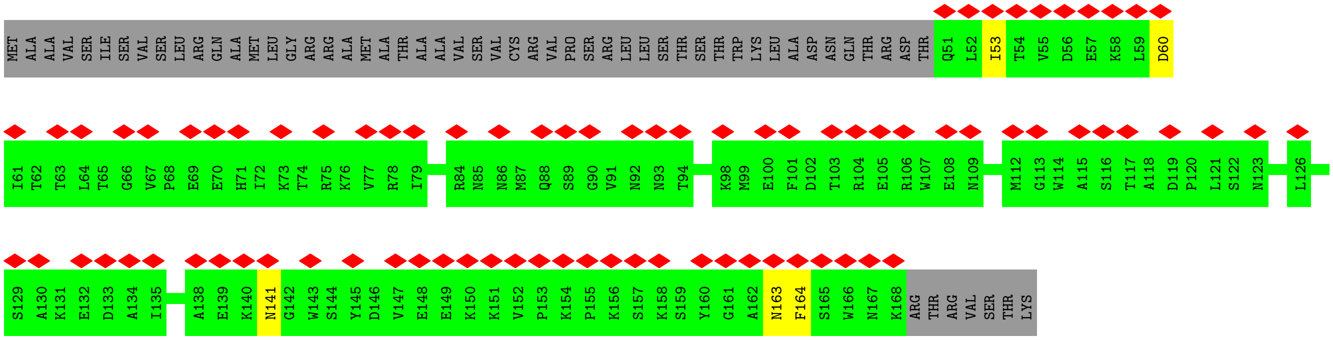
Chain P:





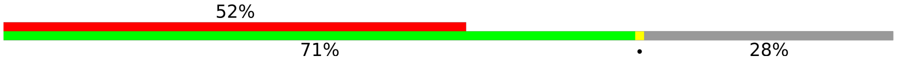
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

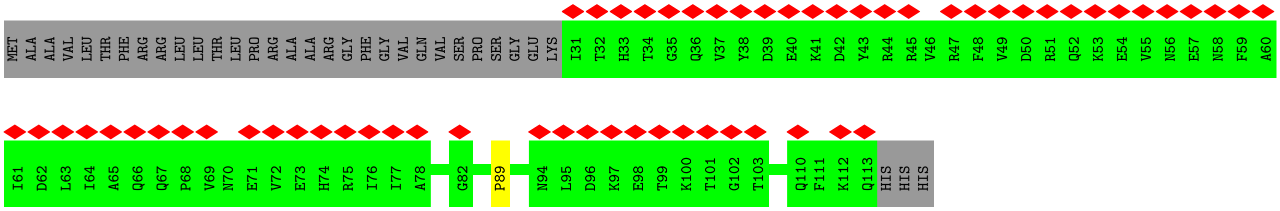
Chain Q:



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

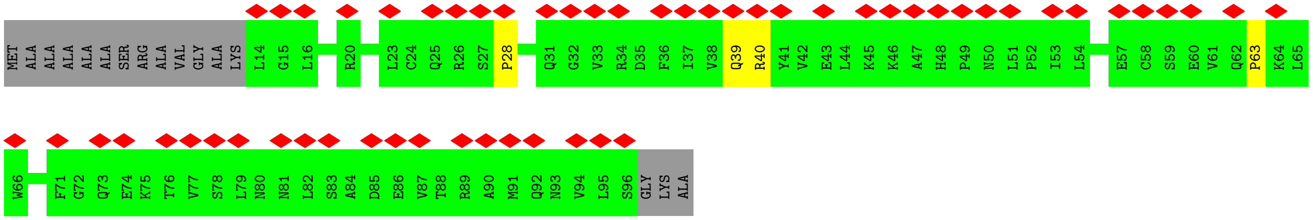
Chain R:



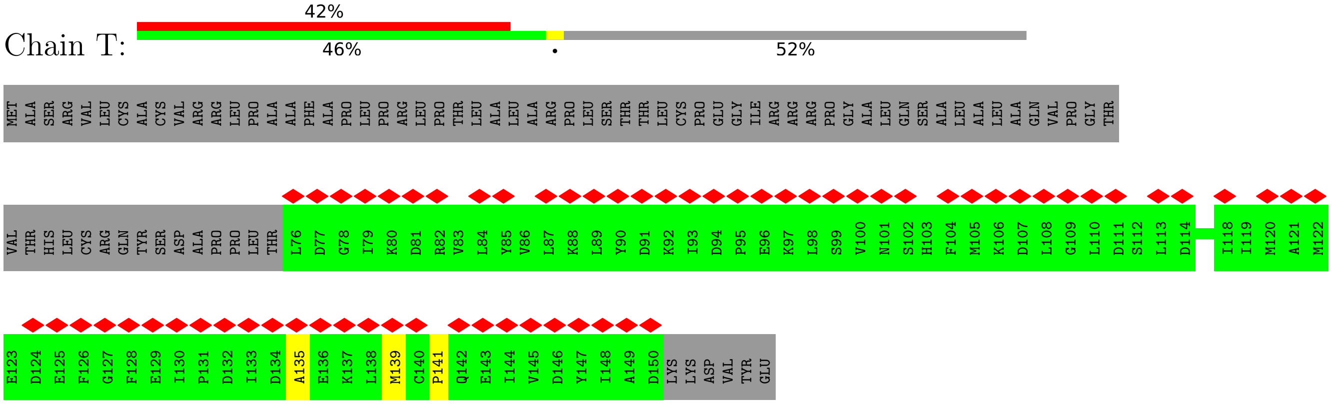


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

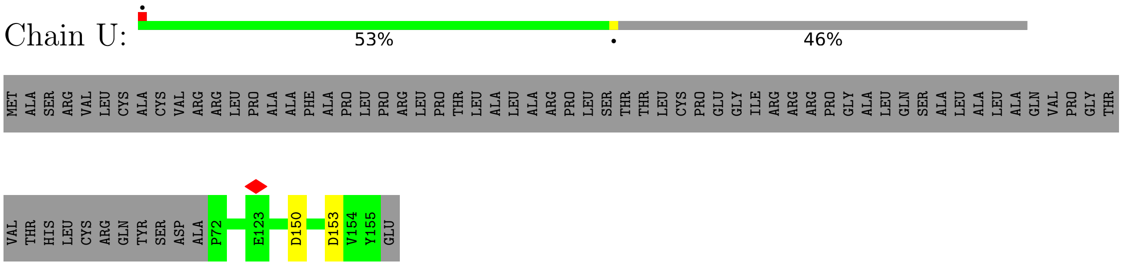
Chain S:



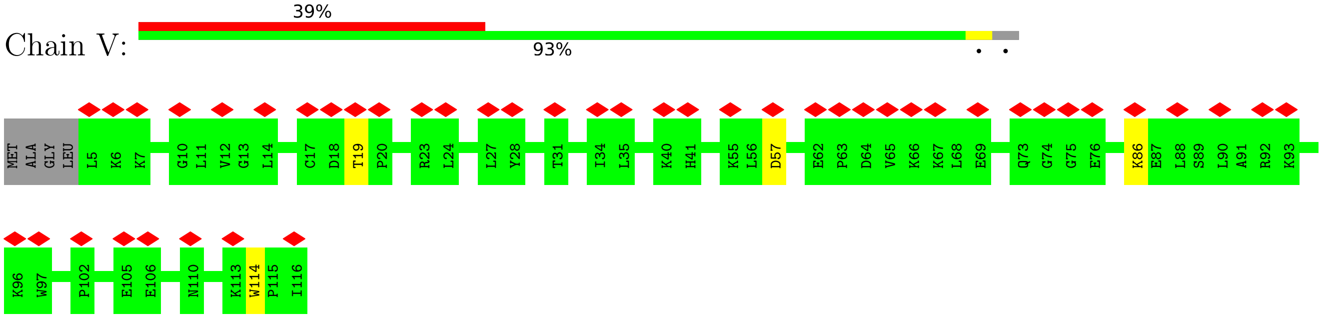
- Molecule 20: Acyl carrier protein, mitochondrial



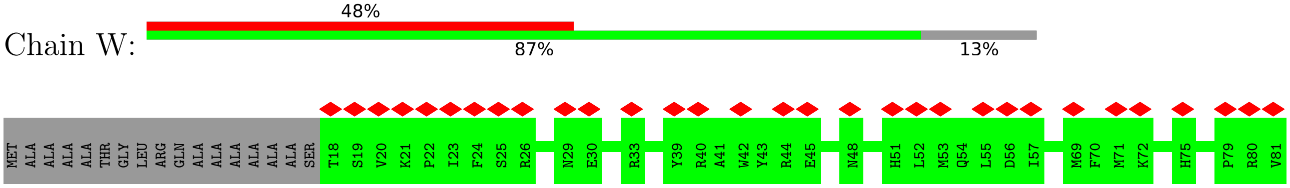
- Molecule 20: Acyl carrier protein, mitochondrial

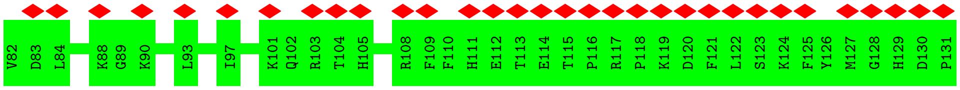


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



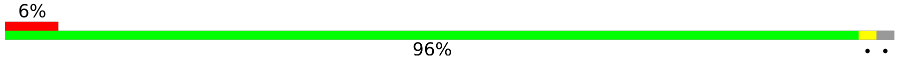
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

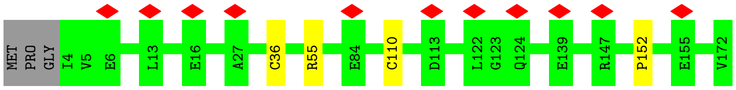




- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

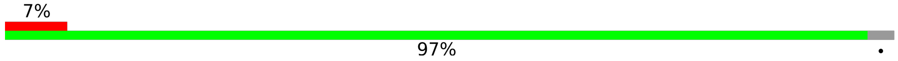
Chain X:

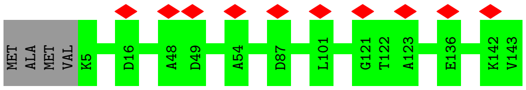




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

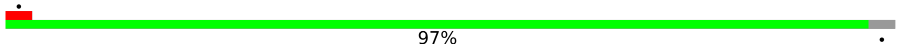
Chain Y:

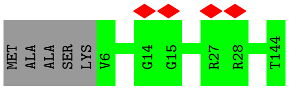




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

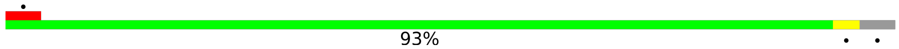
Chain Z:

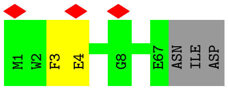




- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

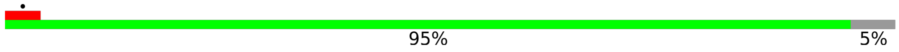
Chain a:

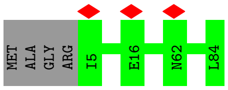




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

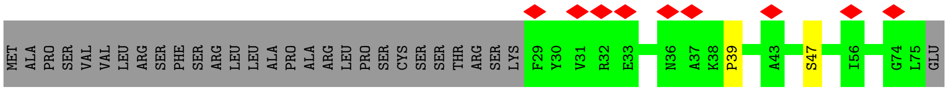
Chain b:





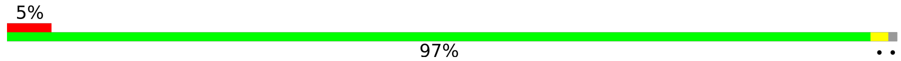
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

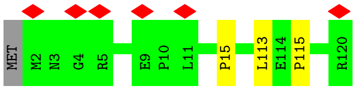
Chain c:



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

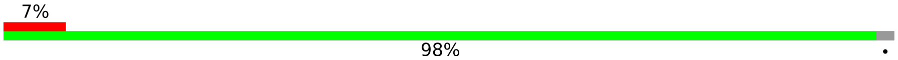
Chain d:

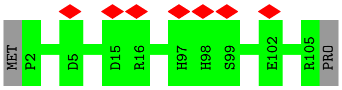




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

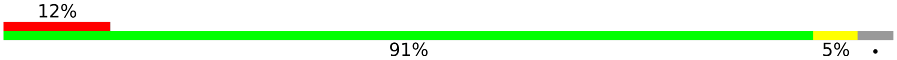
Chain e:

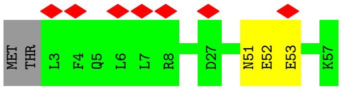




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

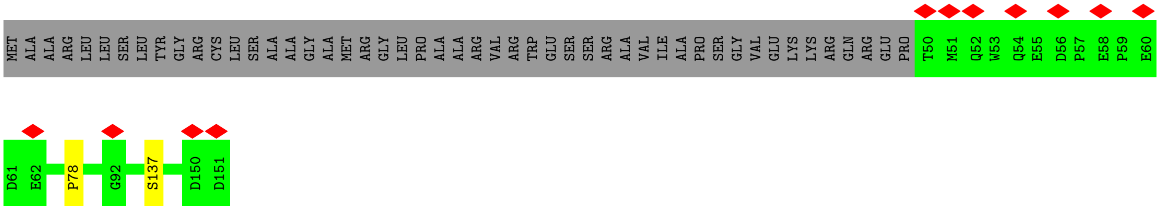
Chain f:





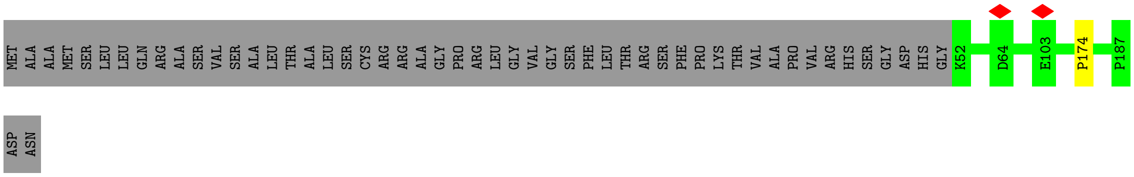
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



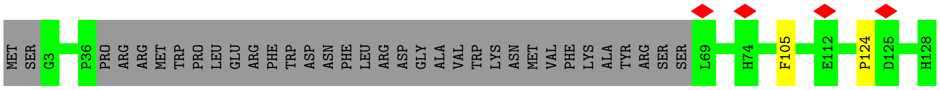
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



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

Chain i:

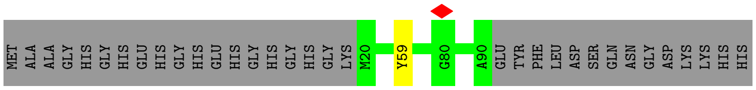


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:

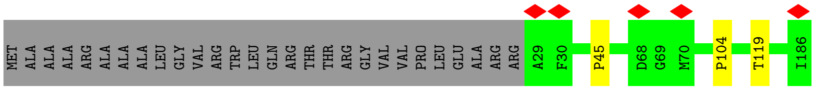
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



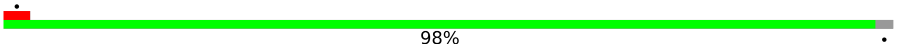
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

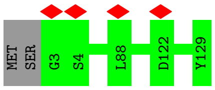
Chain l:



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

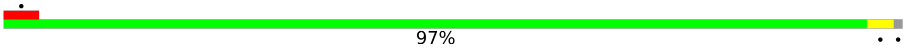
Chain m:

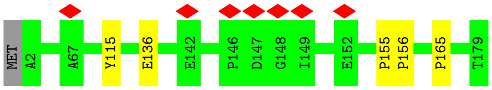




- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

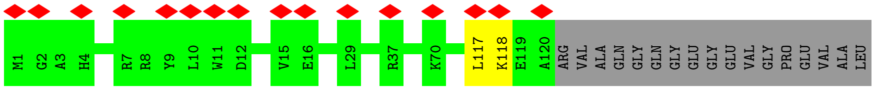
Chain n:



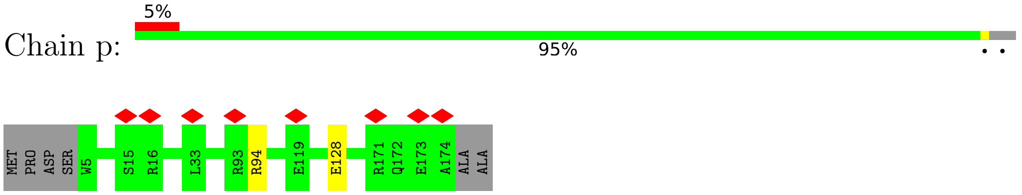


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

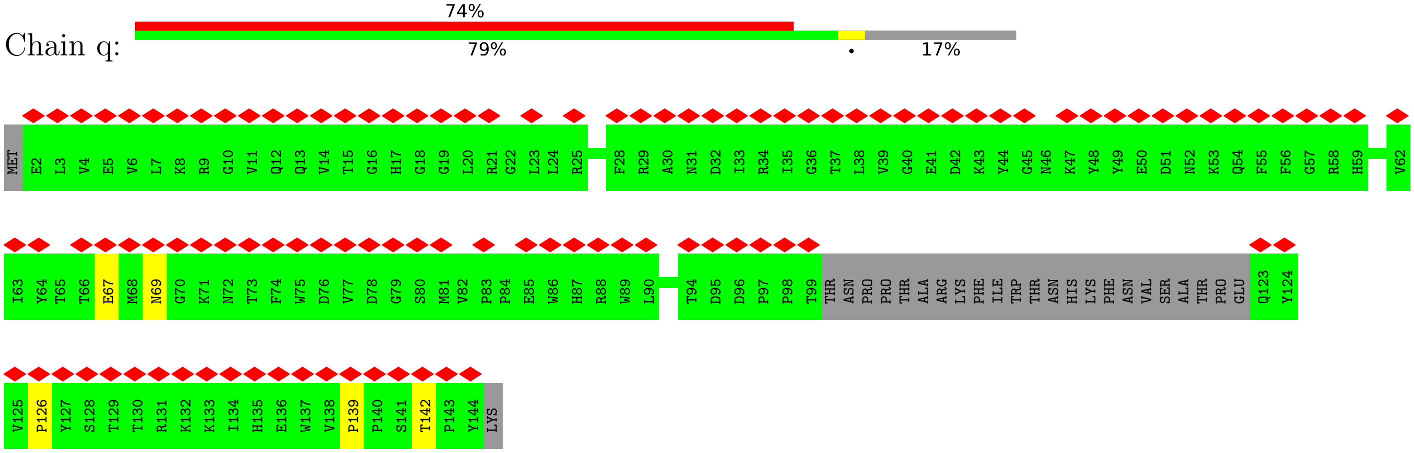
Chain o:



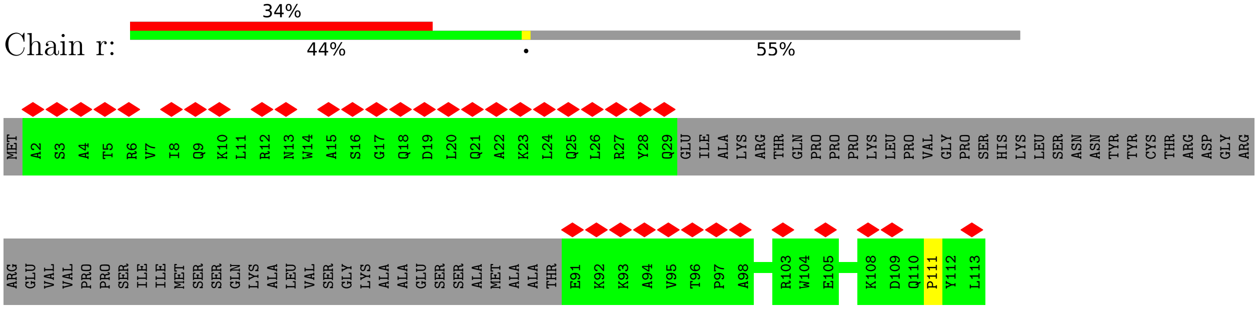
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



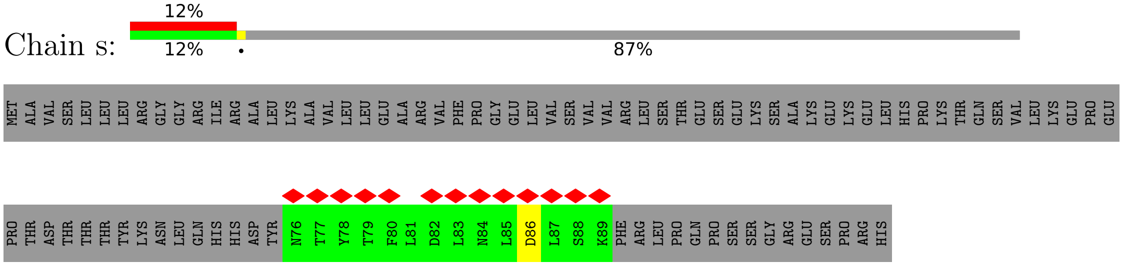
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



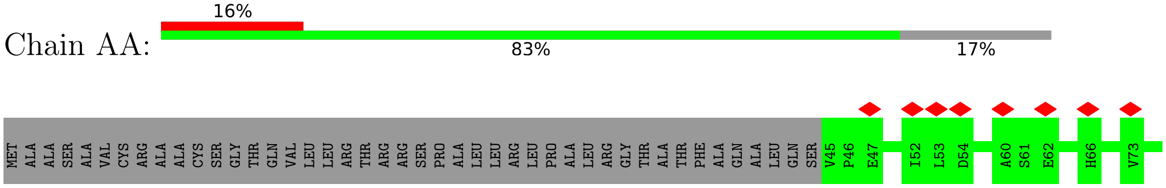
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

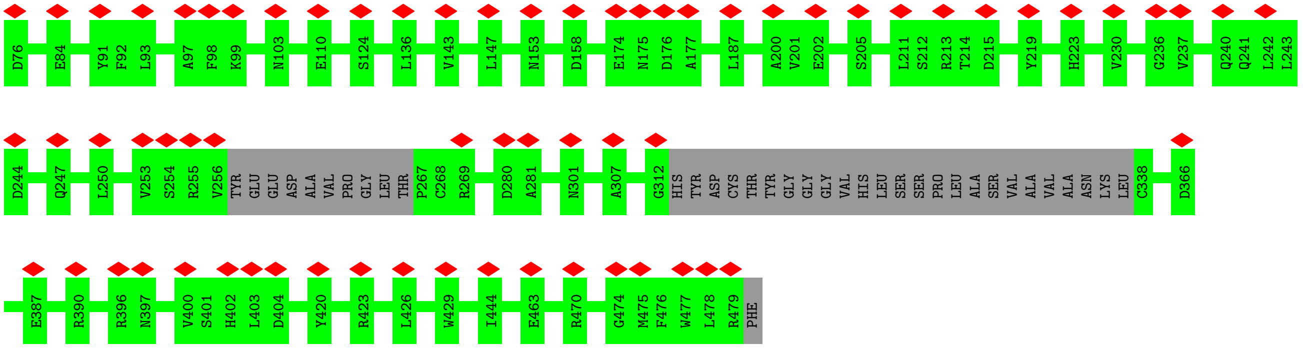


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



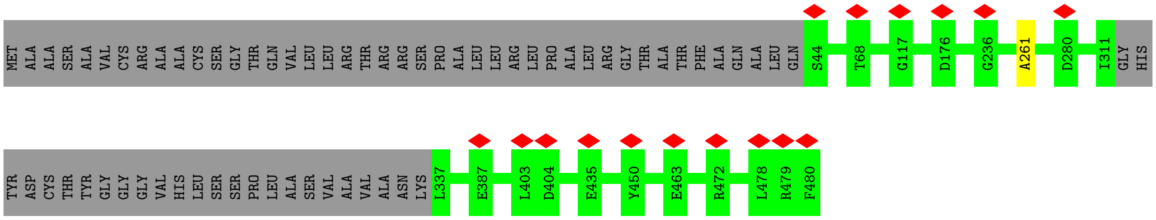
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial





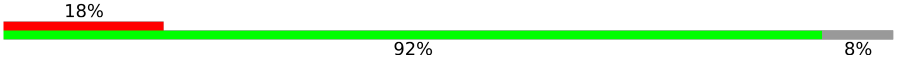
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

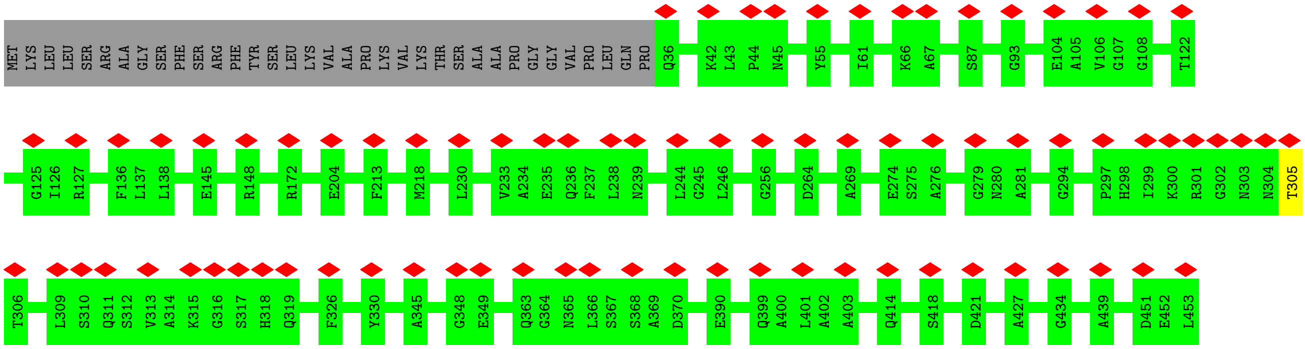
Chain Aa:



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

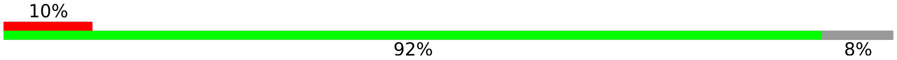
Chain AB:

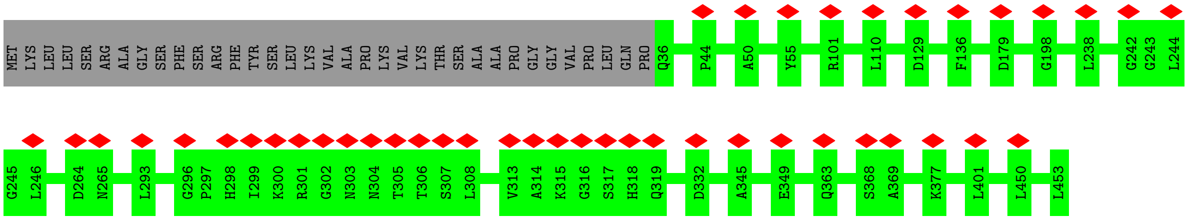




- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

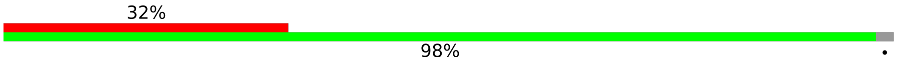
Chain Ab:

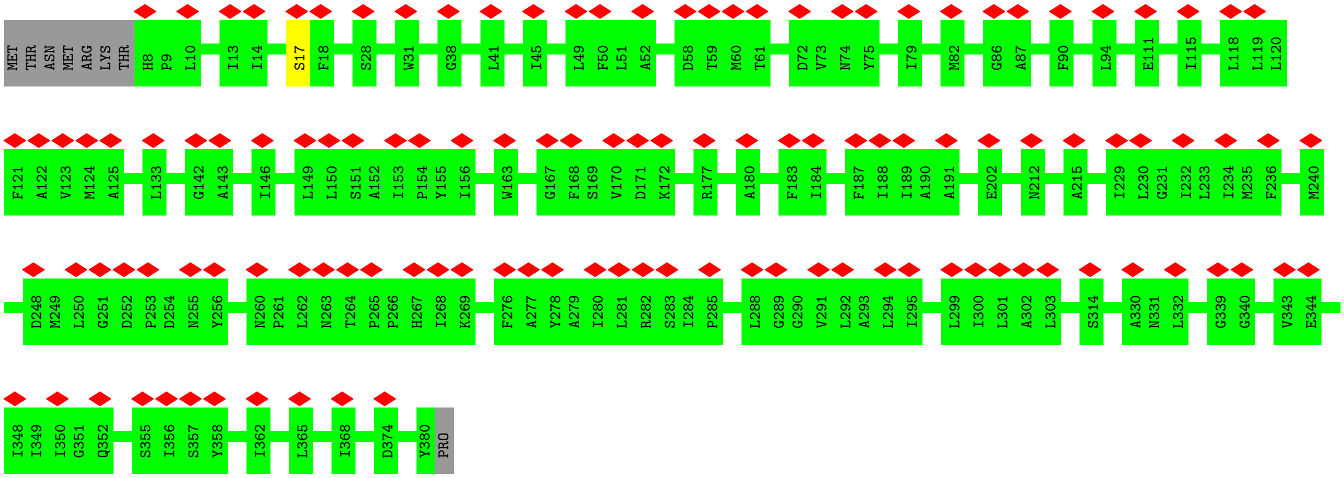




- Molecule 47: Cytochrome b

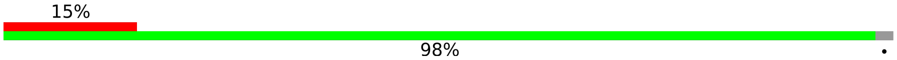
Chain AC:

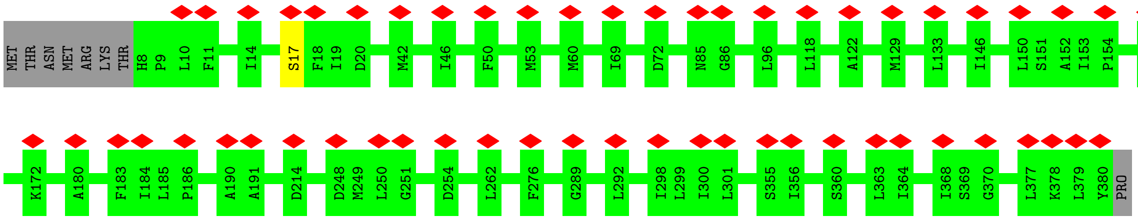




- Molecule 47: Cytochrome b

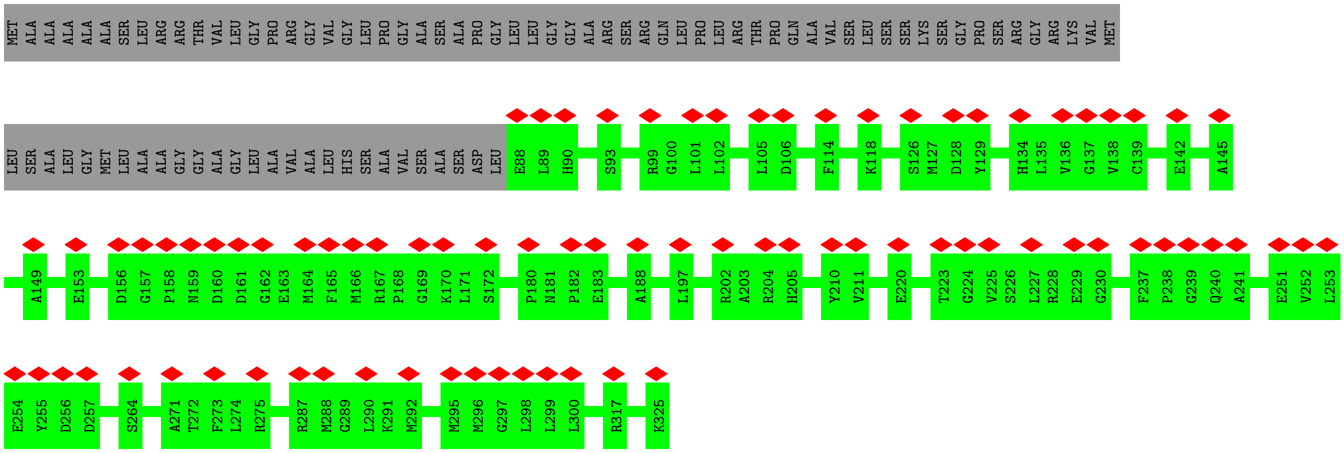
Chain Ac:





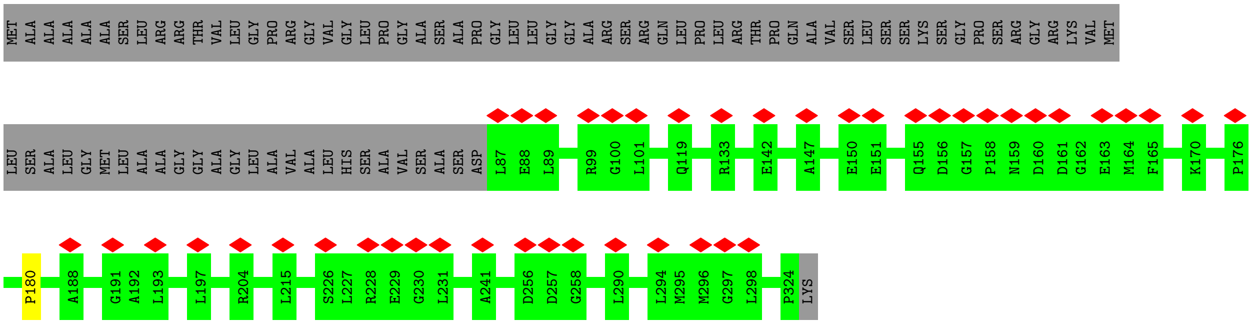
- Molecule 48: Cytochrome c1, heme protein, mitochondrial

Chain AD:



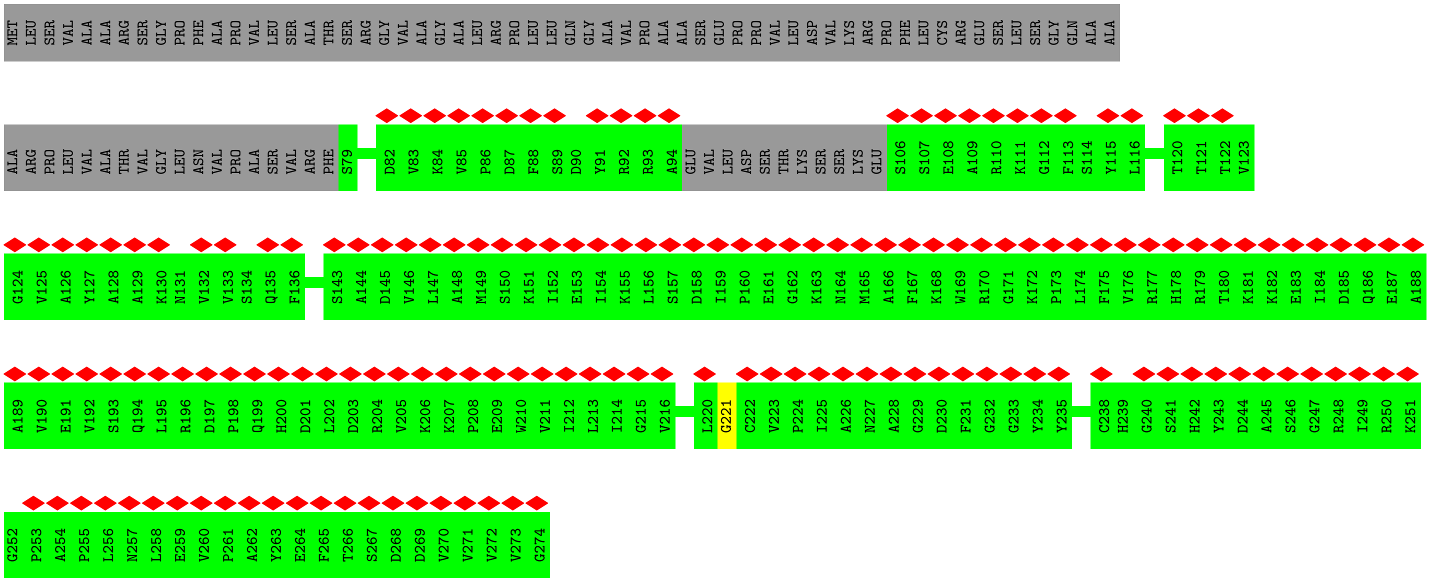
- Molecule 48: Cytochrome c1, heme protein, mitochondrial

Chain Ad:



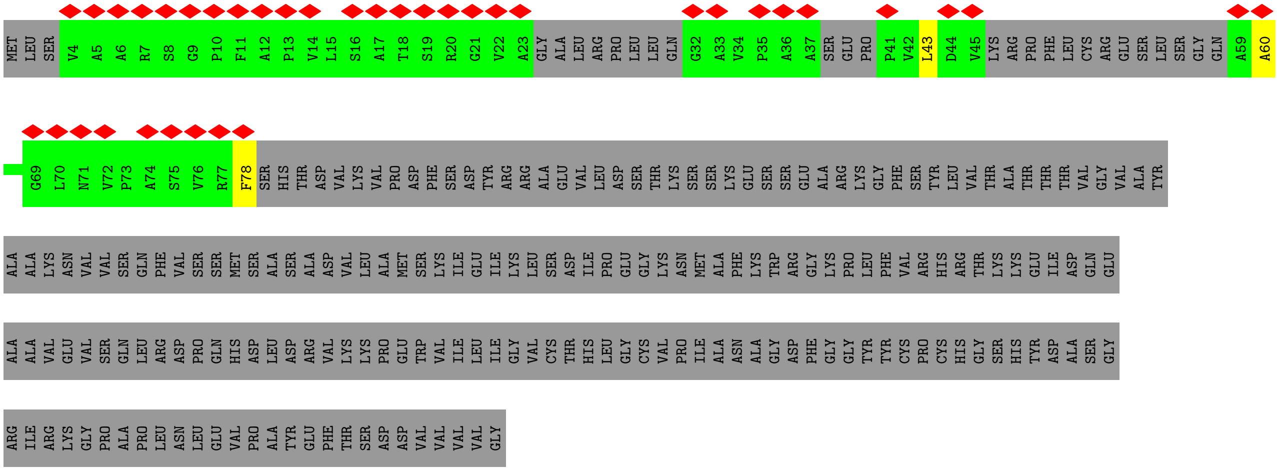
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE:

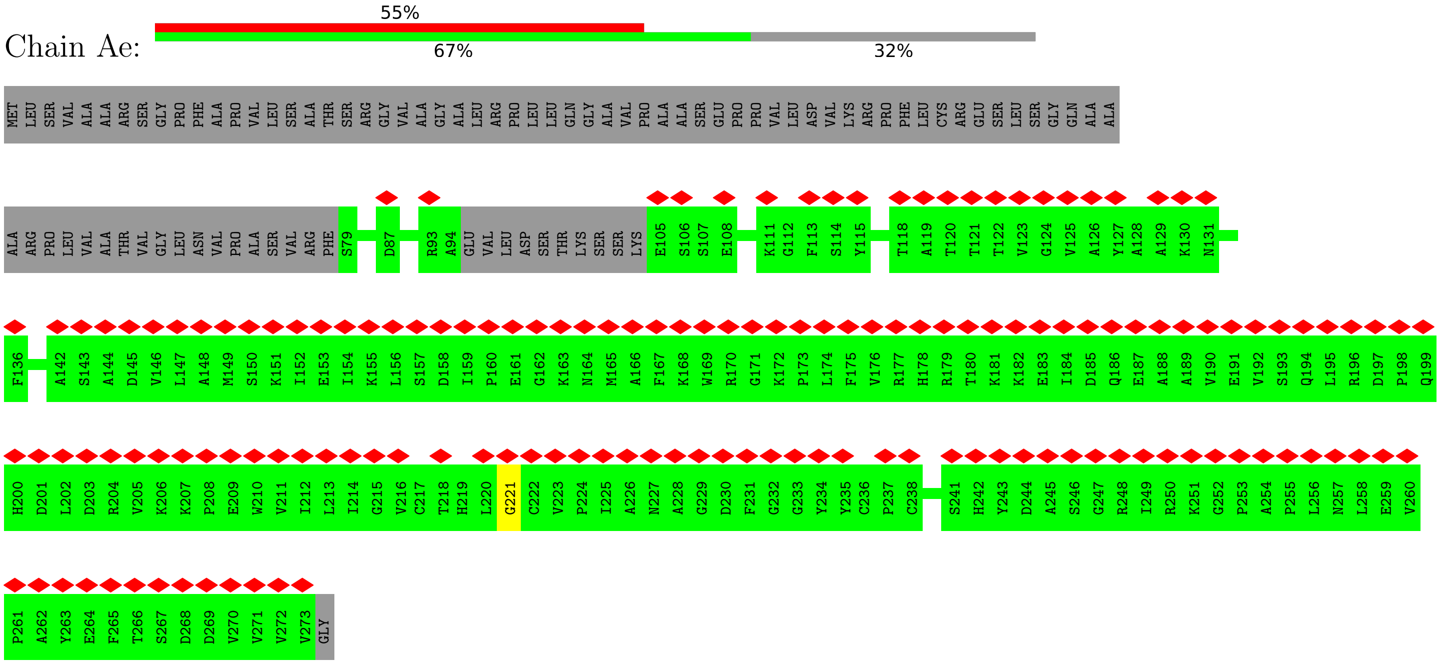


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

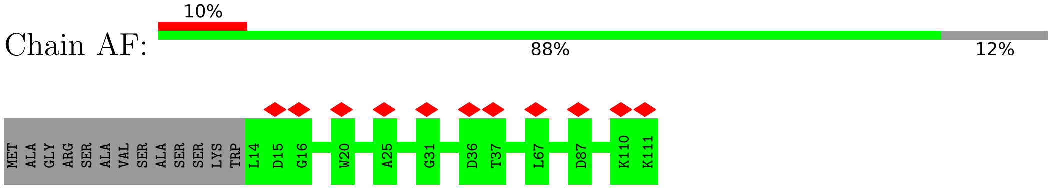
Chain AI:



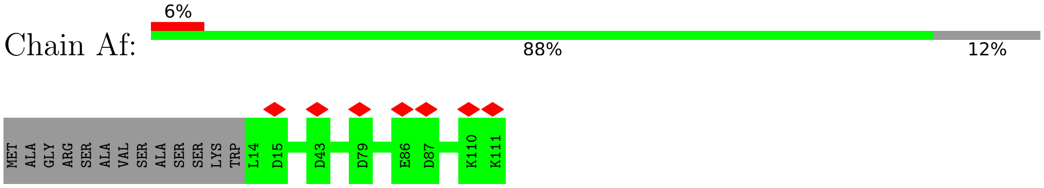
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



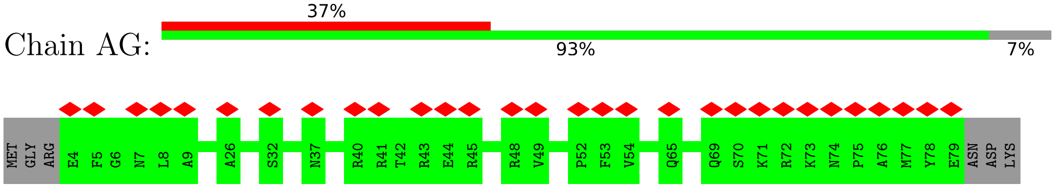
- Molecule 50: Cytochrome b-c1 complex subunit 7



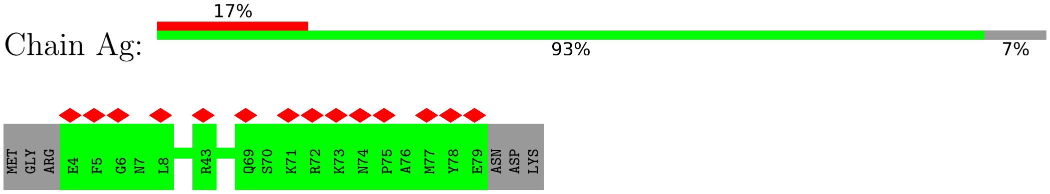
- Molecule 50: Cytochrome b-c1 complex subunit 7



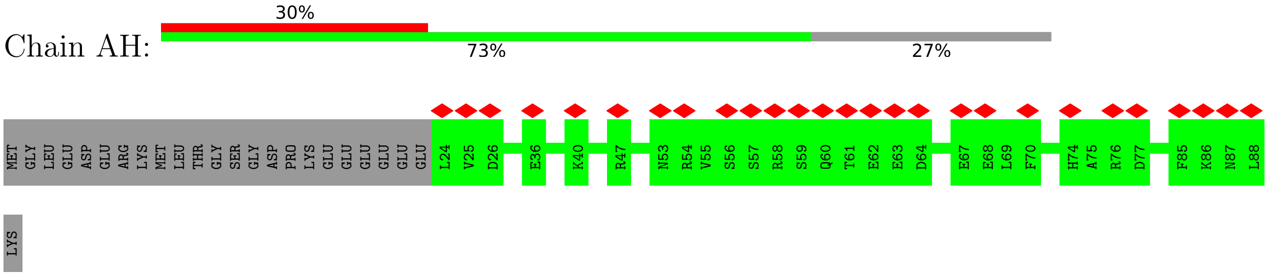
- Molecule 51: Cytochrome b-c1 complex subunit 8



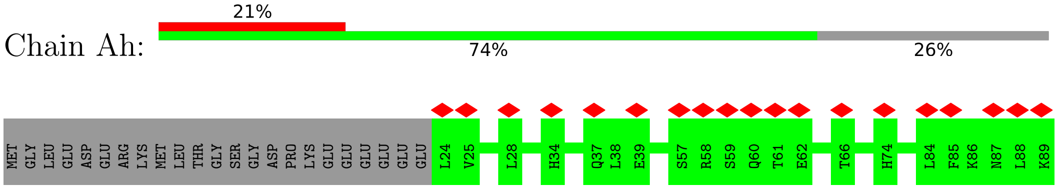
- Molecule 51: Cytochrome b-c1 complex subunit 8



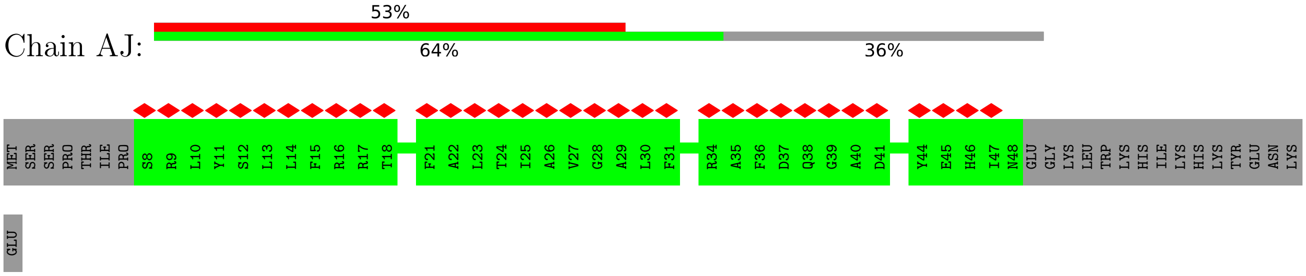
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



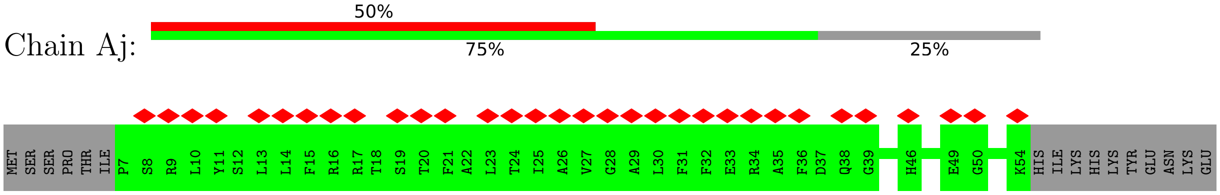
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



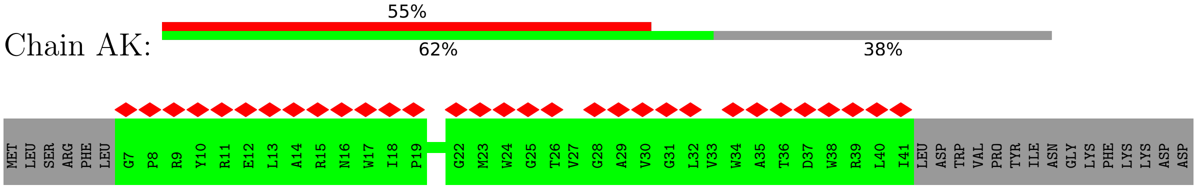
- Molecule 53: Cytochrome b-c1 complex subunit 9



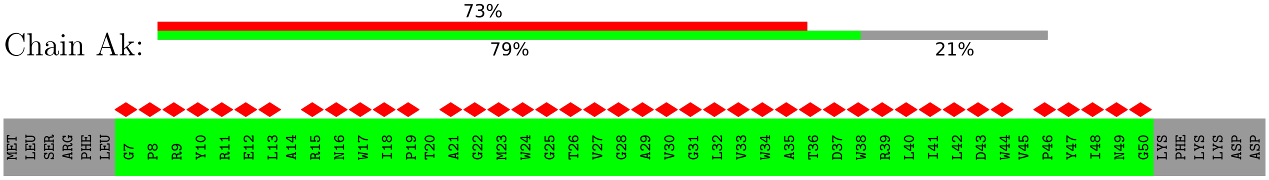
- Molecule 53: Cytochrome b-c1 complex subunit 9



- Molecule 54: Cytochrome b-c1 complex subunit 10



- Molecule 54: Cytochrome b-c1 complex subunit 10



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49613	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 $(e^-/\text{Å}^2)$	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	0.080	Depositor
Minimum map value	-0.033	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PH, HEC, UQ1, SF4, FES, UQ6, ADP, U10, FMN, EHZ, HEM, 3PE, ZN, NDP, PC1, 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	0.54	0/774	0.79	0/1056
2	B	0.63	0/1289	0.94	5/1744 (0.3%)
3	C	0.55	0/1687	0.81	1/2297 (0.0%)
4	D	0.63	3/3504 (0.1%)	0.84	6/4747 (0.1%)
5	E	0.56	2/1675 (0.1%)	0.83	6/2282 (0.3%)
6	F	0.65	5/3363 (0.1%)	0.89	8/4543 (0.2%)
7	G	0.65	5/5374 (0.1%)	0.99	19/7281 (0.3%)
8	H	0.68	3/2585 (0.1%)	0.90	9/3529 (0.3%)
9	I	0.63	1/1427 (0.1%)	0.89	2/1927 (0.1%)
10	J	0.53	0/1233	0.77	1/1672 (0.1%)
11	K	0.59	0/740	0.83	2/1005 (0.2%)
12	L	0.69	5/4921 (0.1%)	0.91	19/6696 (0.3%)
13	M	0.69	4/3709 (0.1%)	0.89	10/5052 (0.2%)
14	N	0.71	4/2756 (0.1%)	0.91	8/3751 (0.2%)
15	O	0.78	7/2666 (0.3%)	0.92	18/3615 (0.5%)
16	P	0.61	2/2804 (0.1%)	0.82	9/3802 (0.2%)
17	Q	0.58	1/980 (0.1%)	0.80	4/1324 (0.3%)
18	R	0.72	1/671 (0.1%)	0.74	1/903 (0.1%)
19	S	0.83	2/678 (0.3%)	1.08	5/915 (0.5%)
20	T	0.75	1/613 (0.2%)	0.90	4/826 (0.5%)
20	U	0.61	0/690	0.90	3/931 (0.3%)
21	V	0.56	0/937	0.85	4/1270 (0.3%)
22	W	0.53	0/993	0.72	0/1335
23	X	0.60	1/1422 (0.1%)	0.88	7/1921 (0.4%)
24	Y	0.53	0/1054	0.59	0/1429
25	Z	0.50	0/1183	0.62	0/1597
26	a	0.54	0/561	0.86	2/755 (0.3%)
27	b	0.47	0/651	0.53	0/895
28	c	0.81	1/400 (0.2%)	0.95	3/544 (0.6%)
29	d	0.77	2/1020 (0.2%)	0.74	5/1377 (0.4%)
30	e	0.44	0/885	0.60	0/1178
31	f	0.59	0/488	0.81	3/657 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.67	1/886 (0.1%)	0.92	3/1207 (0.2%)
33	h	0.54	1/1181 (0.1%)	0.79	0/1599
34	i	0.52	0/823	0.76	1/1119 (0.1%)
35	j	0.56	0/588	0.82	2/805 (0.2%)
36	k	0.58	0/587	0.80	1/794 (0.1%)
37	l	0.68	2/1384 (0.1%)	0.76	2/1889 (0.1%)
38	m	0.54	0/1083	0.73	0/1468
39	n	0.62	1/1596 (0.1%)	0.79	3/2162 (0.1%)
40	o	0.52	0/1052	0.72	3/1411 (0.2%)
41	p	0.50	0/1471	0.73	3/1988 (0.2%)
42	q	0.77	2/1037 (0.2%)	0.97	5/1408 (0.4%)
43	r	0.73	1/426 (0.2%)	0.98	1/573 (0.2%)
44	s	0.64	0/116	1.01	1/157 (0.6%)
45	AA	0.41	0/3187	0.61	0/4320
45	Aa	0.42	0/3288	0.61	1/4462 (0.0%)
46	AB	0.35	0/3187	0.58	1/4308 (0.0%)
46	Ab	0.36	0/3187	0.56	0/4308
47	AC	0.35	0/3089	0.55	1/4221 (0.0%)
47	Ac	0.36	0/3089	0.56	1/4221 (0.0%)
48	AD	0.38	0/1955	0.53	0/2655
48	Ad	0.44	1/1954 (0.1%)	0.55	0/2655
49	AE	0.47	0/1459	0.63	1/1976 (0.1%)
49	AI	0.47	0/349	0.73	3/476 (0.6%)
49	Ae	0.47	0/1464	0.63	1/1983 (0.1%)
50	AF	0.32	0/884	0.50	0/1184
50	Af	0.32	0/884	0.50	0/1184
51	AG	0.37	0/662	0.55	0/895
51	Ag	0.42	0/662	0.53	0/895
52	AH	0.34	0/542	0.61	0/728
52	Ah	0.44	0/551	0.60	0/739
53	AJ	0.35	0/339	0.48	0/457
53	Aj	0.42	0/402	0.61	0/541
54	AK	0.31	0/291	0.49	0/399
54	Ak	0.41	0/371	0.55	0/511
All	All	0.57	59/97759 (0.1%)	0.78	198/132554 (0.1%)

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	247	PRO	N-CD	16.59	1.71	1.47
18	R	89	PRO	N-CD	-15.12	1.26	1.47
29	d	115	PRO	N-CD	-14.05	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	265	PRO	N-CD	13.77	1.67	1.47
14	N	255	PRO	N-CD	-13.61	1.28	1.47

The worst 5 of 198 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	83	MET	O-C-N	11.12	140.50	122.70
26	a	3	PHE	CB-CA-C	-10.42	89.56	110.40
14	N	255	PRO	CA-N-CD	9.91	125.58	111.70
15	O	206	TYR	N-CA-CB	-9.89	92.81	110.60
42	q	139	PRO	CA-N-CD	9.58	125.12	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	79 (90%)	9 (10%)	0	100	100
2	B	155/224 (69%)	145 (94%)	9 (6%)	1 (1%)	22	59
3	C	196/263 (74%)	185 (94%)	11 (6%)	0	100	100
4	D	420/463 (91%)	391 (93%)	29 (7%)	0	100	100
5	E	208/248 (84%)	189 (91%)	19 (9%)	0	100	100
6	F	424/464 (91%)	408 (96%)	16 (4%)	0	100	100
7	G	685/727 (94%)	629 (92%)	56 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	308/318 (97%)	288 (94%)	19 (6%)	1 (0%)	37	72
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	J	153/172 (89%)	144 (94%)	9 (6%)	0	100	100
11	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
12	L	604/607 (100%)	573 (95%)	30 (5%)	1 (0%)	44	78
13	M	456/459 (99%)	438 (96%)	18 (4%)	0	100	100
14	N	342/345 (99%)	330 (96%)	11 (3%)	1 (0%)	37	72
15	O	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
16	P	338/377 (90%)	317 (94%)	21 (6%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	77 (95%)	4 (5%)	0	100	100
19	S	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	82/156 (53%)	76 (93%)	6 (7%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
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%)	129 (94%)	8 (6%)	0	100	100
26	a	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
27	b	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
30	e	102/106 (96%)	97 (95%)	5 (5%)	0	100	100
31	f	53/57 (93%)	50 (94%)	3 (6%)	0	100	100
32	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
33	h	134/189 (71%)	127 (95%)	7 (5%)	0	100	100
34	i	90/128 (70%)	76 (84%)	13 (14%)	1 (1%)	12	46
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	69/104 (66%)	67 (97%)	2 (3%)	0	100	100
37	l	156/186 (84%)	143 (92%)	13 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	m	125/129 (97%)	117 (94%)	8 (6%)	0	100	100
39	n	176/179 (98%)	162 (92%)	13 (7%)	1 (1%)	22	59
40	o	118/137 (86%)	109 (92%)	9 (8%)	0	100	100
41	p	168/176 (96%)	153 (91%)	15 (9%)	0	100	100
42	q	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
43	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
44	s	12/104 (12%)	12 (100%)	0	0	100	100
45	AA	394/480 (82%)	381 (97%)	13 (3%)	0	100	100
45	Aa	408/480 (85%)	388 (95%)	20 (5%)	0	100	100
46	AB	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
46	Ab	416/453 (92%)	405 (97%)	11 (3%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
48	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
48	Ad	236/325 (73%)	220 (93%)	16 (7%)	0	100	100
49	AE	181/274 (66%)	169 (93%)	12 (7%)	0	100	100
49	AI	43/274 (16%)	39 (91%)	4 (9%)	0	100	100
49	Ae	181/274 (66%)	166 (92%)	15 (8%)	0	100	100
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	63/89 (71%)	62 (98%)	1 (2%)	0	100	100
52	Ah	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	46/64 (72%)	44 (96%)	2 (4%)	0	100	100
54	AK	33/56 (59%)	33 (100%)	0	0	100	100
54	Ak	42/56 (75%)	40 (95%)	2 (5%)	0	100	100
All	All	11769/14118 (83%)	11186 (95%)	577 (5%)	6 (0%)	50	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
14	N	109	ALA
34	i	124	PRO
2	B	195	PRO
39	n	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	79	85
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	366/395 (93%)	366 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	579 (100%)	0	100	100
8	H	276/280 (99%)	276 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	J	127/138 (92%)	127 (100%)	0	100	100
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	549 (100%)	0	100	100
13	M	414/415 (100%)	414 (100%)	0	100	100
14	N	307/308 (100%)	307 (100%)	0	100	100
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	297/325 (91%)	297 (100%)	0	100	100
17	Q	105/153 (69%)	105 (100%)	0	100	100
18	R	70/96 (73%)	70 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	69/135 (51%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	U	78/135 (58%)	78 (100%)	0	100	100
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%)	120 (100%)	0	100	100
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	106/107 (99%)	106 (100%)	0	100	100
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	51/53 (96%)	51 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	121/162 (75%)	121 (100%)	0	100	100
34	i	89/120 (74%)	89 (100%)	0	100	100
35	j	61/87 (70%)	61 (100%)	0	100	100
36	k	54/78 (69%)	54 (100%)	0	100	100
37	l	142/161 (88%)	142 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	163 (100%)	0	100	100
40	o	110/121 (91%)	110 (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	14/95 (15%)	14 (100%)	0	100	100
45	AA	338/398 (85%)	338 (100%)	0	100	100
45	Aa	349/398 (88%)	349 (100%)	0	100	100
46	AB	328/356 (92%)	328 (100%)	0	100	100
46	Ab	328/356 (92%)	328 (100%)	0	100	100
47	AC	325/333 (98%)	325 (100%)	0	100	100
47	Ac	325/333 (98%)	325 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	AD	203/260 (78%)	203 (100%)	0	100	100
48	Ad	203/260 (78%)	203 (100%)	0	100	100
49	AE	155/224 (69%)	155 (100%)	0	100	100
49	AI	34/224 (15%)	33 (97%)	1 (3%)	37	58
49	Ae	156/224 (70%)	156 (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	62/83 (75%)	62 (100%)	0	100	100
52	Ah	63/83 (76%)	63 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (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	10334/12037 (86%)	10332 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	170	TYR
49	AI	78	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 200 such sidechains are listed below:

Mol	Chain	Res	Type
22	W	54	GLN
39	n	14	GLN
53	Aj	48	ASN
24	Y	21	HIS
33	h	170	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 60 ligands modelled in this entry, 1 is monoatomic - leaving 59 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	$\#\|Z\| > 2$
66	EHZ	n	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.85	11 (29%)
55	3PE	L	707	-	44,44,50	0.96	2 (4%)	47,49,55	1.08	3 (6%)
62	CDL	Ag	101	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	6 (9%)
59	FES	G	803	7	0,4,4	-	-	-		
58	PC1	J	201	-	41,41,53	1.07	2 (4%)	47,49,61	1.08	4 (8%)
57	UQ1	B	302	-	18,18,18	1.07	2 (11%)	22,25,25	0.70	0
61	UQ9	H	400	-	35,35,58	0.81	2 (5%)	42,45,73	0.49	0
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
55	3PE	AF	201	-	41,41,50	1.00	2 (4%)	44,46,55	0.98	2 (4%)
59	FES	E	301	5	0,4,4	-	-	-		
56	SF4	I	303	9	0,12,12	-	-	-		
70	HEC	AD	401	48	32,50,50	2.16	10 (31%)	24,82,82	2.57	6 (25%)
71	3PH	AD	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.21	3 (7%)
55	3PE	b	201	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
62	CDL	AC	406	-	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
63	ADP	O	402	-	24,29,29	0.98	1 (4%)	29,45,45	1.42	4 (13%)
56	SF4	G	801	7	0,12,12	-	-	-		
70	HEC	Ad	401	48	32,50,50	2.18	11 (34%)	24,82,82	2.45	6 (25%)
55	3PE	J	202	-	45,45,50	0.96	2 (4%)	48,50,55	1.06	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
64	NDP	P	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.21	4 (7%)
67	HEM	Ac	402	47	41,50,50	1.42	6 (14%)	45,82,82	2.15	11 (24%)
69	UQ6	AC	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.80	10 (30%)
71	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.13	3 (7%)
55	3PE	M	503	-	50,50,50	0.93	2 (4%)	53,55,55	1.11	3 (5%)
68	U10	Ac	405	-	38,38,63	1.37	2 (5%)	46,49,79	1.71	12 (26%)
55	3PE	Ac	401	-	22,22,50	0.38	0	25,27,55	0.48	0
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
68	U10	AC	404	-	23,23,63	1.78	2 (8%)	28,31,79	1.49	5 (17%)
69	UQ6	Ac	406	-	28,28,43	2.51	6 (21%)	33,37,55	1.59	9 (27%)
55	3PE	L	703	-	50,50,50	0.90	2 (4%)	53,55,55	1.12	3 (5%)
56	SF4	I	304	9	0,12,12	-	-	-		
55	3PE	Ac	404	-	34,34,50	1.09	2 (5%)	37,39,55	1.23	4 (10%)
55	3PE	O	401	-	30,30,50	1.16	2 (6%)	33,35,55	1.27	3 (9%)
66	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
60	FMN	F	501	-	33,33,33	1.40	5 (15%)	48,50,50	1.22	7 (14%)
55	3PE	L	704	-	46,46,50	0.95	2 (4%)	49,51,55	1.08	3 (6%)
56	SF4	B	301	2	0,12,12	-	-	-		
55	3PE	M	501	-	50,50,50	0.91	2 (4%)	53,55,55	1.11	4 (7%)
67	HEM	AC	401	47	41,50,50	1.36	5 (12%)	45,82,82	1.88	10 (22%)
55	3PE	Ag	102	-	38,38,50	1.04	2 (5%)	41,43,55	1.13	4 (9%)
55	3PE	Y	201	-	39,39,50	1.02	2 (5%)	42,44,55	1.14	3 (7%)
55	3PE	L	701	-	41,41,50	0.99	2 (4%)	44,46,55	1.03	2 (4%)
62	CDL	L	705	-	76,76,99	1.02	4 (5%)	82,88,111	1.17	5 (6%)
62	CDL	L	706	-	85,85,99	0.99	4 (4%)	91,97,111	1.13	5 (5%)
62	CDL	Aa	501	-	45,45,99	0.36	0	51,57,111	0.42	0
55	3PE	A	401	-	45,45,50	0.94	2 (4%)	48,50,55	1.01	2 (4%)
62	CDL	Ac	407	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
56	SF4	G	802	7	0,12,12	-	-	-		
62	CDL	X	201	-	66,66,99	1.09	4 (6%)	72,78,111	1.26	6 (8%)
56	SF4	F	502	6	0,12,12	-	-	-		
55	3PE	N	401	-	36,36,50	1.06	2 (5%)	39,41,55	1.18	4 (10%)
58	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.08	3 (5%)
58	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	3 (7%)
55	3PE	AC	403	-	34,34,50	1.10	2 (5%)	37,39,55	1.18	3 (8%)
55	3PE	I	301	-	50,50,50	0.89	2 (4%)	53,55,55	1.03	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
67	HEM	AC	402	47	41,50,50	1.47	8 (19%)	45,82,82	2.43	16 (35%)
55	3PE	L	702	-	39,39,50	1.03	2 (5%)	42,44,55	1.10	4 (9%)
55	3PE	M	502	-	50,50,50	0.89	2 (4%)	53,55,55	1.15	4 (7%)
67	HEM	Ac	403	47	41,50,50	1.42	6 (14%)	45,82,82	1.84	11 (24%)

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
59	FES	G	803	7	-	-	0/1/1/1
66	EHZ	n	201	-	-	21/39/39/45	-
55	3PE	L	707	-	-	13/48/48/54	-
62	CDL	Ag	101	-	-	12/66/66/110	-
68	U10	AC	404	-	-	0/15/39/87	0/1/1/1
58	PC1	J	201	-	-	14/45/45/57	-
57	UQ1	B	302	-	-	3/9/33/33	0/1/1/1
61	UQ9	H	400	-	-	13/30/54/81	0/1/1/1
62	CDL	a	101	-	-	14/67/67/110	-
55	3PE	AF	201	-	-	9/45/45/54	-
68	U10	Ac	405	-	-	9/33/57/87	0/1/1/1
70	HEC	AD	401	48	-	3/10/54/54	-
71	3PH	AD	402	-	-	8/37/37/49	-
56	SF4	I	303	9	-	-	0/6/5/5
55	3PE	b	201	-	-	8/49/49/54	-
62	CDL	AC	406	-	-	18/66/66/110	-
63	ADP	O	402	-	-	4/12/32/32	0/3/3/3
70	HEC	Ad	401	48	-	2/10/54/54	-
56	SF4	G	801	7	-	-	0/6/5/5
55	3PE	J	202	-	-	12/49/49/54	-
64	NDP	P	401	-	-	6/30/77/77	0/5/5/5
67	HEM	Ac	402	47	-	3/12/54/54	-
69	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
71	3PH	Ad	402	-	-	8/37/37/49	-
55	3PE	M	503	-	-	17/54/54/54	-
55	3PE	Ac	401	-	-	10/26/26/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	CDL	h	201	-	-	23/80/80/110	-
69	UQ6	Ac	406	-	-	7/21/21/39	0/1/1/1
55	3PE	L	703	-	-	13/54/54/54	-
56	SF4	I	304	9	-	-	0/6/5/5
55	3PE	Ac	404	-	-	8/38/38/54	-
55	3PE	O	401	-	-	10/34/34/54	-
66	EHZ	W	201	-	-	22/39/39/45	-
60	FMN	F	501	-	-	4/18/18/18	0/3/3/3
55	3PE	L	704	-	-	13/50/50/54	-
56	SF4	B	301	2	-	-	0/6/5/5
55	3PE	M	501	-	-	15/54/54/54	-
67	HEM	AC	401	47	-	6/12/54/54	-
55	3PE	Ag	102	-	-	5/42/42/54	-
55	3PE	Y	201	-	-	5/43/43/54	-
55	3PE	L	701	-	-	13/45/45/54	-
62	CDL	L	705	-	-	24/87/87/110	-
62	CDL	L	706	-	-	27/96/96/110	-
62	CDL	Aa	501	-	-	16/56/56/110	-
55	3PE	A	401	-	-	14/49/49/54	-
62	CDL	Ac	407	-	-	11/52/52/110	-
62	CDL	X	201	-	-	27/77/77/110	-
56	SF4	G	802	7	-	-	0/6/5/5
56	SF4	F	502	6	-	-	0/6/5/5
59	FES	E	301	5	-	-	0/1/1/1
55	3PE	N	401	-	-	8/40/40/54	-
58	PC1	I	302	-	-	13/50/50/57	-
58	PC1	B	303	-	-	11/38/38/57	-
55	3PE	AC	403	-	-	12/38/38/54	-
55	3PE	I	301	-	-	17/54/54/54	-
67	HEM	AC	402	47	-	4/12/54/54	-
55	3PE	L	702	-	-	8/43/43/54	-
55	3PE	M	502	-	-	14/54/54/54	-
67	HEM	Ac	403	47	-	8/12/54/54	-

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	AC	404	U10	C6-C1	7.59	1.49	1.35
68	Ac	405	U10	C6-C1	7.42	1.48	1.35
70	Ad	401	HEC	C3C-C2C	6.23	1.47	1.40
69	AC	405	UQ6	C2-C3	5.95	1.49	1.39
69	Ac	406	UQ6	C2-C3	5.90	1.49	1.39

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	AD	401	HEC	CMC-C2C-C3C	7.21	134.30	125.82
67	Ac	402	HEM	C4B-C3B-C2B	-6.98	101.57	107.11
70	Ad	401	HEC	C1D-C2D-C3D	-6.40	102.54	107.00
66	W	201	EHZ	C8-C9-S1	6.32	121.44	113.63
66	n	201	EHZ	C8-C9-S1	6.30	121.43	113.63

There are no chirality outliers.

5 of 568 torsion outliers are listed below:

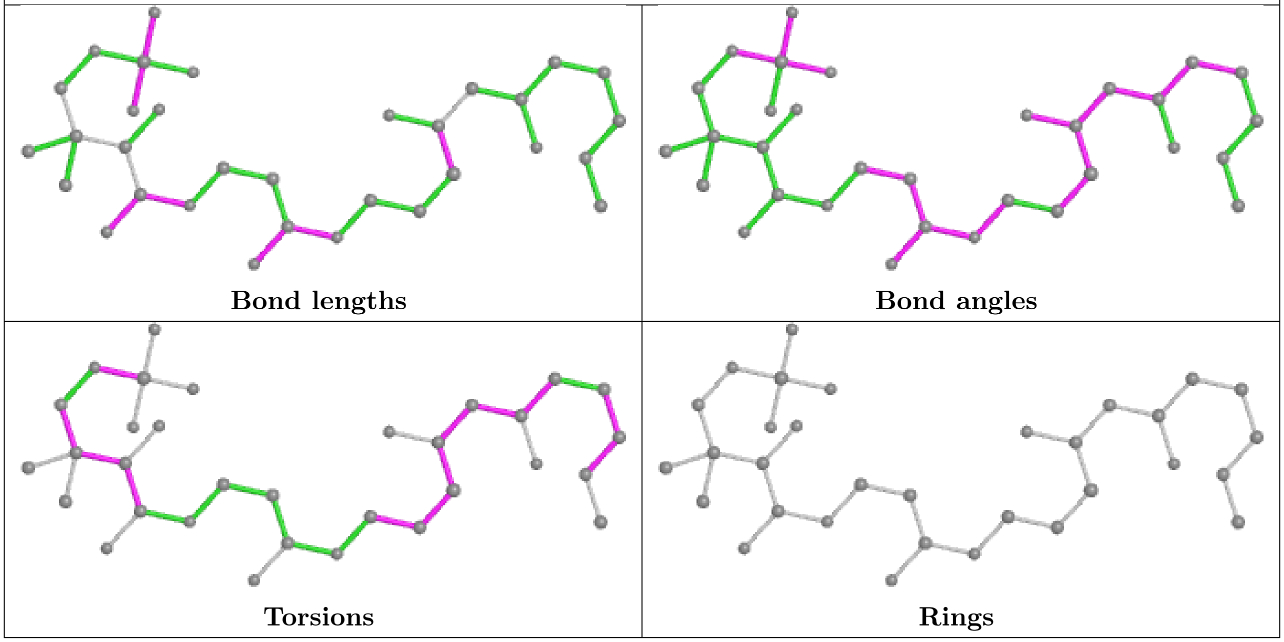
Mol	Chain	Res	Type	Atoms
55	A	401	3PE	C12-C11-O13-P
55	A	401	3PE	O32-C31-O31-C3
55	A	401	3PE	C32-C31-O31-C3
55	I	301	3PE	C11-O13-P-O12
55	L	701	3PE	C1-O11-P-O12

There are no ring outliers.

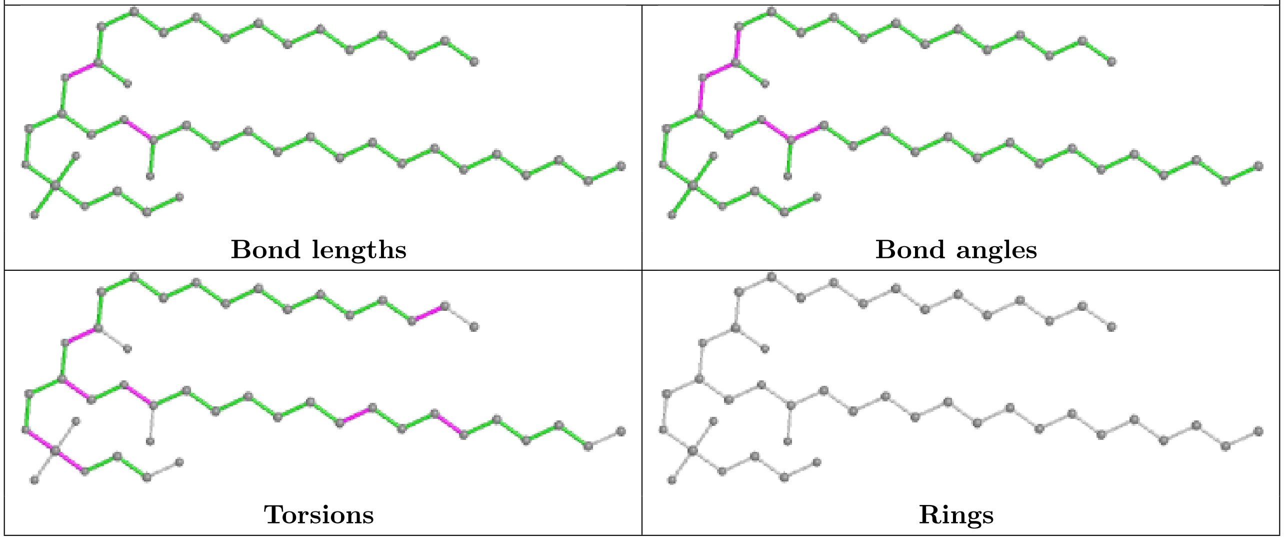
No monomer is involved in short contacts.

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.

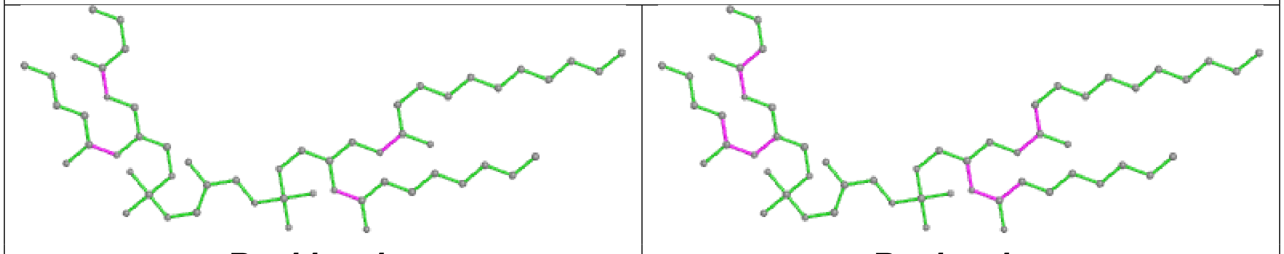
Ligand EHZ n 201


Bond lengths
Bond angles
Torsions
Rings

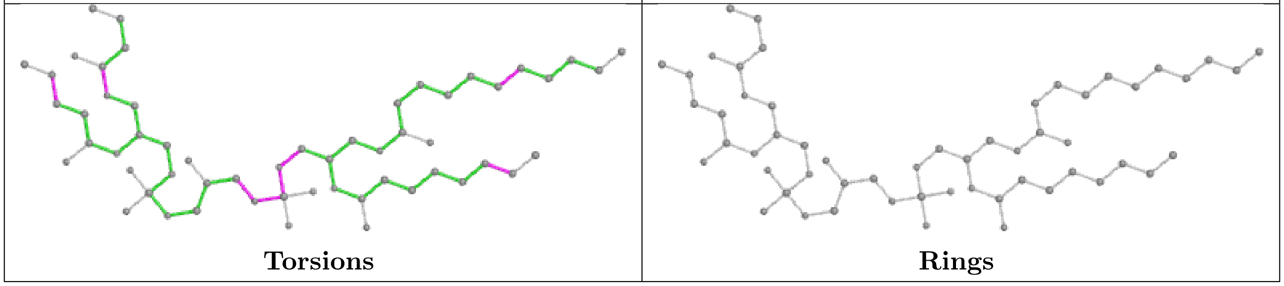
Ligand 3PE L 707


Bond lengths
Bond angles
Torsions
Rings

Ligand CDL Ag 101

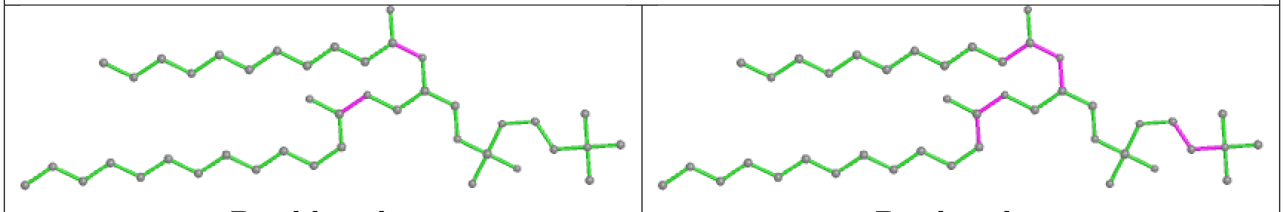


Bond lengths Bond angles

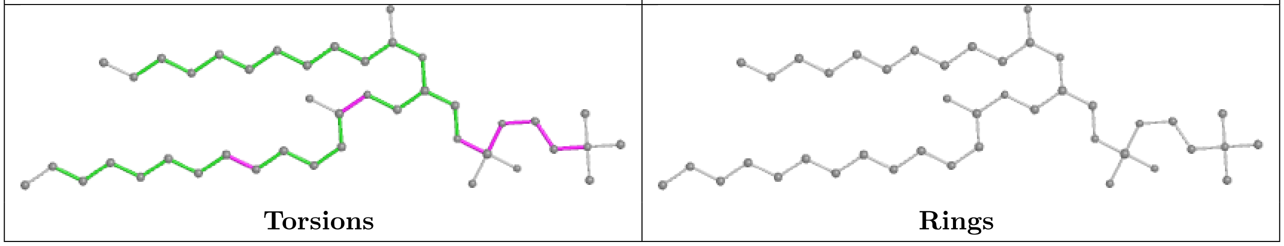


Torsions Rings

Ligand PC1 J 201

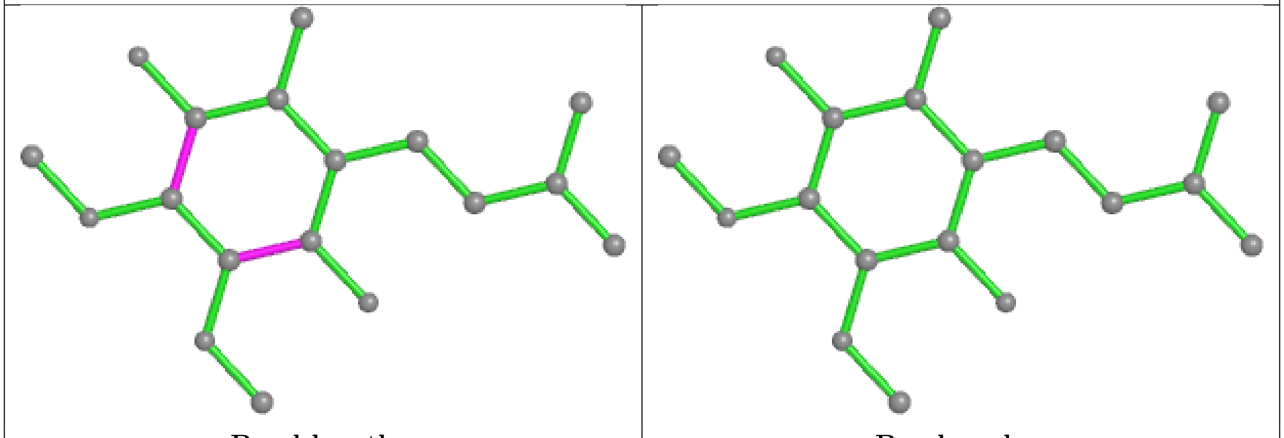


Bond lengths Bond angles

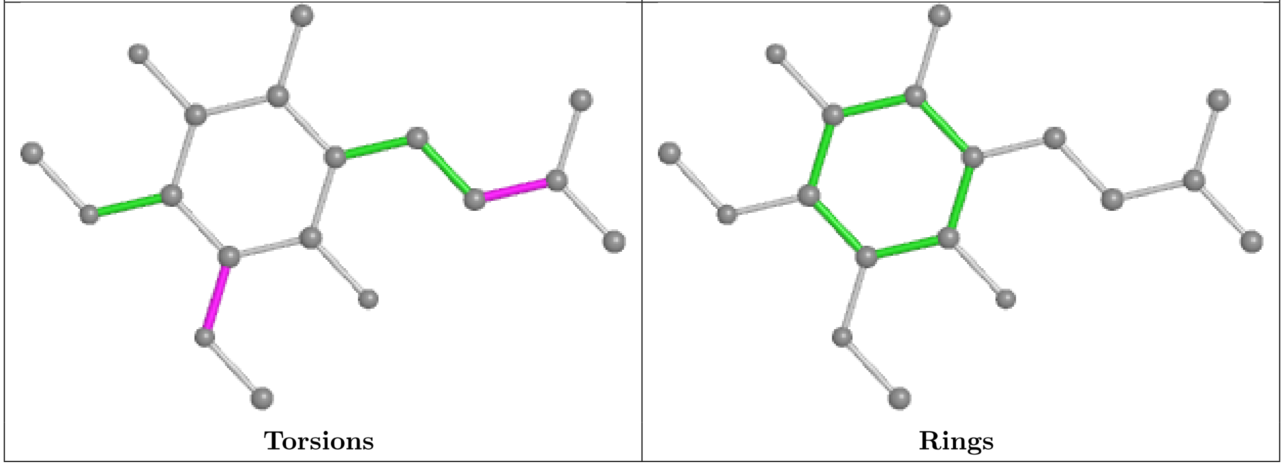


Torsions Rings

Ligand UQ1 B 302

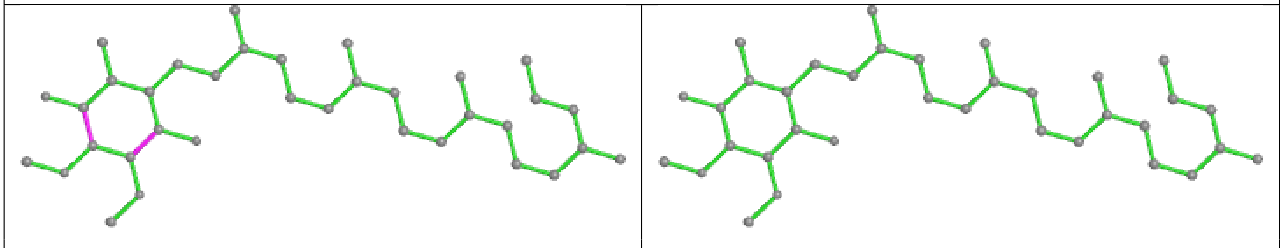


Bond lengths Bond angles

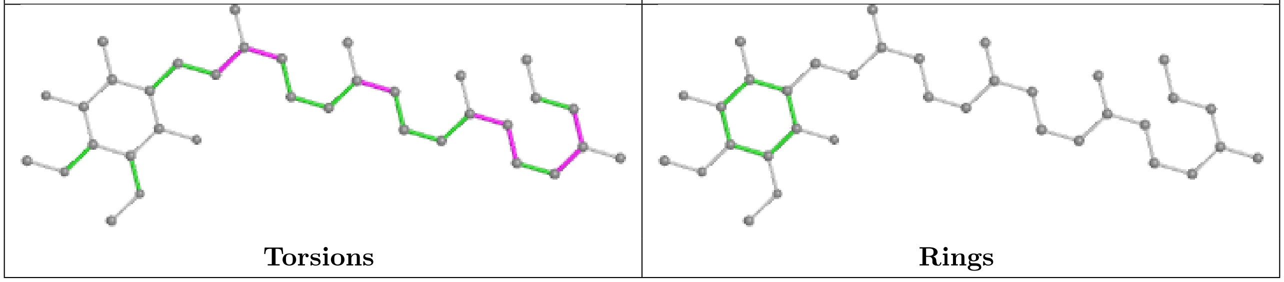


Torsions Rings

Ligand UQ9 H 400

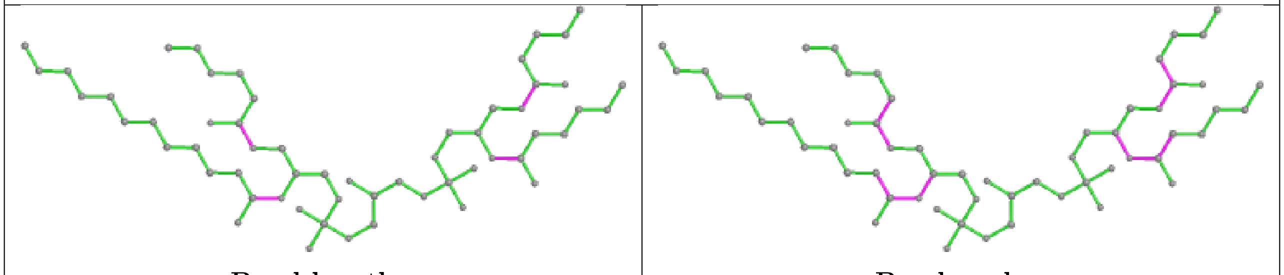


Bond lengths Bond angles



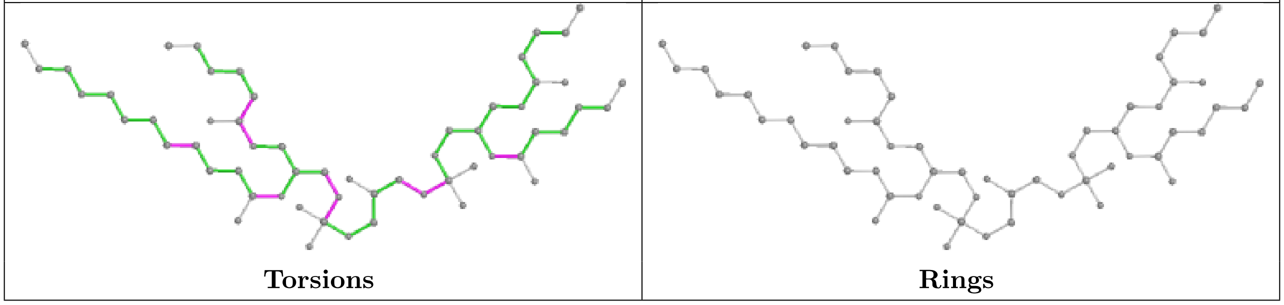
Torsions Rings

Ligand CDL a 101



Bond lengths

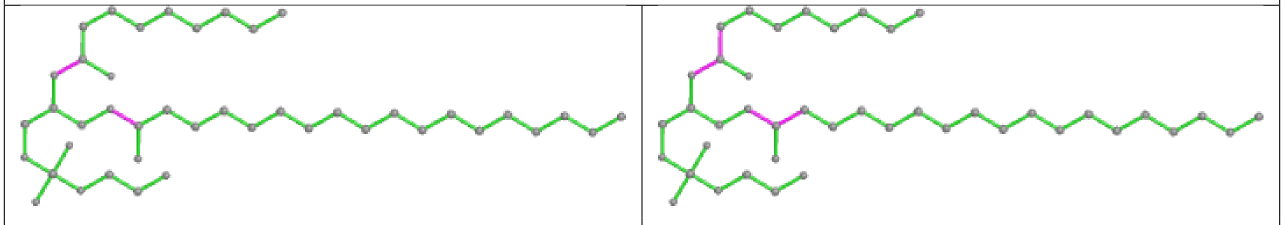
Bond angles



Torsions

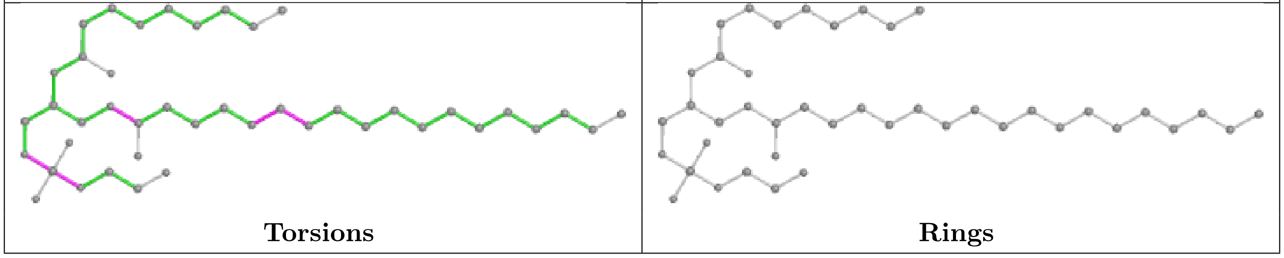
Rings

Ligand 3PE AF 201



Bond lengths

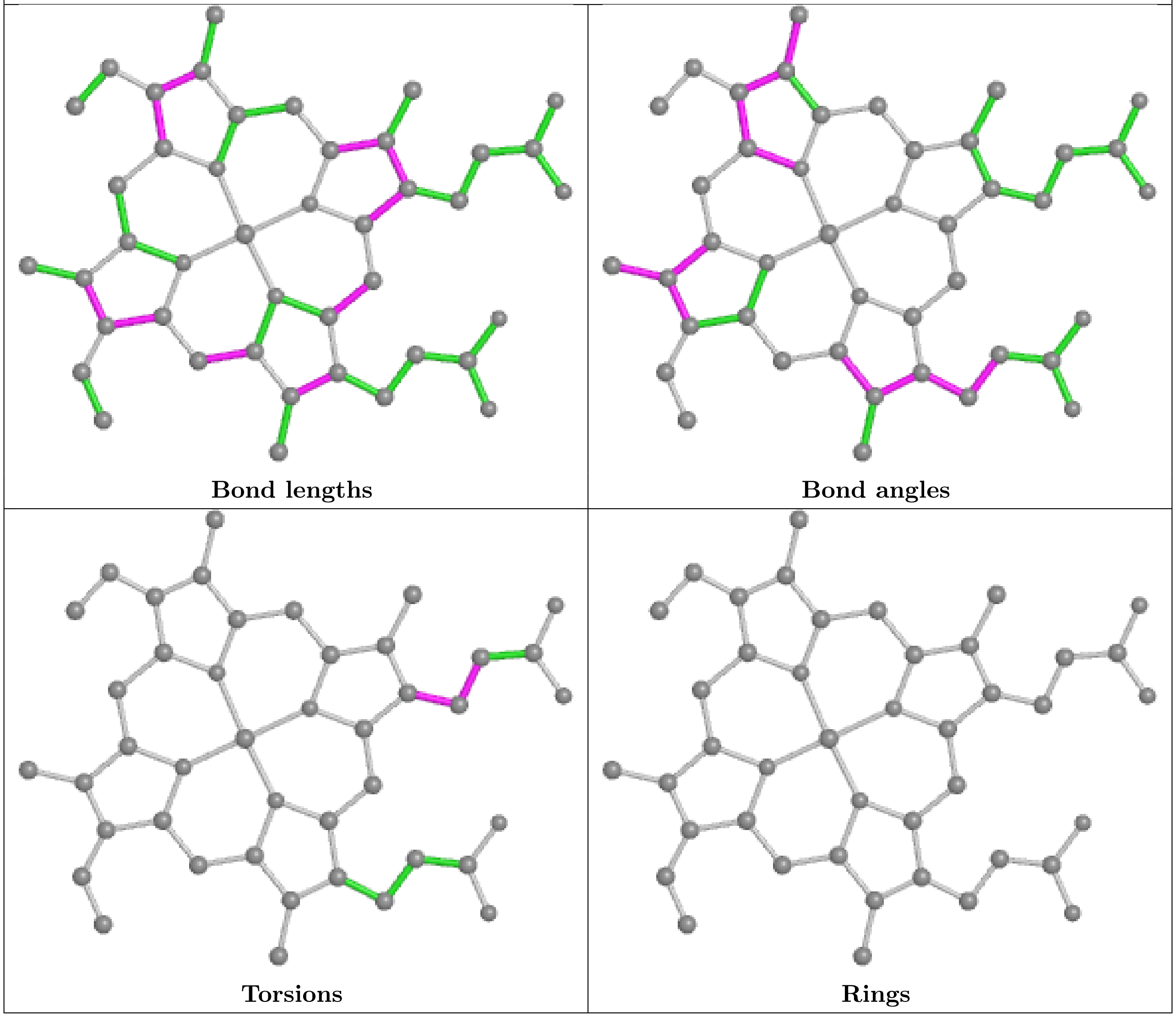
Bond angles



Torsions

Rings

Ligand HEC AD 401



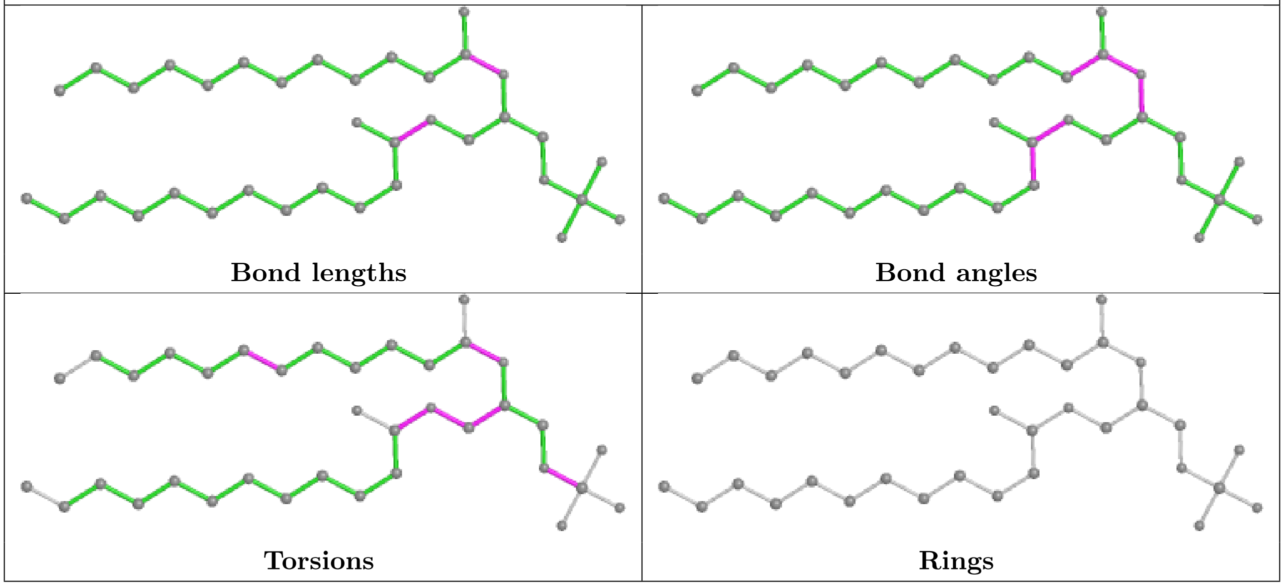
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PH AD 402



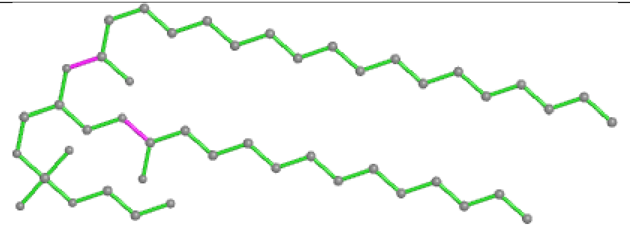
Bond lengths

Bond angles

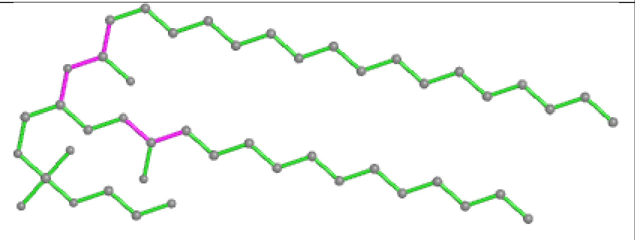
Torsions

Rings

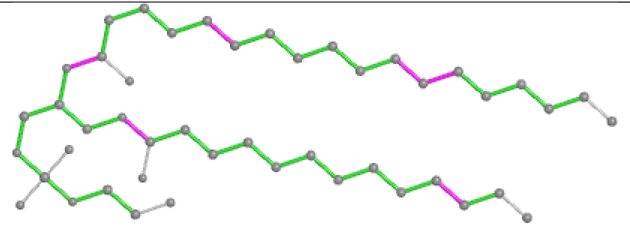
Ligand 3PE b 201



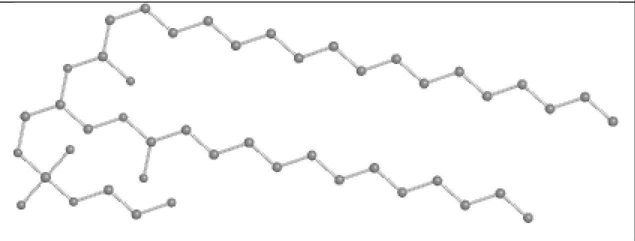
Bond lengths



Bond angles

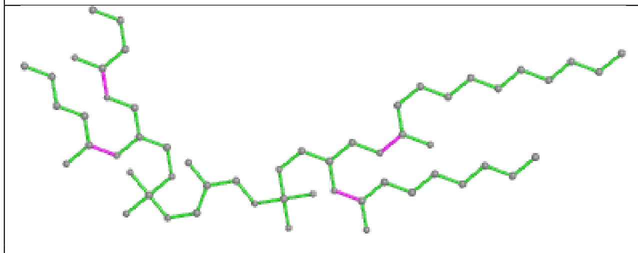


Torsions

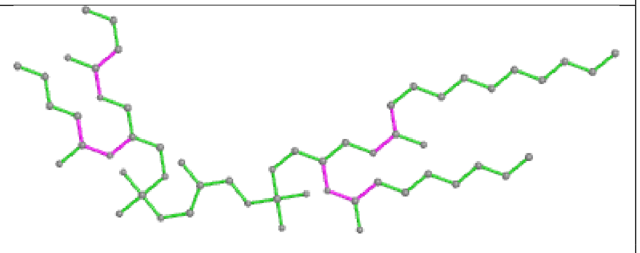


Rings

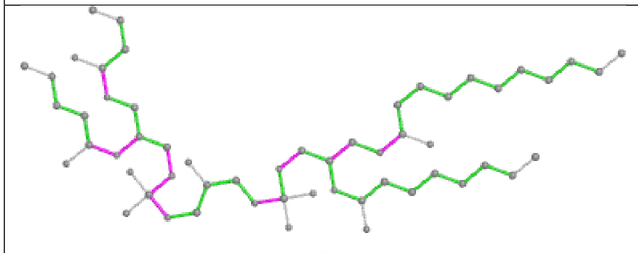
Ligand CDL AC 406



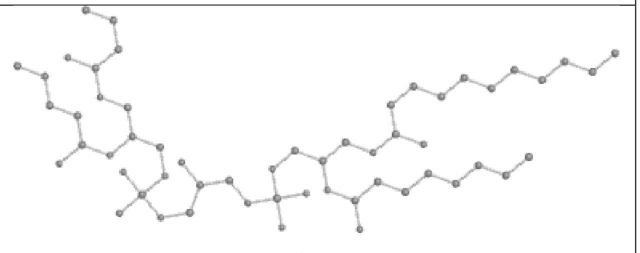
Bond lengths



Bond angles

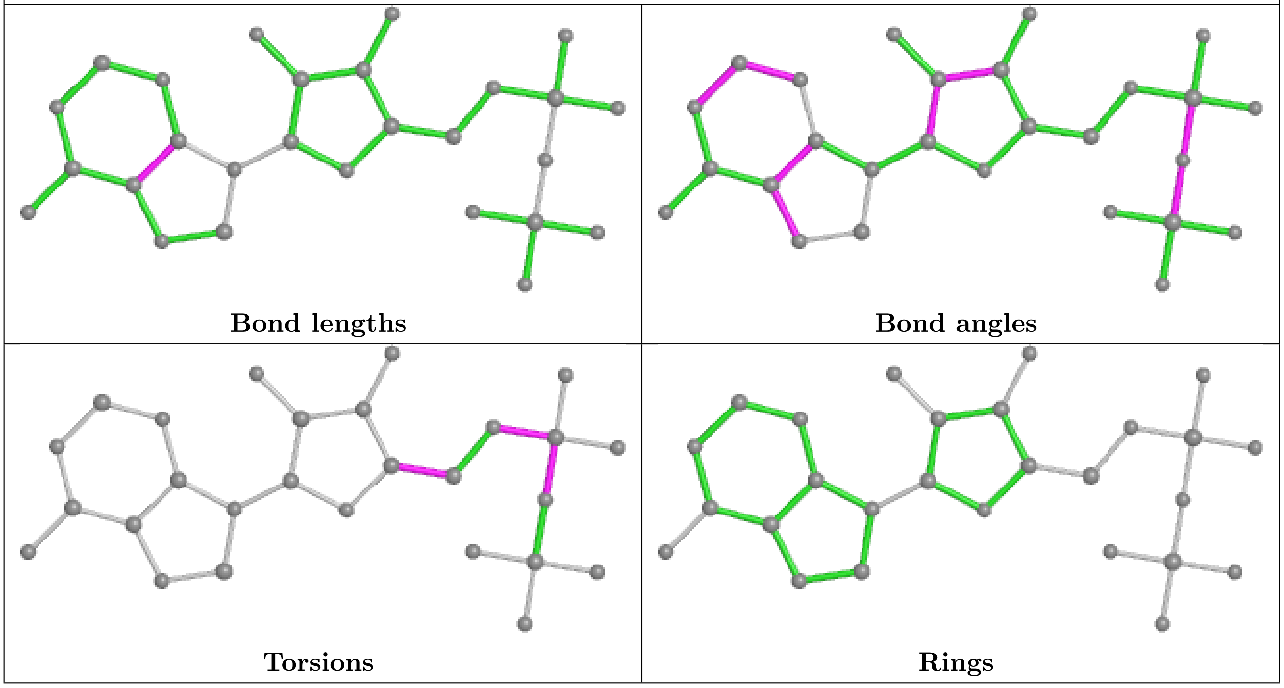


Torsions



Rings

Ligand ADP O 402



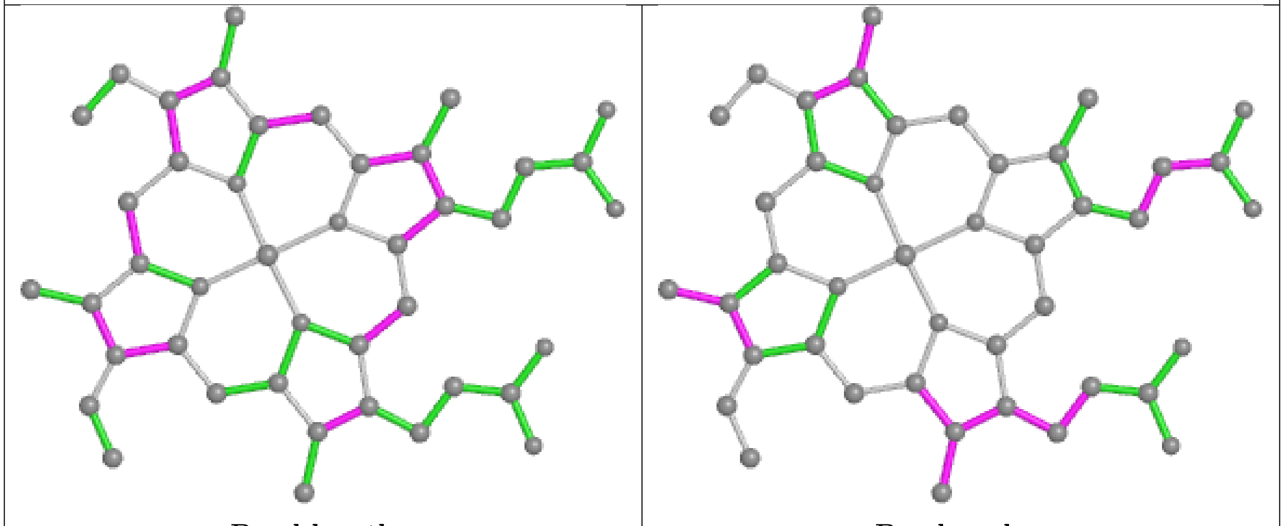
Bond lengths

Bond angles

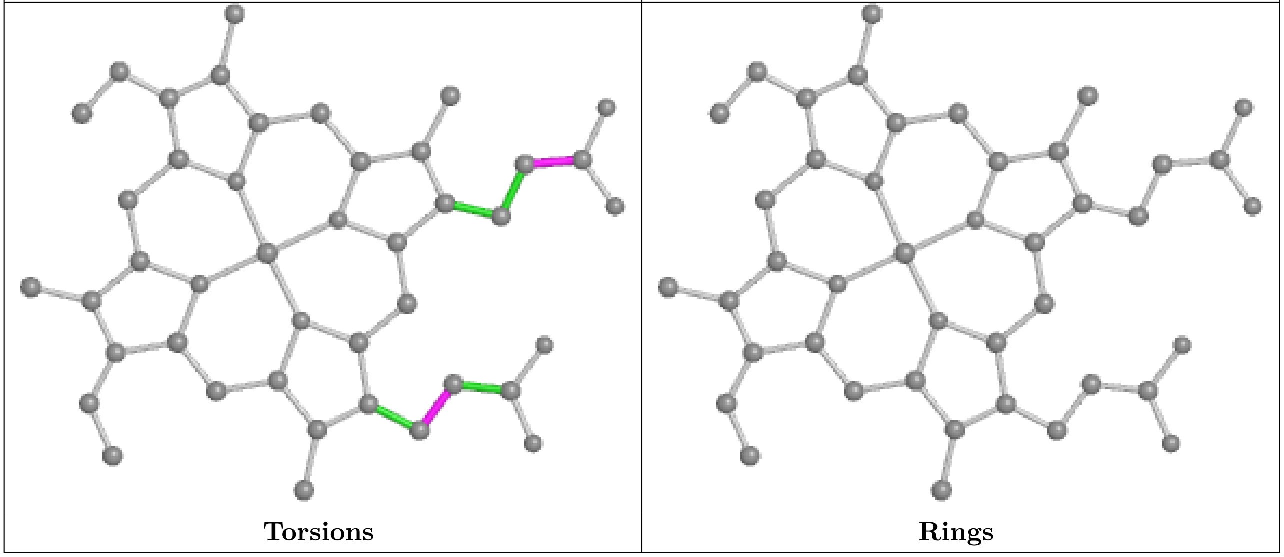
Torsions

Rings

Ligand HEC Ad 401

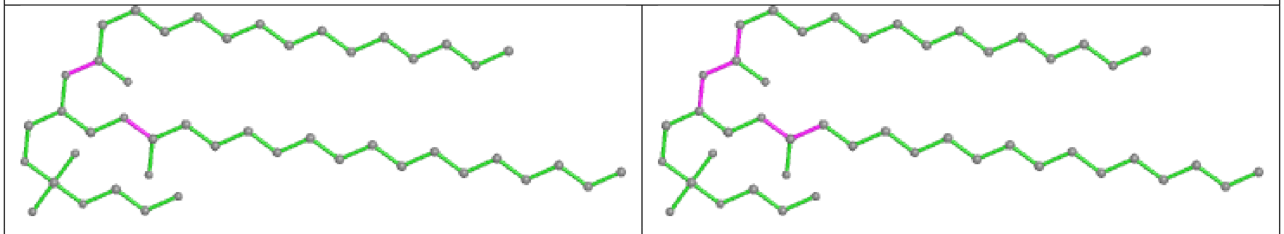


Bond lengths Bond angles

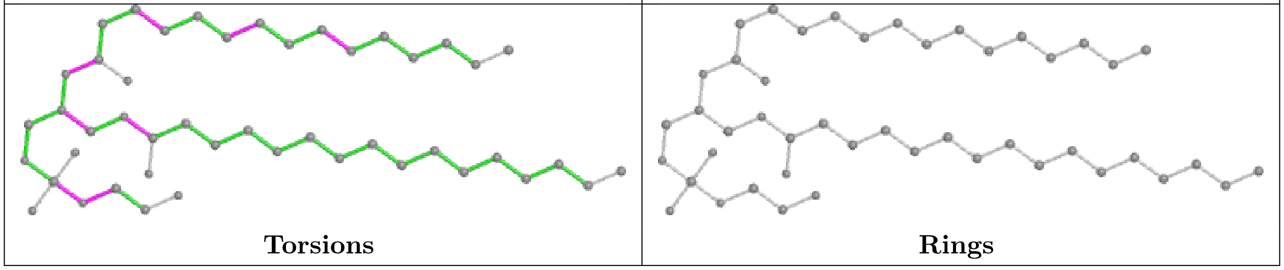


Torsions Rings

Ligand 3PE J 202

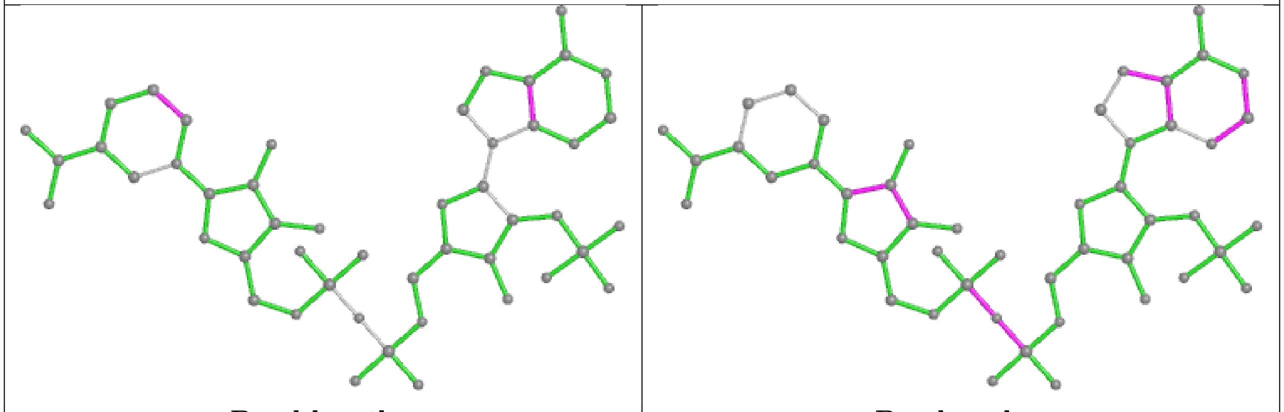


Bond lengths Bond angles



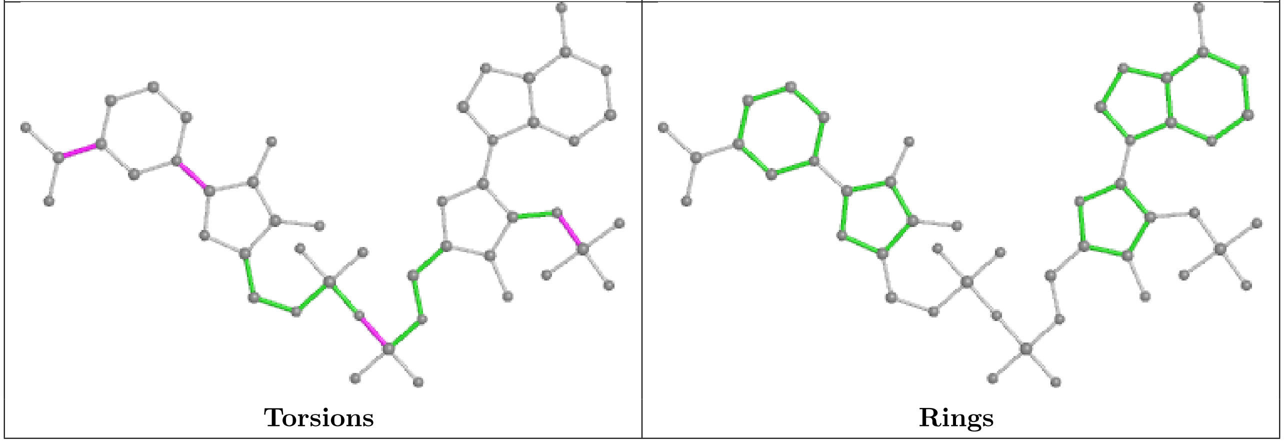
Torsions Rings

Ligand NDP P 401



Bond lengths

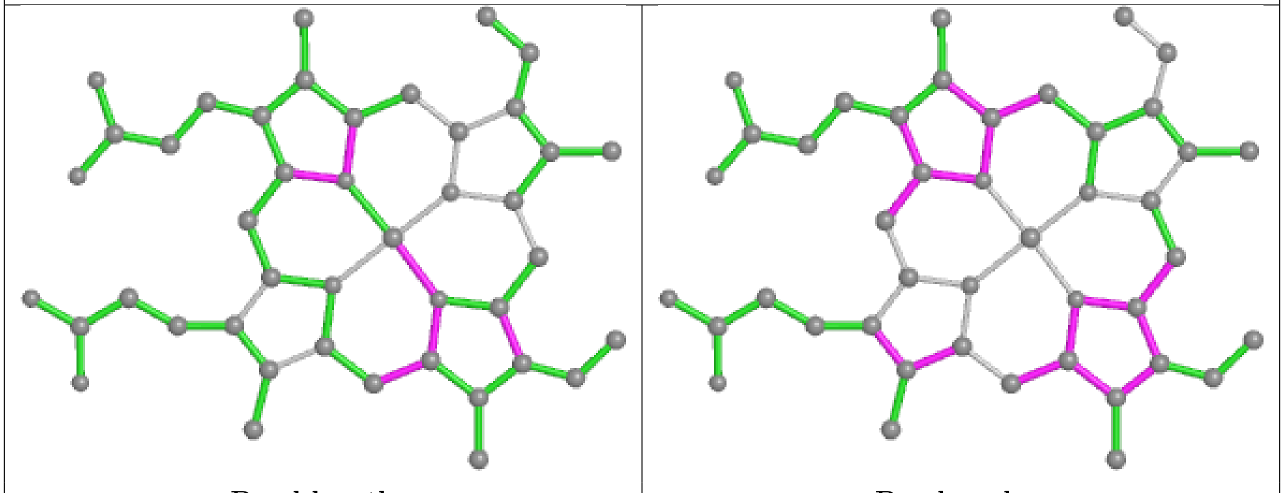
Bond angles



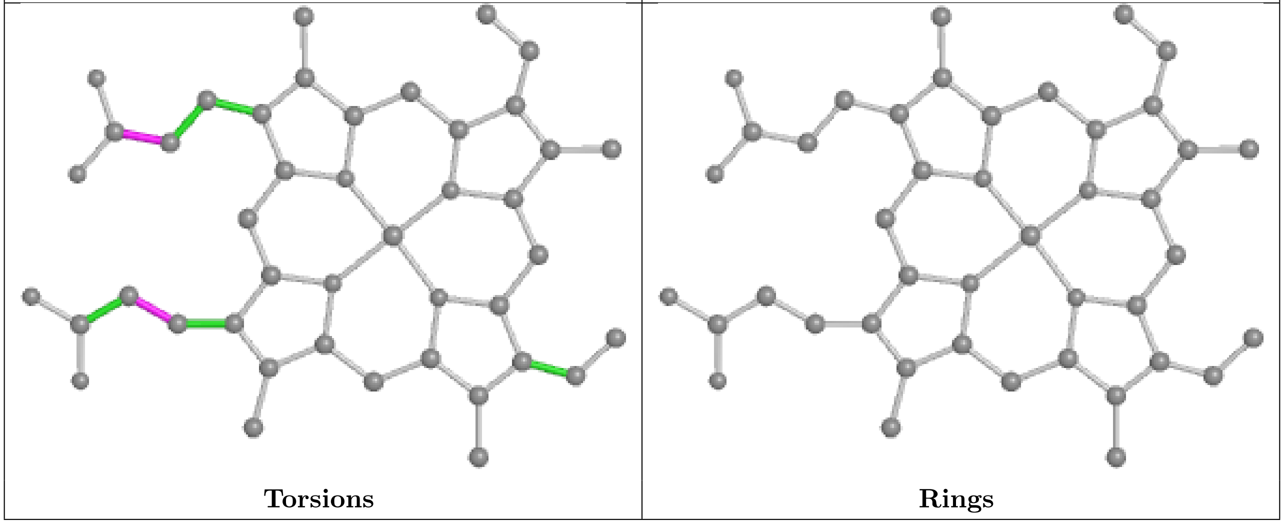
Torsions

Rings

Ligand HEM Ac 402

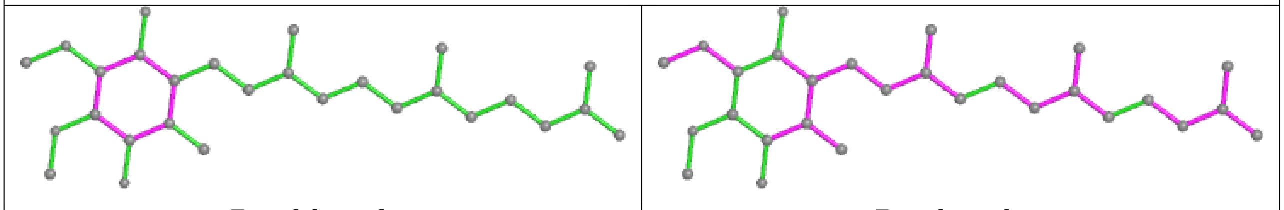


Bond lengths Bond angles

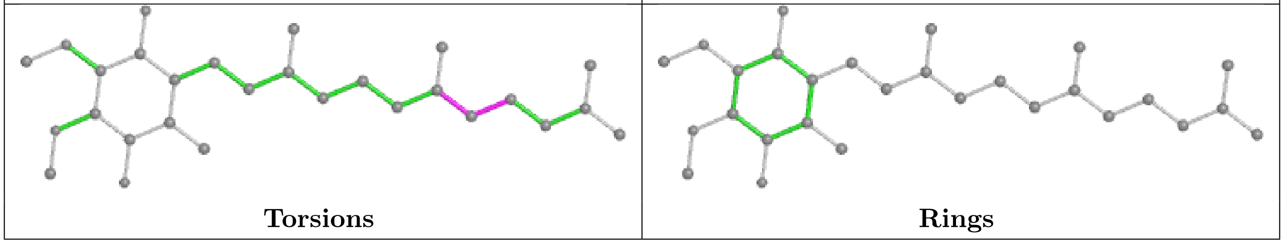


Torsions Rings

Ligand UQ6 AC 405

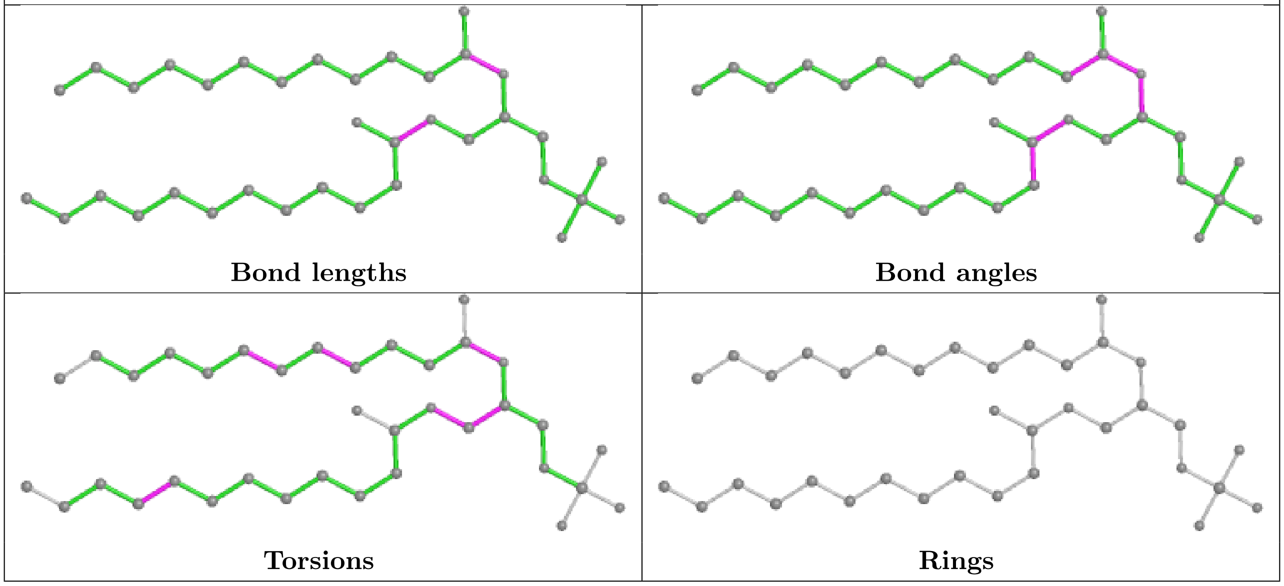


Bond lengths Bond angles

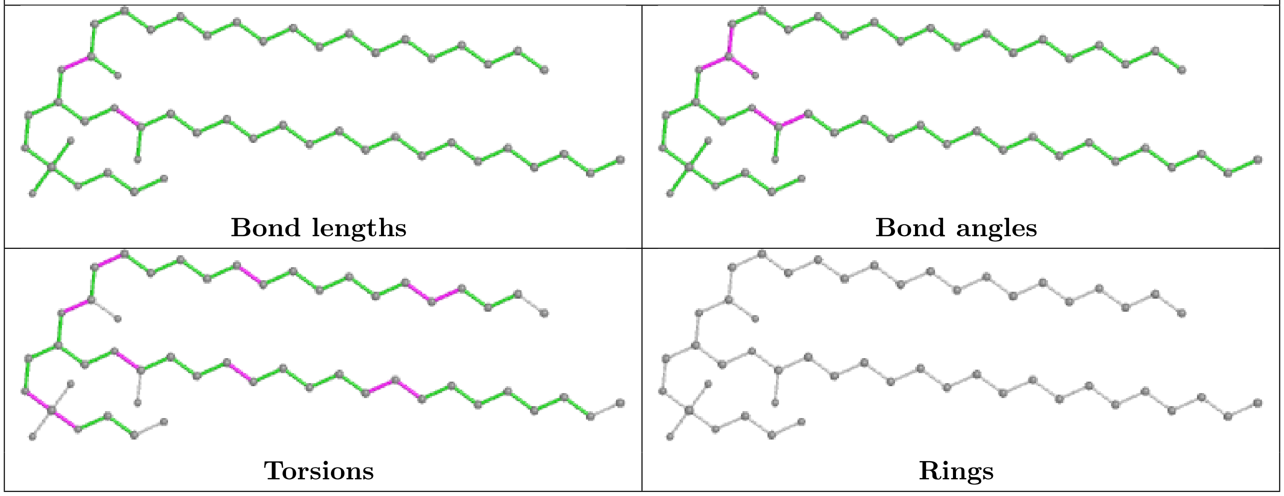


Torsions Rings

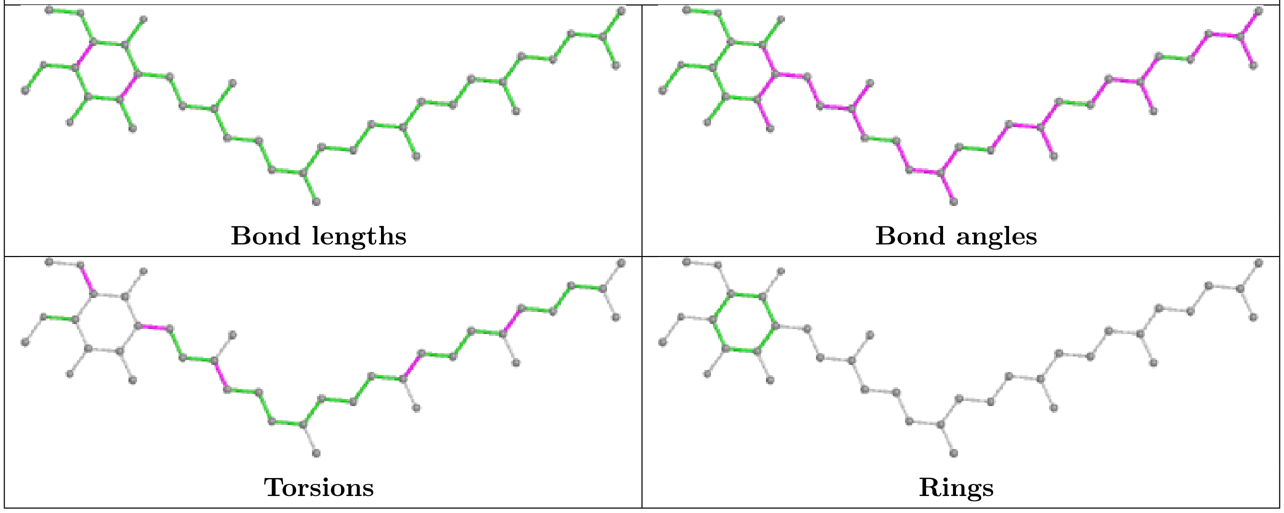
Ligand 3PH Ad 402



Ligand 3PE M 503



Ligand U10 Ac 405



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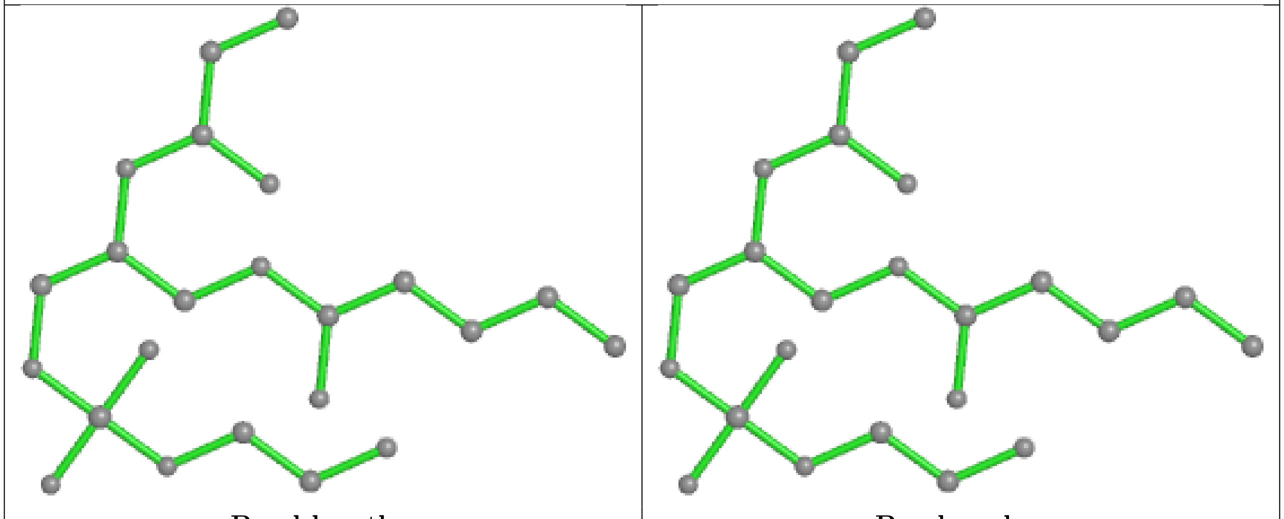
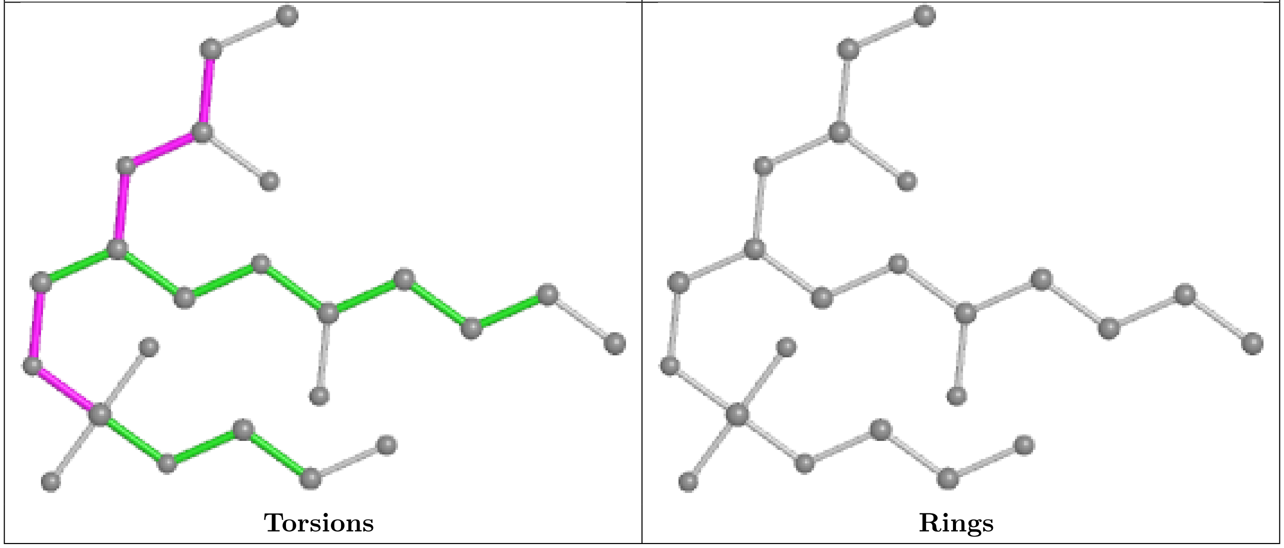
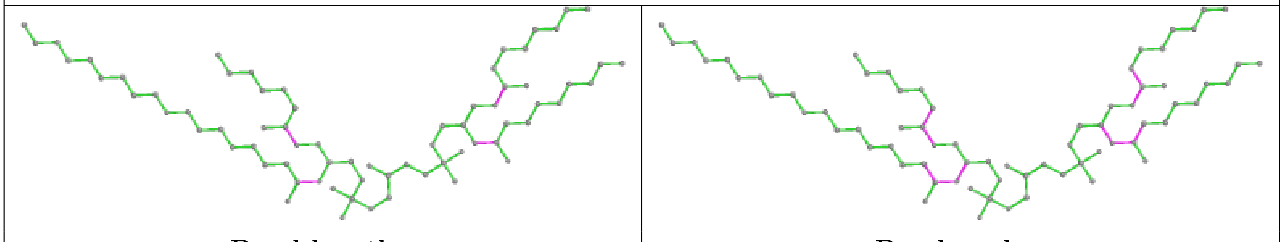


Bond lengths Bond angles

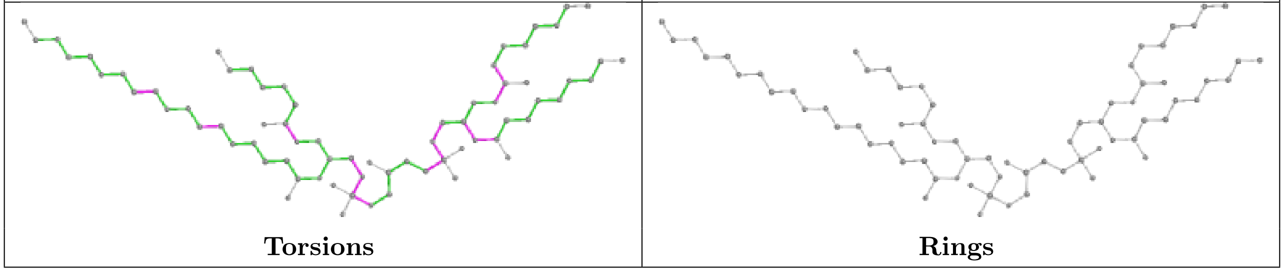


Torsions Rings

Ligand CDL h 201



Bond lengths Bond angles



Torsions Rings

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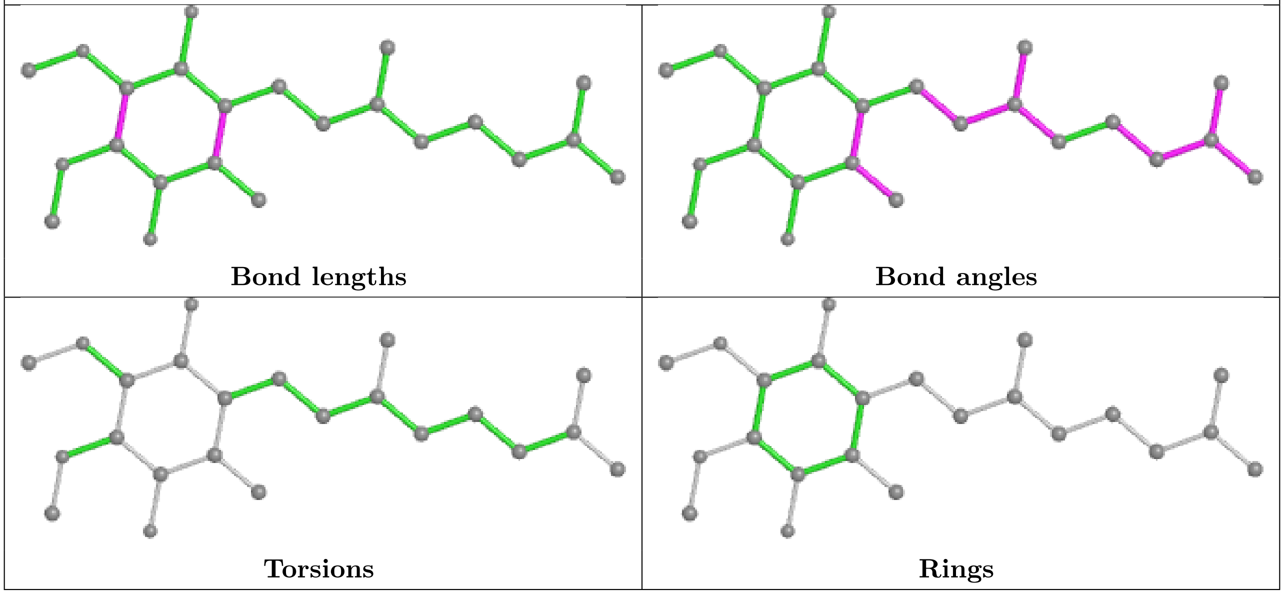
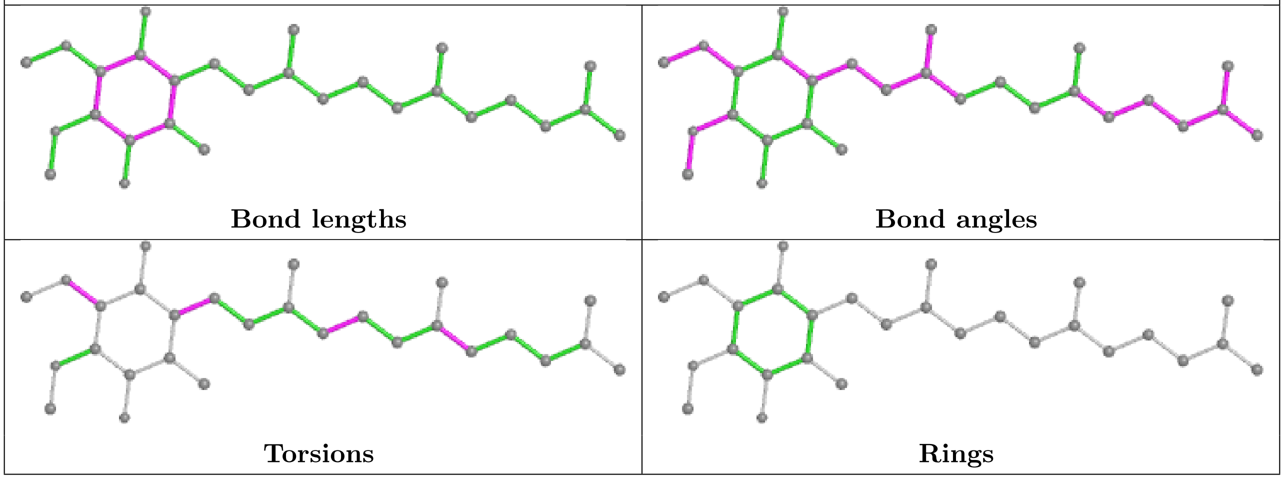
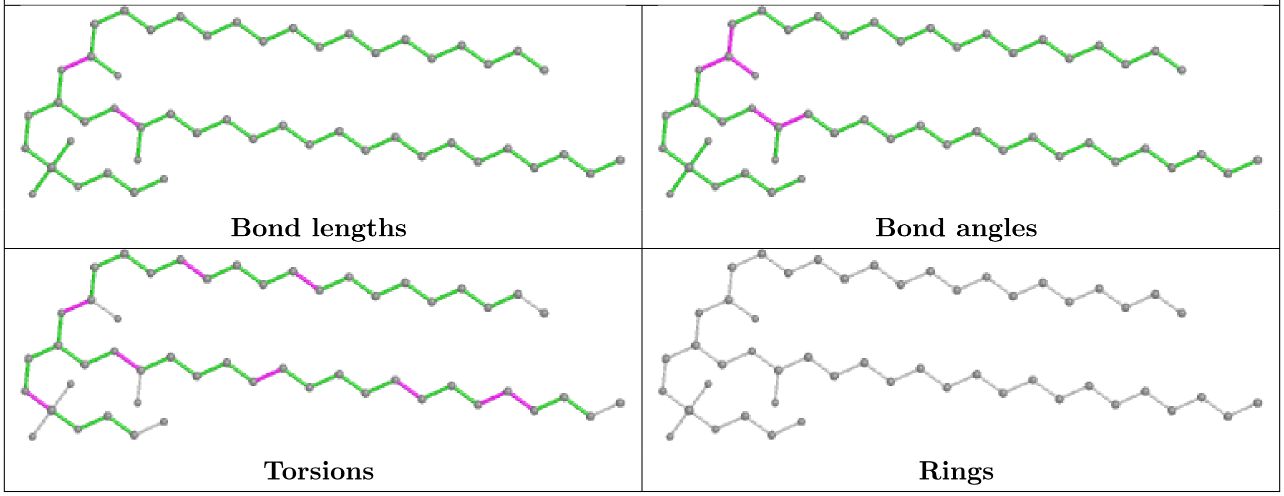


Ligand UQ6 Ac 406



Ligand 3PE L 703



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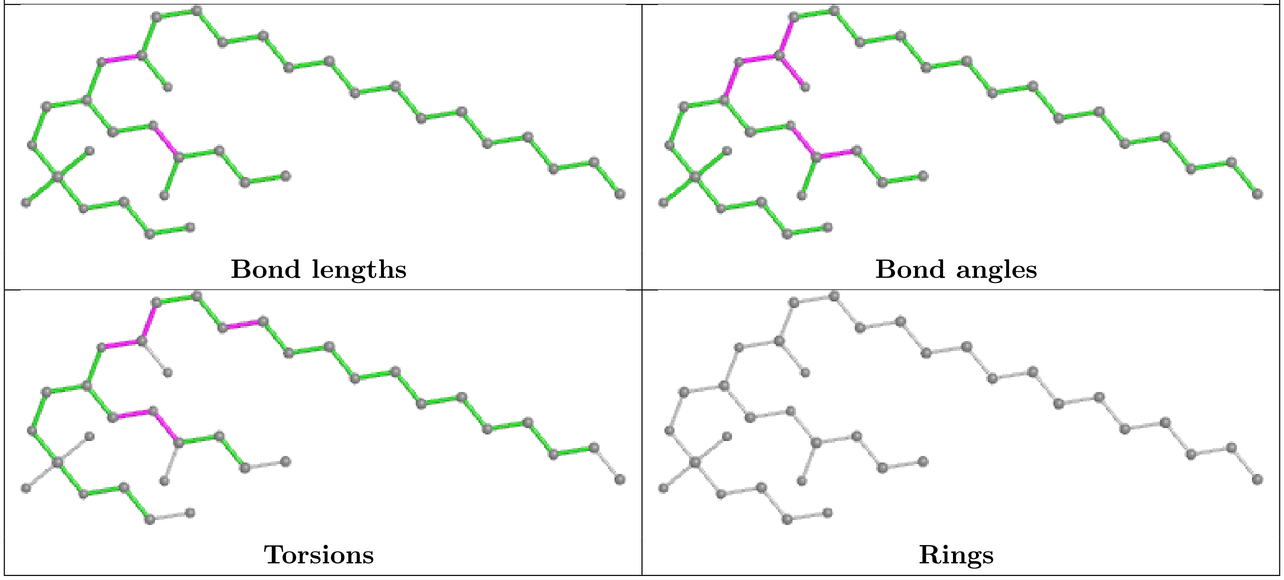


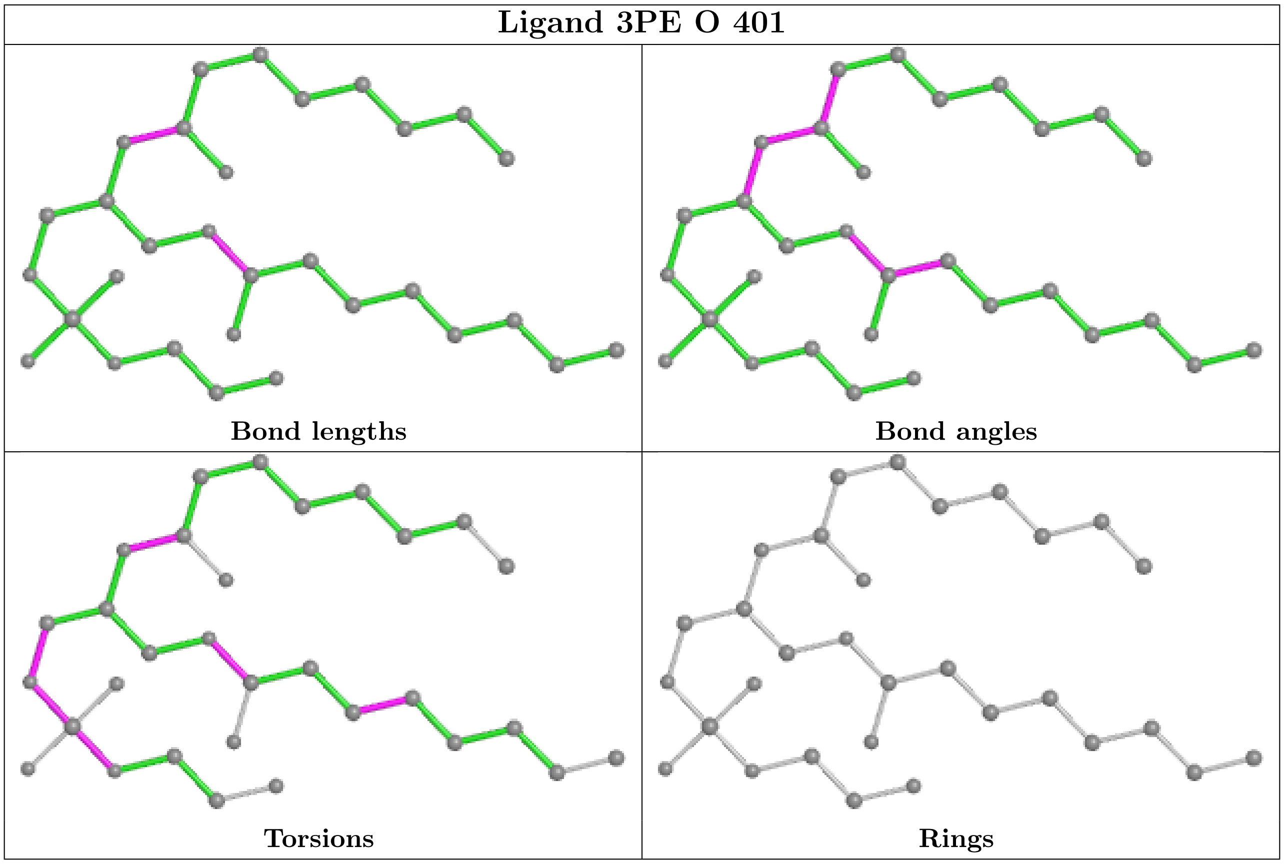
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE O 401



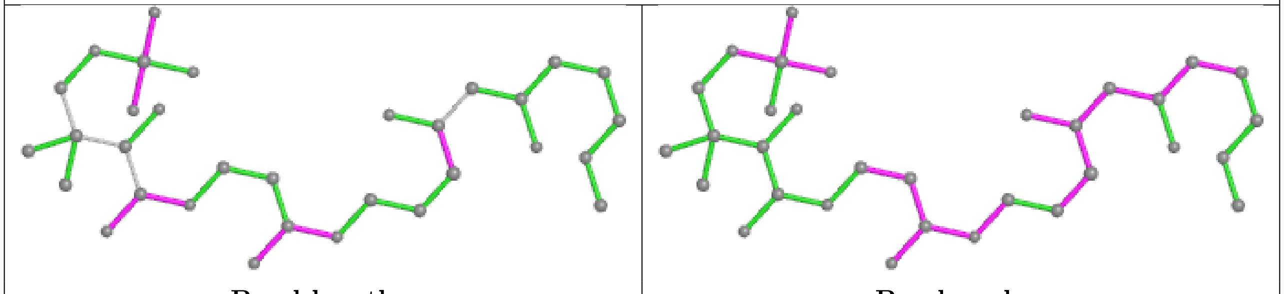
Bond lengths

Bond angles

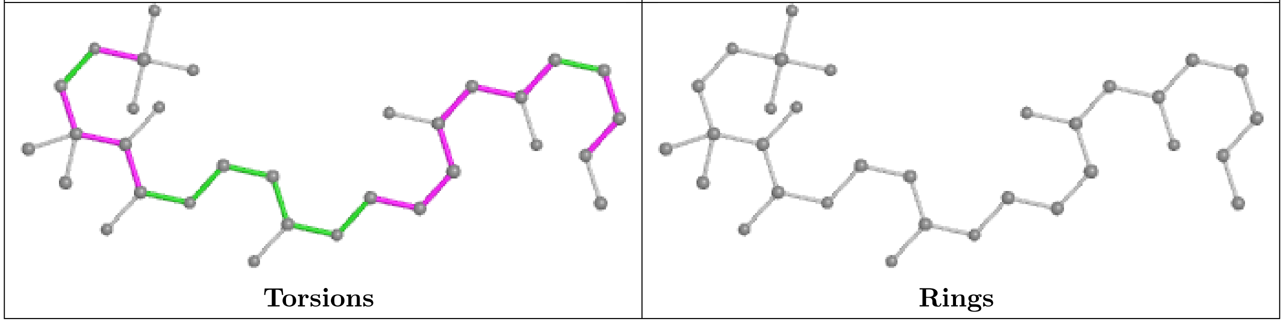
Torsions

Rings

Ligand EHZ W 201

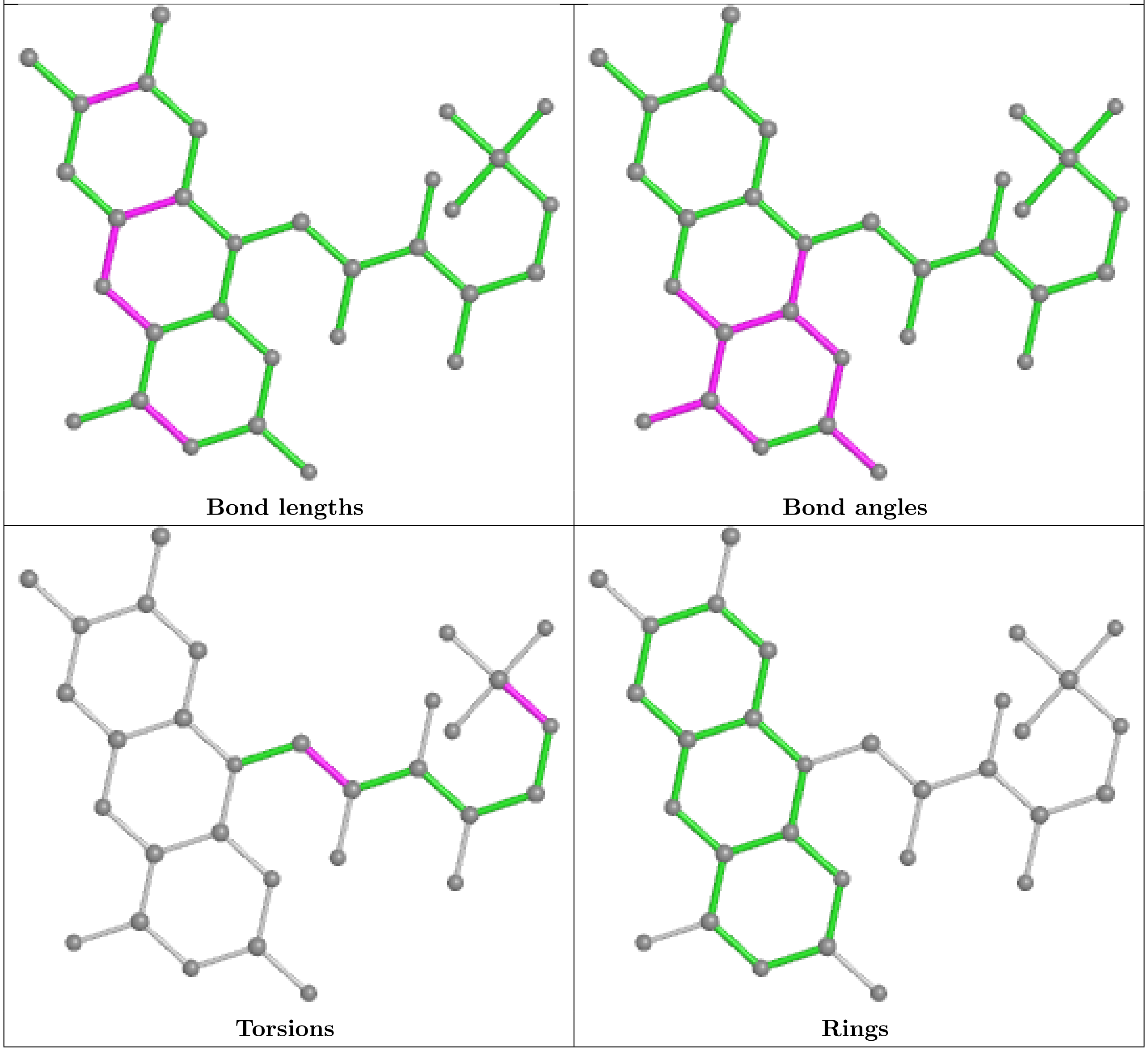


Bond lengths Bond angles



Torsions Rings

Ligand FMN F 501



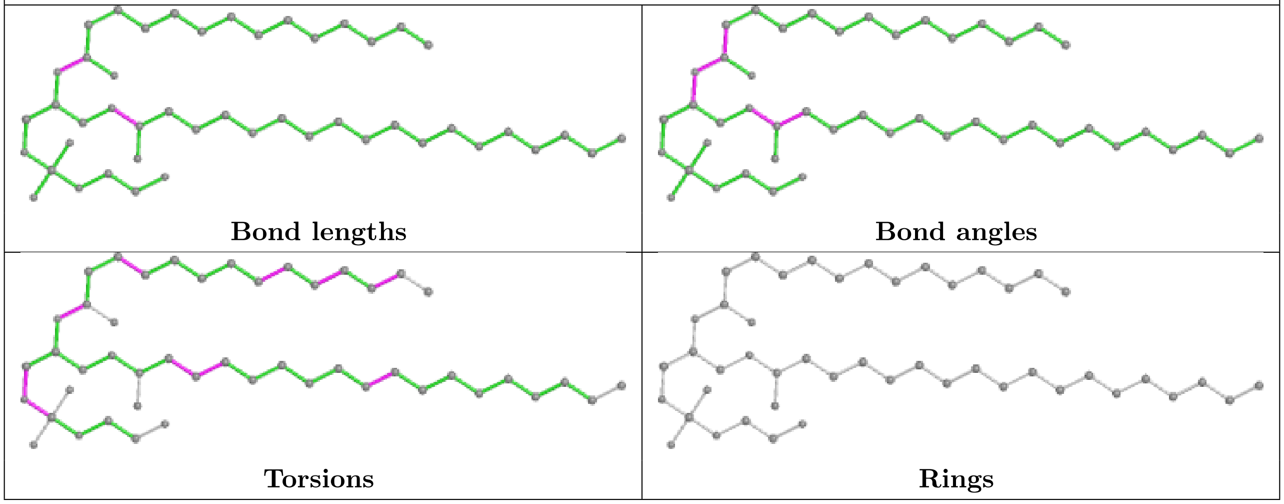
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE L 704



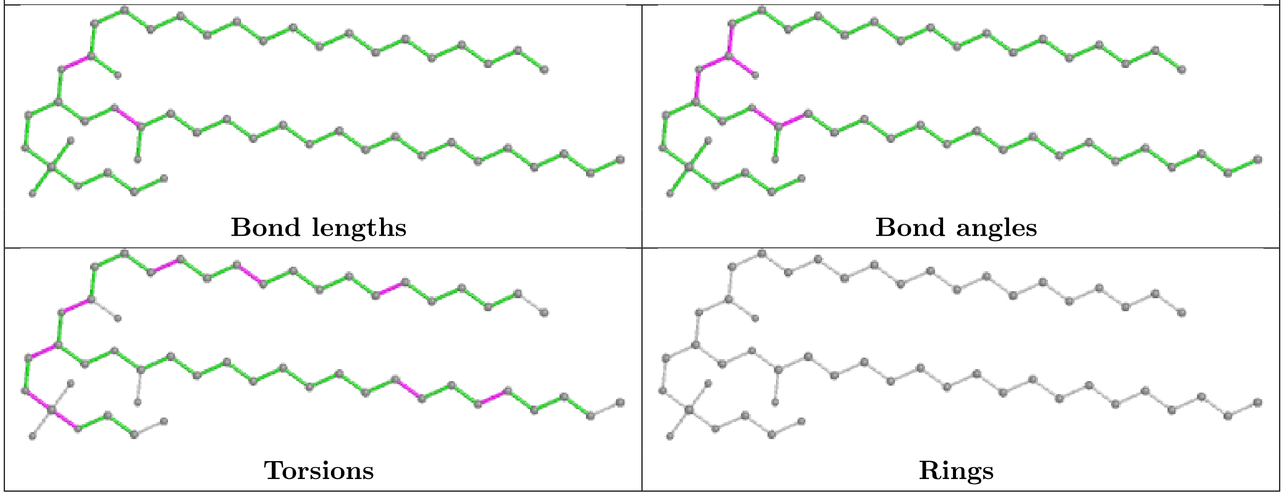
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE M 501



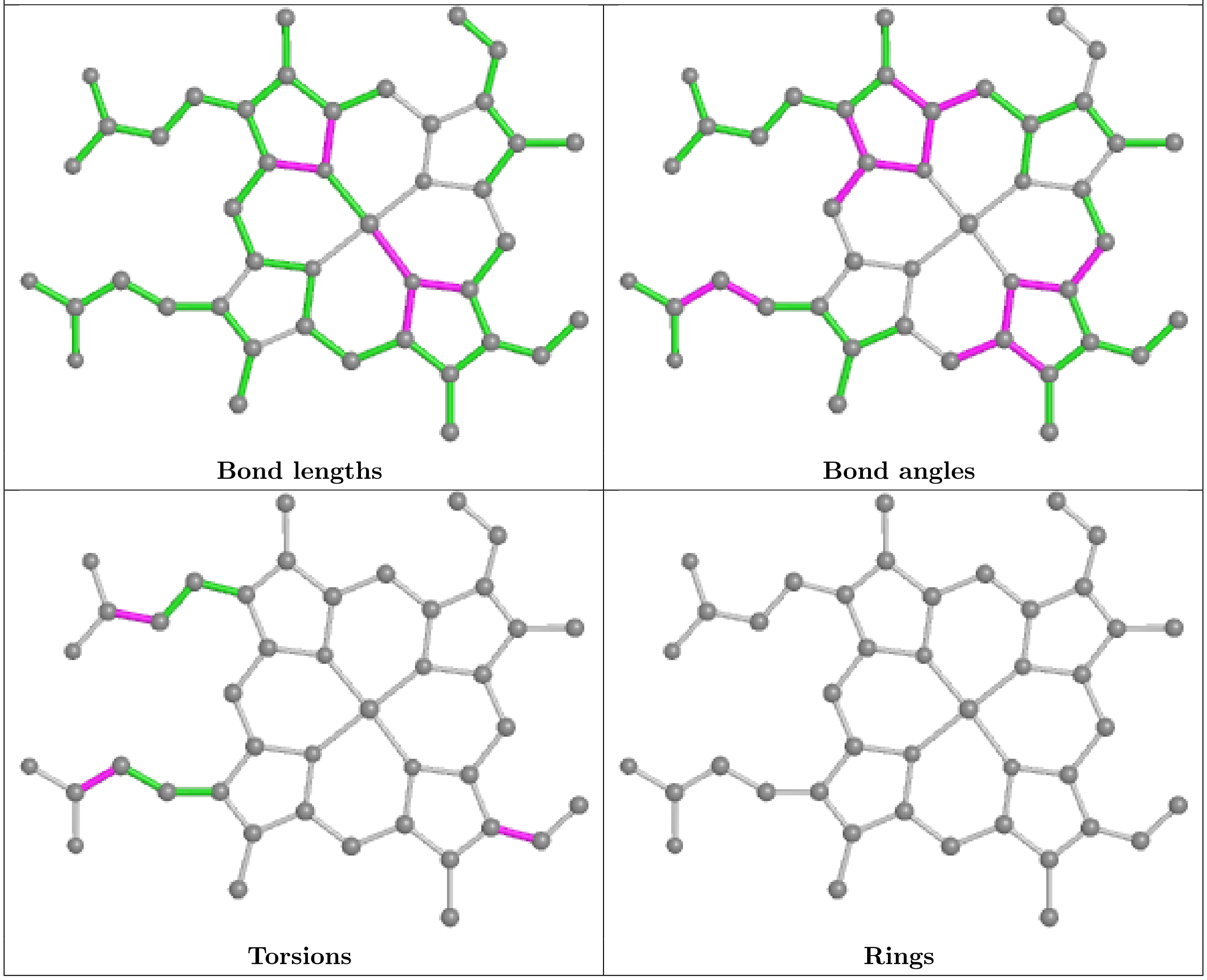
Bond lengths

Bond angles

Torsions

Rings

Ligand HEM AC 401



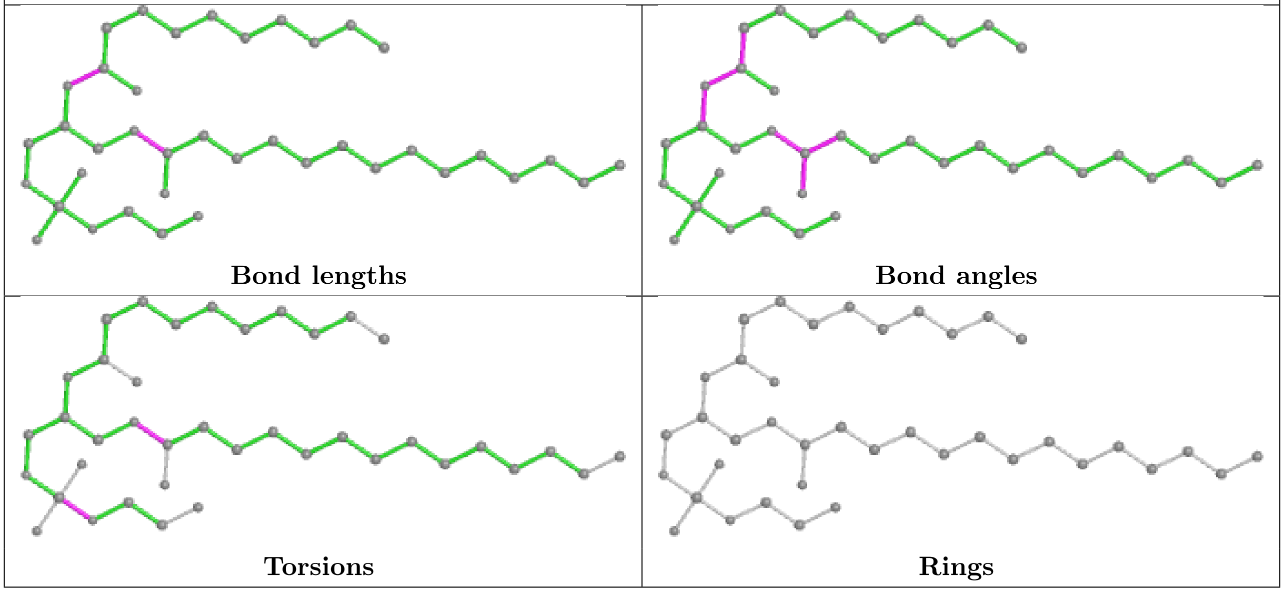
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Ag 102



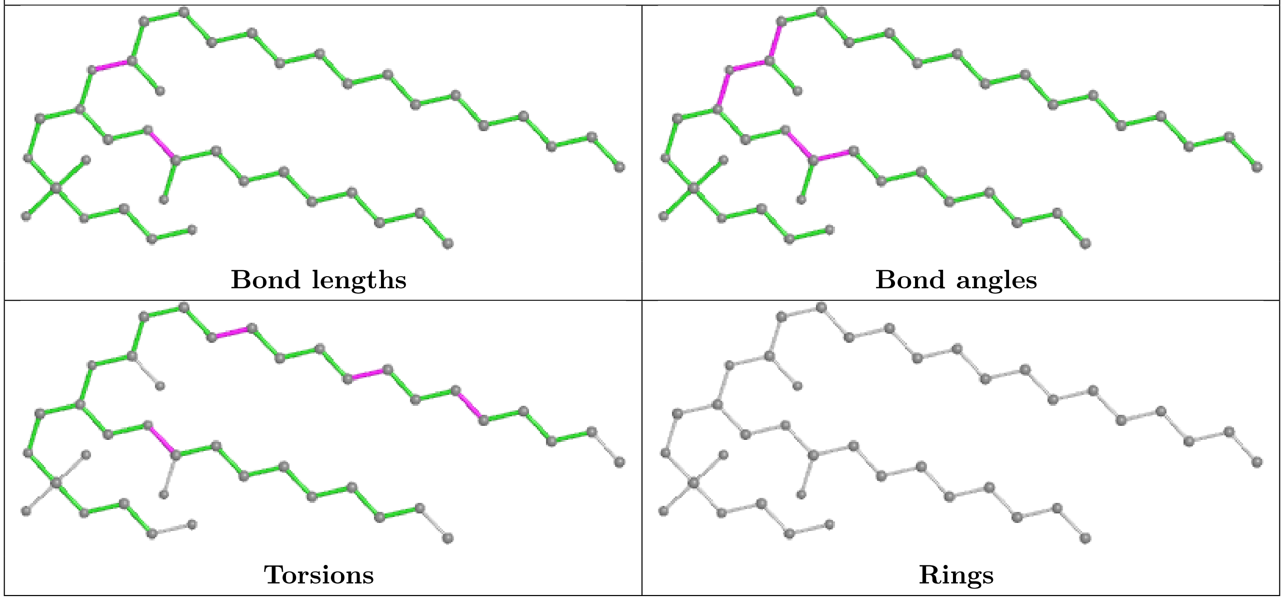
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Y 201



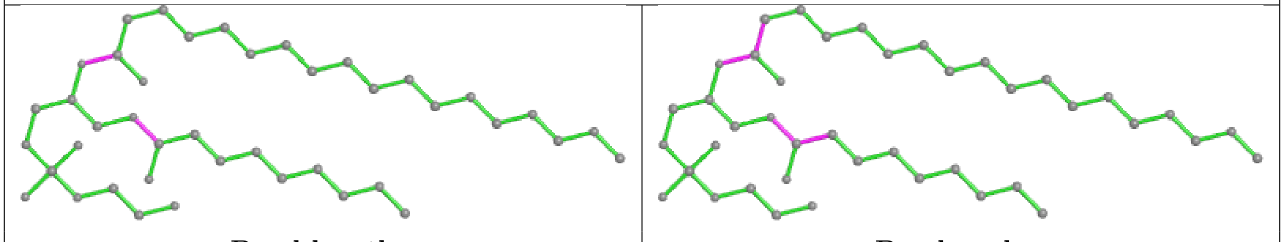
Bond lengths

Bond angles

Torsions

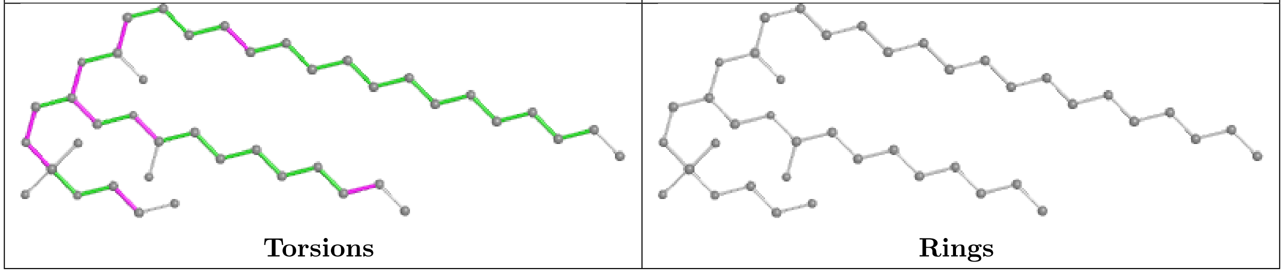
Rings

Ligand 3PE L 701



Bond lengths

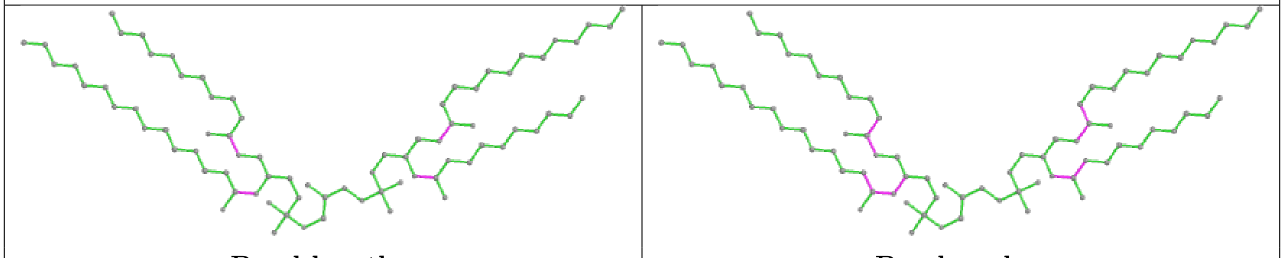
Bond angles



Torsions

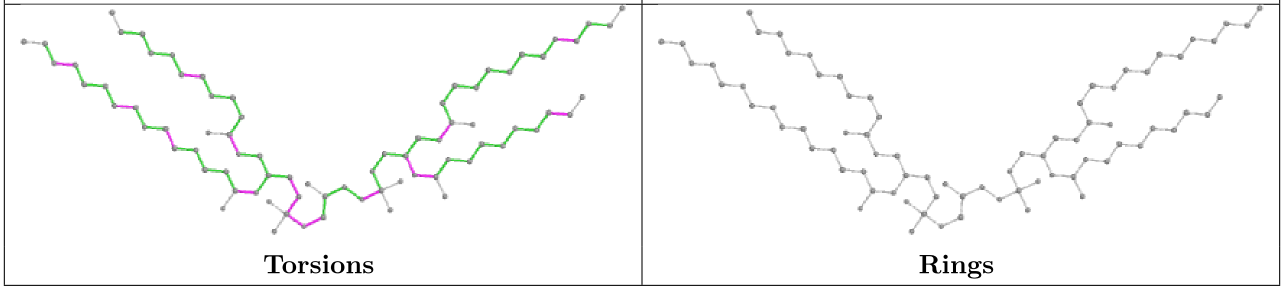
Rings

Ligand CDL L 705



Bond lengths

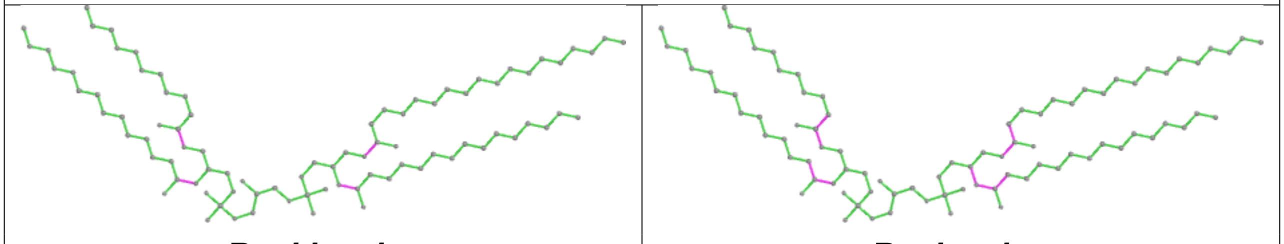
Bond angles



Torsions

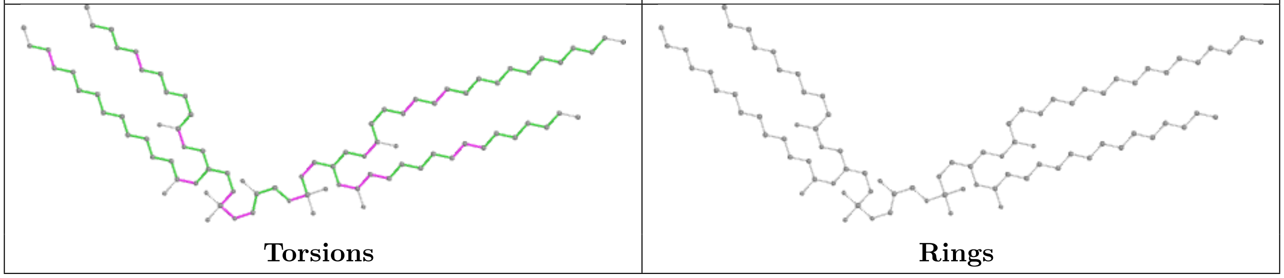
Rings

Ligand CDL L 706



Bond lengths

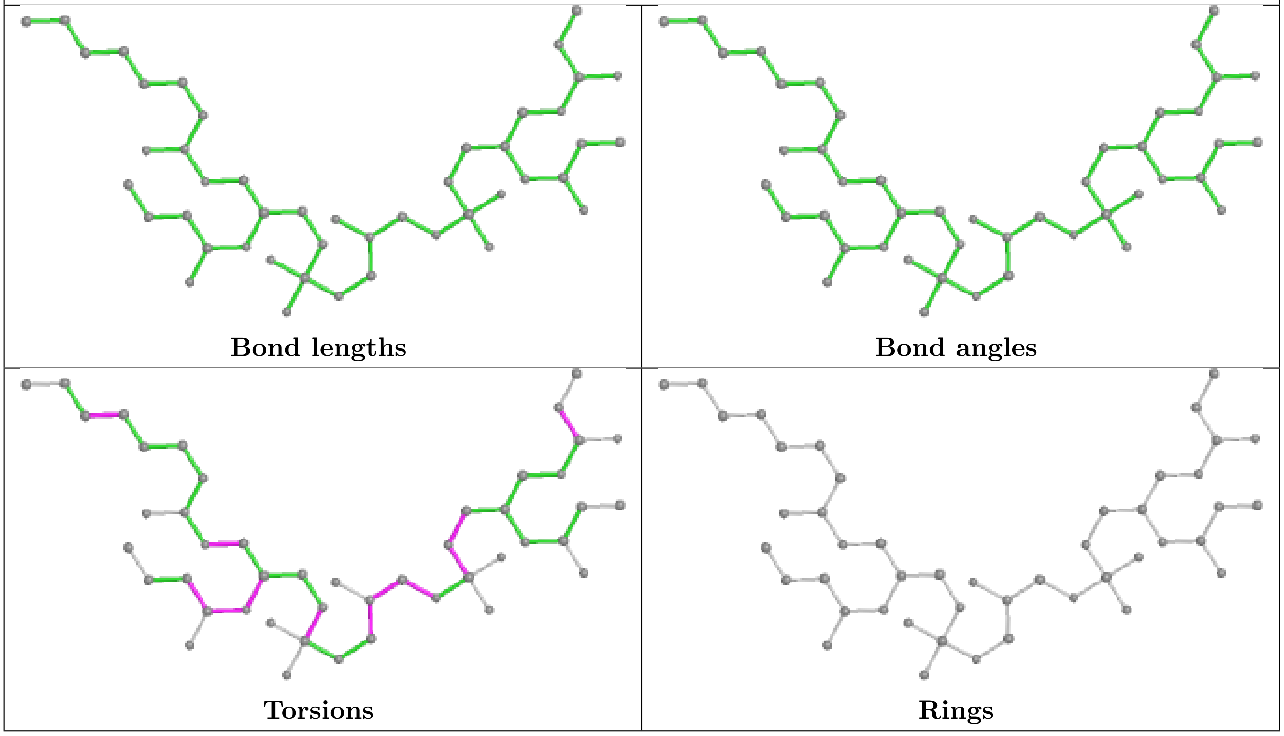
Bond angles



Torsions

Rings

Ligand CDL Aa 501



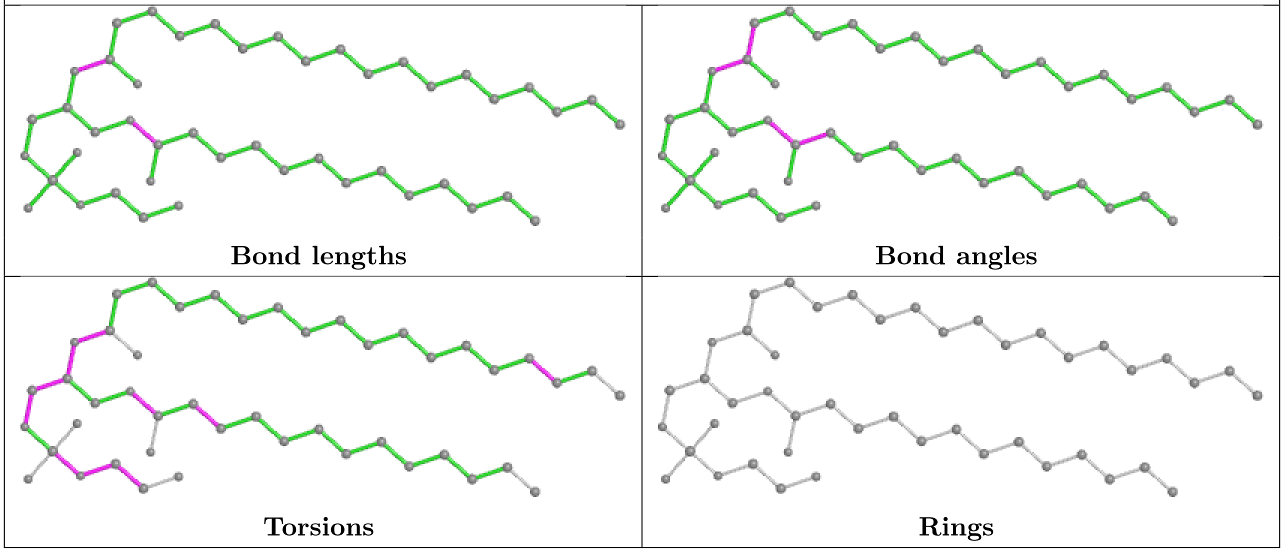
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE A 401



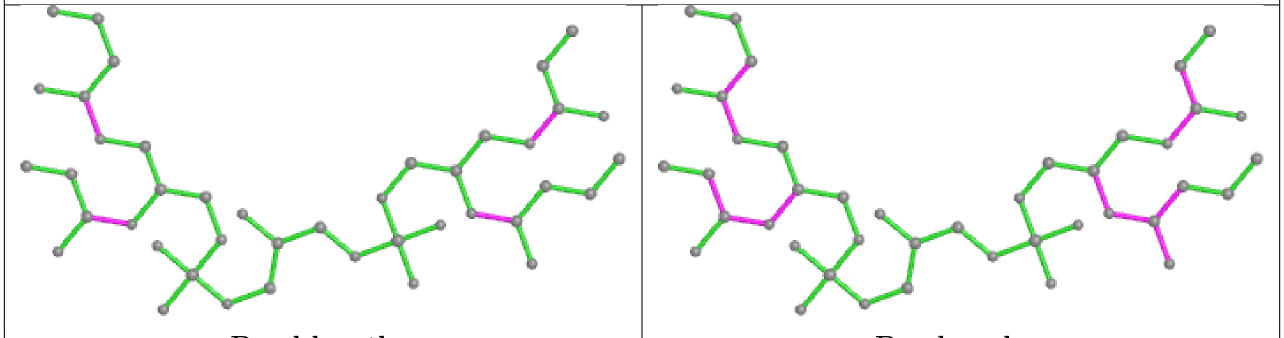
Bond lengths

Bond angles

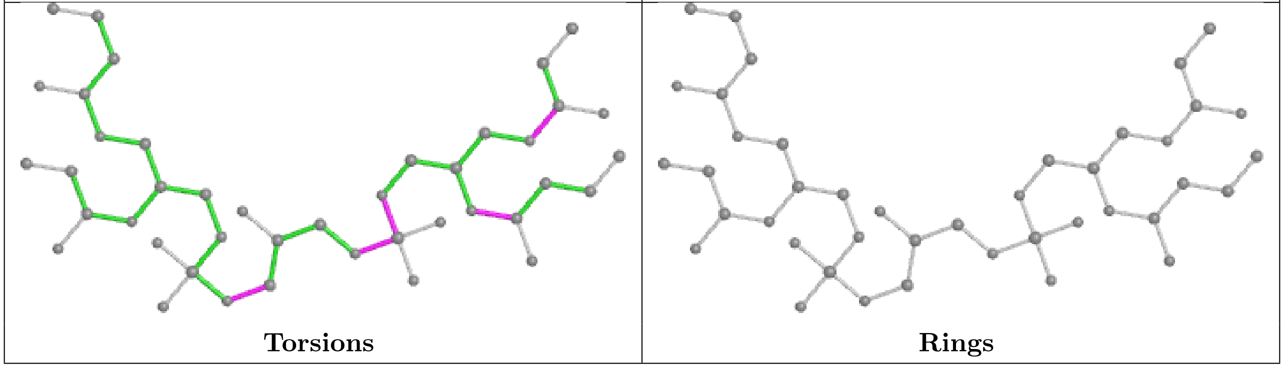
Torsions

Rings

Ligand CDL Ac 407

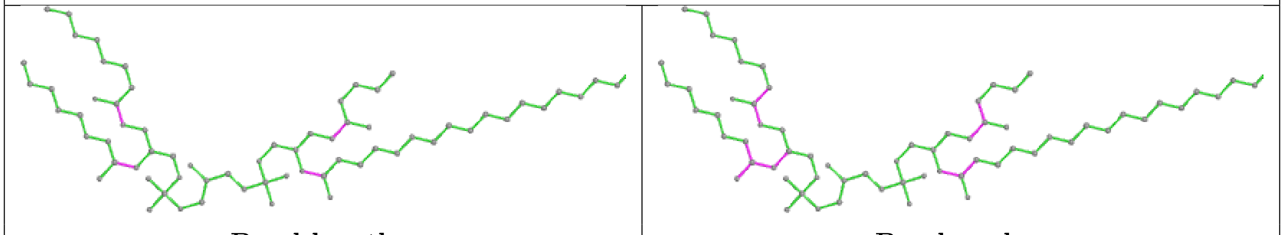


Bond lengths **Bond angles**

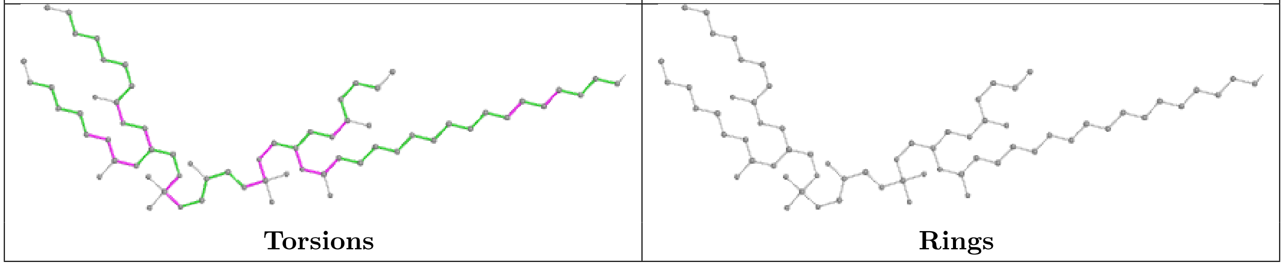


Torsions **Rings**

Ligand CDL X 201

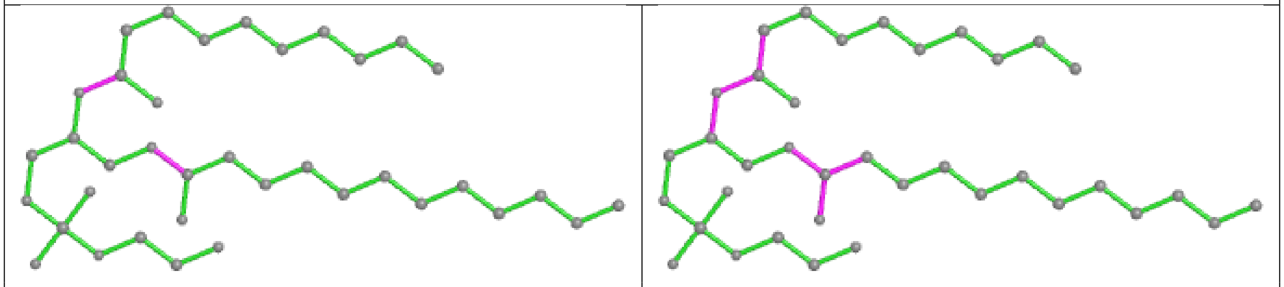


Bond lengths **Bond angles**



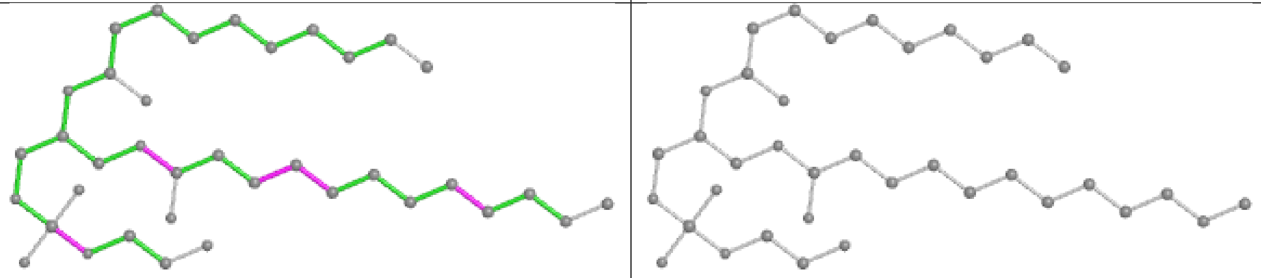
Torsions **Rings**

Ligand 3PE N 401



Bond lengths

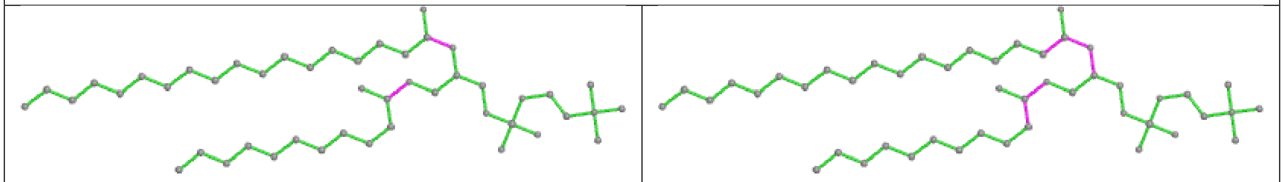
Bond angles



Torsions

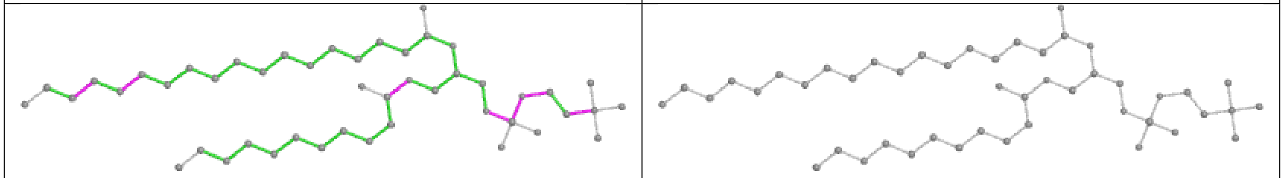
Rings

Ligand PC1 I 302



Bond lengths

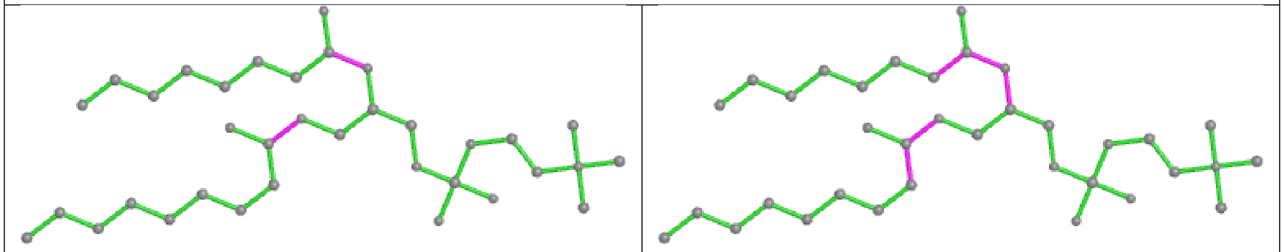
Bond angles



Torsions

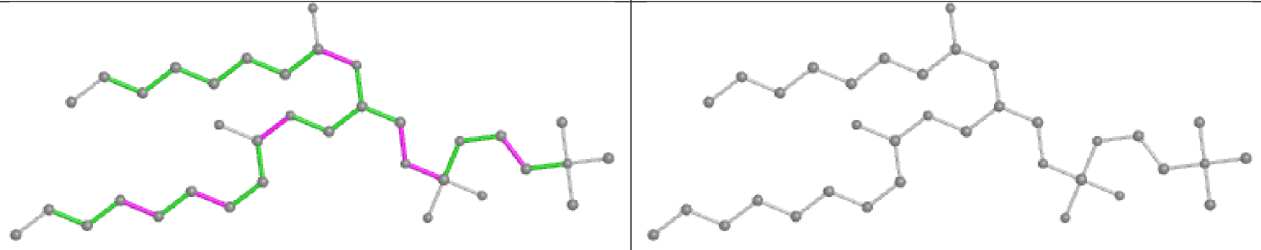
Rings

Ligand PC1 B 303



Bond lengths

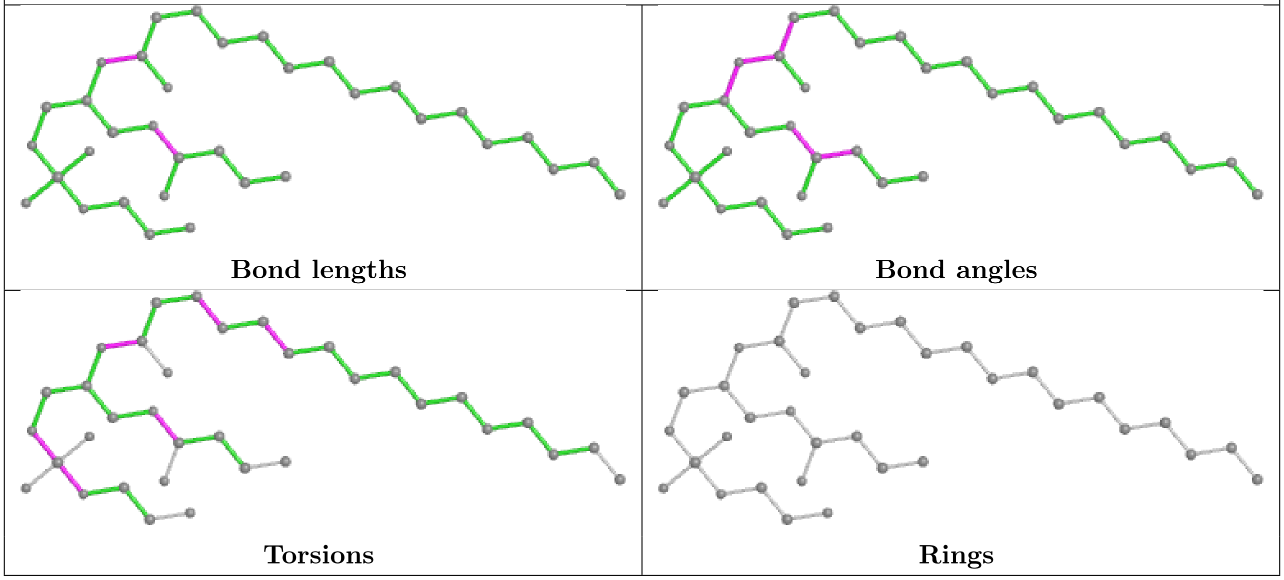
Bond angles



Torsions

Rings

Ligand 3PE AC 403



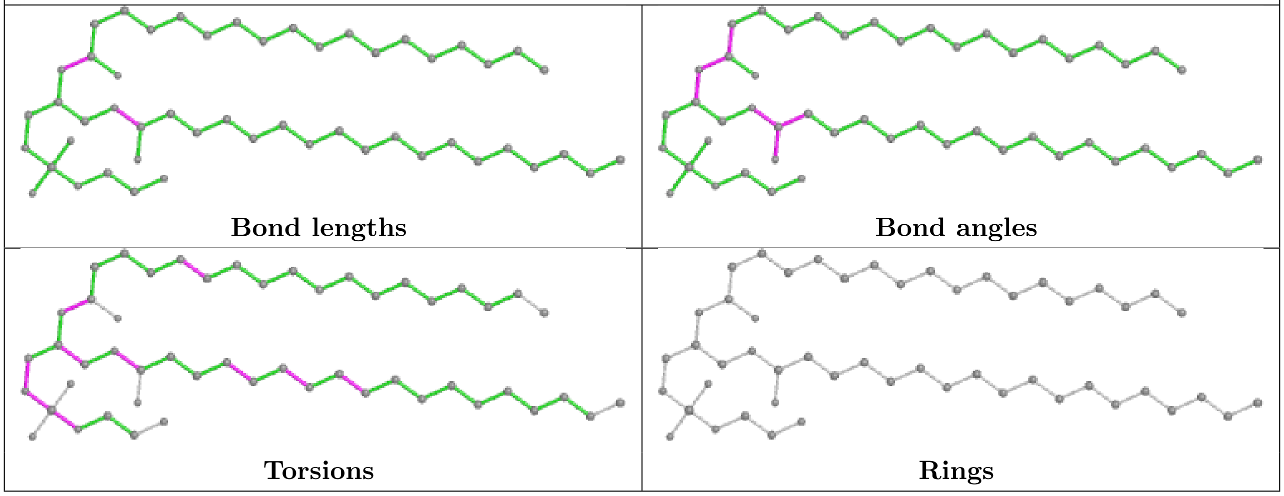
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE I 301



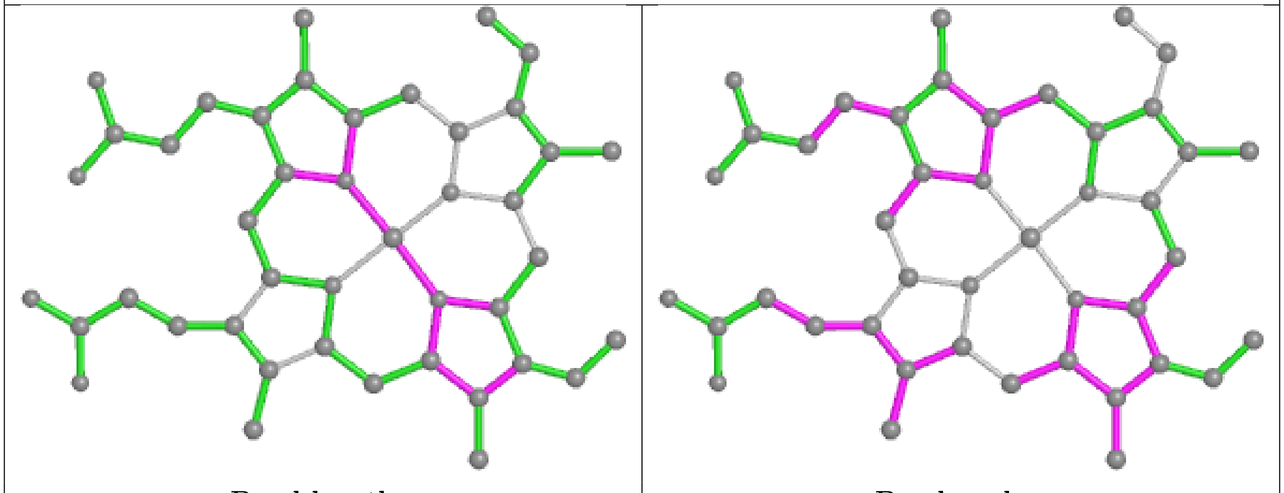
Bond lengths

Bond angles

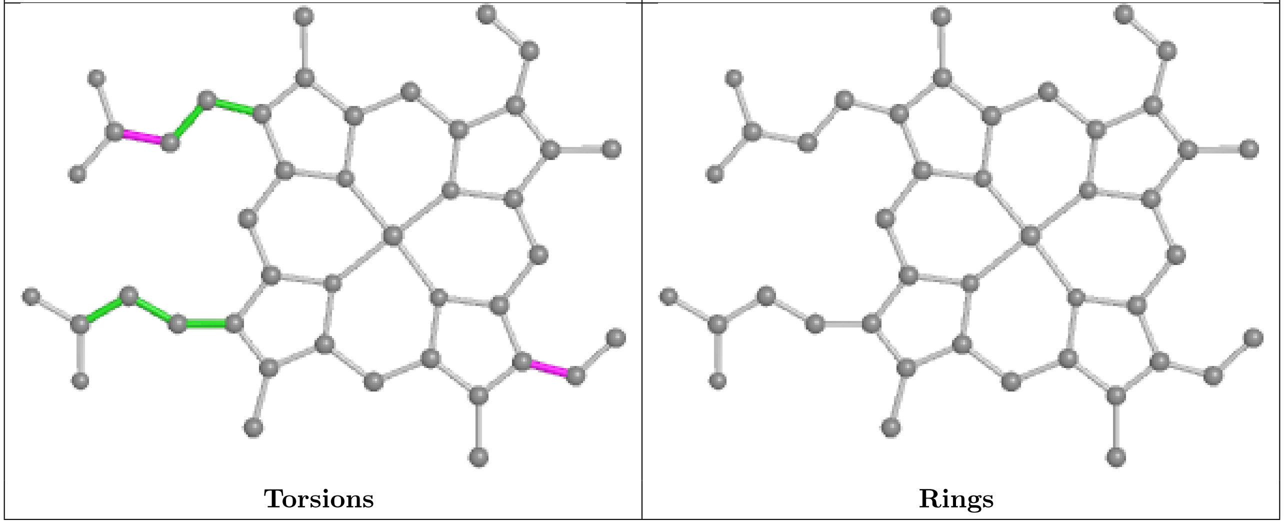
Torsions

Rings

Ligand HEM AC 402

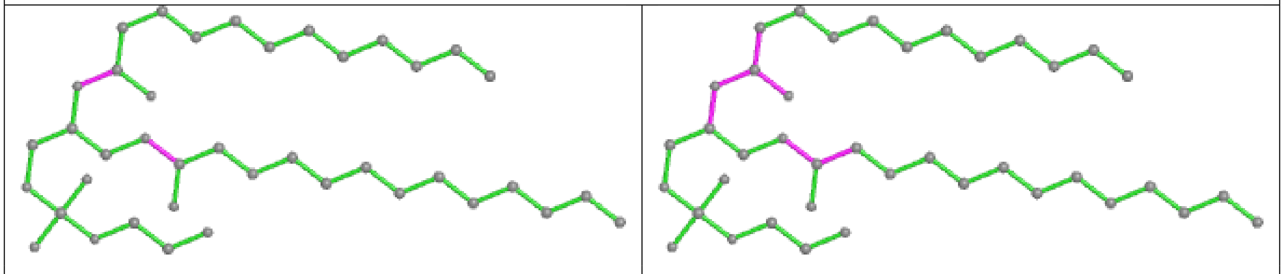


Bond lengths **Bond angles**

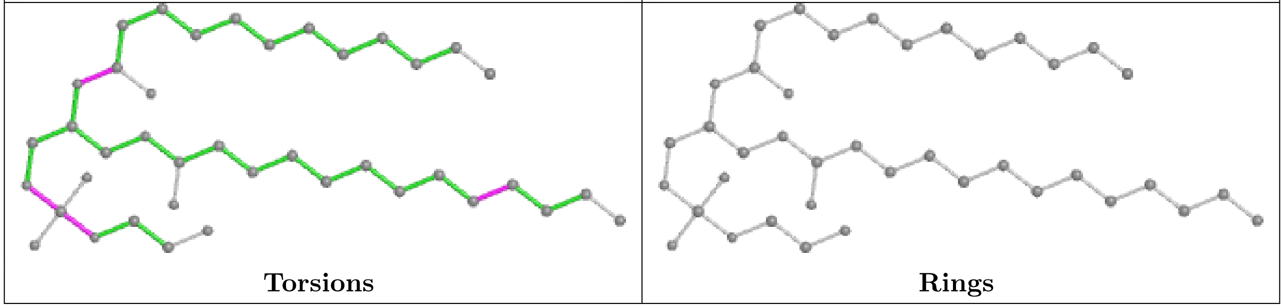


Torsions **Rings**

Ligand 3PE L 702

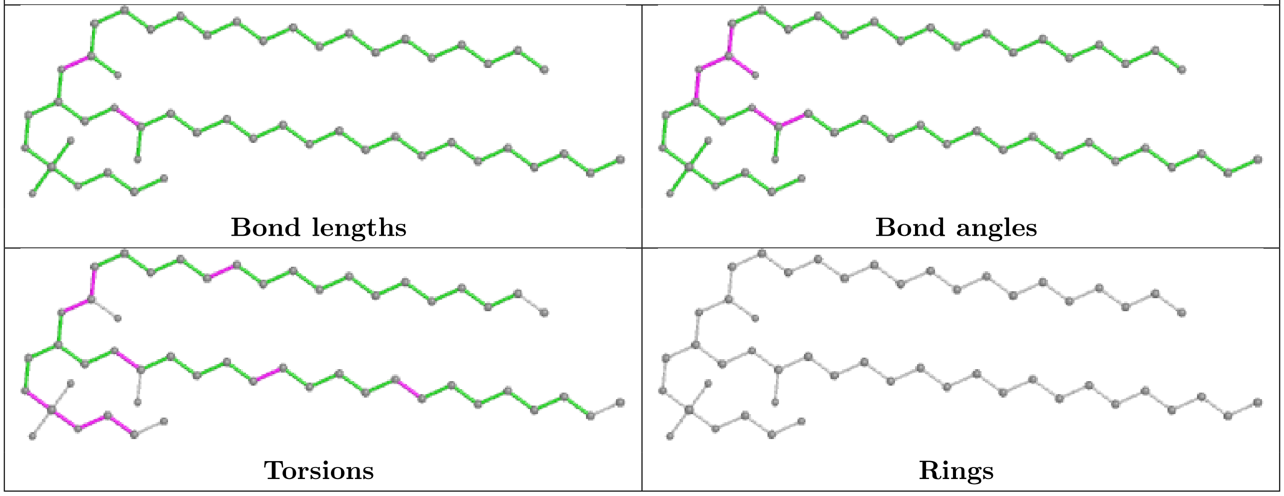


Bond lengths **Bond angles**



Torsions **Rings**

Ligand 3PE M 502



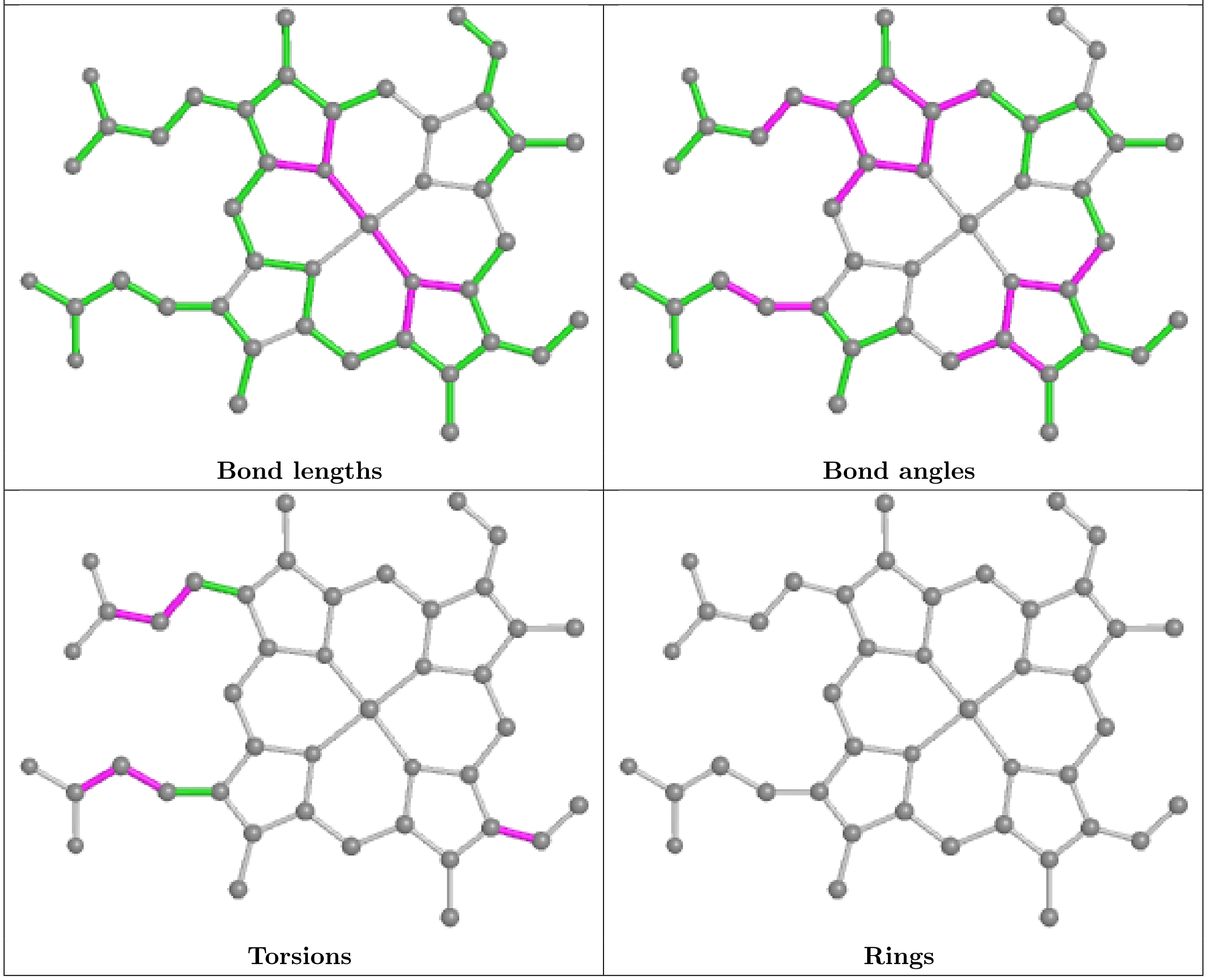
Bond lengths

Bond angles

Torsions

Rings

Ligand HEM Ac 403



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

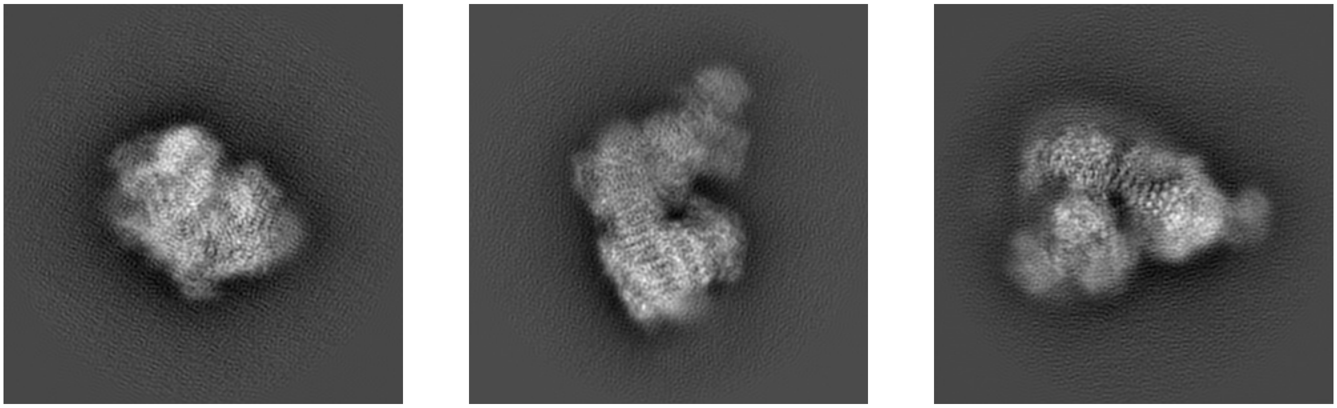
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-35331. 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.

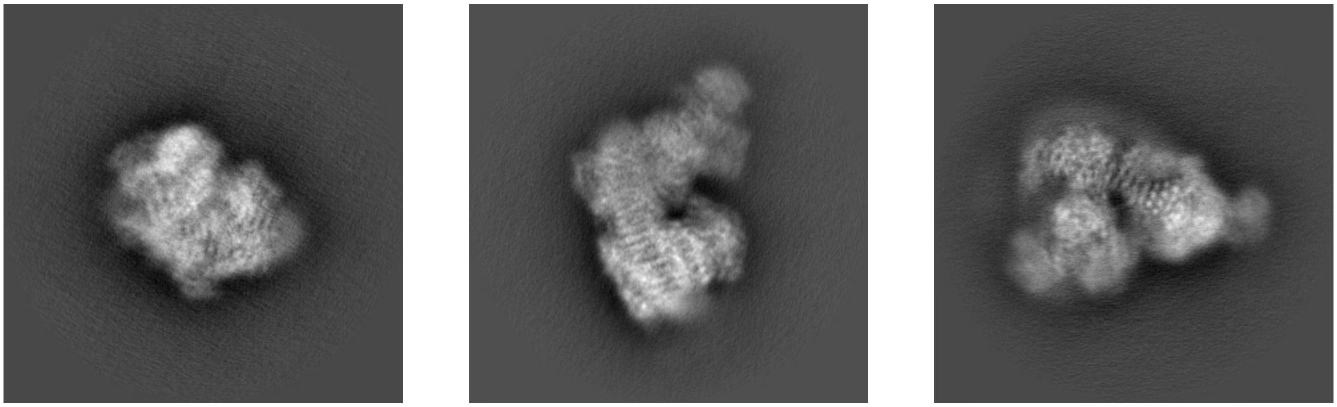
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

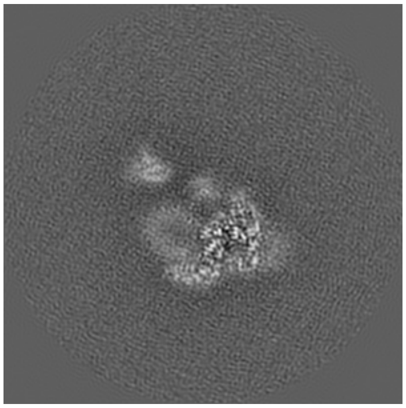


X Y Z

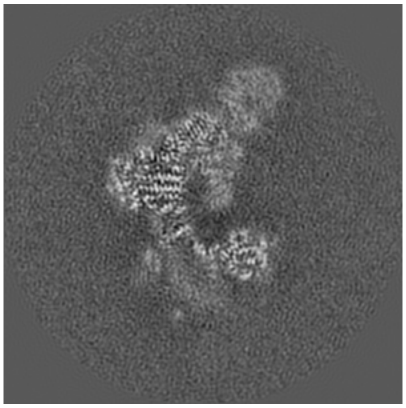
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

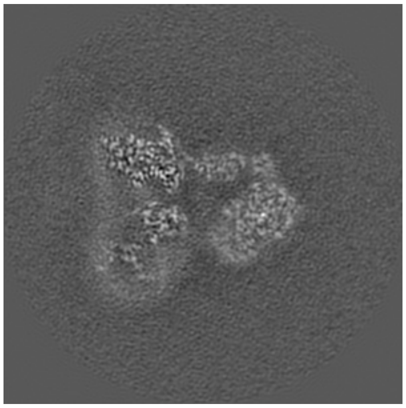
6.2.1 Primary map



X Index: 192

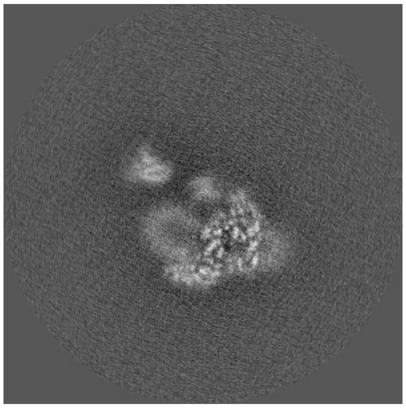


Y Index: 192

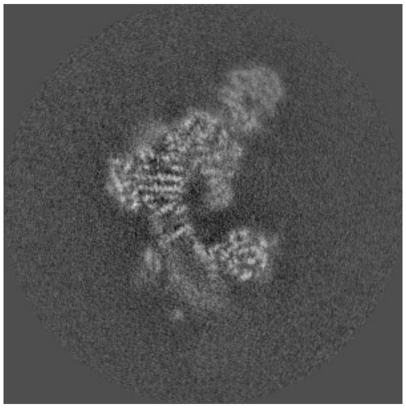


Z Index: 192

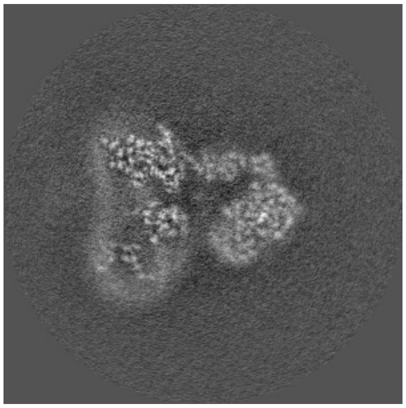
6.2.2 Raw map



X Index: 192



Y Index: 192

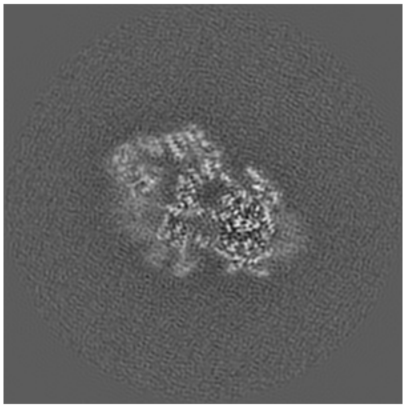


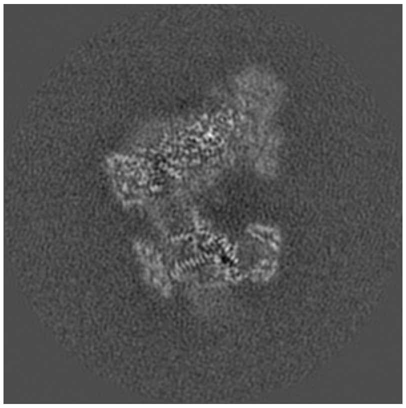
Z Index: 192

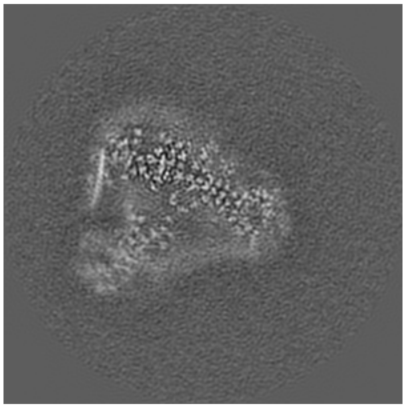
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

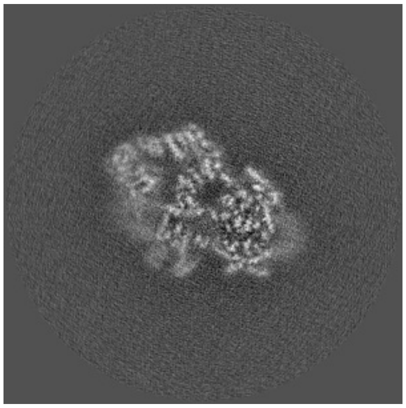
6.3.1 Primary map

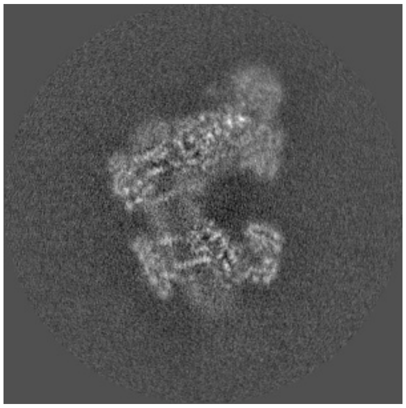

X Index: 154

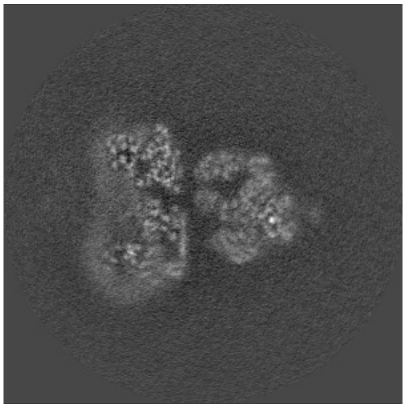

Y Index: 177


Z Index: 167

6.3.2 Raw map


X Index: 154

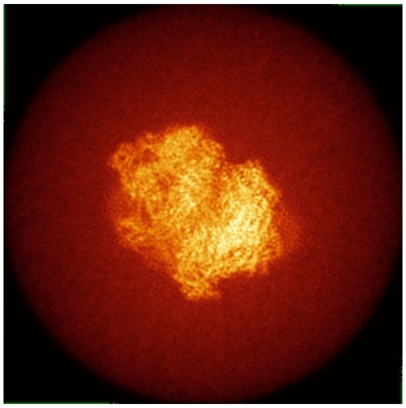

Y Index: 174

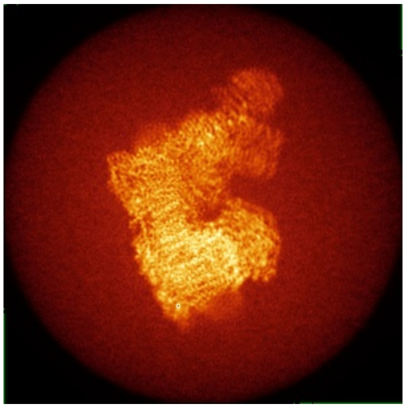

Z Index: 198

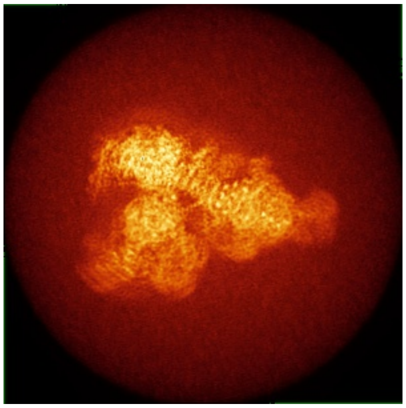
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

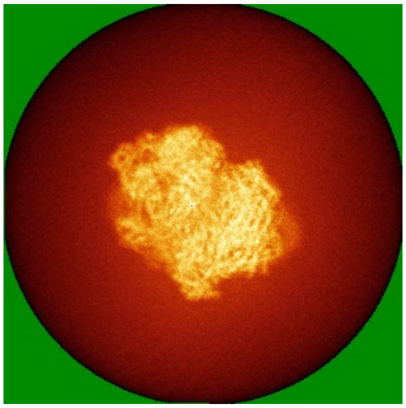
6.4.1 Primary map

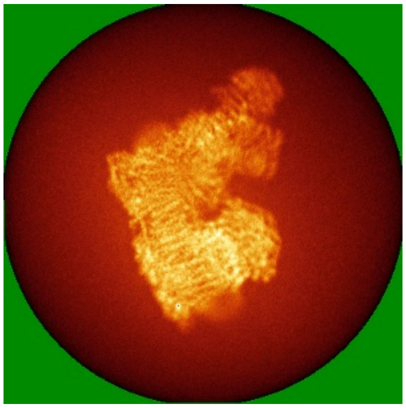

X

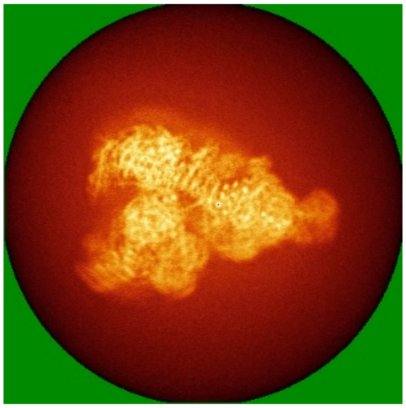

Y


Z

6.4.2 Raw map


X


Y


Z

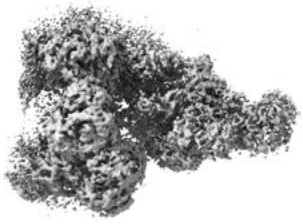
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

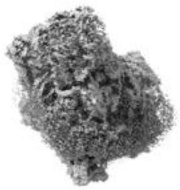

X


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.

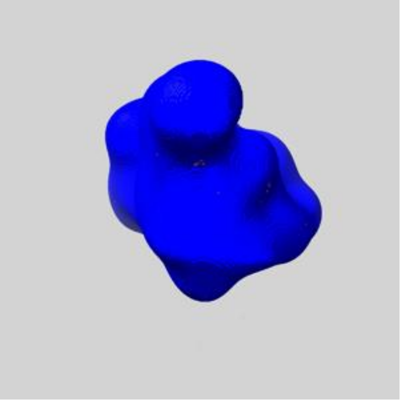
6.6 Mask visualisation

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

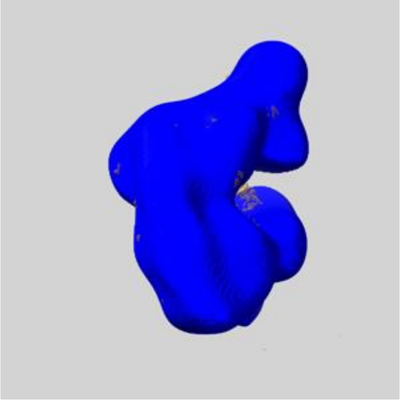
A mask typically either:

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

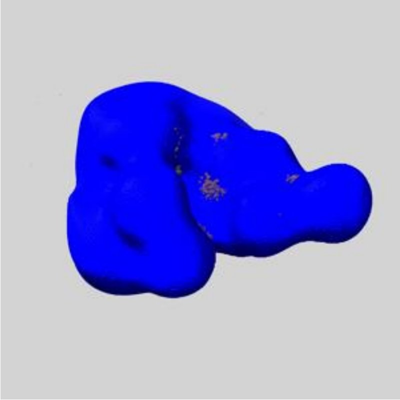
6.6.1 emd_35331_msk_1.map



X



Y

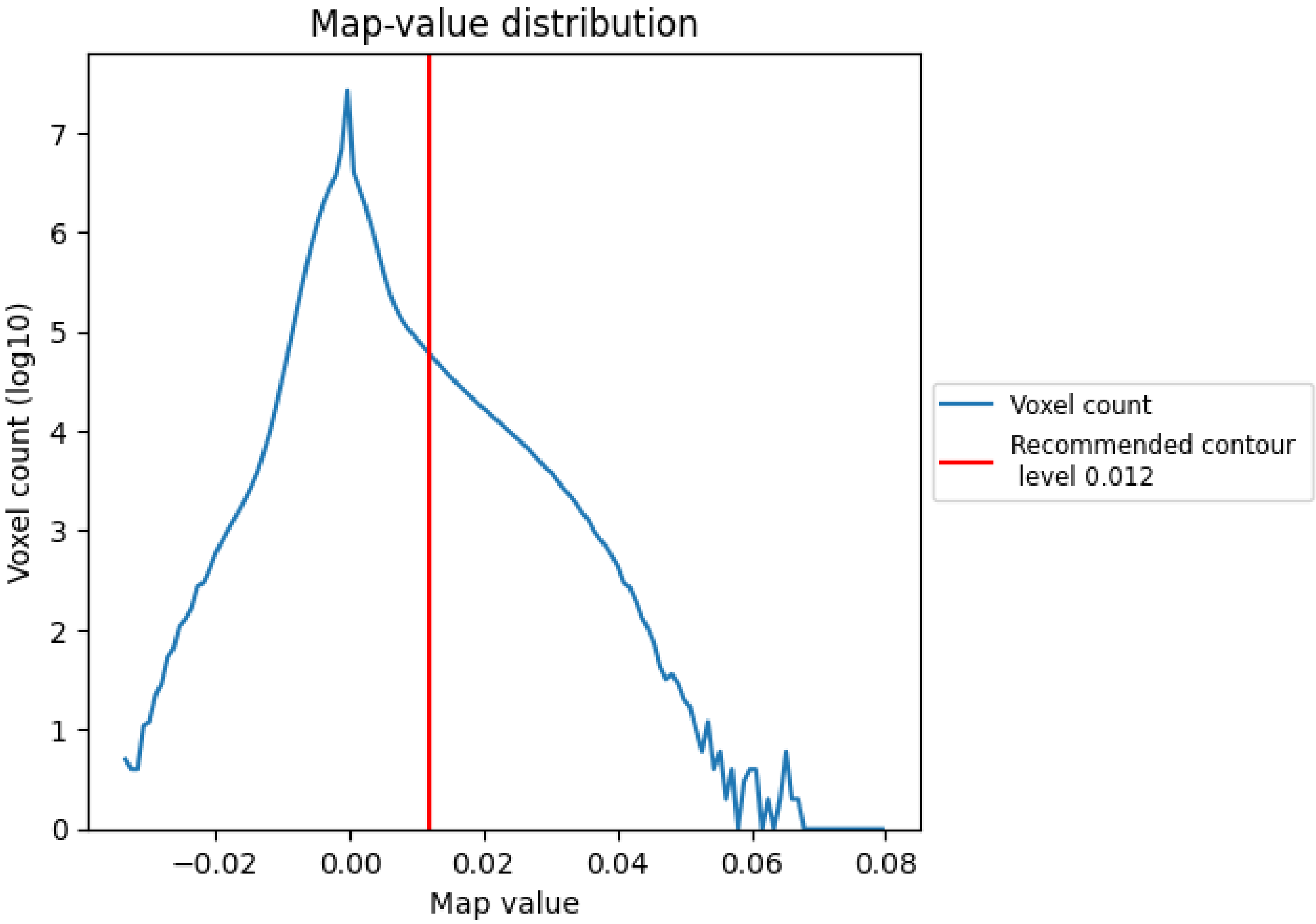


Z

7 Map analysis ⓘ

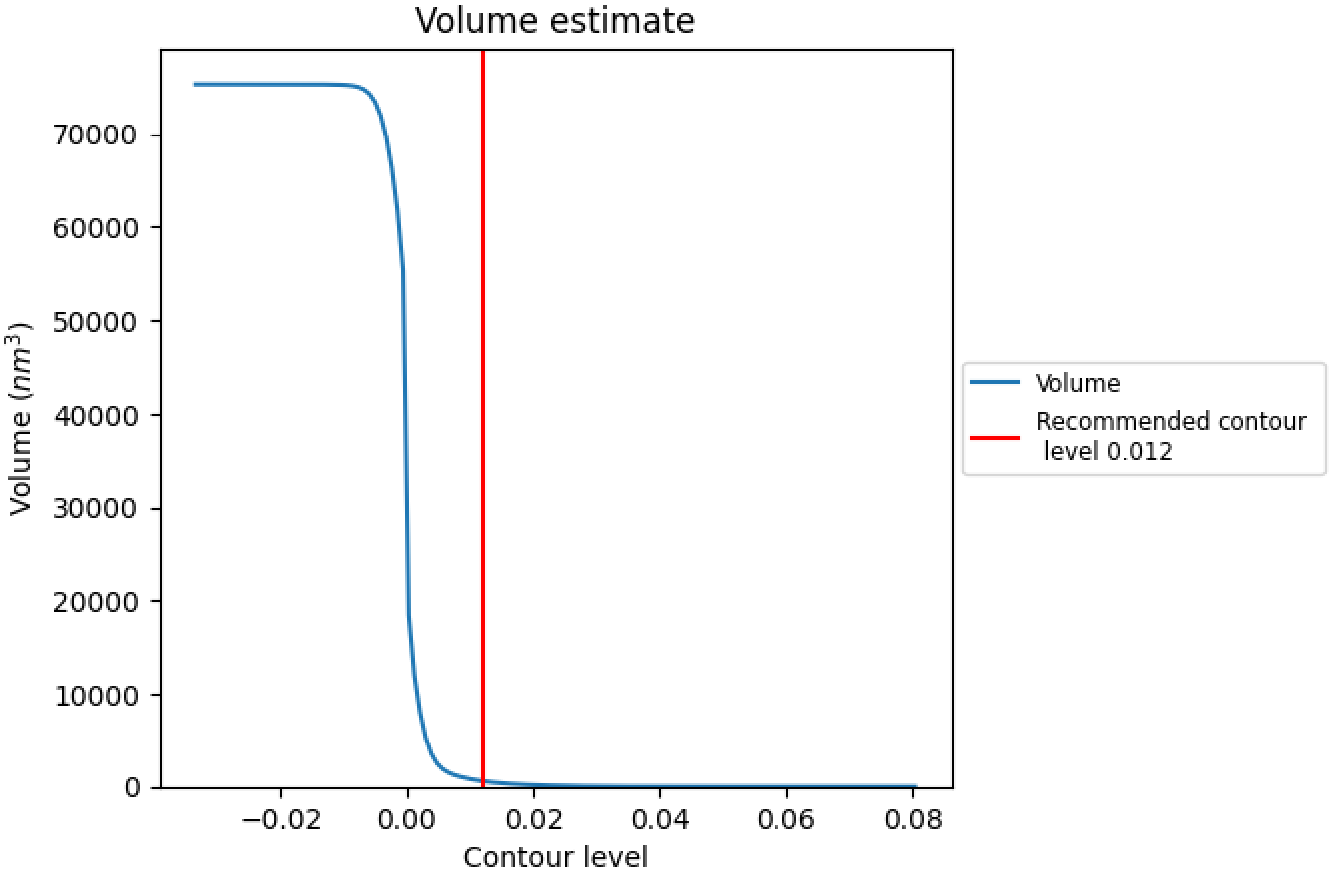
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

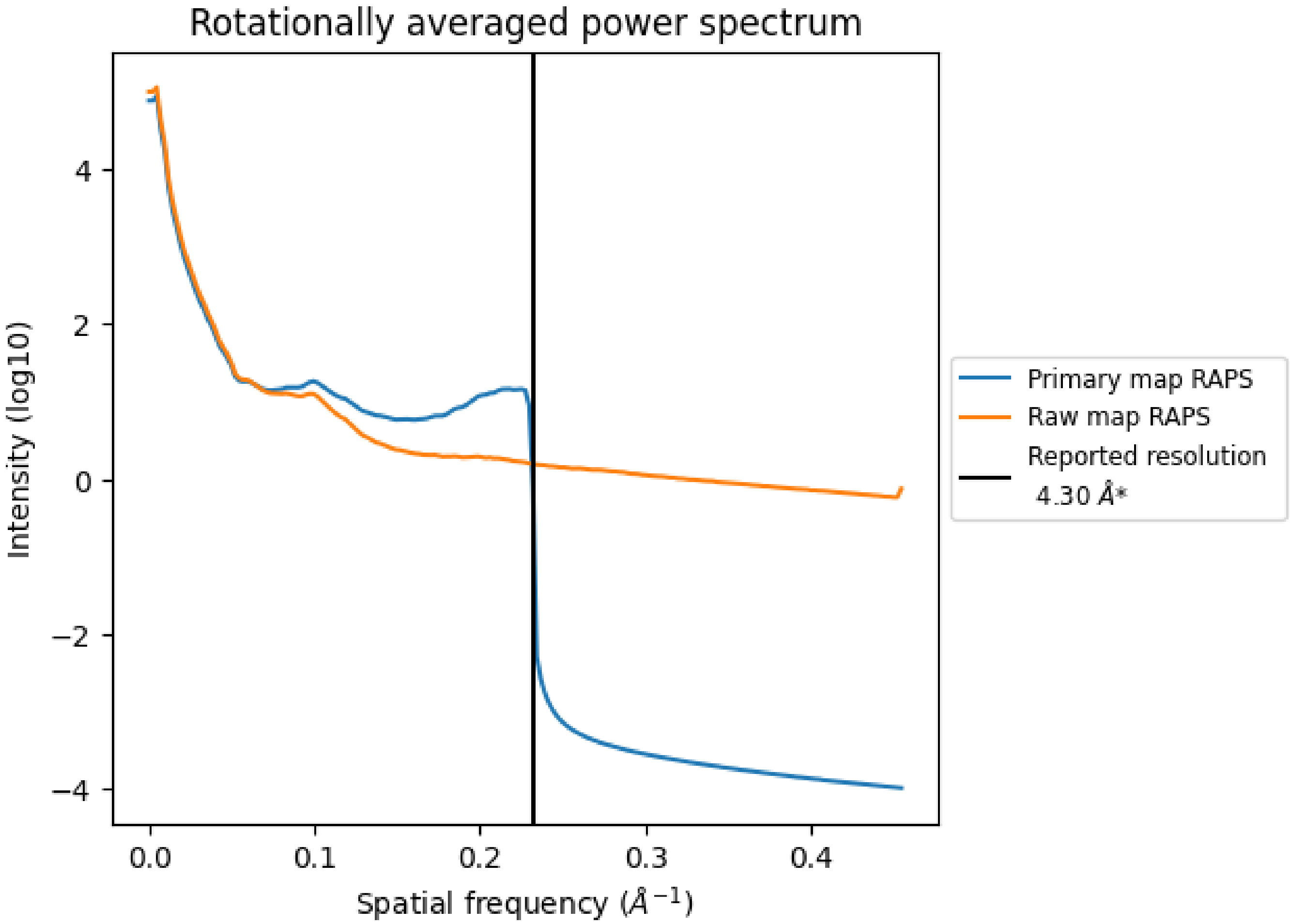
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 593 nm^3; this corresponds to an approximate mass of 536 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

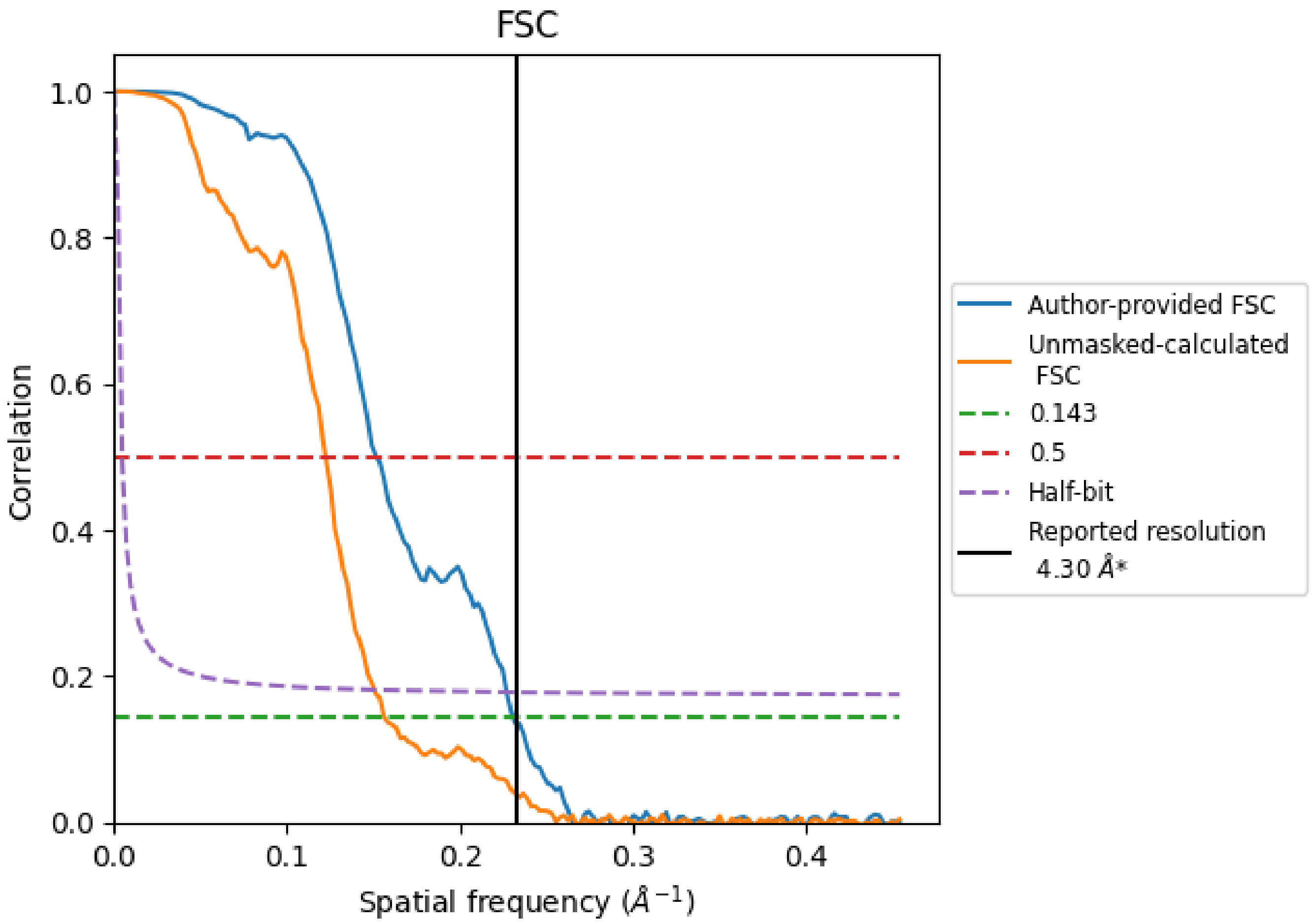


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



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

8.2 Resolution estimates

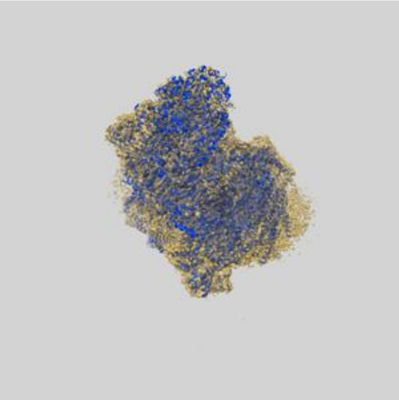
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.33	6.59	4.40
Unmasked-calculated*	6.39	8.17	6.64

*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 6.39 differs from the reported value 4.3 by more than 10 %

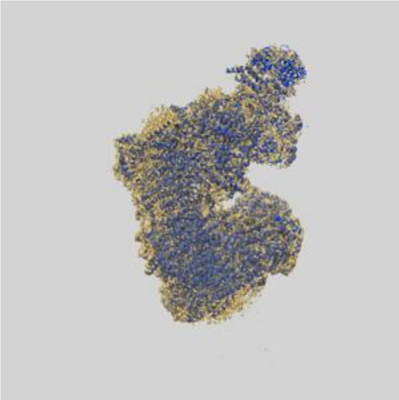
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-35331 and PDB model 8IB4. Per-residue inclusion information can be found in section 3 on page 27.

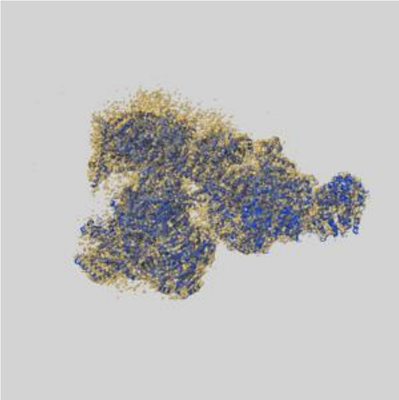
9.1 Map-model overlay ⓘ



X



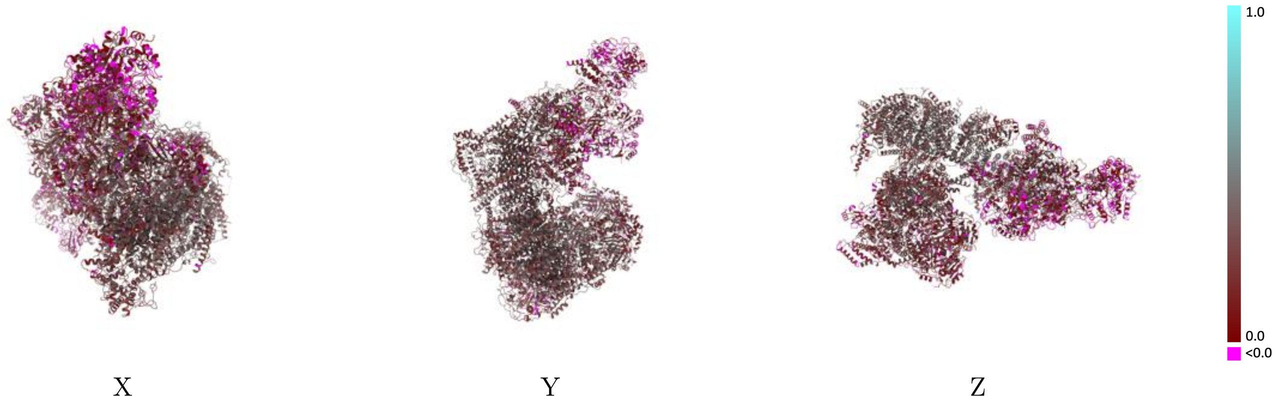
Y



Z

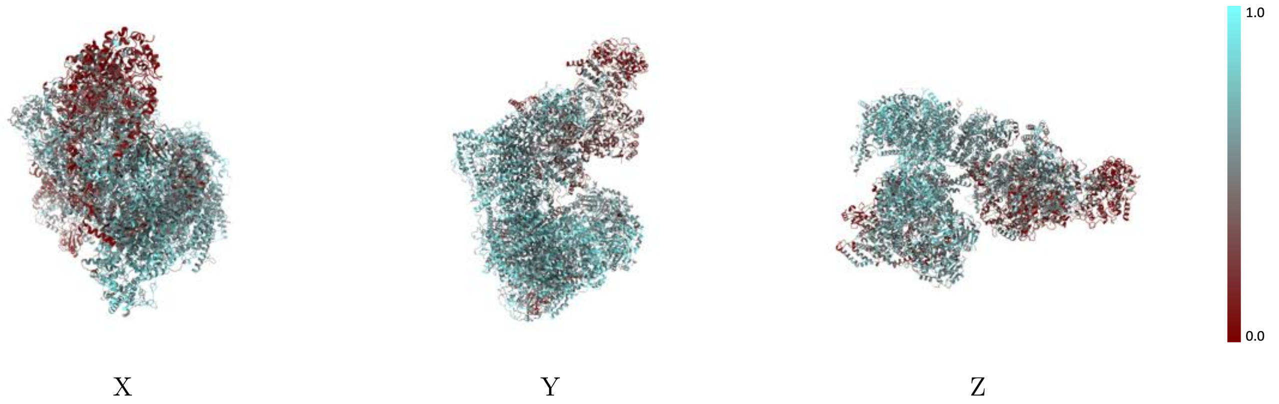
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



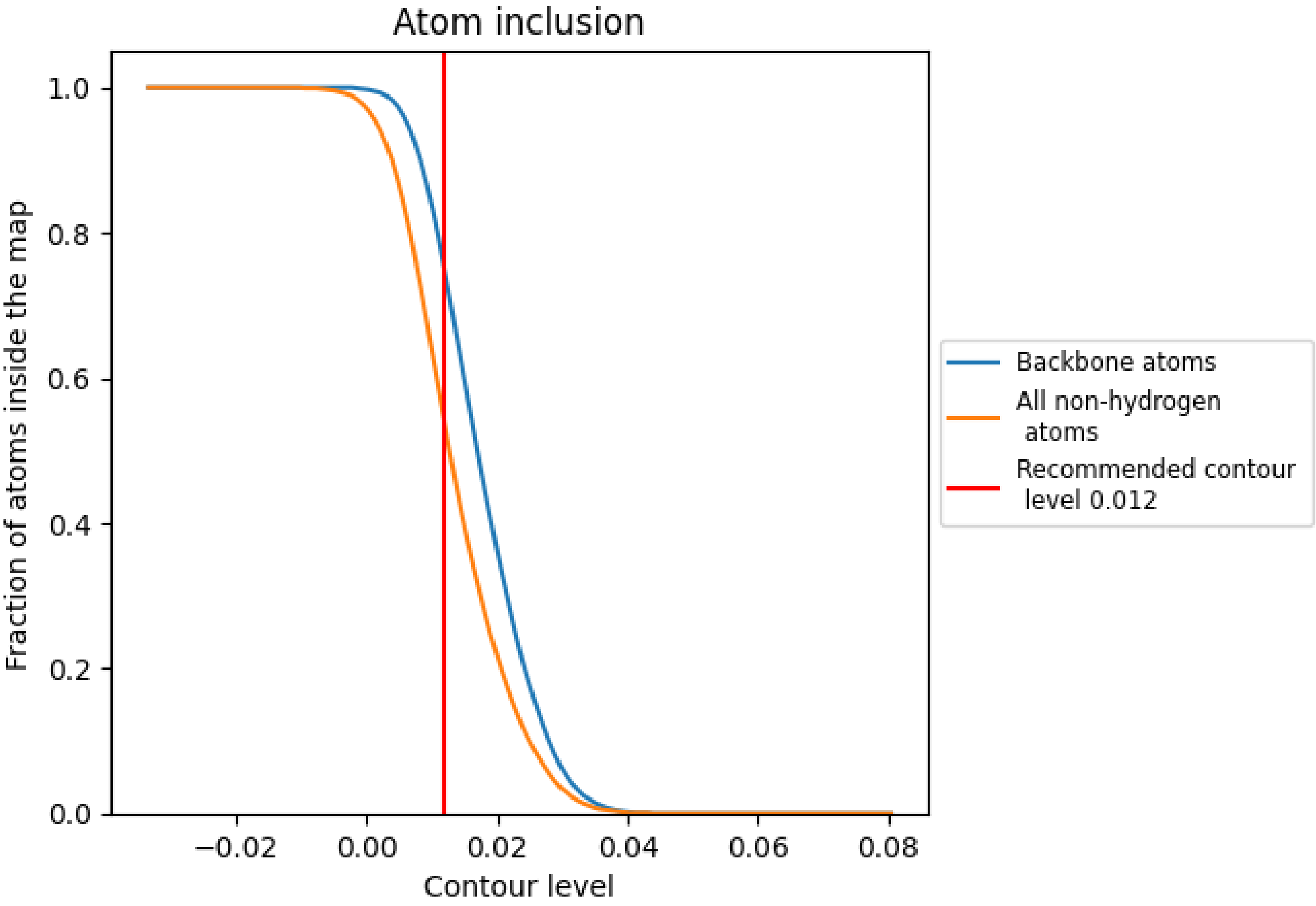
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 75% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.5370	0.2580
A	0.5630	0.3210
AA	0.5930	0.2210
AB	0.5900	0.2290
AC	0.4970	0.2570
AD	0.5020	0.1900
AE	0.1630	0.1300
AF	0.6180	0.2580
AG	0.4350	0.1990
AH	0.4400	0.1220
AI	0.2820	0.2100
AJ	0.1830	0.1680
AK	0.1720	0.1620
Aa	0.6900	0.3210
Ab	0.6560	0.2690
Ac	0.5620	0.2860
Ad	0.5900	0.2170
Ae	0.1790	0.1480
Af	0.6290	0.2990
Ag	0.5350	0.2910
Ah	0.5510	0.1690
Aj	0.3540	0.2340
Ak	0.1580	0.1740
B	0.6170	0.3110
C	0.5140	0.2050
D	0.6100	0.3010
E	0.1830	0.0850
F	0.2410	0.1140
G	0.3630	0.1480
H	0.6240	0.3380
I	0.6400	0.2880
J	0.5270	0.2930
K	0.6230	0.3560
L	0.6340	0.3490
M	0.6740	0.3770

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Chain	Atom inclusion	Q-score
N	0.6600	0.3700
O	0.5300	0.2840
P	0.3430	0.1390
Q	0.3060	0.1770
R	0.2130	0.1200
S	0.2980	0.1030
T	0.2020	0.0800
U	0.7410	0.3560
V	0.4580	0.1640
W	0.3570	0.1420
X	0.6760	0.2990
Y	0.6030	0.3310
Z	0.6950	0.3090
a	0.6500	0.3120
b	0.6520	0.2950
c	0.5930	0.2730
d	0.7040	0.3470
e	0.6680	0.3140
f	0.6080	0.2920
g	0.6530	0.3140
h	0.6790	0.3300
i	0.7090	0.3220
j	0.6840	0.3020
k	0.7380	0.3450
l	0.7390	0.3840
m	0.7130	0.3500
n	0.7500	0.3470
o	0.6400	0.2640
p	0.7140	0.3320
q	0.1600	0.1780
r	0.2320	0.1530
s	0.1050	0.0160