wwPDB EM Validation Summary Report

Nov 20, 2022 – 02:06 pm GMT

PDB ID	:	6QC2
EMDB ID	:	EMD-4494
Title	:	Ovine respiratory supercomplex I+III2 open class 2
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-26
Resolution	:	4.20 Å(reported)
Based on initial models	:	1PPJ, 5LNK

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

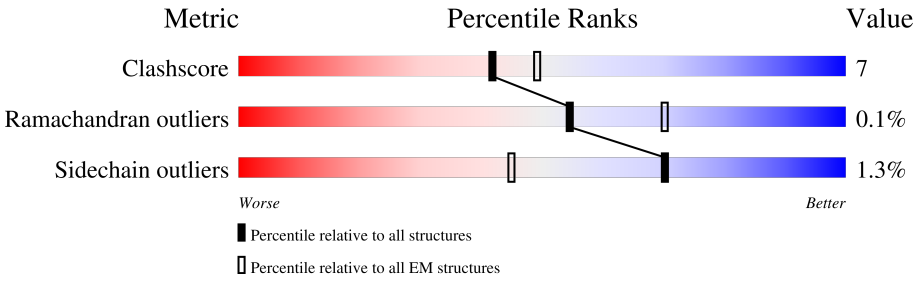
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	D3	115	48% 68% 10% 22%
2	D1	318	37% 68% 24% • 7%
3	D6	175	56% 75% 21% •
4	4L	98	42% 80% 20%
5	D5	606	34% 79% 21%
6	D4	459	28% 80% 19% •
7	D2	347	26% 77% 22% •
8	AK	140	57% 81% 18% •

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Mol	Chain	Length	Quality of chain
9	B5	143	22% 77% 19%
10	AA	88	72% 77% 14% 9%
10	AB	88	25% 84% 15%
11	A8	171	30% 77% 21%
12	BJ	175	30% 77% 20%
13	AJ	320	34% 78% 21%
14	S5	105	25% 72% 22% 6%
15	A3	83	36% 66% 22% 11%
16	B3	97	33% 63% 11% 25%
17	C2	120	29% 82% 15%
18	B4	128	32% 79% 20%
19	AM	143	27% 75% 22%
20	B6	127	22% 53% 18% 26%
21	B7	119	39% 77% 20%
22	B9	178	19% 78% 21%
23	B2	72	36% 69% 21% 10%
24	B8	158	34% 77% 22%
25	BK	125	29% 62% 20% 18%
26	C1	49	29% 84% 10% 6%
27	B1	57	32% 77% 14% 9%
28	A1	70	43% 87% 13%
29	a1	446	42% 97%
29	a3	446	28% 98%
30	a2	439	50% 93% 6%
30	a4	439	31% 93% 6%

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Mol	Chain	Length	Quality of chain
31	b1	379	42% 99%
31	b2	379	32% 99%
32	c1	240	45% 98%
32	c2	240	35% 98%
33	f1	196	88% 99%
33	f2	196	88% 98%
34	d1	110	32% 88% 9%
34	d2	110	42% 89% 8%
35	q1	81	51% 90% 10%
35	q2	81	36% 91% 7%
36	h1	78	58% 81% 17%
36	h2	78	56% 81% 17%
37	x1	78	37% 42% 58%
37	x2	78	26% 38% 62%
38	i1	63	62% 86% 13%
38	i2	63	60% 90% 10%
39	V1	445	38% 74% 22%
40	V2	217	37% 75% 23%
41	S1	704	42% 72% 26%
42	S2	430	31% 78% 21%
43	S3	228	27% 74% 17% 9%
44	S7	179	21% 63% 23% 13%
45	S8	176	19% 69% 28%
46	V3	75	25% 39% 12% 45%
47	S6	96	33% 83% 15%

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Mol	Chain	Length	Quality of chain
48	S4	133	38% 72% 22% 5%
49	A9	338	52% 67% 18% 14%
50	A2	98	46% 67% 15% 16%
51	A5	115	43% 79% 16%
52	A6	127	50% 76% 13% 10%
53	A7	112	47% 69% 15% 15%
54	AL	145	50% 68% 28%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
62	SF4	S8	202	-	-	X	-
62	SF4	V1	500	-	-	X	-

2 Entry composition (i)

There are 65 unique types of molecules in this entry. The entry contains 96938 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D3	90	728	500	103	120	5	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D1	296	2362	1599	358	386	19	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D6	168	1280	859	183	225	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4L	98	748	489	112	132	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D5	606	4805	3187	746	828	44	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D4	459	3646	2428	571	607	40	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D2	347	Total	C	N	O	S	0	0
			2724	1808	416	460	40		

- Molecule 8 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AK	140	Total	C	N	O	S	0	0
			1025	654	175	190	6		

- Molecule 9 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B5	139	Total	C	N	O	S	0	0
			1156	761	194	199	2		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AB	87	Total	C	N	O	S	0	0
			702	451	103	143	5		
10	AA	80	Total	C	N	O	S	0	0
			645	416	96	128	5		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A8	171	Total	C	N	O	S	0	0
			1404	889	253	252	10		

- Molecule 12 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BJ	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	319	Total	C	N	O	S	0	0
			2583	1653	430	490	10		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S5	99	Total	C	N	O	S	0	0
			822	520	154	142	6		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A3	74	Total	C	N	O	S	0	0
			582	379	96	105	2		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B3	73	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C2	119	Total	C	N	O	S	0	0
			997	647	174	172	4		

- Molecule 18 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B4	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 19 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AM	139	Total	C	N	O	S	0	0
			1143	733	200	201	9		

- Molecule 20 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B6	94	Total	C	N	O	S	0	0
			797	525	134	137	1		

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B7	119	Total	C	N	O	S	0	0
			1026	641	196	181	8		

- Molecule 22 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B9	176	Total	C	N	O	S	0	0
			1515	970	278	261	6		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B2	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B8	157	Total	C	N	O	S	0	0
			1324	855	217	243	9		

- Molecule 25 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BK	102	Total	C	N	O	S	0	0
			853	547	141	161	4		

- Molecule 26 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	C1	46	Total	C	N	O	0	0
			391	258	67	66		

- Molecule 27 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	B1	52	Total	C	N	O	0	0
			449	296	79	74		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 28 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 29 is a protein called UQCRC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a1	439	Total	C	N	O	S	0	0
			3409	2132	603	654	20		
29	a3	444	Total	C	N	O	S	0	0
			3447	2153	608	666	20		

- Molecule 30 is a protein called Ubiquinol-cytochrome c reductase core protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a2	414	Total	C	N	O	S	0	0
			3126	1963	554	601	8		
30	a4	413	Total	C	N	O	S	0	0
			3122	1961	553	600	8		

- Molecule 31 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b1	378	Total	C	N	O	S	0	0
			3019	2029	471	498	21		
31	b2	378	Total	C	N	O	S	0	0
			3019	2029	471	498	21		

- Molecule 32 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c1	239	Total	C	N	O	S	0	0
			1909	1219	330	345	15		
32	c2	238	Total	C	N	O	S	0	0
			1903	1216	329	343	15		

- Molecule 33 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f1	196	Total	C	N	O	S	0	0
			1520	958	263	291	8		
33	f2	195	Total	C	N	O	S	0	0
			1514	955	262	289	8		

- Molecule 34 is a protein called UQCRB.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d1	100	Total	C	N	O	S	0	0
			886	566	159	159	2		
34	d2	101	Total	C	N	O	S	0	0
			888	566	159	161	2		

- Molecule 35 is a protein called Ubiquinol-cytochrome c reductase complex III subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q1	73	Total	C	N	O	S	0	0
			618	404	116	97	1		
35	q2	75	Total	C	N	O	S	0	0
			631	413	118	99	1		

- Molecule 36 is a protein called UQCRQH.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h1	65	Total	C	N	O	S	0	0
			532	324	96	107	5		
36	h2	65	Total	C	N	O	S	0	0
			532	324	96	107	5		

- Molecule 37 is a protein called UQCRFS1N.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	x1	33	Total	C	N	O	0	0
			164	98	33	33		

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Mol	Chain	Residues	Atoms				AltConf	Trace
37	x2	30	Total 150	C 90	N 30	O 30	0	0

- Molecule 38 is a protein called Ubiquinol-cytochrome c reductase, complex III subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	i1	55	Total 459	C 303	N 80	O 76	0	0
38	i2	57	Total 473	C 312	N 82	O 79	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	V1	430	Total 3312	C 2086	N 593	O 613	S 20	0	0

- Molecule 40 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	V2	212	Total 1647	C 1052	N 277	O 308	S 10	0	0

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S1	688	Total 5275	C 3301	N 922	O 1011	S 41	0	0

- Molecule 42 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	S2	427	Total 3435	C 2193	N 589	O 628	S 25	0	0

- Molecule 43 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	S3	208	Total 1726	C 1112	N 296	O 315	S 3	0	0

- Molecule 44 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S7	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 45 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	S8	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 46 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	V3	41	Total	C	N	O	S	0	0
			345	215	63	66	1		

- Molecule 47 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S6	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 48 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S4	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 49 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	A9	291	Total	C	N	O	S	0	0
			2301	1470	416	410	5		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	A2	82	Total	C	N	O	S	0	0
			665	419	124	120	2		

- Molecule 51 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A5	111	Total	C	N	O	S	0	0
			901	583	151	165	2		

- Molecule 52 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A6	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

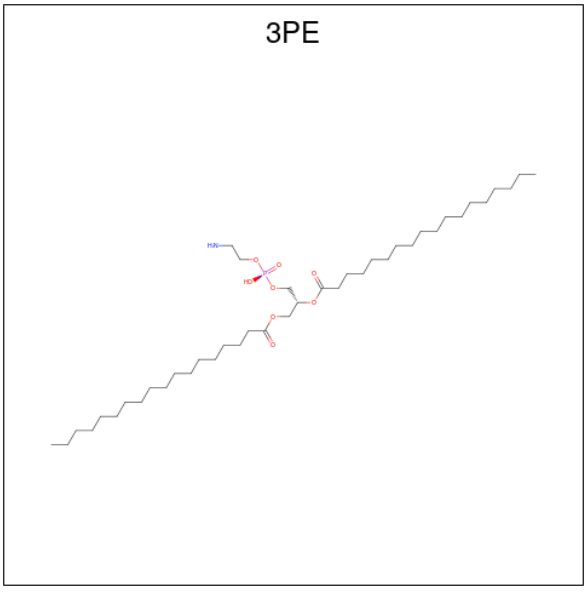
- Molecule 53 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A7	95	Total	C	N	O	S	0	0
			757	473	144	137	3		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

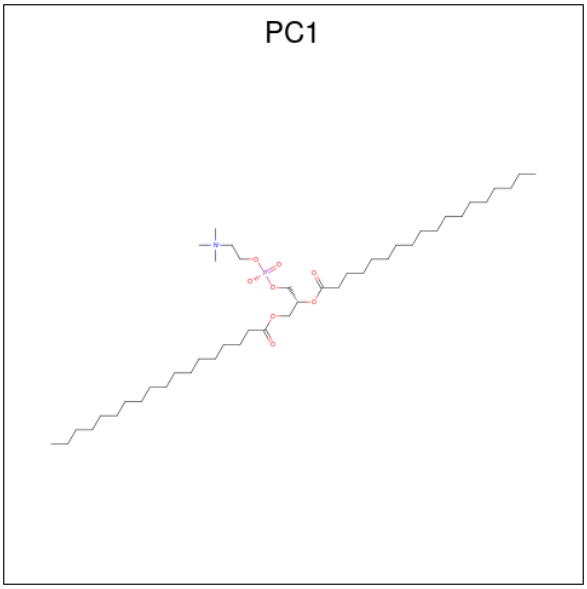
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AL	139	Total	C	N	O	S	0	0
			1160	746	209	201	4		

- Molecule 55 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



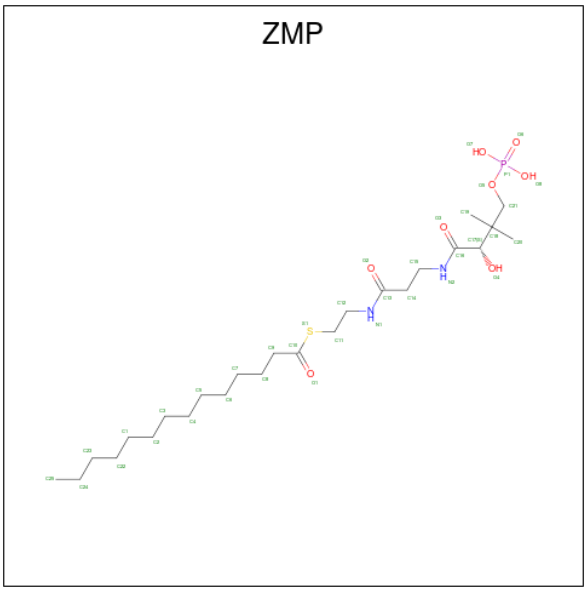
Mol	Chain	Residues	Atoms					AltConf
55	D1	1	Total	C	N	O	P	0
			32	22	1	8	1	
55	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	
55	D4	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	b2	1	Total	C	N	O	P	0
			29	19	1	8	1	
55	f2	1	Total	C	N	O	P	0
			23	13	1	8	1	

- Molecule 56 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



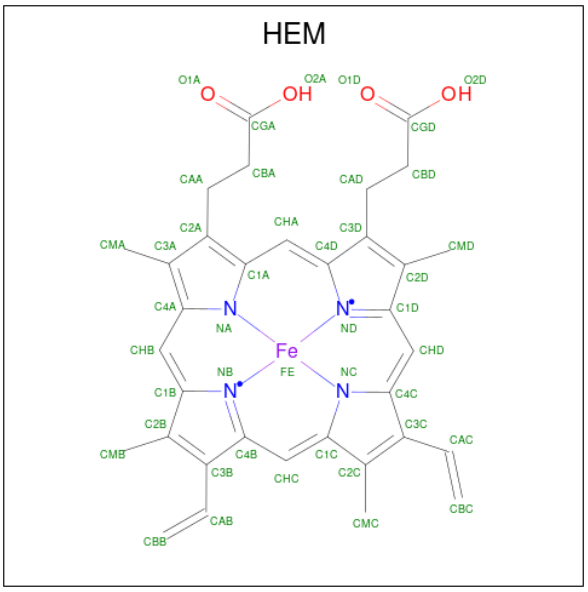
Mol	Chain	Residues	Atoms					AltConf
56	D4	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 57 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
57	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
57	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 58 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
58	b1	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

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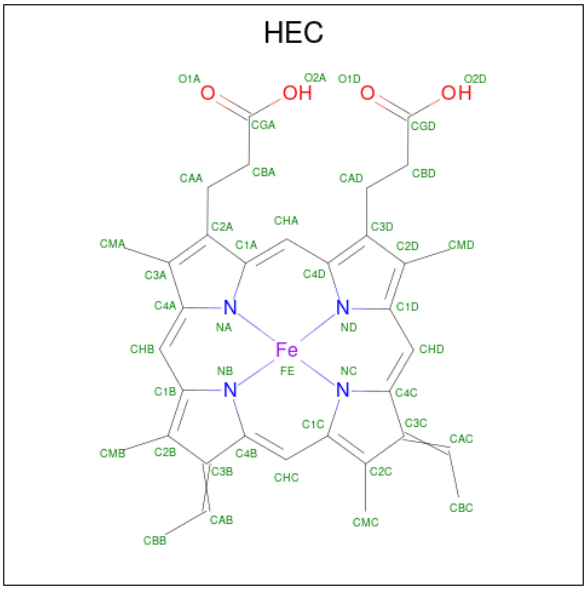
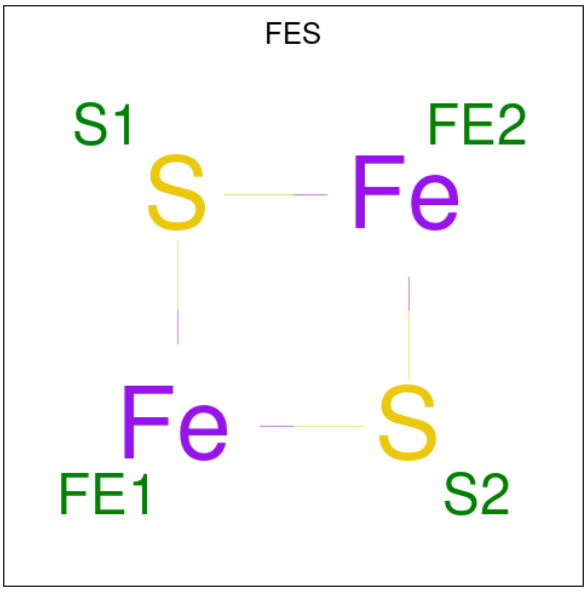
Mol	Chain	Residues	Atoms					AltConf
58	b1	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
58	b2	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
58	b2	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 59 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



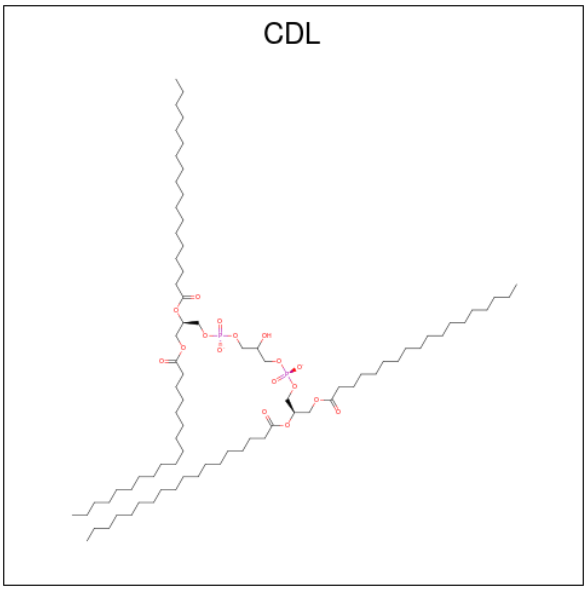
Mol	Chain	Residues	Atoms					AltConf
59	c1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
59	c2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 60 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



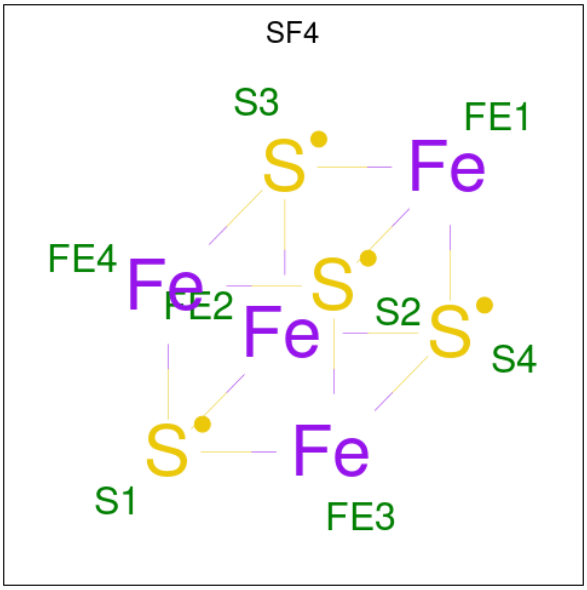
Mol	Chain	Residues	Atoms			AltConf
60	f1	1	Total	Fe	S	0
			4	2	2	
60	f2	1	Total	Fe	S	0
			4	2	2	
60	V2	1	Total	Fe	S	0
			4	2	2	
60	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 61 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



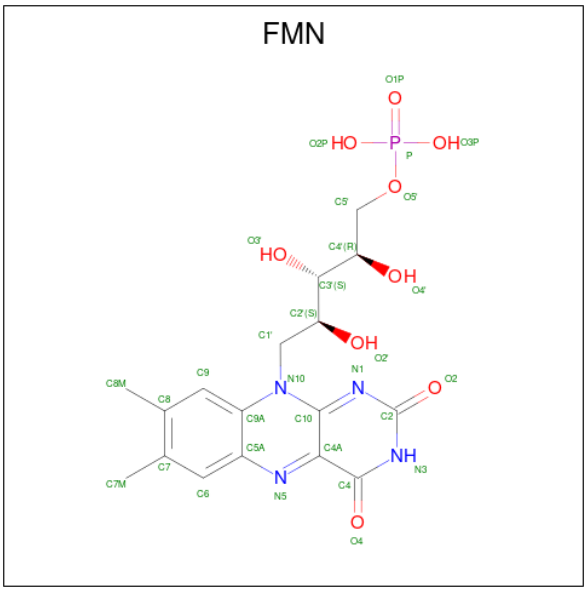
Mol	Chain	Residues	Atoms				AltConf
61	b2	1	Total	C	O	P	0
			79	41	34	4	
61	b2	1	Total	C	O	P	0
			79	41	34	4	
61	c2	1	Total	C	O	P	0
			41	22	17	2	

- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
62	V1	1	Total	Fe	S	0
			8	4	4	
62	S1	1	Total	Fe	S	0
			16	8	8	
62	S1	1	Total	Fe	S	0
			16	8	8	
62	S7	1	Total	Fe	S	0
			8	4	4	
62	S8	1	Total	Fe	S	0
			16	8	8	
62	S8	1	Total	Fe	S	0
			16	8	8	

- Molecule 63 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

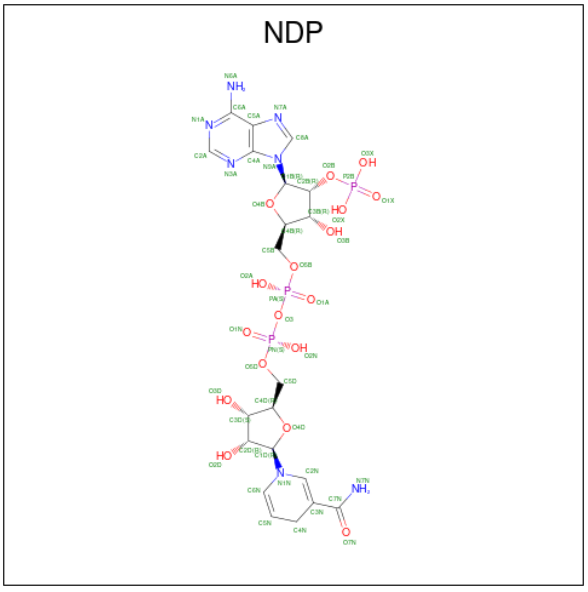


Mol	Chain	Residues	Atoms					AltConf
63	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	S6	1	Total	Zn	0
			1	1	

- Molecule 65 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



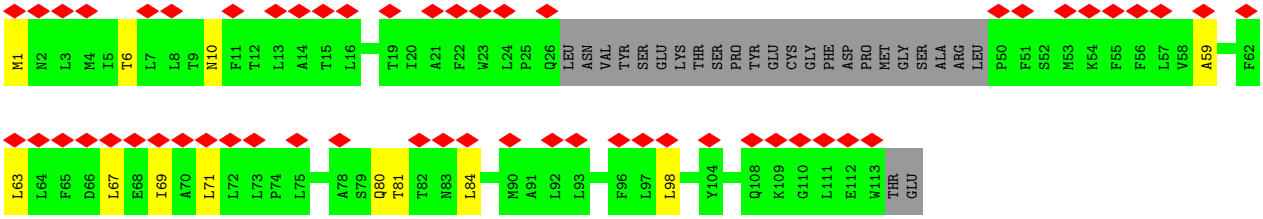
Mol	Chain	Residues	Atoms					AltConf
65	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

3 Residue-property plots (i)

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

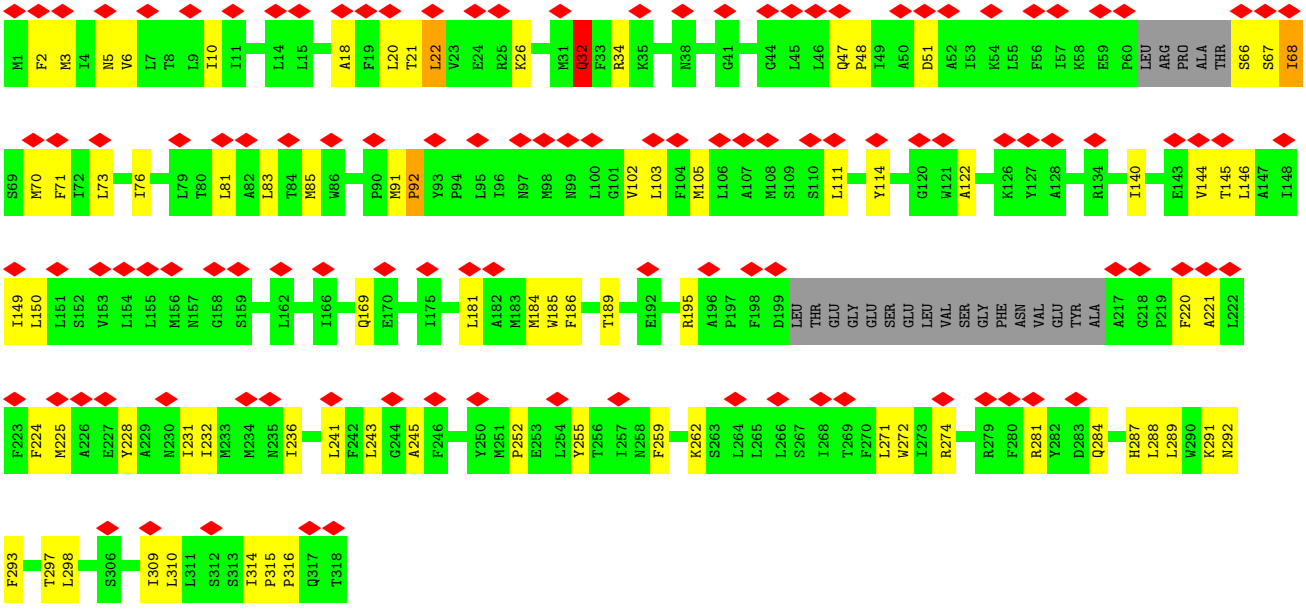
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain D3:



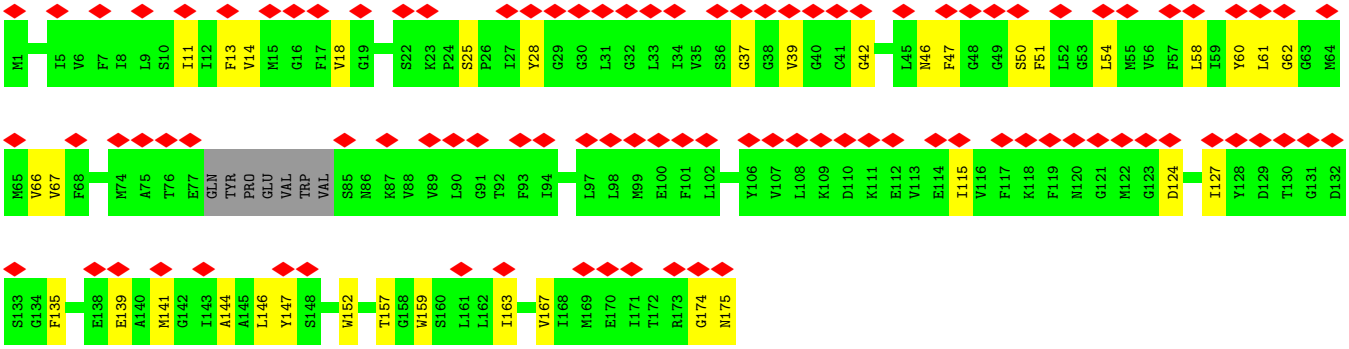
• Molecule 2: NADH-ubiquinone oxidoreductase chain 1

Chain D1:



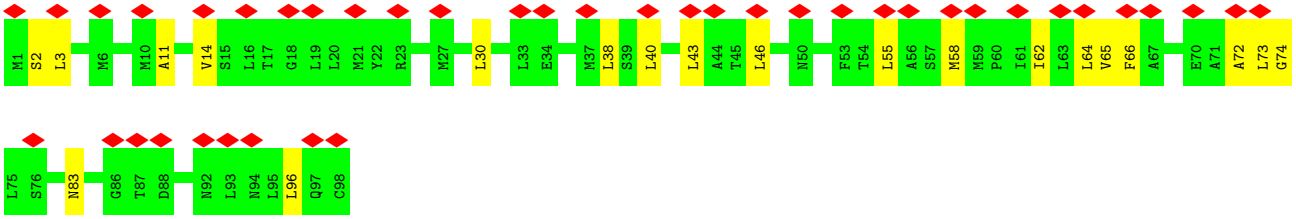
• Molecule 3: NADH-ubiquinone oxidoreductase chain 6

Chain D6:



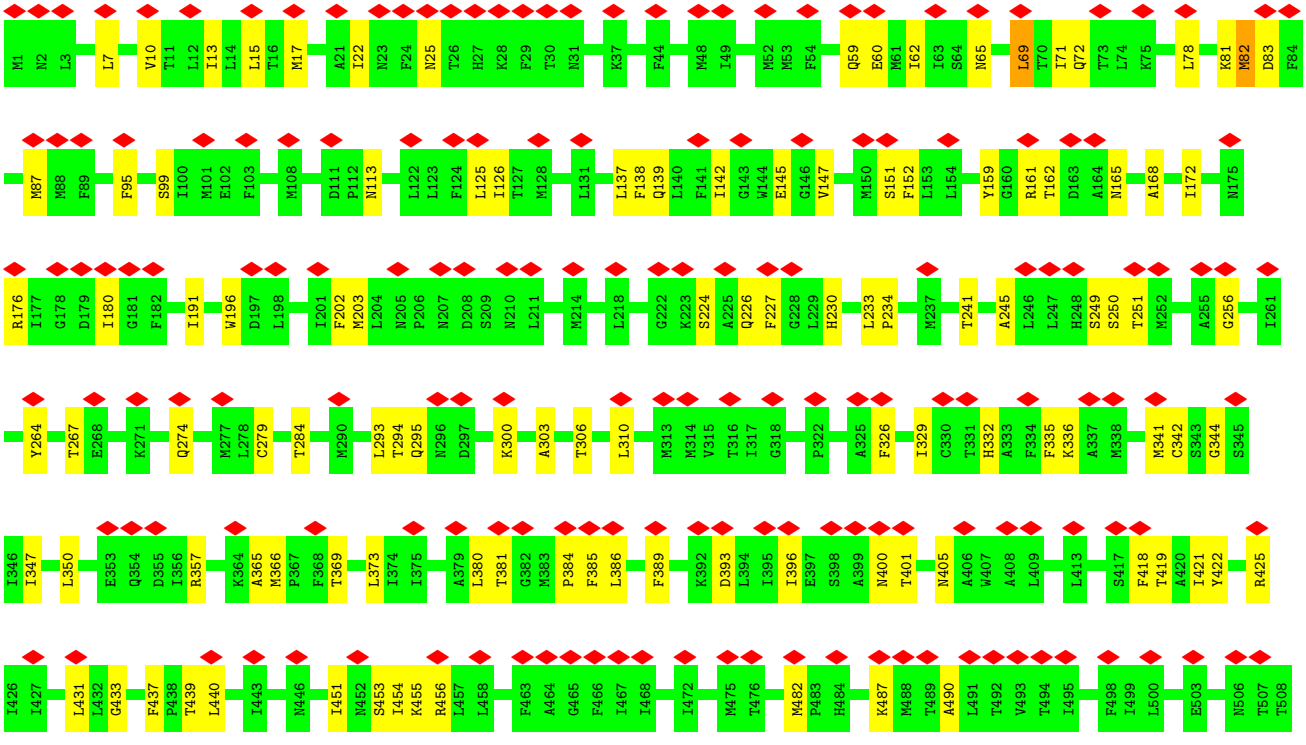
• Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

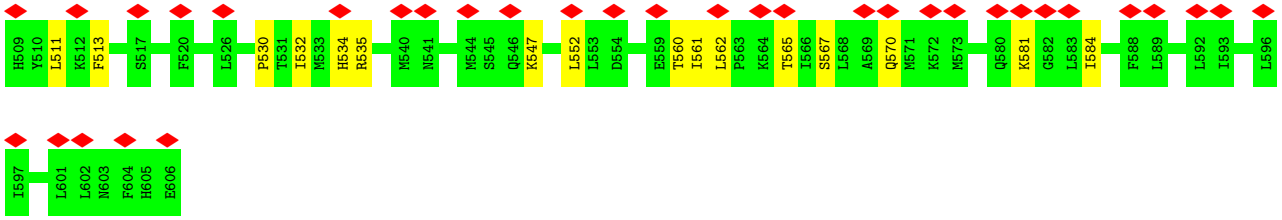
Chain 4L:



• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

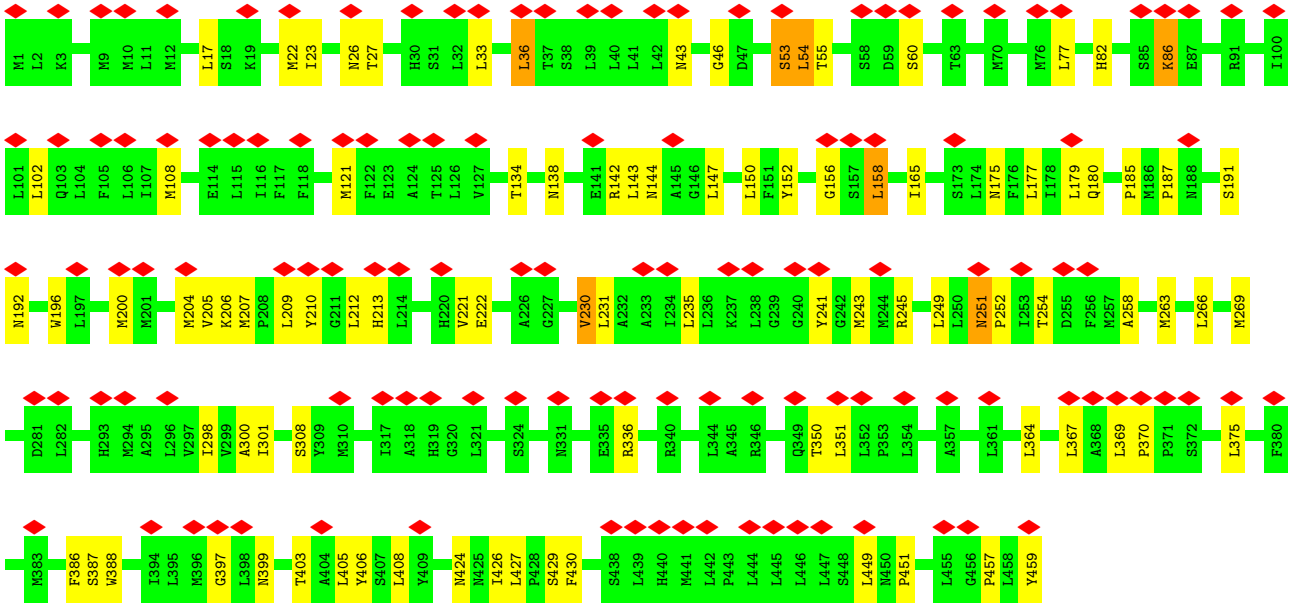
Chain D5:





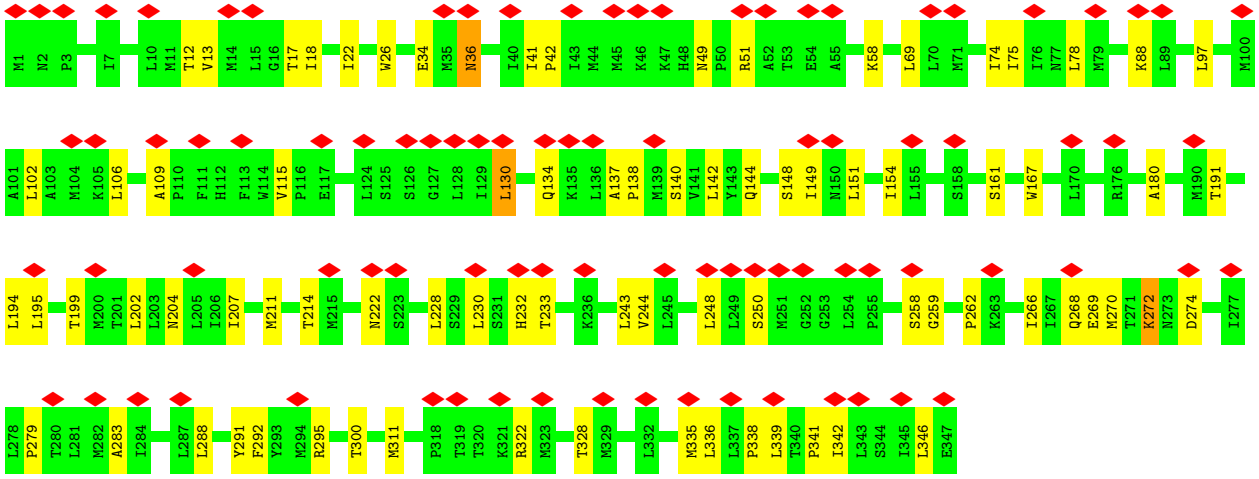
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4

Chain D4:



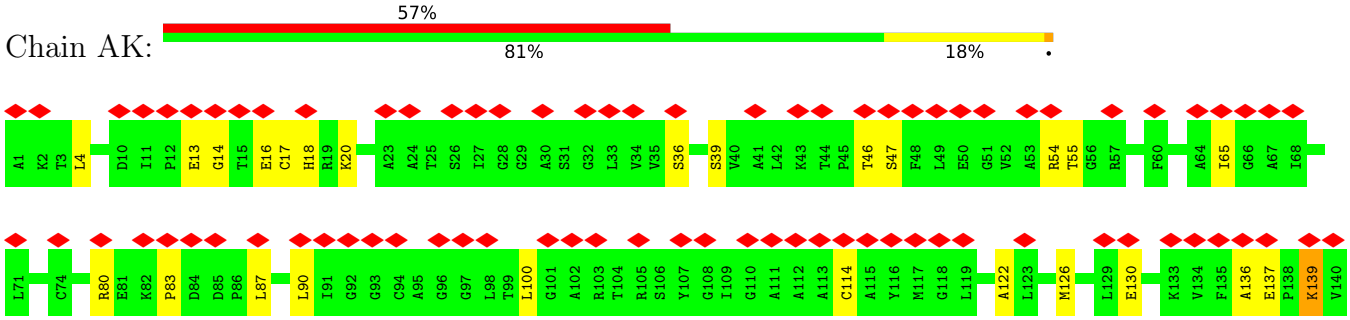
• Molecule 7: NADH-ubiquinone oxidoreductase chain 2

Chain D2:



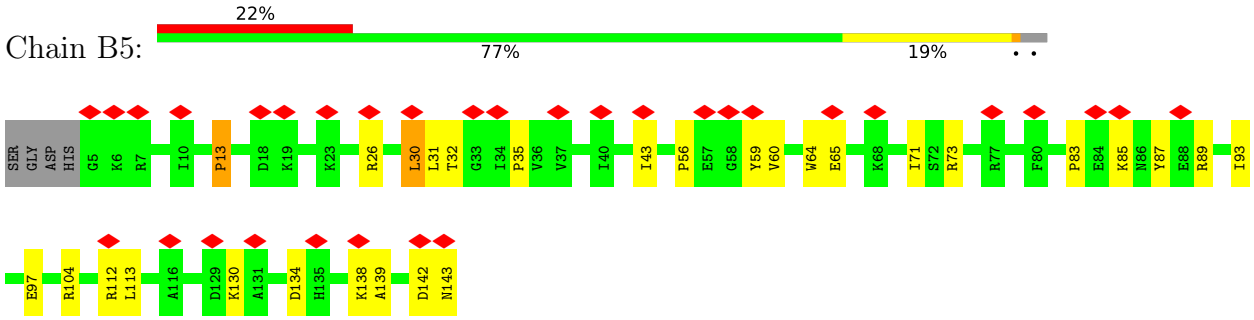
• Molecule 8: NDUFA11

Chain AK:



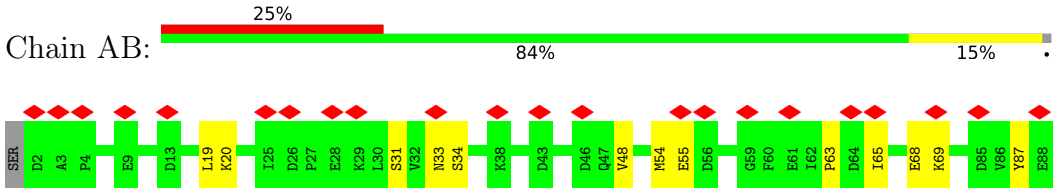
• Molecule 9: NADH:ubiquinone oxidoreductase subunit B5

Chain B5:



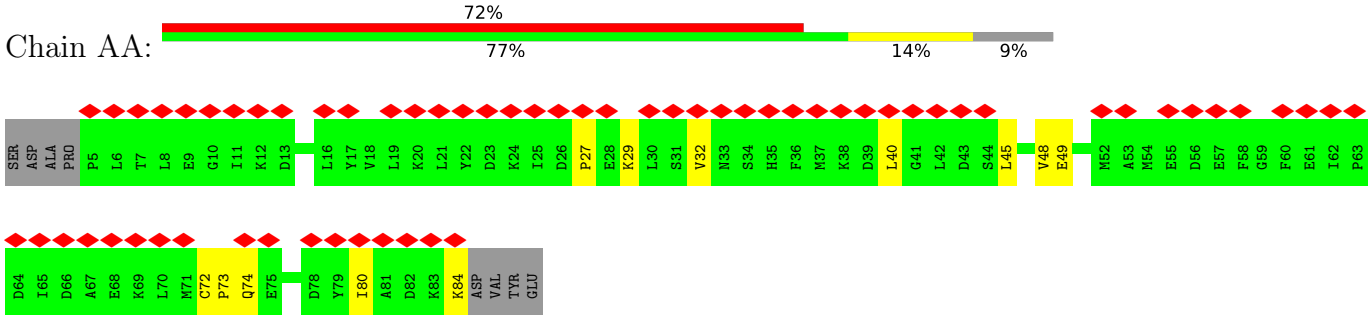
• Molecule 10: Acyl carrier protein

Chain AB:



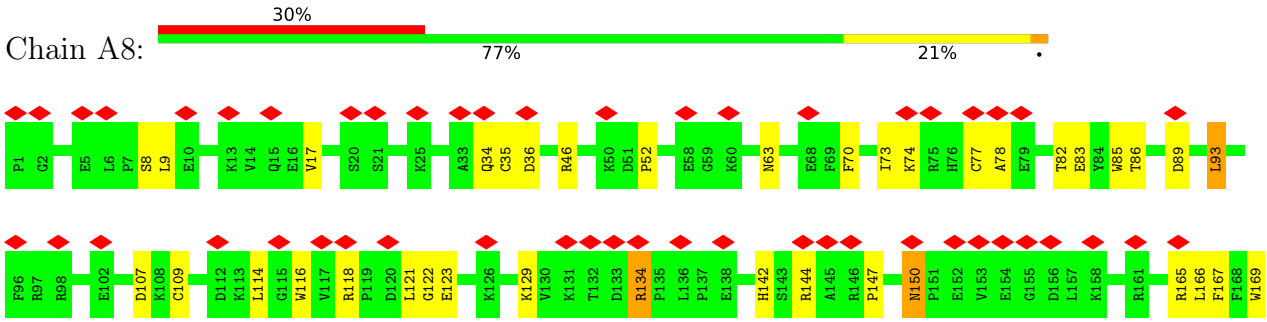
• Molecule 10: Acyl carrier protein

Chain AA:



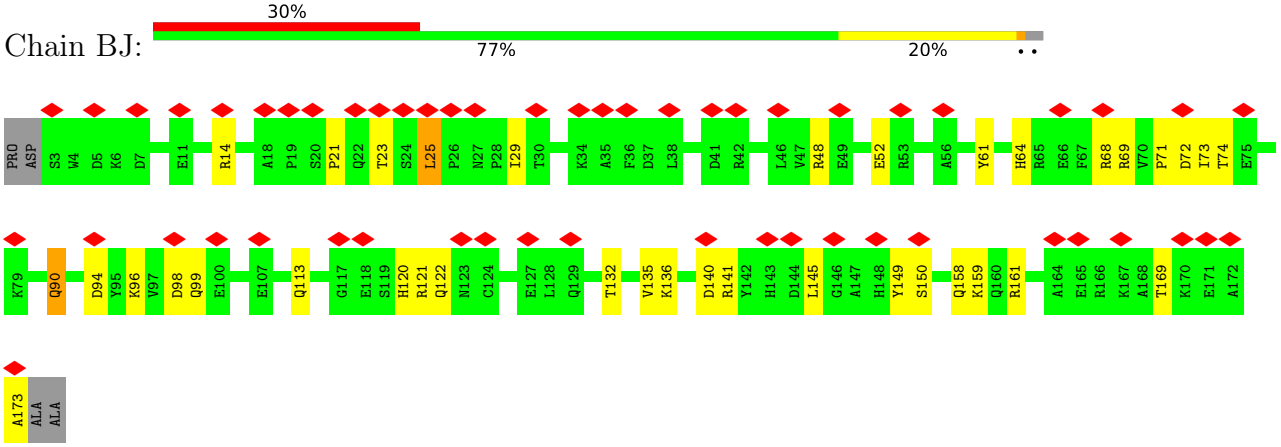
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:



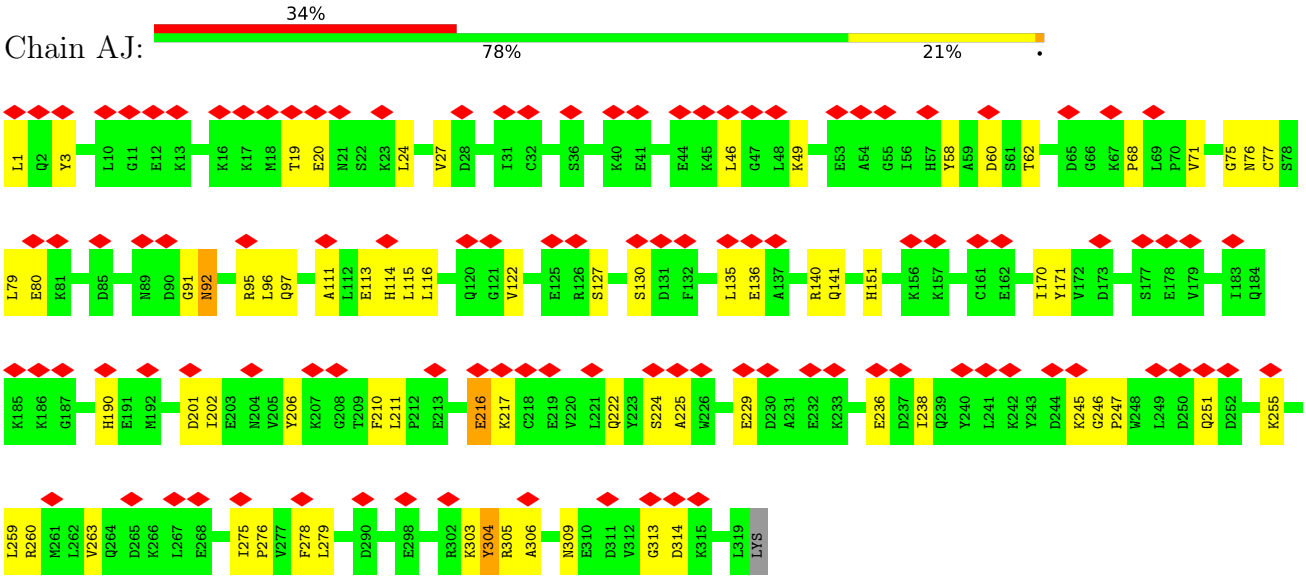
• Molecule 12: NDUFB10

Chain BJ:



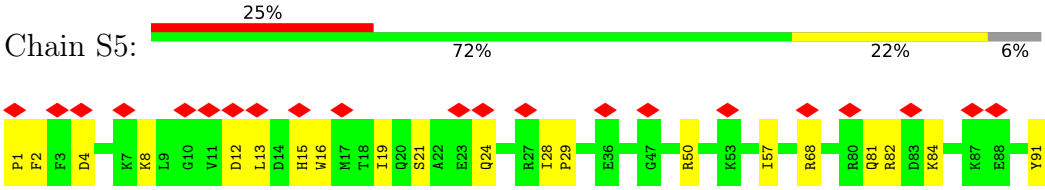
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

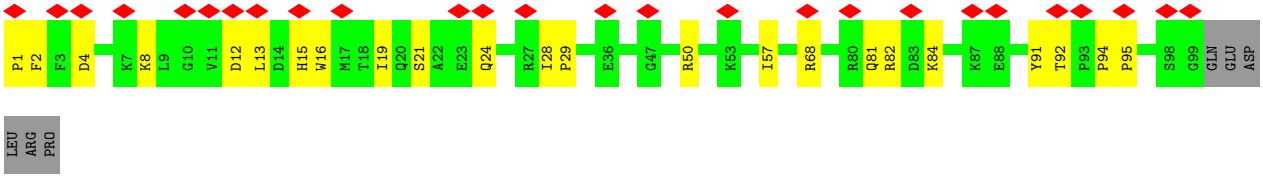
Chain AJ:



• Molecule 14: NADH:ubiquinone oxidoreductase subunit S5

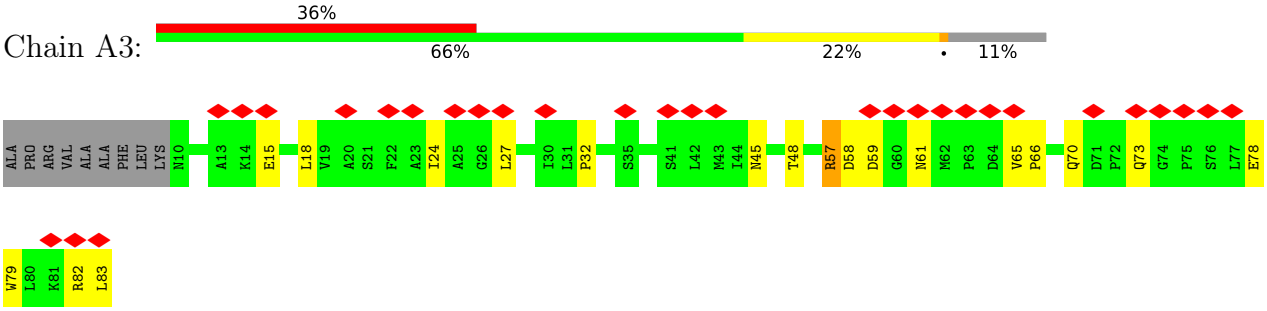
Chain S5:





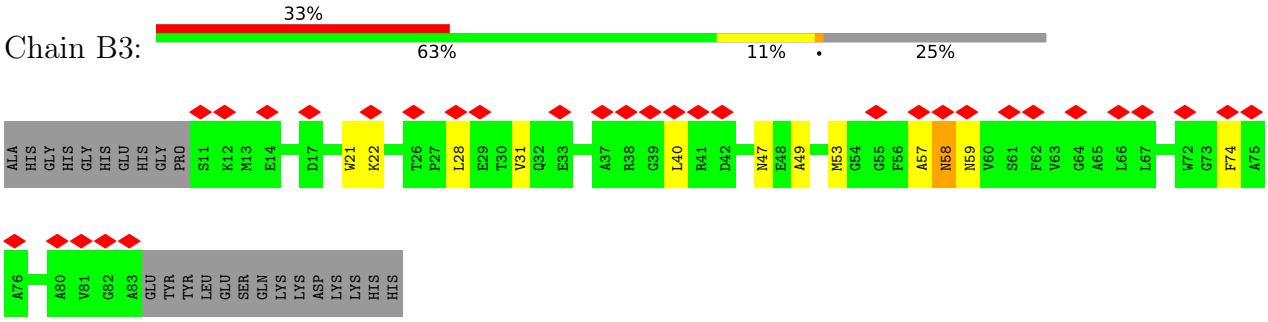
• Molecule 15: NADH:ubiquinone oxidoreductase subunit A3

Chain A3:



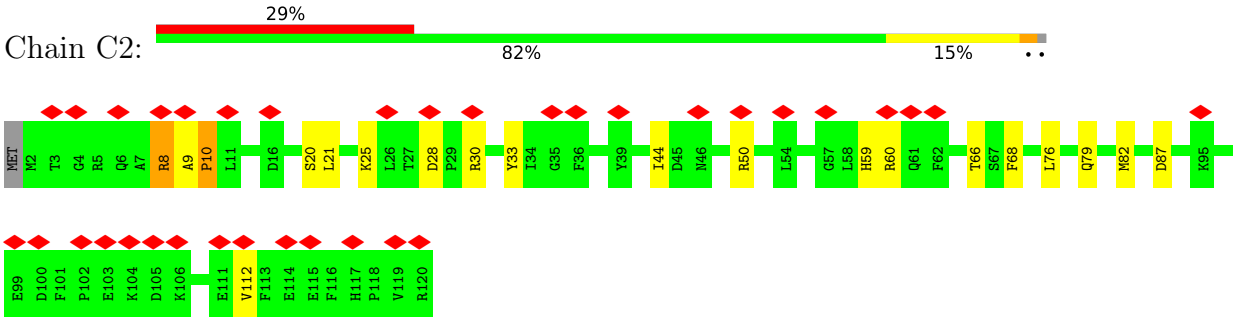
• Molecule 16: NADH:ubiquinone oxidoreductase subunit B3

Chain B3:



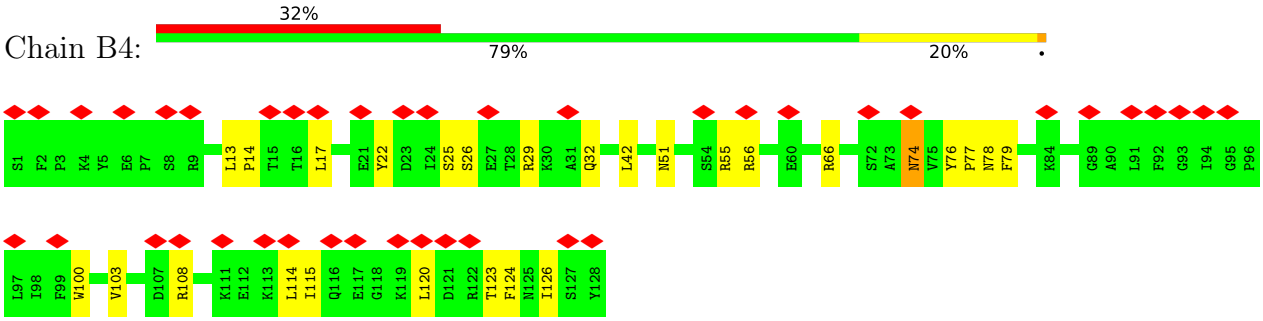
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain C2:



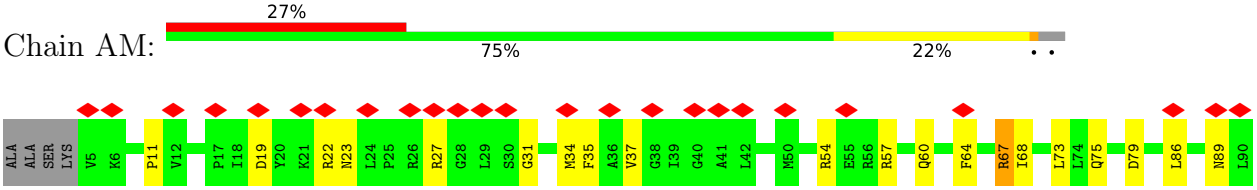
• Molecule 18: NADH:ubiquinone oxidoreductase subunit B4

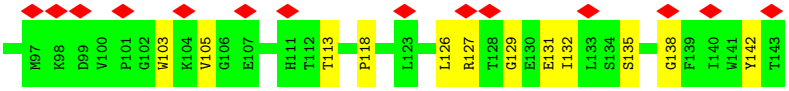
Chain B4:



• Molecule 19: NDUFA13

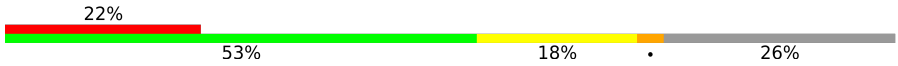
Chain AM:

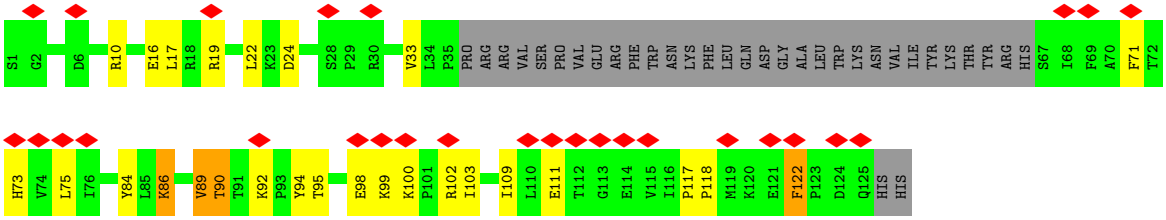




• Molecule 20: NDUFB6

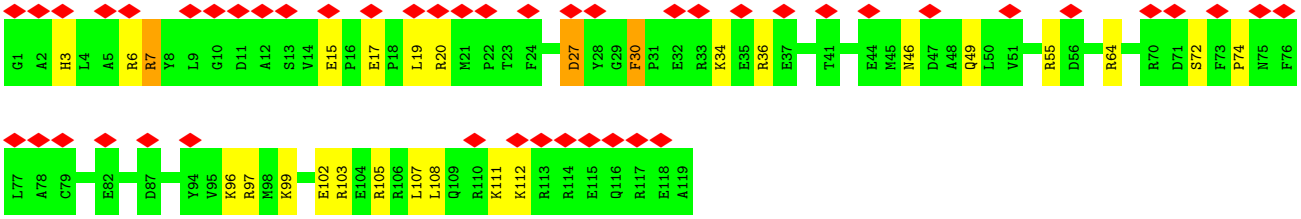
Chain B6:





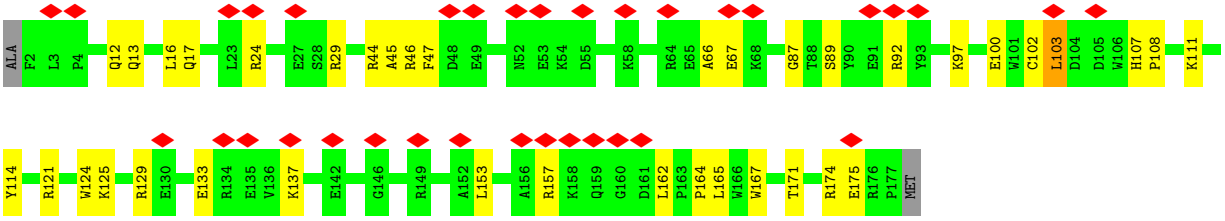
• Molecule 21: NADH:ubiquinone oxidoreductase subunit B7

Chain B7:



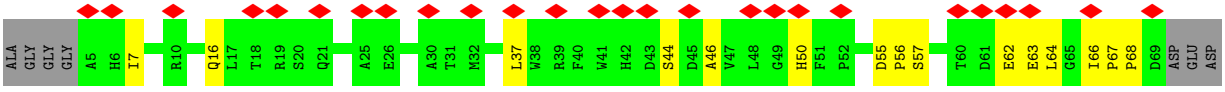
• Molecule 22: NADH:ubiquinone oxidoreductase subunit B9

Chain B9:



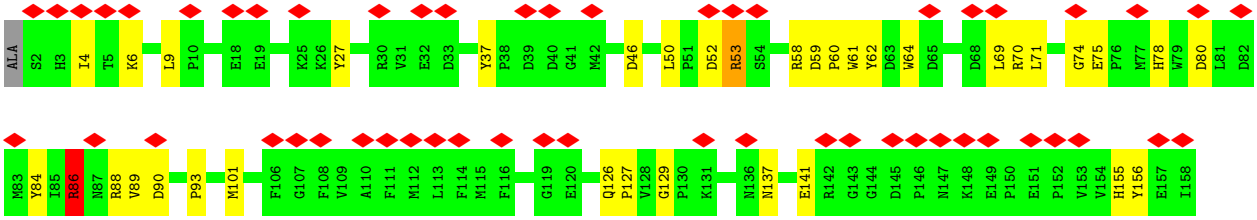
• Molecule 23: NADH:ubiquinone oxidoreductase subunit B2

Chain B2:

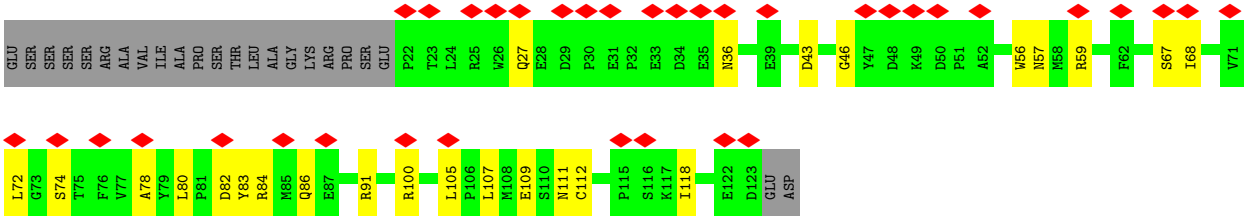


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

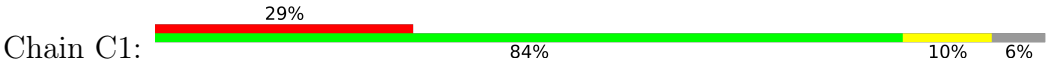
Chain B8:

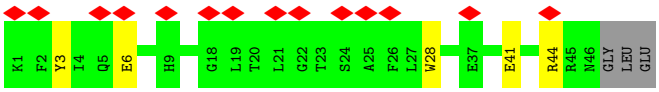


• Molecule 25: NDUFB11

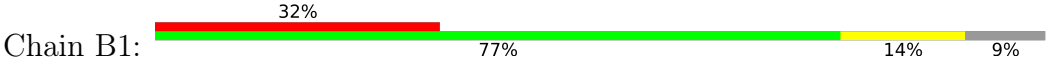


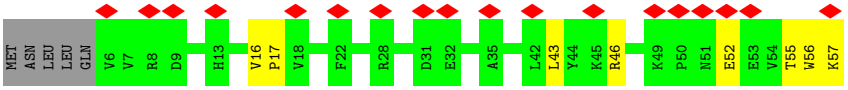
• Molecule 26: NDUFC1



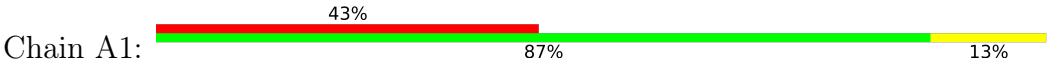


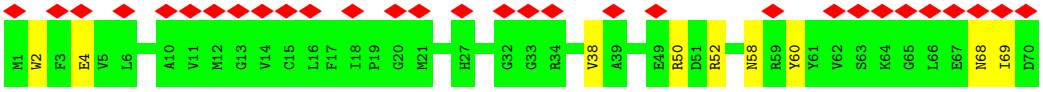
• Molecule 27: NDUFB1



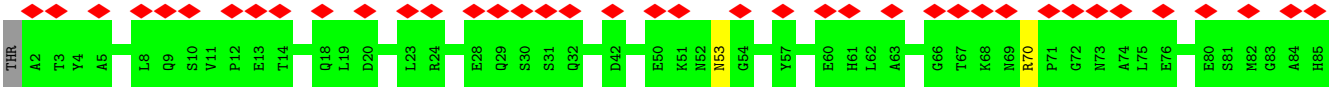


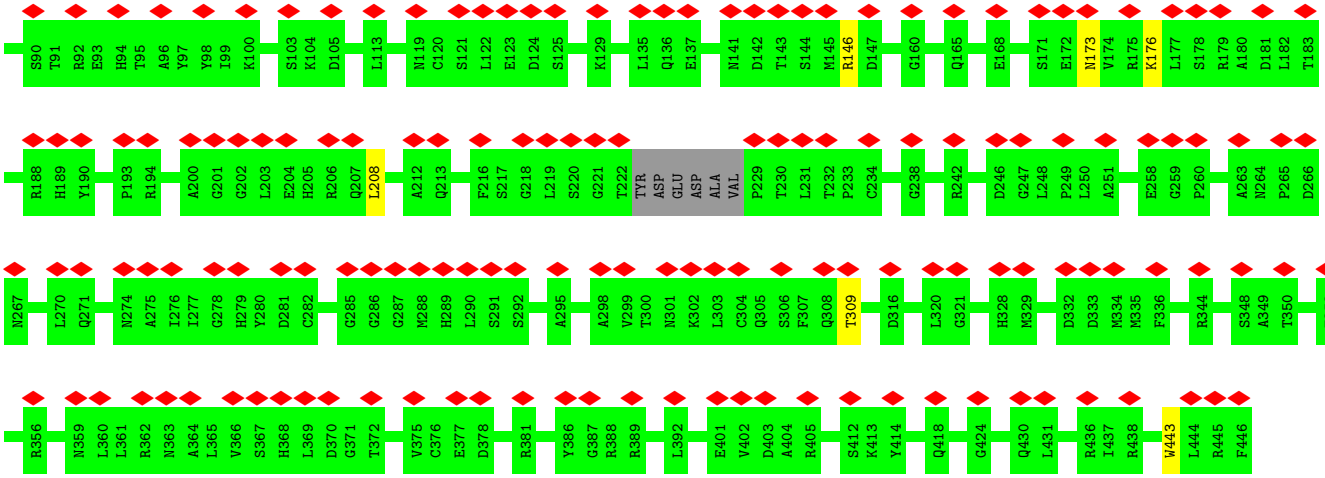
• Molecule 28: NDUFA1





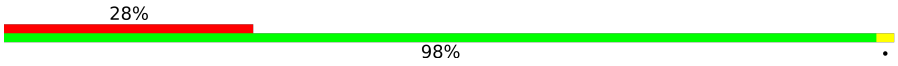
• Molecule 29: UQCRC1

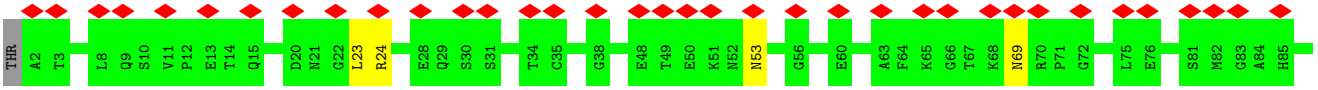


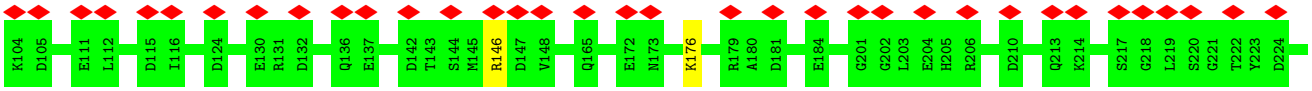


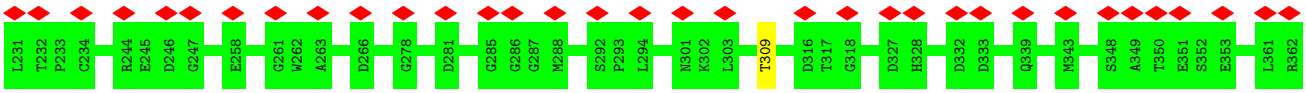
- Molecule 29: UQCRC1

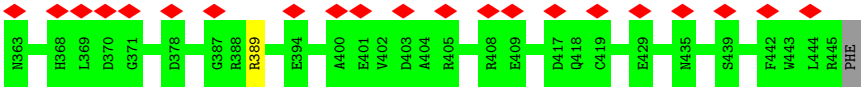
Chain a3:





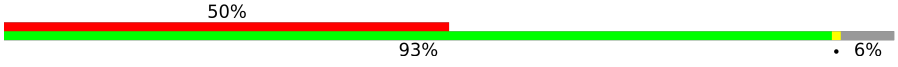


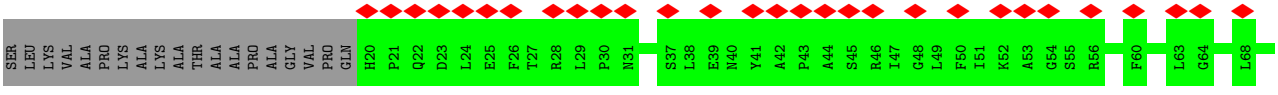


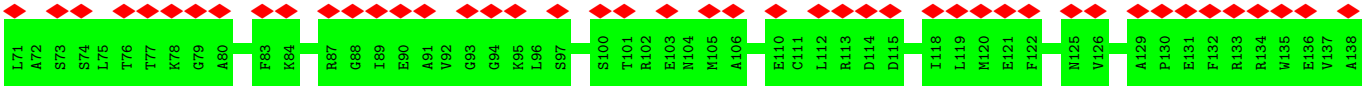


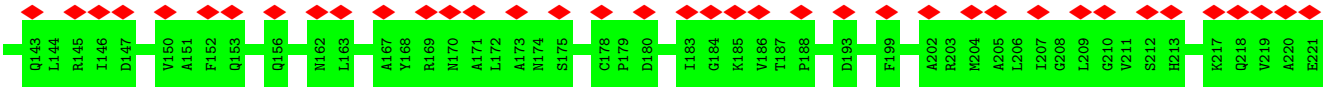
- Molecule 30: Ubiquinol-cytochrome c reductase core protein 2

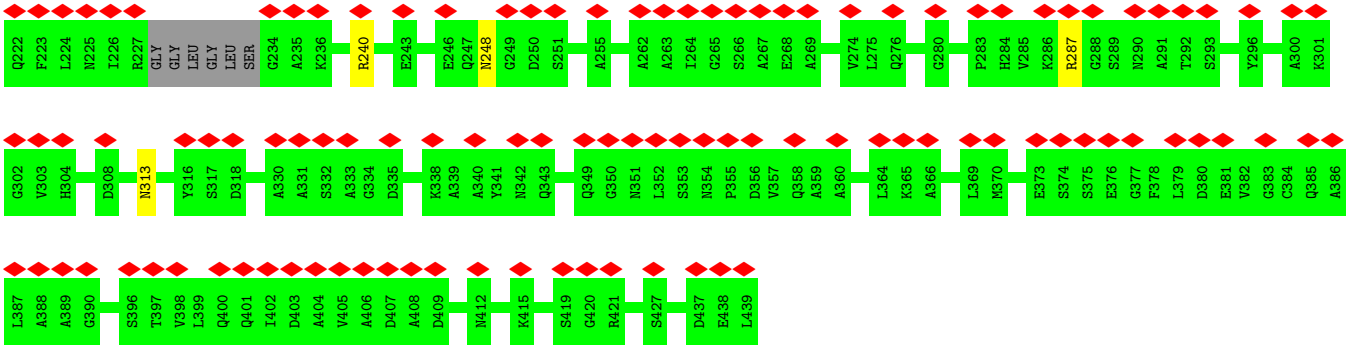
Chain a2:





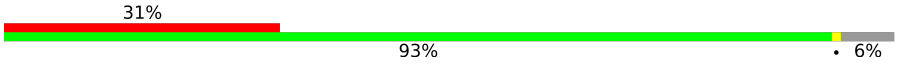


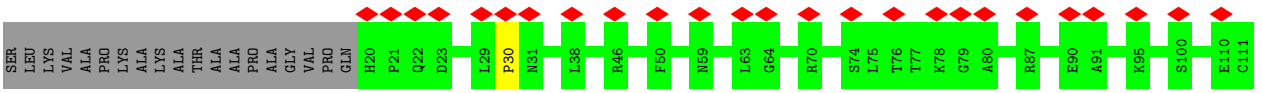




• Molecule 30: Ubiquinol-cytochrome c reductase core protein 2

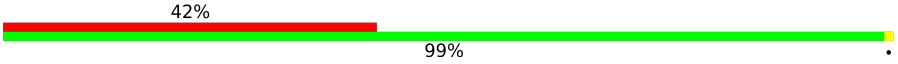
Chain a4:

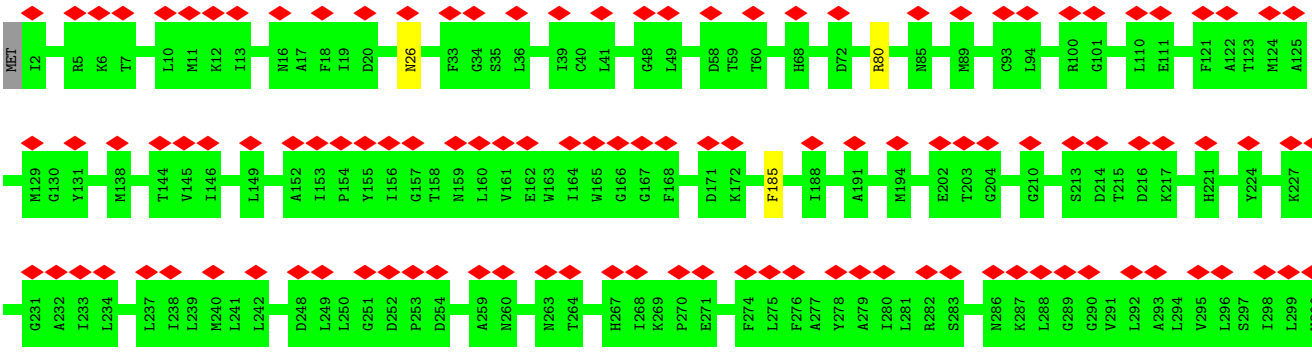


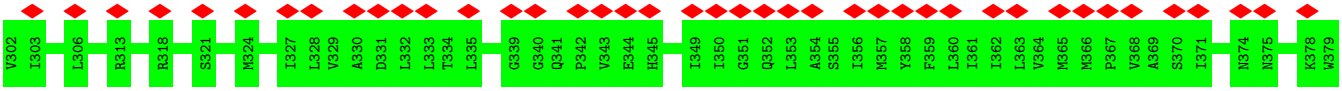


• Molecule 31: Cytochrome b

Chain b1:

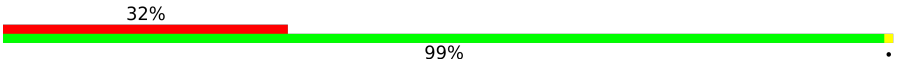


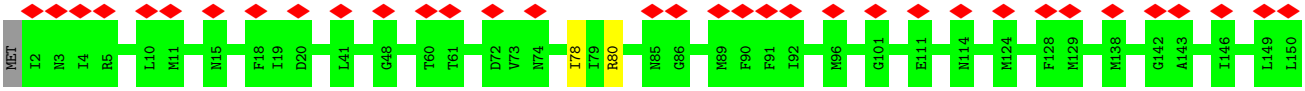


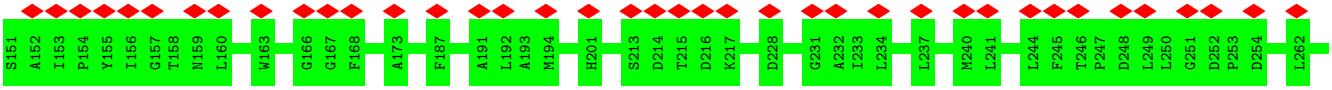


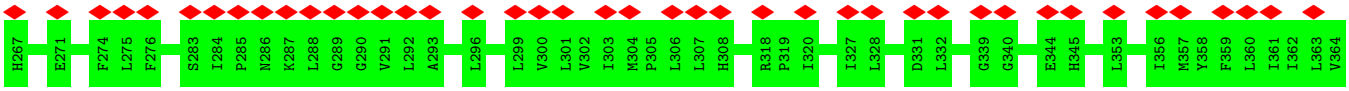
• Molecule 31: Cytochrome b

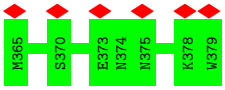
Chain b2:





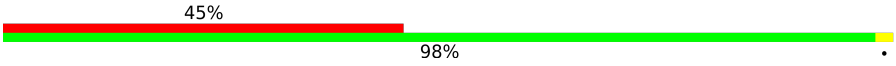


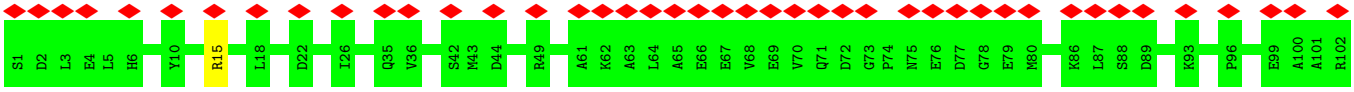


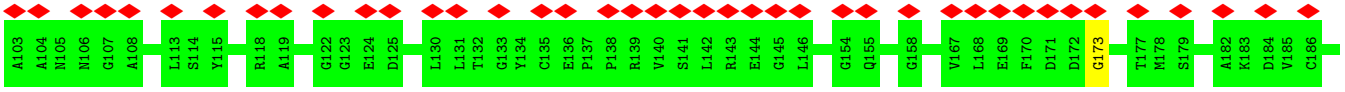


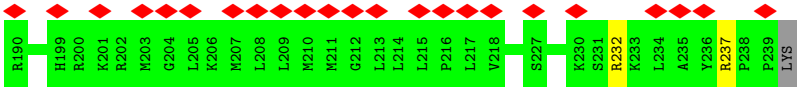
• Molecule 32: Cytochrome c1

Chain c1:



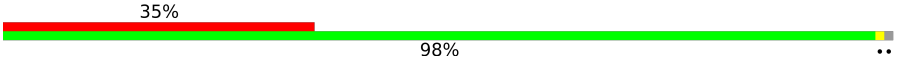


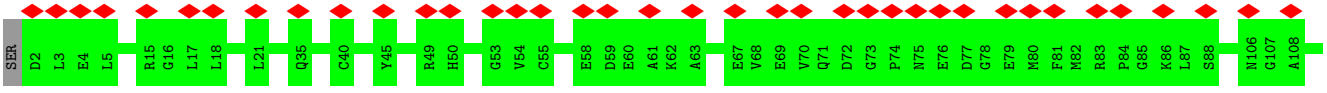


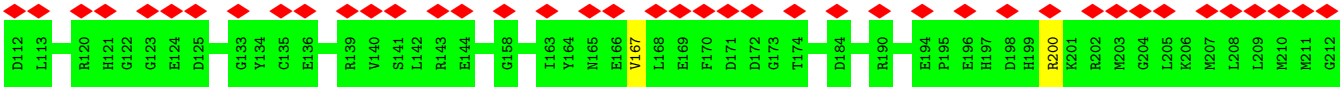


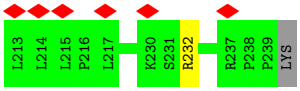
• Molecule 32: Cytochrome c1

Chain c2:



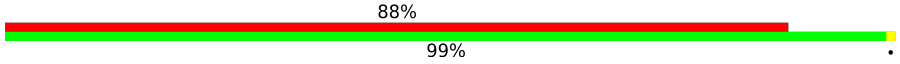


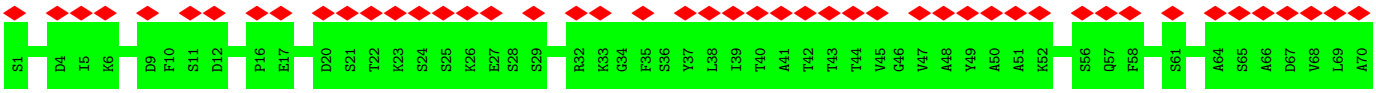


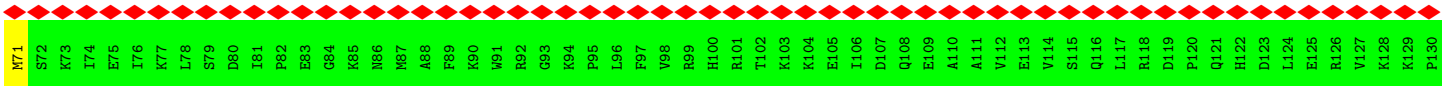


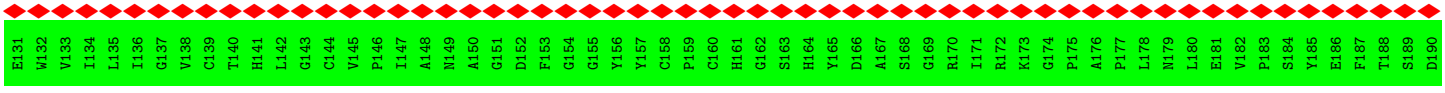
• Molecule 33: Cytochrome b-c1 complex subunit Rieske, mitochondrial

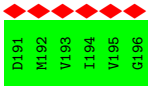
Chain f1:





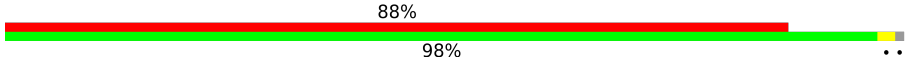


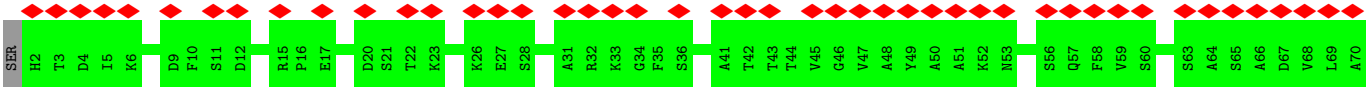


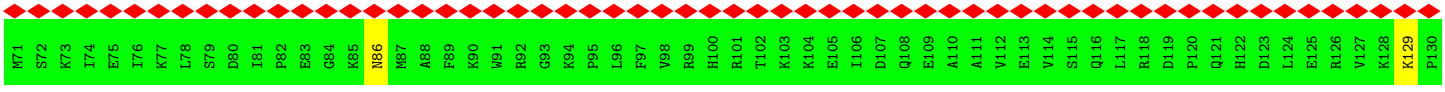


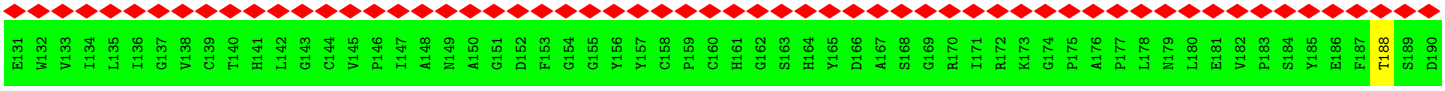
• Molecule 33: Cytochrome b-c1 complex subunit Rieske, mitochondrial

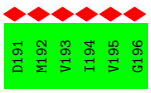
Chain f2:





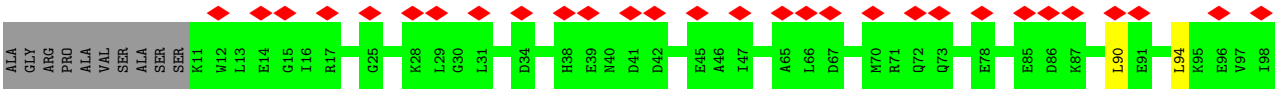


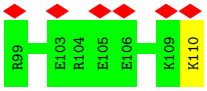




• Molecule 34: UQCRB

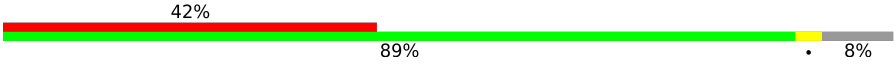
Chain d1:

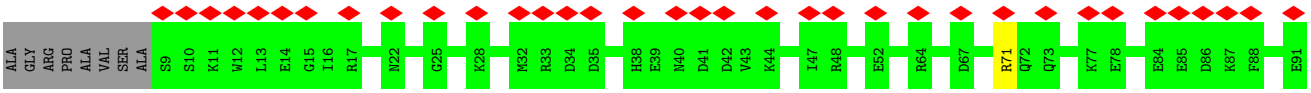


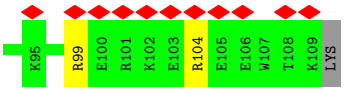


• Molecule 34: UQCRB

Chain d2:

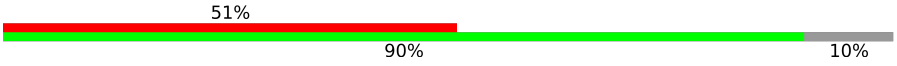


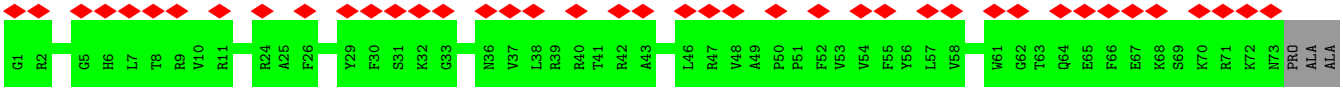




• Molecule 35: Ubiquinol-cytochrome c reductase complex III subunit VII

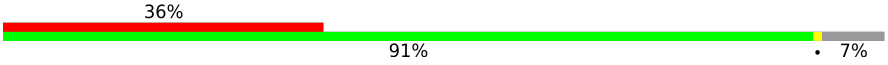
Chain q1:

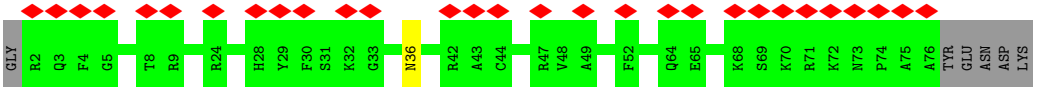




• Molecule 35: Ubiquinol-cytochrome c reductase complex III subunit VII

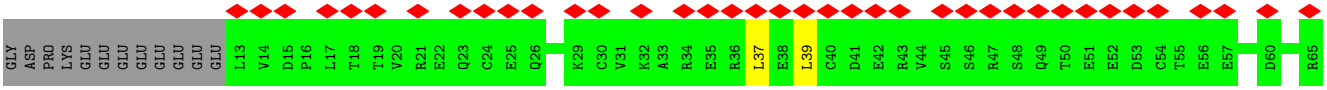
Chain q2:

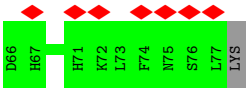




• Molecule 36: UQCRQH

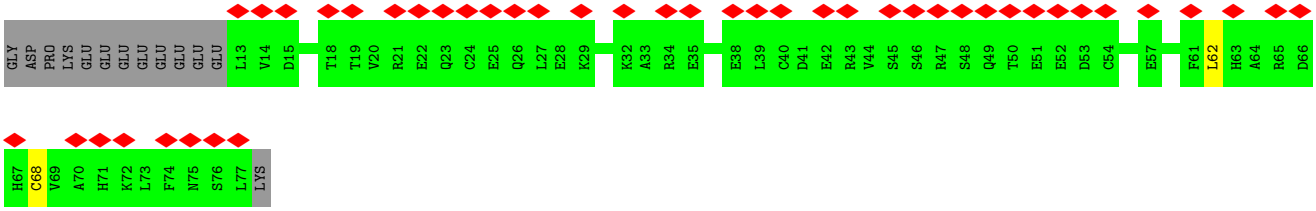
Chain h1:



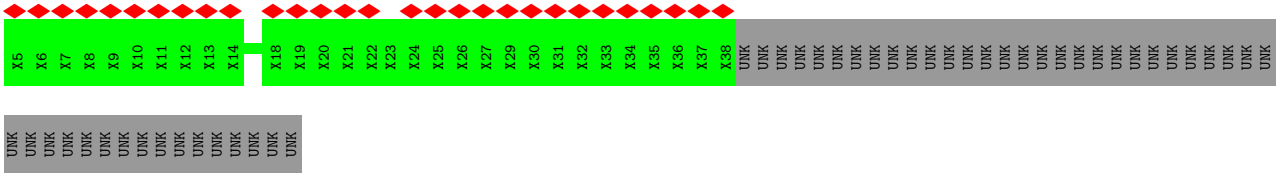


• Molecule 36: UQCRQH

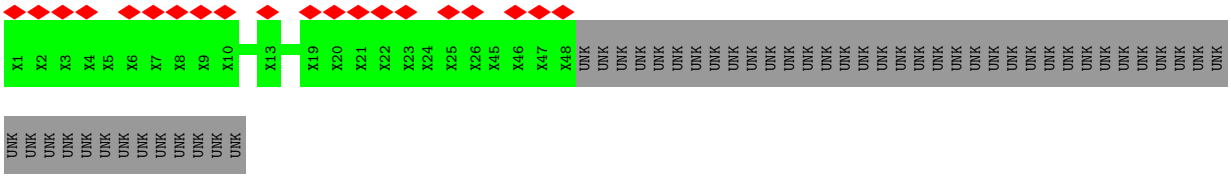
Chain h2:



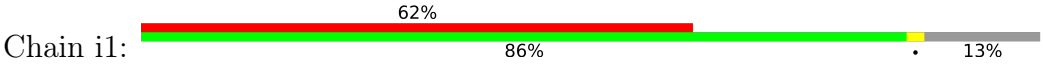
• Molecule 37: UQCRFS1N

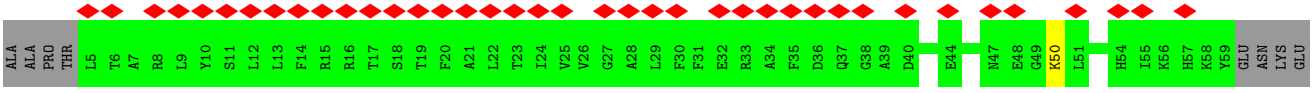


• Molecule 37: UQCRFS1N

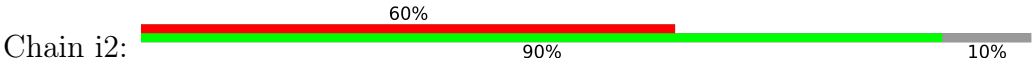


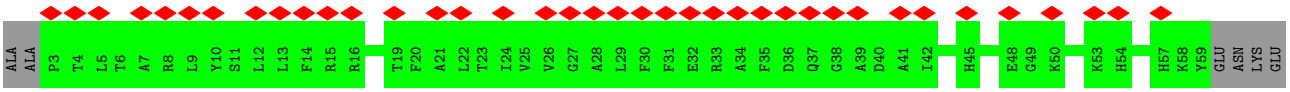
• Molecule 38: Ubiquinol-cytochrome c reductase, complex III subunit X



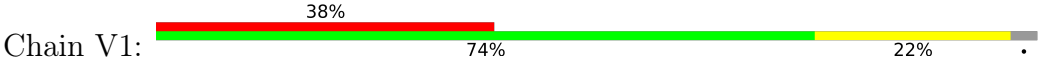


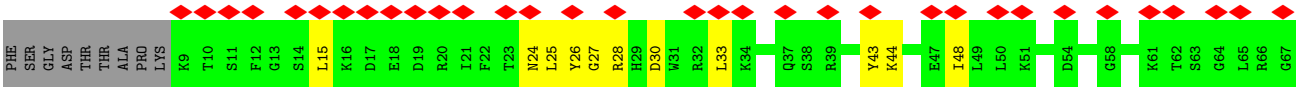
• Molecule 38: Ubiquinol-cytochrome c reductase, complex III subunit X

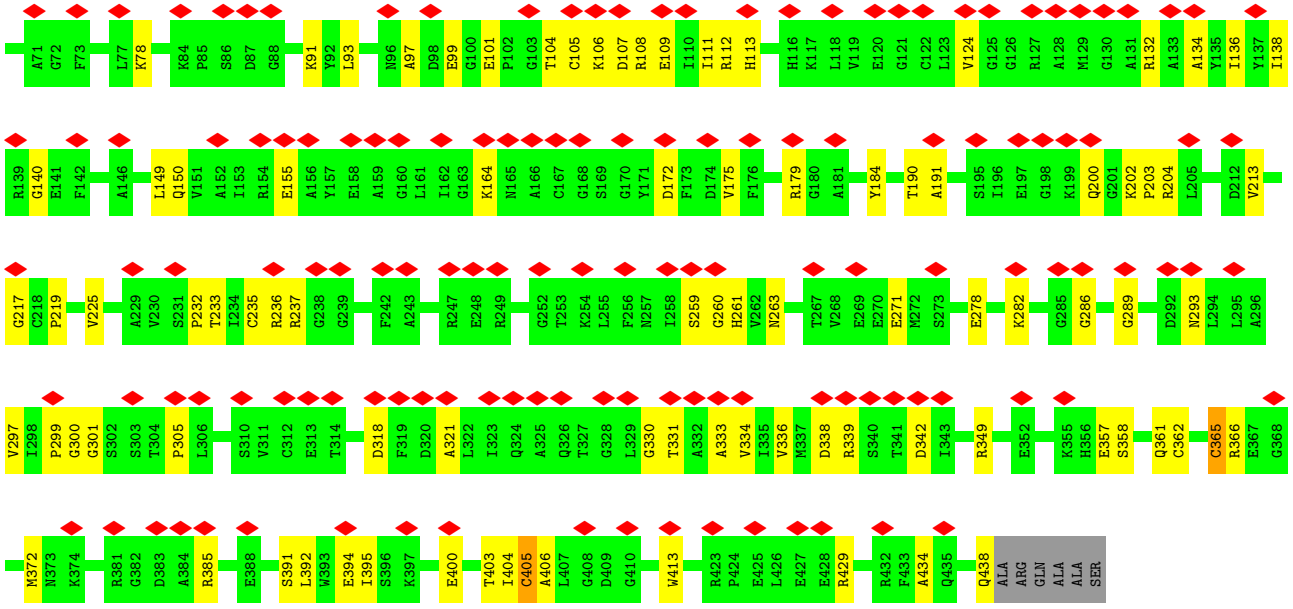




• Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

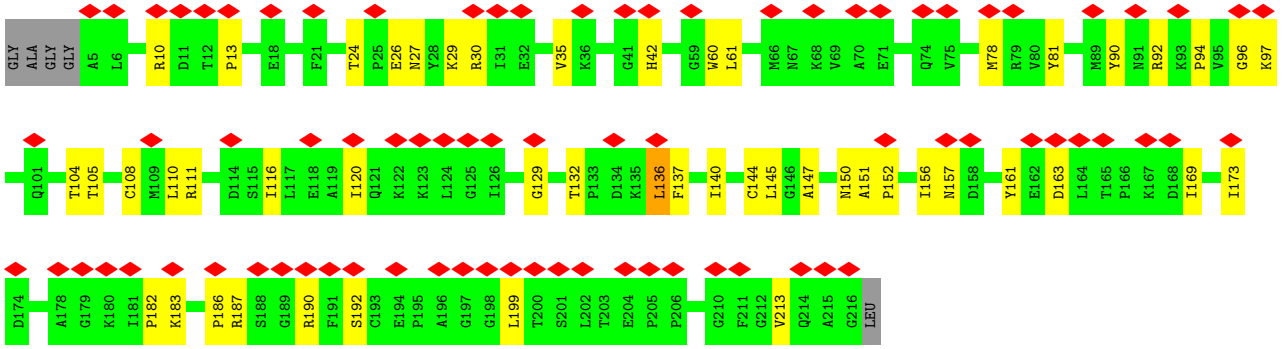






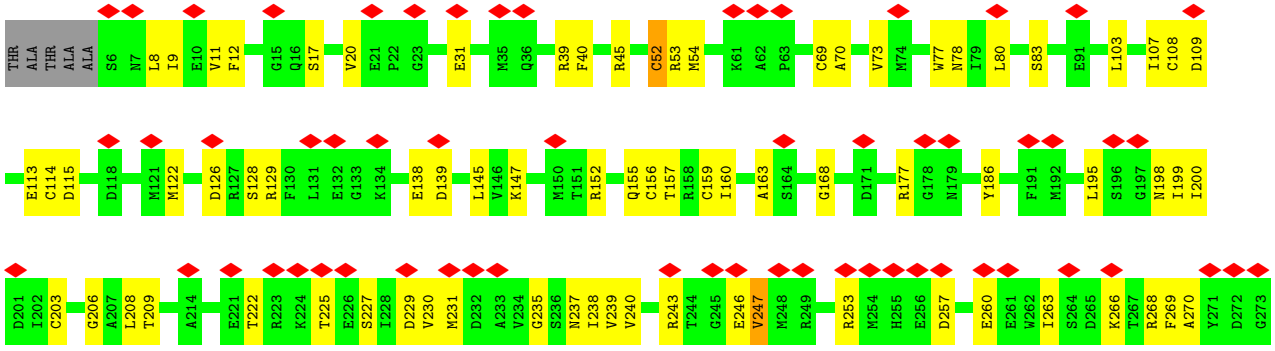
• Molecule 40: NDUFV2

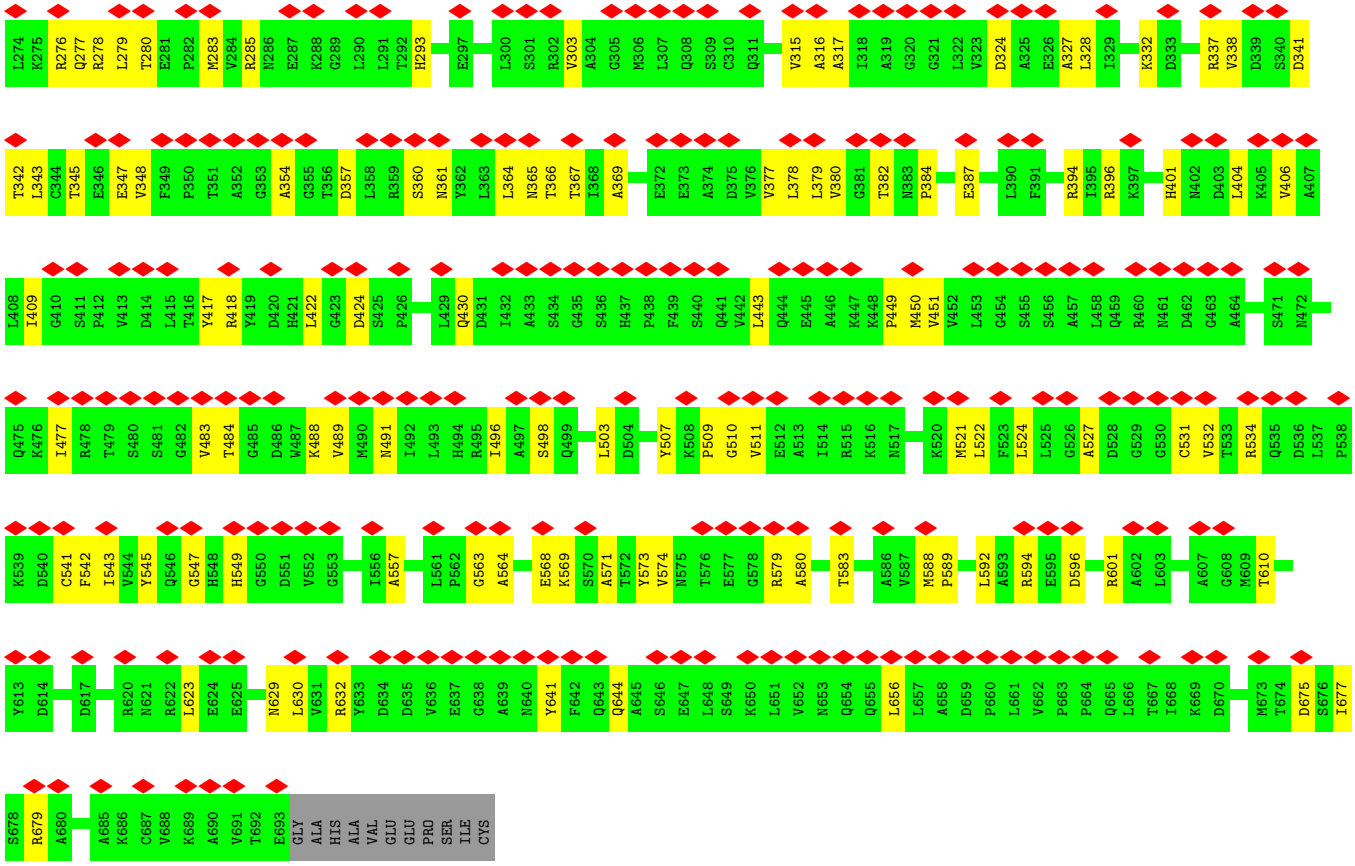
Chain V2:



• Molecule 41: NADH:ubiquinone oxidoreductase core subunit S1

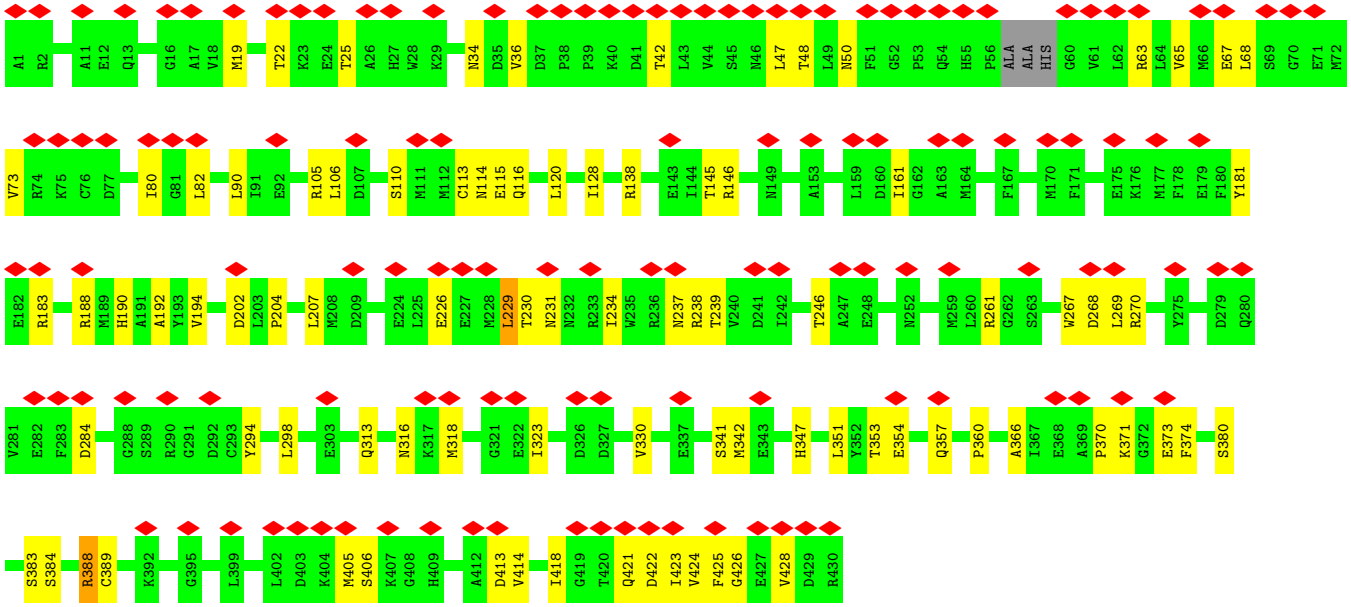
Chain S1:





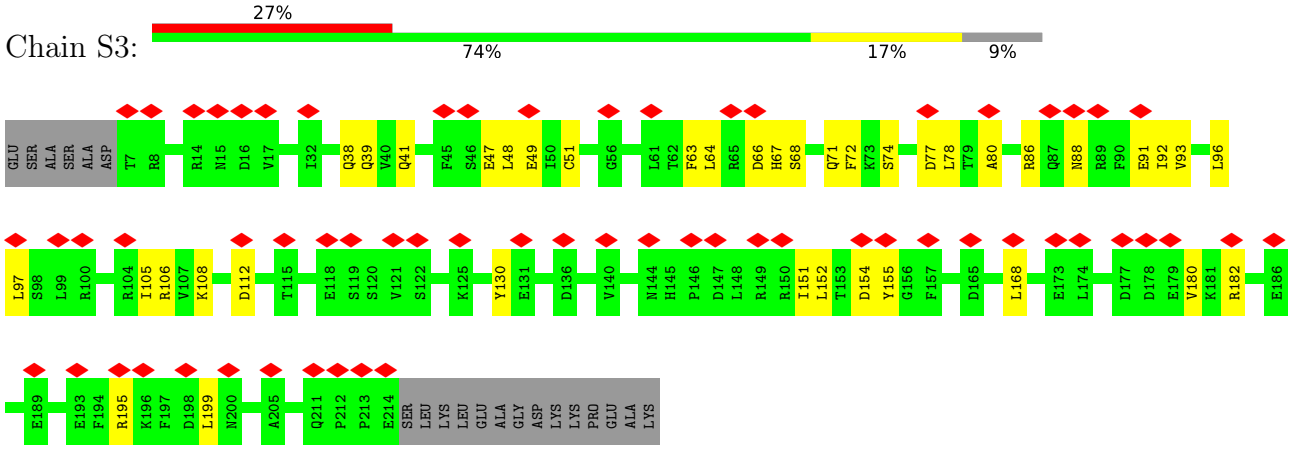
• Molecule 42: NDUFS2

Chain S2:



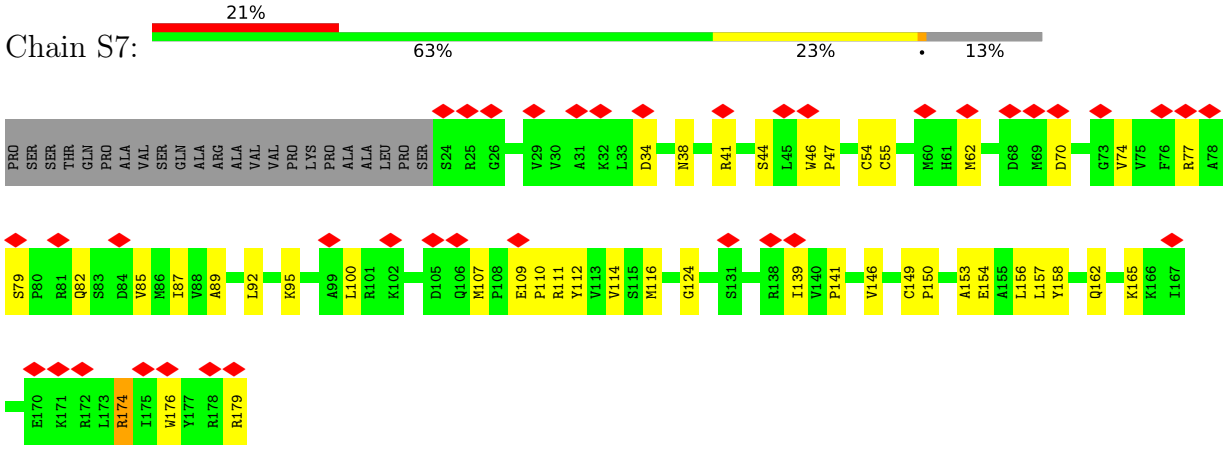
• Molecule 43: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:



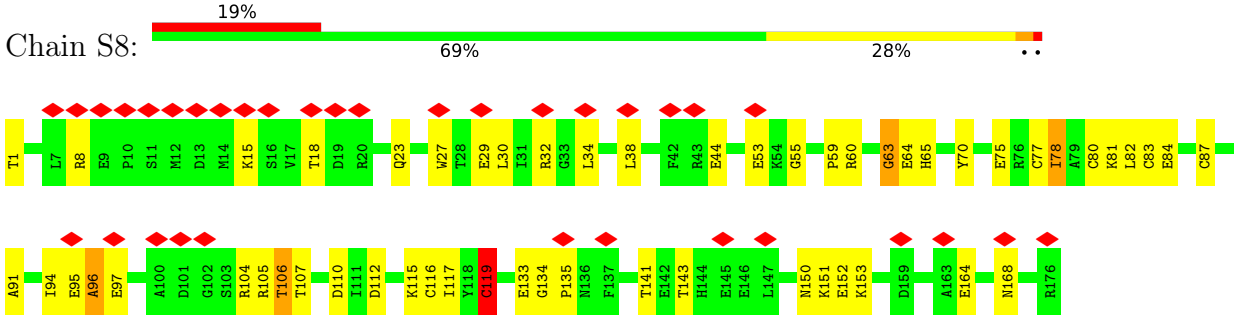
- Molecule 44: NDUFS7

Chain S7:



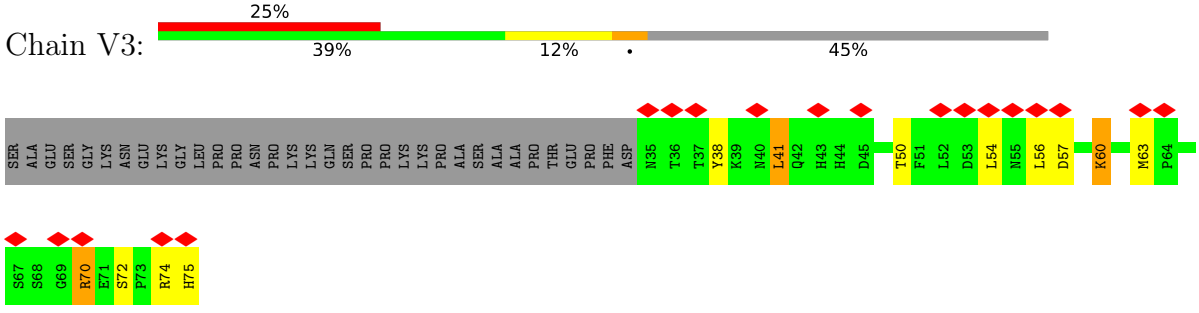
- Molecule 45: NDUFS8

Chain S8:



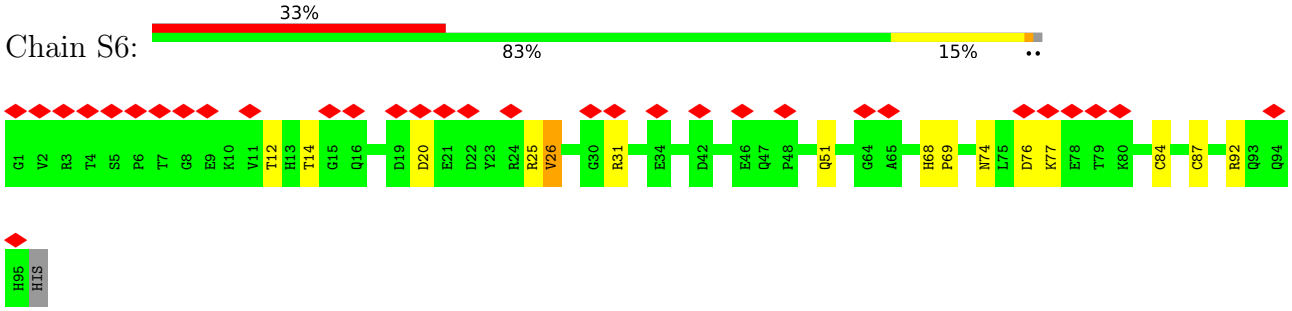
- Molecule 46: NDUFV3

Chain V3:



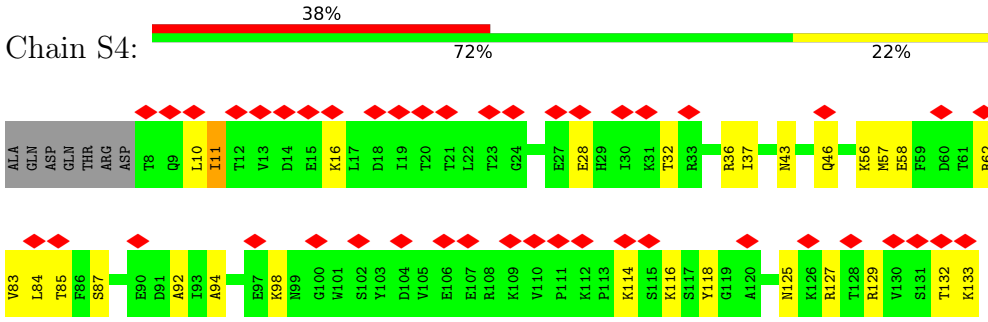
- Molecule 47: NDUFS6

Chain S6:



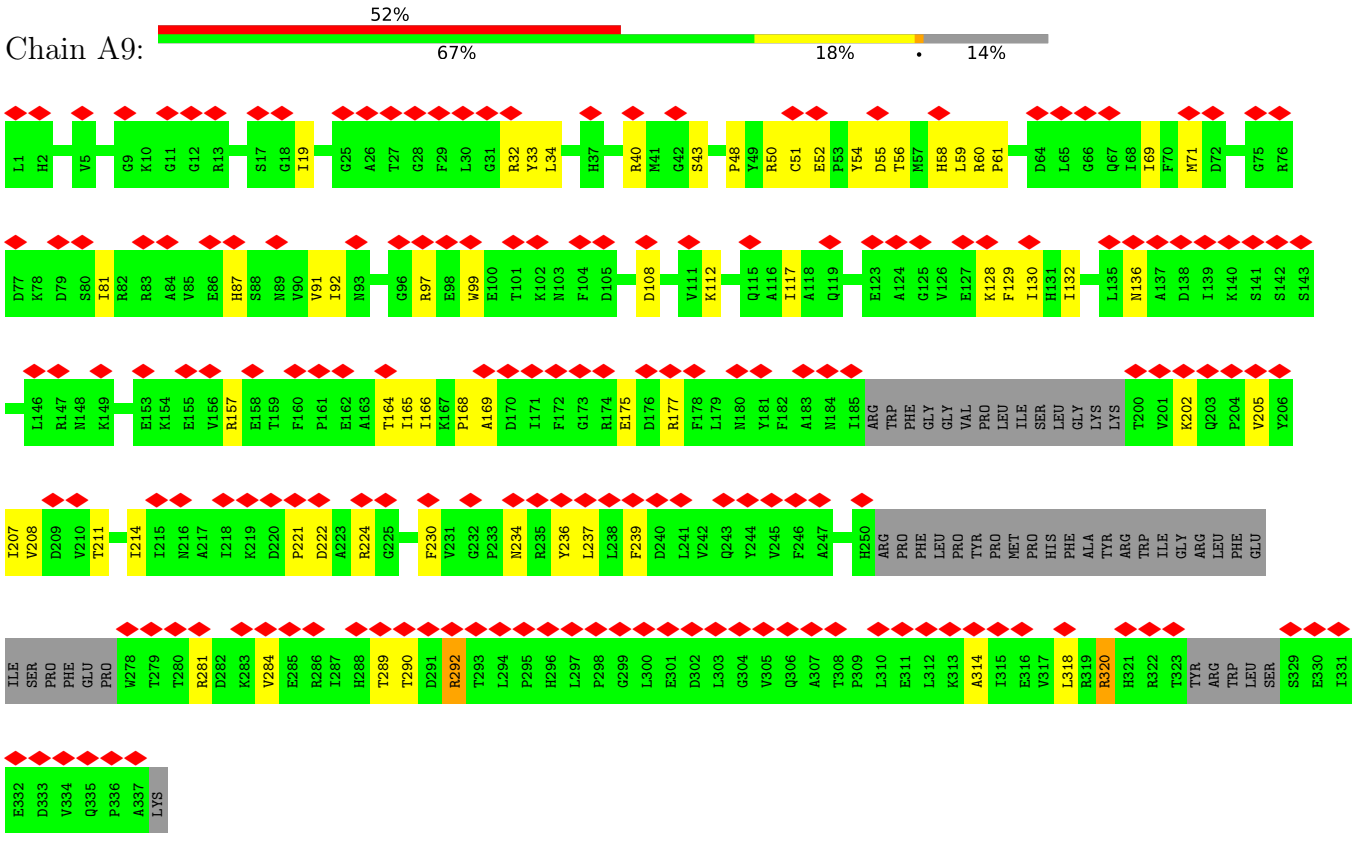
• Molecule 48: NADH:ubiquinone oxidoreductase subunit S4

Chain S4:



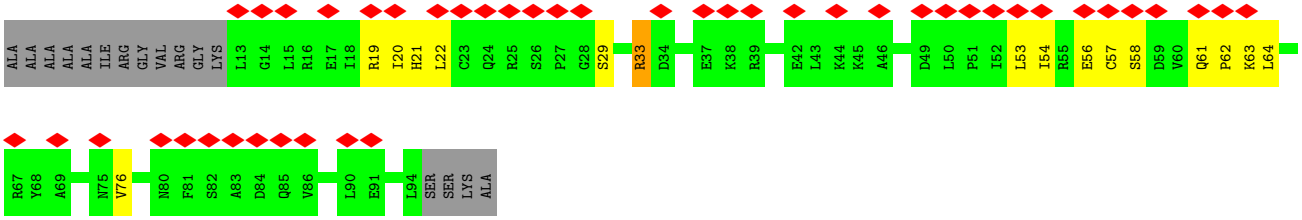
• Molecule 49: NADH:ubiquinone oxidoreductase subunit A9

Chain A9:



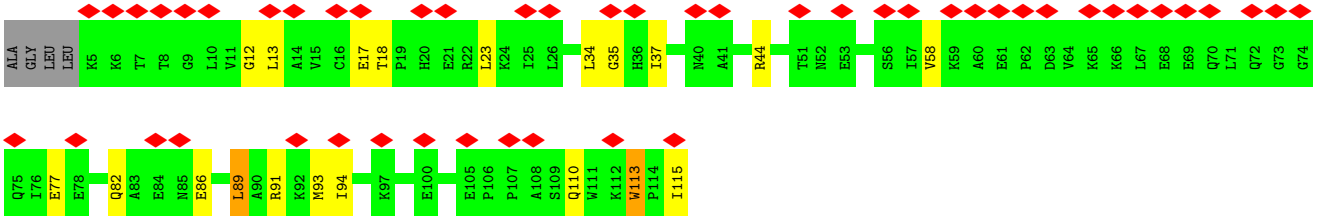
• Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:



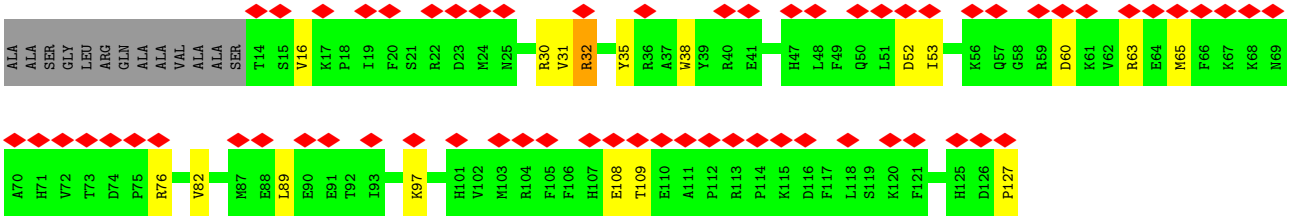
• Molecule 51: NDUFA5

Chain A5:



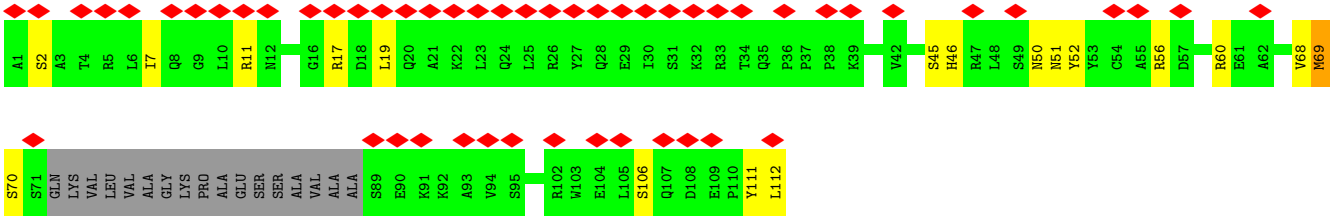
• Molecule 52: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



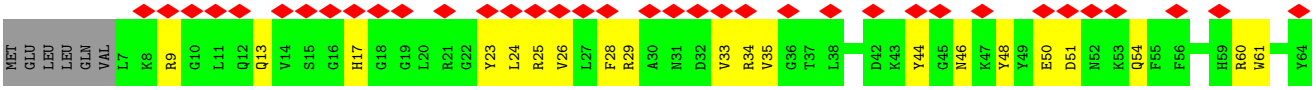
• Molecule 53: NDUFA7

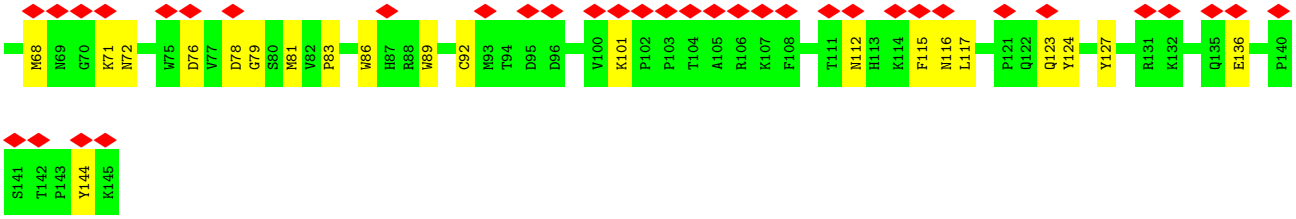
Chain A7:



• Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:




M68
N69
G70
K71
N72
W75
D76
V77
D78
G79
S80
N81
V82
P83
W86
H87
R88
W89
C92
M93
T94
D95
D96
V100
K101
P102
P103
T104
A105
R106
K107
F108
T111
N112
H113
K114
F115
N116
L117
P121
Q122
Q123
Y124
Y127
R131
K132
Q135
E136
P140
S141
T142
P143
Y144
K145

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.153	Depositor
Minimum map value	-0.304	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	D3	0.38	0/747	0.68	0/1022
2	D1	0.48	0/2432	0.74	1/3323 (0.0%)
3	D6	0.43	0/1309	0.72	1/1768 (0.1%)
4	4L	0.45	0/758	0.76	0/1024
5	D5	0.46	0/4933	0.76	5/6710 (0.1%)
6	D4	0.49	0/3740	0.77	5/5095 (0.1%)
7	D2	0.51	0/2788	0.73	1/3795 (0.0%)
8	AK	0.39	0/1046	0.69	1/1419 (0.1%)
9	B5	0.44	0/1189	0.63	1/1607 (0.1%)
10	AA	0.32	0/655	0.66	0/881
10	AB	0.42	0/714	0.66	0/963
11	A8	0.40	0/1441	0.70	1/1942 (0.1%)
12	BJ	0.43	0/1475	0.62	2/1989 (0.1%)
13	AJ	0.45	0/2644	0.69	3/3579 (0.1%)
14	S5	0.42	0/843	0.68	1/1128 (0.1%)
15	A3	0.37	0/602	0.70	0/828
16	B3	0.45	0/595	0.75	0/803
17	C2	0.48	0/1028	0.67	0/1388
18	B4	0.47	0/1085	0.68	1/1467 (0.1%)
19	AM	0.44	0/1172	0.66	1/1579 (0.1%)
20	B6	0.44	0/822	0.77	0/1118
21	B7	0.40	0/1051	0.68	2/1408 (0.1%)
22	B9	0.45	0/1568	0.64	1/2123 (0.0%)
23	B2	0.41	0/590	0.71	0/810
24	B8	0.51	1/1379 (0.1%)	0.75	2/1884 (0.1%)
25	BK	0.47	0/880	0.67	0/1196
26	C1	0.40	0/404	0.55	0/548
27	B1	0.39	0/462	0.59	0/624
28	A1	0.42	0/592	0.68	0/795
29	a1	0.38	0/3479	0.61	1/4719 (0.0%)
29	a3	0.42	0/3518	0.61	1/4776 (0.0%)
30	a2	0.35	0/3183	0.56	0/4313

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	a4	0.38	0/3179	0.60	0/4308
31	b1	0.42	0/3119	0.60	0/4268
31	b2	0.45	0/3119	0.62	0/4268
32	c1	0.39	0/1968	0.59	0/2672
32	c2	0.41	0/1962	0.59	0/2664
33	f1	0.32	0/1554	0.52	0/2101
33	f2	0.35	0/1548	0.57	0/2093
34	d1	0.38	0/906	0.60	2/1213 (0.2%)
34	d2	0.41	0/908	0.60	0/1218
35	q1	0.41	0/638	0.56	0/862
35	q2	0.47	0/652	0.63	0/883
36	h1	0.34	0/538	0.64	1/723 (0.1%)
36	h2	0.37	0/538	0.75	1/723 (0.1%)
38	i1	0.36	0/471	0.52	0/634
38	i2	0.35	0/486	0.53	0/655
39	V1	0.41	0/3386	0.66	0/4575
40	V2	0.39	0/1687	0.74	1/2295 (0.0%)
41	S1	0.41	0/5362	0.64	0/7266
42	S2	0.50	0/3525	0.67	1/4776 (0.0%)
43	S3	0.47	0/1776	0.64	0/2417
44	S7	0.51	0/1278	0.63	0/1728
45	S8	0.59	1/1445 (0.1%)	0.72	3/1956 (0.2%)
46	V3	0.38	0/355	0.69	0/480
47	S6	0.44	0/749	0.62	0/1009
48	S4	0.38	0/1047	0.60	0/1415
49	A9	0.37	0/2351	0.67	3/3181 (0.1%)
50	A2	0.33	0/676	0.65	0/911
51	A5	0.38	0/921	0.66	2/1249 (0.2%)
52	A6	0.37	0/993	0.59	0/1336
53	A7	0.33	0/775	0.65	0/1048
54	AL	0.41	0/1201	0.67	0/1632
All	All	0.43	2/98237 (0.0%)	0.66	45/133183 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D1	0	3
3	D6	0	2
5	D5	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	D4	0	1
7	D2	0	1
8	AK	0	1
10	AB	0	1
11	A8	0	1
12	BJ	0	1
13	AJ	0	2
14	S5	0	1
15	A3	0	1
16	B3	0	4
17	C2	0	1
18	B4	0	2
20	B6	0	2
21	B7	0	1
23	B2	0	4
24	B8	0	2
26	C1	0	1
27	B1	0	1
29	a1	0	2
29	a3	0	1
30	a4	0	2
32	c1	0	2
32	c2	0	1
33	f2	0	2
39	V1	0	2
40	V2	0	2
41	S1	0	3
42	S2	0	4
45	S8	0	2
48	S4	0	1
51	A5	0	2
53	A7	0	2
All	All	0	63

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S8	119	CYS	CB-SG	-7.04	1.70	1.82
24	B8	46	ASP	C-N	-6.11	1.20	1.34

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D5	69	LEU	CA-CB-CG	7.97	133.64	115.30
22	B9	103	LEU	CA-CB-CG	7.63	132.85	115.30
40	V2	136	LEU	CA-CB-CG	7.56	132.70	115.30
51	A5	89	LEU	CA-CB-CG	7.55	132.68	115.30
45	S8	78	ILE	CG1-CB-CG2	-7.37	95.19	111.40

There are no chirality outliers.

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D1	316	PRO	Peptide
2	D1	32	GLN	Peptide
2	D1	91	MET	Peptide
3	D6	115	ILE	Peptide
3	D6	51	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D3	728	0	773	12	0
2	D1	2362	0	2480	54	0
3	D6	1280	0	1305	28	0
4	4L	748	0	794	16	0
5	D5	4805	0	4950	89	0
6	D4	3646	0	3850	66	0
7	D2	2724	0	2930	59	0
8	AK	1025	0	1033	13	0
9	B5	1156	0	1177	22	0
10	AA	645	0	649	8	0
10	AB	702	0	692	9	0
11	A8	1404	0	1384	28	0
12	BJ	1441	0	1417	28	0
13	AJ	2583	0	2547	40	0
14	S5	822	0	820	19	0
15	A3	582	0	583	17	0
16	B3	578	0	570	5	0
17	C2	997	0	983	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B4	1059	0	1062	19	0
19	AM	1143	0	1137	25	0
20	B6	797	0	817	19	0
21	B7	1026	0	995	22	0
22	B9	1515	0	1469	29	0
23	B2	563	0	509	10	0
24	B8	1324	0	1218	24	0
25	BK	853	0	800	21	0
26	C1	391	0	391	3	0
27	B1	449	0	453	6	0
28	A1	577	0	570	5	0
29	a1	3409	0	3322	0	0
29	a3	3447	0	3350	0	0
30	a2	3126	0	3093	0	0
30	a4	3122	0	3090	0	0
31	b1	3019	0	3082	0	0
31	b2	3019	0	3082	0	0
32	c1	1909	0	1858	0	0
32	c2	1903	0	1850	0	0
33	f1	1520	0	1505	0	0
33	f2	1514	0	1497	0	0
34	d1	886	0	883	0	0
34	d2	888	0	880	0	0
35	q1	618	0	628	0	0
35	q2	631	0	639	0	0
36	h1	532	0	509	0	0
36	h2	532	0	509	0	0
37	x1	164	0	40	0	0
37	x2	150	0	45	0	0
38	i1	459	0	462	0	0
38	i2	473	0	477	0	0
39	V1	3312	0	3266	68	0
40	V2	1647	0	1657	32	0
41	S1	5275	0	5300	128	0
42	S2	3435	0	3377	60	0
43	S3	1726	0	1676	36	0
44	S7	1247	0	1256	35	0
45	S8	1414	0	1371	41	0
46	V3	345	0	323	9	0
47	S6	737	0	710	13	0
48	S4	1024	0	1023	23	0
49	A9	2301	0	2291	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	A2	665	0	678	10	0
51	A5	901	0	936	19	0
52	A6	969	0	980	21	0
53	A7	757	0	771	14	0
54	AL	1160	0	1125	26	0
55	D1	32	0	38	1	0
55	D4	40	0	54	3	0
55	D5	38	0	50	1	0
55	b2	29	0	32	0	0
55	f2	23	0	20	0	0
56	D4	28	0	30	0	0
57	AA	34	0	40	4	0
57	AB	31	0	34	6	0
58	b1	86	0	60	0	0
58	b2	86	0	60	0	0
59	c1	43	0	30	0	0
59	c2	43	0	30	0	0
60	S1	4	0	0	1	0
60	V2	4	0	0	0	0
60	f1	4	0	0	0	0
60	f2	4	0	0	0	0
61	b2	79	0	46	0	0
61	c2	41	0	26	0	0
62	S1	16	0	0	2	0
62	S7	8	0	0	0	0
62	S8	16	0	0	2	0
62	V1	8	0	0	3	0
63	V1	31	0	19	1	0
64	S6	1	0	0	0	0
65	A9	48	0	26	4	0
All	All	96938	0	96494	1034	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1034 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S3:80:ALA:HA	43:S3:91:GLU:O	1.13	1.25
43:S3:38:GLN:HA	53:A7:70:SER:O	1.35	1.25
41:S1:449:PRO:O	41:S1:489:VAL:HA	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S3:80:ALA:CA	43:S3:91:GLU:O	2.08	1.00
50:A2:21:HIS:O	50:A2:62:PRO:HA	1.64	0.95

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D3	86/115 (75%)	80 (93%)	6 (7%)	0	100	100
2	D1	290/318 (91%)	264 (91%)	23 (8%)	3 (1%)	15	54
3	D6	164/175 (94%)	140 (85%)	24 (15%)	0	100	100
4	4L	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
5	D5	604/606 (100%)	533 (88%)	71 (12%)	0	100	100
6	D4	457/459 (100%)	424 (93%)	32 (7%)	1 (0%)	47	80
7	D2	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
8	AK	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
9	B5	137/143 (96%)	117 (85%)	19 (14%)	1 (1%)	22	62
10	AA	78/88 (89%)	69 (88%)	9 (12%)	0	100	100
10	AB	85/88 (97%)	77 (91%)	8 (9%)	0	100	100
11	A8	169/171 (99%)	142 (84%)	26 (15%)	1 (1%)	25	64
12	BJ	169/175 (97%)	153 (90%)	15 (9%)	1 (1%)	25	64
13	AJ	317/320 (99%)	270 (85%)	47 (15%)	0	100	100
14	S5	97/105 (92%)	78 (80%)	19 (20%)	0	100	100
15	A3	72/83 (87%)	60 (83%)	12 (17%)	0	100	100
16	B3	71/97 (73%)	52 (73%)	19 (27%)	0	100	100
17	C2	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	B4	126/128 (98%)	105 (83%)	21 (17%)	0	100	100
19	AM	137/143 (96%)	121 (88%)	16 (12%)	0	100	100
20	B6	90/127 (71%)	74 (82%)	16 (18%)	0	100	100
21	B7	117/119 (98%)	99 (85%)	18 (15%)	0	100	100
22	B9	174/178 (98%)	144 (83%)	30 (17%)	0	100	100
23	B2	63/72 (88%)	51 (81%)	12 (19%)	0	100	100
24	B8	155/158 (98%)	118 (76%)	37 (24%)	0	100	100
25	BK	100/125 (80%)	79 (79%)	21 (21%)	0	100	100
26	C1	44/49 (90%)	40 (91%)	4 (9%)	0	100	100
27	B1	50/57 (88%)	43 (86%)	7 (14%)	0	100	100
28	A1	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
29	a1	435/446 (98%)	393 (90%)	42 (10%)	0	100	100
29	a3	442/446 (99%)	405 (92%)	37 (8%)	0	100	100
30	a2	410/439 (93%)	383 (93%)	27 (7%)	0	100	100
30	a4	409/439 (93%)	367 (90%)	42 (10%)	0	100	100
31	b1	376/379 (99%)	350 (93%)	26 (7%)	0	100	100
31	b2	376/379 (99%)	349 (93%)	27 (7%)	0	100	100
32	c1	237/240 (99%)	201 (85%)	36 (15%)	0	100	100
32	c2	236/240 (98%)	200 (85%)	36 (15%)	0	100	100
33	f1	194/196 (99%)	176 (91%)	18 (9%)	0	100	100
33	f2	193/196 (98%)	170 (88%)	23 (12%)	0	100	100
34	d1	98/110 (89%)	94 (96%)	4 (4%)	0	100	100
34	d2	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
35	q1	71/81 (88%)	64 (90%)	7 (10%)	0	100	100
35	q2	73/81 (90%)	67 (92%)	6 (8%)	0	100	100
36	h1	63/78 (81%)	57 (90%)	6 (10%)	0	100	100
36	h2	63/78 (81%)	59 (94%)	4 (6%)	0	100	100
38	i1	53/63 (84%)	48 (91%)	5 (9%)	0	100	100
38	i2	55/63 (87%)	50 (91%)	5 (9%)	0	100	100
39	V1	428/445 (96%)	379 (89%)	49 (11%)	0	100	100
40	V2	210/217 (97%)	171 (81%)	39 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	S1	686/704 (97%)	611 (89%)	74 (11%)	1 (0%)	51 85
42	S2	423/430 (98%)	378 (89%)	45 (11%)	0	100 100
43	S3	206/228 (90%)	183 (89%)	23 (11%)	0	100 100
44	S7	154/179 (86%)	137 (89%)	17 (11%)	0	100 100
45	S8	174/176 (99%)	152 (87%)	22 (13%)	0	100 100
46	V3	39/75 (52%)	29 (74%)	10 (26%)	0	100 100
47	S6	93/96 (97%)	82 (88%)	11 (12%)	0	100 100
48	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100 100
49	A9	283/338 (84%)	237 (84%)	46 (16%)	0	100 100
50	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100 100
51	A5	109/115 (95%)	97 (89%)	12 (11%)	0	100 100
52	A6	112/127 (88%)	104 (93%)	8 (7%)	0	100 100
53	A7	91/112 (81%)	74 (81%)	16 (18%)	1 (1%)	14 52
54	AL	137/145 (94%)	111 (81%)	26 (19%)	0	100 100
All	All	11848/12556 (94%)	10487 (88%)	1351 (11%)	10 (0%)	54 85

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D4	54	LEU
2	D1	32	GLN
53	A7	69	MET
17	C2	10	PRO
2	D1	68	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D3	81/103 (79%)	80 (99%)	1 (1%)	71 83
2	D1	260/278 (94%)	259 (100%)	1 (0%)	91 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D6	137/144 (95%)	137 (100%)	0	100	100
4	4L	87/87 (100%)	83 (95%)	4 (5%)	27	54
5	D5	539/539 (100%)	533 (99%)	6 (1%)	73	84
6	D4	412/412 (100%)	404 (98%)	8 (2%)	57	74
7	D2	315/315 (100%)	309 (98%)	6 (2%)	57	74
8	AK	101/101 (100%)	98 (97%)	3 (3%)	41	63
9	B5	122/125 (98%)	121 (99%)	1 (1%)	81	89
10	AA	74/81 (91%)	74 (100%)	0	100	100
10	AB	80/81 (99%)	78 (98%)	2 (2%)	47	68
11	A8	154/154 (100%)	149 (97%)	5 (3%)	39	62
12	BJ	155/157 (99%)	154 (99%)	1 (1%)	86	92
13	AJ	283/284 (100%)	282 (100%)	1 (0%)	91	94
14	S5	88/94 (94%)	88 (100%)	0	100	100
15	A3	65/71 (92%)	65 (100%)	0	100	100
16	B3	55/75 (73%)	52 (94%)	3 (6%)	21	49
17	C2	106/107 (99%)	106 (100%)	0	100	100
18	B4	114/114 (100%)	113 (99%)	1 (1%)	78	87
19	AM	119/121 (98%)	116 (98%)	3 (2%)	47	68
20	B6	90/121 (74%)	86 (96%)	4 (4%)	28	54
21	B7	108/108 (100%)	105 (97%)	3 (3%)	43	65
22	B9	159/160 (99%)	156 (98%)	3 (2%)	57	74
23	B2	59/62 (95%)	59 (100%)	0	100	100
24	B8	142/142 (100%)	140 (99%)	2 (1%)	67	80
25	BK	93/112 (83%)	91 (98%)	2 (2%)	52	70
26	C1	42/44 (96%)	42 (100%)	0	100	100
27	B1	48/53 (91%)	48 (100%)	0	100	100
28	A1	59/59 (100%)	56 (95%)	3 (5%)	24	51
29	a1	366/372 (98%)	361 (99%)	5 (1%)	67	80
29	a3	370/372 (100%)	364 (98%)	6 (2%)	62	79
30	a2	326/341 (96%)	322 (99%)	4 (1%)	71	83
30	a4	326/341 (96%)	324 (99%)	2 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	b1	330/331 (100%)	327 (99%)	3 (1%)	78 87
31	b2	330/331 (100%)	328 (99%)	2 (1%)	86 92
32	c1	205/206 (100%)	203 (99%)	2 (1%)	76 86
32	c2	204/206 (99%)	202 (99%)	2 (1%)	76 86
33	f1	168/168 (100%)	167 (99%)	1 (1%)	86 92
33	f2	167/168 (99%)	166 (99%)	1 (1%)	86 92
34	d1	93/99 (94%)	92 (99%)	1 (1%)	73 84
34	d2	94/99 (95%)	91 (97%)	3 (3%)	39 62
35	q1	66/72 (92%)	66 (100%)	0	100 100
35	q2	67/72 (93%)	66 (98%)	1 (2%)	65 80
36	h1	62/74 (84%)	61 (98%)	1 (2%)	62 79
36	h2	62/74 (84%)	61 (98%)	1 (2%)	62 79
38	i1	46/52 (88%)	45 (98%)	1 (2%)	52 70
38	i2	48/52 (92%)	48 (100%)	0	100 100
39	V1	344/354 (97%)	340 (99%)	4 (1%)	71 83
40	V2	182/183 (100%)	181 (100%)	1 (0%)	88 93
41	S1	578/588 (98%)	574 (99%)	4 (1%)	84 90
42	S2	370/371 (100%)	366 (99%)	4 (1%)	73 84
43	S3	189/204 (93%)	189 (100%)	0	100 100
44	S7	132/150 (88%)	130 (98%)	2 (2%)	65 80
45	S8	151/151 (100%)	149 (99%)	2 (1%)	69 82
46	V3	40/68 (59%)	36 (90%)	4 (10%)	7 28
47	S6	79/80 (99%)	78 (99%)	1 (1%)	69 82
48	S4	113/119 (95%)	112 (99%)	1 (1%)	78 87
49	A9	242/292 (83%)	238 (98%)	4 (2%)	60 78
50	A2	73/81 (90%)	72 (99%)	1 (1%)	67 80
51	A5	99/101 (98%)	99 (100%)	0	100 100
52	A6	107/113 (95%)	106 (99%)	1 (1%)	78 87
53	A7	83/94 (88%)	83 (100%)	0	100 100
54	AL	125/131 (95%)	121 (97%)	4 (3%)	39 62
All	All	10384/10814 (96%)	10252 (99%)	132 (1%)	70 82

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	S8	119	CYS
46	V3	70	ARG
54	AL	72	ASN
20	B6	90	THR
20	B6	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
42	S2	34	ASN
42	S2	316	ASN
51	A5	82	GLN
19	AM	60	GLN
18	B4	51	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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	$\#\|Z\|>2$
58	HEM	b2	402	31	41,50,50	1.42	4 (9%)	45,82,82	1.83	10 (22%)
57	ZMP	AB	101	10	24,30,36	0.72	1 (4%)	29,37,45	1.01	1 (3%)
60	FES	f2	202	33	0,4,4	-	-	-		
62	SF4	S8	202	45	0,12,12	-	-	-		
65	NDP	A9	401	-	45,52,52	0.65	0	53,80,80	0.71	1 (1%)
62	SF4	S8	201	45	0,12,12	-	-	-		
59	HEC	c2	501	32	32,50,50	2.11	4 (12%)	24,82,82	2.81	13 (54%)
58	HEM	b1	401	31	41,50,50	1.43	5 (12%)	45,82,82	2.11	13 (28%)
55	3PE	b2	404	-	28,28,50	0.40	0	31,33,55	0.39	0
62	SF4	V1	500	39	0,12,12	-	-	-		
62	SF4	S7	300	44	0,12,12	-	-	-		
61	CDL	b2	401	-	37,37,99	0.45	0	43,49,111	0.41	0
63	FMN	V1	501	-	33,33,33	0.36	0	48,50,50	0.43	0
55	3PE	D1	501	-	31,31,50	0.38	0	34,36,55	0.46	0
56	PC1	D4	502	-	27,27,53	0.40	0	33,35,61	0.44	0
60	FES	V2	300	40	0,4,4	-	-	-		
55	3PE	D4	501	-	39,39,50	0.34	0	42,44,55	0.36	0
61	CDL	c2	502	-	40,40,99	0.42	0	46,52,111	0.63	1 (2%)
57	ZMP	AA	101	10	27,33,36	0.69	1 (3%)	32,40,45	1.07	1 (3%)
55	3PE	D5	701	-	37,37,50	0.35	0	40,42,55	0.39	0
60	FES	S1	803	41	0,4,4	-	-	-		
58	HEM	b2	403	31	41,50,50	1.55	6 (14%)	45,82,82	1.94	11 (24%)
59	HEC	c1	501	32	32,50,50	2.20	4 (12%)	24,82,82	2.60	15 (62%)
62	SF4	S1	801	41	0,12,12	-	-	-		
62	SF4	S1	802	41	0,12,12	-	-	-		
60	FES	f1	501	33	0,4,4	-	-	-		
55	3PE	f2	201	-	22,22,50	0.44	0	25,27,55	0.48	0
61	CDL	b2	405	-	40,40,99	0.47	0	46,52,111	0.59	1 (2%)
58	HEM	b1	402	31	41,50,50	1.49	5 (12%)	45,82,82	1.85	10 (22%)

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
58	HEM	b2	402	31	-	5/12/54/54	-
57	ZMP	AB	101	10	-	13/35/37/43	-
60	FES	f2	202	33	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	NDP	A9	401	-	-	15/30/77/77	0/5/5/5
62	SF4	S8	202	45	-	-	0/6/5/5
62	SF4	S8	201	45	-	-	0/6/5/5
59	HEC	c2	501	32	-	4/10/54/54	-
58	HEM	b1	401	31	-	3/12/54/54	-
55	3PE	b2	404	-	-	10/32/32/54	-
62	SF4	V1	500	39	-	-	0/6/5/5
62	SF4	S7	300	44	-	-	0/6/5/5
61	CDL	b2	401	-	-	17/46/46/110	-
63	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
55	3PE	D1	501	-	-	9/35/35/54	-
56	PC1	D4	502	-	-	11/31/31/57	-
60	FES	V2	300	40	-	-	0/1/1/1
55	3PE	D4	501	-	-	9/43/43/54	-
61	CDL	c2	502	-	-	14/48/48/110	-
57	ZMP	AA	101	10	-	12/38/40/43	-
55	3PE	D5	701	-	-	13/41/41/54	-
59	HEC	c1	501	32	-	5/10/54/54	-
58	HEM	b2	403	31	-	4/12/54/54	-
60	FES	S1	803	41	-	-	0/1/1/1
62	SF4	S1	801	41	-	-	0/6/5/5
62	SF4	S1	802	41	-	-	0/6/5/5
60	FES	f1	501	33	-	-	0/1/1/1
55	3PE	f2	201	-	-	5/26/26/54	-
61	CDL	b2	405	-	-	17/51/51/110	-
58	HEM	b1	402	31	-	6/12/54/54	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	c1	501	HEC	C2B-C3B	-7.27	1.33	1.40
59	c1	501	HEC	C3C-C2C	-7.08	1.33	1.40
59	c2	501	HEC	C3C-C2C	-7.03	1.33	1.40
59	c2	501	HEC	C2B-C3B	-6.63	1.33	1.40
58	b1	401	HEM	C4D-ND	-4.42	1.32	1.40

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	c2	501	HEC	CBA-CAA-C2A	6.42	123.43	112.60
58	b2	403	HEM	CHC-C4B-NB	5.87	130.81	124.43
58	b1	401	HEM	CHC-C4B-NB	5.60	130.52	124.43
58	b1	402	HEM	CHC-C4B-NB	5.25	130.14	124.43
58	b2	402	HEM	CHC-C4B-NB	5.07	129.94	124.43

There are no chirality outliers.

5 of 177 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	D1	501	3PE	C1-O11-P-O12
55	D1	501	3PE	C1-O11-P-O13
55	D1	501	3PE	C1-O11-P-O14
55	D5	701	3PE	C1-O11-P-O12
55	D5	701	3PE	C1-O11-P-O14

There are no ring outliers.

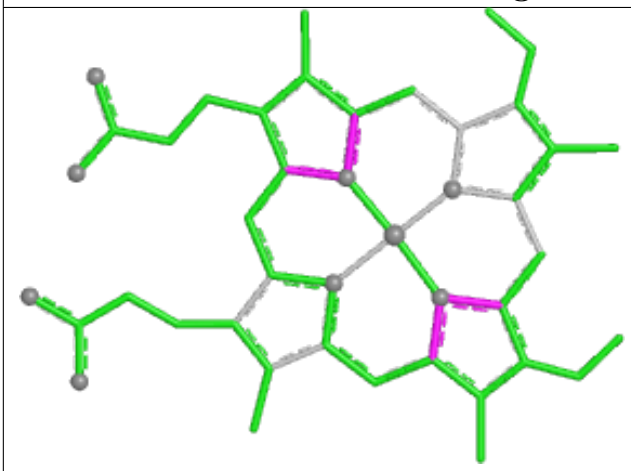
12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AB	101	ZMP	6	0
62	S8	202	SF4	2	0
65	A9	401	NDP	4	0
62	V1	500	SF4	3	0
63	V1	501	FMN	1	0
55	D1	501	3PE	1	0
55	D4	501	3PE	3	0
57	AA	101	ZMP	4	0
55	D5	701	3PE	1	0
60	S1	803	FES	1	0
62	S1	801	SF4	1	0
62	S1	802	SF4	1	0

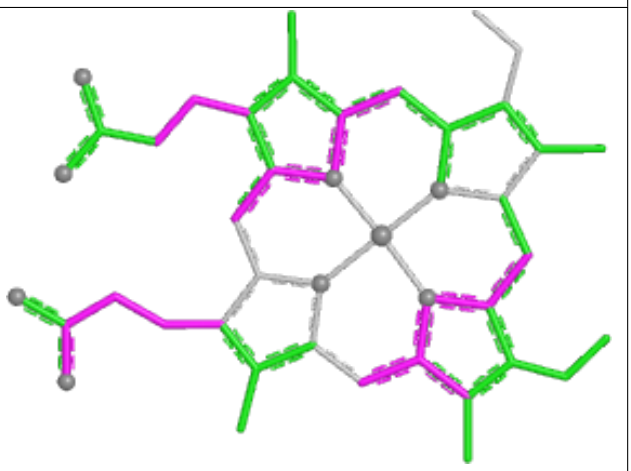
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

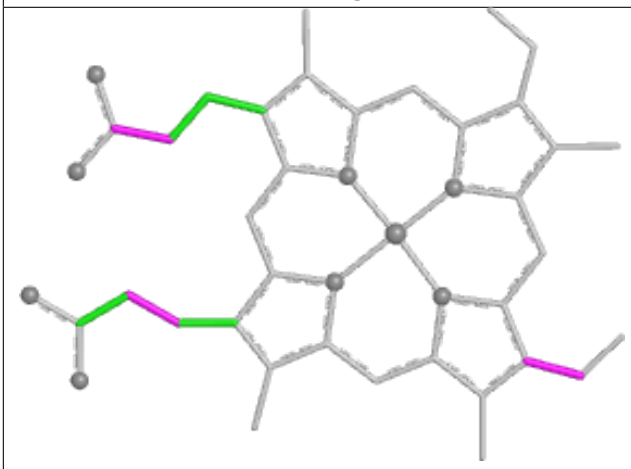
Ligand HEM b2 402



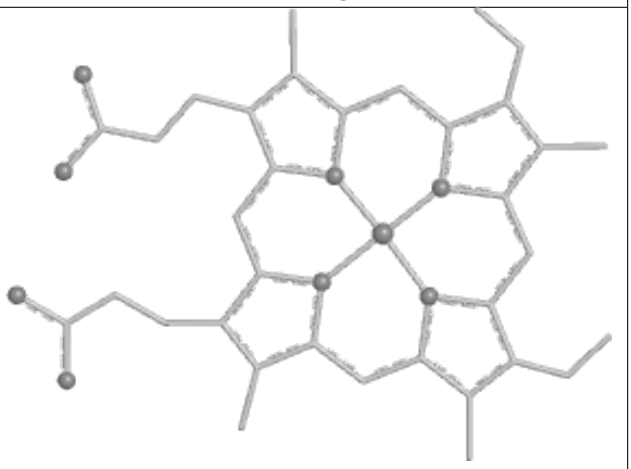
Bond lengths



Bond angles

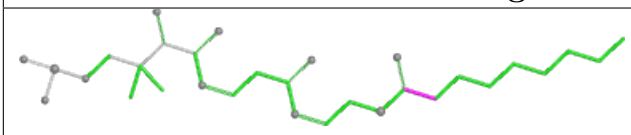


Torsions

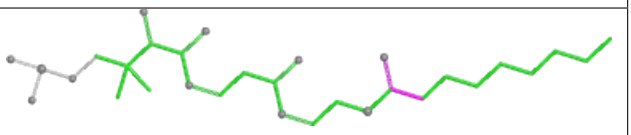


Rings

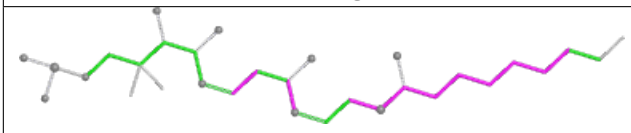
Ligand ZMP AB 101



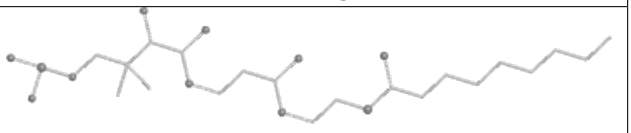
Bond lengths



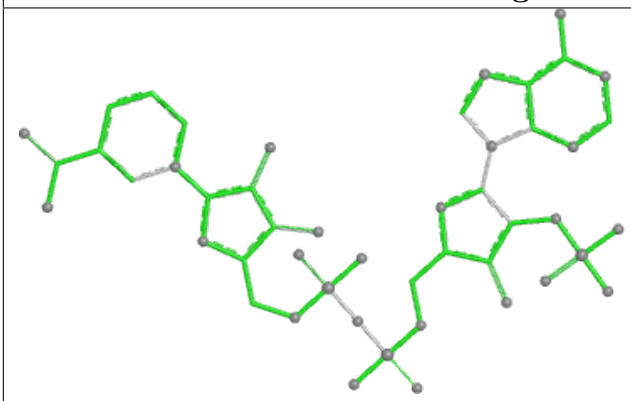
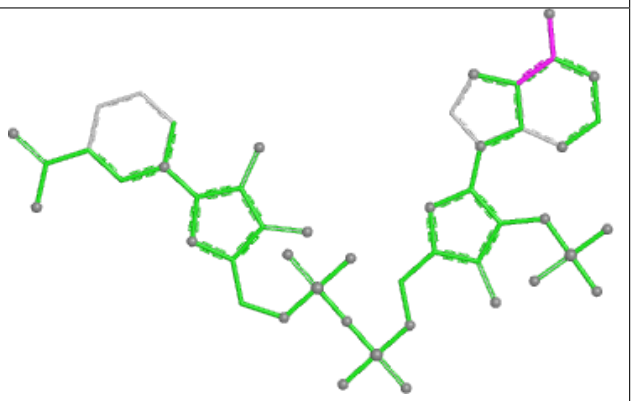
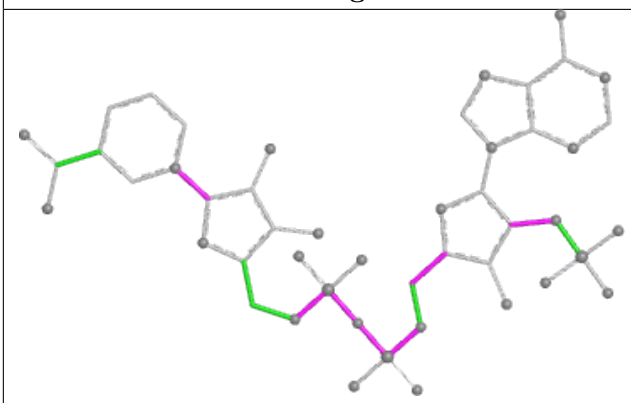
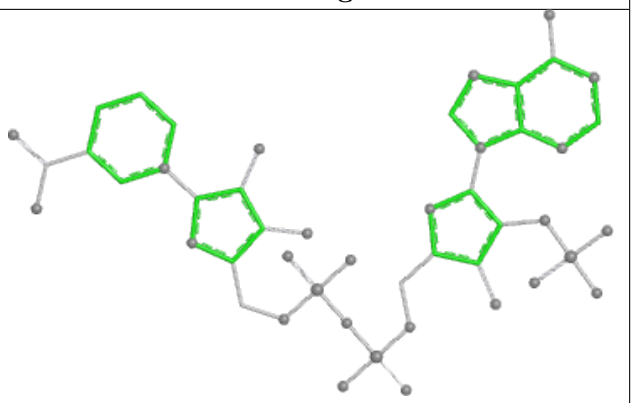
Bond angles



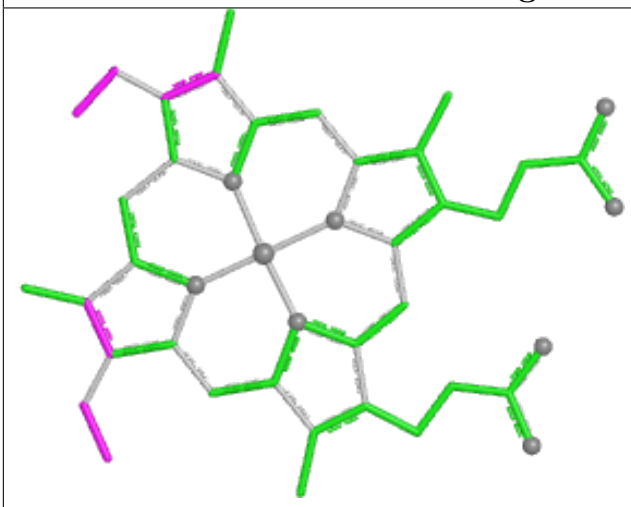
Torsions



Rings

Ligand NDP A9 401	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand HEC c2 501



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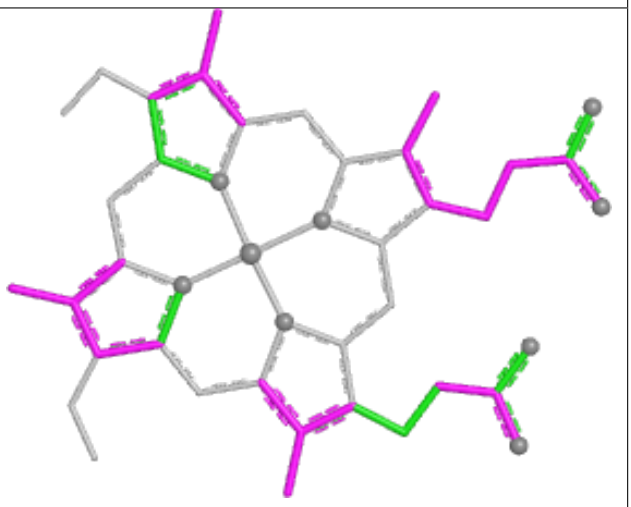
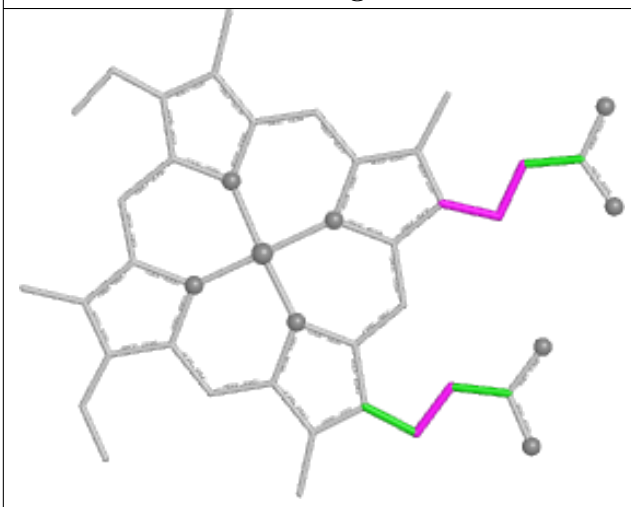
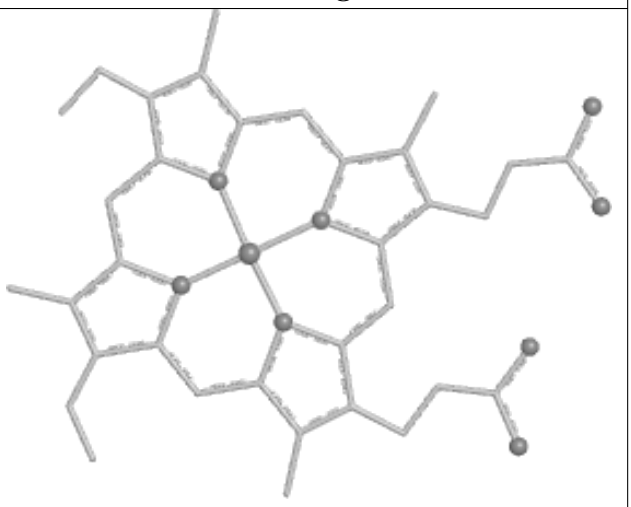


Bond angles

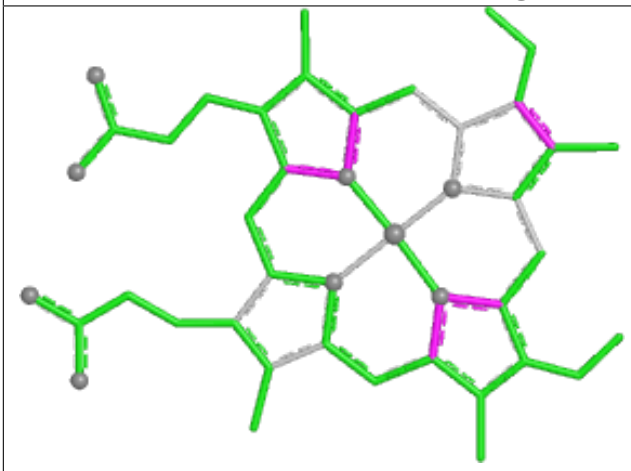


Torsions



Rings

Ligand HEM b1 401



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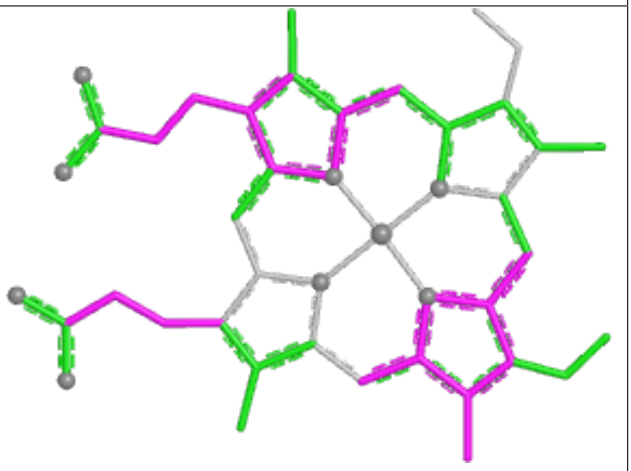

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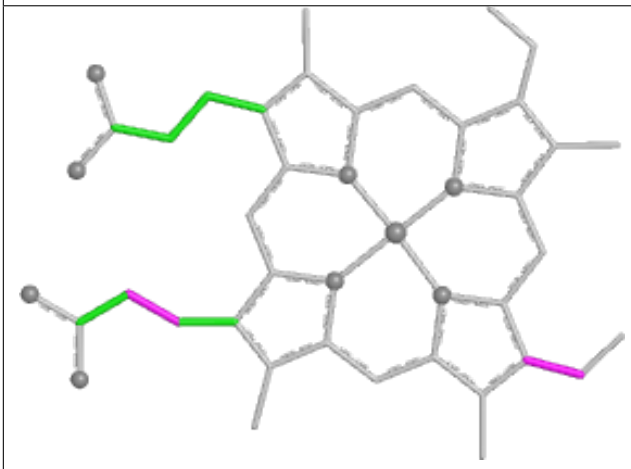

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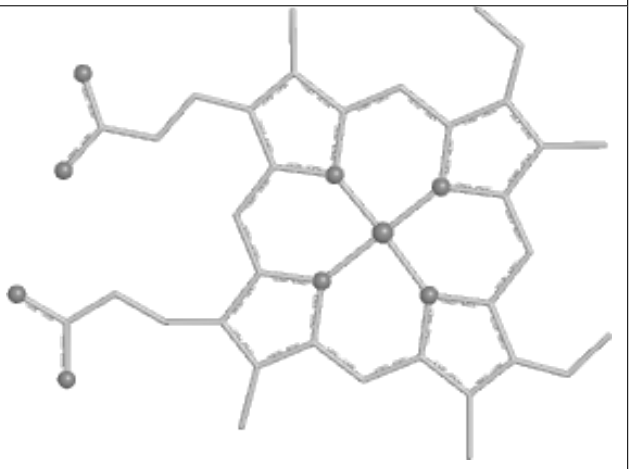
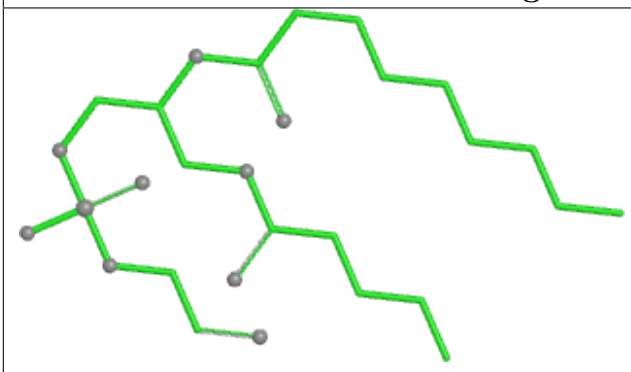
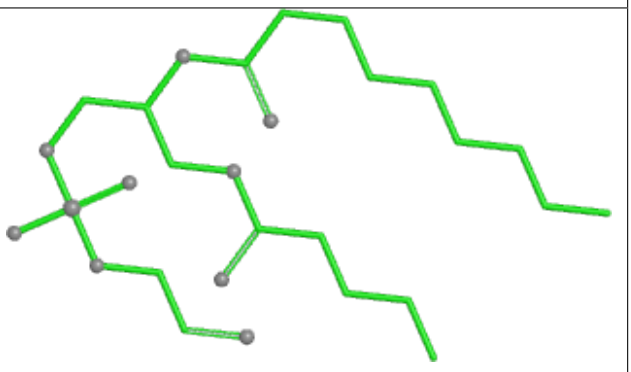
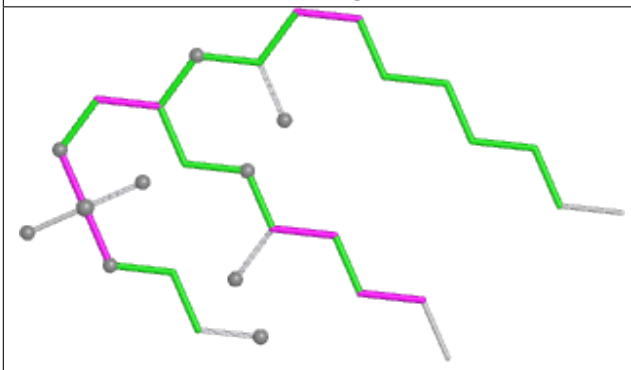
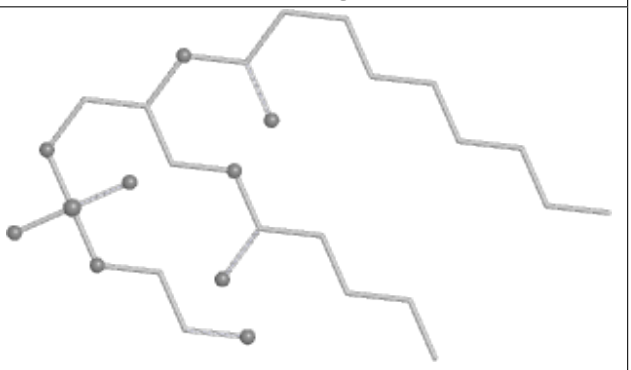
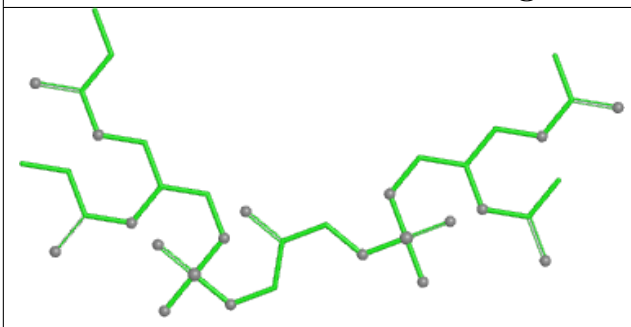
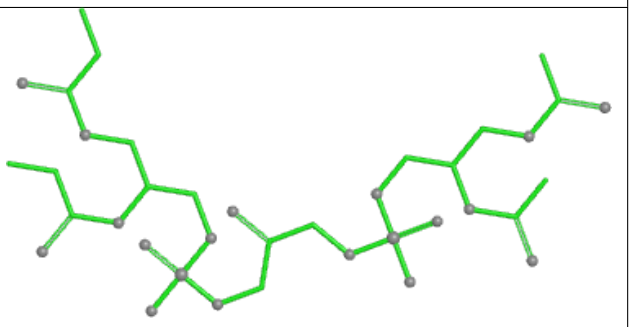
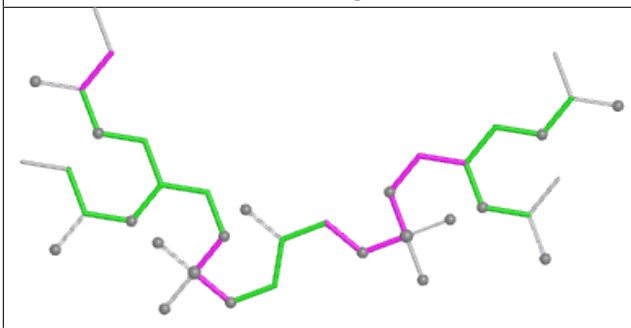
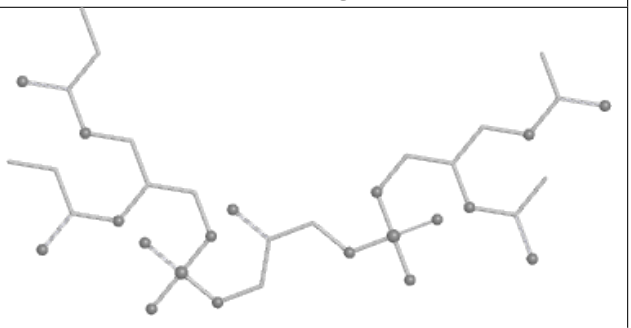
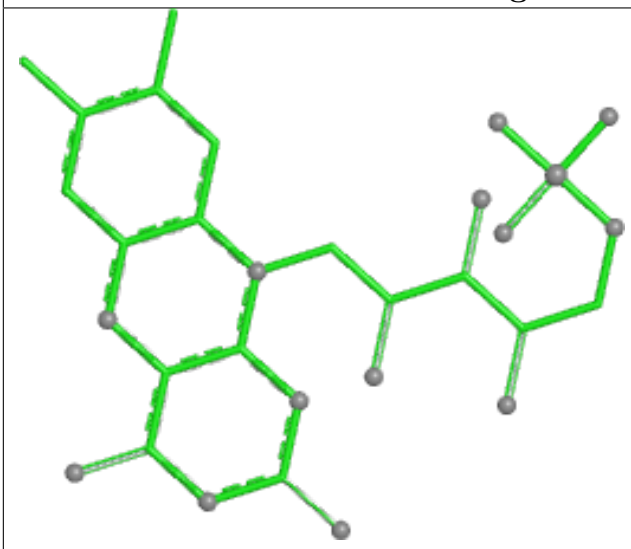


Rings

Ligand 3PE b2 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL b2 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN V1 501



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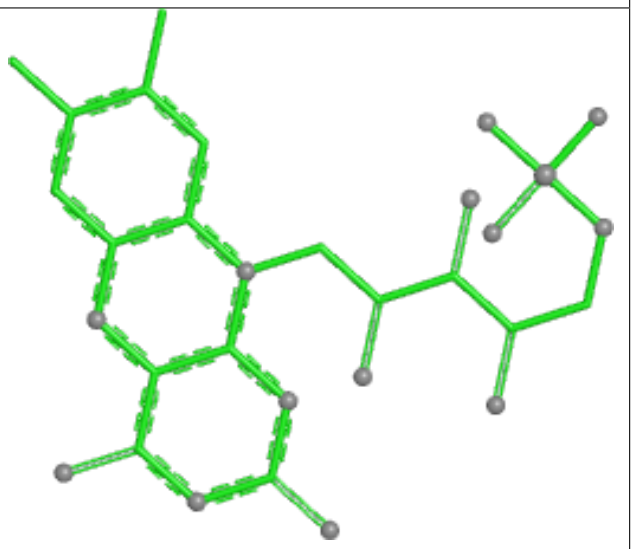
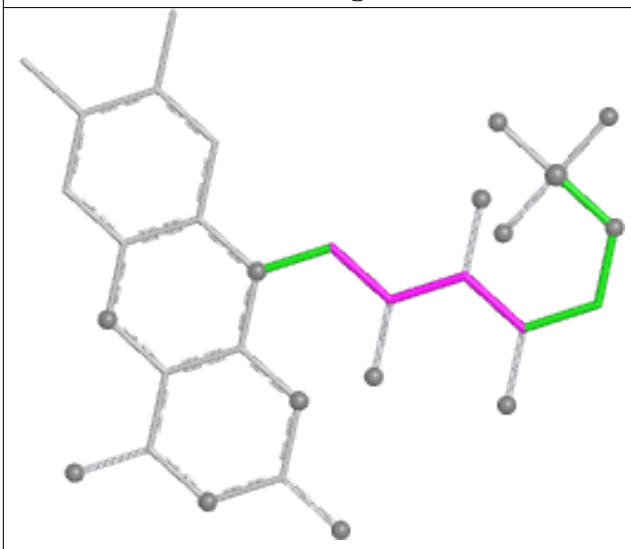


Bond angles



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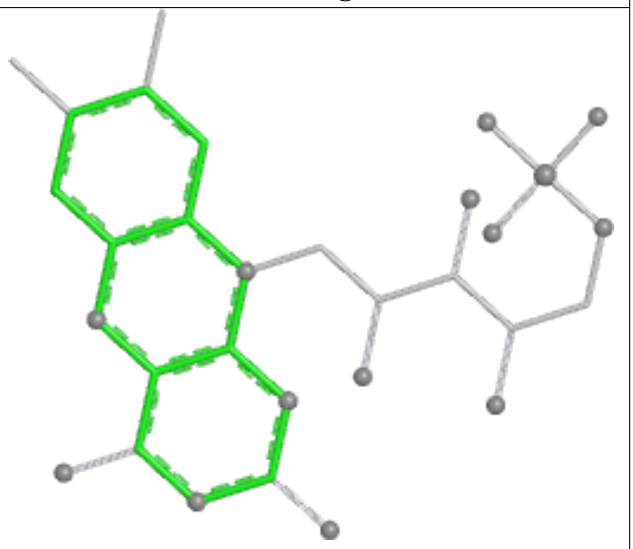
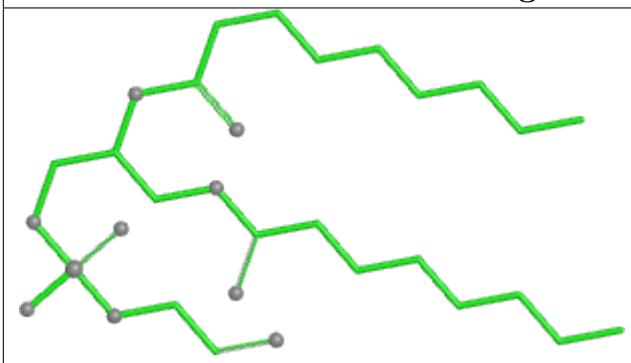


Rings

Ligand 3PE D1 501



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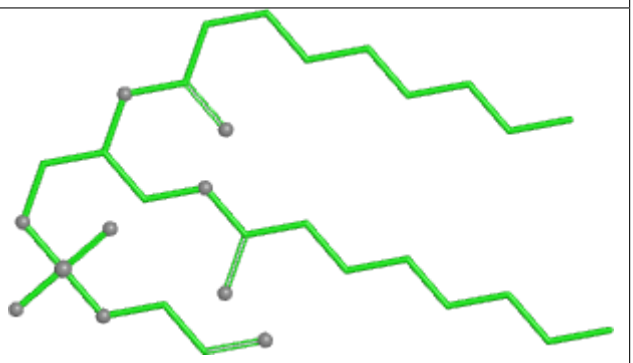

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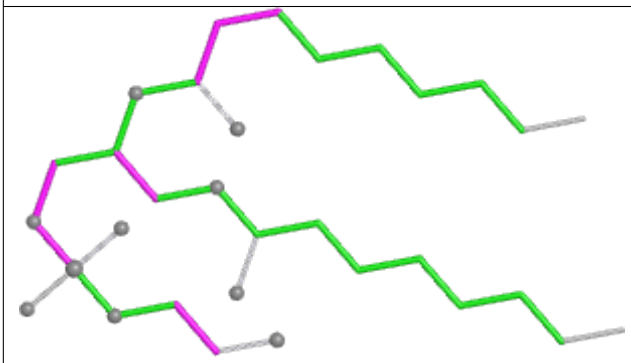

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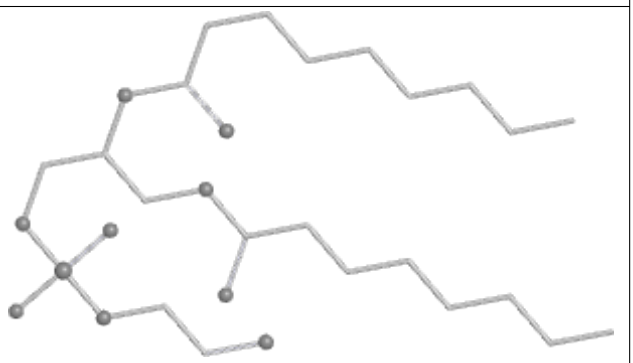
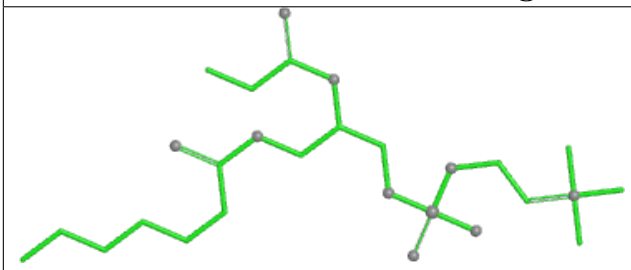


Rings

Ligand PC1 D4 502



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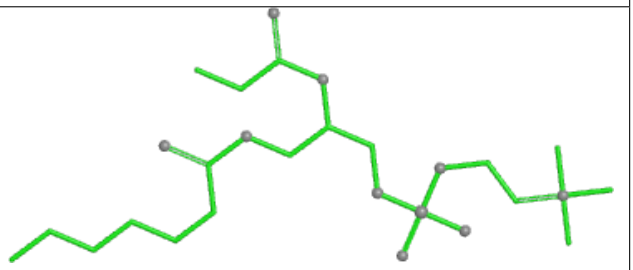
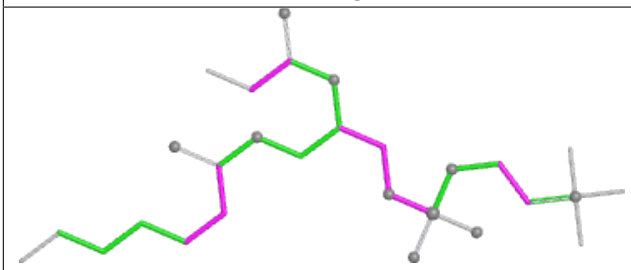


Bond angles



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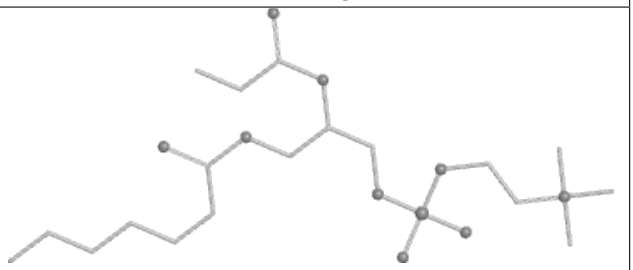
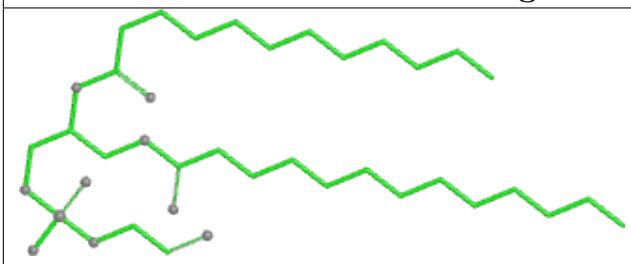


Rings

Ligand 3PE D4 501



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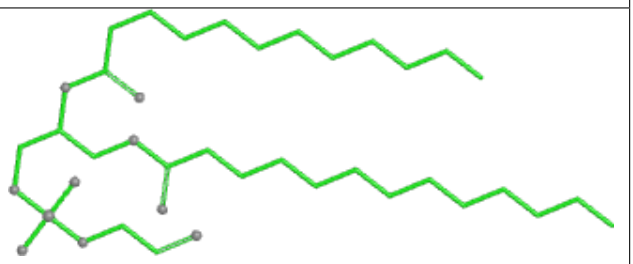
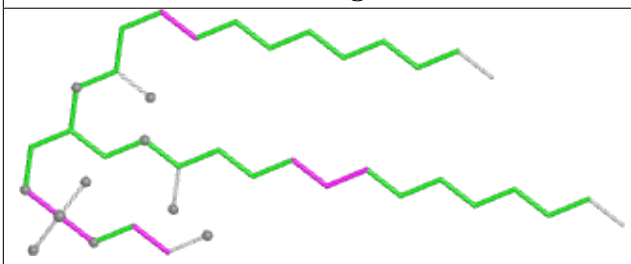


Bond angles



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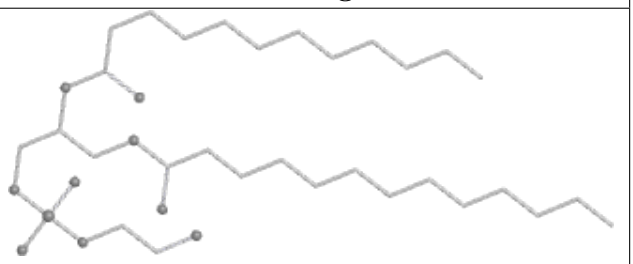
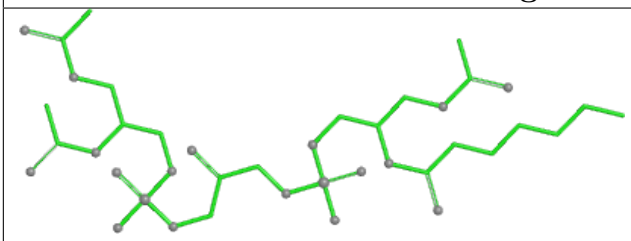


Rings

Ligand CDL c2 502



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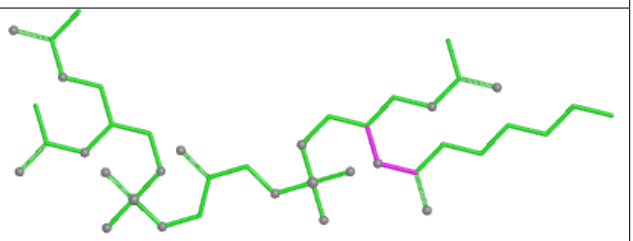

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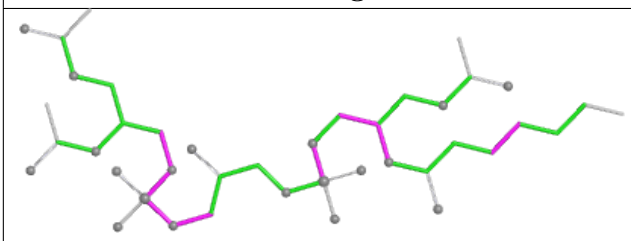

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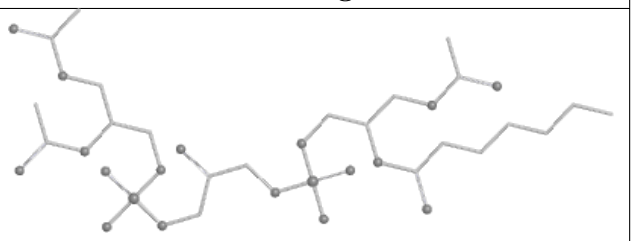
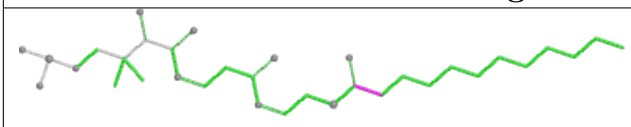


Rings

Ligand ZMP AA 101



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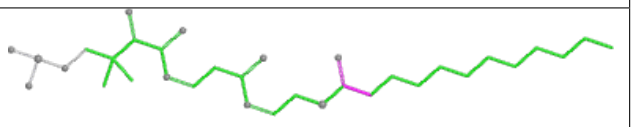
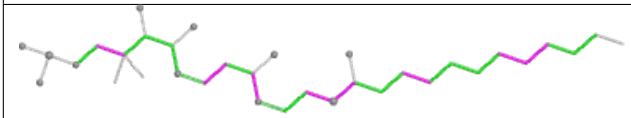


Bond angles



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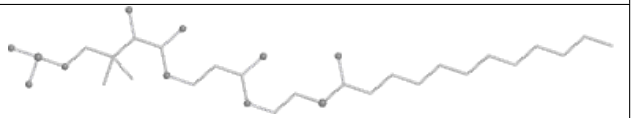
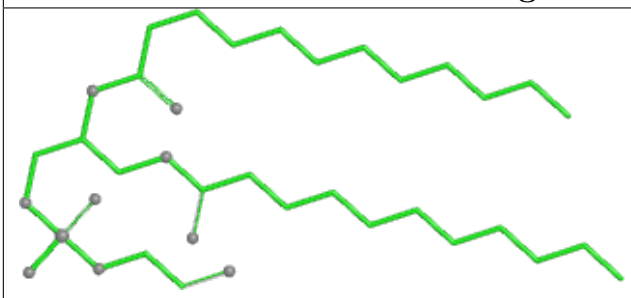


Rings

Ligand 3PE D5 701



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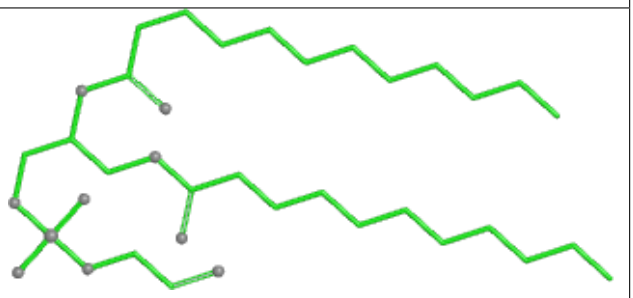
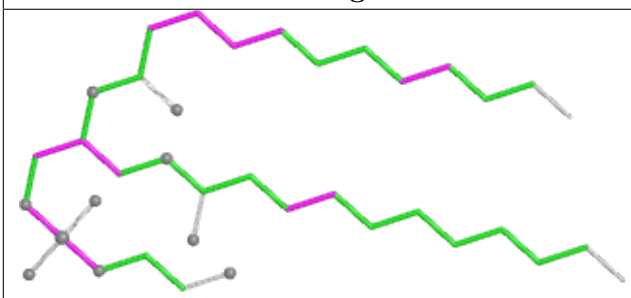


Bond angles



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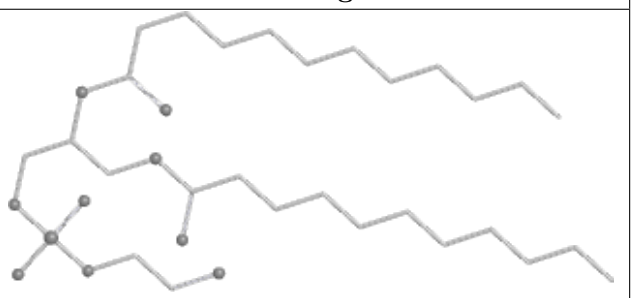
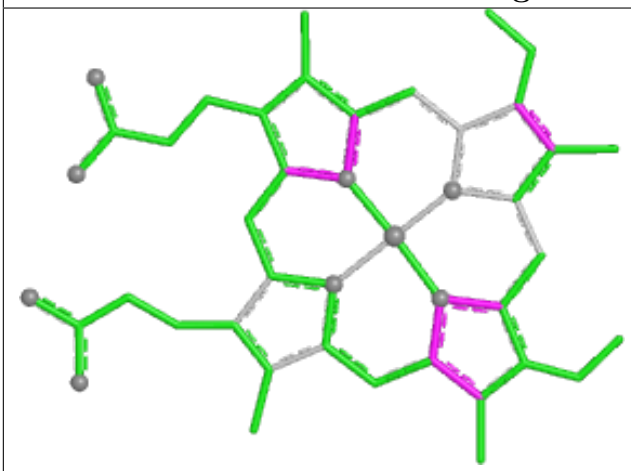


Rings

Ligand HEM b2 403



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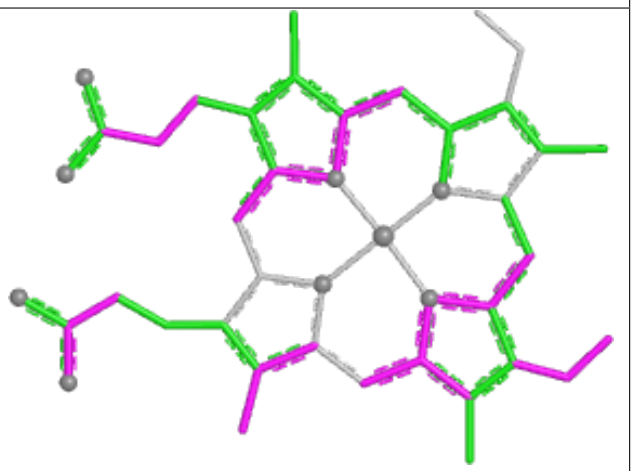
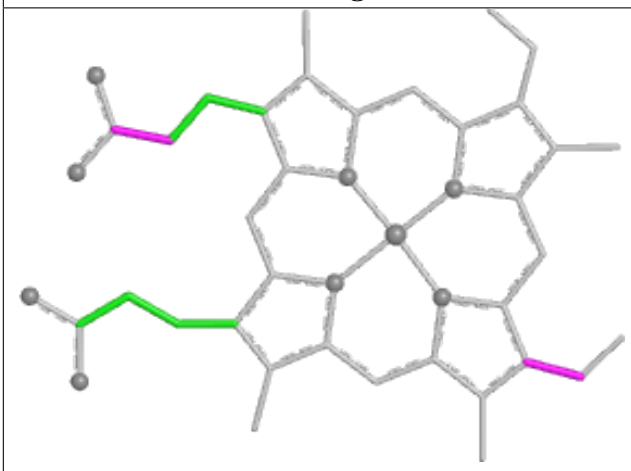


Bond angles



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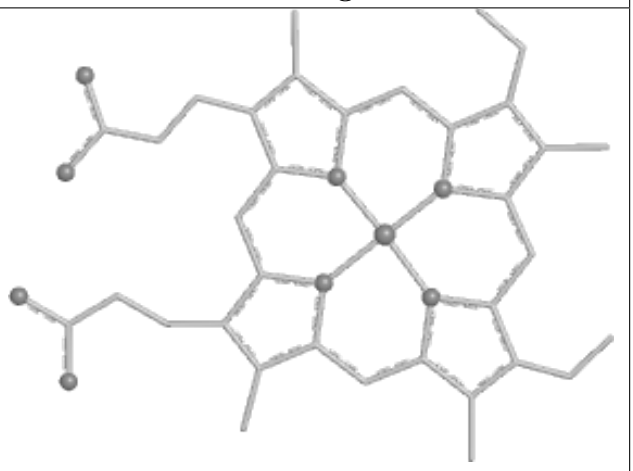
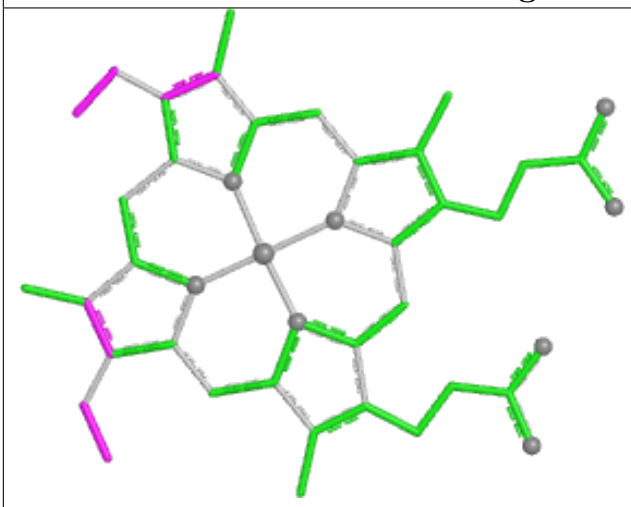
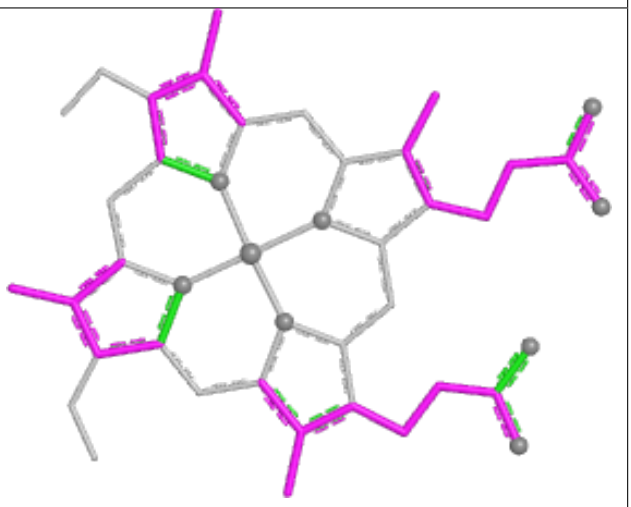


Rings

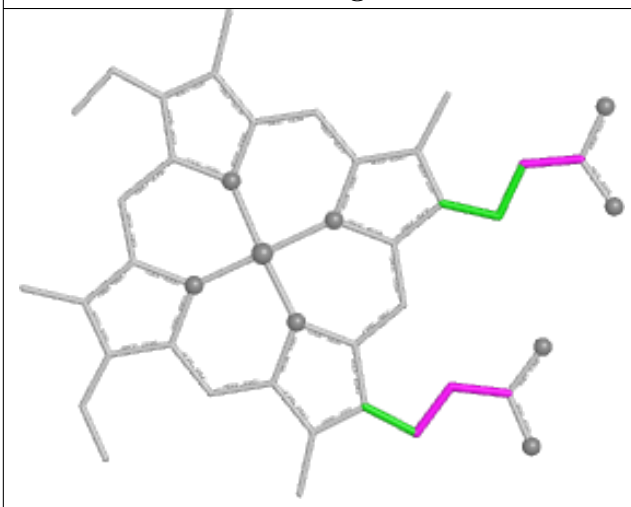
Ligand HEC c1 501



Bond lengths



Bond angles



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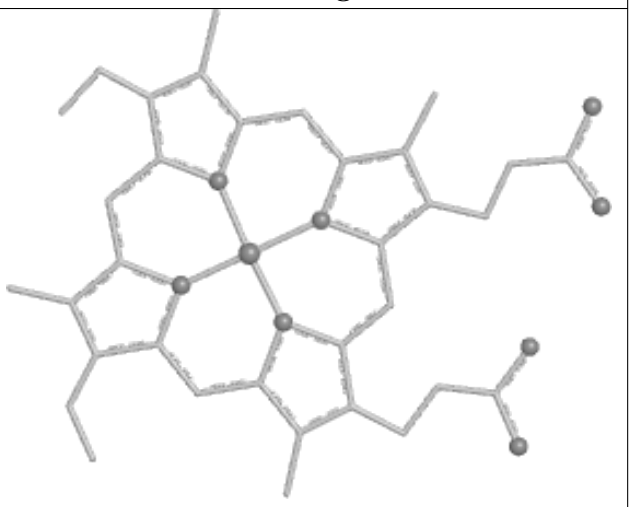
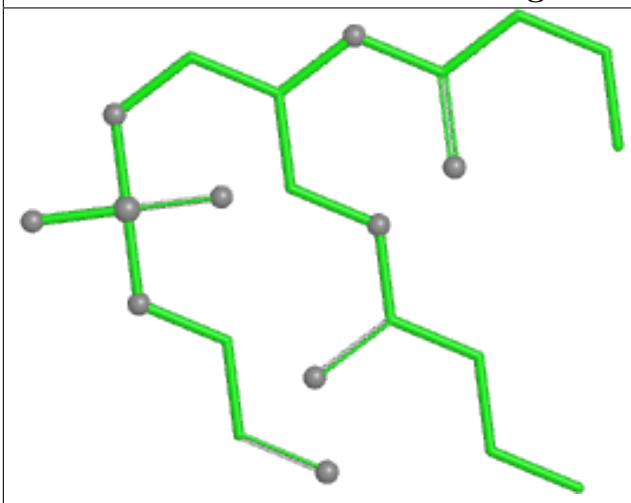
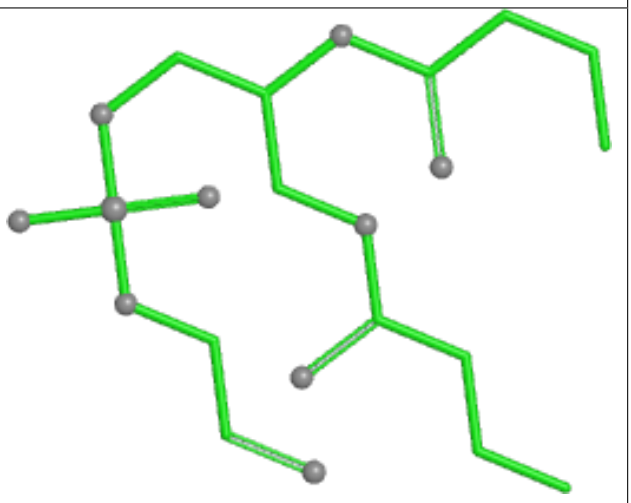


Rings

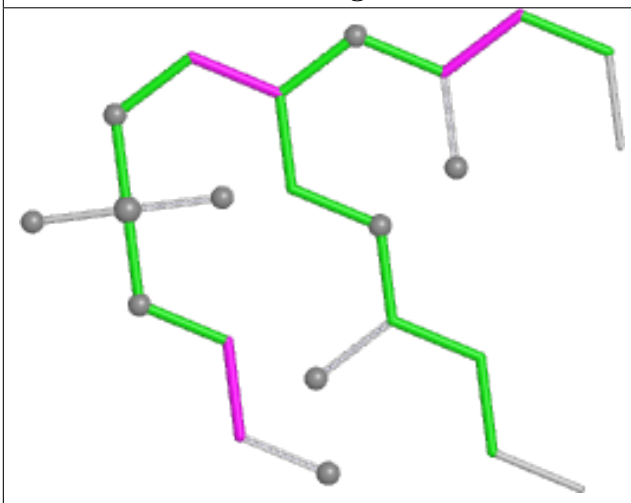
Ligand 3PE f2 201



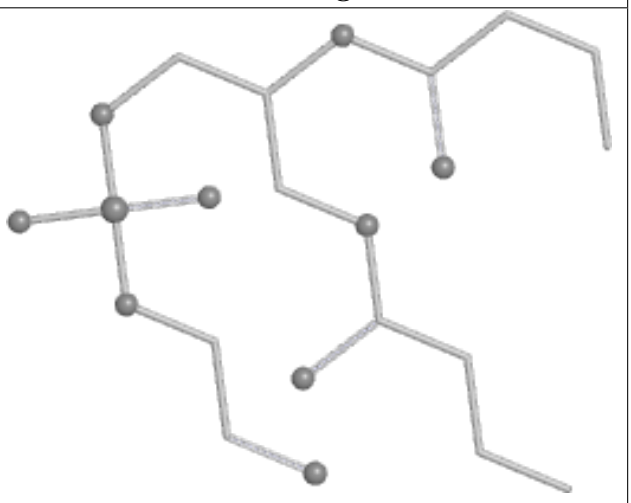
Bond lengths



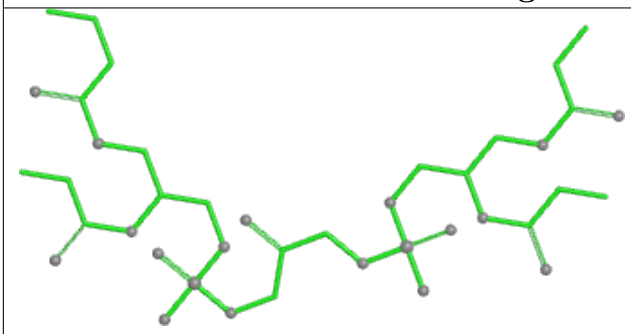
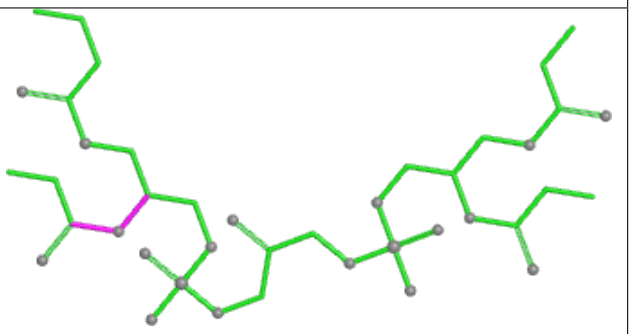
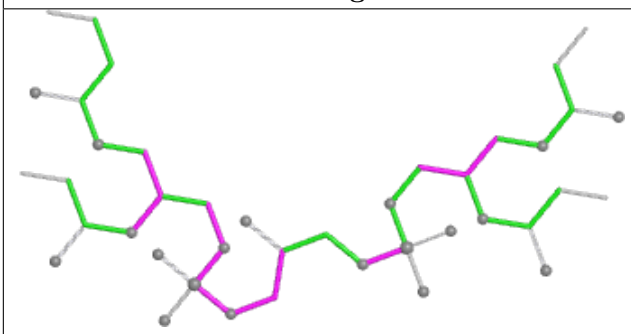
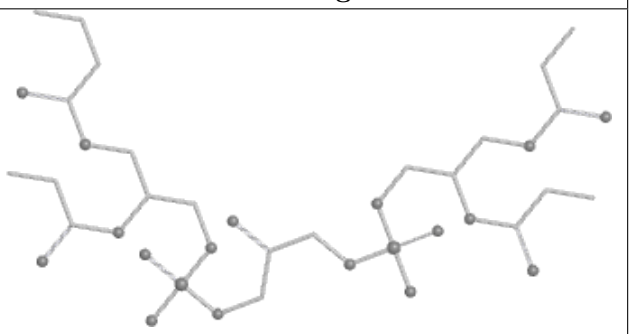
Bond angles



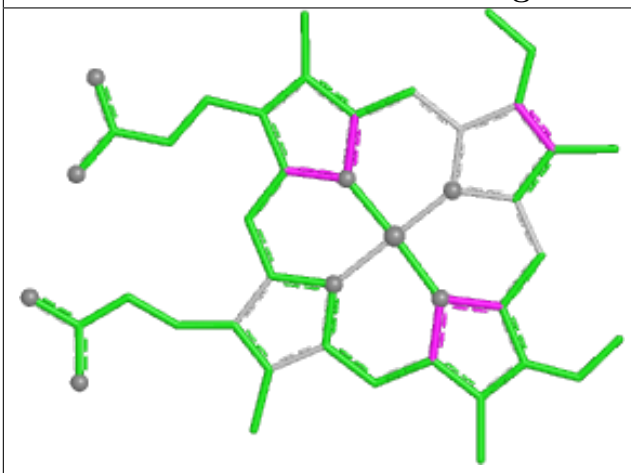
Torsions



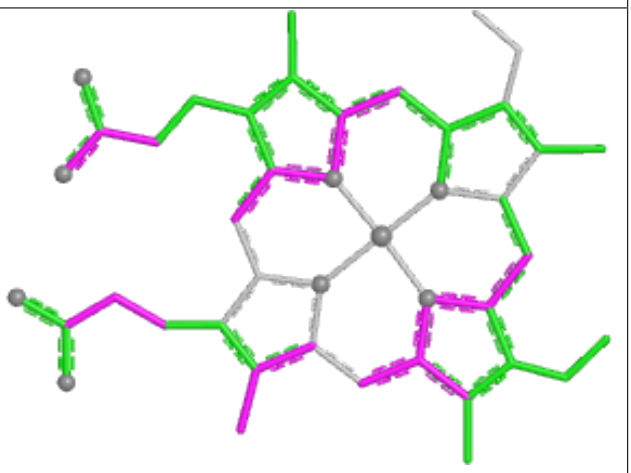
Rings

Ligand CDL b2 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

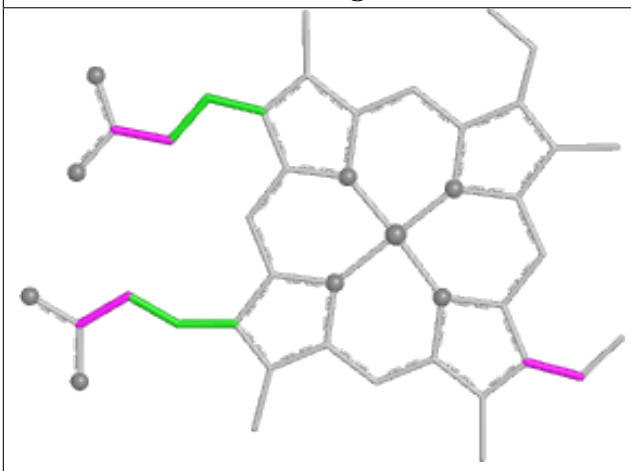
Ligand HEM b1 402



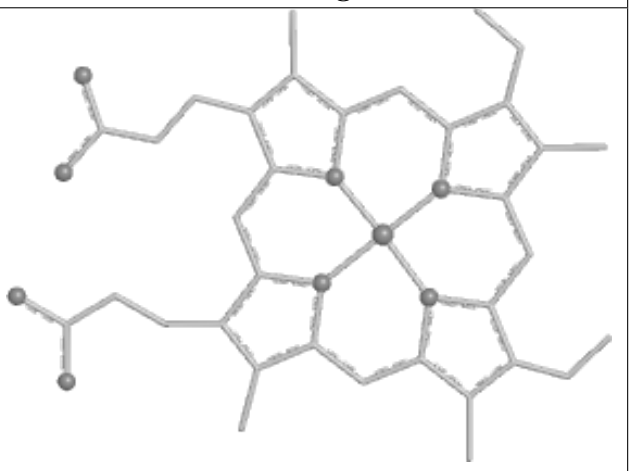
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	x2	1
37	x1	1
24	B8	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x2	26:UNK	C	45:UNK	N	27.65
1	x1	27:UNK	C	29:UNK	N	5.59
1	B8	46:ASP	C	47:TYR	N	1.20

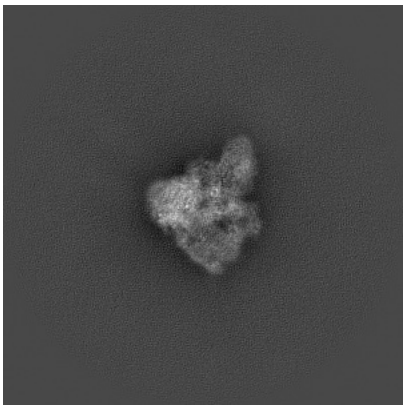
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4494. These allow visual inspection of the internal detail of the map and identification of artifacts.

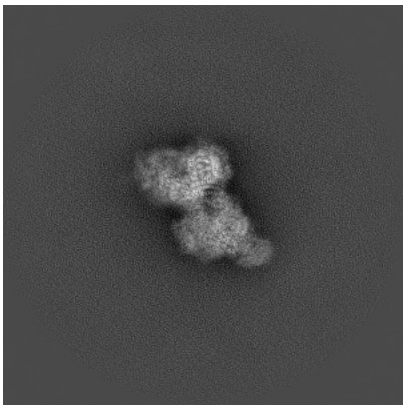
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

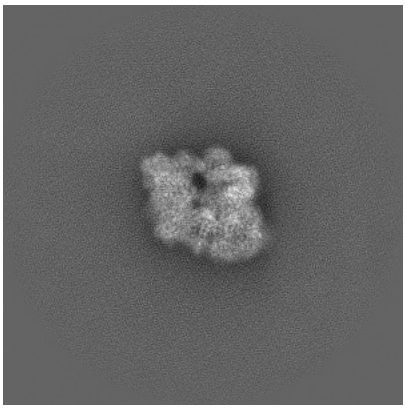
6.1.1 Primary map



X

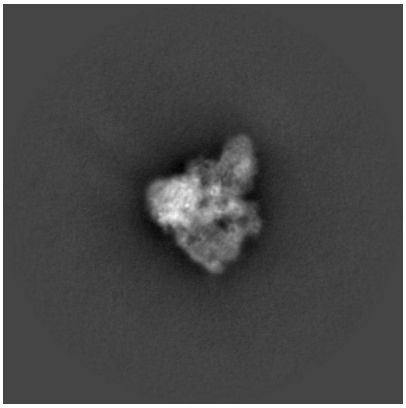


Y

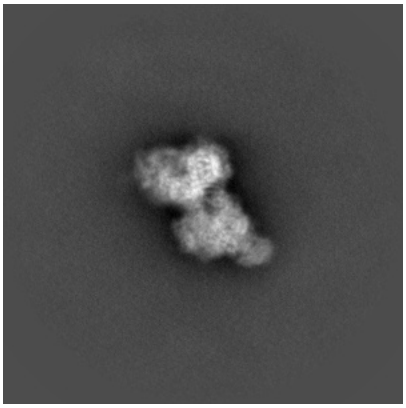


Z

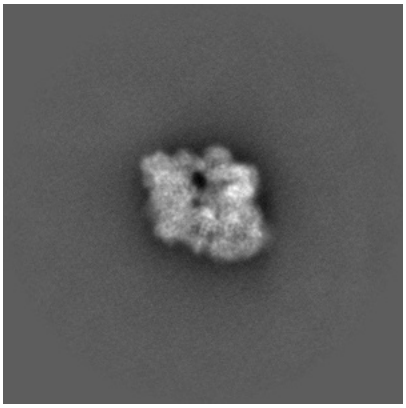
6.1.2 Raw map



X



Y

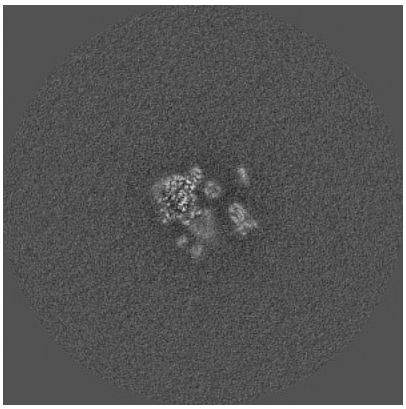


Z

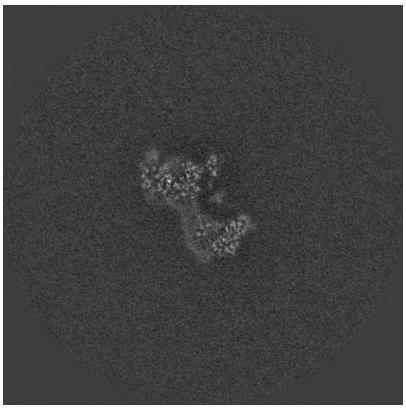
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

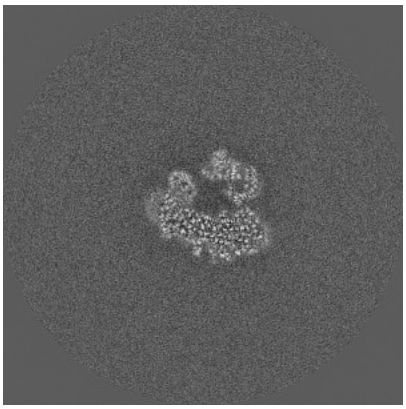
6.2.1 Primary map



X Index: 256

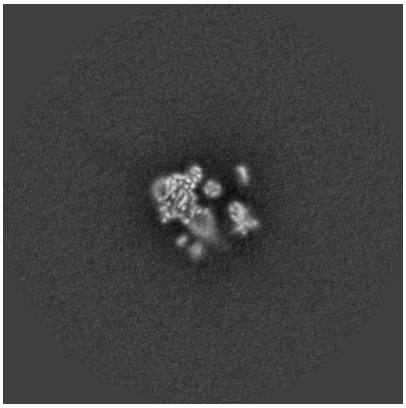


Y Index: 256

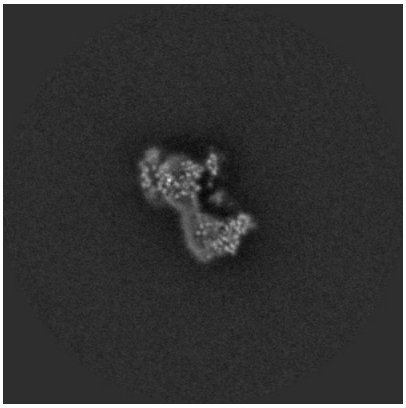


Z Index: 256

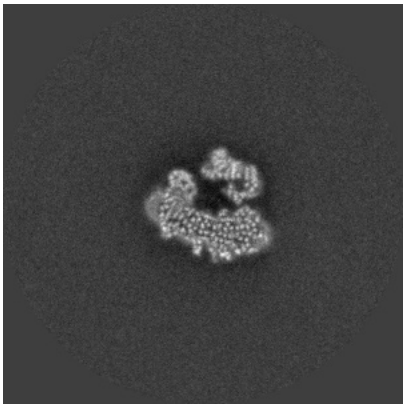
6.2.2 Raw map



X Index: 256



Y Index: 256

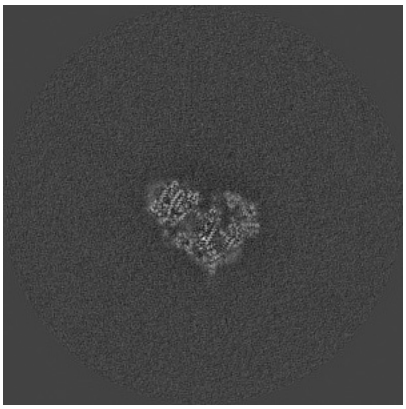


Z Index: 256

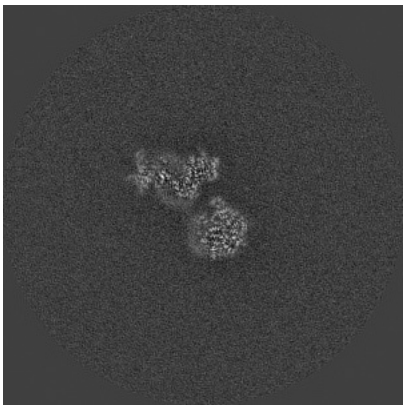
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

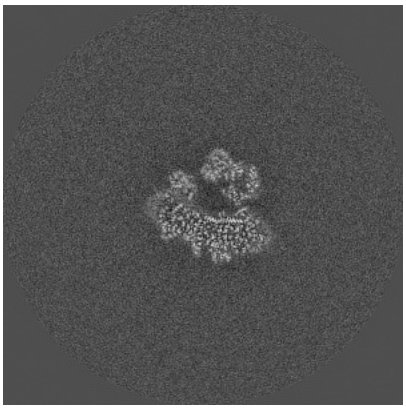
6.3.1 Primary map



X Index: 285

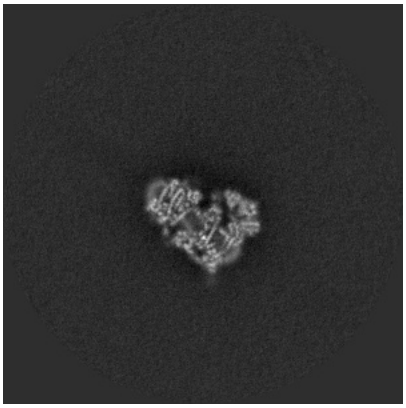


Y Index: 267

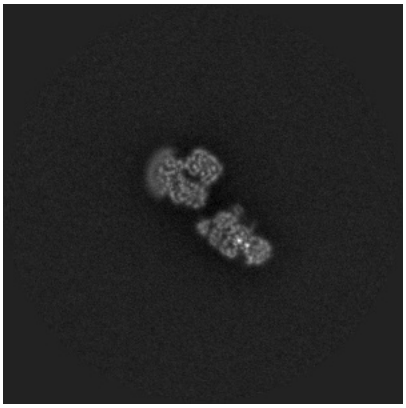


Z Index: 254

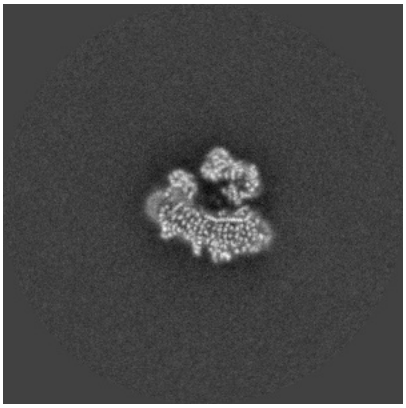
6.3.2 Raw map



X Index: 285



Y Index: 296



Z Index: 254

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

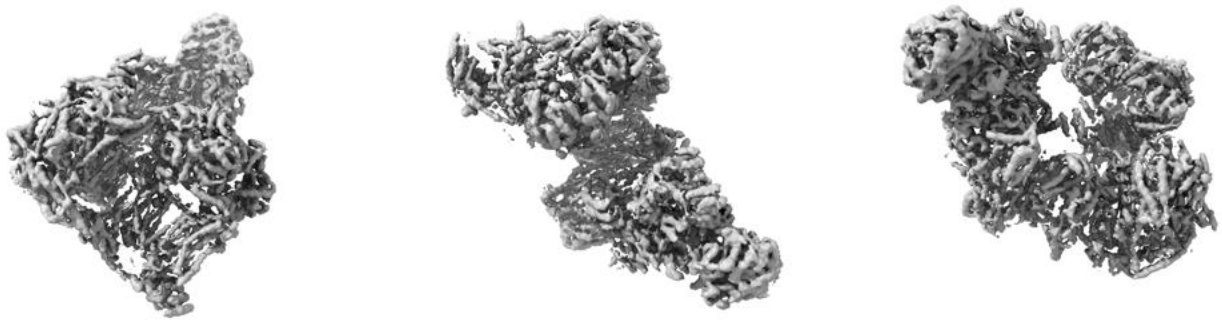
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

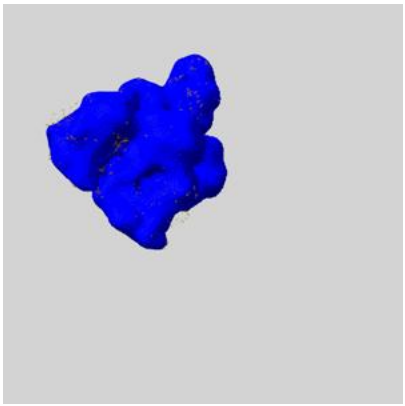
6.5 Mask visualisation (i)

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

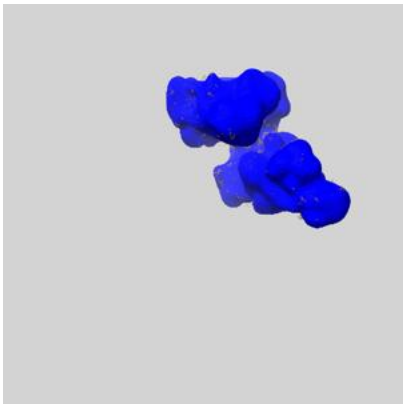
A mask typically either:

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

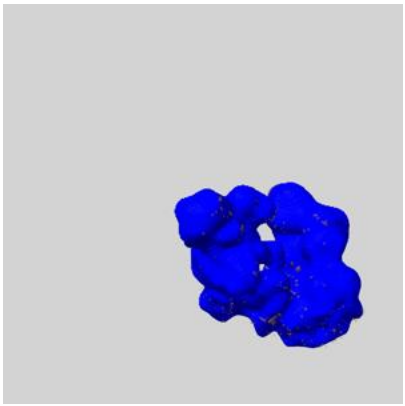
6.5.1 emd_4494_msk_1.map (i)



X



Y

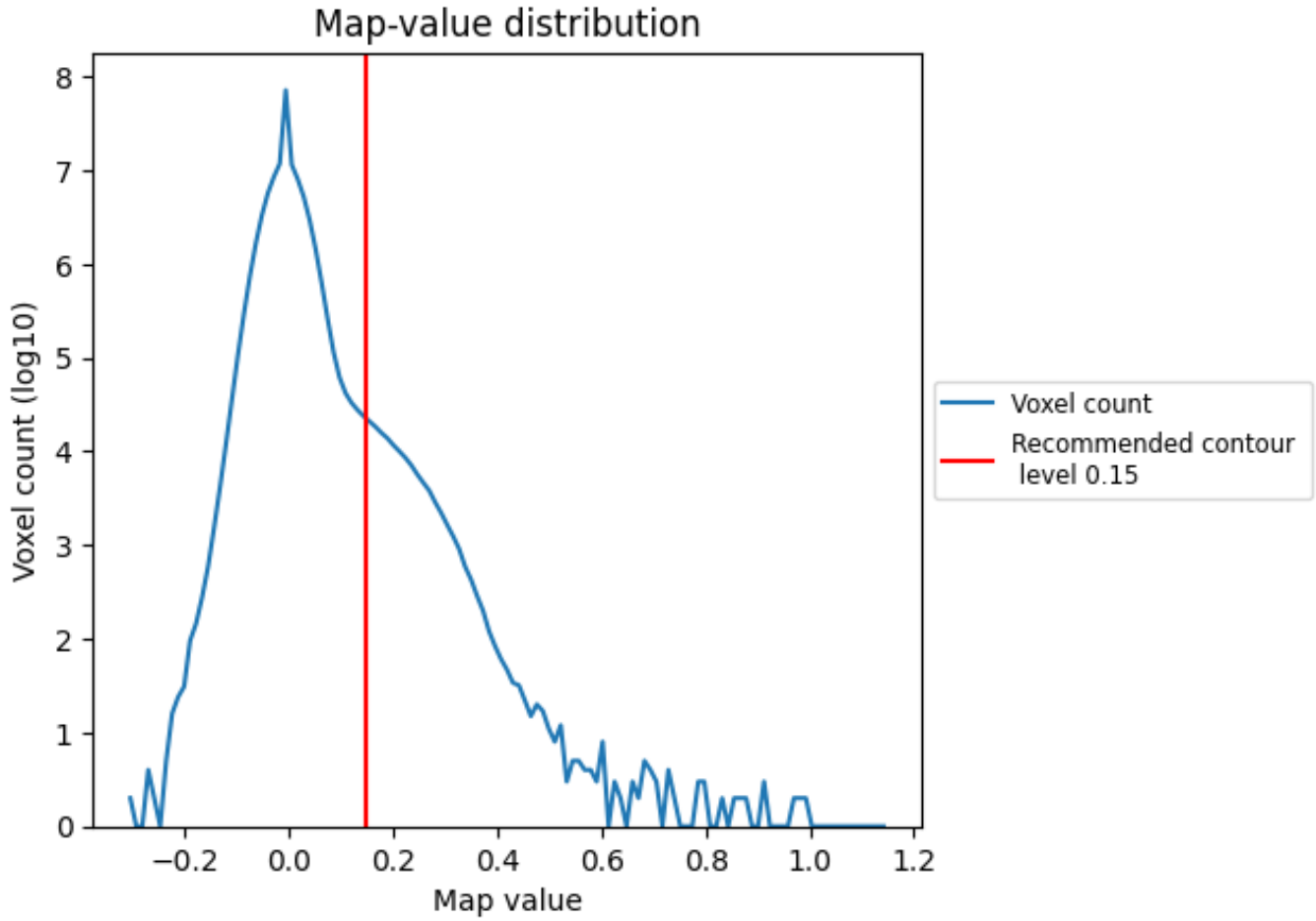


Z

7 Map analysis

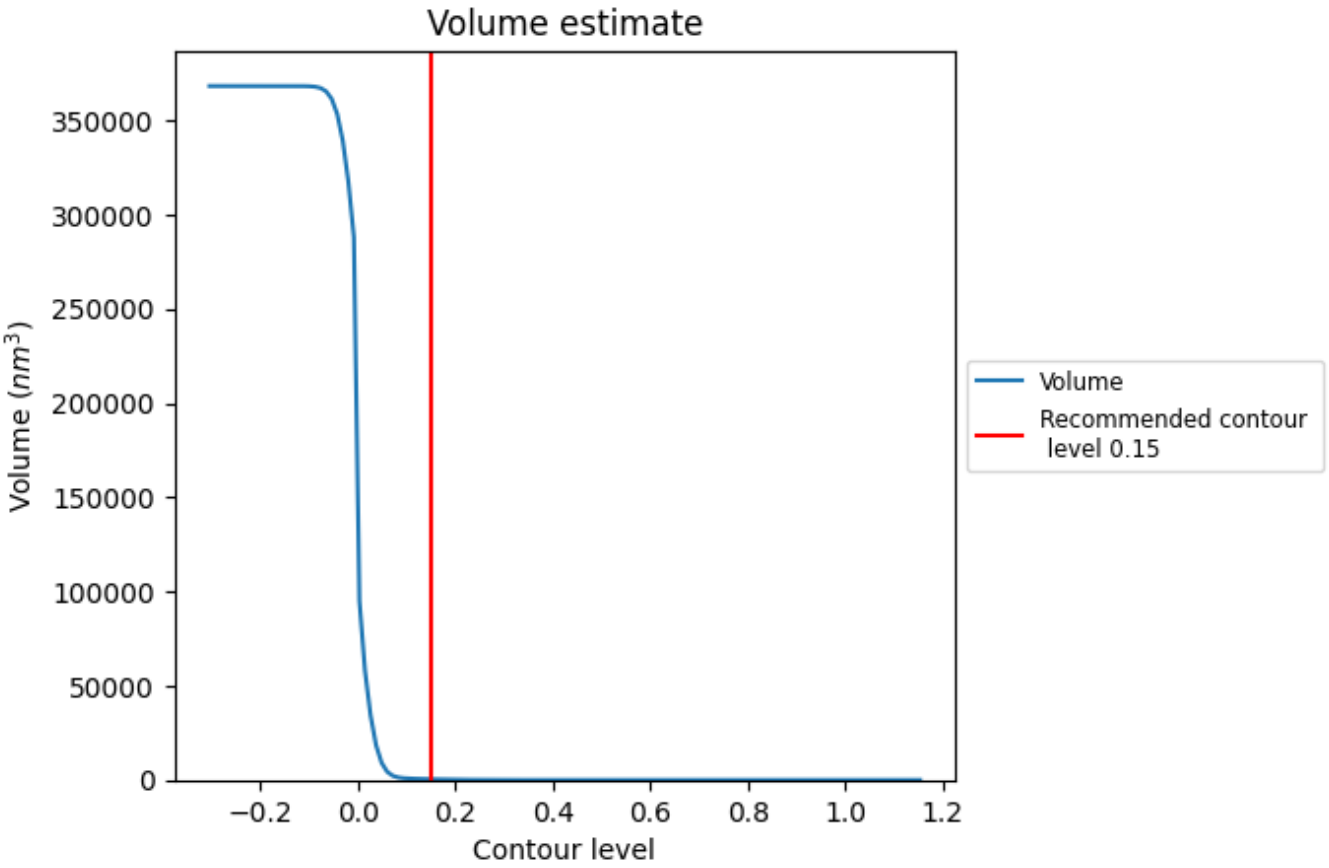
This section contains the results of statistical analysis of the map.

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.

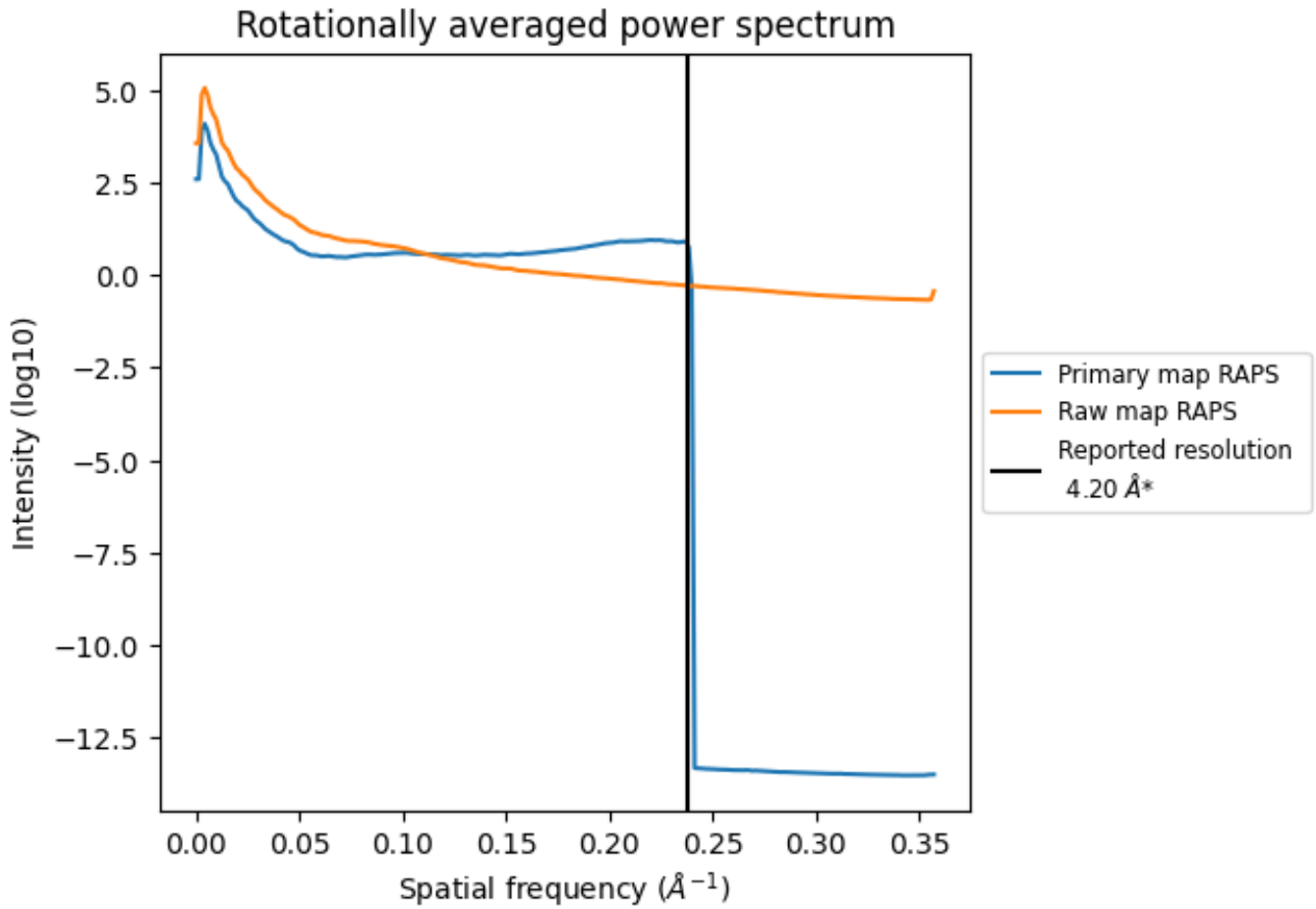
7.2 Volume estimate (i)



The volume at the recommended contour level is 389 nm^3; this corresponds to an approximate mass of 351 kDa.

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

7.3 Rotationally averaged power spectrum (i)

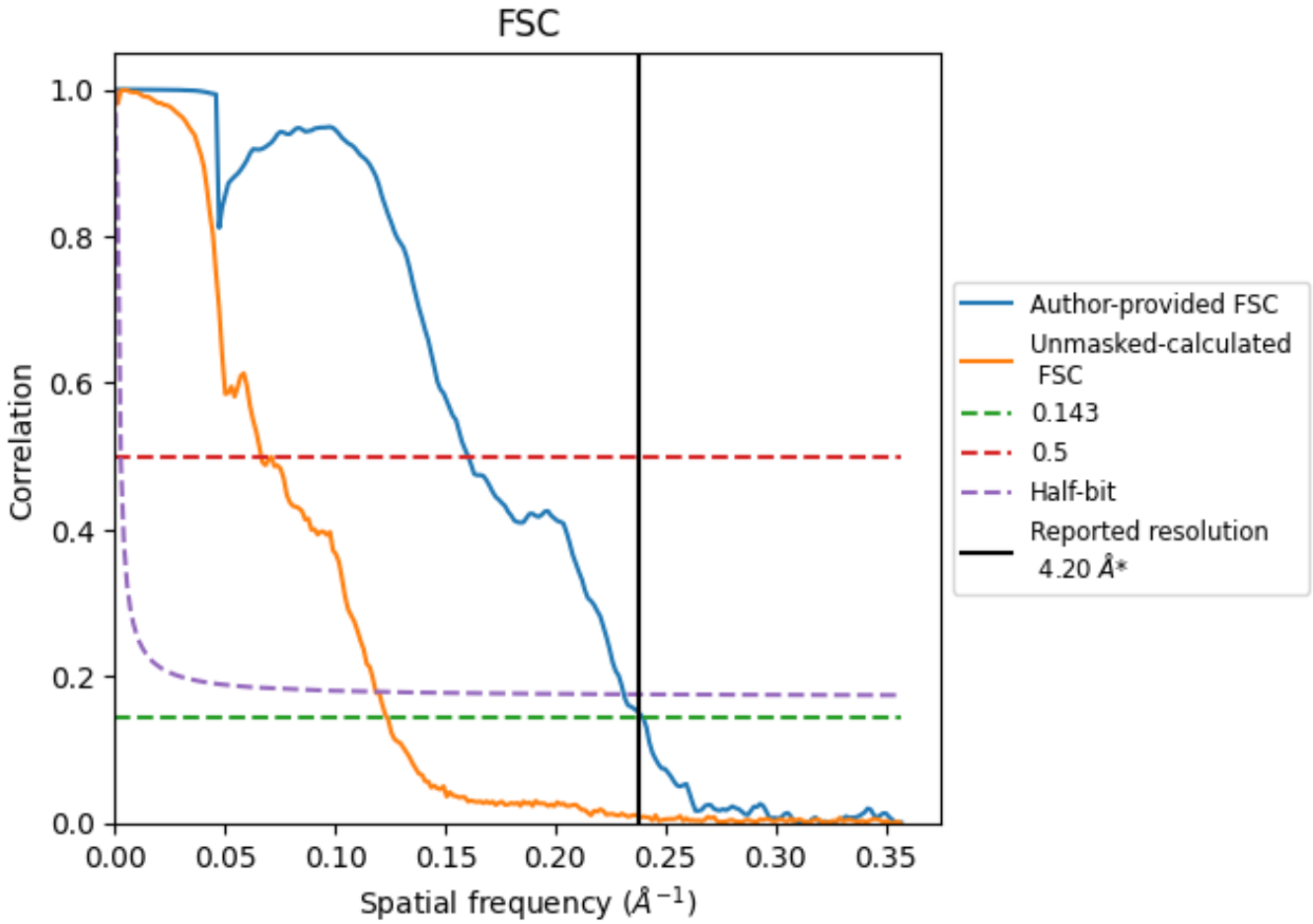


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

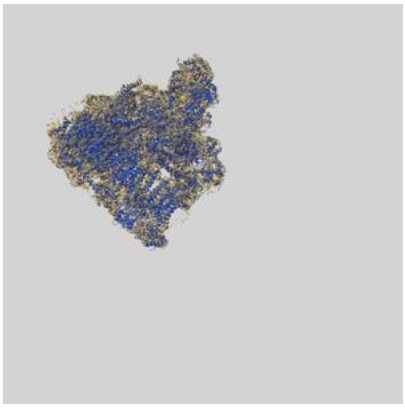
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.17	6.23	4.33
Unmasked-calculated*	8.09	15.06	8.44

*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 8.09 differs from the reported value 4.2 by more than 10 %

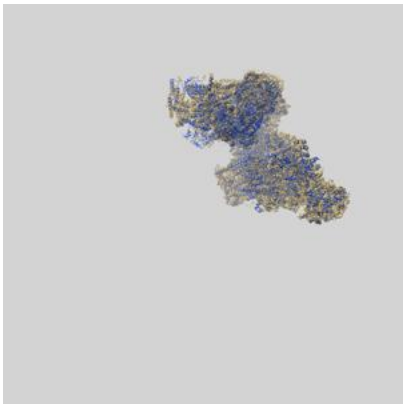
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4494 and PDB model 6QC2. Per-residue inclusion information can be found in section 3 on page 22.

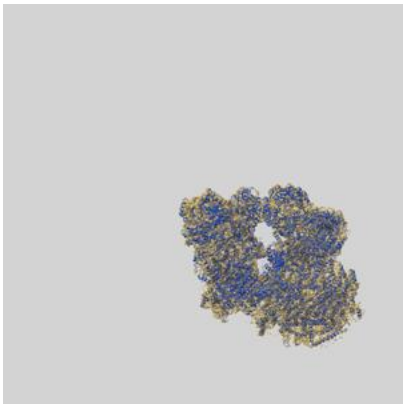
9.1 Map-model overlay



X



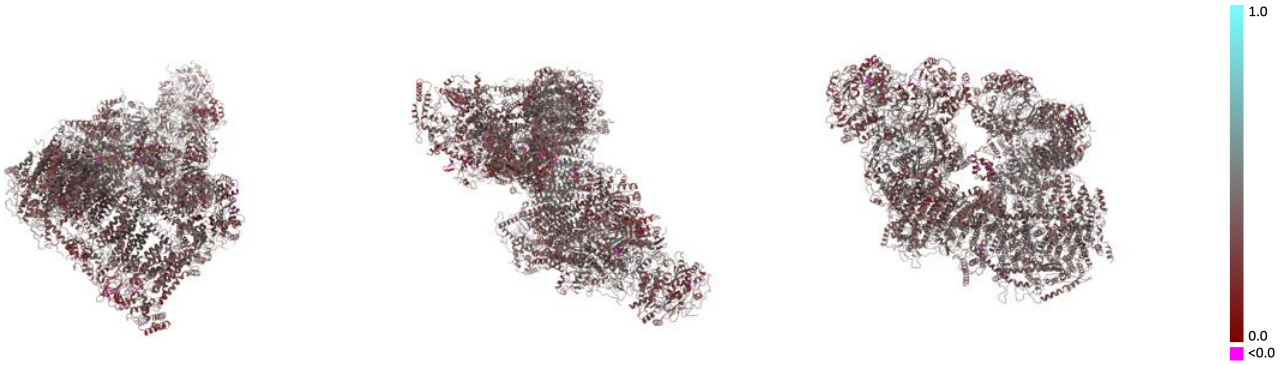
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

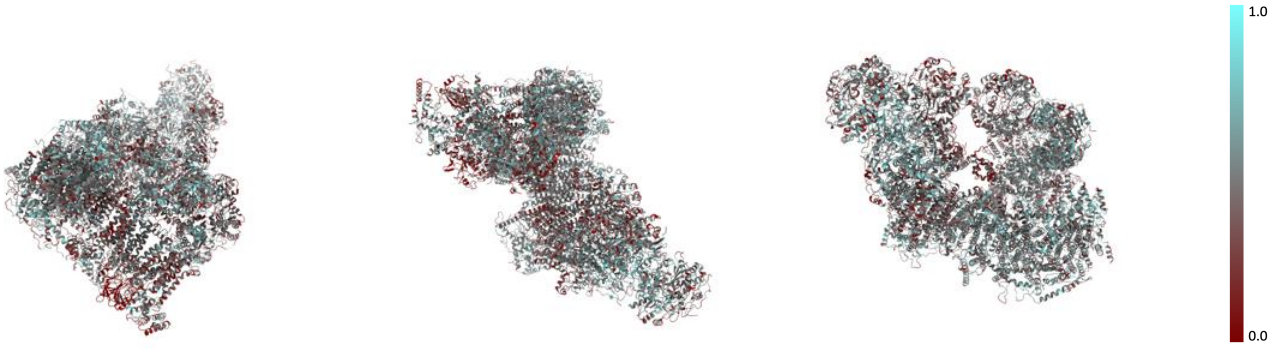
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

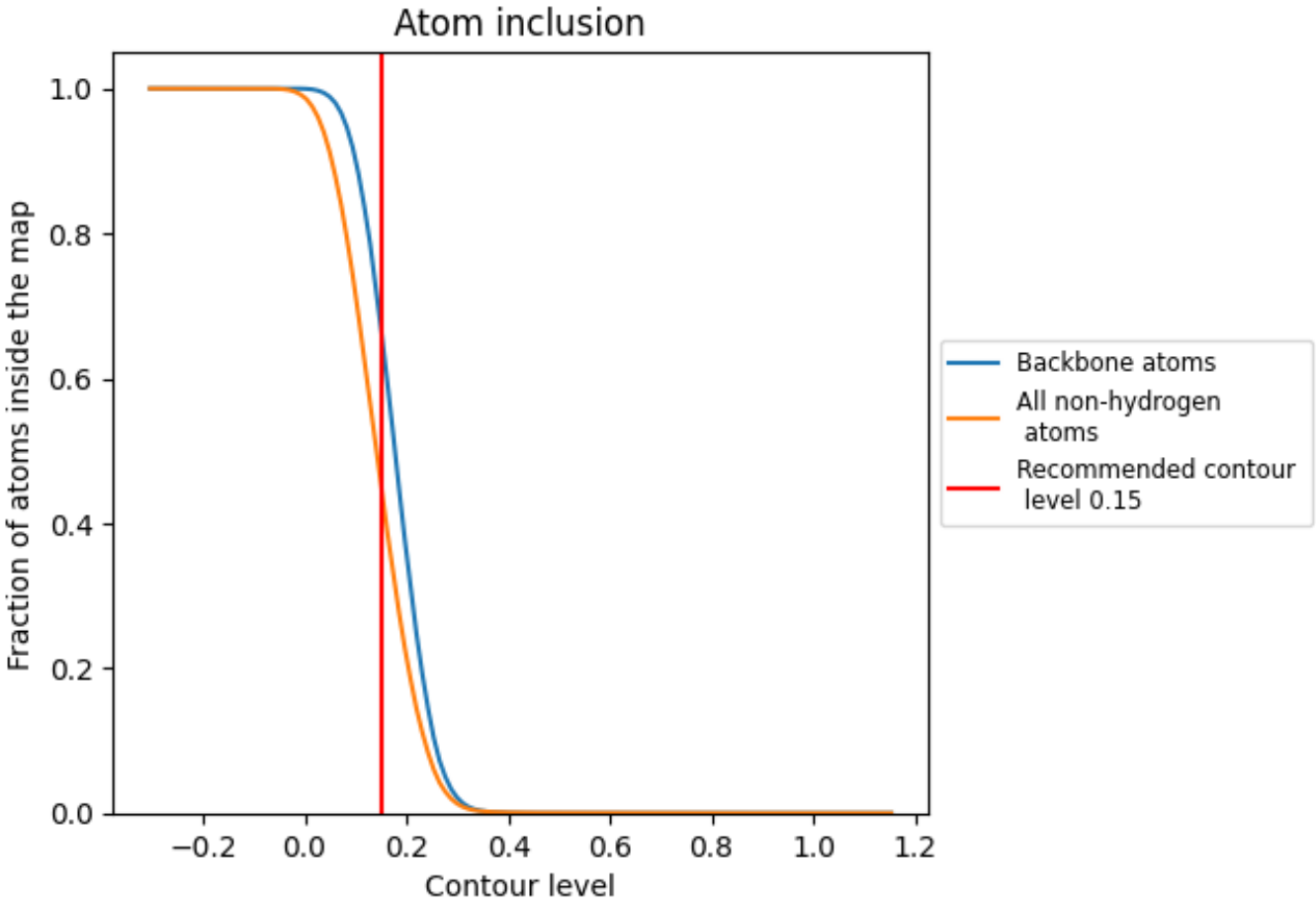
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 45% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4527	0.3600
4L	0.4299	0.3770
A1	0.4910	0.3620
A2	0.4102	0.3080
A3	0.4386	0.3380
A5	0.4392	0.3260
A6	0.3777	0.3480
A7	0.3461	0.3720
A8	0.5110	0.3660
A9	0.3502	0.3480
AA	0.2107	0.2710
AB	0.5034	0.3740
AJ	0.4961	0.3740
AK	0.4014	0.3630
AL	0.4014	0.3690
AM	0.5186	0.3570
B1	0.4610	0.3890
B2	0.4818	0.3600
B3	0.4805	0.3520
B4	0.4946	0.3840
B5	0.5448	0.3910
B6	0.4936	0.3620
B7	0.4640	0.3030
B8	0.4891	0.3790
B9	0.5793	0.3880
BJ	0.5211	0.3600
BK	0.4633	0.3570
C1	0.4974	0.3620
C2	0.5176	0.3840
D1	0.4394	0.3660
D2	0.5074	0.4000
D3	0.3804	0.3470
D4	0.4995	0.4000
D5	0.4719	0.3790
D6	0.3594	0.3540

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S1	0.4441	0.3450
S2	0.5025	0.3910
S3	0.5146	0.3880
S4	0.4386	0.3810
S5	0.5056	0.3610
S6	0.4889	0.3840
S7	0.5318	0.3870
S8	0.5712	0.3950
V1	0.4701	0.3270
V2	0.4545	0.3260
V3	0.4554	0.3090
a1	0.4376	0.3370
a2	0.3919	0.3360
a3	0.5230	0.3900
a4	0.4897	0.3670
b1	0.4545	0.3710
b2	0.4750	0.3810
c1	0.4473	0.3510
c2	0.4728	0.3720
d1	0.4859	0.3670
d2	0.4650	0.3710
f1	0.1304	0.2700
f2	0.1356	0.2640
h1	0.3058	0.2590
h2	0.3404	0.2690
i1	0.3221	0.2930
i2	0.3297	0.3570
q1	0.3966	0.3240
q2	0.4605	0.3880
x1	0.1951	0.3380
x2	0.3000	0.3960