wwPDB EM Validation Summary Report

Oct 28, 2024 – 07:49 pm GMT

PDB ID	:	6QBX
EMDB ID	:	EMD-4493
Title	:	Ovine respiratory supercomplex I+III2 closed class.
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-24
Resolution	:	4.20 Å(reported)
Based on initial model	:	1PPJ

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:

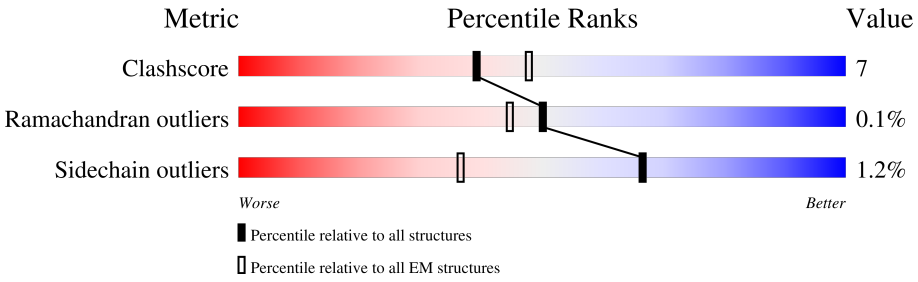
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a1	446	58% 97%
1	a3	446	31% 98%
2	a2	439	58% 93% 6%
2	a4	439	38% 93% 6%
3	b1	379	59% 99%
3	b2	379	41% 99%
4	c1	240	62% 97%
4	c2	240	48% 98%

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Mol	Chain	Length	Quality of chain
5	f1	196	96% 99%
5	f2	196	92% 98%
6	d1	110	46% 89% 9%
6	d2	110	42% 89% 8%
7	q1	81	69% 89% 10%
7	q2	81	35% 91% 7%
8	h1	78	71% 81% 17%
8	h2	78	59% 81% 17%
9	x1	78	21% 29% 71%
9	x2	78	21% 33% 67%
10	i1	63	75% 86% 13%
10	i2	63	73% 90% 10%
11	V1	445	44% 76% 20%
12	V2	217	49% 74% 23%
13	S1	704	48% 75% 22%
14	S2	430	37% 79% 20%
15	S3	228	36% 77% 14% 9%
16	S7	179	26% 60% 27% 13%
17	S8	176	32% 74% 25%
18	V3	75	27% 40% 13% 45%
19	S6	96	43% 82% 17%
20	S4	133	42% 77% 18% 5%
21	A9	338	53% 66% 20% 14%
22	A2	98	55% 57% 26% 16%
23	A5	115	57% 82% 14%

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Mol	Chain	Length	Quality of chain
24	A6	127	44% 77% 13% 10%
25	A7	112	60% 68% 15% 14%
26	AL	145	62% 63% 21% 15%
27	AA	88	72% 74% 17% 9%
27	AB	88	33% 85% 13%
28	AM	143	37% 78% 17%
29	D3	115	68% 74% 26%
30	D1	318	55% 71% 28%
31	D6	175	58% 86% 13%
32	4L	98	49% 83% 16%
33	D5	606	44% 80% 20%
34	D4	459	31% 76% 23%
35	D2	347	32% 76% 24%
36	AK	140	50% 84% 16%
37	B5	143	22% 76% 21%
38	A8	171	39% 81% 19%
39	BJ	175	29% 77% 20%
40	AJ	320	32% 79% 21%
41	S5	105	27% 73% 19% 6%
42	A3	83	53% 70% 18% 11%
43	B3	97	38% 62% 11% 25%
44	C2	120	40% 93% 6%
45	B4	128	31% 88% 12%
46	B6	127	25% 58% 15% 25%
47	B7	119	42% 83% 16%

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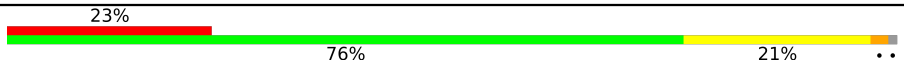
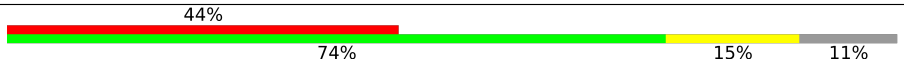
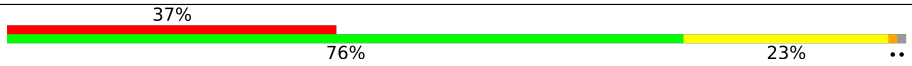
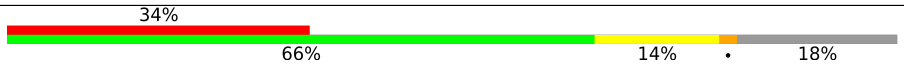
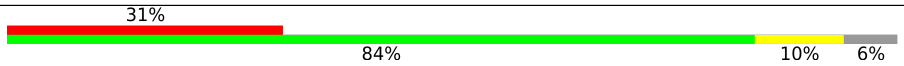
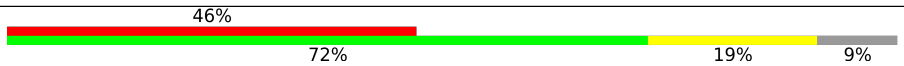
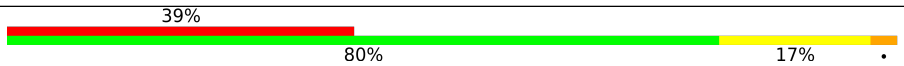
Mol	Chain	Length	Quality of chain
48	B9	178	
49	B2	72	
50	B8	158	
51	BK	125	
52	C1	49	
53	B1	57	
54	A1	70	

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 97049 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 Ubiquinol-cytochrome c reductase core protein 1.

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

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a1	241	ILE	LEU	conflict	UNP W5Q5G6
a1	242	ARG	CYS	conflict	UNP W5Q5G6
a1	244	ARG	PRO	conflict	UNP W5Q5G6
a1	245	GLU	TRP	conflict	UNP W5Q5G6
a1	246	ASP	GLY	conflict	UNP W5Q5G6
a1	?	-	ALA	deletion	UNP W5Q5G6
a1	?	-	VAL	deletion	UNP W5Q5G6
a1	?	-	PRO	deletion	UNP W5Q5G6
a1	249	PRO	GLN	conflict	UNP W5Q5G6
a1	251	ALA	TRP	conflict	UNP W5Q5G6
a1	254	ALA	PRO	conflict	UNP W5Q5G6
a1	255	ILE	PHE	conflict	UNP W5Q5G6
a1	256	ALA	GLN	conflict	UNP W5Q5G6
a1	257	VAL	ILE	conflict	UNP W5Q5G6
a1	258	GLU	ARG	conflict	UNP W5Q5G6
a1	259	GLY	HIS	conflict	UNP W5Q5G6
a3	241	ILE	LEU	conflict	UNP W5Q5G6
a3	242	ARG	CYS	conflict	UNP W5Q5G6
a3	244	ARG	PRO	conflict	UNP W5Q5G6
a3	245	GLU	TRP	conflict	UNP W5Q5G6
a3	246	ASP	GLY	conflict	UNP W5Q5G6
a3	?	-	ALA	deletion	UNP W5Q5G6
a3	?	-	VAL	deletion	UNP W5Q5G6
a3	?	-	PRO	deletion	UNP W5Q5G6
a3	249	PRO	GLN	conflict	UNP W5Q5G6
a3	251	ALA	TRP	conflict	UNP W5Q5G6

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Chain	Residue	Modelled	Actual	Comment	Reference
a3	254	ALA	PRO	conflict	UNP W5Q5G6
a3	255	ILE	PHE	conflict	UNP W5Q5G6
a3	256	ALA	GLN	conflict	UNP W5Q5G6
a3	257	VAL	ILE	conflict	UNP W5Q5G6
a3	258	GLU	ARG	conflict	UNP W5Q5G6
a3	259	GLY	HIS	conflict	UNP W5Q5G6

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

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

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called Cytochrome c1.

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

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d1	1	ALA	-	insertion	UNP W5P642
d1	2	GLY	SER	conflict	UNP W5P642
d1	3	ARG	ASP	conflict	UNP W5P642
d1	4	PRO	LEU	conflict	UNP W5P642
d1	5	ALA	SER	conflict	UNP W5P642
d2	1	ALA	-	insertion	UNP W5P642
d2	2	GLY	SER	conflict	UNP W5P642
d2	3	ARG	ASP	conflict	UNP W5P642
d2	4	PRO	LEU	conflict	UNP W5P642
d2	5	ALA	SER	conflict	UNP W5P642

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex III subunit VII.

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

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

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

- Molecule 9 is a protein called UQCRFS1N.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	x1	23	Total	C	N	O	0	0
			114	68	23	23		
9	x2	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase, complex III subunit X.

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

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

- Molecule 12 is a protein called NDUFV2.

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

- Molecule 13 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

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

- Molecule 14 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S2	430	Total	C	N	O	S	0	0
			3455	2205	594	631	25		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

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

- Molecule 16 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S7	156	Total	C	N	O	S	0	0
			1248	795	225	214	14		

- Molecule 17 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S8	176	Total	C	N	O	S	0	0
			1415	889	243	271	12		

- Molecule 18 is a protein called NDUFV3.

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

- Molecule 19 is a protein called NDUFS6.

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

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S4	126	Total	C	N	O	S	0	0
			1025	646	182	194	3		

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A9	292	Total	C	N	O	S	0	0
			2344	1498	428	413	5		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 23 is a protein called NDUFA5.

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

- Molecule 24 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

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

- Molecule 25 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A7	96	Total	C	N	O	S	0	0
			766	478	146	139	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AL	123	Total	C	N	O	S	0	0
			1044	676	182	182	4		

- Molecule 27 is a protein called Acyl carrier protein.

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

- Molecule 28 is a protein called NDUFA13.

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

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D3	115	Total	C	N	O	S	0	0
			923	621	133	162	7		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	D1	318	Total	C	N	O	S	0	0
			2529	1704	384	422	19		

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D6	175	Total	C	N	O	S	0	0
			1345	904	192	236	13		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 36 is a protein called NDUFA11.

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

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 39 is a protein called NDUFB10.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 42 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 43 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 45 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 46 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	B6	95	Total	C	N	O	S	0	0
			804	530	135	138	1		

- Molecule 47 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 48 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 49 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B2	64	Total	C	N	O	S	0	0
			555	368	92	94	1		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 51 is a protein called NDUFB11.

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

- Molecule 52 is a protein called NDUFC1.

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

- Molecule 53 is a protein called NDUFB1.

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

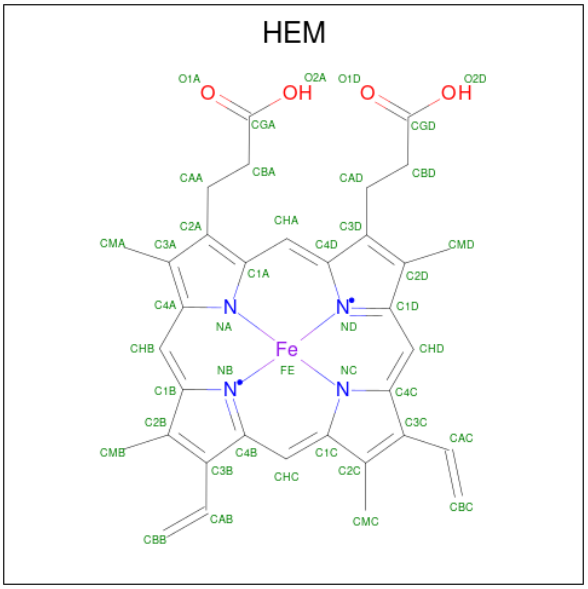
There are 3 discrepancies between the modelled and reference sequences:

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 54 is a protein called NDUFA1.

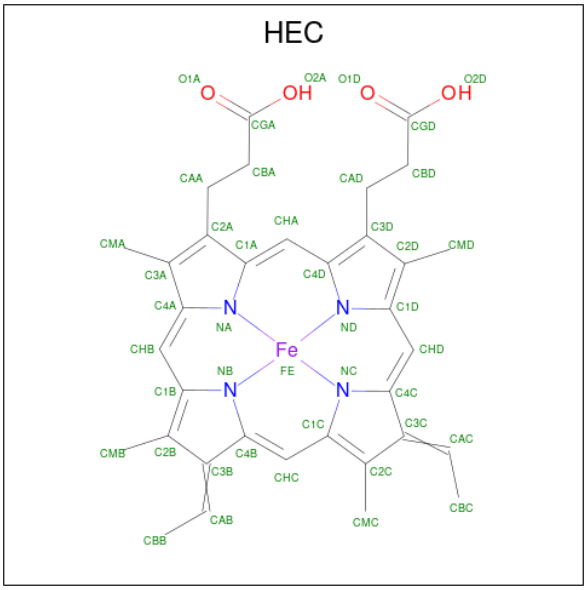
Mol	Chain	Residues	Atoms					AltConf	Trace
54	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 55 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



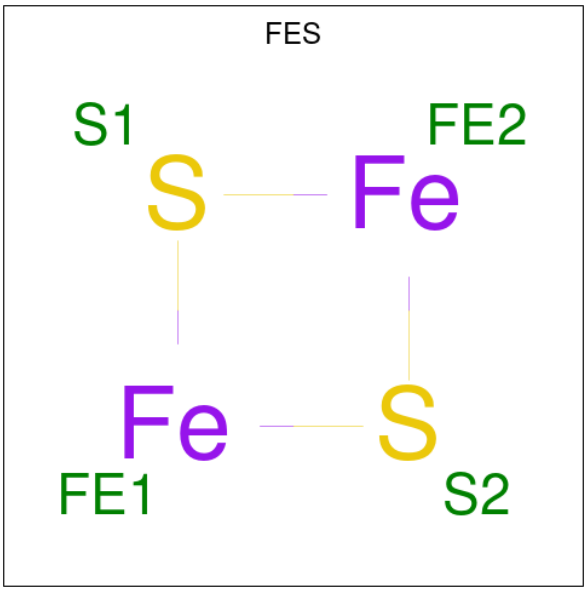
Mol	Chain	Residues	Atoms					AltConf
55	b1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
55	b1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
55	b2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
55	b2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 56 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



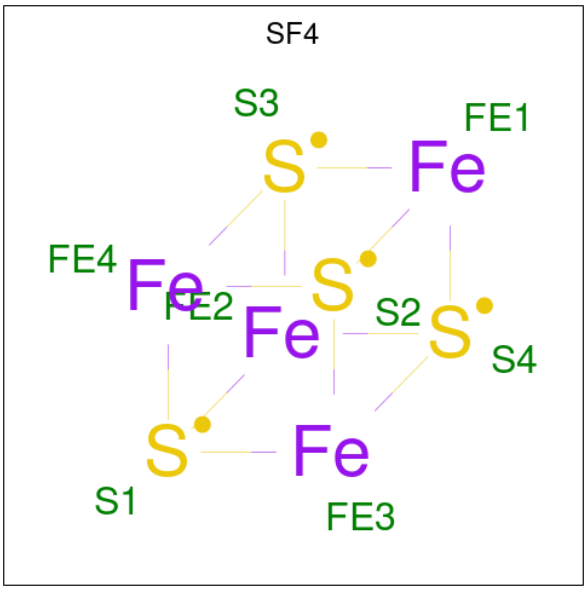
Mol	Chain	Residues	Atoms					AltConf
56	c1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	c2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 57 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



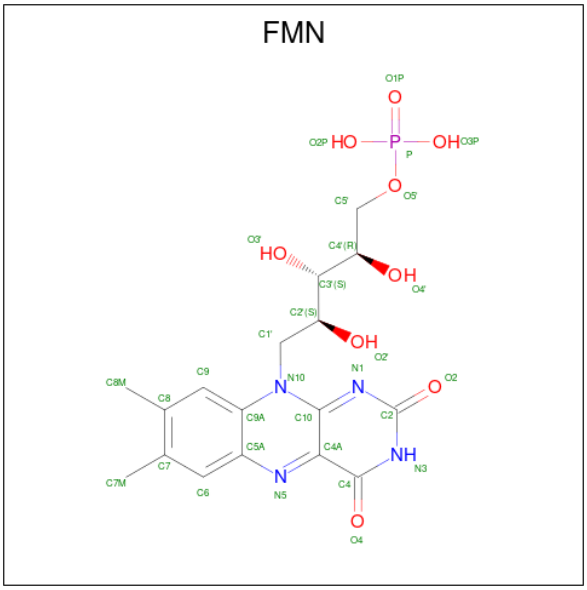
Mol	Chain	Residues	Atoms	AltConf
57	f1	1	Total Fe S 4 2 2	0
57	f2	1	Total Fe S 4 2 2	0
57	V2	1	Total Fe S 4 2 2	0
57	S1	1	Total Fe S 4 2 2	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



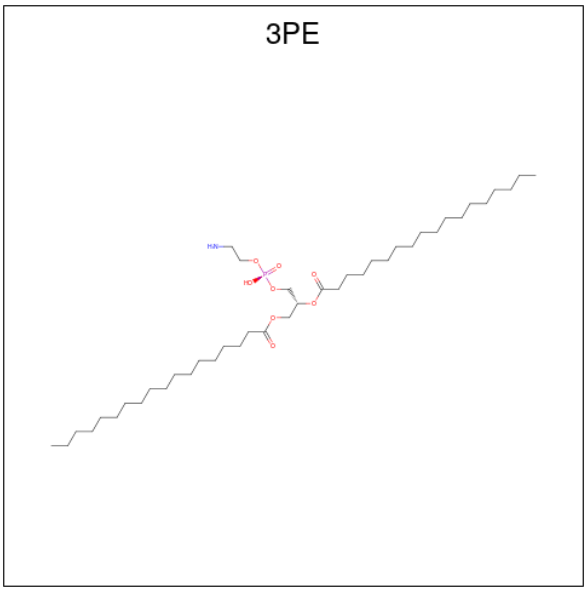
Mol	Chain	Residues	Atoms	AltConf
58	V1	1	Total Fe S 8 4 4	0
58	S1	1	Total Fe S 8 4 4	0
58	S1	1	Total Fe S 8 4 4	0
58	S7	1	Total Fe S 8 4 4	0
58	S8	1	Total Fe S 8 4 4	0
58	S8	1	Total Fe S 8 4 4	0

- Molecule 59 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 60 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).

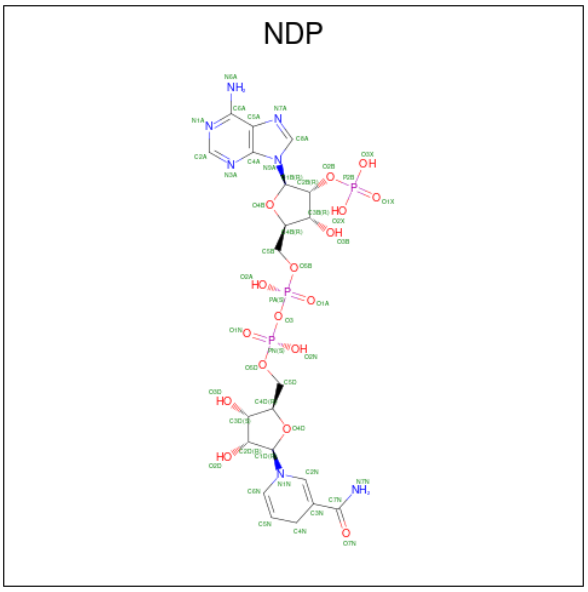


Mol	Chain	Residues	Atoms					AltConf
60	S2	1	Total	C	N	O	P	0
			40	30	1	8	1	
60	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

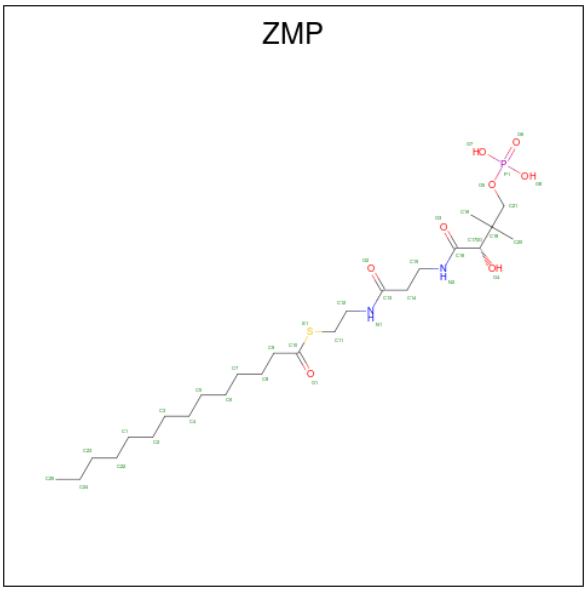
Mol	Chain	Residues	Atoms		AltConf
61	S6	1	Total	Zn	0
			1	1	

- Molecule 62 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



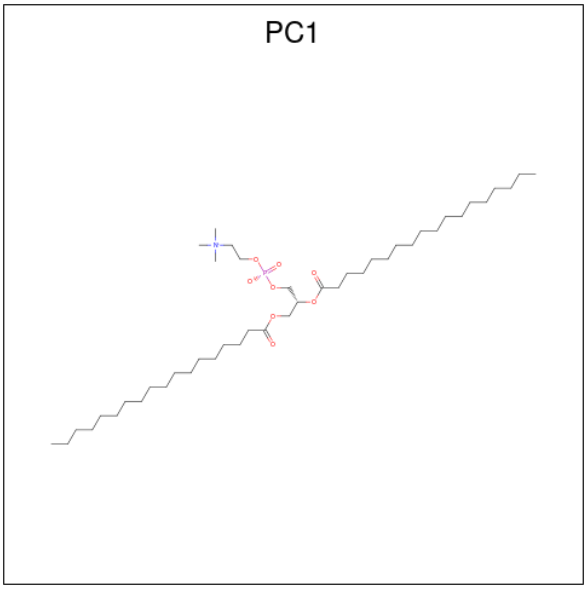
Mol	Chain	Residues	Atoms					AltConf
62	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 63 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
63	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
63	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 64 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



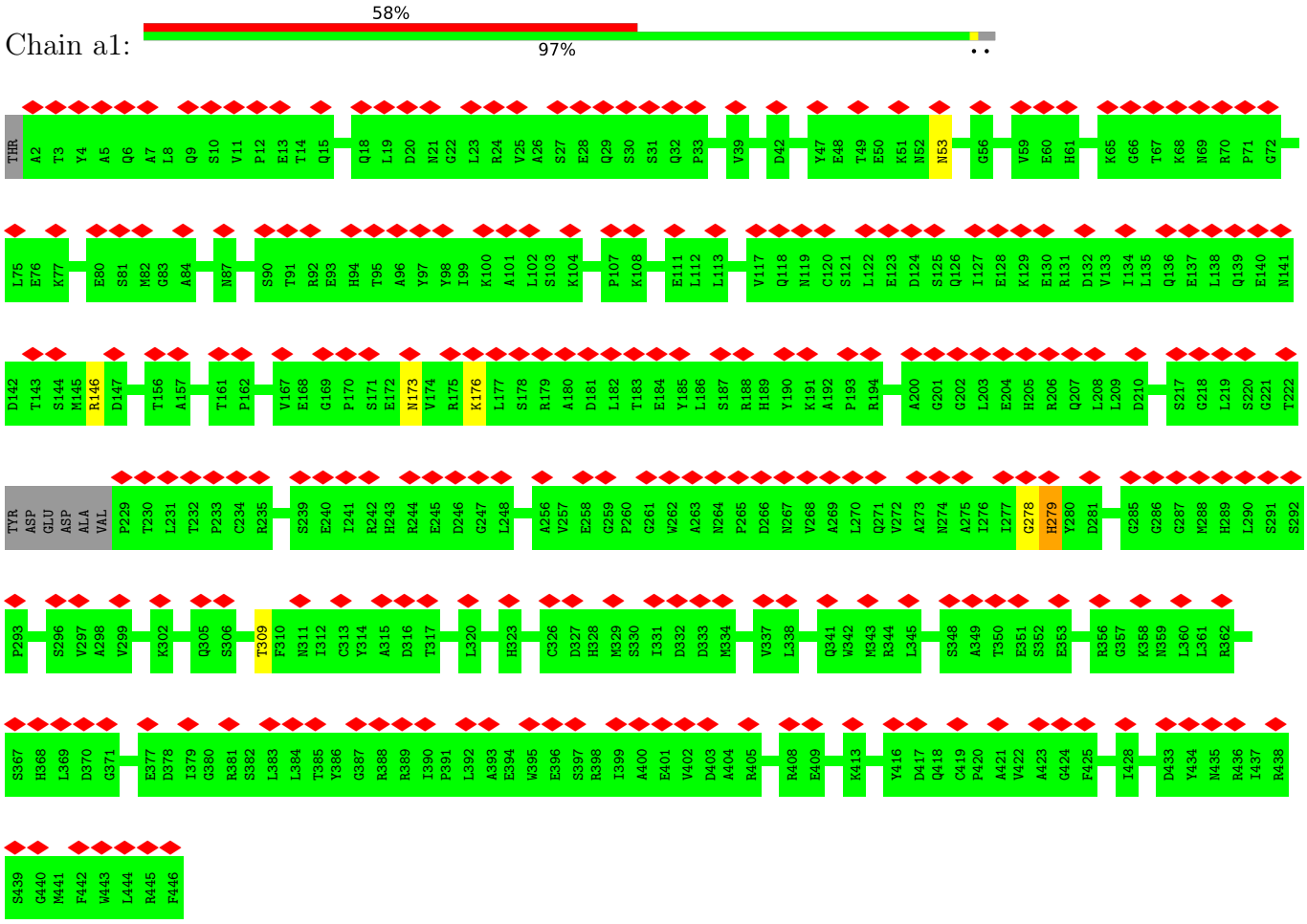
Mol	Chain	Residues	Atoms					AltConf
64	AK	1	Total	C	N	O	P	0
			28	18	1	8	1	

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.

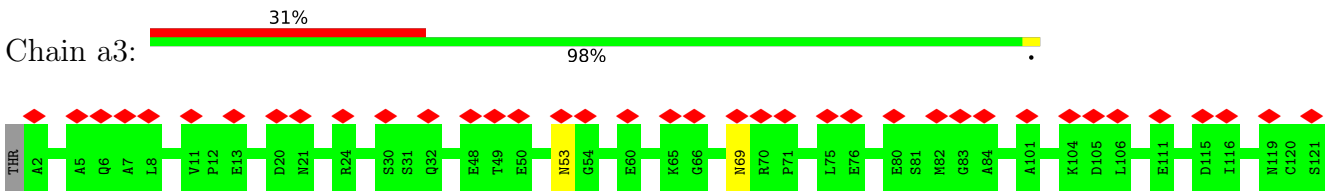
• Molecule 1: Ubiquinol-cytochrome c reductase core protein 1

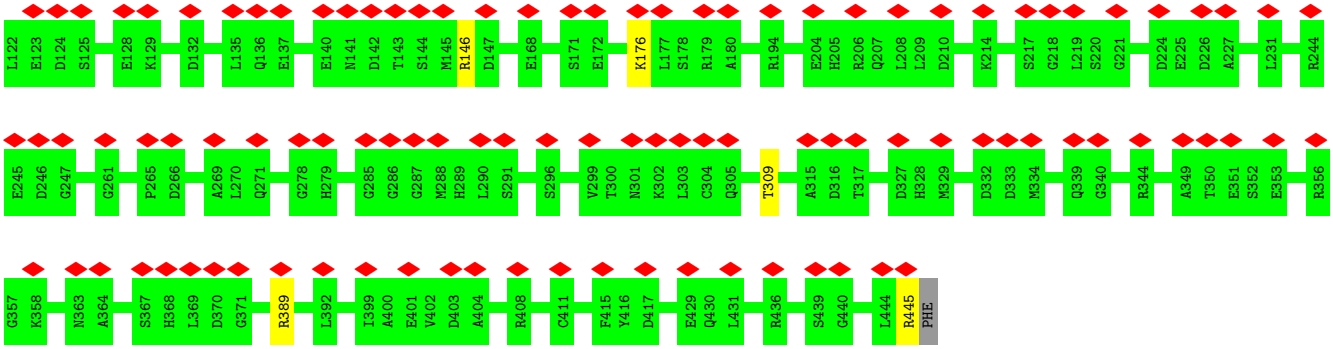
Chain a1:



• Molecule 1: Ubiquinol-cytochrome c reductase core protein 1

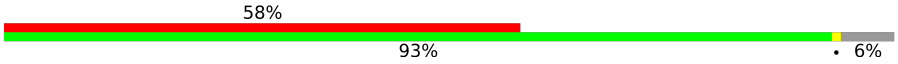
Chain a3:

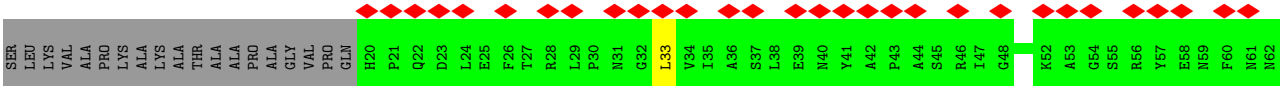


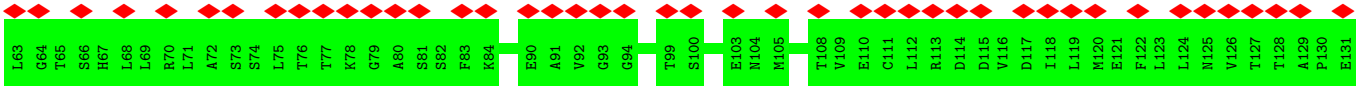


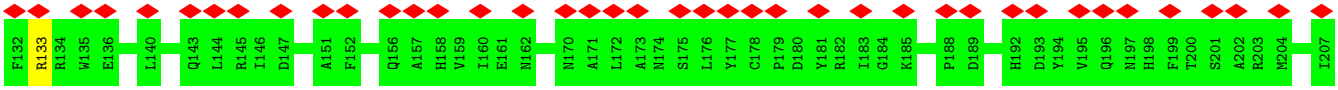
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

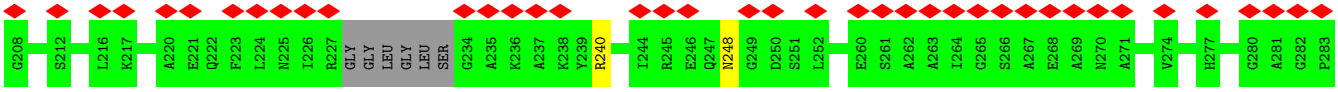
Chain a2:

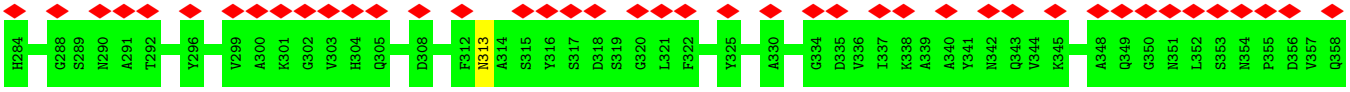


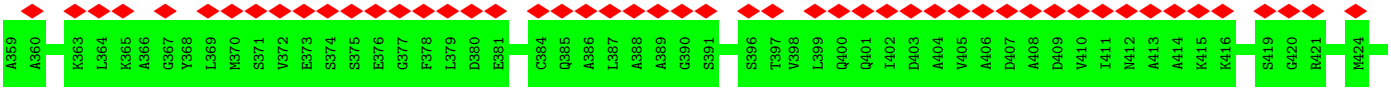


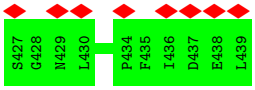






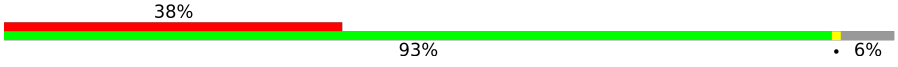


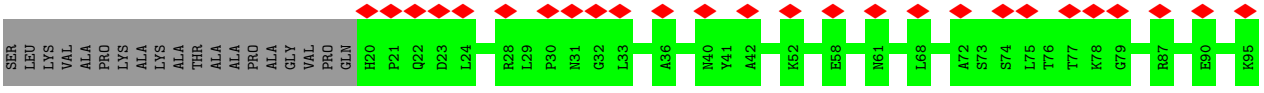


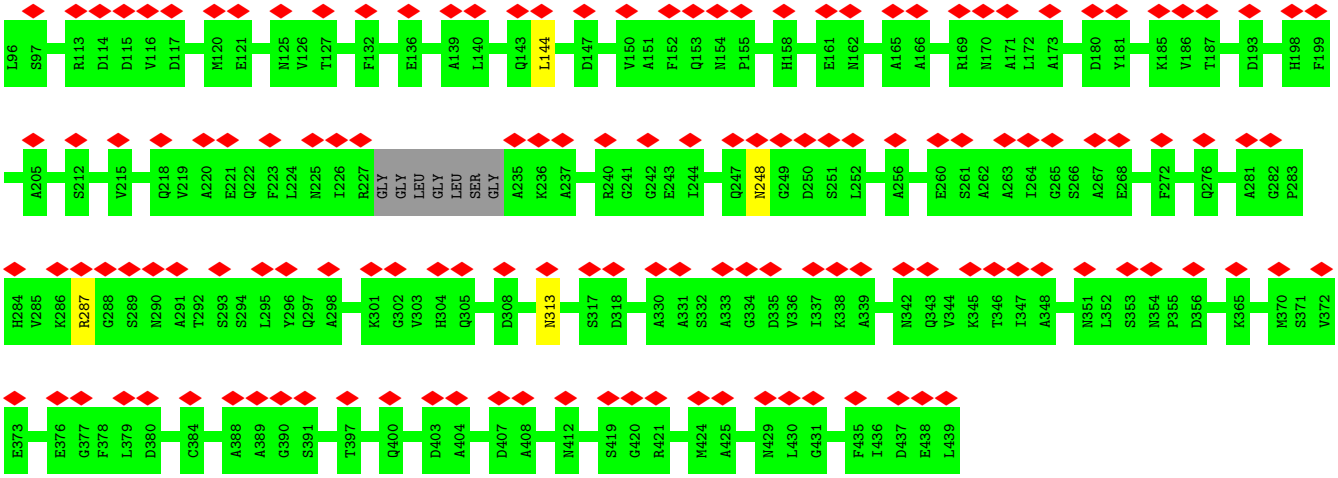


• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

Chain a4:

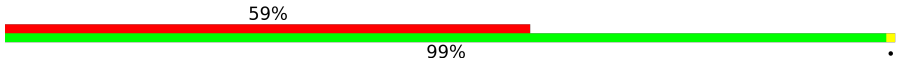


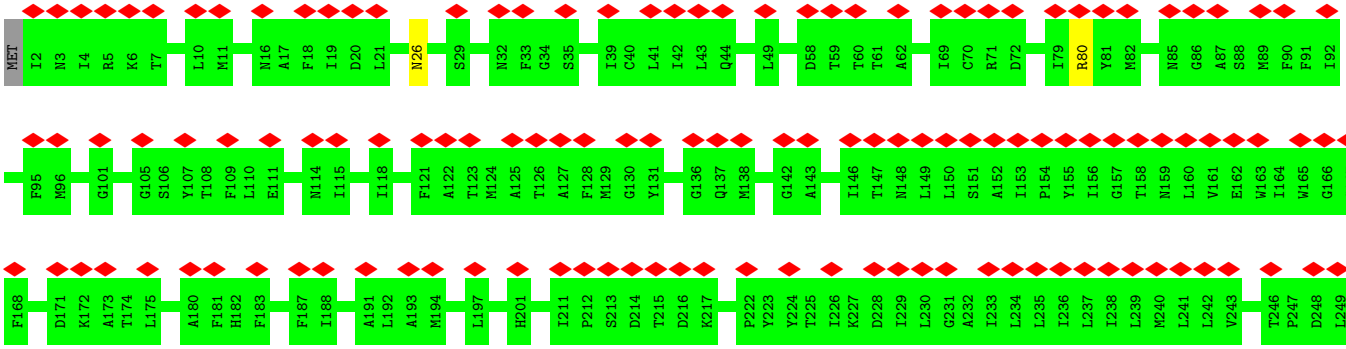




• Molecule 3: Cytochrome b

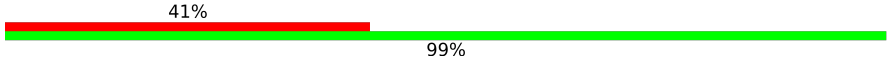
Chain b1:

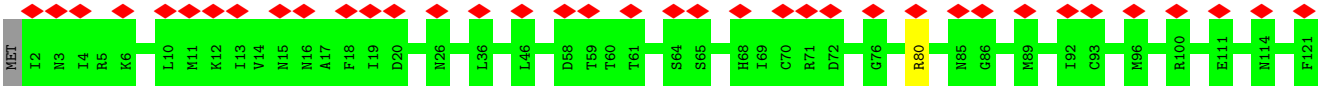


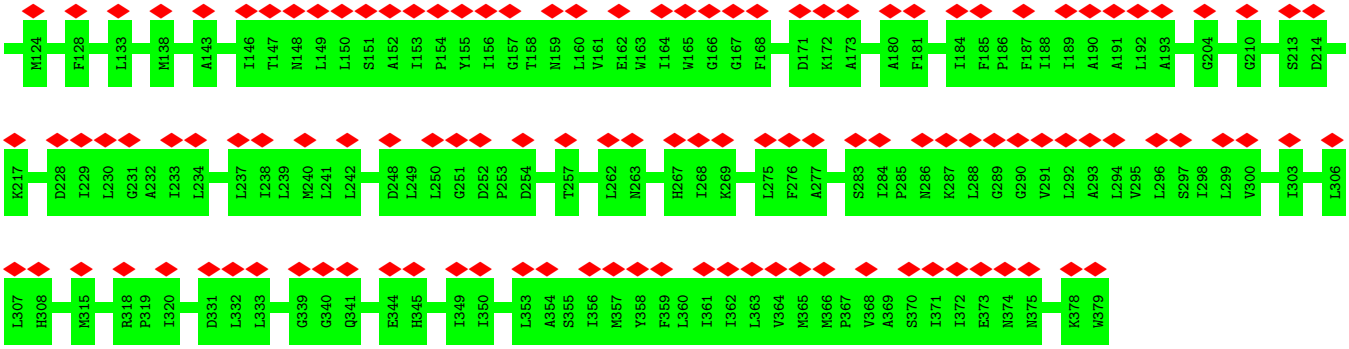


• Molecule 3: Cytochrome b

Chain b2:

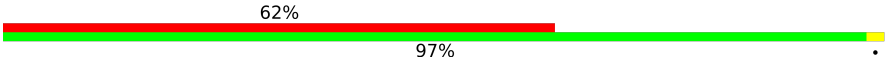


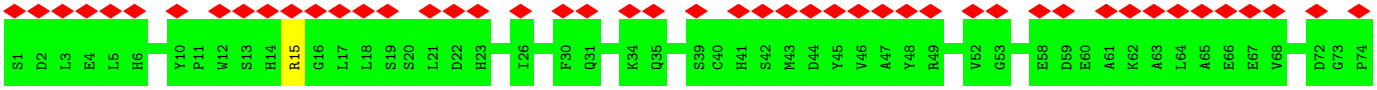




• Molecule 4: Cytochrome c1

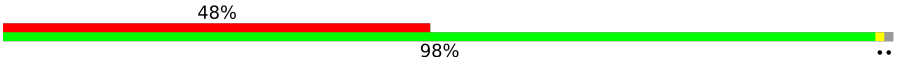
Chain c1:

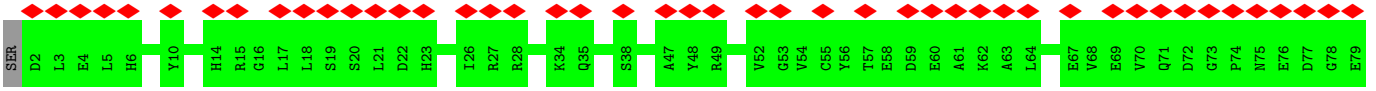




• Molecule 4: Cytochrome c1

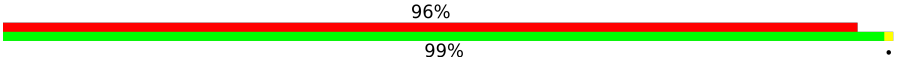
Chain c2:

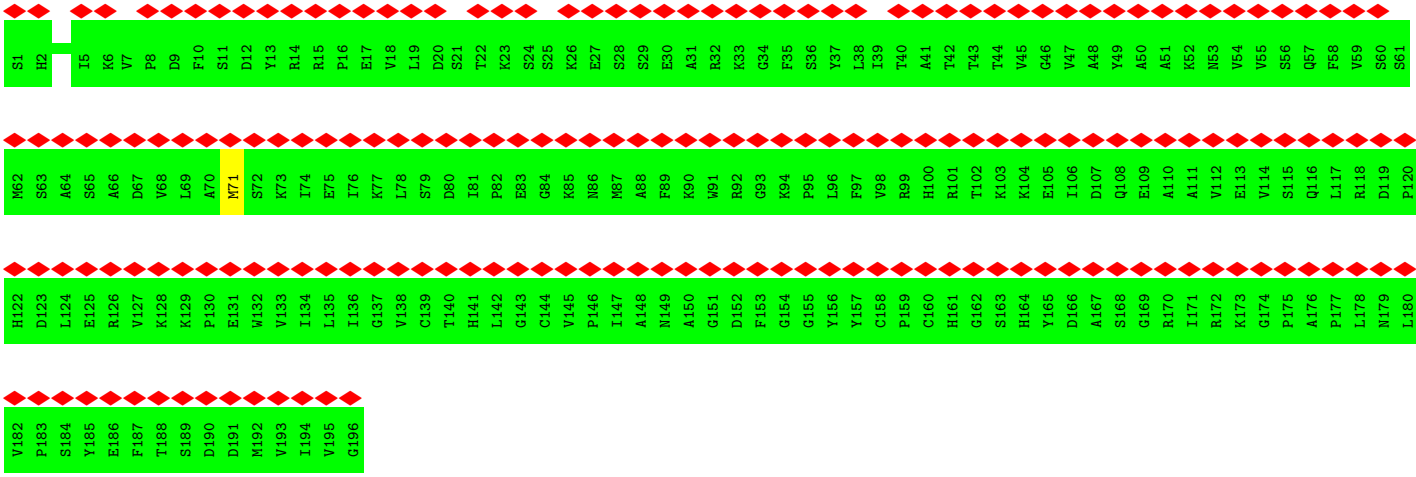




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

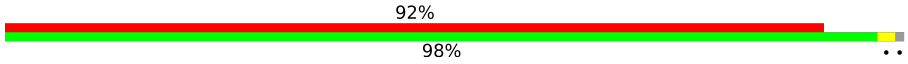
Chain f1:

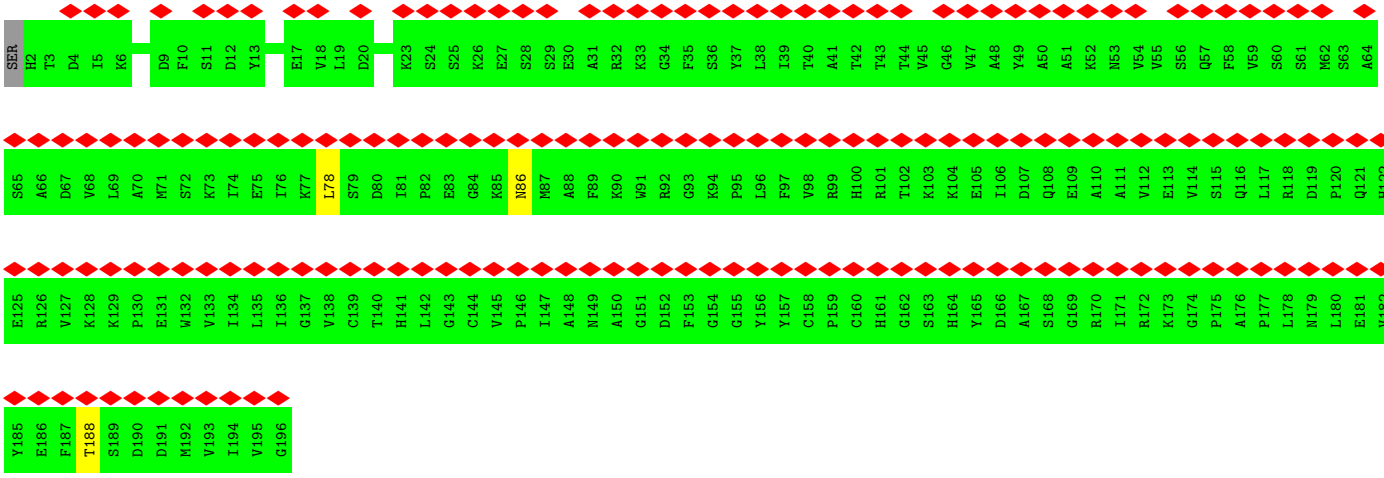




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

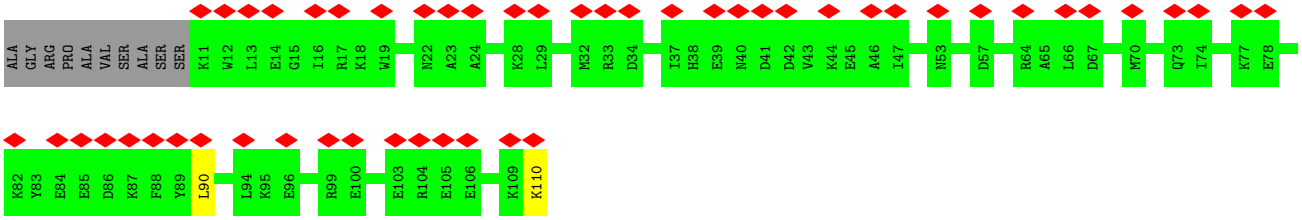
Chain f2:





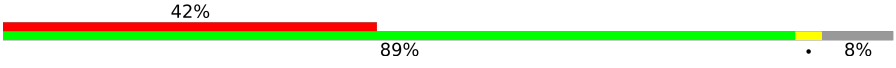
• Molecule 6: Cytochrome b-c1 complex subunit 7

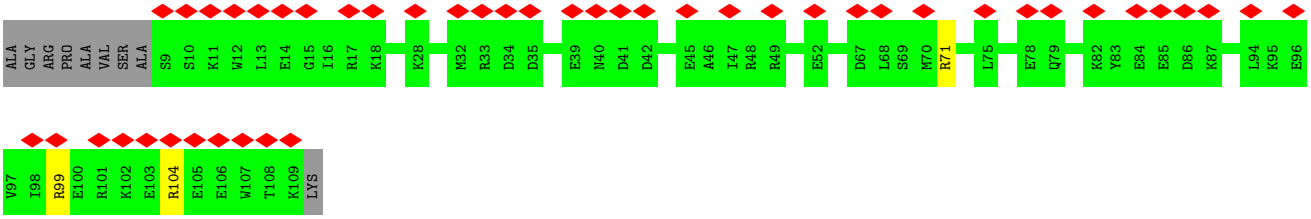
Chain d1:



• Molecule 6: Cytochrome b-c1 complex subunit 7

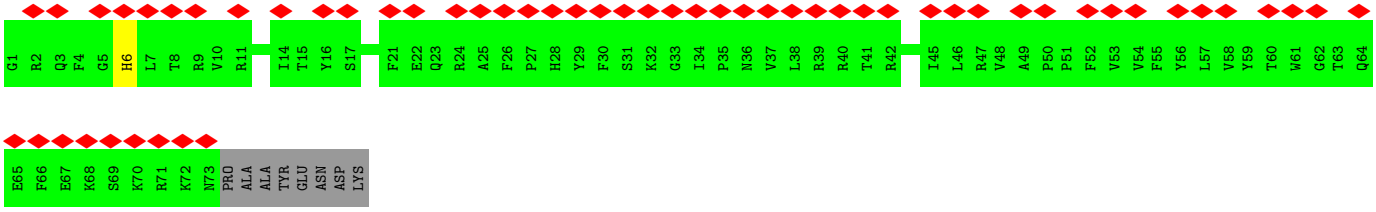
Chain d2:





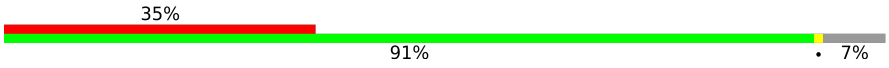
• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII

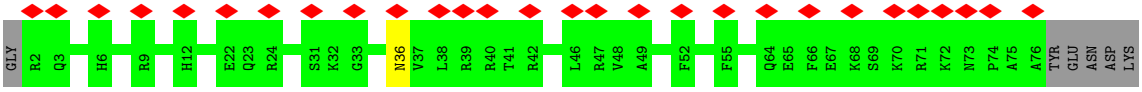
Chain q1:



• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII

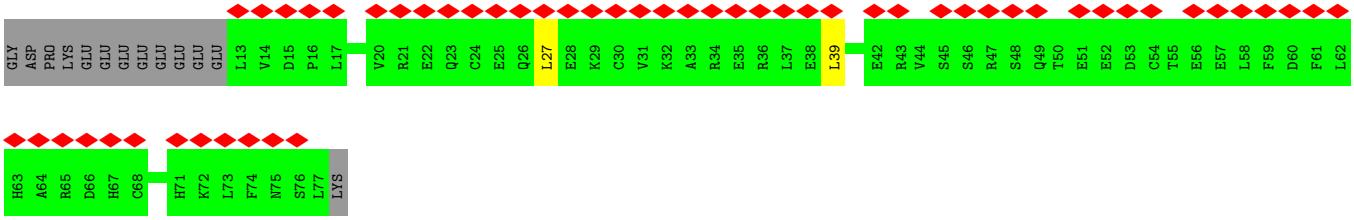
Chain q2:





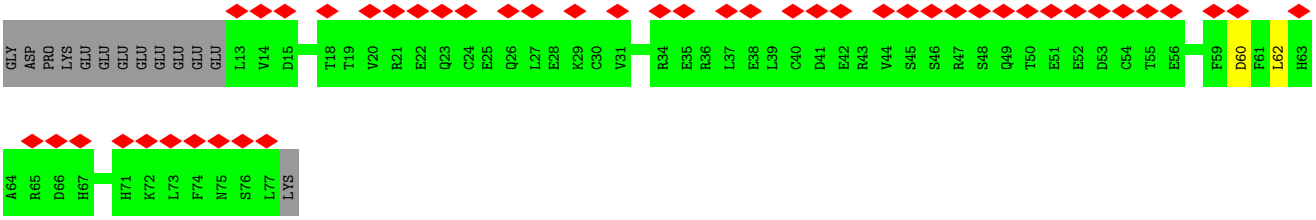
• Molecule 8: Cytochrome b-c1 complex subunit 6

Chain h1:



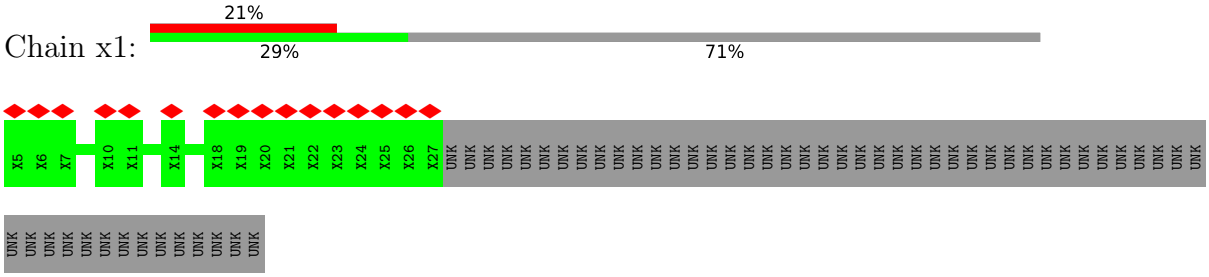
• Molecule 8: Cytochrome b-c1 complex subunit 6

Chain h2:



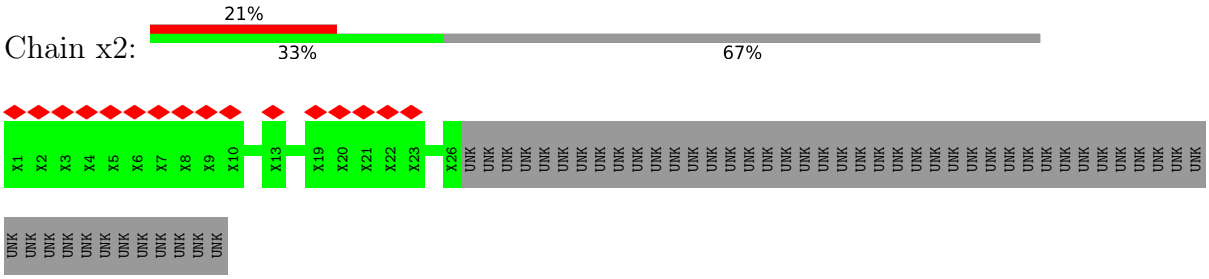
• Molecule 9: UQCRFS1N

Chain x1:



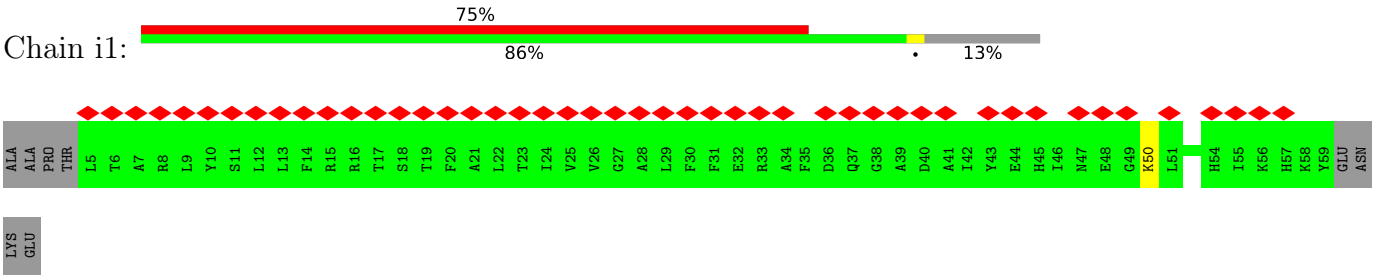
• Molecule 9: UQCRFS1N

Chain x2:



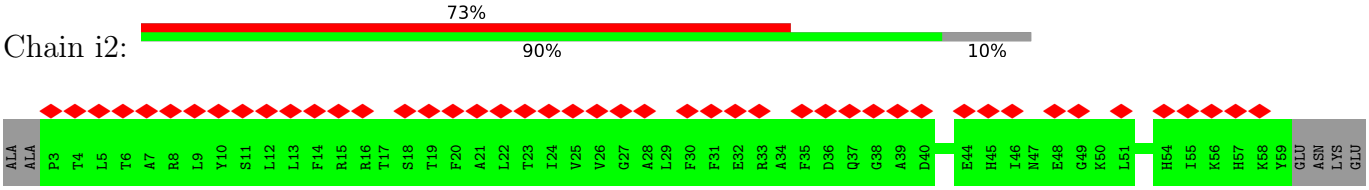
• Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

Chain i1:



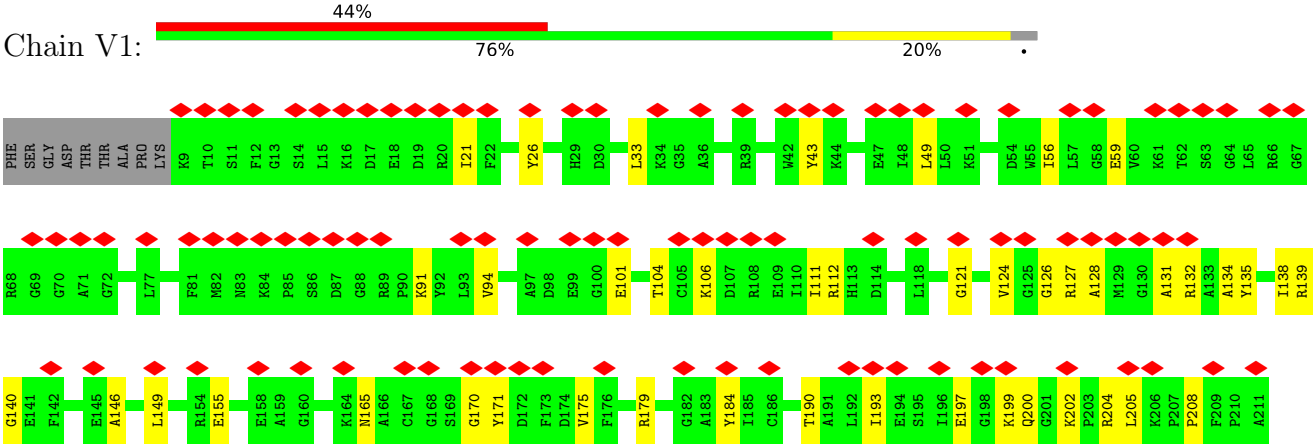
• Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

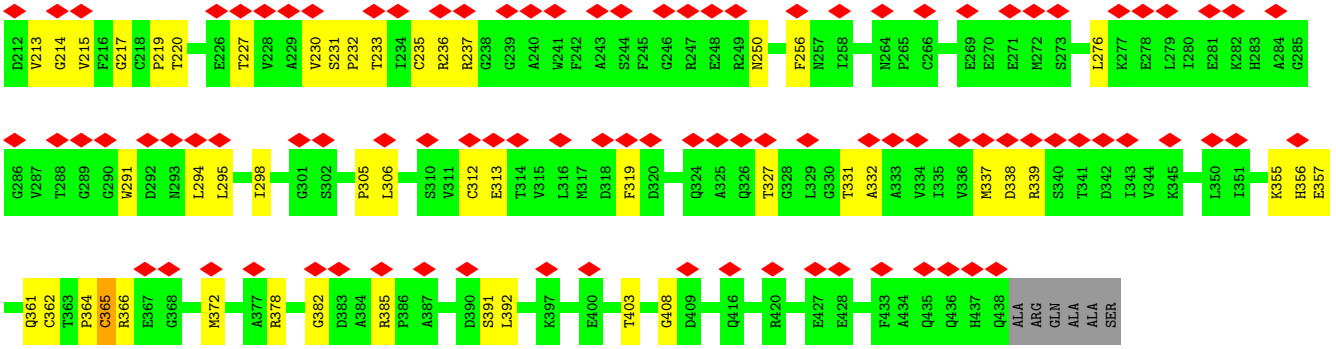
Chain i2:



• Molecule 11: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

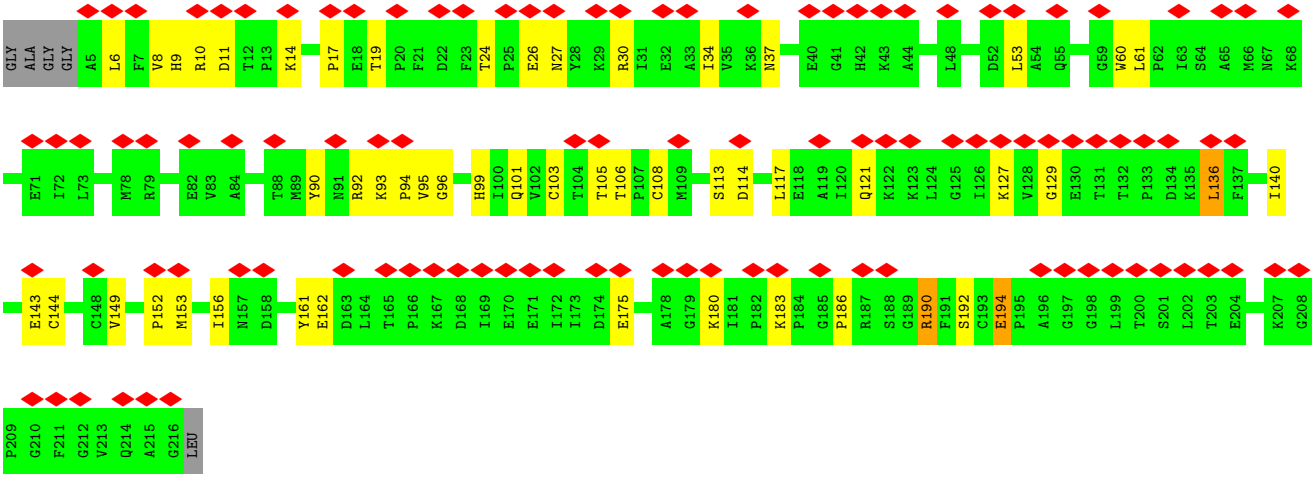
Chain V1:





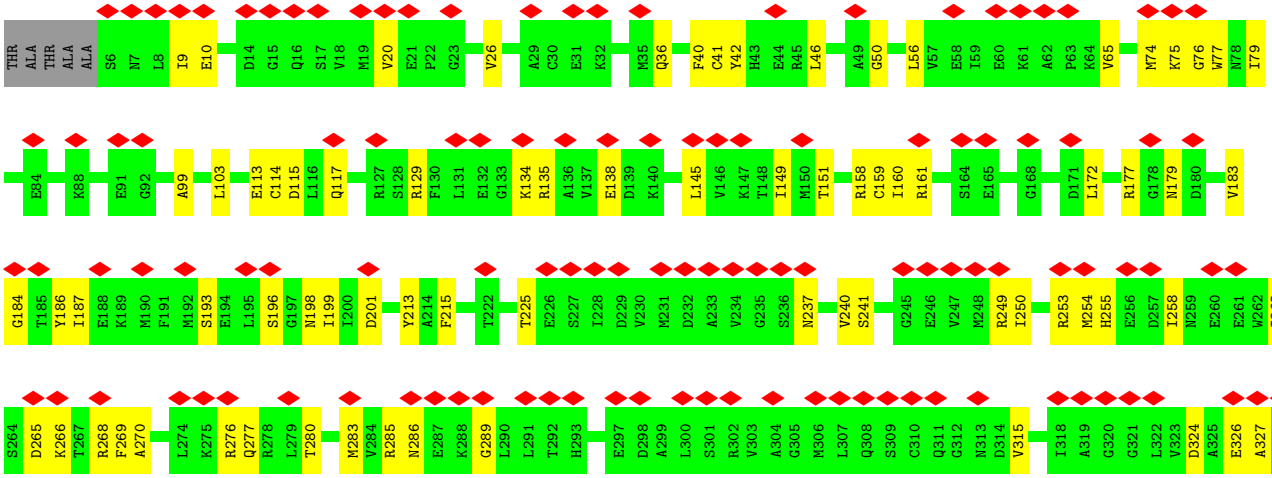
• Molecule 12: NDUFV2

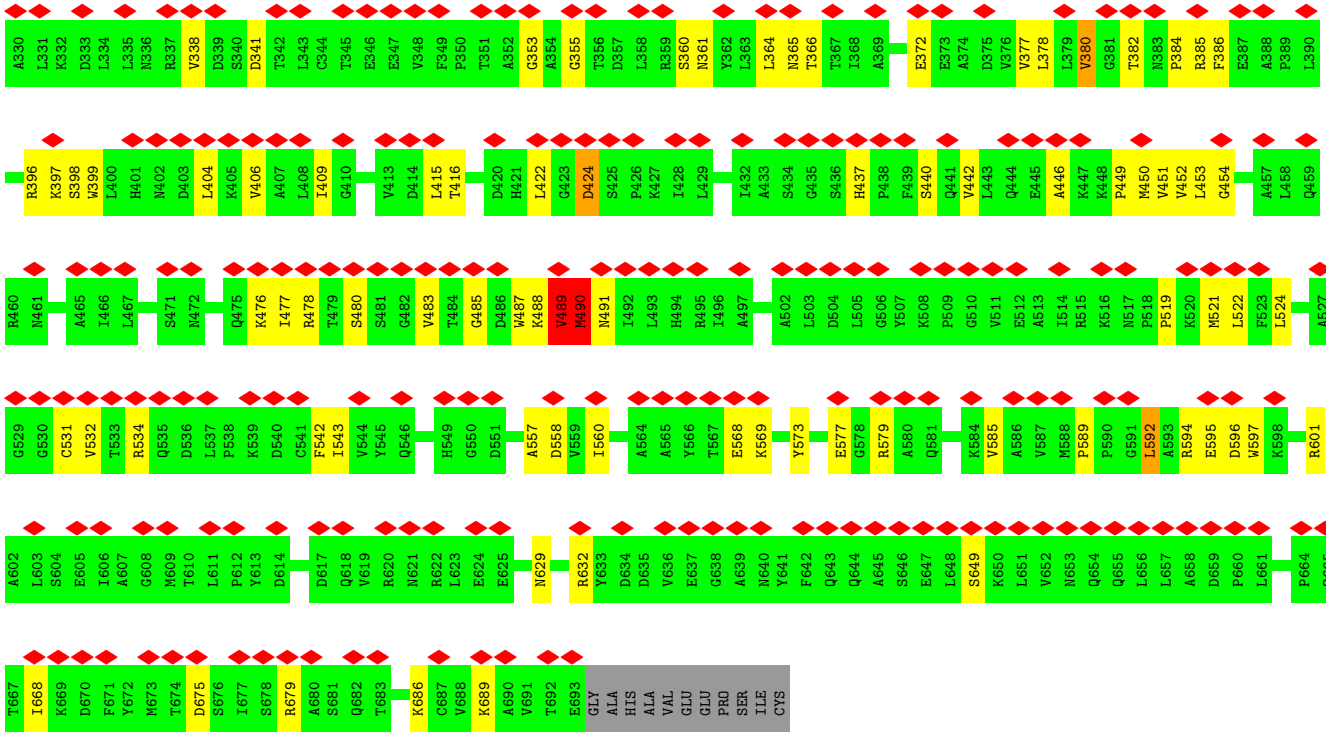
Chain V2:



• Molecule 13: NADH:ubiquinone oxidoreductase core subunit S1

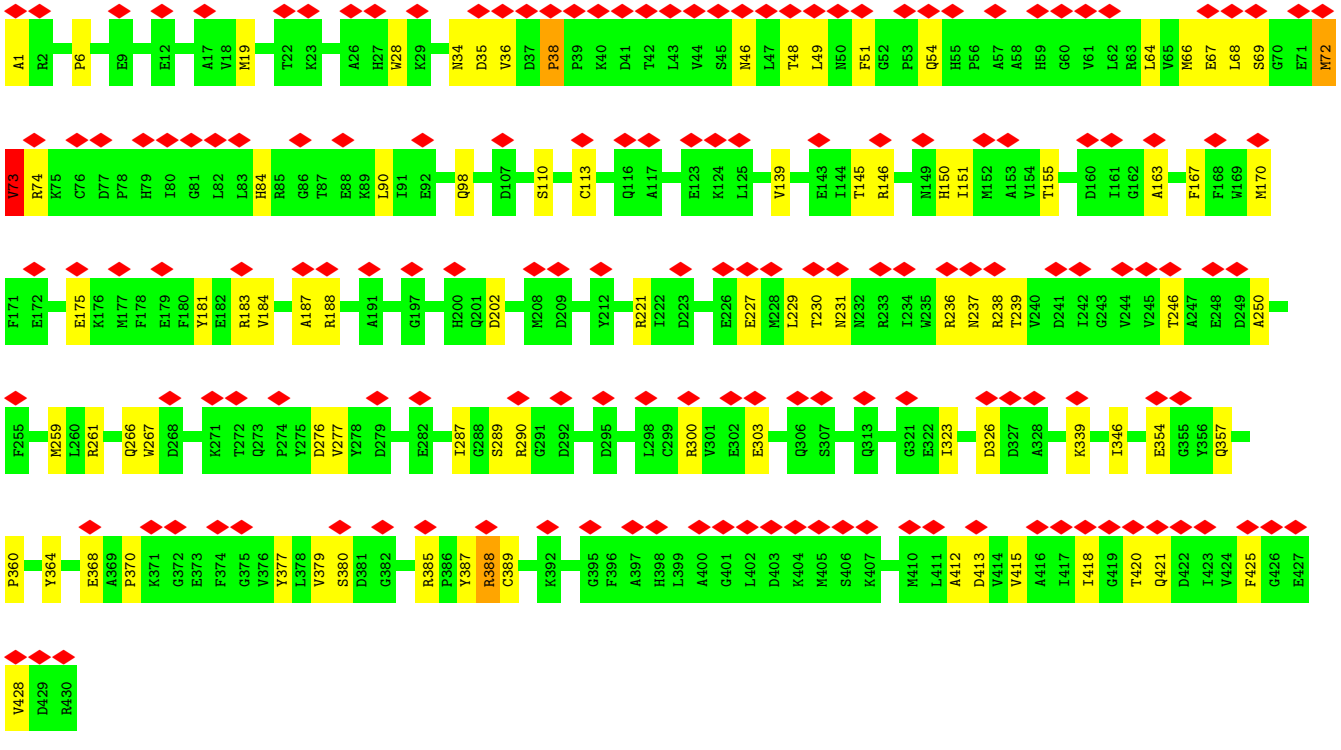
Chain S1:





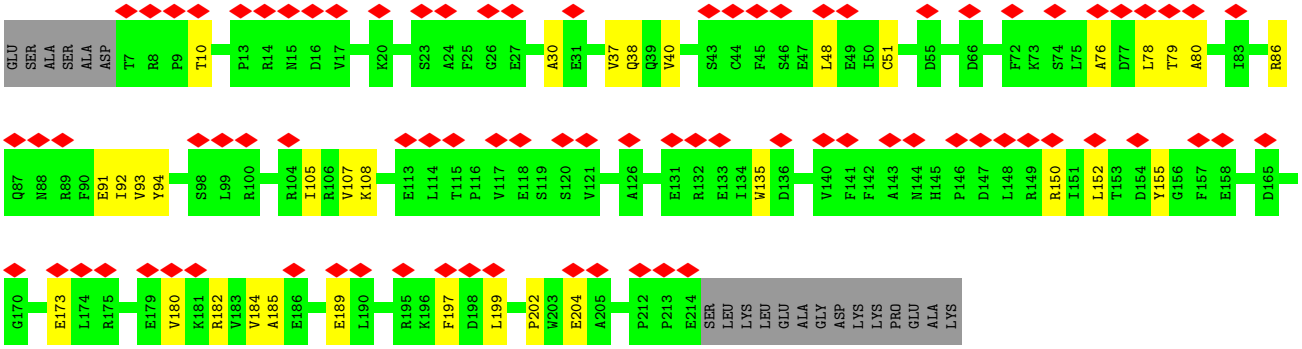
• Molecule 14: NDUFS2

Chain S2:



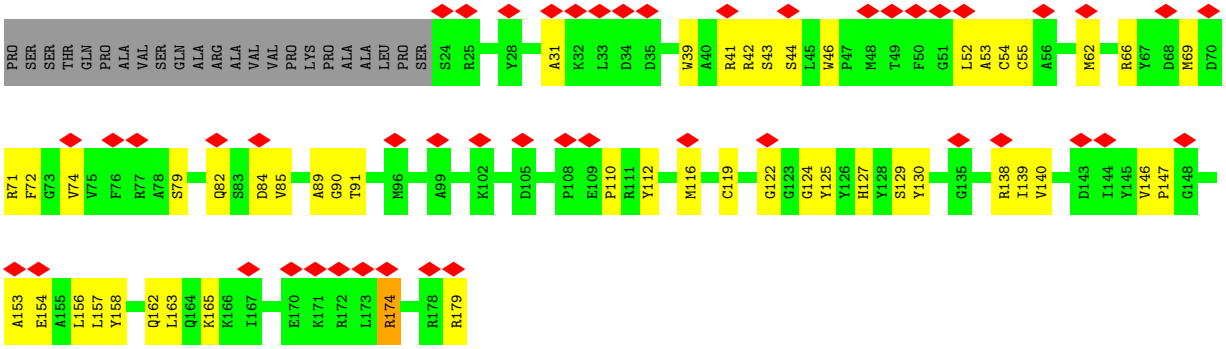
• Molecule 15: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:



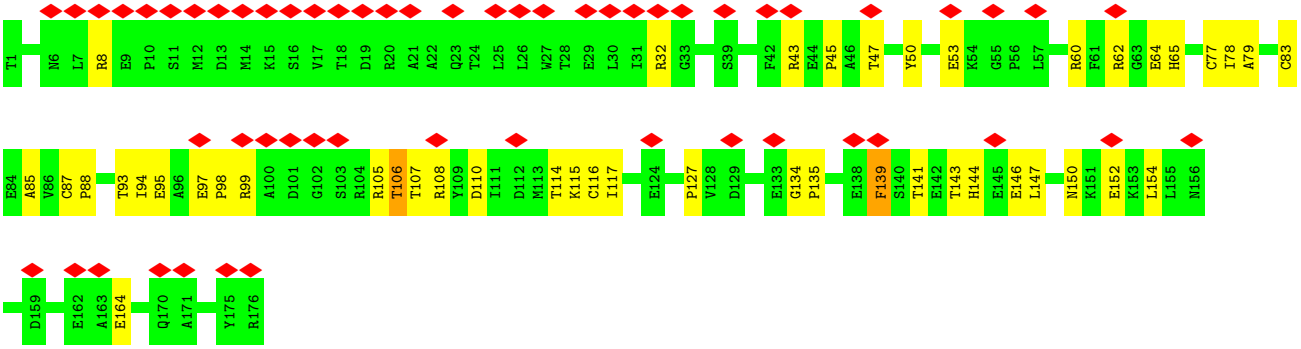
- Molecule 16: NDUFS7

Chain S7:



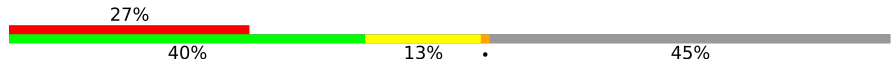
- Molecule 17: NDUFS8

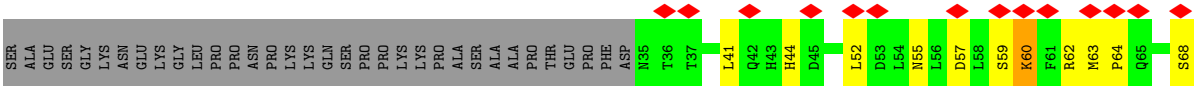
Chain S8:

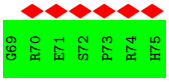


- Molecule 18: NDUFV3

Chain V3:

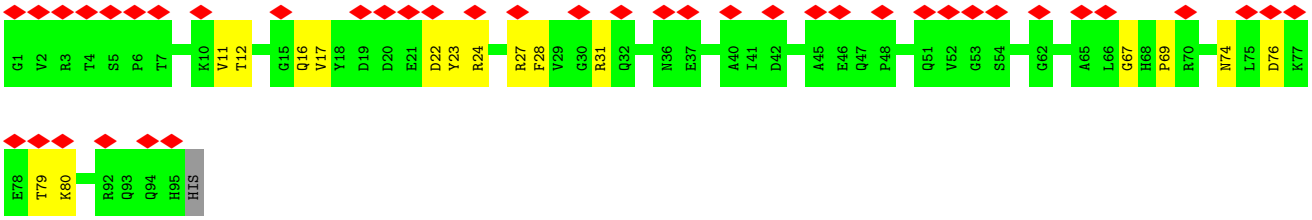






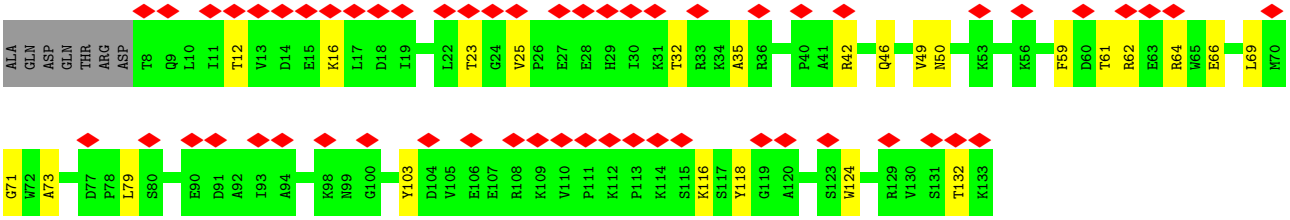
• Molecule 19: NDUFS6

Chain S6:



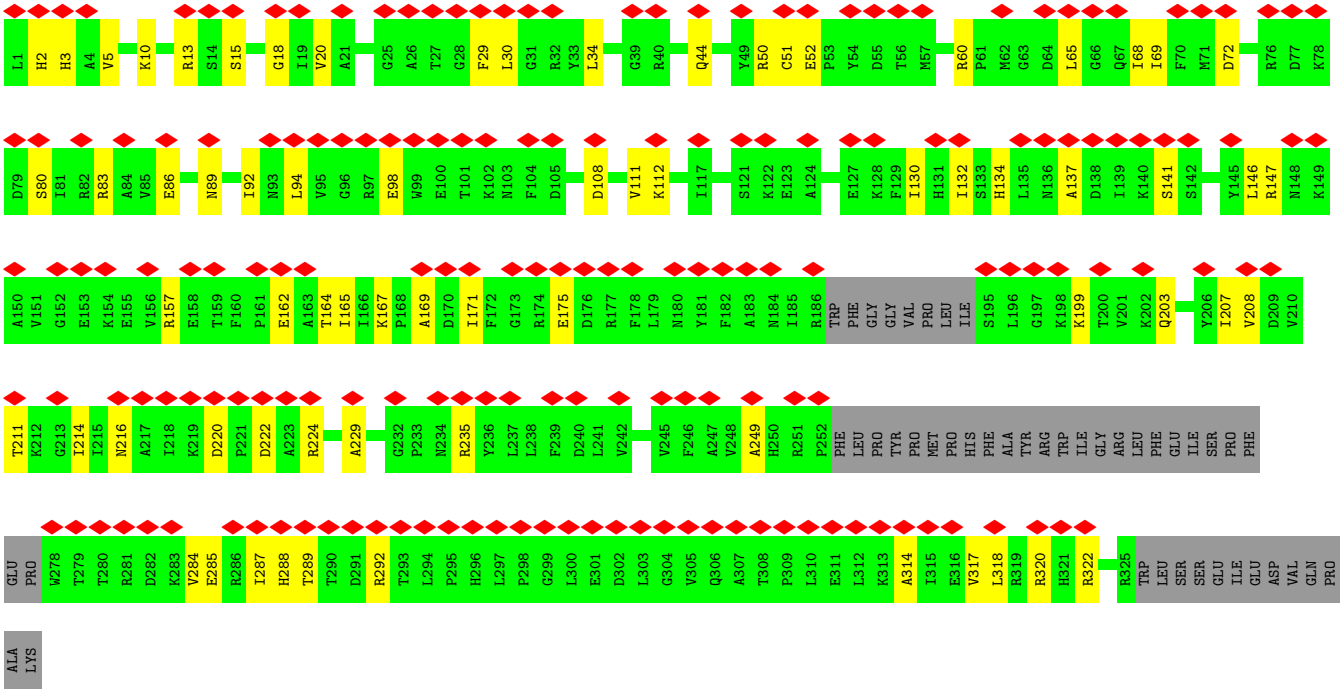
• Molecule 20: NADH:ubiquinone oxidoreductase subunit S4

Chain S4:



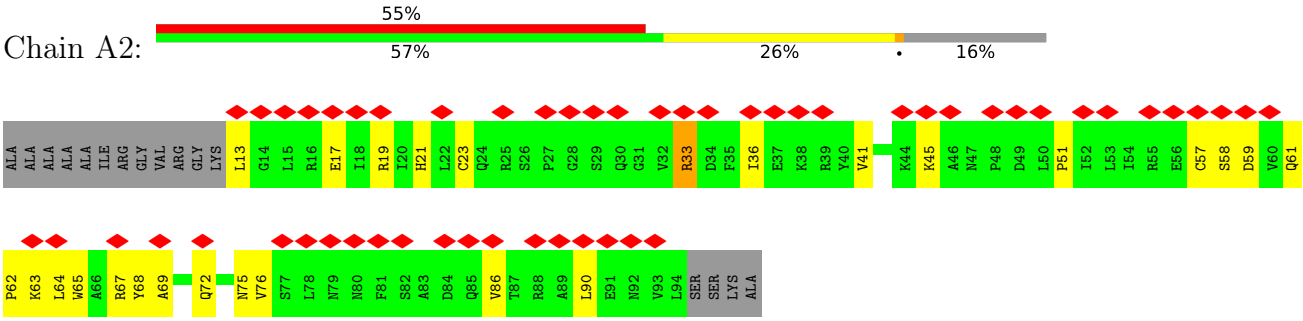
• Molecule 21: NADH:ubiquinone oxidoreductase subunit A9

Chain A9:



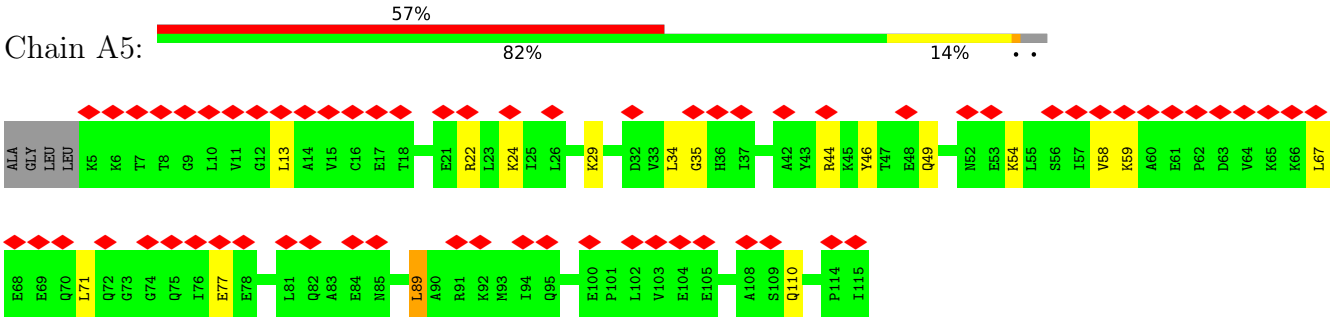
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:



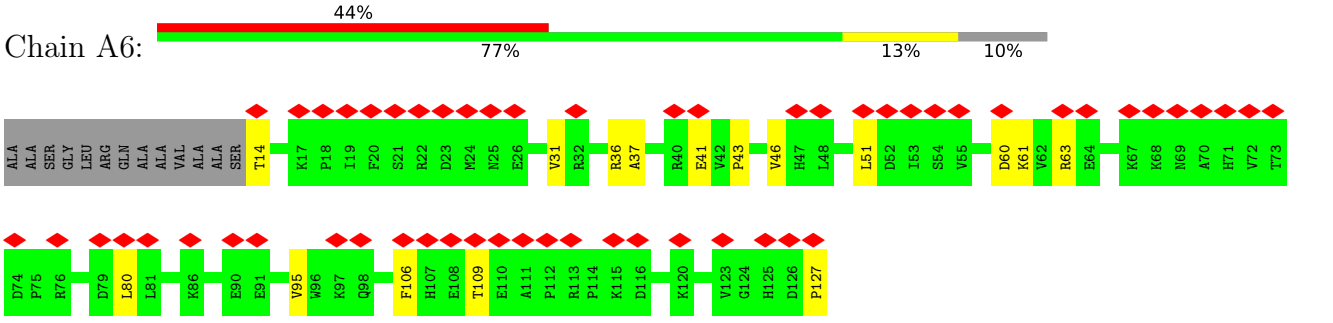
• Molecule 23: NDUFA5

Chain A5:



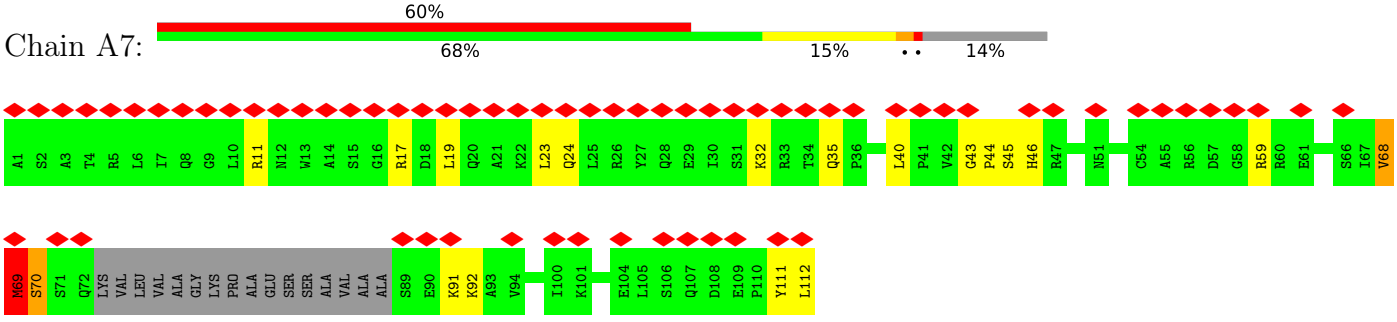
• Molecule 24: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



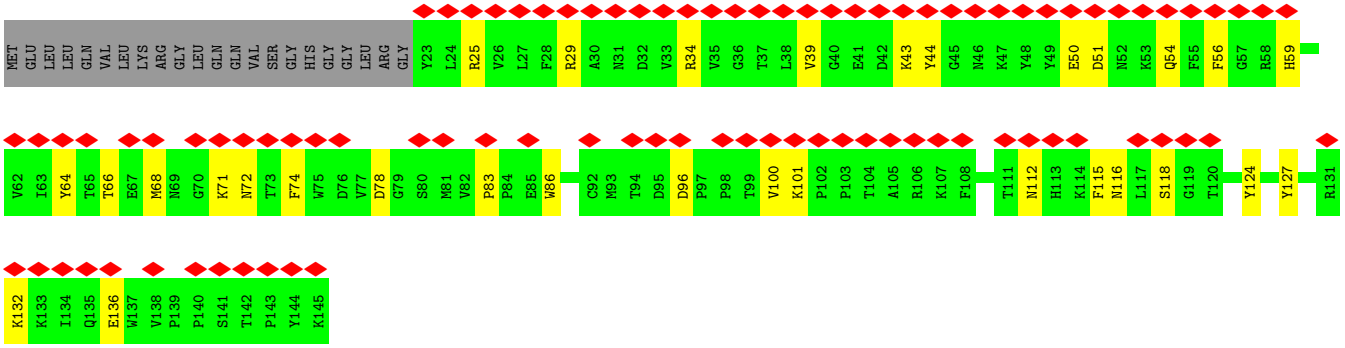
• Molecule 25: NDUFA7

Chain A7:

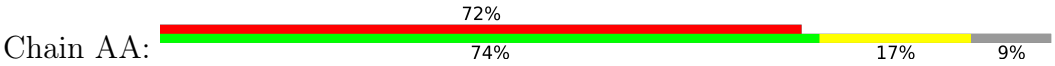


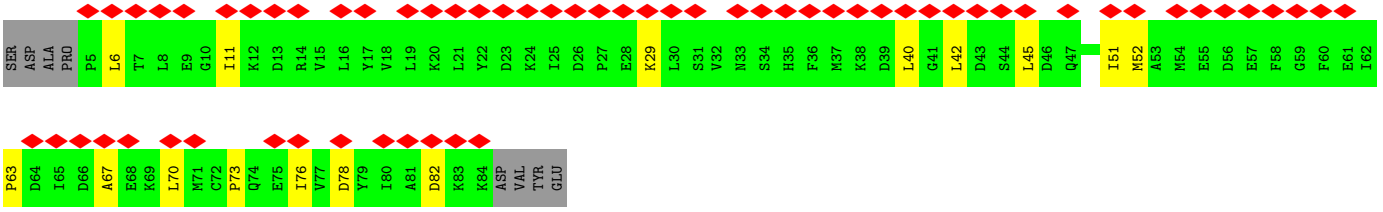
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:

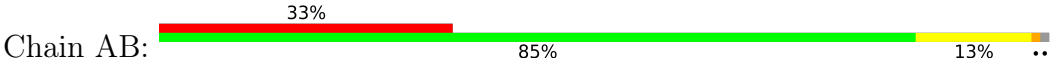


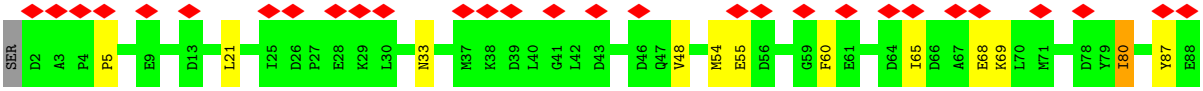
• Molecule 27: Acyl carrier protein



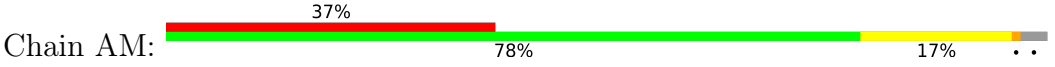


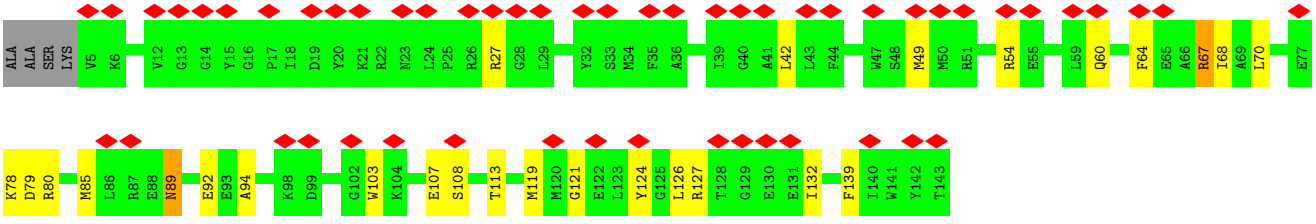
• Molecule 27: Acyl carrier protein



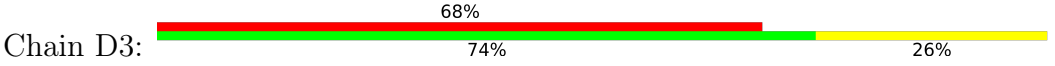


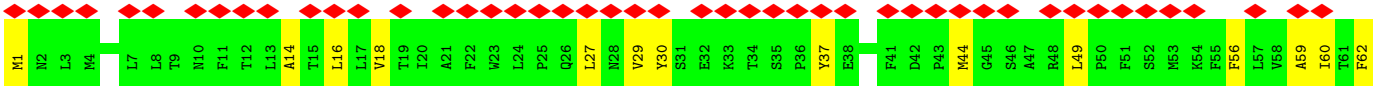
• Molecule 28: NDUFA13

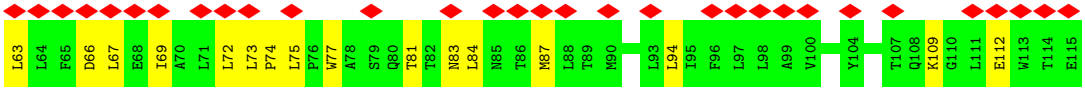




• Molecule 29: NADH-ubiquinone oxidoreductase chain 3

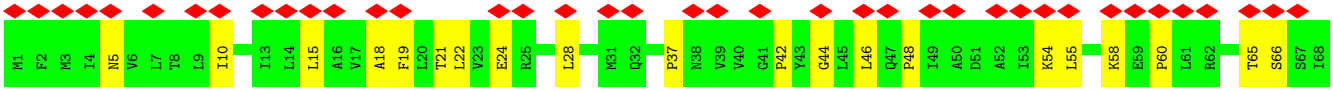


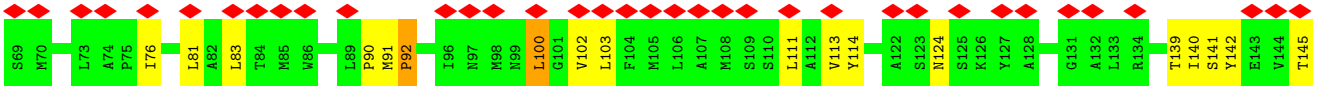


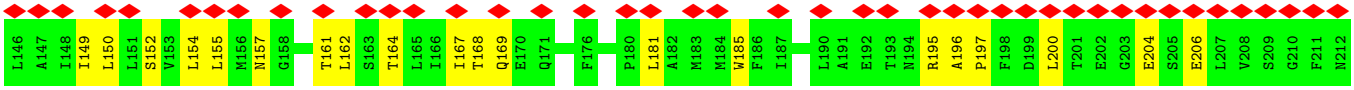


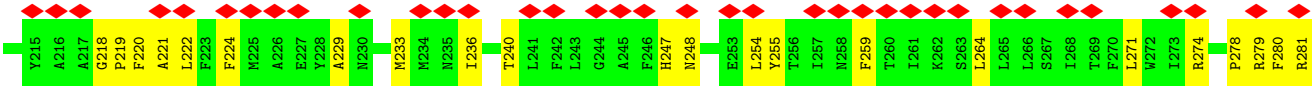
• Molecule 30: NADH-ubiquinone oxidoreductase chain 1

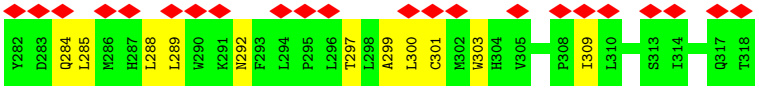
Chain D1:





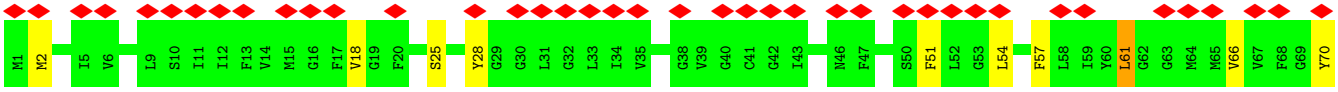


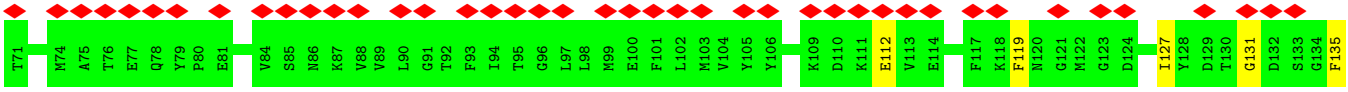


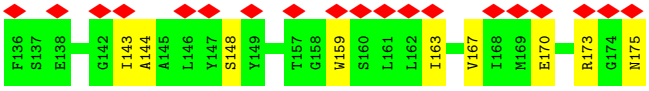


• Molecule 31: NADH-ubiquinone oxidoreductase chain 6

Chain D6:

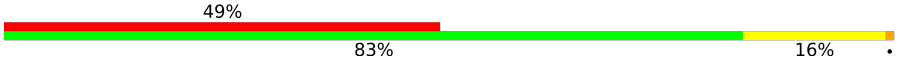


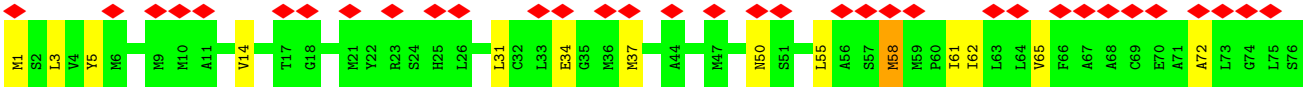


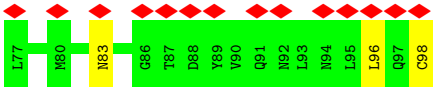


• Molecule 32: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:

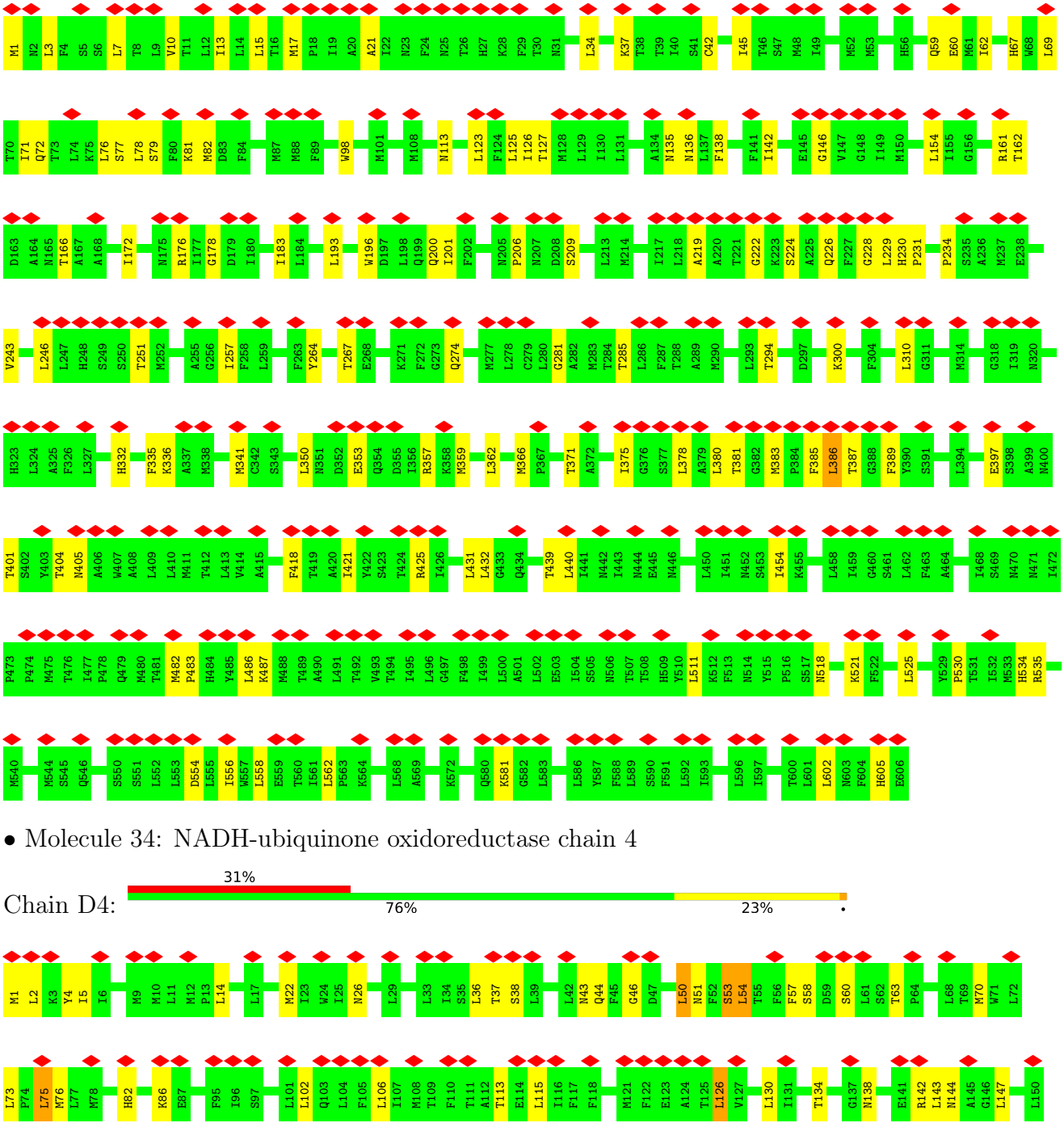






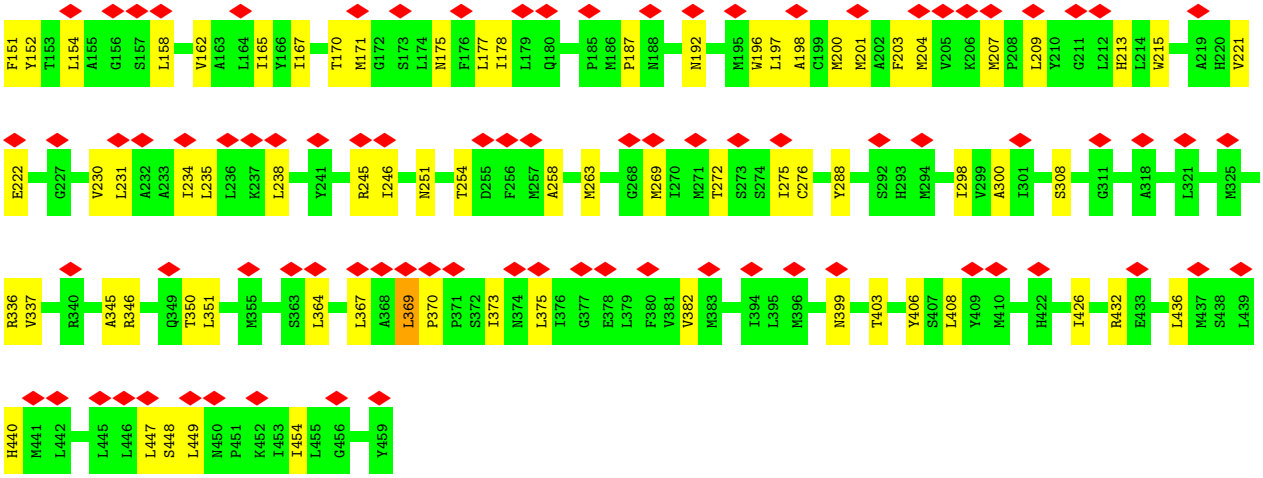
• Molecule 33: NADH-ubiquinone oxidoreductase chain 5

Chain D5:



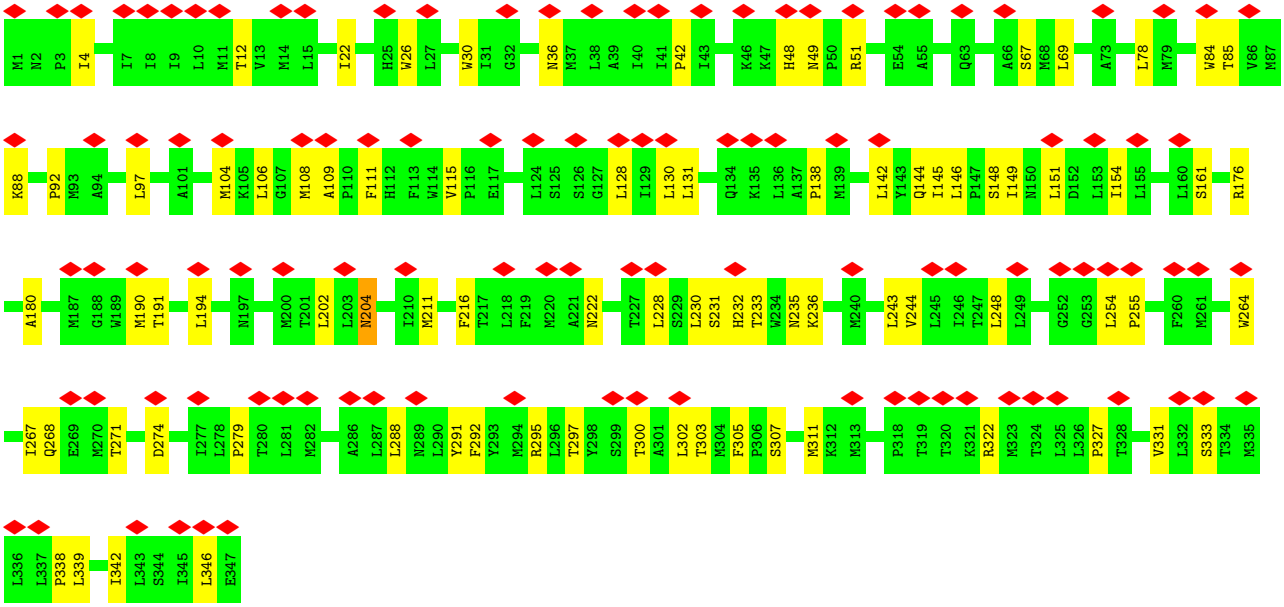
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4

Chain D4:



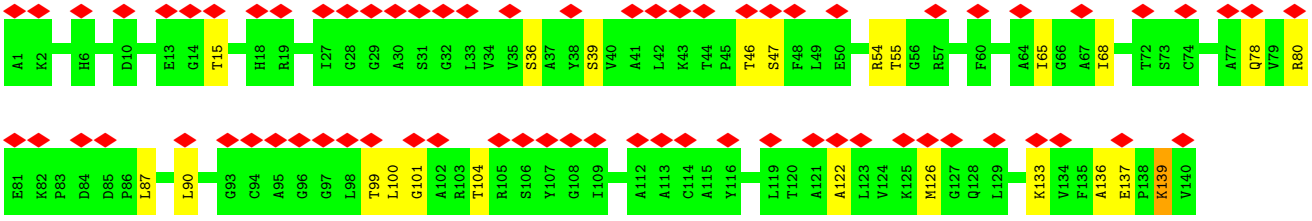
• Molecule 35: NADH-ubiquinone oxidoreductase chain 2

Chain D2:



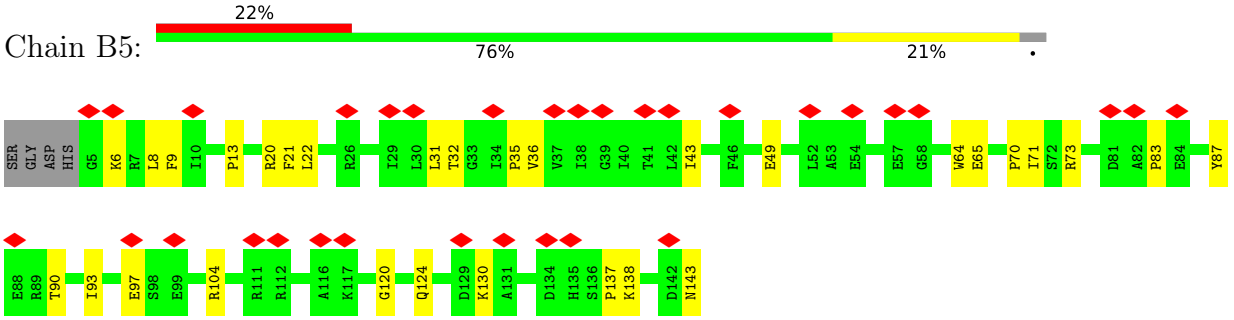
• Molecule 36: NDUFA11

Chain AK:



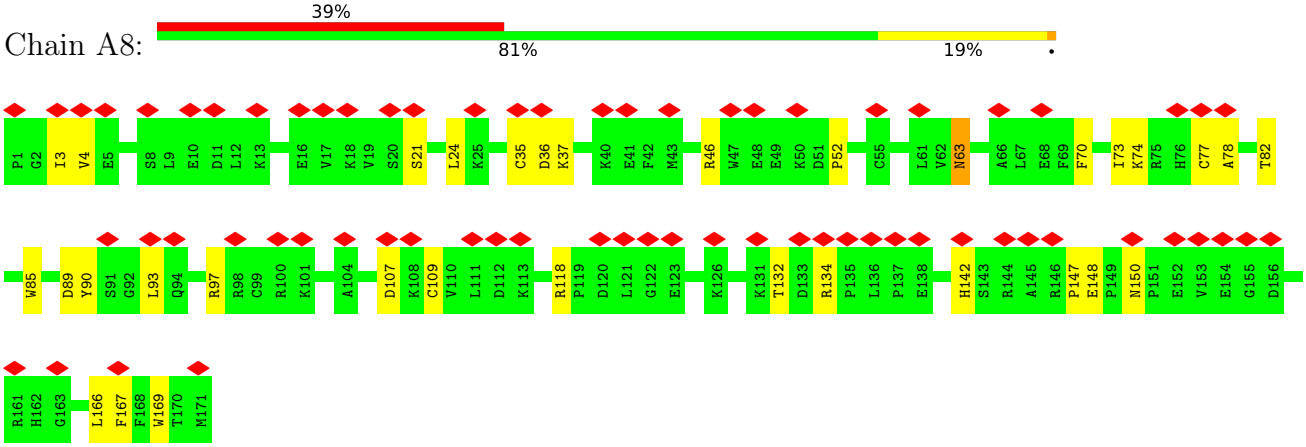
• Molecule 37: NADH:ubiquinone oxidoreductase subunit B5

Chain B5:



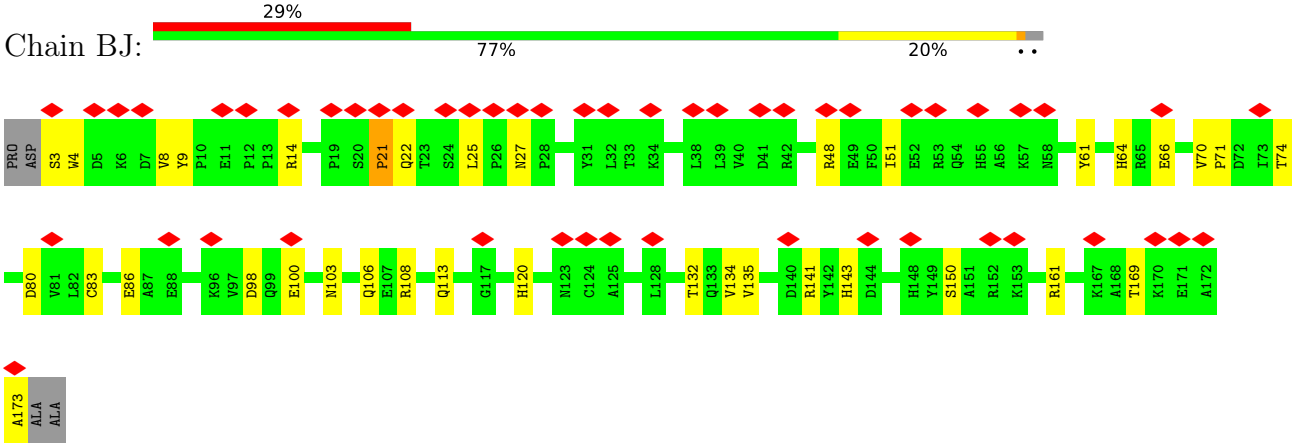
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:



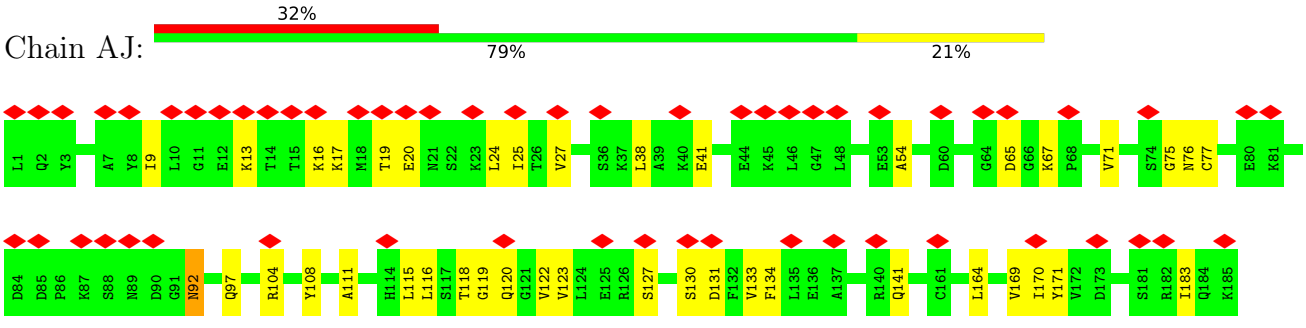
• Molecule 39: NDUFB10

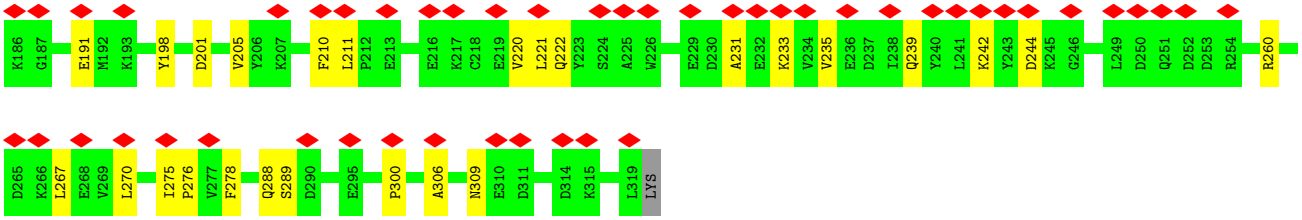
Chain BJ:



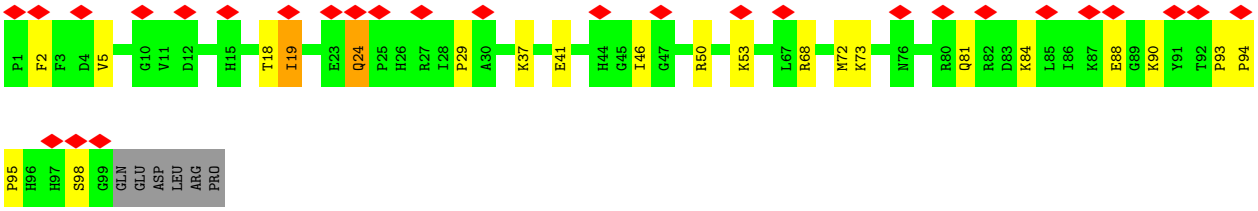
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AJ:

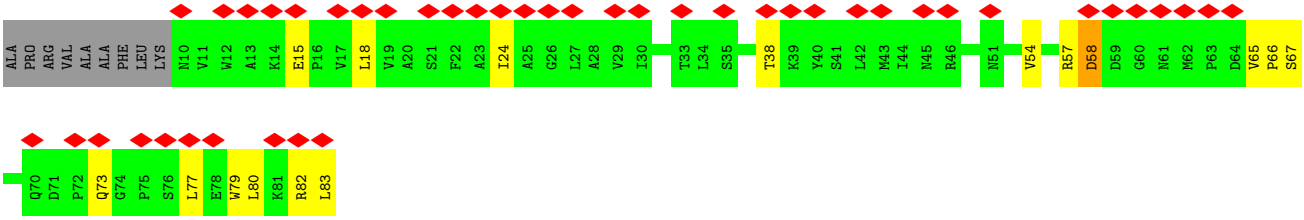




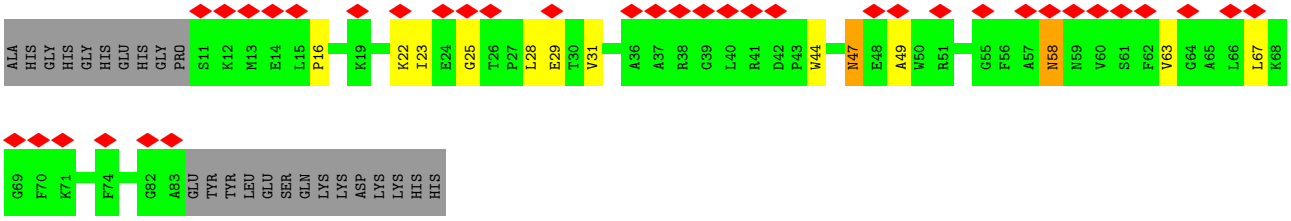
• Molecule 41: NADH:ubiquinone oxidoreductase subunit S5



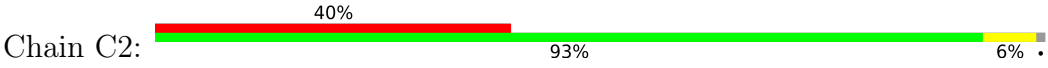
• Molecule 42: NADH:ubiquinone oxidoreductase subunit A3

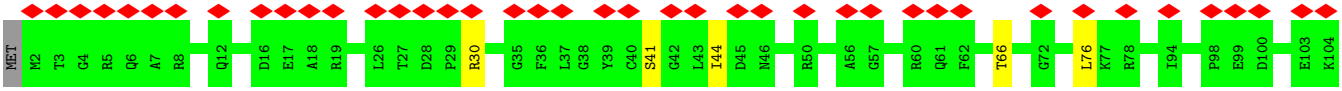


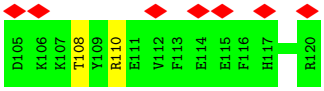
• Molecule 43: NADH:ubiquinone oxidoreductase subunit B3



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 subunit C2

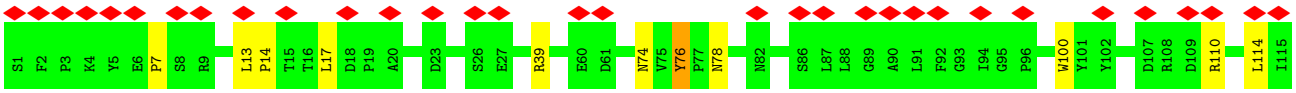


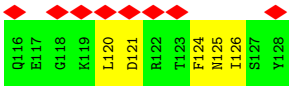




• Molecule 45: NADH:ubiquinone oxidoreductase subunit B4

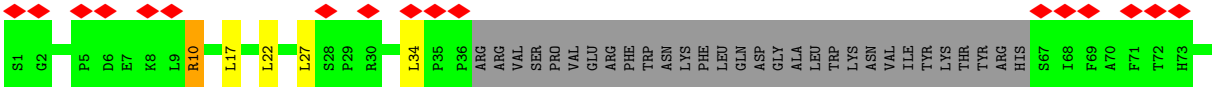
Chain B4:





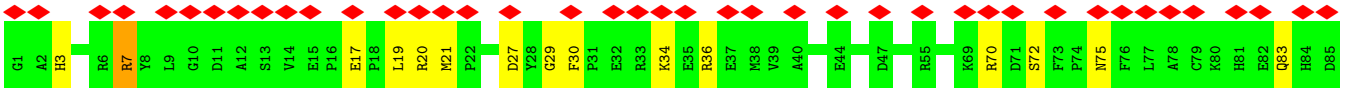
• Molecule 46: NDUFB6

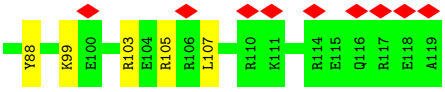
Chain B6:



• Molecule 47: NADH:ubiquinone oxidoreductase subunit B7

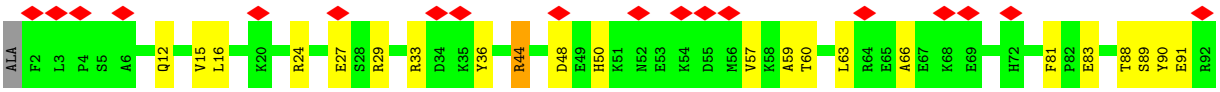
Chain B7:

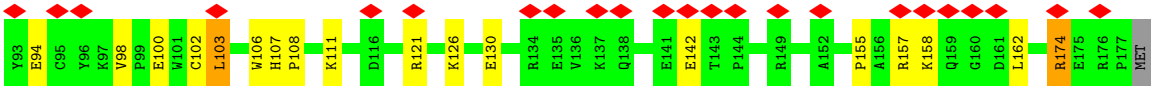




• Molecule 48: NADH:ubiquinone oxidoreductase subunit B9

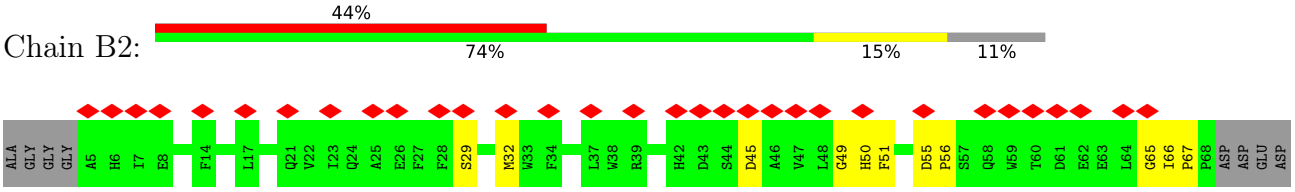
Chain B9:





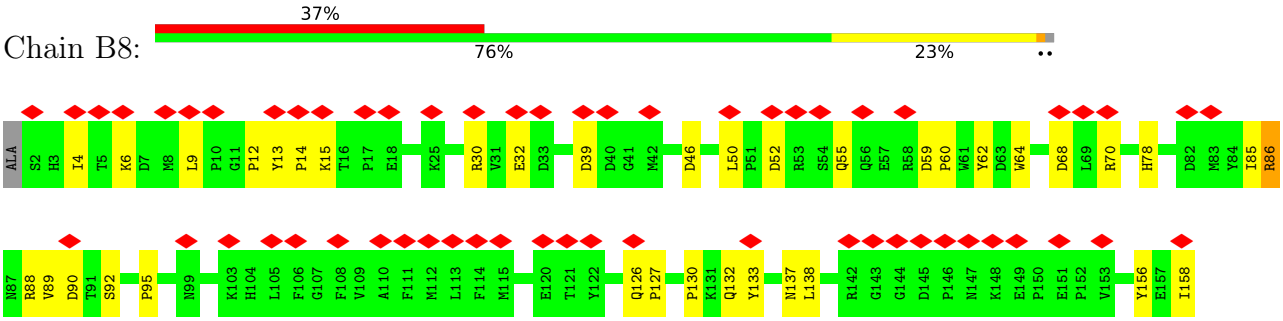
• Molecule 49: NADH:ubiquinone oxidoreductase subunit B2

Chain B2:



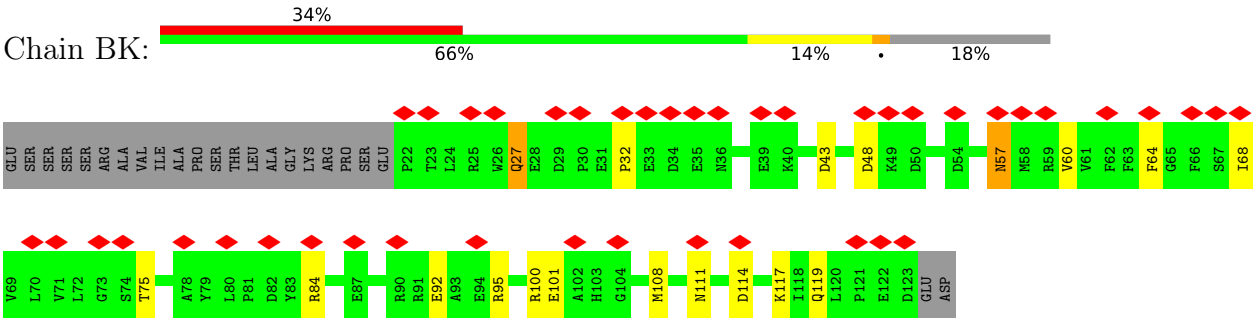
• Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



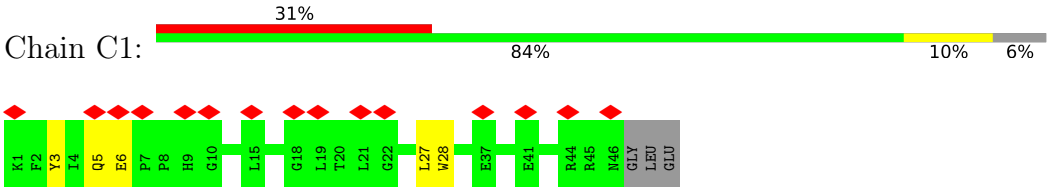
• Molecule 51: NDUFB11

Chain BK:



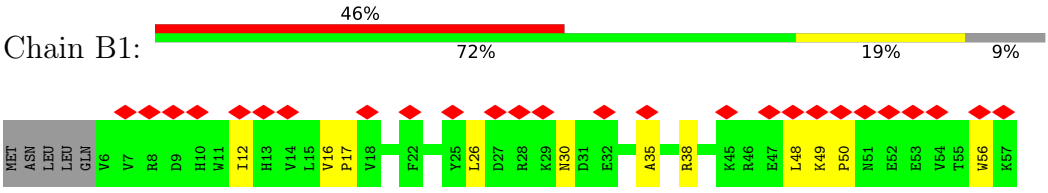
• Molecule 52: NDUFC1

Chain C1:



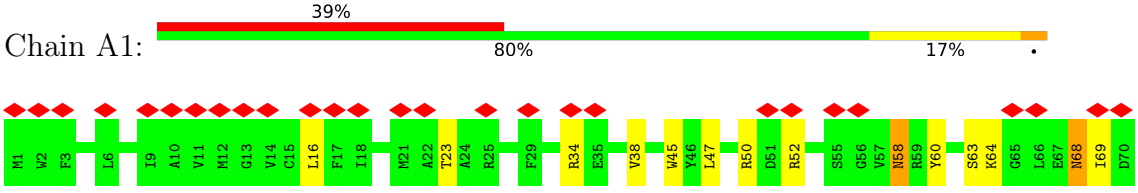
• Molecule 53: NDUFB1

Chain B1:



• Molecule 54: NDUFA1

Chain A1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39863	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	1.049	Depositor
Minimum map value	-0.332	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	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: SF4, ZN, 3PE, FES, PC1, HEM, NDP, ZMP, HEC, FMN

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	a1	0.32	0/3479	0.60	0/4719
1	a3	0.33	0/3518	0.56	0/4776
2	a2	0.31	0/3183	0.55	0/4313
2	a4	0.32	0/3179	0.56	1/4308 (0.0%)
3	b1	0.34	0/3119	0.58	0/4268
3	b2	0.35	0/3119	0.56	0/4268
4	c1	0.30	0/1968	0.54	0/2672
4	c2	0.33	0/1962	0.56	0/2664
5	f1	0.30	0/1554	0.52	0/2101
5	f2	0.29	0/1548	0.54	1/2093 (0.0%)
6	d1	0.32	0/906	0.54	1/1213 (0.1%)
6	d2	0.32	0/908	0.53	0/1218
7	q1	0.33	0/638	0.53	0/862
7	q2	0.36	0/652	0.63	0/883
8	h1	0.29	0/538	0.64	2/723 (0.3%)
8	h2	0.32	0/538	0.70	2/723 (0.3%)
10	i1	0.31	0/471	0.53	0/634
10	i2	0.30	0/486	0.53	0/655
11	V1	0.34	0/3386	0.59	0/4575
12	V2	0.33	0/1687	0.69	1/2295 (0.0%)
13	S1	0.34	0/5362	0.61	2/7266 (0.0%)
14	S2	0.38	0/3547	0.61	1/4808 (0.0%)
15	S3	0.36	0/1776	0.63	0/2417
16	S7	0.40	0/1279	0.61	0/1728
17	S8	0.42	0/1446	0.62	0/1956
18	V3	0.31	0/355	0.73	1/480 (0.2%)
19	S6	0.33	0/749	0.57	0/1009
20	S4	0.33	0/1048	0.54	0/1415
21	A9	0.33	0/2397	0.66	1/3239 (0.0%)
22	A2	0.29	0/676	0.63	0/911
23	A5	0.33	0/921	0.71	2/1249 (0.2%)
24	A6	0.33	0/993	0.56	0/1336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
25	A7	0.29	0/784	0.65	0/1060
26	AL	0.35	0/1084	0.62	0/1478
27	AA	0.30	0/655	0.67	0/881
27	AB	0.33	0/714	0.61	0/963
28	AM	0.35	0/1172	0.64	2/1579 (0.1%)
29	D3	0.39	0/948	0.73	4/1296 (0.3%)
30	D1	0.41	0/2604	0.68	1/3561 (0.0%)
31	D6	0.39	0/1379	0.70	1/1868 (0.1%)
32	4L	0.37	0/758	0.73	1/1024 (0.1%)
33	D5	0.38	0/4933	0.73	5/6710 (0.1%)
34	D4	0.40	0/3740	0.72	8/5095 (0.2%)
35	D2	0.40	0/2788	0.69	2/3795 (0.1%)
36	AK	0.34	0/1046	0.70	1/1419 (0.1%)
37	B5	0.34	0/1189	0.55	0/1607
38	A8	0.34	0/1441	0.69	1/1942 (0.1%)
39	BJ	0.36	0/1475	0.59	2/1989 (0.1%)
40	AJ	0.37	0/2644	0.62	1/3579 (0.0%)
41	S5	0.36	0/843	0.64	1/1128 (0.1%)
42	A3	0.34	0/602	0.72	0/828
43	B3	0.36	0/595	0.72	0/803
44	C2	0.38	0/1028	0.58	0/1388
45	B4	0.37	0/1085	0.64	1/1467 (0.1%)
46	B6	0.35	0/830	0.74	1/1130 (0.1%)
47	B7	0.33	0/1051	0.68	3/1408 (0.2%)
48	B9	0.37	0/1568	0.63	1/2123 (0.0%)
49	B2	0.39	0/582	0.63	0/799
50	B8	0.38	0/1379	0.70	1/1884 (0.1%)
51	BK	0.36	0/880	0.65	1/1196 (0.1%)
52	C1	0.32	0/404	0.59	0/548
53	B1	0.34	0/462	0.60	1/624 (0.2%)
54	A1	0.34	0/592	0.60	0/795
All	All	0.35	0/98643	0.63	54/133744 (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
1	a1	0	4
1	a3	0	1
2	a2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	c1	0	2
5	f2	0	1
7	q1	0	1
12	V2	0	1
13	S1	0	5
14	S2	0	2
15	S3	0	1
17	S8	0	2
25	A7	0	3
26	AL	0	1
30	D1	0	4
33	D5	0	1
34	D4	0	1
39	BJ	0	1
40	AJ	0	1
41	S5	0	1
42	A3	0	2
43	B3	0	3
45	B4	0	1
46	B6	0	1
48	B9	0	1
49	B2	0	1
52	C1	0	2
54	A1	0	1
All	All	0	46

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A5	89	LEU	CA-CB-CG	8.71	135.33	115.30
33	D5	69	LEU	CA-CB-CG	8.09	133.90	115.30
23	A5	89	LEU	CB-CG-CD2	-7.78	97.77	111.00
47	B7	27	ASP	CB-CG-OD1	7.65	125.19	118.30
48	B9	103	LEU	CA-CB-CG	7.61	132.79	115.30

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a1	278	GLY	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	a1	279	HIS	Peptide
1	a1	309	THR	Peptide
2	a2	133	ARG	Peptide
4	c1	170	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	a1	3409	0	3322	0	0
1	a3	3447	0	3350	0	0
2	a2	3126	0	3093	0	0
2	a4	3122	0	3090	0	0
3	b1	3019	0	3082	0	0
3	b2	3019	0	3082	0	0
4	c1	1909	0	1858	0	0
4	c2	1903	0	1850	0	0
5	f1	1520	0	1505	0	0
5	f2	1514	0	1497	0	0
6	d1	886	0	883	0	0
6	d2	888	0	880	0	0
7	q1	618	0	628	0	0
7	q2	631	0	639	0	0
8	h1	532	0	509	0	0
8	h2	532	0	509	0	0
9	x1	114	0	29	0	0
9	x2	130	0	34	0	0
10	i1	459	0	462	0	0
10	i2	473	0	477	0	0
11	V1	3312	0	3266	59	0
12	V2	1647	0	1657	36	0
13	S1	5275	0	5300	105	0
14	S2	3455	0	3395	71	0
15	S3	1726	0	1676	32	0
16	S7	1248	0	1256	37	0
17	S8	1415	0	1371	38	0
18	V3	345	0	323	8	0
19	S6	737	0	710	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	S4	1025	0	1023	19	0
21	A9	2344	0	2372	43	0
22	A2	665	0	678	18	0
23	A5	901	0	936	12	0
24	A6	969	0	980	14	0
25	A7	766	0	779	19	0
26	AL	1044	0	1001	21	0
27	AA	645	0	649	9	0
27	AB	702	0	692	10	0
28	AM	1143	0	1137	20	0
29	D3	923	0	953	22	0
30	D1	2529	0	2641	63	0
31	D6	1345	0	1364	22	0
32	4L	748	0	794	15	0
33	D5	4805	0	4950	76	0
34	D4	3646	0	3850	72	0
35	D2	2724	0	2930	61	0
36	AK	1025	0	1033	14	0
37	B5	1156	0	1177	25	0
38	A8	1404	0	1384	24	0
39	BJ	1441	0	1417	23	0
40	AJ	2583	0	2547	41	0
41	S5	822	0	820	19	0
42	A3	582	0	583	12	0
43	B3	578	0	570	7	0
44	C2	997	0	983	8	0
45	B4	1059	0	1062	10	0
46	B6	804	0	824	15	0
47	B7	1026	0	995	12	0
48	B9	1515	0	1469	29	0
49	B2	555	0	505	8	0
50	B8	1324	0	1219	28	0
51	BK	853	0	800	17	0
52	C1	391	0	391	3	0
53	B1	449	0	453	7	0
54	A1	577	0	570	11	0
55	b1	86	0	60	0	0
55	b2	86	0	60	0	0
56	c1	43	0	30	0	0
56	c2	43	0	30	0	0
57	S1	4	0	0	0	0
57	V2	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	f1	4	0	0	0	0
57	f2	4	0	0	0	0
58	S1	16	0	0	1	0
58	S7	8	0	0	0	0
58	S8	16	0	0	0	0
58	V1	8	0	0	0	0
59	V1	31	0	19	0	0
60	D5	38	0	50	1	0
60	S2	40	0	54	3	0
61	S6	1	0	0	0	0
62	A9	48	0	26	5	0
63	AA	34	0	40	1	0
63	AB	31	0	34	4	0
64	AK	28	0	30	1	0
All	All	97049	0	96697	969	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 969 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)
15:S3:38:GLN:O	25:A7:70:SER:HA	1.14	1.25
15:S3:80:ALA:HA	15:S3:91:GLU:O	1.39	1.20
15:S3:38:GLN:O	25:A7:70:SER:CA	2.00	1.09
13:S1:237:ASN:O	13:S1:253:ARG:HB2	1.70	0.91
22:A2:21:HIS:O	22:A2:62:PRO:HA	1.70	0.91

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	a1	435/446 (98%)	397 (91%)	37 (8%)	1 (0%)	44	77
1	a3	442/446 (99%)	407 (92%)	35 (8%)	0	100	100
2	a2	410/439 (93%)	373 (91%)	37 (9%)	0	100	100
2	a4	409/439 (93%)	376 (92%)	33 (8%)	0	100	100
3	b1	376/379 (99%)	355 (94%)	21 (6%)	0	100	100
3	b2	376/379 (99%)	352 (94%)	24 (6%)	0	100	100
4	c1	237/240 (99%)	206 (87%)	31 (13%)	0	100	100
4	c2	236/240 (98%)	203 (86%)	33 (14%)	0	100	100
5	f1	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
5	f2	193/196 (98%)	180 (93%)	13 (7%)	0	100	100
6	d1	98/110 (89%)	95 (97%)	3 (3%)	0	100	100
6	d2	99/110 (90%)	95 (96%)	4 (4%)	0	100	100
7	q1	71/81 (88%)	66 (93%)	5 (7%)	0	100	100
7	q2	73/81 (90%)	67 (92%)	6 (8%)	0	100	100
8	h1	63/78 (81%)	57 (90%)	6 (10%)	0	100	100
8	h2	63/78 (81%)	59 (94%)	4 (6%)	0	100	100
10	i1	53/63 (84%)	49 (92%)	4 (8%)	0	100	100
10	i2	55/63 (87%)	51 (93%)	4 (7%)	0	100	100
11	V1	428/445 (96%)	383 (90%)	45 (10%)	0	100	100
12	V2	210/217 (97%)	174 (83%)	36 (17%)	0	100	100
13	S1	686/704 (97%)	595 (87%)	87 (13%)	4 (1%)	22	59
14	S2	428/430 (100%)	374 (87%)	53 (12%)	1 (0%)	44	77
15	S3	206/228 (90%)	169 (82%)	36 (18%)	1 (0%)	25	62
16	S7	154/179 (86%)	133 (86%)	20 (13%)	1 (1%)	22	59
17	S8	174/176 (99%)	158 (91%)	16 (9%)	0	100	100
18	V3	39/75 (52%)	31 (80%)	8 (20%)	0	100	100
19	S6	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
20	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
21	A9	286/338 (85%)	245 (86%)	41 (14%)	0	100	100
22	A2	80/98 (82%)	67 (84%)	13 (16%)	0	100	100
23	A5	109/115 (95%)	100 (92%)	9 (8%)	0	100	100
24	A6	112/127 (88%)	105 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	A7	92/112 (82%)	71 (77%)	20 (22%)	1 (1%)	12 46
26	AL	121/145 (83%)	100 (83%)	21 (17%)	0	100 100
27	AA	78/88 (89%)	64 (82%)	14 (18%)	0	100 100
27	AB	85/88 (97%)	75 (88%)	10 (12%)	0	100 100
28	AM	137/143 (96%)	123 (90%)	14 (10%)	0	100 100
29	D3	113/115 (98%)	91 (80%)	22 (20%)	0	100 100
30	D1	316/318 (99%)	274 (87%)	41 (13%)	1 (0%)	37 71
31	D6	173/175 (99%)	151 (87%)	22 (13%)	0	100 100
32	4L	96/98 (98%)	88 (92%)	7 (7%)	1 (1%)	13 48
33	D5	604/606 (100%)	532 (88%)	72 (12%)	0	100 100
34	D4	457/459 (100%)	423 (93%)	33 (7%)	1 (0%)	44 77
35	D2	345/347 (99%)	314 (91%)	31 (9%)	0	100 100
36	AK	138/140 (99%)	128 (93%)	10 (7%)	0	100 100
37	B5	137/143 (96%)	123 (90%)	14 (10%)	0	100 100
38	A8	169/171 (99%)	137 (81%)	31 (18%)	1 (1%)	22 59
39	BJ	169/175 (97%)	153 (90%)	15 (9%)	1 (1%)	22 59
40	AJ	317/320 (99%)	271 (86%)	46 (14%)	0	100 100
41	S5	97/105 (92%)	83 (86%)	14 (14%)	0	100 100
42	A3	72/83 (87%)	61 (85%)	11 (15%)	0	100 100
43	B3	71/97 (73%)	55 (78%)	16 (22%)	0	100 100
44	C2	117/120 (98%)	108 (92%)	9 (8%)	0	100 100
45	B4	126/128 (98%)	107 (85%)	19 (15%)	0	100 100
46	B6	91/127 (72%)	79 (87%)	11 (12%)	1 (1%)	12 46
47	B7	117/119 (98%)	102 (87%)	15 (13%)	0	100 100
48	B9	174/178 (98%)	147 (84%)	27 (16%)	0	100 100
49	B2	62/72 (86%)	58 (94%)	4 (6%)	0	100 100
50	B8	155/158 (98%)	110 (71%)	45 (29%)	0	100 100
51	BK	100/125 (80%)	83 (83%)	17 (17%)	0	100 100
52	C1	44/49 (90%)	41 (93%)	3 (7%)	0	100 100
53	B1	50/57 (88%)	45 (90%)	5 (10%)	0	100 100
54	A1	68/70 (97%)	60 (88%)	8 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11903/12556 (95%)	10550 (89%)	1338 (11%)	15 (0%)	50 82

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a1	279	HIS
13	S1	490	MET
16	S7	130	TYR
34	D4	54	LEU
32	4L	3	LEU

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	a1	366/372 (98%)	362 (99%)	4 (1%)	70 79
1	a3	370/372 (100%)	364 (98%)	6 (2%)	58 73
2	a2	326/341 (96%)	322 (99%)	4 (1%)	67 78
2	a4	326/341 (96%)	323 (99%)	3 (1%)	75 83
3	b1	330/331 (100%)	328 (99%)	2 (1%)	84 88
3	b2	330/331 (100%)	329 (100%)	1 (0%)	91 92
4	c1	205/206 (100%)	200 (98%)	5 (2%)	44 63
4	c2	204/206 (99%)	202 (99%)	2 (1%)	73 81
5	f1	168/168 (100%)	167 (99%)	1 (1%)	84 88
5	f2	167/168 (99%)	166 (99%)	1 (1%)	84 88
6	d1	93/99 (94%)	92 (99%)	1 (1%)	70 79
6	d2	94/99 (95%)	91 (97%)	3 (3%)	34 55
7	q1	66/72 (92%)	66 (100%)	0	100 100
7	q2	67/72 (93%)	66 (98%)	1 (2%)	60 74
8	h1	62/74 (84%)	62 (100%)	0	100 100
8	h2	62/74 (84%)	62 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	i1	46/52 (88%)	45 (98%)	1 (2%)	47	65
10	i2	48/52 (92%)	48 (100%)	0	100	100
11	V1	344/354 (97%)	340 (99%)	4 (1%)	67	78
12	V2	182/183 (100%)	179 (98%)	3 (2%)	58	73
13	S1	578/588 (98%)	577 (100%)	1 (0%)	92	94
14	S2	371/371 (100%)	367 (99%)	4 (1%)	70	79
15	S3	189/204 (93%)	189 (100%)	0	100	100
16	S7	132/150 (88%)	130 (98%)	2 (2%)	60	74
17	S8	151/151 (100%)	150 (99%)	1 (1%)	81	86
18	V3	40/68 (59%)	39 (98%)	1 (2%)	42	62
19	S6	79/80 (99%)	79 (100%)	0	100	100
20	S4	113/119 (95%)	112 (99%)	1 (1%)	75	83
21	A9	251/292 (86%)	246 (98%)	5 (2%)	50	68
22	A2	73/81 (90%)	72 (99%)	1 (1%)	62	75
23	A5	99/101 (98%)	98 (99%)	1 (1%)	73	81
24	A6	107/113 (95%)	107 (100%)	0	100	100
25	A7	84/94 (89%)	84 (100%)	0	100	100
26	AL	114/131 (87%)	111 (97%)	3 (3%)	41	61
27	AA	74/81 (91%)	74 (100%)	0	100	100
27	AB	80/81 (99%)	77 (96%)	3 (4%)	28	50
28	AM	119/121 (98%)	116 (98%)	3 (2%)	42	62
29	D3	103/103 (100%)	102 (99%)	1 (1%)	73	81
30	D1	278/278 (100%)	275 (99%)	3 (1%)	70	79
31	D6	144/144 (100%)	142 (99%)	2 (1%)	62	75
32	4L	87/87 (100%)	85 (98%)	2 (2%)	45	64
33	D5	539/539 (100%)	532 (99%)	7 (1%)	65	76
34	D4	412/412 (100%)	406 (98%)	6 (2%)	60	74
35	D2	315/315 (100%)	309 (98%)	6 (2%)	52	69
36	AK	101/101 (100%)	100 (99%)	1 (1%)	73	81
37	B5	122/125 (98%)	121 (99%)	1 (1%)	79	84
38	A8	154/154 (100%)	150 (97%)	4 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BJ	155/157 (99%)	155 (100%)	0	100	100
40	AJ	283/284 (100%)	281 (99%)	2 (1%)	81	86
41	S5	88/94 (94%)	88 (100%)	0	100	100
42	A3	65/71 (92%)	65 (100%)	0	100	100
43	B3	55/75 (73%)	53 (96%)	2 (4%)	30	52
44	C2	106/107 (99%)	106 (100%)	0	100	100
45	B4	114/114 (100%)	113 (99%)	1 (1%)	75	83
46	B6	91/121 (75%)	90 (99%)	1 (1%)	70	79
47	B7	108/108 (100%)	104 (96%)	4 (4%)	29	51
48	B9	159/160 (99%)	156 (98%)	3 (2%)	52	69
49	B2	58/62 (94%)	58 (100%)	0	100	100
50	B8	142/142 (100%)	139 (98%)	3 (2%)	48	66
51	BK	93/112 (83%)	91 (98%)	2 (2%)	47	65
52	C1	42/44 (96%)	42 (100%)	0	100	100
53	B1	48/53 (91%)	48 (100%)	0	100	100
54	A1	59/59 (100%)	56 (95%)	3 (5%)	20	44
All	All	10431/10814 (96%)	10309 (99%)	122 (1%)	66	78

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	A2	33	ARG
47	B7	105	ARG
32	4L	58	MET
47	B7	103	ARG
51	BK	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
39	BJ	103	ASN
40	AJ	97	GLN
47	B7	75	ASN
7	q2	23	GLN
5	f2	179	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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	$\#\|Z\| > 2$
57	FES	f1	501	5	0,4,4	-	-	-		
58	SF4	S7	300	16	0,12,12	-	-	-		
57	FES	S1	803	13	0,4,4	-	-	-		
64	PC1	AK	201	-	27,27,53	0.40	0	33,35,61	0.38	0
56	HEC	c1	501	4	32,50,50	1.90	4 (12%)	24,82,82	2.73	14 (58%)
56	HEC	c2	501	4	32,50,50	2.12	4 (12%)	24,82,82	2.44	13 (54%)
58	SF4	S1	802	13	0,12,12	-	-	-		
57	FES	V2	300	12	0,4,4	-	-	-		
58	SF4	S8	202	17	0,12,12	-	-	-		
55	HEM	b1	402	3	41,50,50	1.33	4 (9%)	45,82,82	1.82	8 (17%)
55	HEM	b1	401	3	41,50,50	1.31	4 (9%)	45,82,82	1.82	11 (24%)
60	3PE	D5	701	-	37,37,50	0.35	0	40,42,55	0.30	0
58	SF4	V1	500	11	0,12,12	-	-	-		
58	SF4	S1	801	13	0,12,12	-	-	-		
58	SF4	S8	201	17	0,12,12	-	-	-		
60	3PE	S2	501	-	39,39,50	0.34	0	42,44,55	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
63	ZMP	AA	101	27	27,33,36	0.70	1 (3%)	32,40,45	0.95	1 (3%)
59	FMN	V1	501	-	33,33,33	0.24	0	48,50,50	0.42	0
63	ZMP	AB	101	27	24,30,36	0.69	0	29,37,45	1.01	2 (6%)
55	HEM	b2	402	3	41,50,50	1.38	5 (12%)	45,82,82	1.85	10 (22%)
55	HEM	b2	401	3	41,50,50	1.27	4 (9%)	45,82,82	1.81	11 (24%)
57	FES	f2	501	5	0,4,4	-	-	-		
62	NDP	A9	401	-	45,52,52	0.60	0	53,80,80	0.64	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	FES	f1	501	5	-	-	0/1/1/1
58	SF4	S7	300	16	-	-	0/6/5/5
57	FES	S1	803	13	-	-	0/1/1/1
64	PC1	AK	201	-	-	6/31/31/57	-
56	HEC	c1	501	4	-	4/10/54/54	-
56	HEC	c2	501	4	-	0/10/54/54	-
58	SF4	S1	802	13	-	-	0/6/5/5
57	FES	V2	300	12	-	-	0/1/1/1
58	SF4	S8	202	17	-	-	0/6/5/5
55	HEM	b1	402	3	-	5/12/54/54	-
55	HEM	b1	401	3	-	5/12/54/54	-
60	3PE	D5	701	-	-	16/41/41/54	-
58	SF4	V1	500	11	-	-	0/6/5/5
60	3PE	S2	501	-	-	8/43/43/54	-
58	SF4	S1	801	13	-	-	0/6/5/5
58	SF4	S8	201	17	-	-	0/6/5/5
63	ZMP	AA	101	27	-	12/38/40/43	-
59	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
63	ZMP	AB	101	27	-	11/35/37/43	-
55	HEM	b2	402	3	-	7/12/54/54	-
55	HEM	b2	401	3	-	3/12/54/54	-
57	FES	f2	501	5	-	-	0/1/1/1
62	NDP	A9	401	-	-	12/30/77/77	0/5/5/5

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	c2	501	HEC	C3C-C2C	-6.89	1.33	1.40
56	c2	501	HEC	C2B-C3B	-6.69	1.33	1.40
56	c1	501	HEC	C3C-C2C	-5.98	1.34	1.40
56	c1	501	HEC	C2B-C3B	-5.41	1.35	1.40
55	b2	402	HEM	C4D-ND	-4.07	1.33	1.40

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	c1	501	HEC	CMB-C2B-C3B	5.54	132.33	125.82
55	b2	402	HEM	CHC-C4B-NB	5.29	130.18	124.43
55	b1	402	HEM	CHC-C4B-NB	5.17	130.05	124.43
56	c1	501	HEC	CMB-C2B-C1B	-5.10	120.63	128.46
55	b1	401	HEM	CHC-C4B-NB	4.99	129.85	124.43

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	b1	401	HEM	C2B-C3B-CAB-CBB
55	b1	401	HEM	C4B-C3B-CAB-CBB
55	b1	402	HEM	C2B-C3B-CAB-CBB
55	b1	402	HEM	C4B-C3B-CAB-CBB
55	b2	401	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

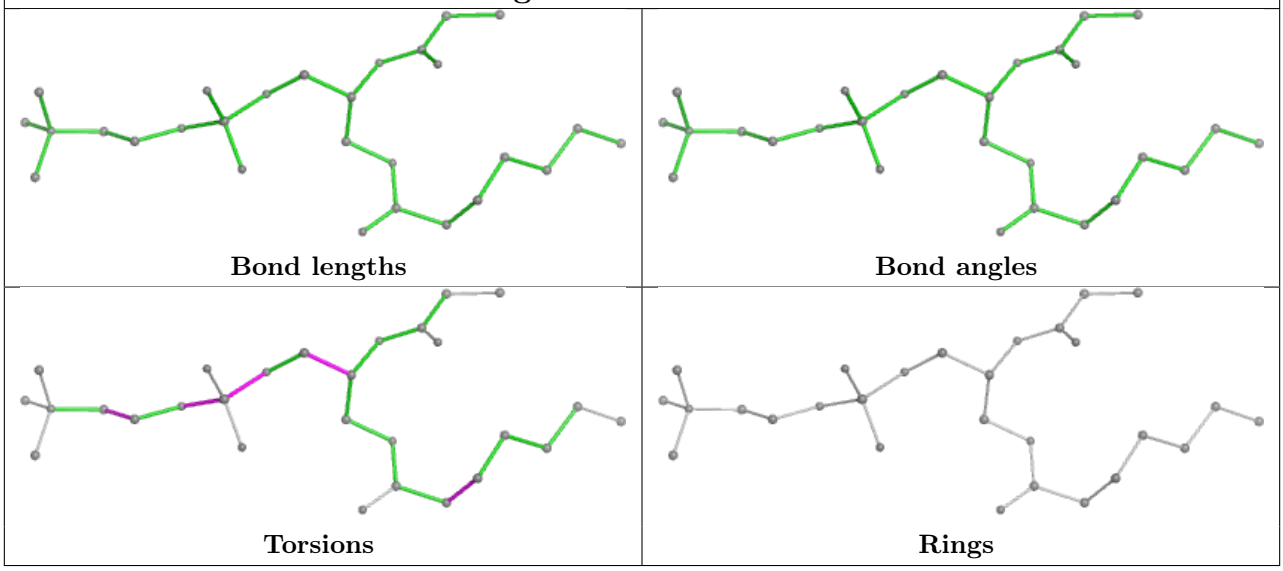
8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	AK	201	PC1	1	0
57	V2	300	FES	1	0
60	D5	701	3PE	1	0
58	S1	801	SF4	1	0
60	S2	501	3PE	3	0
63	AA	101	ZMP	1	0
63	AB	101	ZMP	4	0
62	A9	401	NDP	5	0

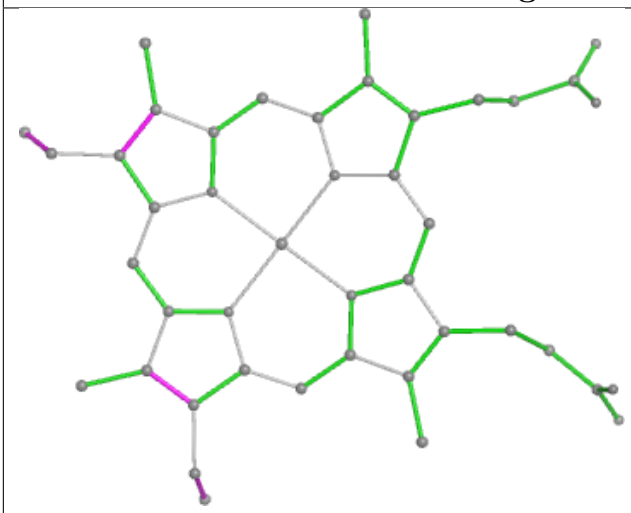
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

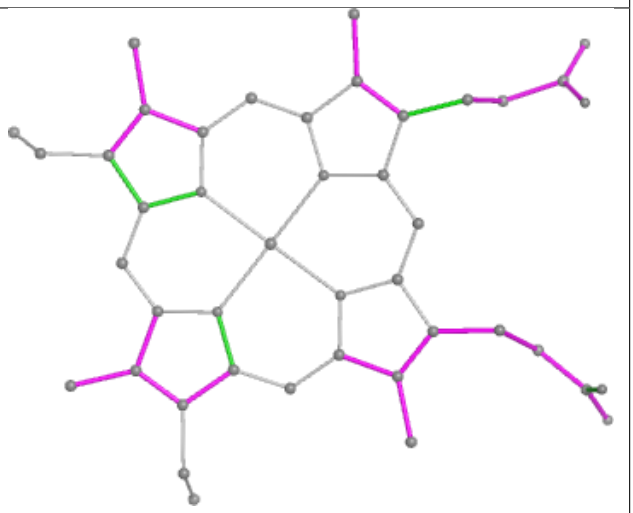
Ligand PC1 AK 201



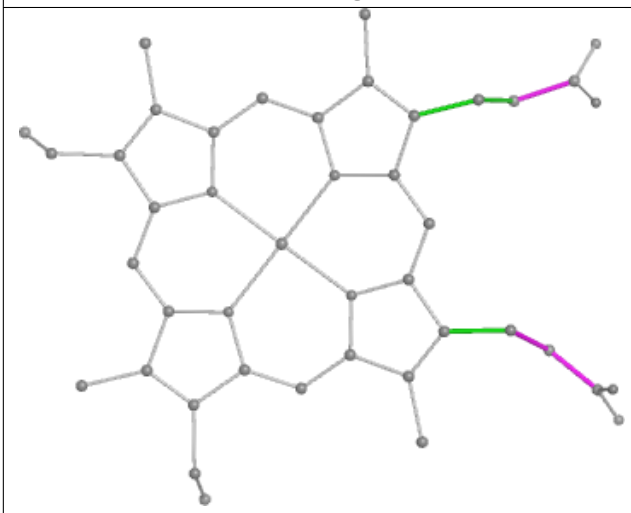
Ligand HEC c1 501



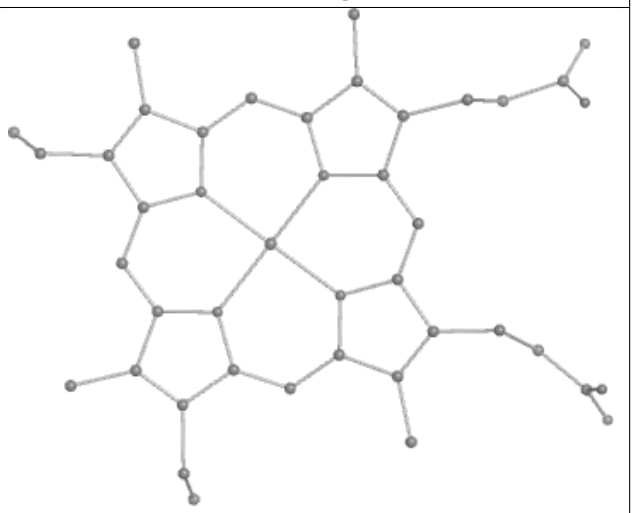
Bond lengths



Bond angles

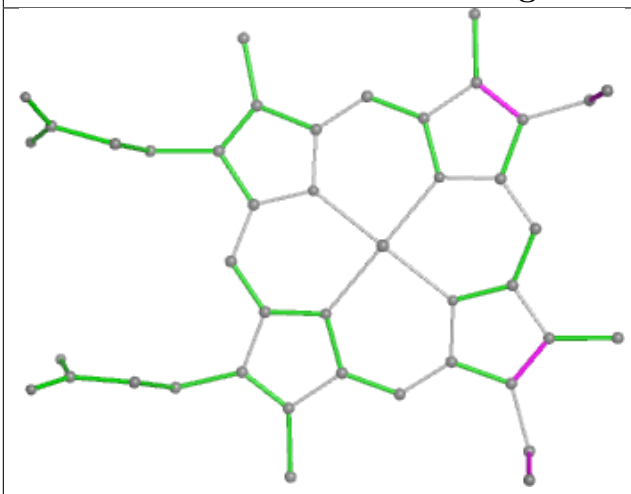


Torsions

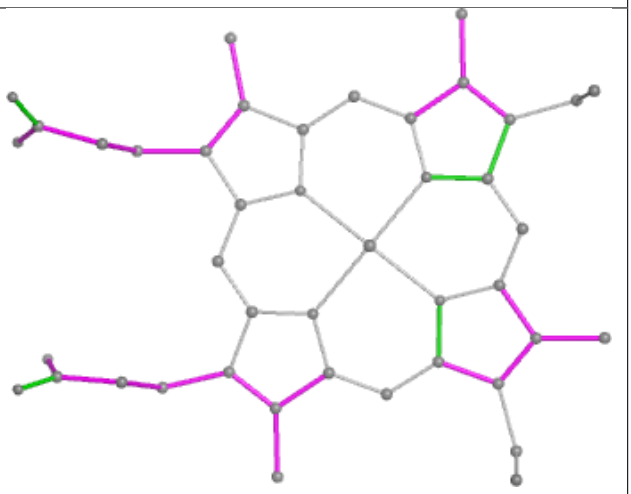


Rings

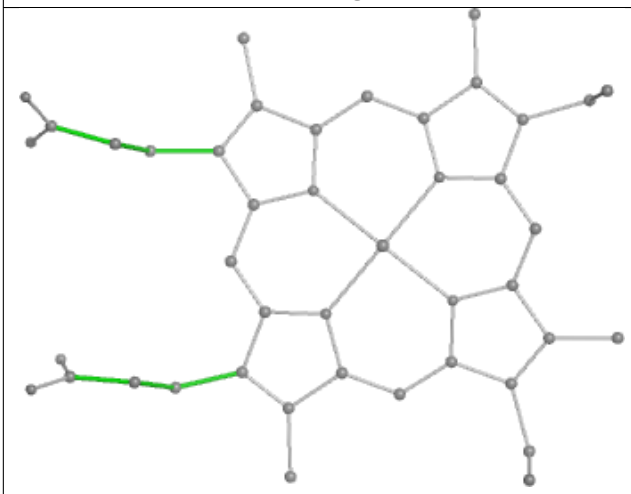
Ligand HEC c2 501



Bond lengths



Bond angles



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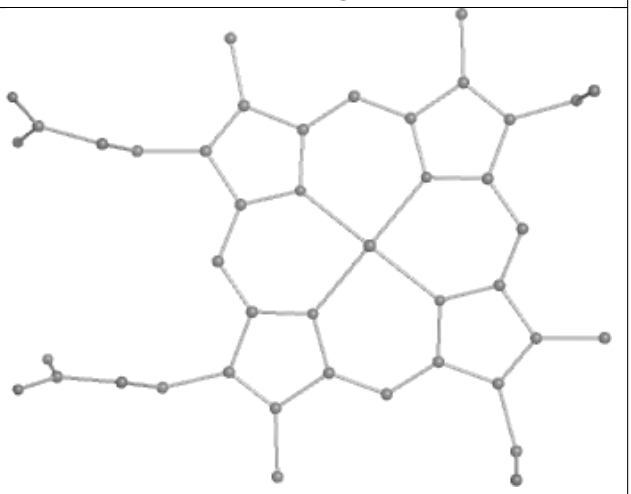
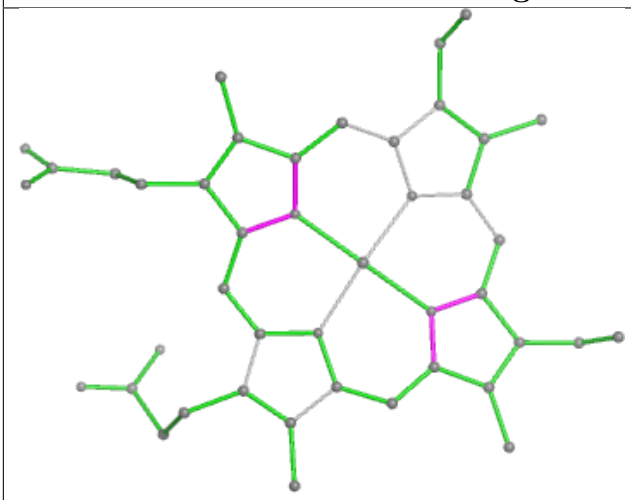
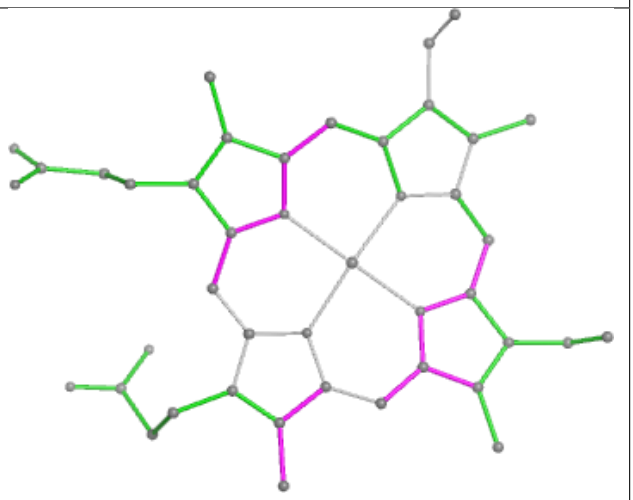


Rings

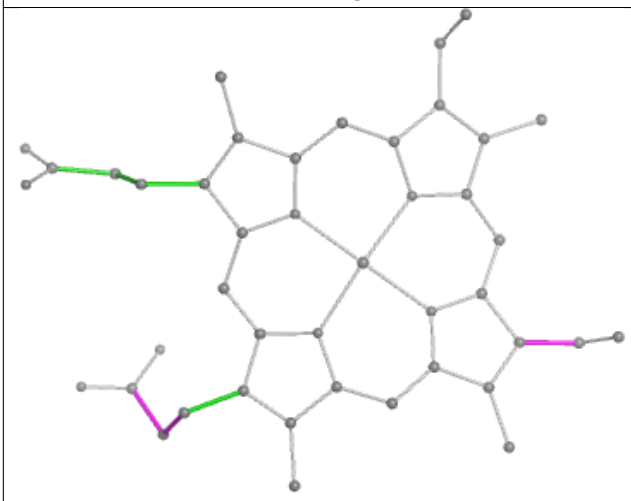
Ligand HEM b1 402



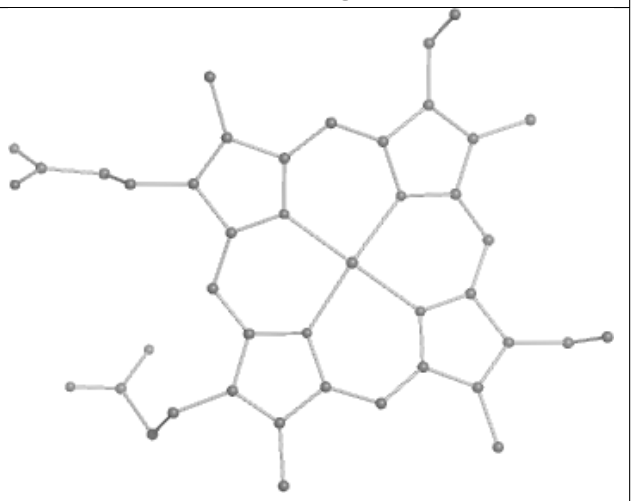
Bond lengths



Bond angles

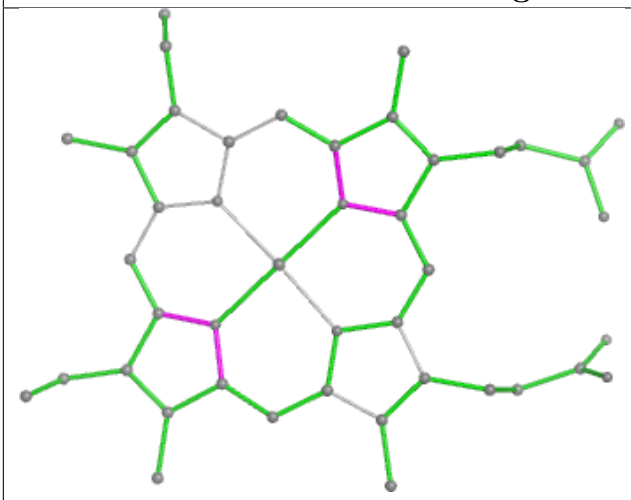


Torsions

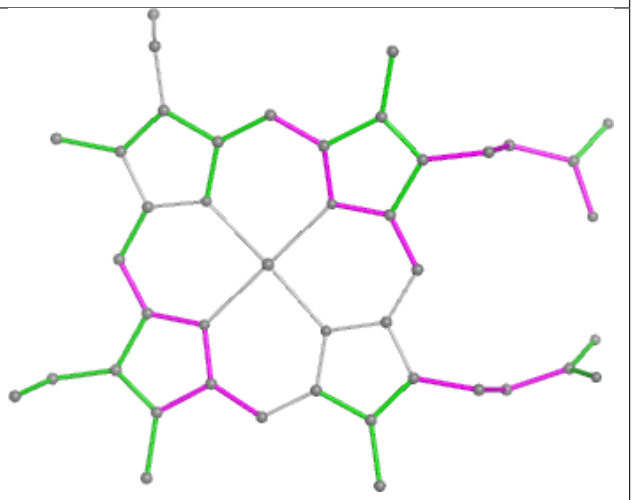


Rings

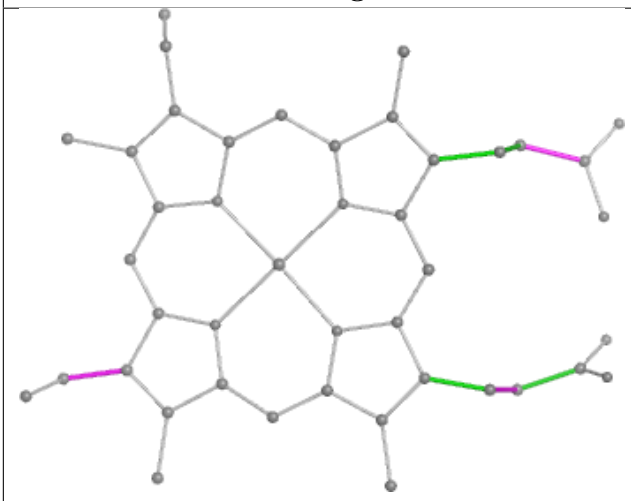
Ligand HEM b1 401



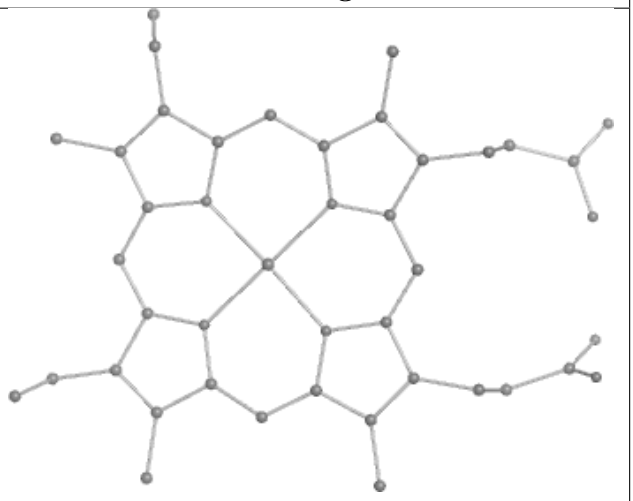
Bond lengths



Bond angles

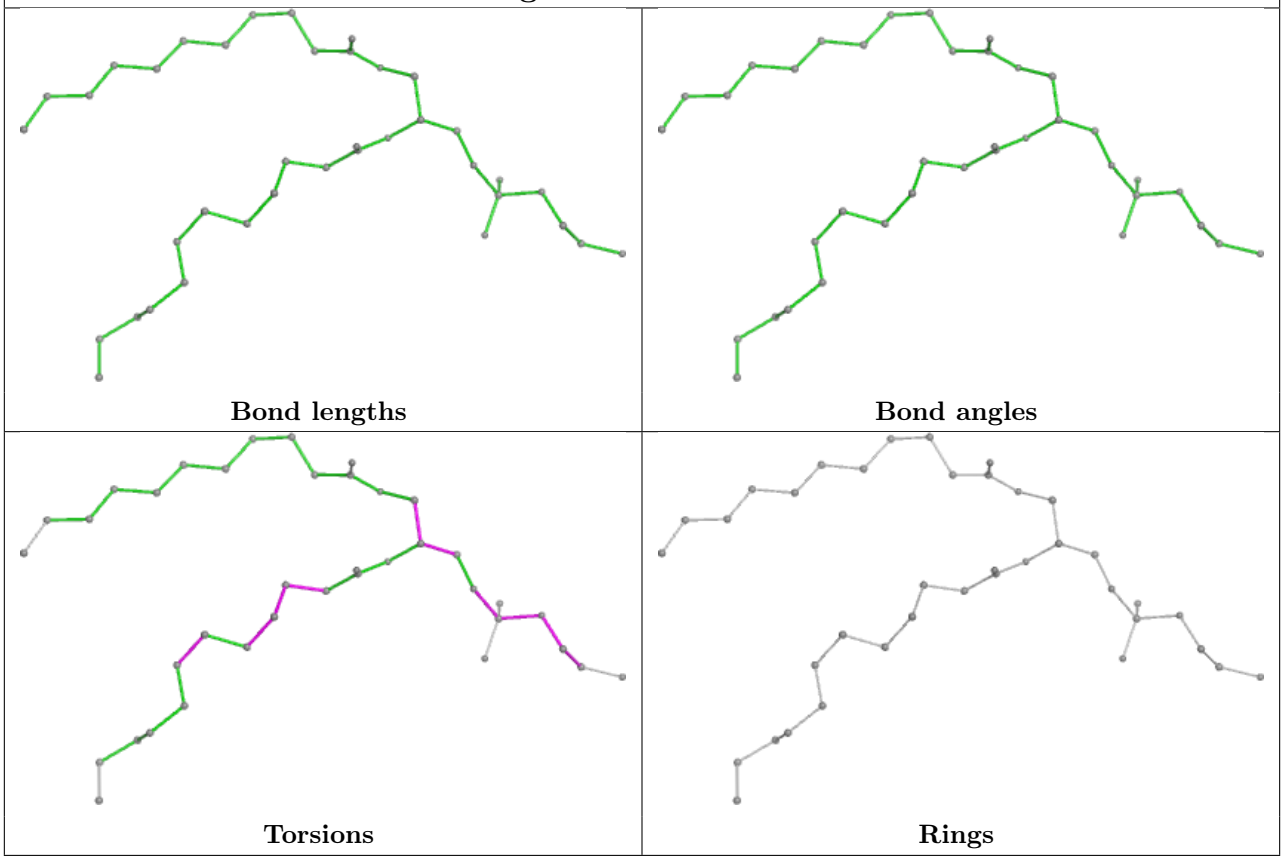


Torsions

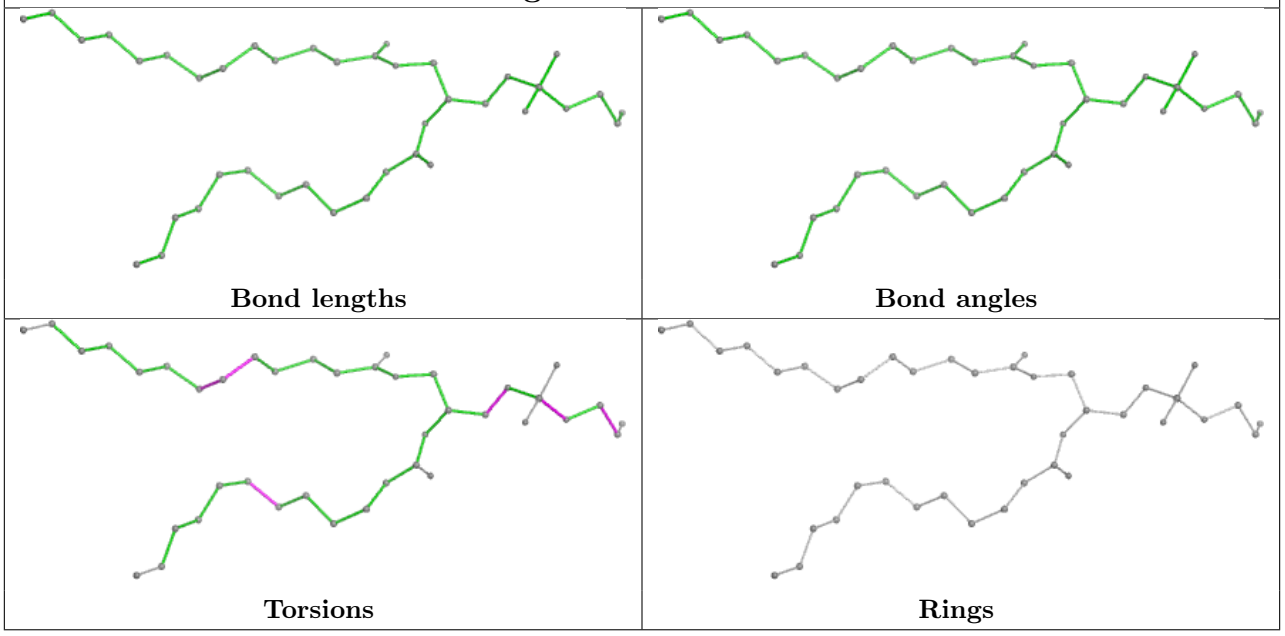


Rings

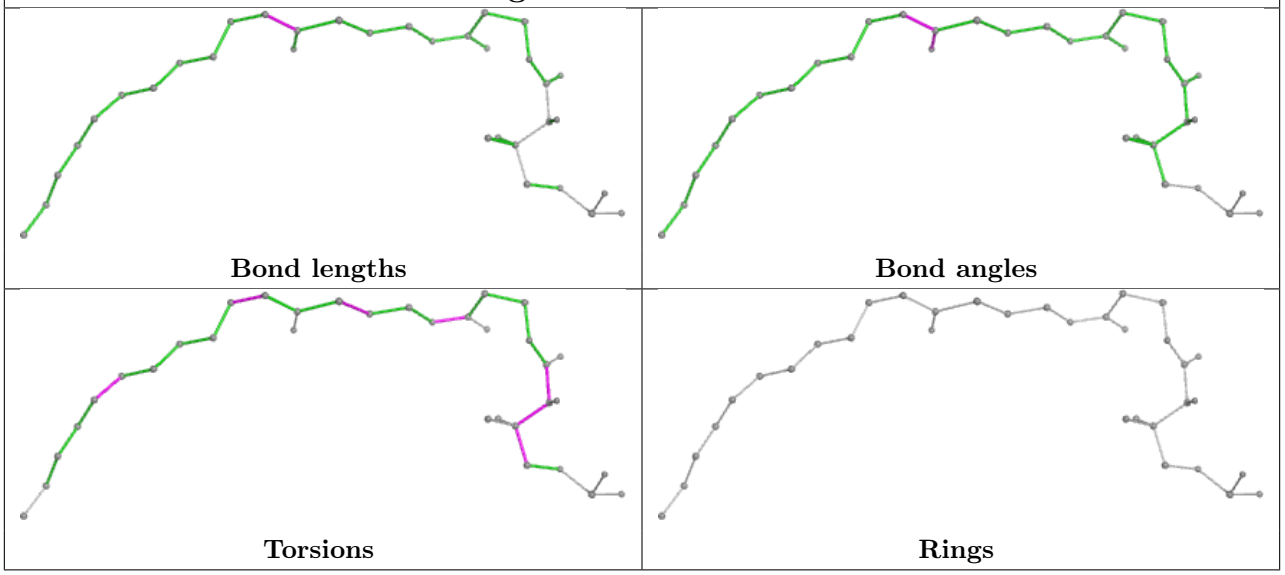
Ligand 3PE D5 701



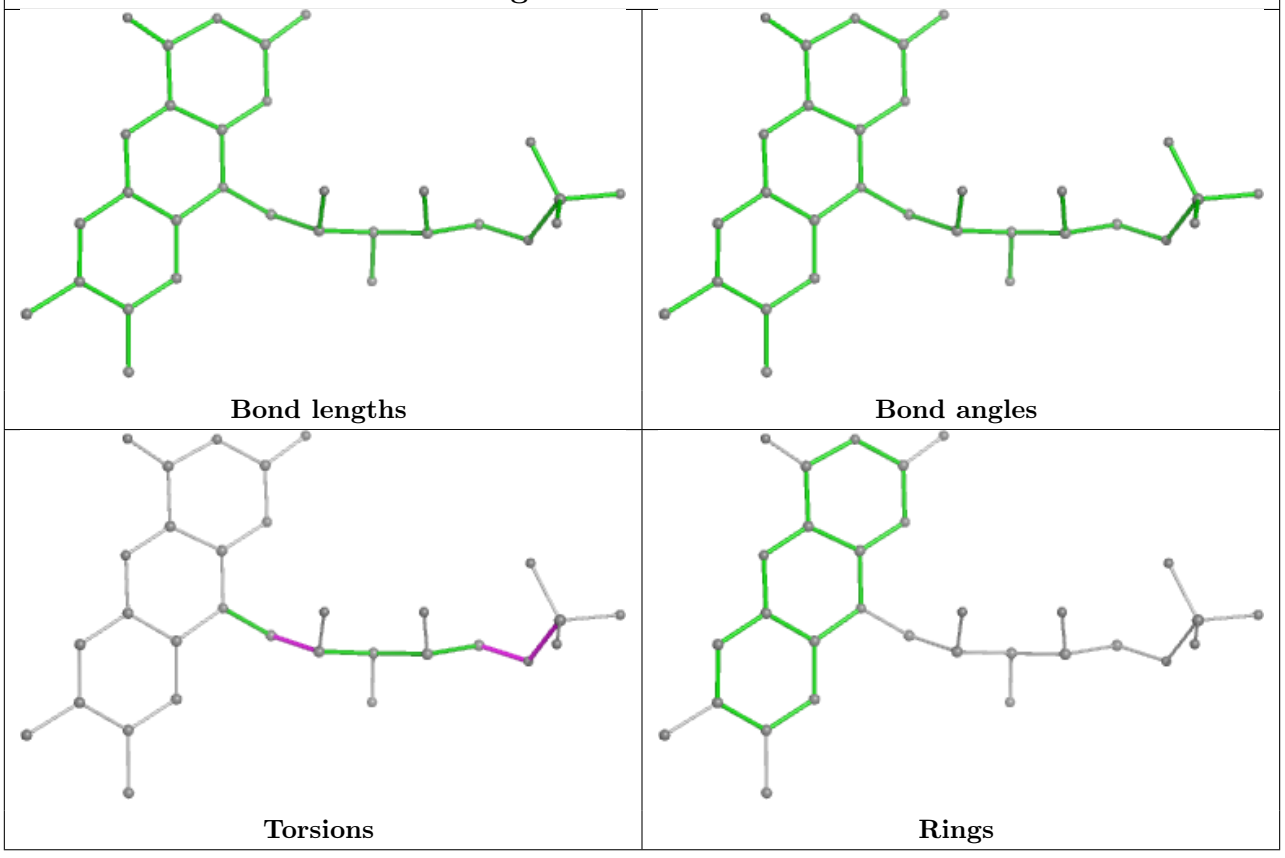
Ligand 3PE S2 501



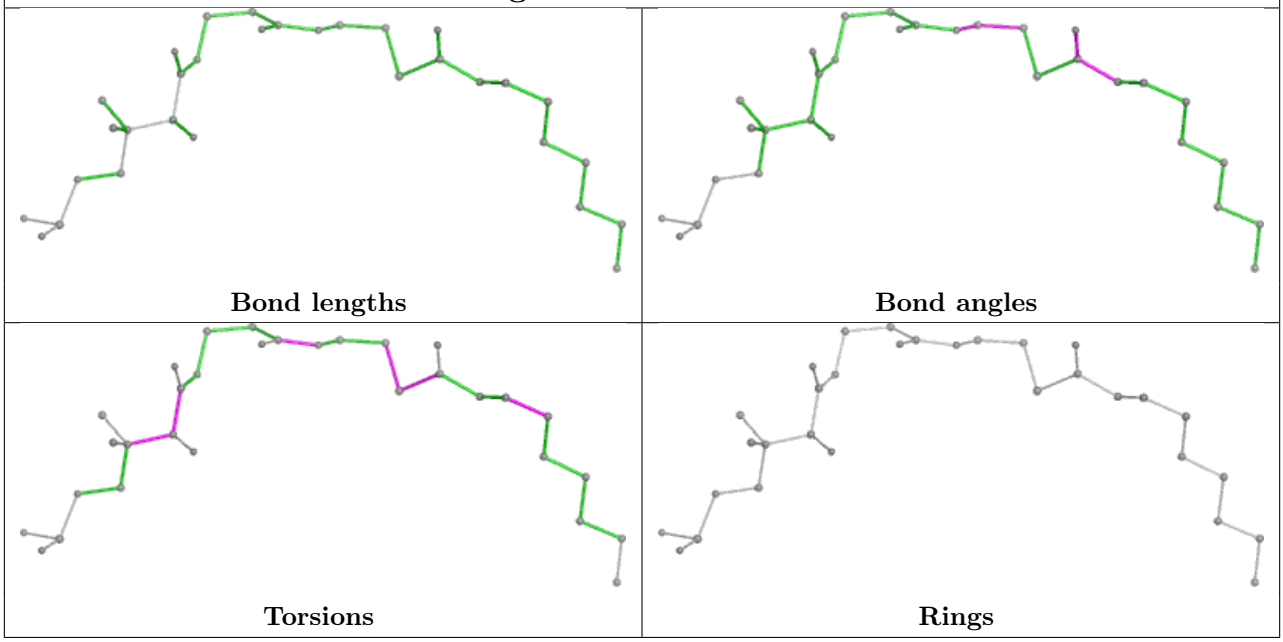
Ligand ZMP AA 101



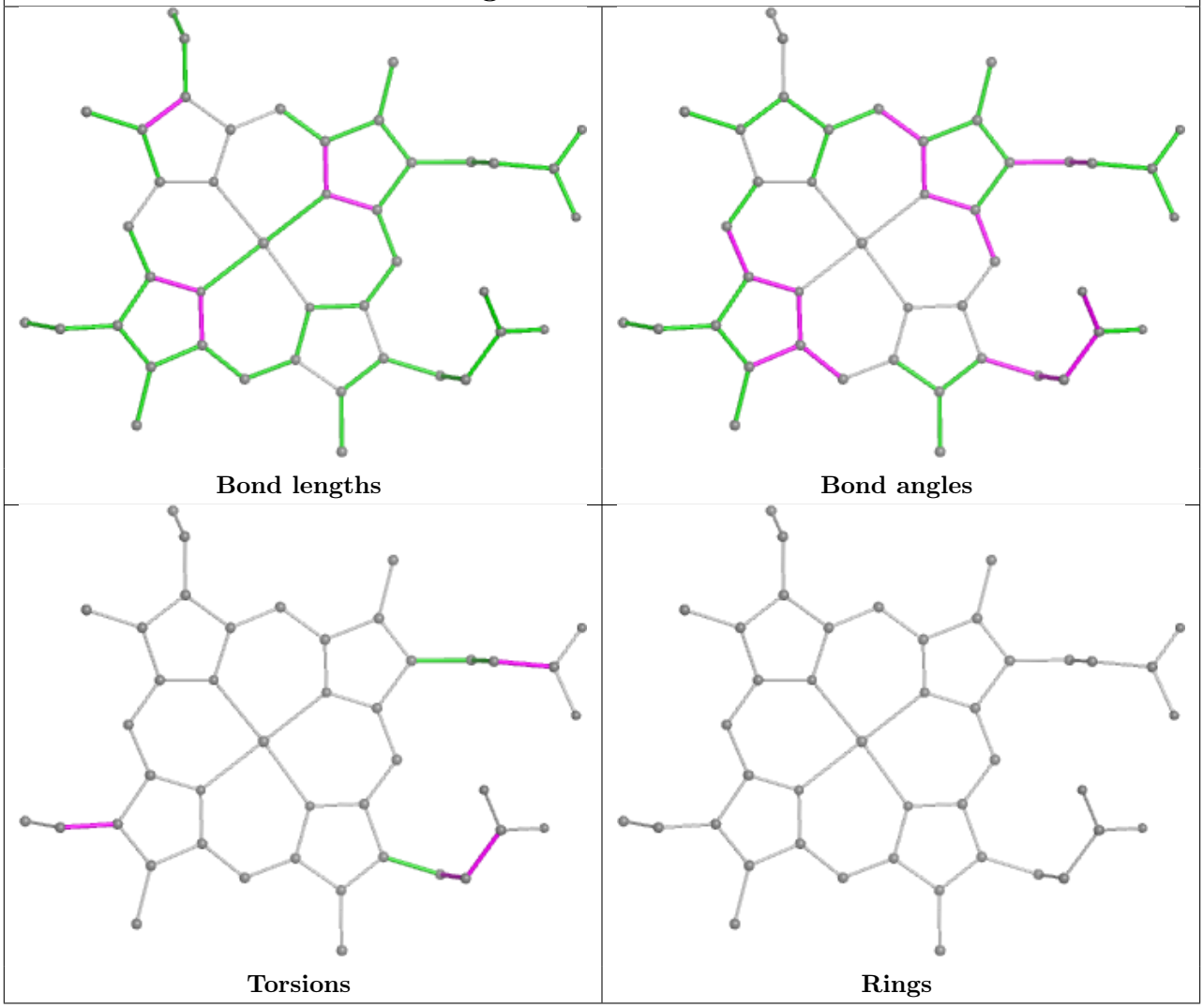
Ligand FMN V1 501



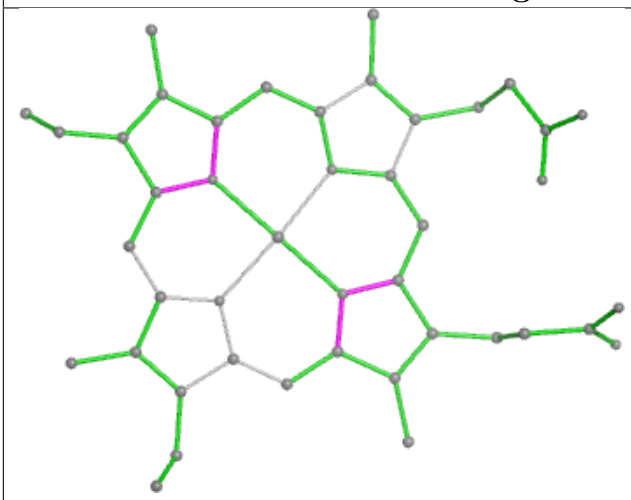
Ligand ZMP AB 101



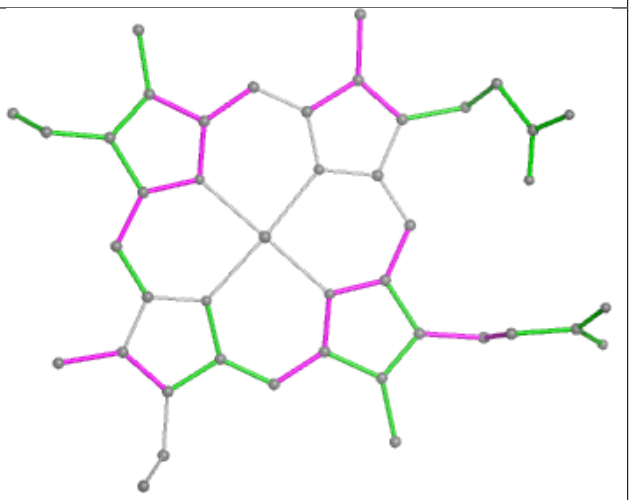
Ligand HEM b2 402



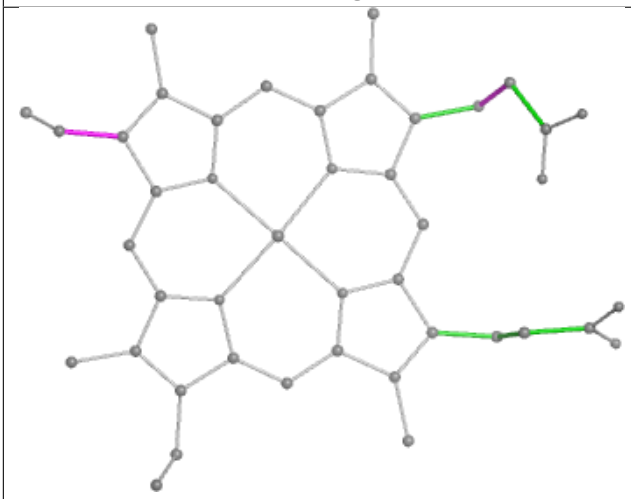
Ligand HEM b2 401



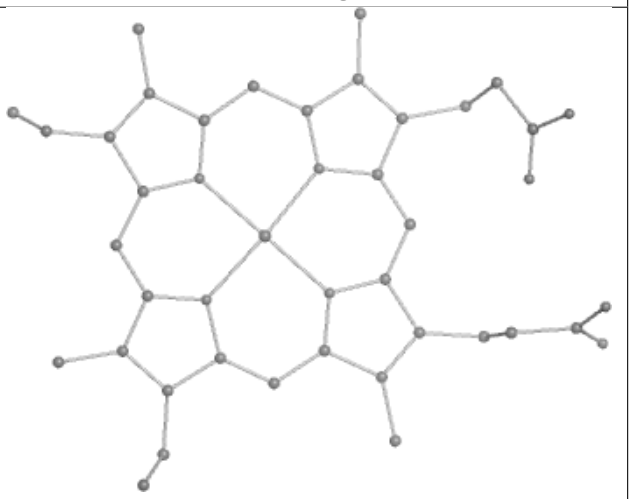
Bond lengths



Bond angles

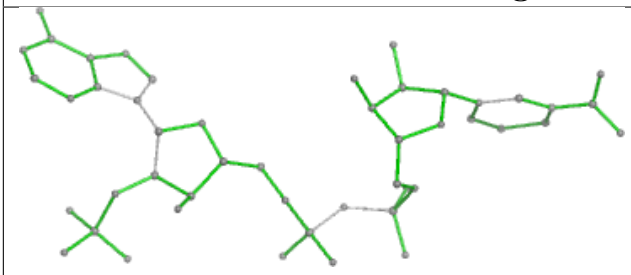


Torsions

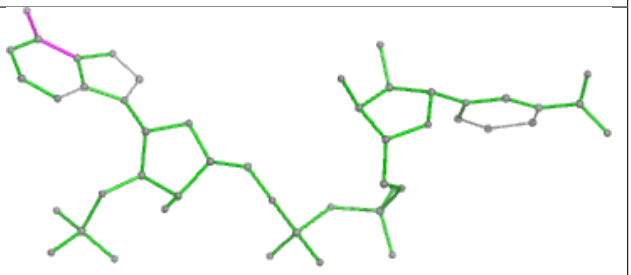


Rings

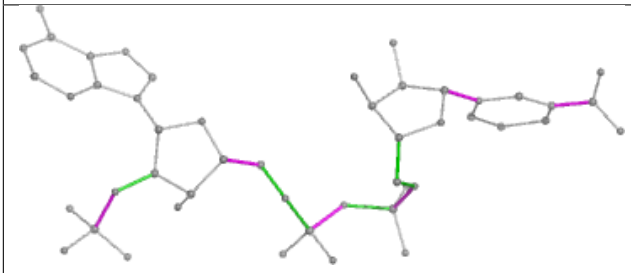
Ligand NDP A9 401



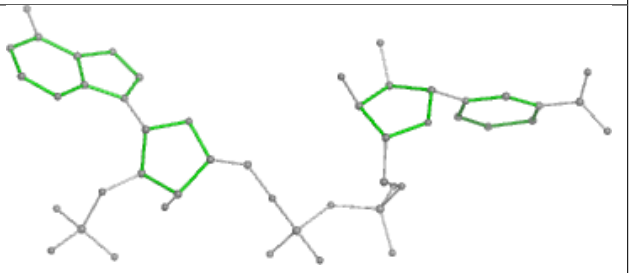
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

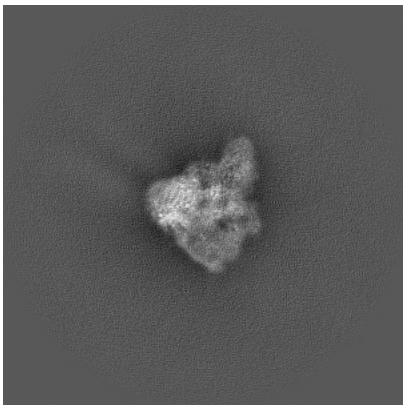
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4493. These allow visual inspection of the internal detail of the map and identification of artifacts.

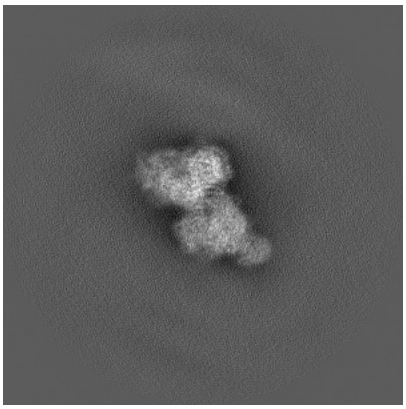
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

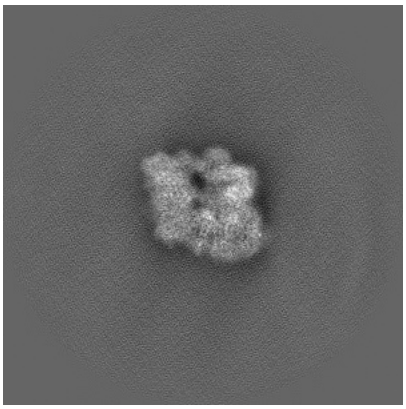
6.1.1 Primary map



X

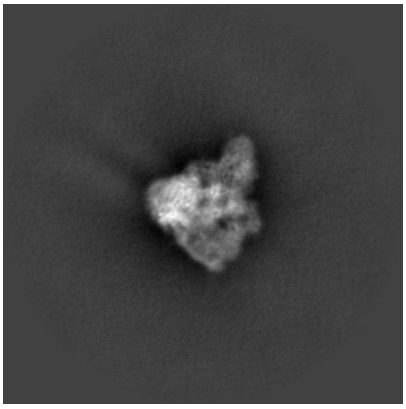


Y

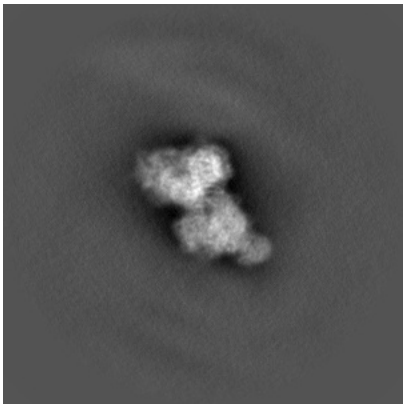


Z

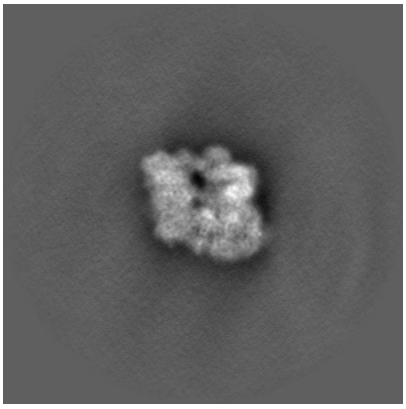
6.1.2 Raw map



X



Y

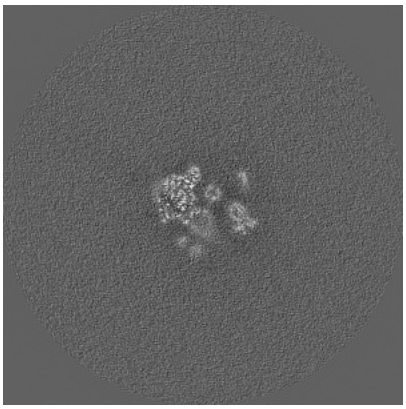


Z

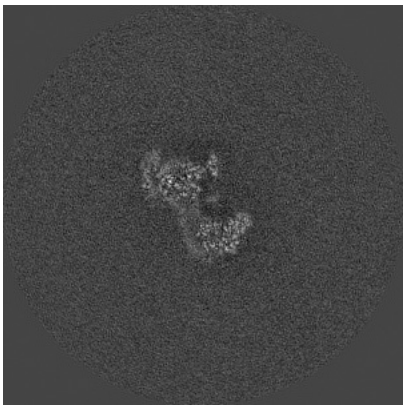
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

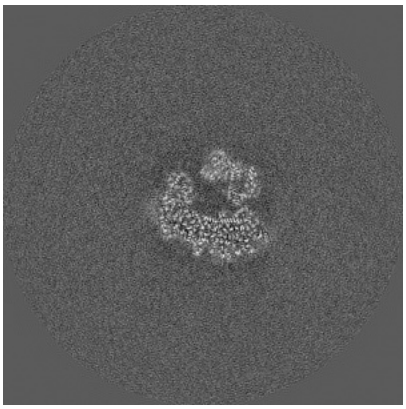
6.2.1 Primary map



X Index: 256

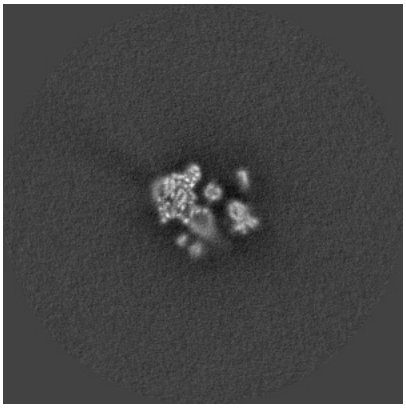


Y Index: 256

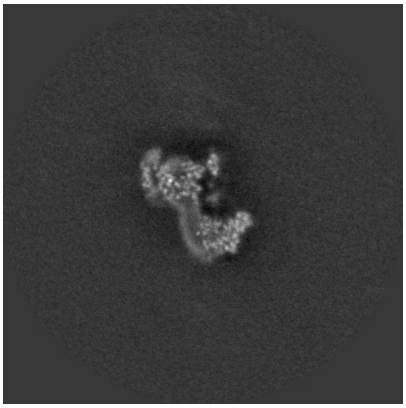


Z Index: 256

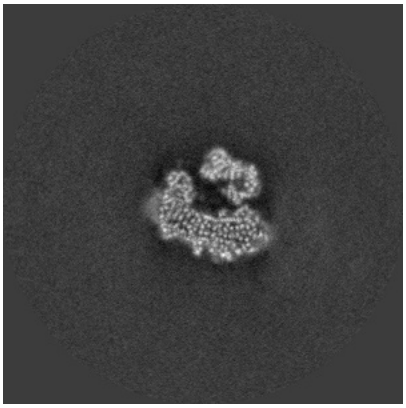
6.2.2 Raw map



X Index: 256



Y Index: 256

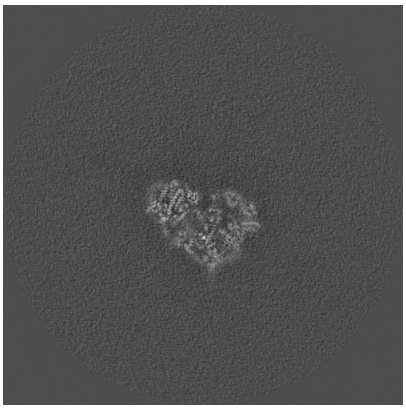


Z Index: 256

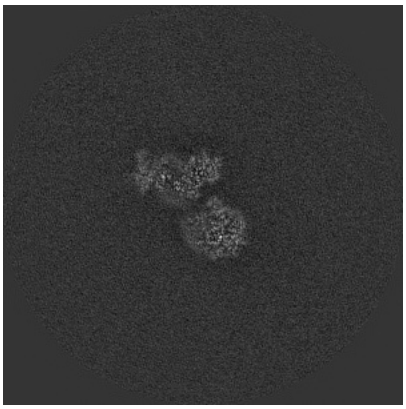
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

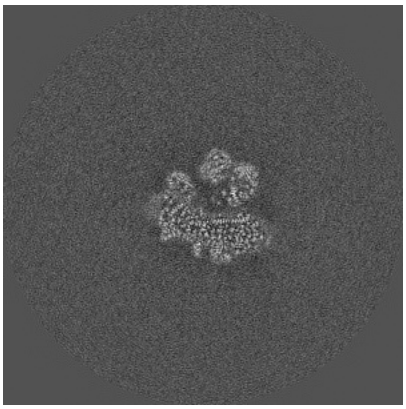
6.3.1 Primary map



X Index: 285

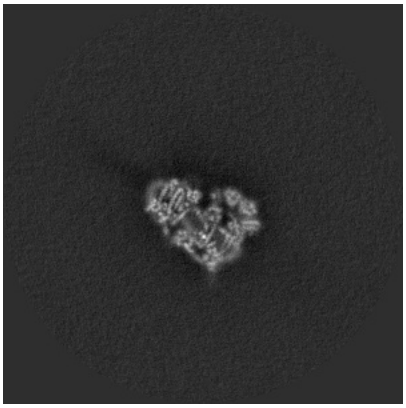


Y Index: 268

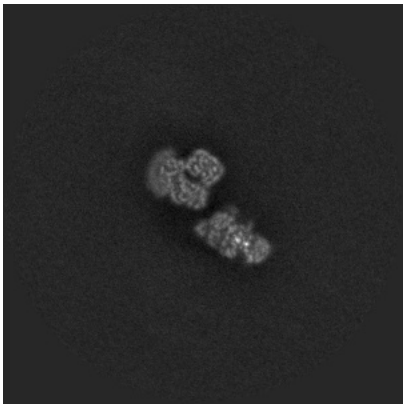


Z Index: 253

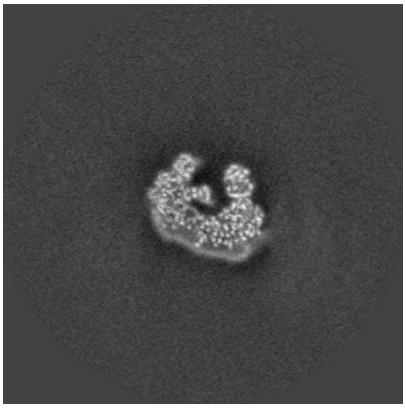
6.3.2 Raw map



X Index: 285



Y Index: 296

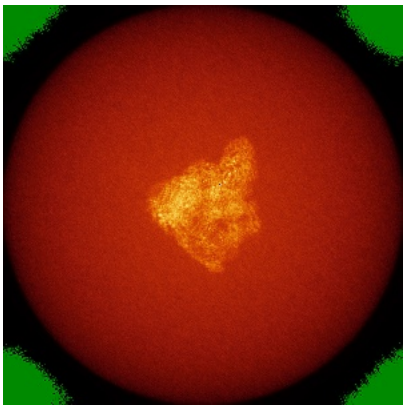


Z Index: 272

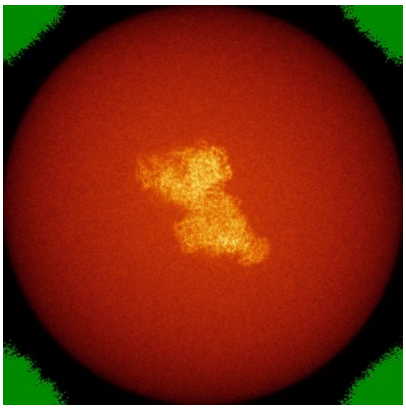
The images above show the largest variance slices of the map in three orthogonal directions.

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

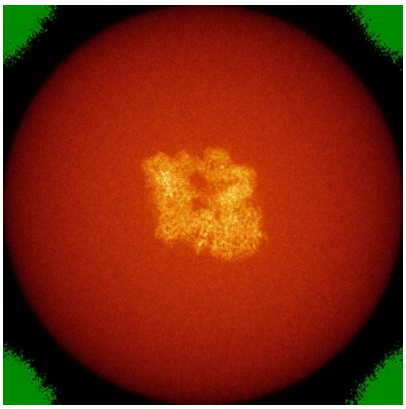
6.4.1 Primary map



X

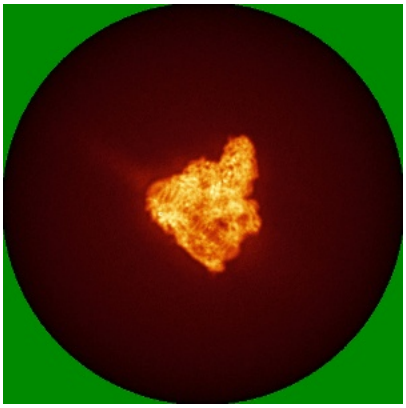


Y

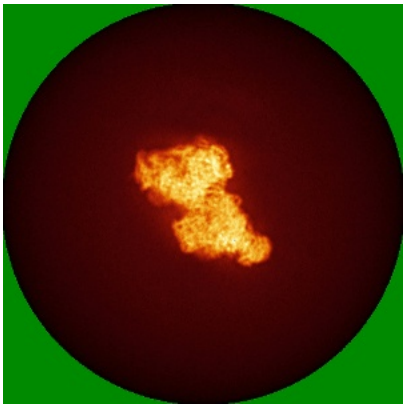


Z

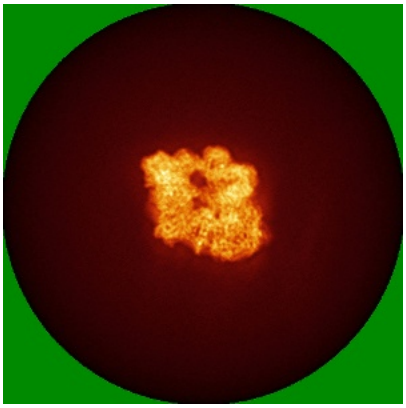
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

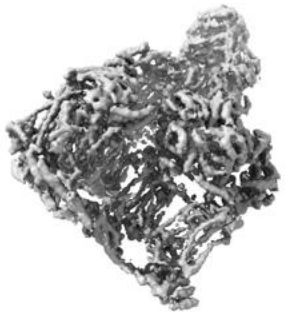
X

Y

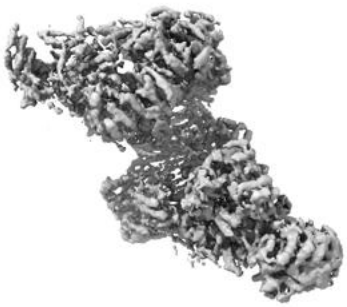
Z

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

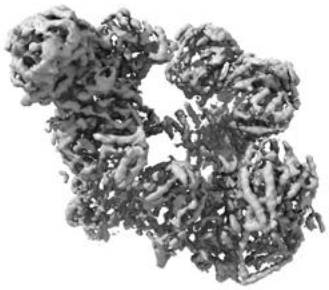
6.5.2 Raw map



X



Y



Z

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

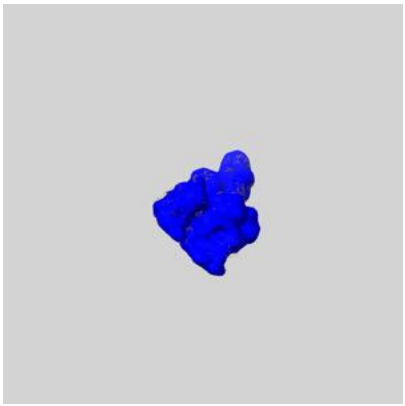
6.6 Mask visualisation (i)

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

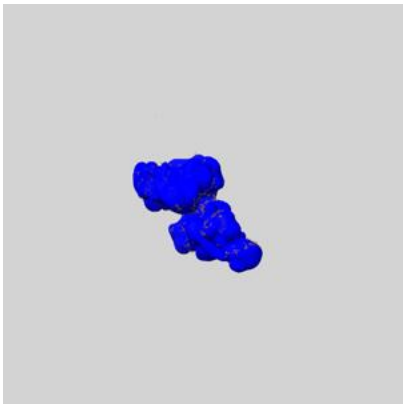
A mask typically either:

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

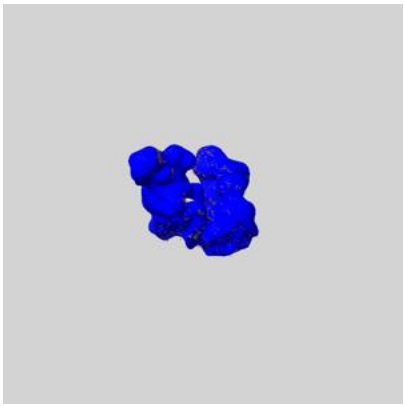
6.6.1 emd_4493_msk_1.map (i)



X



Y

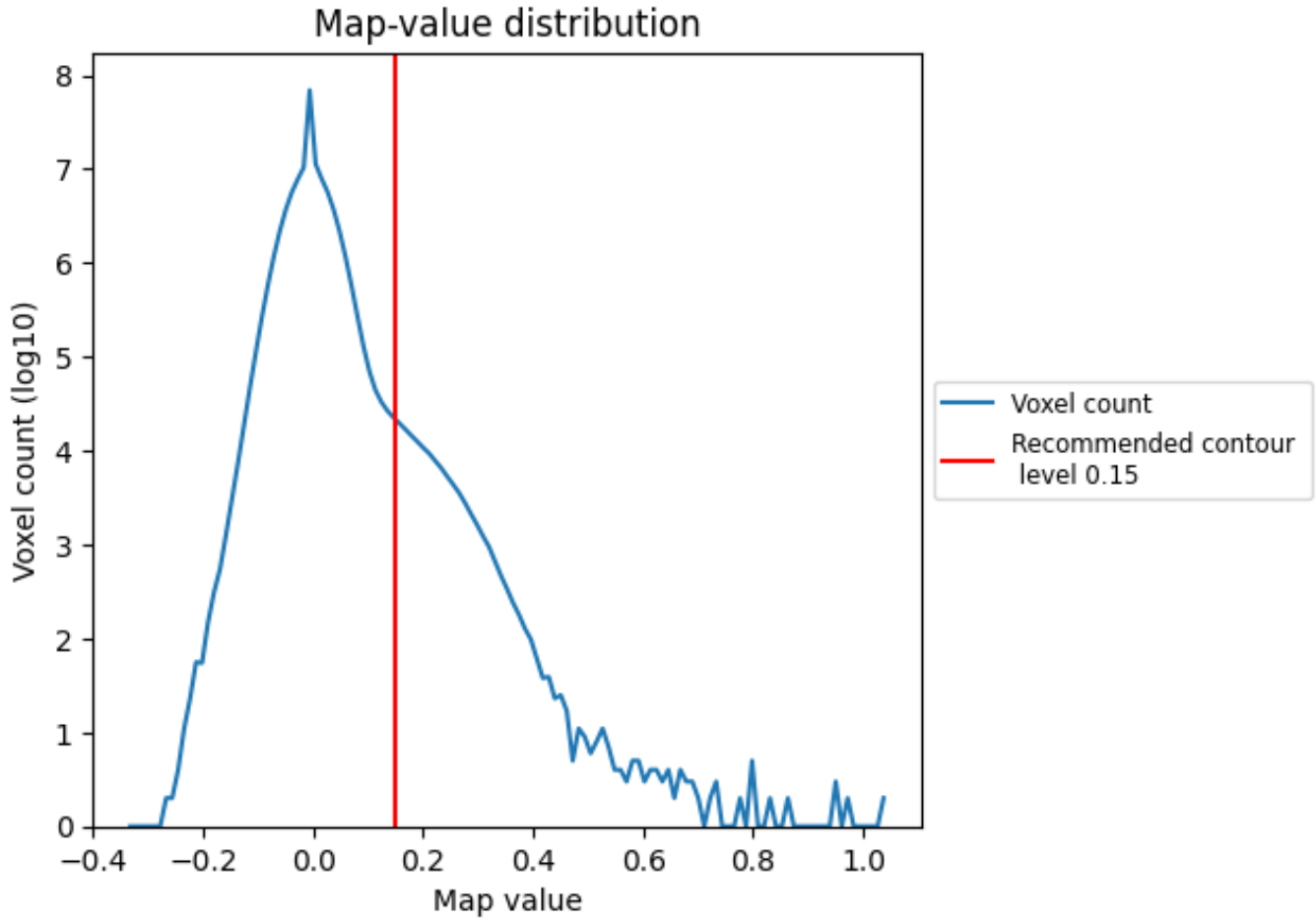


Z

7 Map analysis

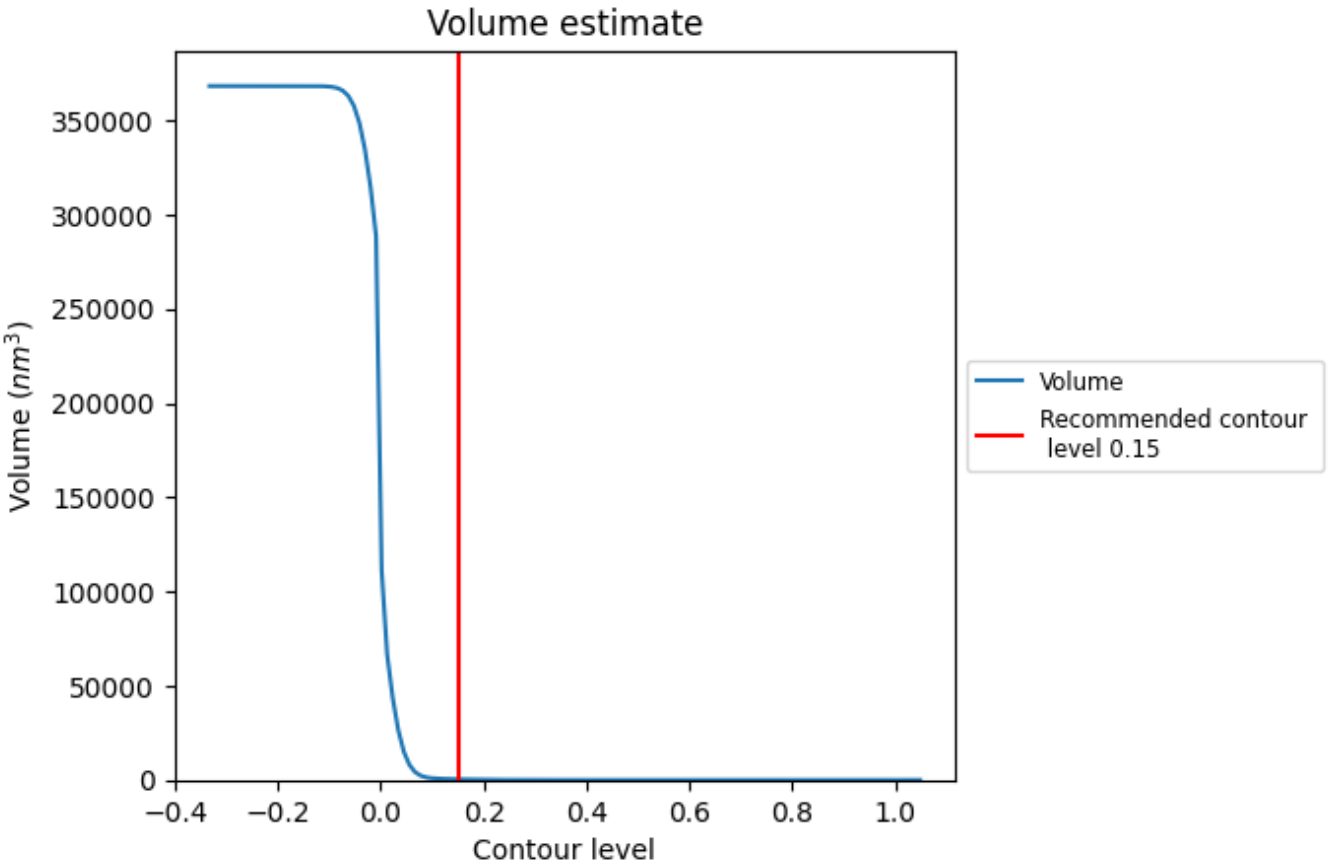
This section contains the results of statistical analysis of the map.

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.

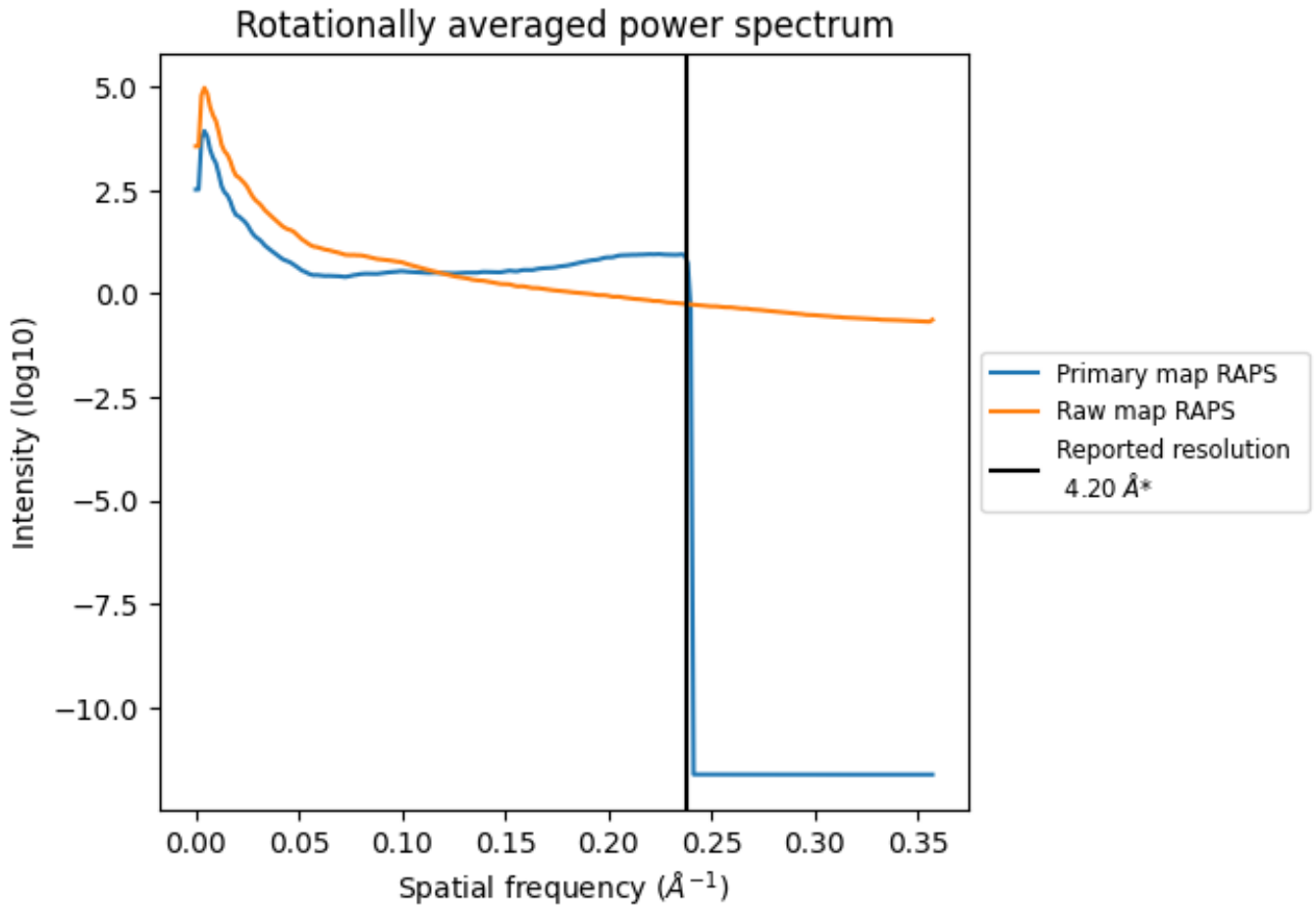
7.2 Volume estimate (i)



The volume at the recommended contour level is 376 nm^3; this corresponds to an approximate mass of 339 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)

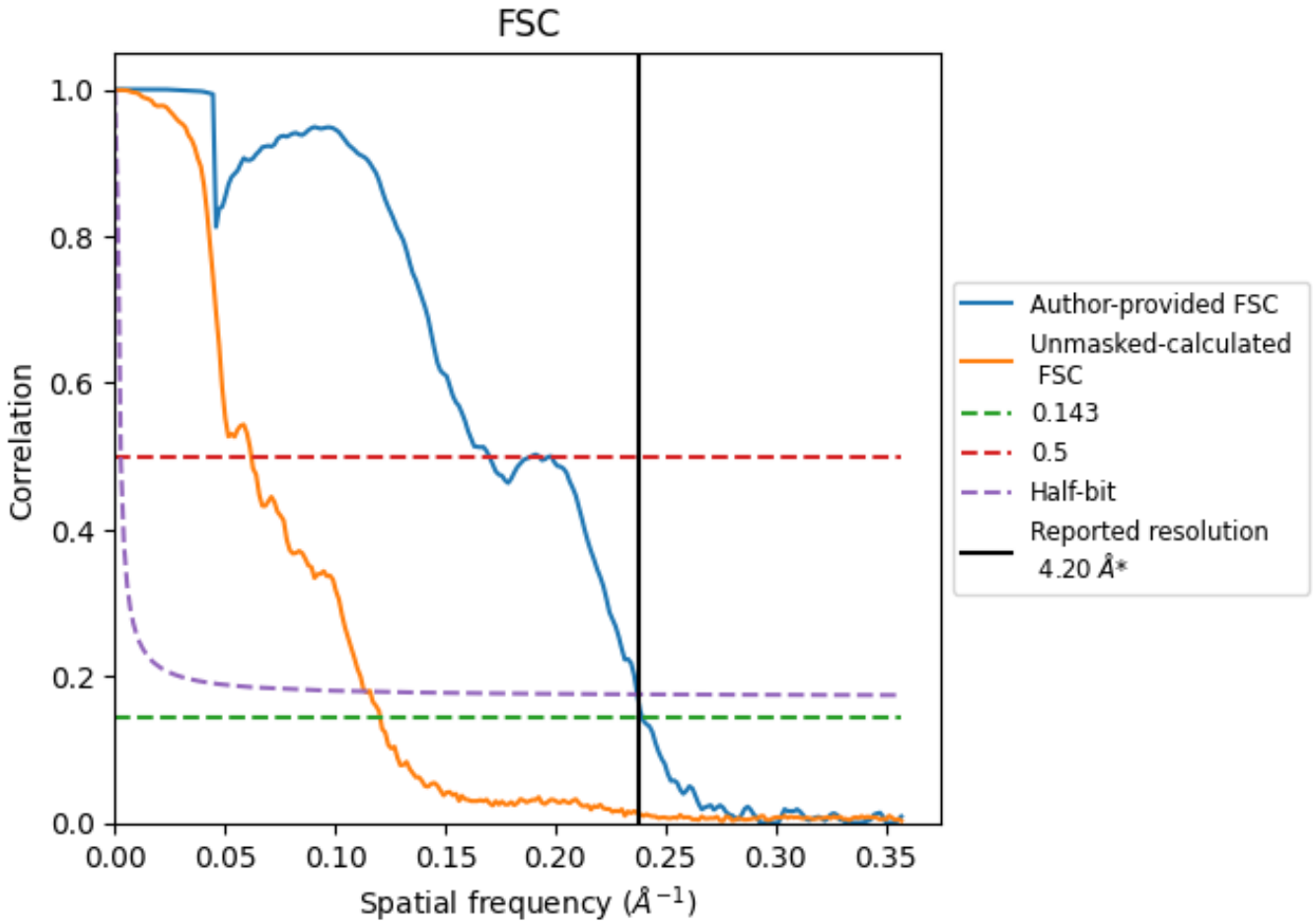


*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

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)

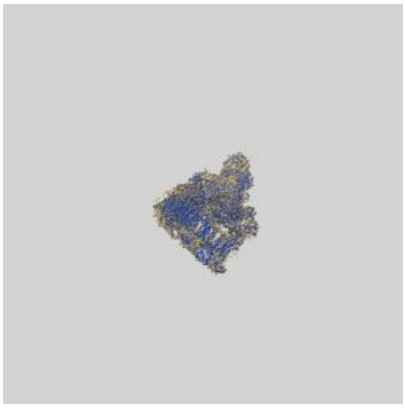
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	5.88	4.22
Unmasked-calculated*	8.30	16.13	8.78

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

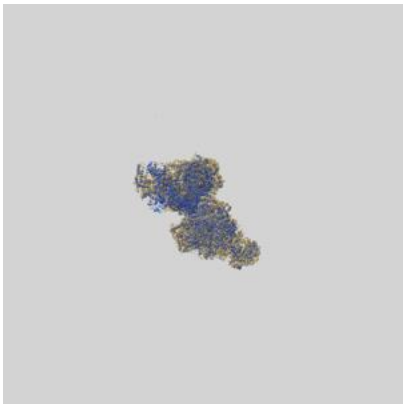
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4493 and PDB model 6QBX. Per-residue inclusion information can be found in section 3 on page 22.

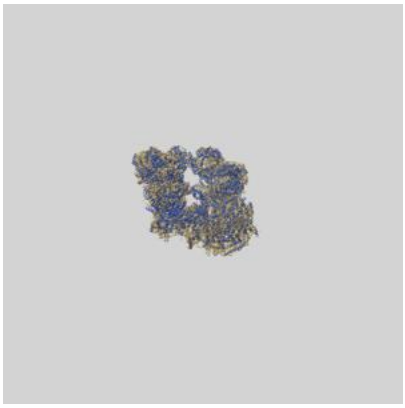
9.1 Map-model overlay



X



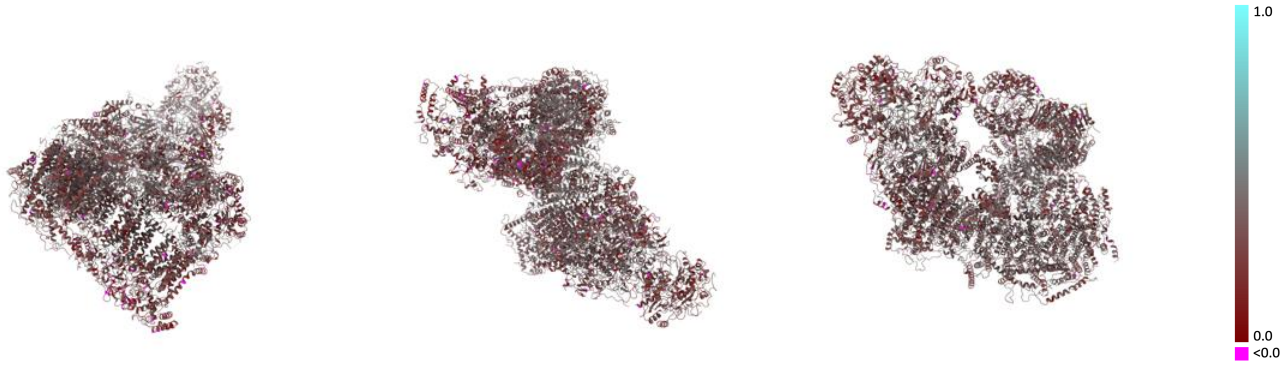
Y



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.

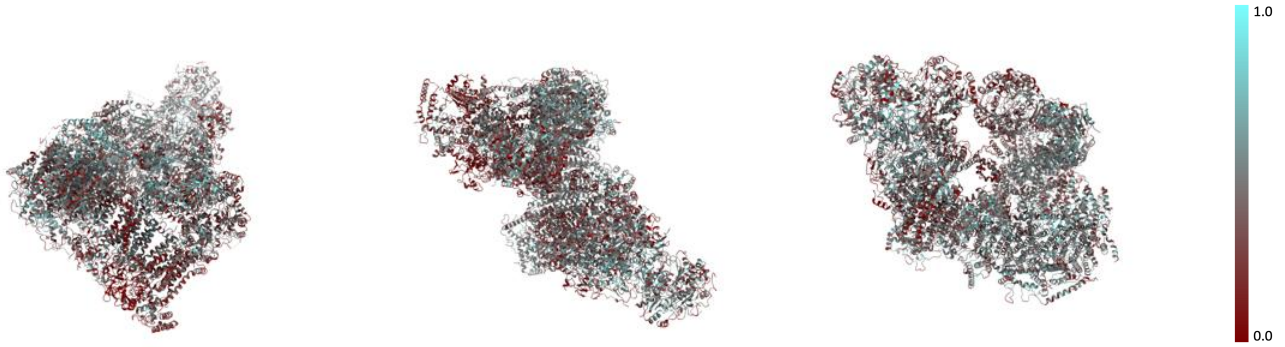
9.2 Q-score mapped to coordinate model (i)



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.

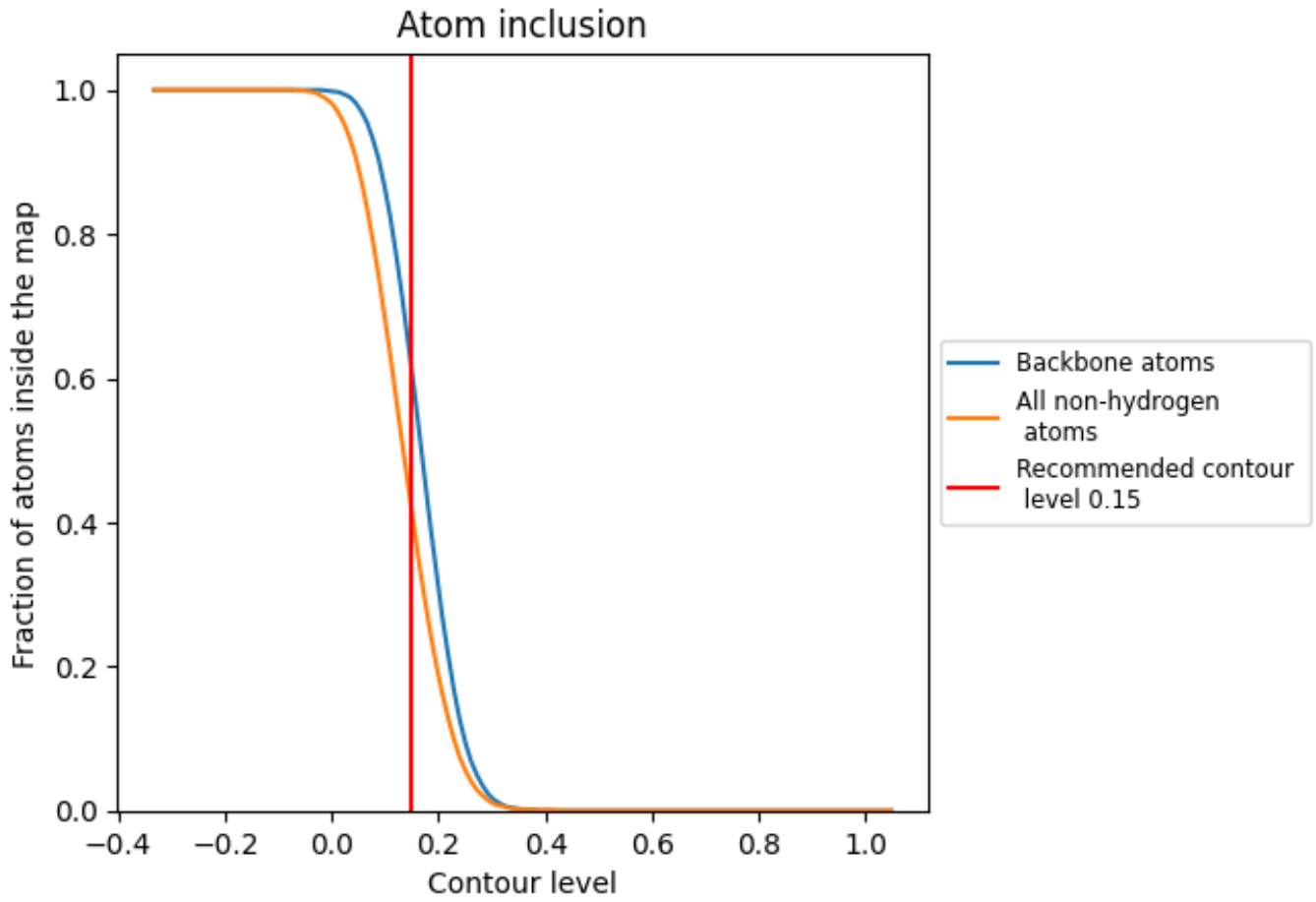
9.3 Atom inclusion mapped to coordinate model (i)



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, 61% of all backbone atoms, 42% 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	0.4150	0.3360
4L	0.3940	0.3590
A1	0.4710	0.3330
A2	0.3130	0.2780
A3	0.3460	0.3120
A5	0.3690	0.3210
A6	0.3800	0.3320
A7	0.2700	0.3190
A8	0.4650	0.3360
A9	0.3600	0.3290
AA	0.2200	0.3030
AB	0.4910	0.3530
AJ	0.4870	0.3520
AK	0.3740	0.3480
AL	0.2680	0.3110
AM	0.4490	0.3210
B1	0.3990	0.3530
B2	0.4180	0.3390
B3	0.4310	0.3280
B4	0.5210	0.3750
B5	0.5340	0.3630
B6	0.4670	0.3570
B7	0.4600	0.3100
B8	0.4700	0.3630
B9	0.5570	0.3660
BJ	0.5110	0.3510
BK	0.4740	0.3550
C1	0.4790	0.3430
C2	0.4760	0.3740
D1	0.3900	0.3420
D2	0.4760	0.3750
D3	0.3000	0.3330
D4	0.4820	0.3790
D5	0.4310	0.3550
D6	0.3590	0.3490

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Chain	Atom inclusion	Q-score
S1	0.4230	0.3290
S2	0.4700	0.3640
S3	0.4570	0.3600
S4	0.4310	0.3760
S5	0.4810	0.3670
S6	0.4420	0.3660
S7	0.5160	0.3850
S8	0.5120	0.3620
V1	0.4370	0.3020
V2	0.4110	0.3010
V3	0.4260	0.3080
a1	0.3600	0.2930
a2	0.3340	0.2930
a3	0.5000	0.3690
a4	0.4570	0.3370
b1	0.3720	0.3270
b2	0.4570	0.3590
c1	0.3530	0.2920
c2	0.4200	0.3360
d1	0.4090	0.3150
d2	0.4110	0.3570
f1	0.0740	0.2430
f2	0.1120	0.2470
h1	0.2310	0.2220
h2	0.3020	0.2410
i1	0.2240	0.2760
i2	0.2520	0.2980
q1	0.2820	0.2790
q2	0.4590	0.4030
x1	0.3250	0.3620
x2	0.3460	0.4180