



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 07:33 pm GMT

PDB ID : 6QC4
EMDB ID : EMD-4496
Title : Ovine respiratory supercomplex I+III2 open class 3
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-26
Resolution : 4.60 Å(reported)
Based on initial models : 5LNK, 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

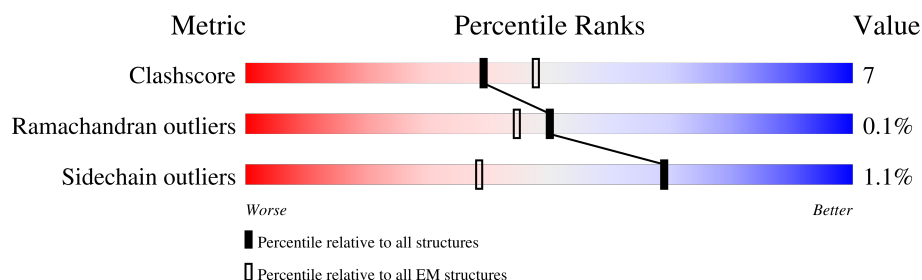
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a1	446	<div> <div>26%</div> <div>97%</div> <div>6%</div> </div>
1	a3	446	<div> <div>25%</div> <div>98%</div> <div>6%</div> </div>
2	a2	439	<div> <div>25%</div> <div>93%</div> <div>6%</div> </div>
2	a4	439	<div> <div>22%</div> <div>93%</div> <div>6%</div> </div>
3	b1	379	<div> <div>33%</div> <div>99%</div> <div>6%</div> </div>
3	b2	379	<div> <div>39%</div> <div>99%</div> <div>6%</div> </div>
4	c1	240	<div> <div>26%</div> <div>98%</div> <div>6%</div> </div>
4	c2	240	<div> <div>30%</div> <div>98%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	f1	196	72% 99% .
5	f2	196	74% 98% ..
6	d1	110	20% 91% 9%
6	d2	110	22% 89% 8%
7	q1	81	28% 90% 10%
7	q2	81	26% 91% 7%
8	h1	78	26% 83% 17%
8	h2	78	38% 82% 17%
9	x1	78	33% 42% 58%
9	x2	78	27% 38% 62%
10	i1	63	35% 86% 13%
10	i2	63	41% 90% 10%
11	D3	115	39% 70% 8% 23%
12	D1	318	37% 73% 20% 6%
13	D6	175	50% 82% 15% ..
14	4L	98	52% 85% 14% .
15	D5	606	36% 77% 22% .
16	D4	459	39% 75% 24%
17	D2	347	32% 80% 20%
18	AK	140	49% 82% 16% .
19	B5	143	22% 82% 15% ..
20	AA	88	53% 77% 14% 9%
20	AB	88	26% 78% 20% .
21	A8	171	24% 81% 19%
22	BJ	175	20% 81% 16% ..

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Mol	Chain	Length	Quality of chain
23	AJ	320	
24	S5	105	
25	A3	83	
26	B3	97	
27	C2	120	
28	B4	128	
29	AM	143	
30	B6	127	
31	B7	119	
32	B9	178	
33	B2	72	
34	B8	158	
35	BK	125	
36	C1	49	
37	B1	57	
38	A1	70	
39	V1	445	
40	V2	217	
41	S1	704	
42	S2	430	
43	S3	228	
44	S7	179	
45	S8	176	
46	V3	75	
47	S6	96	

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Mol	Chain	Length	Quality of chain
48	S4	133	
49	A9	338	
50	A2	98	
51	A5	115	
52	A6	127	
53	A7	112	
54	AL	145	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 96705 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 UQCRC1.

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		

- 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	238	Total	C	N	O	S	0	0
			1902	1214	329	344	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 UQCRB.

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		

- 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	33	Total	C	N	O	0	0
			164	98	33	33		
9	x2	30	Total	C	N	O	0	0
			150	90	30	30		

- 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		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	i2	57	Total	C	N	O	0	0
			473	312	82	79		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D3	89	Total	C	N	O	S	0	0
			719	495	101	118	5		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D1	298	Total	C	N	O	S	0	0
			2372	1605	360	388	19		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D6	171	Total	C	N	O	S	0	0
			1308	878	187	230	13		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 18 is a protein called NDUFA11.

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

- Molecule 19 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 20 is a protein called Acyl carrier protein.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 22 is a protein called NDUF10.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 24 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 28 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 29 is a protein called NDUFA13.

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

- Molecule 30 is a protein called NDUF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B6	96	Total	C	N	O	S	0	0
			809	533	136	139	1		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B2	65	Total	C	N	O	S	0	0
			560	371	93	95	1		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 35 is a protein called NDUFB11.

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

- Molecule 36 is a protein called NDUFC1.

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

- Molecule 37 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	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 38 is a protein called NDUFA1.

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

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

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

- Molecule 40 is a protein called NDUFV2.

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

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

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

- Molecule 42 is a protein called NDUFS2.

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

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

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

- Molecule 44 is a protein called NDUFS7.

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

- Molecule 45 is a protein called NDUFS8.

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

- Molecule 46 is a protein called NDUFV3.

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

- Molecule 47 is a protein called NDUFS6.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	A9	288	Total	C	N	O	S	0	0
			2270	1451	409	405	5		

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

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

- Molecule 51 is a protein called NDUF5A5.

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

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

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

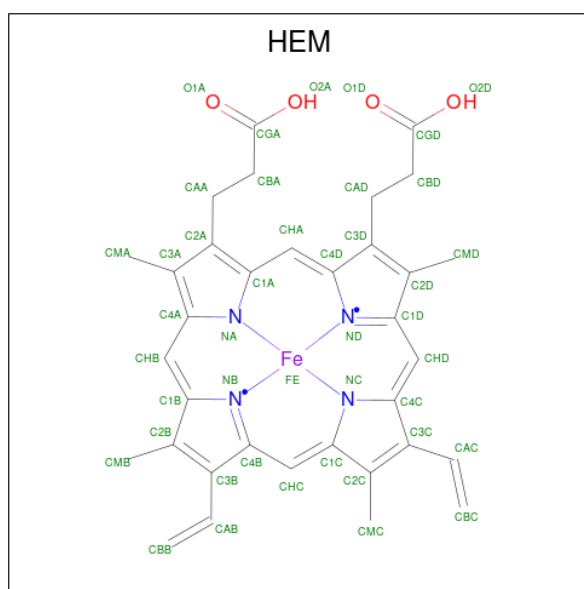
- Molecule 53 is a protein called NDUFA7.

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

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

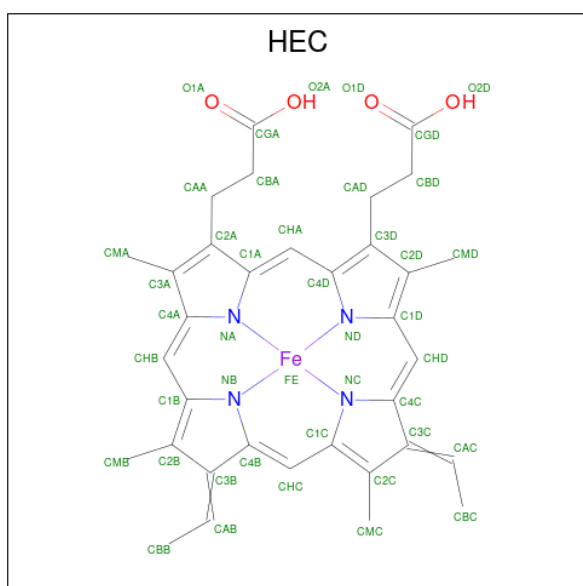
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AL	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- 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 43	C 34	Fe 1	N 4	O 4	0
55	b1	1	Total 43	C 34	Fe 1	N 4	O 4	0
55	b2	1	Total 43	C 34	Fe 1	N 4	O 4	0
55	b2	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 56 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



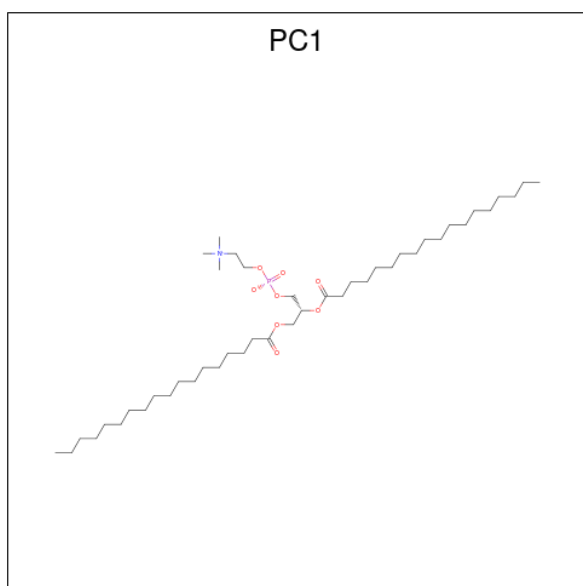
Mol	Chain	Residues	Atoms					AltConf
56	c1	1	Total 43	C 34	Fe 1	N 4	O 4	0
56	c2	1	Total 43	C 34	Fe 1	N 4	O 4	0

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



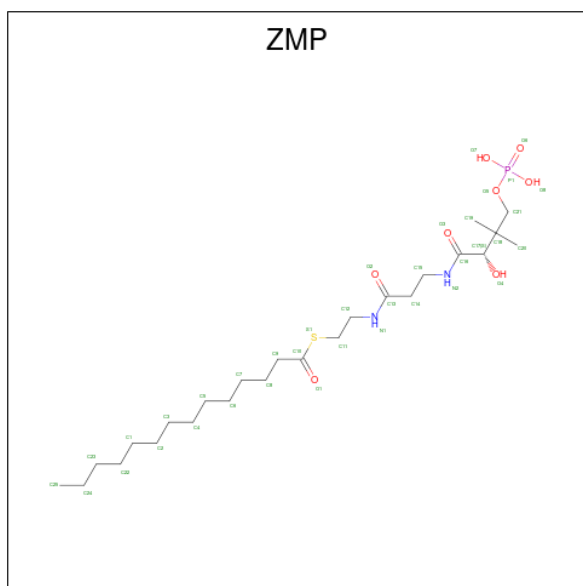
Mol	Chain	Residues	Atoms			AltConf
57	f1	1	Total	Fe	S	0
			4	2	2	
57	f2	1	Total	Fe	S	0
			4	2	2	
57	V2	1	Total	Fe	S	0
			4	2	2	
57	S1	1	Total	Fe	S	0
			4	2	2	

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



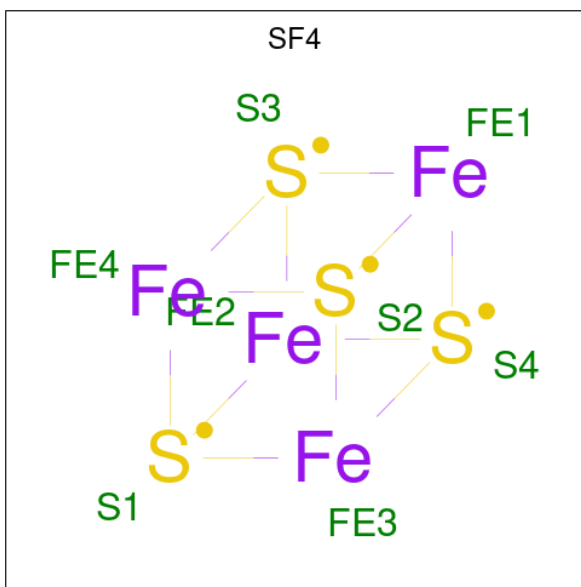
Mol	Chain	Residues	Atoms					AltConf
58	D2	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 59 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



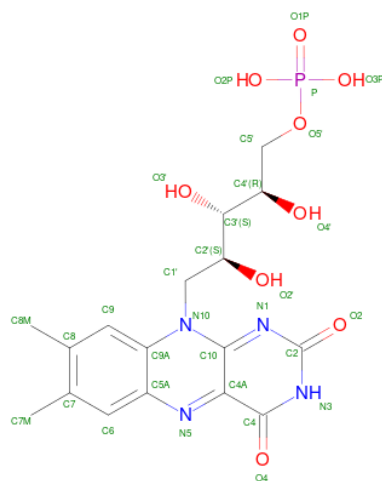
Mol	Chain	Residues	Atoms						AltConf
59	AB	1	Total 31	C 20	N 2	O 7	P 1	S 1	0
59	AA	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

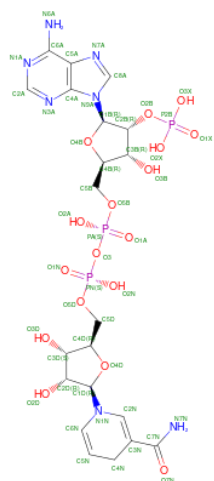


Mol	Chain	Residues	Atoms					AltConf
61	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 63 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

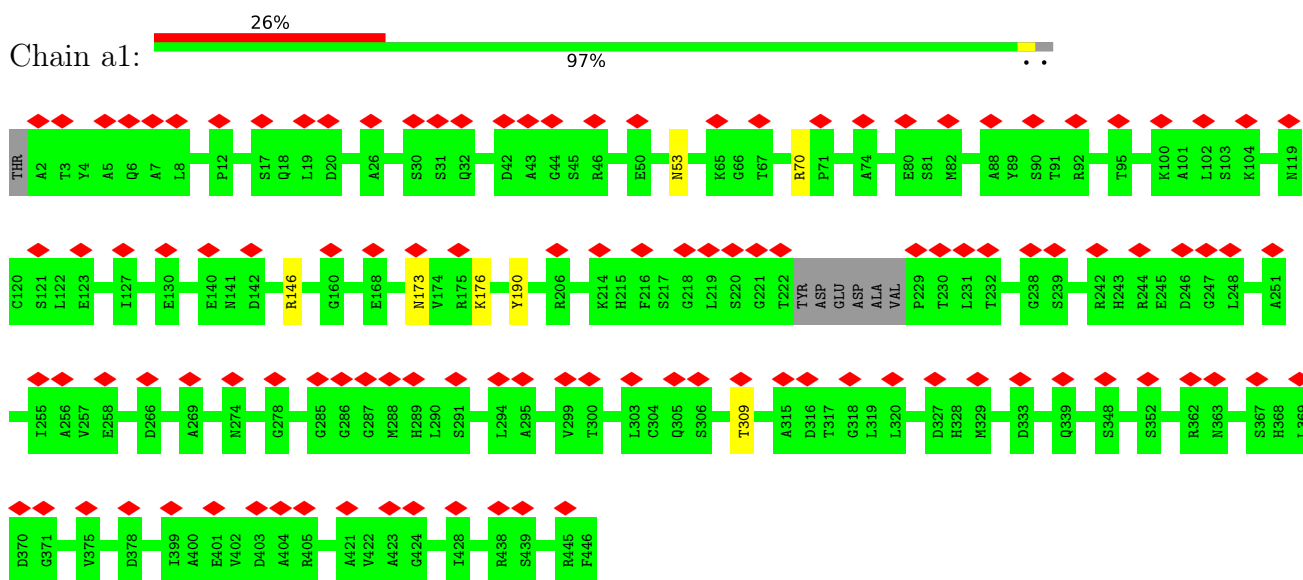


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	A9	1	48	21	7	17	3	0

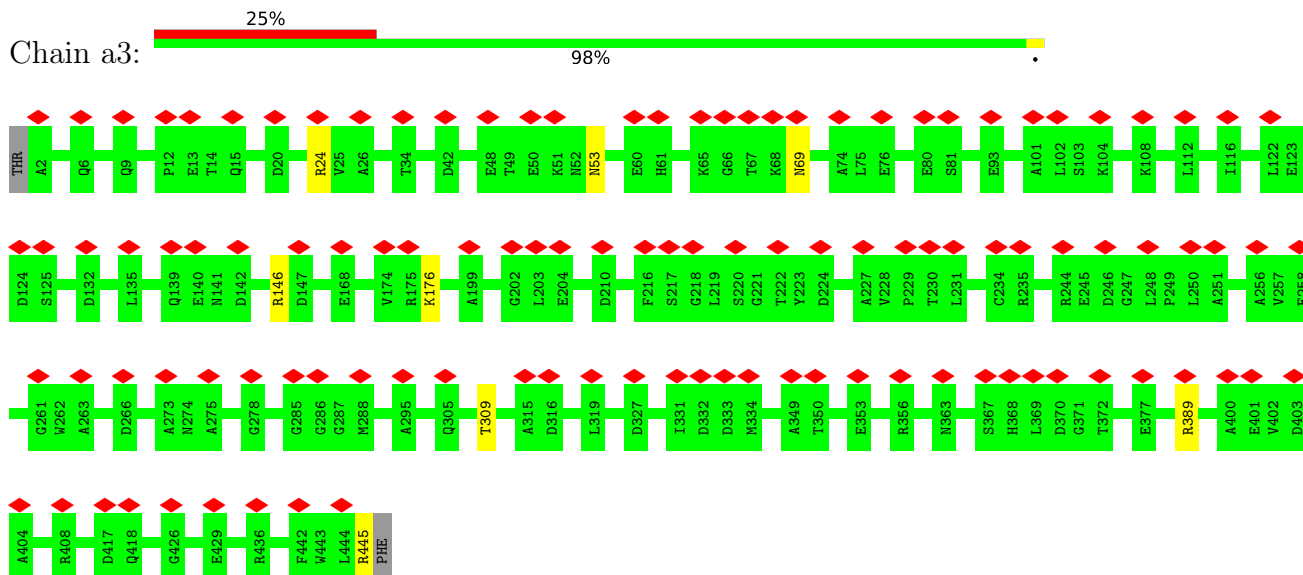
3 Residue-property plots

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

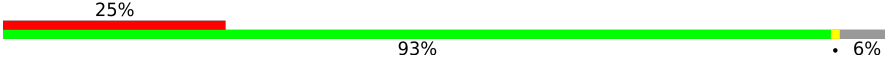
- Molecule 1: UQCRC1

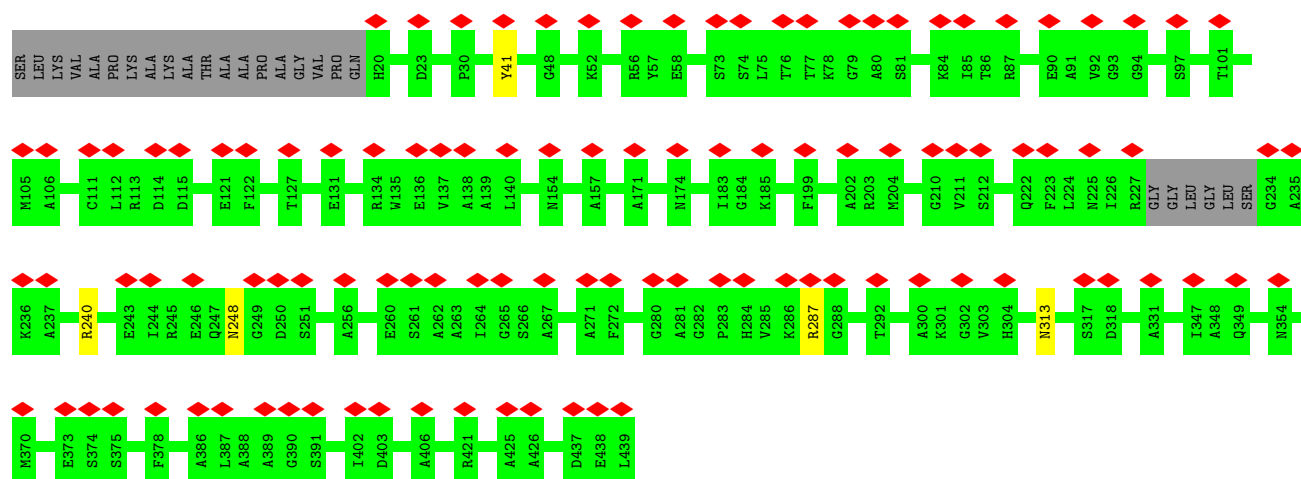


- Molecule 1: UQCRC1

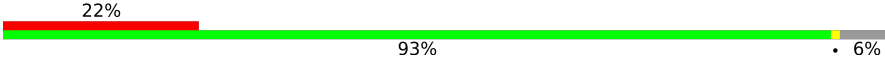


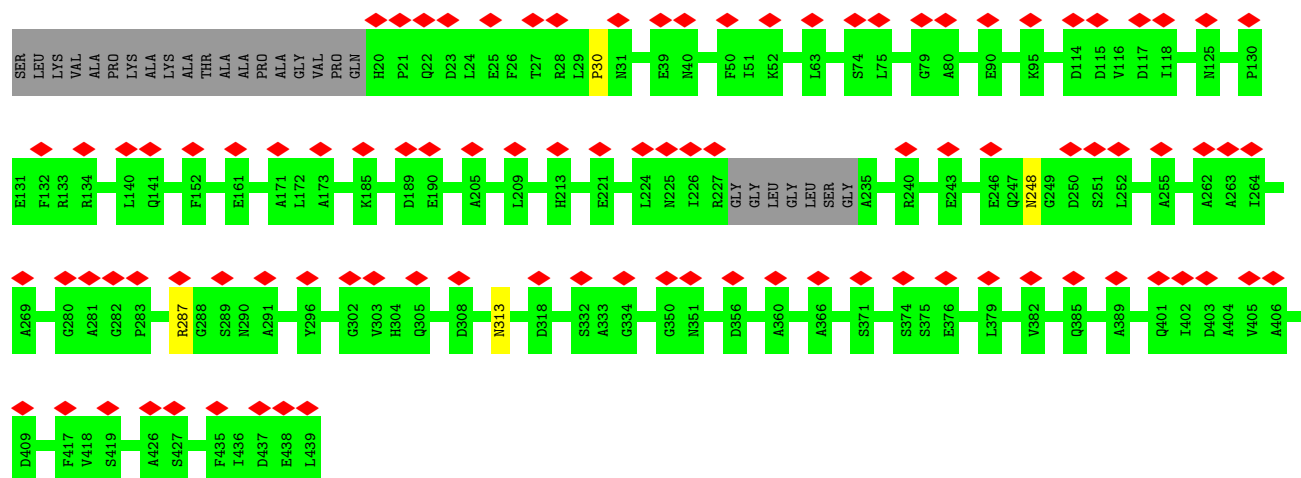
- Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

Chain a2:  25% 93% 6%



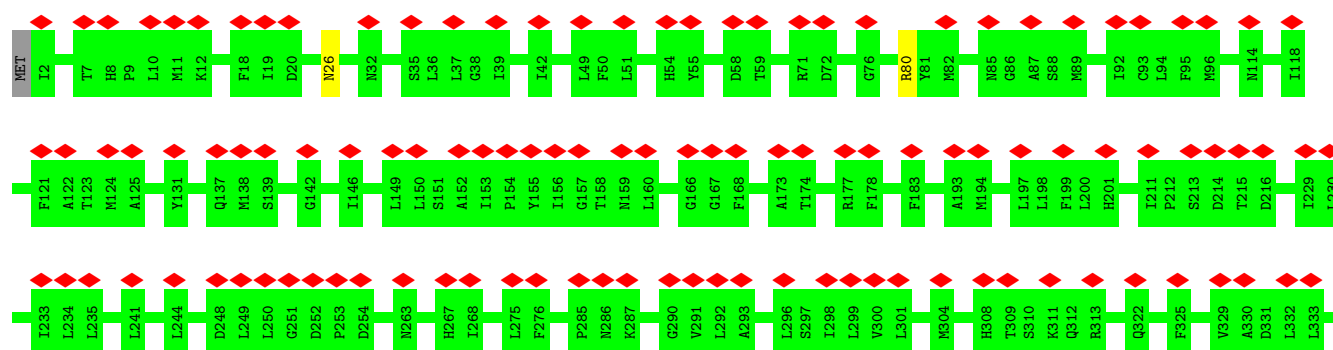
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

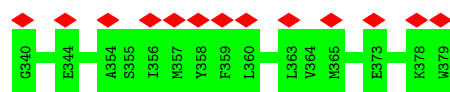
Chain a4:  22% 93% 6%



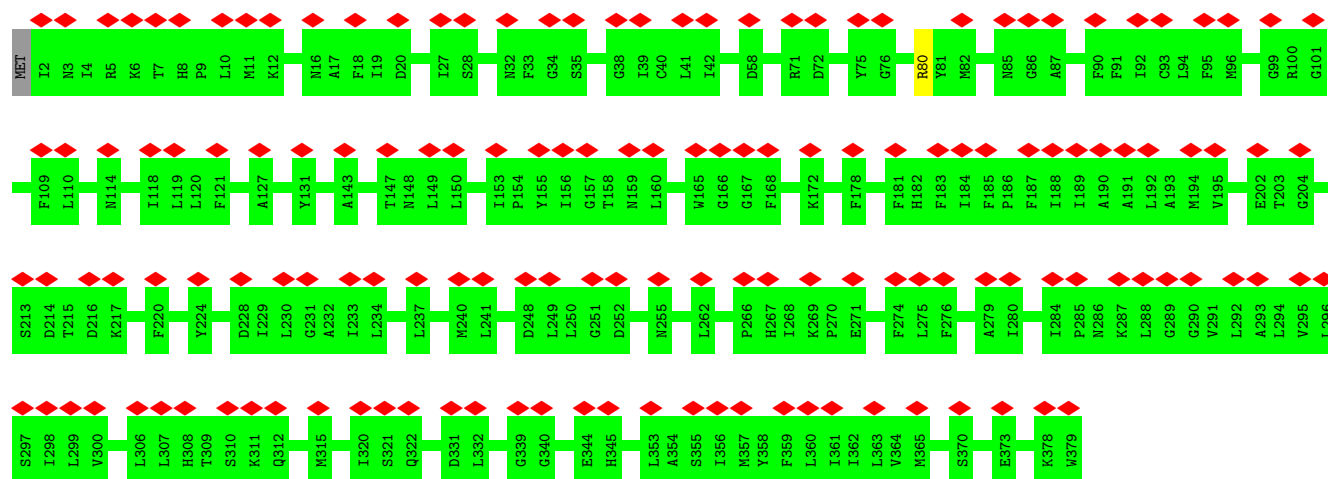
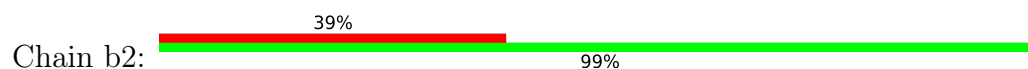
• Molecule 3: Cytochrome b

Chain b1:  33% 99%

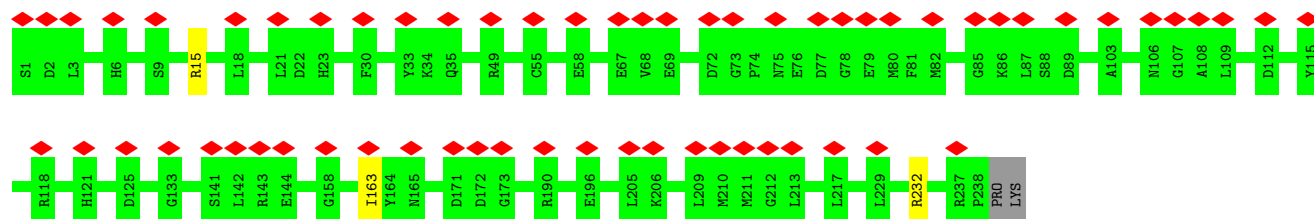




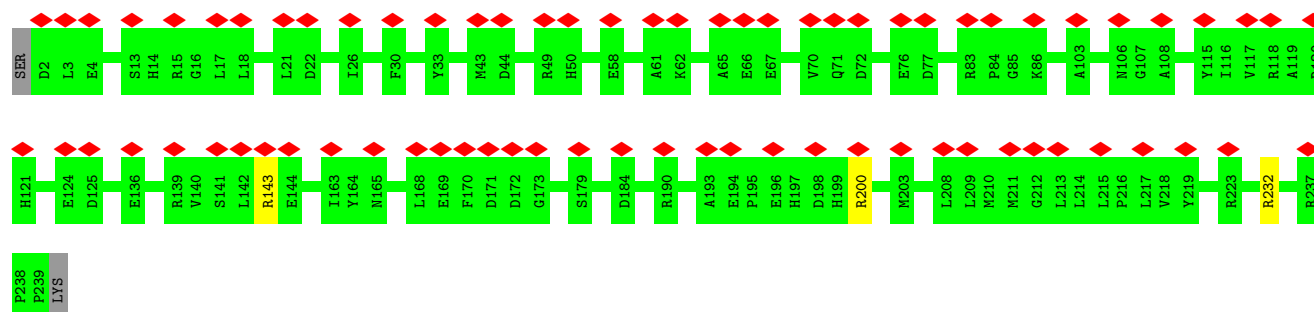
- Molecule 3: Cytochrome b



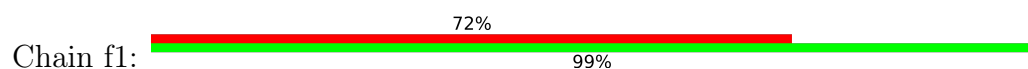
- Molecule 4: Cytochrome c1

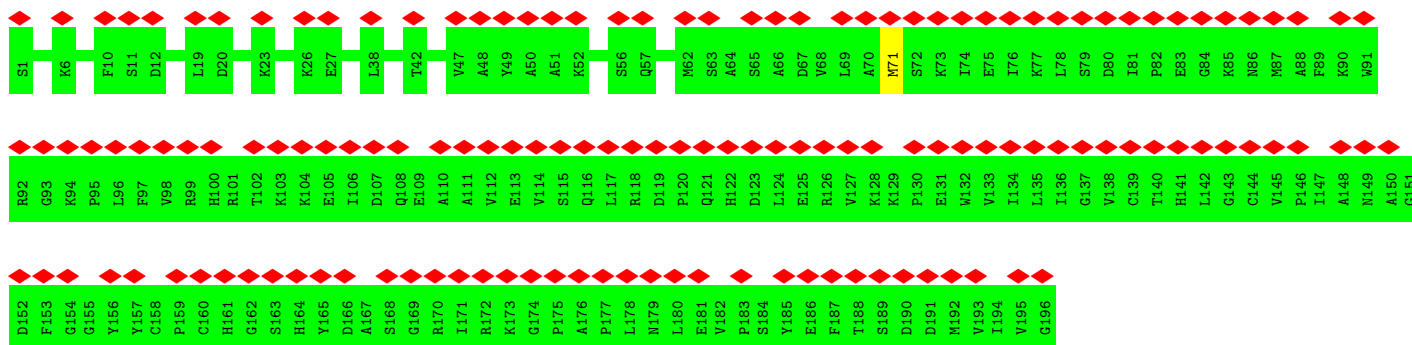


- Molecule 4: Cytochrome c1

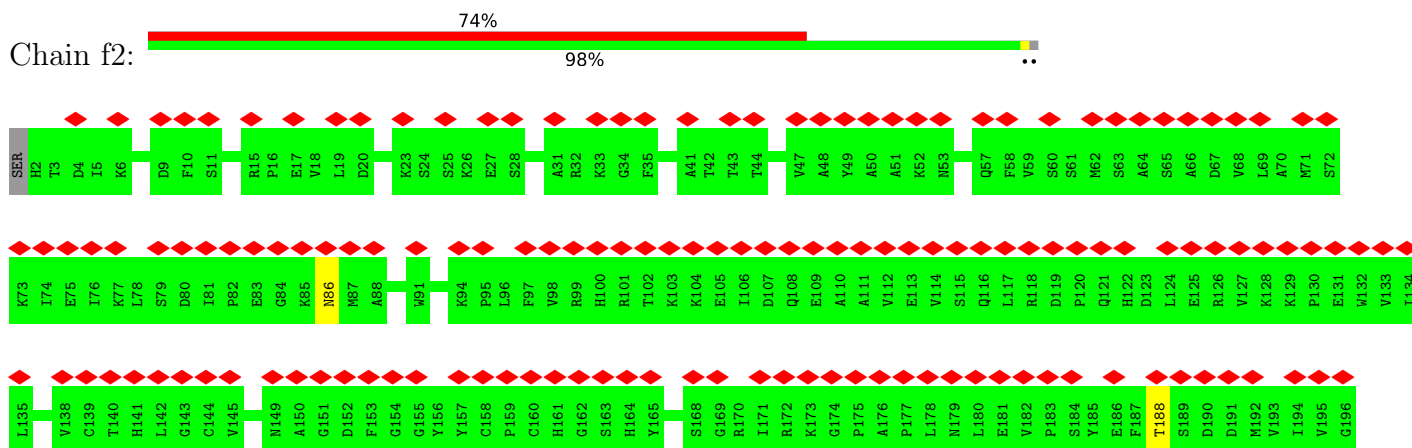


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

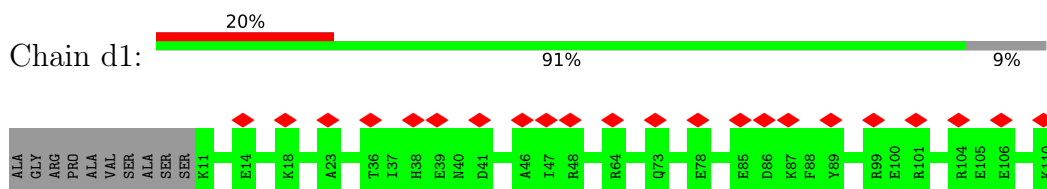




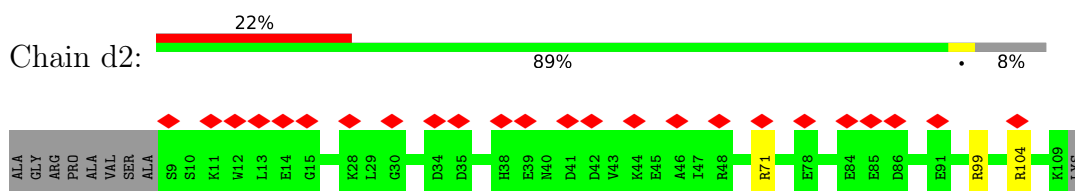
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



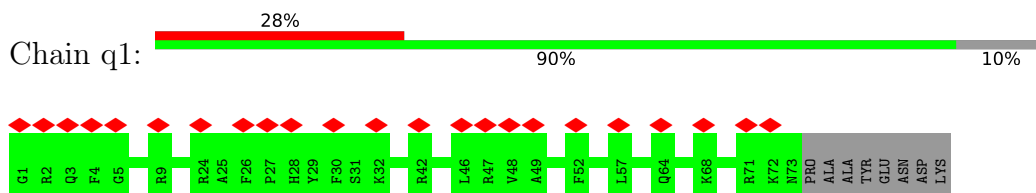
- Molecule 6: UQCRB



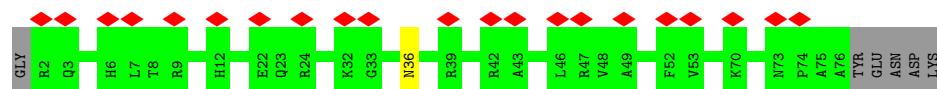
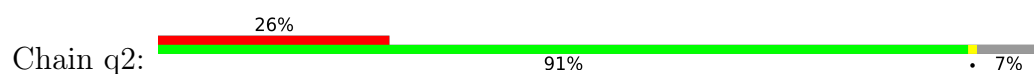
- Molecule 6: UQCRB



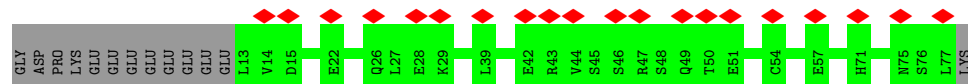
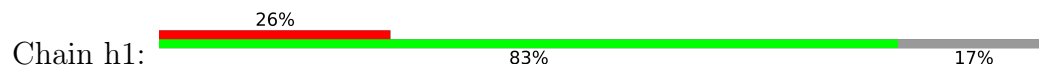
- Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



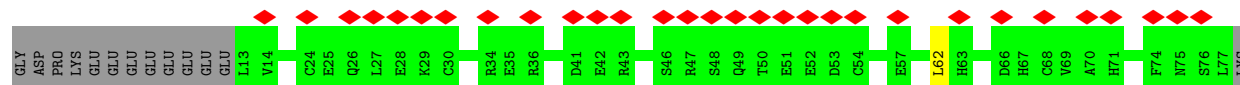
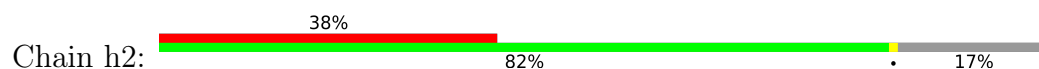
- Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



- Molecule 8: Cytochrome b-c1 complex subunit 6



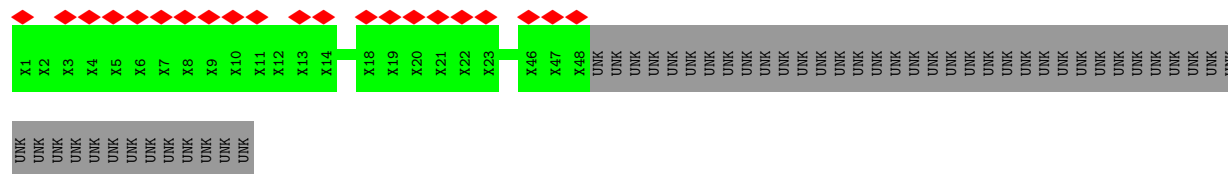
- Molecule 8: Cytochrome b-c1 complex subunit 6



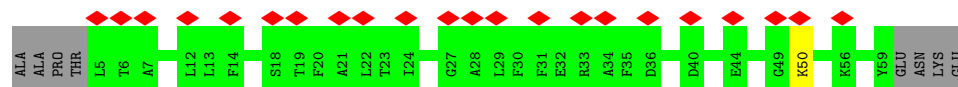
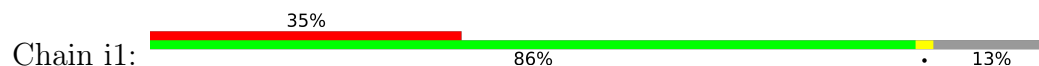
- Molecule 9: UQCRFS1N



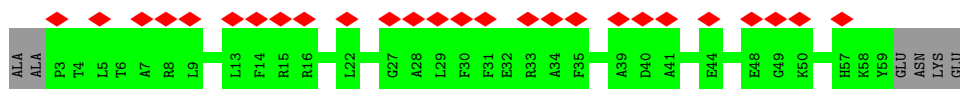
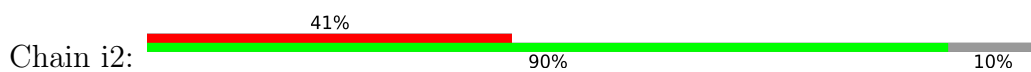
- Molecule 9: UQCRFS1N



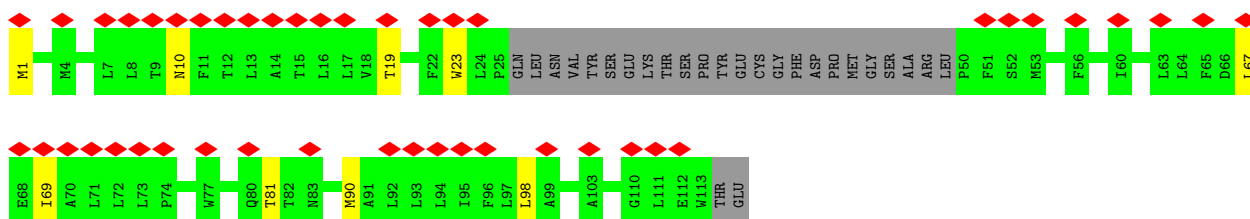
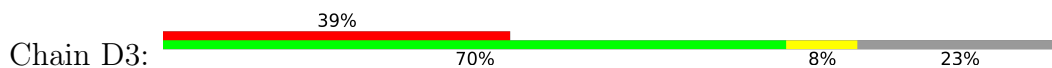
- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X



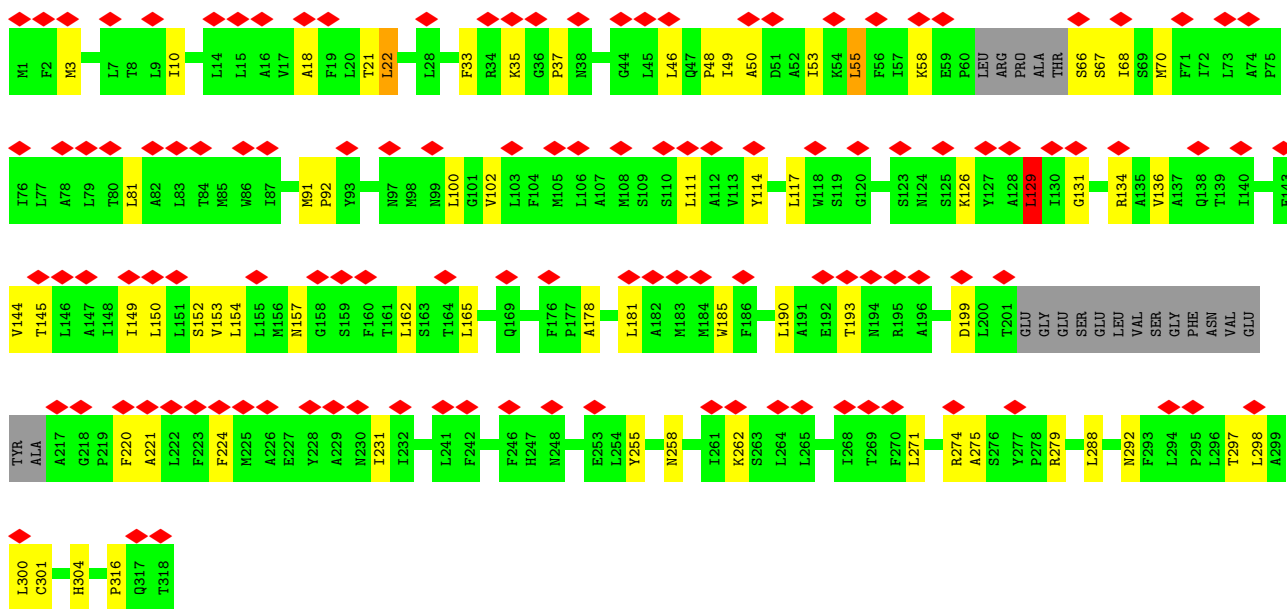
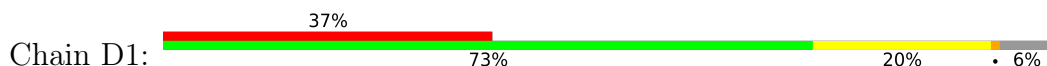
- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X



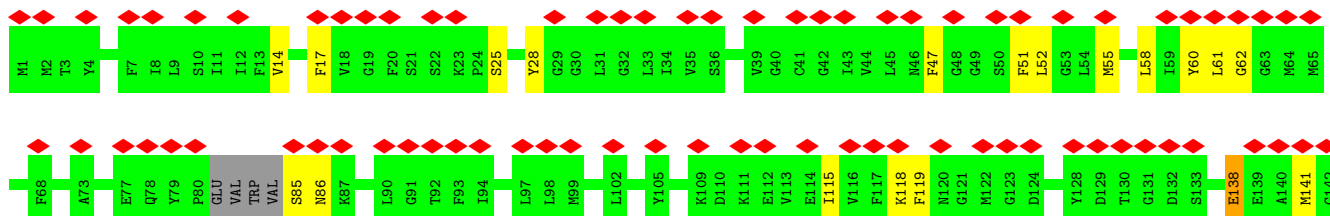
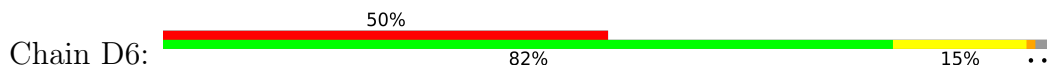
• Molecule 11: NADH-ubiquinone oxidoreductase chain 3

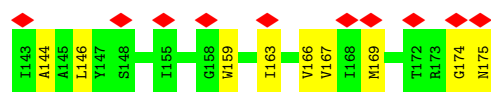


• Molecule 12: NADH-ubiquinone oxidoreductase chain 1

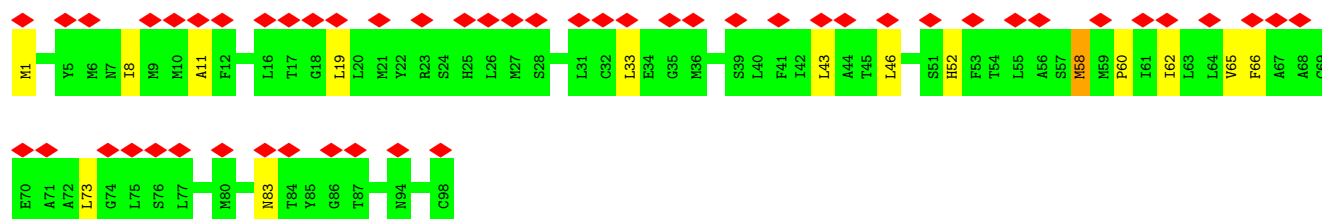
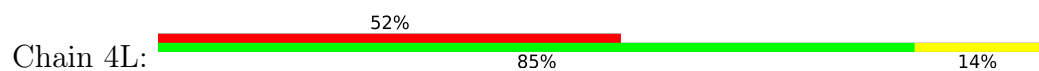


• Molecule 13: NADH-ubiquinone oxidoreductase chain 6

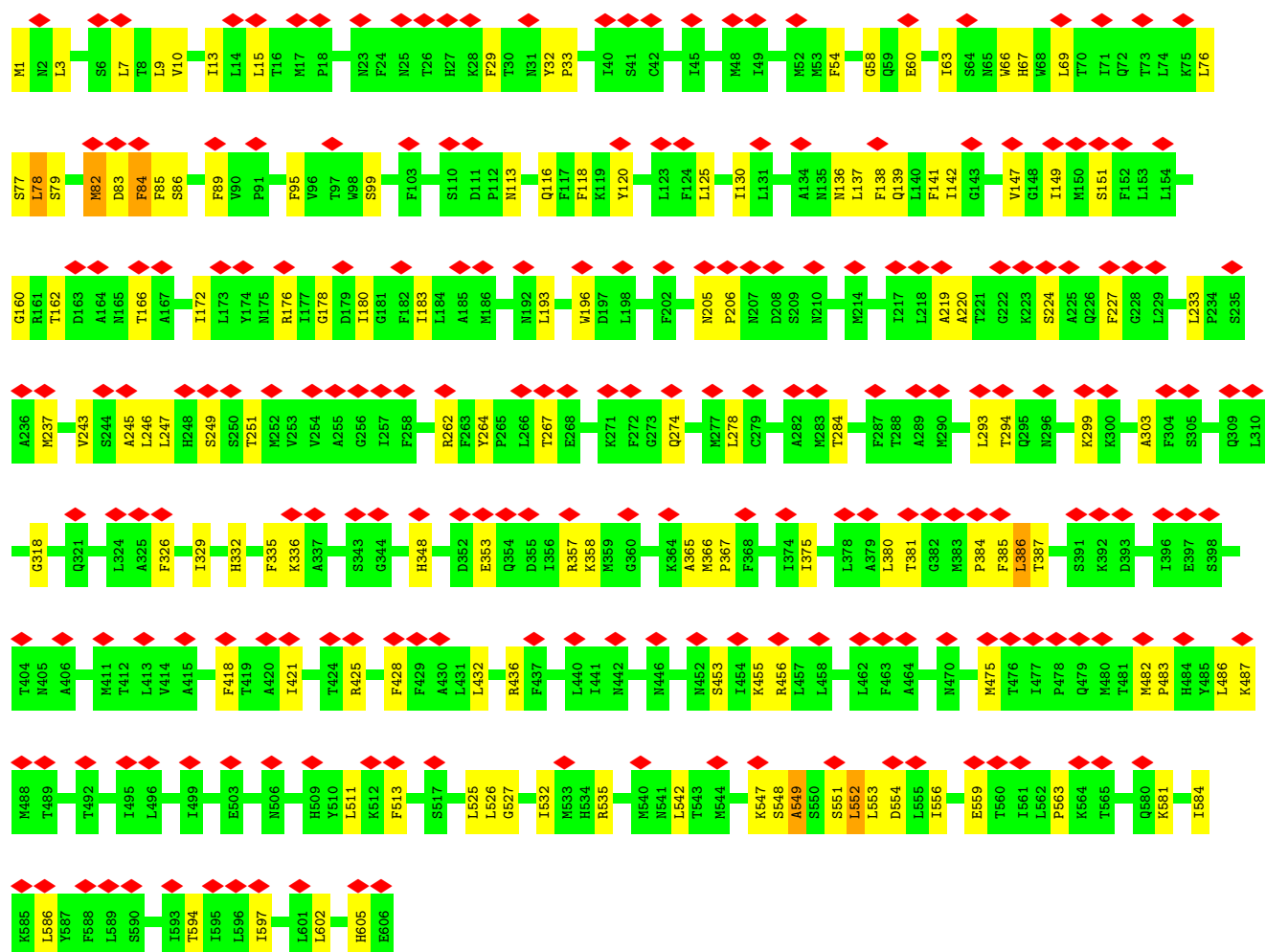
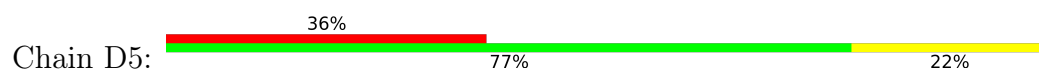




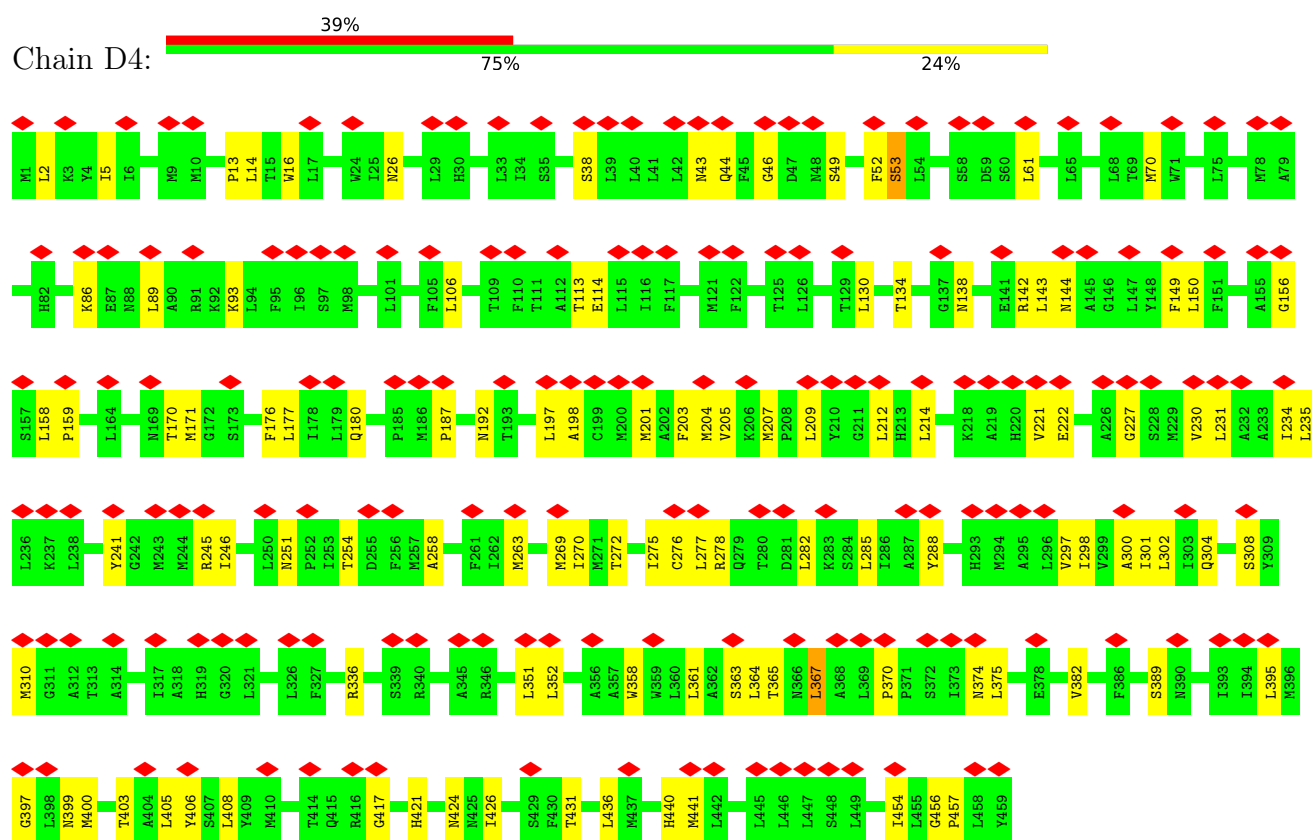
• Molecule 14: NADH-ubiquinone oxidoreductase chain 4L



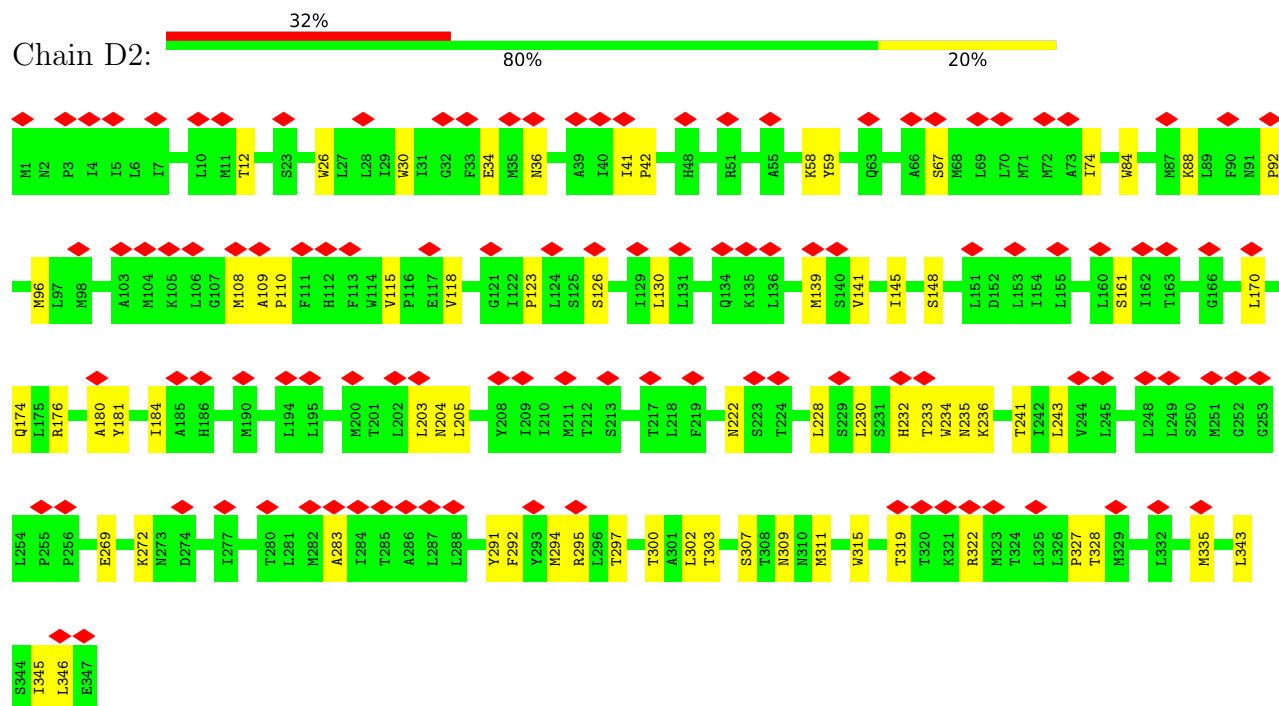
• Molecule 15: NADH-ubiquinone oxidoreductase chain 5



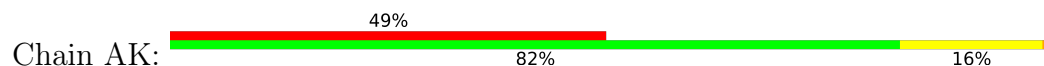
• Molecule 16: NADH-ubiquinone oxidoreductase chain 4

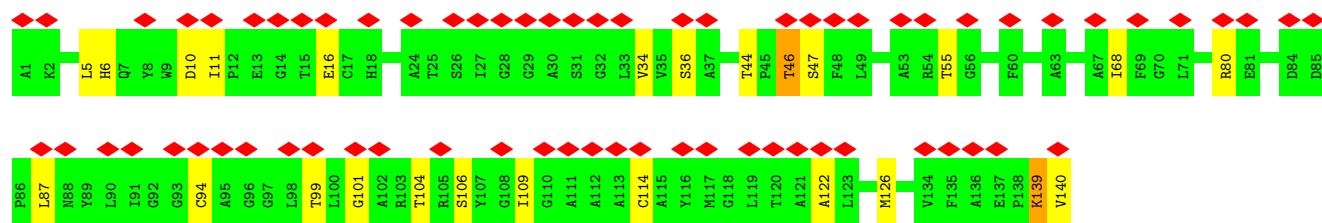


• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

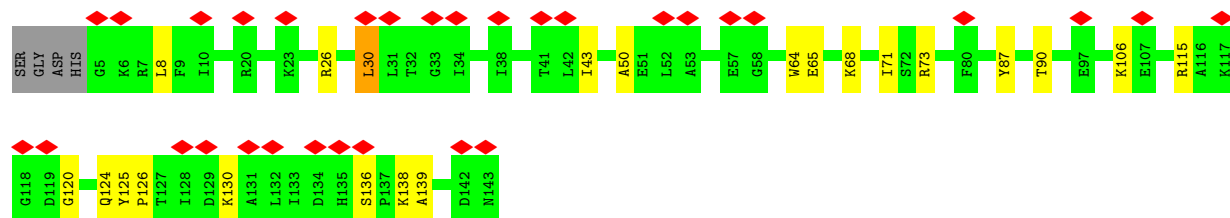
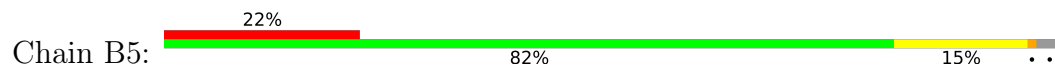


• Molecule 18: NDUFA11

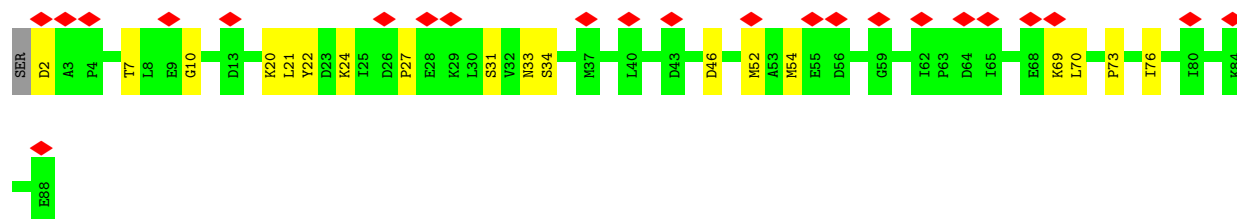
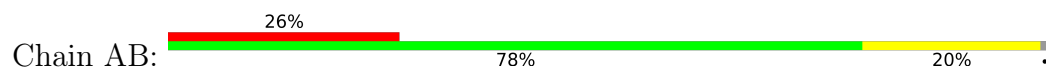




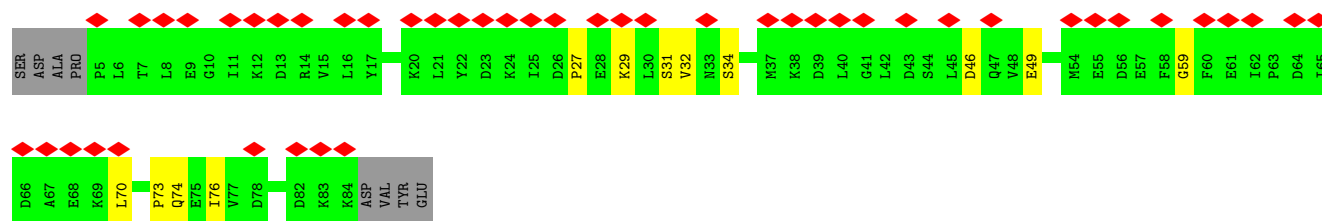
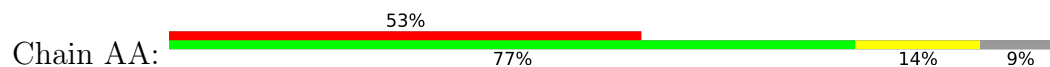
• Molecule 19: NADH:ubiquinone oxidoreductase subunit B5



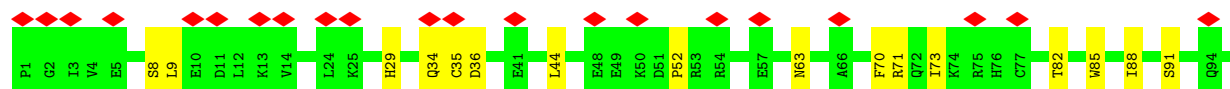
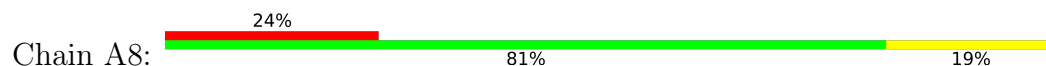
• Molecule 20: Acyl carrier protein

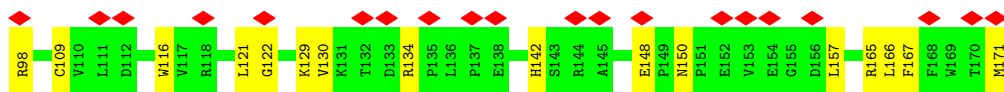


• Molecule 20: Acyl carrier protein

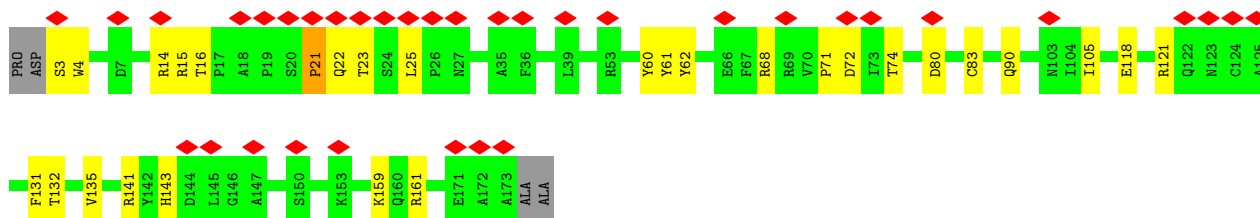
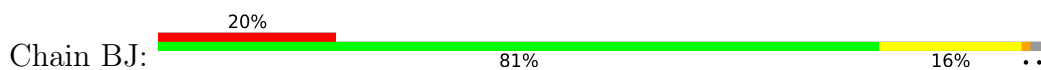


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

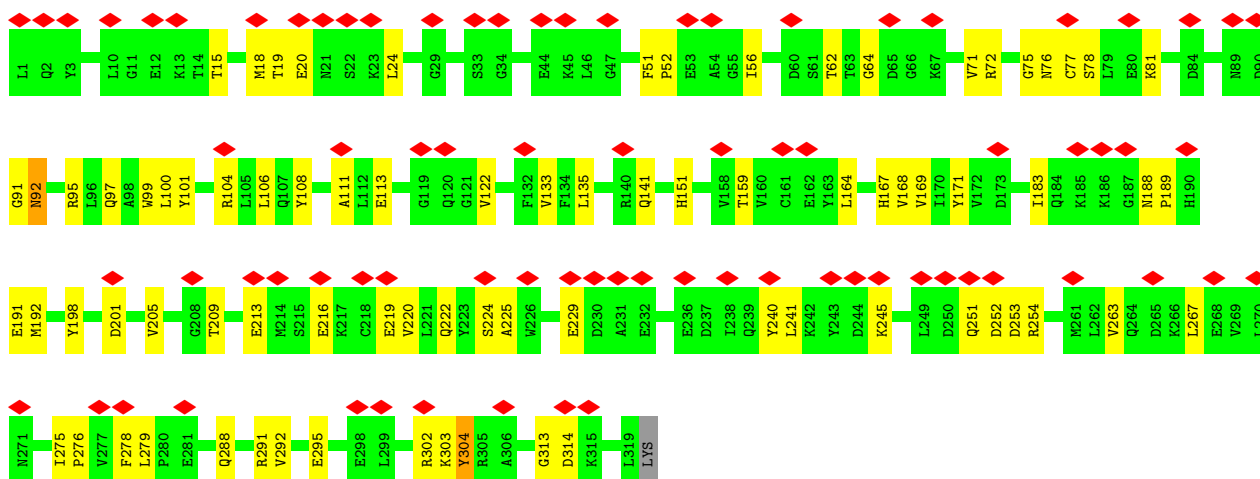
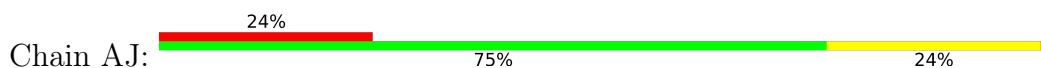




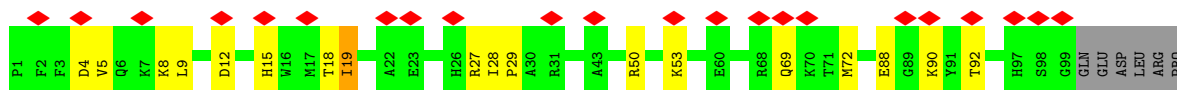
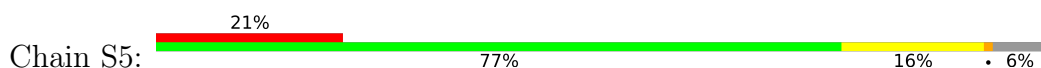
• Molecule 22: NDUFB10



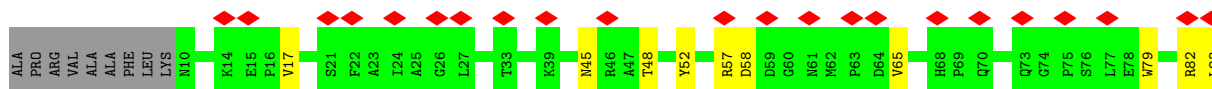
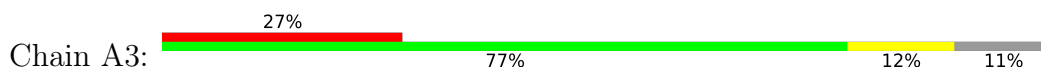
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



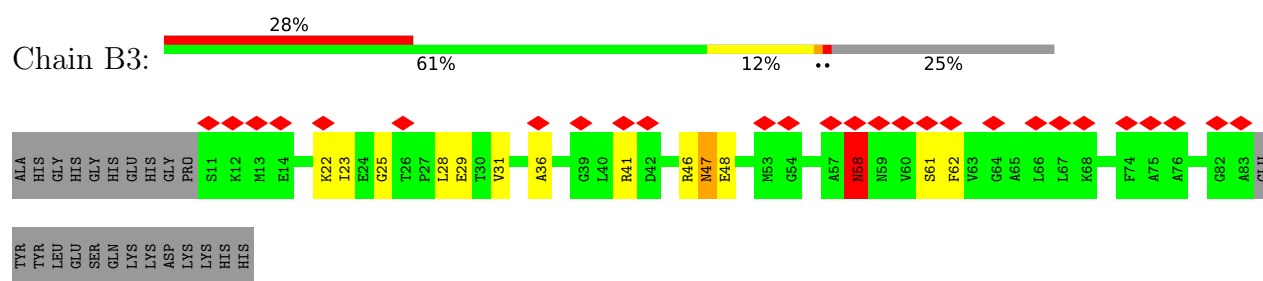
• Molecule 24: NADH:ubiquinone oxidoreductase subunit S5



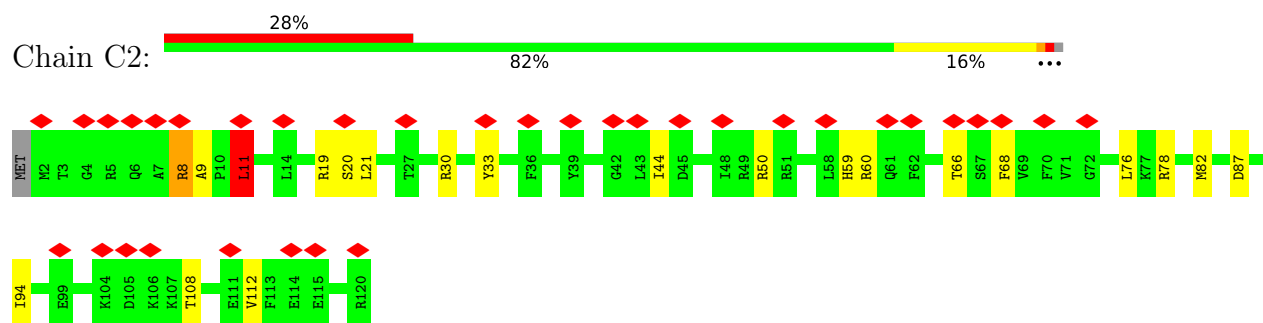
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A3



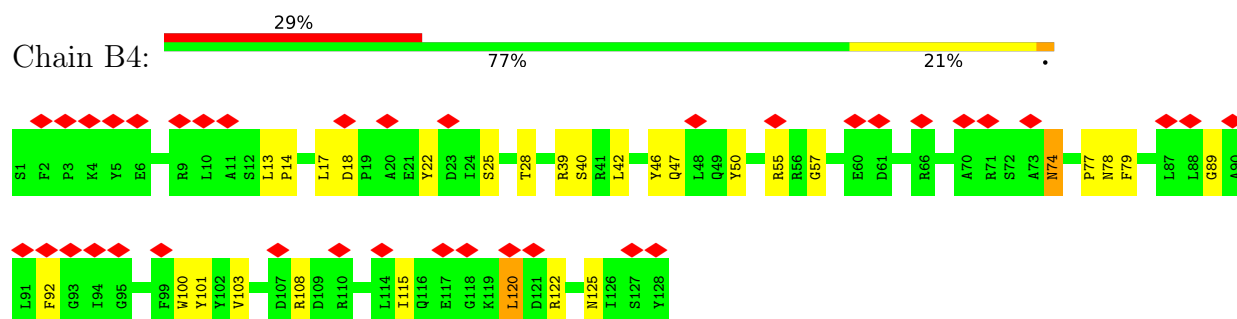
• Molecule 26: NADH:ubiquinone oxidoreductase subunit B3



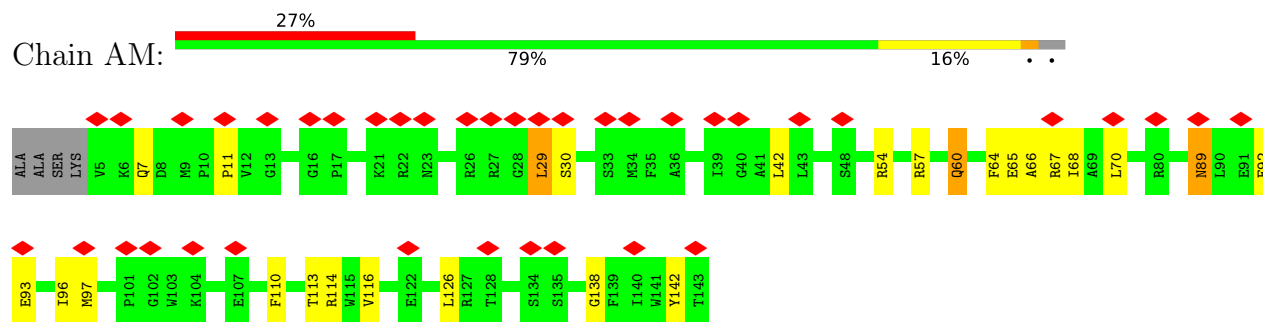
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2



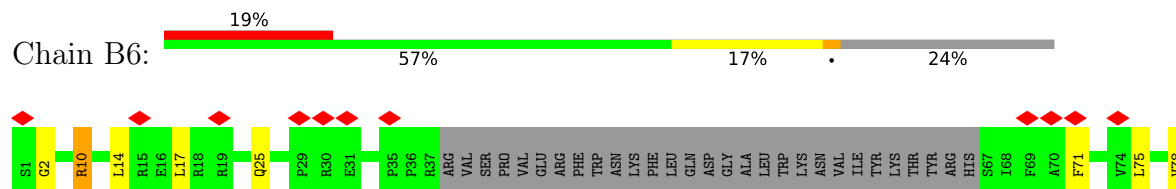
- Molecule 28: NADH:ubiquinone oxidoreductase subunit B4



- Molecule 29: NDUFA13

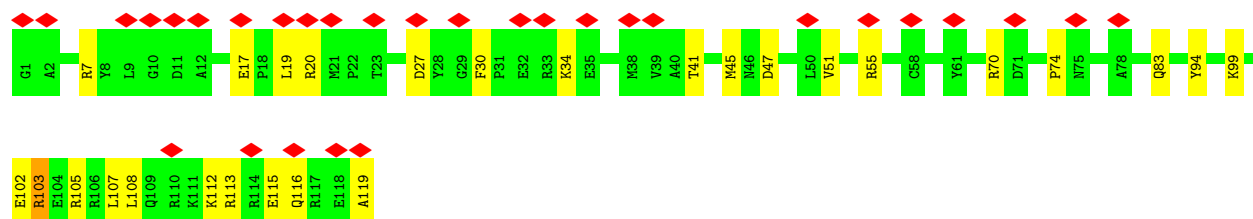
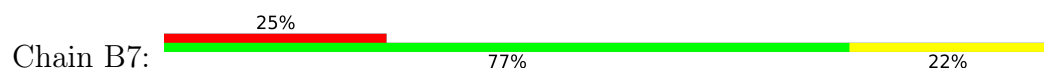


- Molecule 30: NDUF6

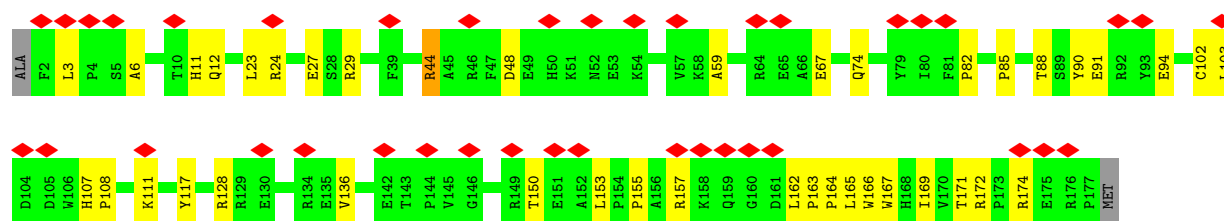
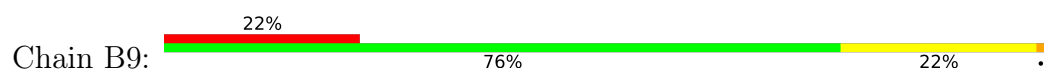




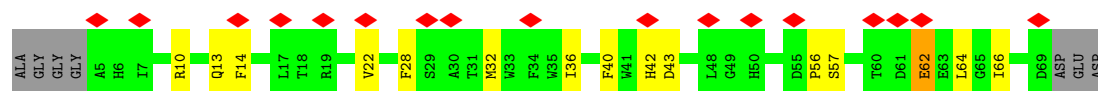
- Molecule 31: NADH:ubiquinone oxidoreductase subunit B7



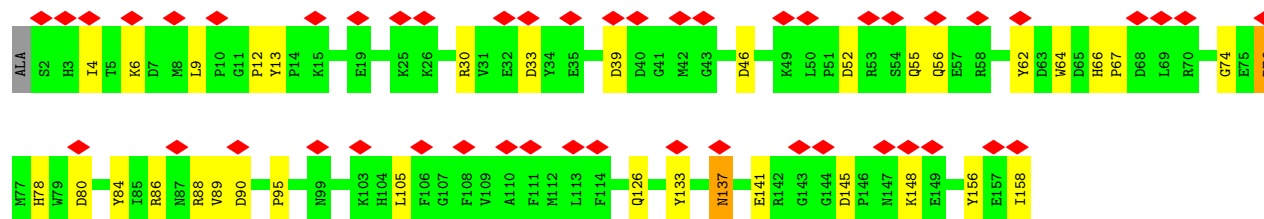
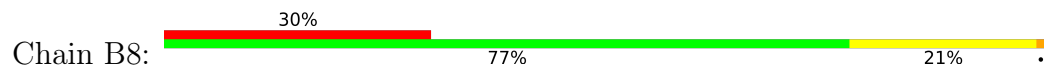
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B9



- Molecule 33: NADH:ubiquinone oxidoreductase subunit B2

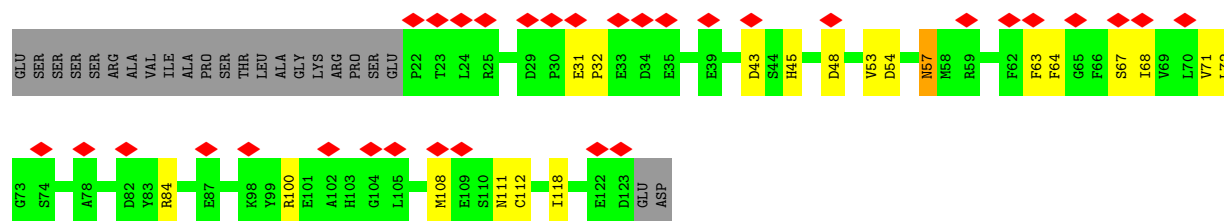


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

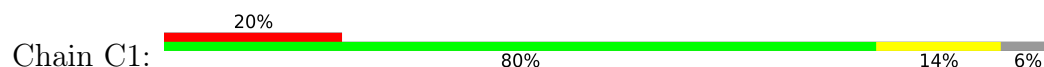


- Molecule 35: NDUFB11

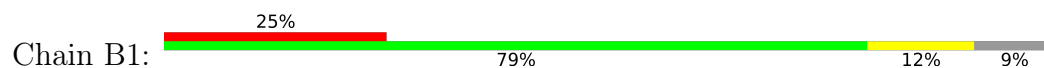




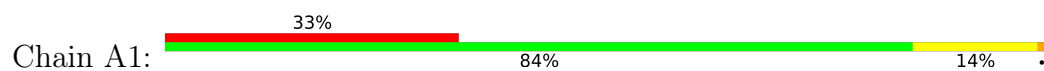
• Molecule 36: NDUFC1



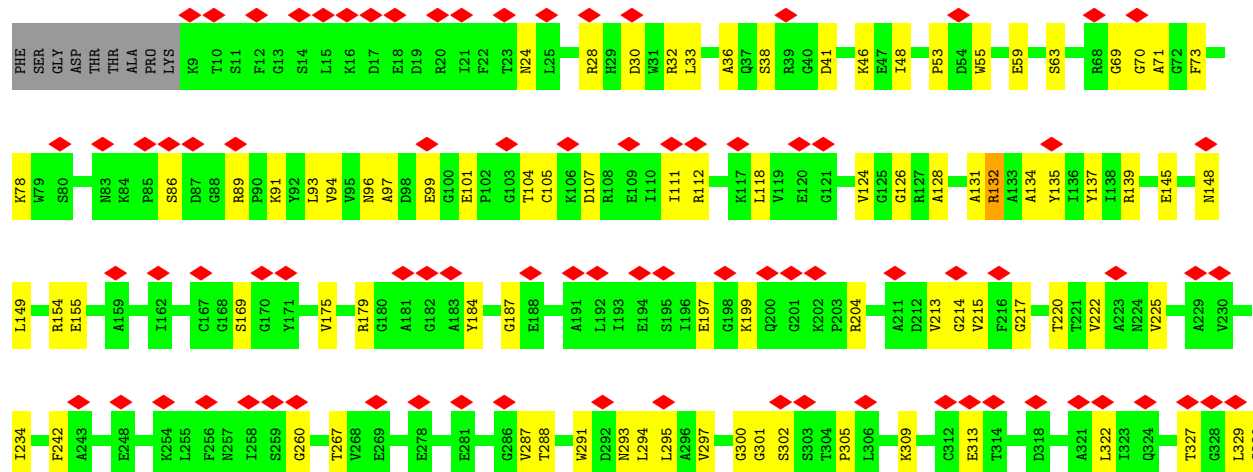
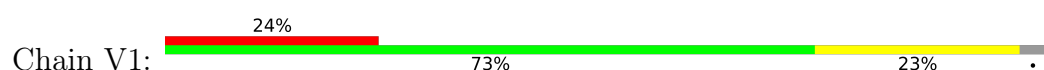
• Molecule 37: NDUFB1

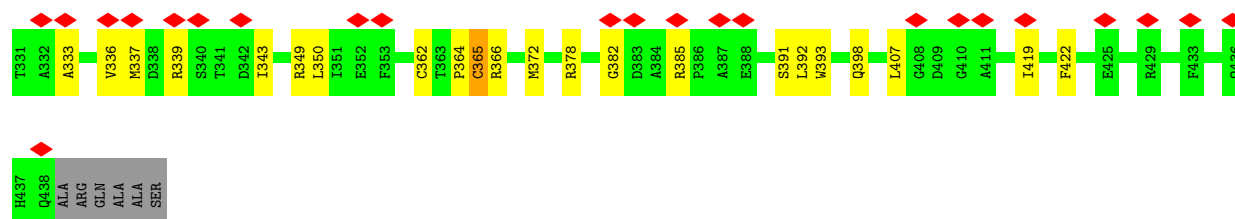


• Molecule 38: NDUFA1

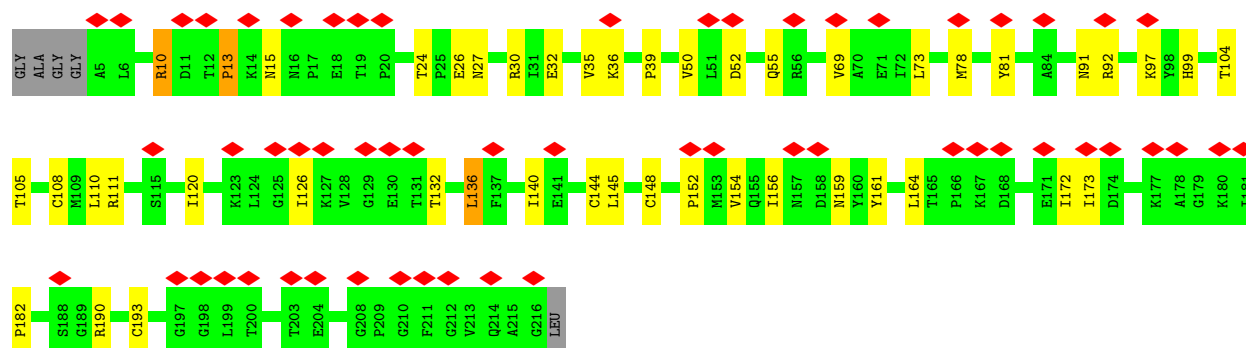
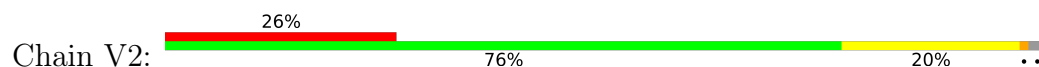


• Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

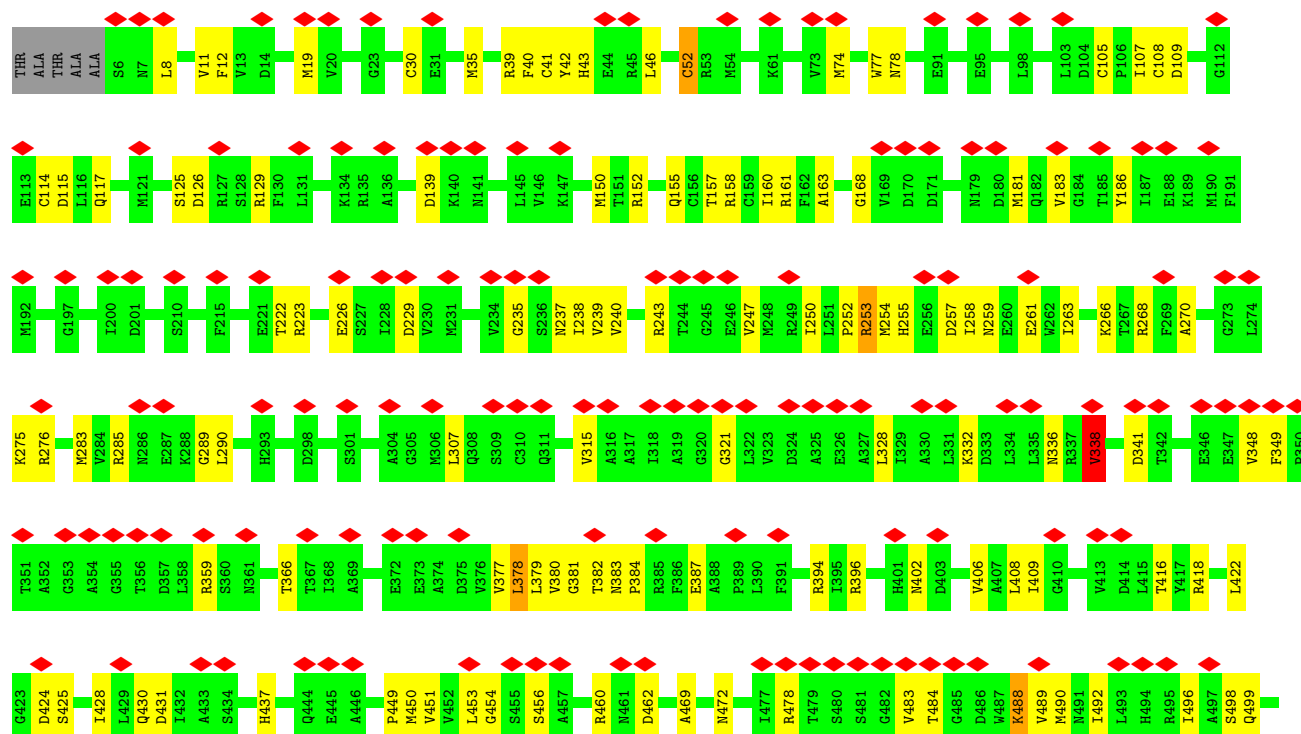
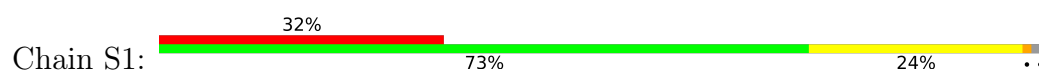


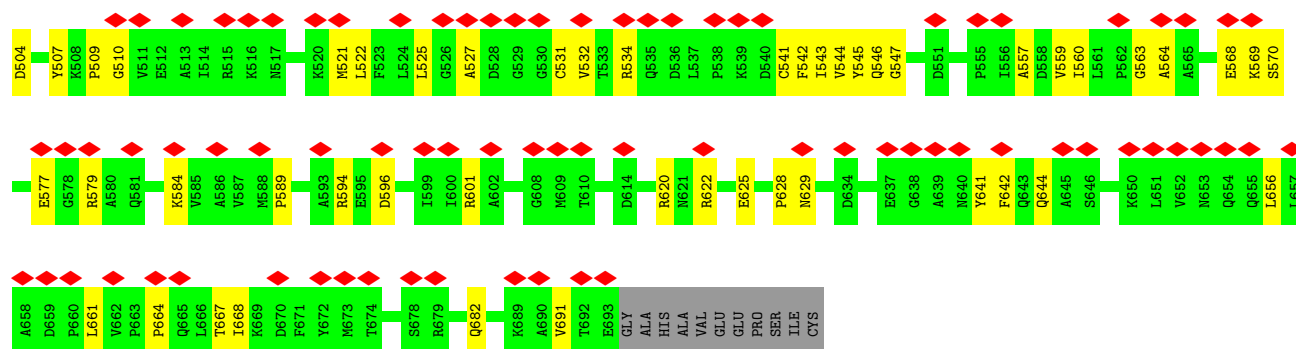


• Molecule 40: NDUFV2

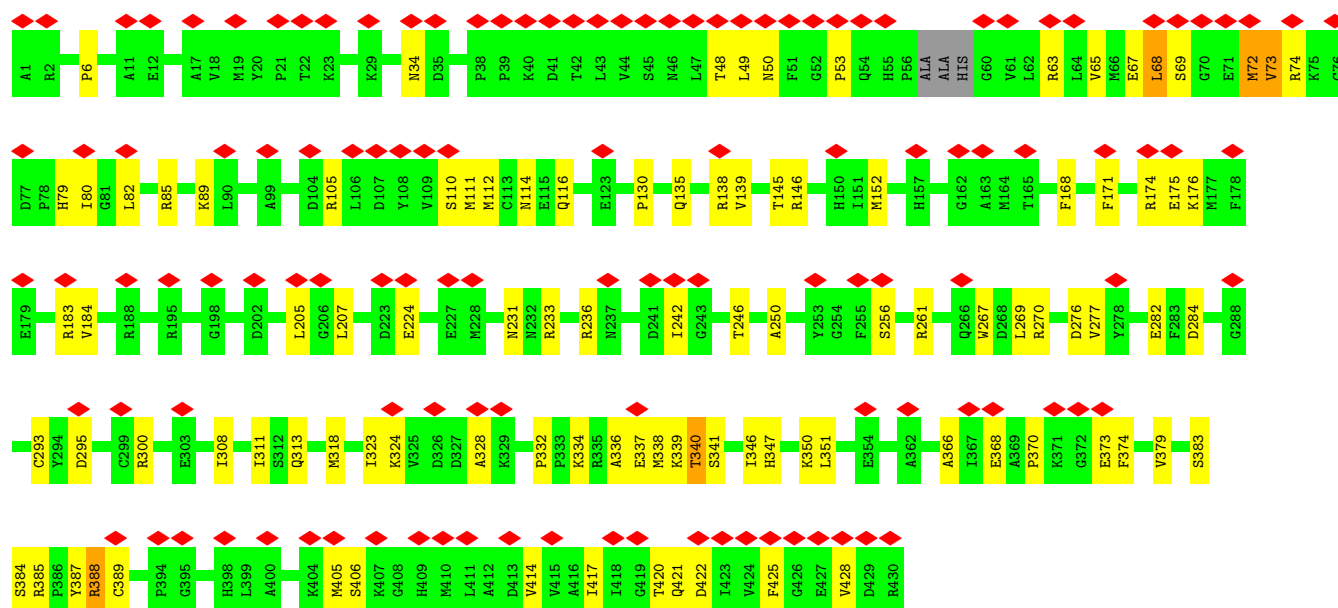
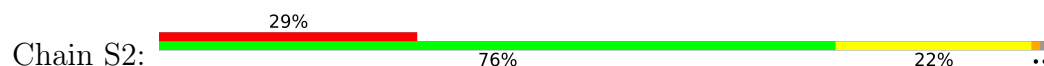


• Molecule 41: NADH:ubiquinone oxidoreductase core subunit S1

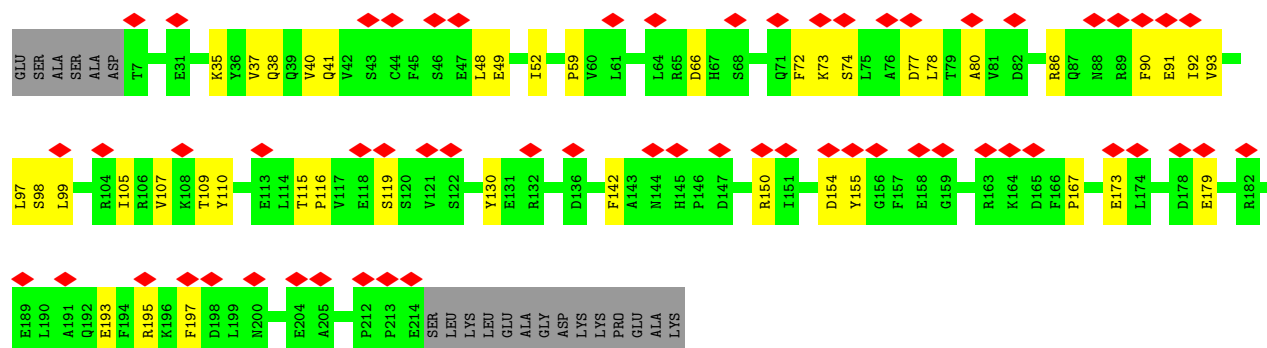
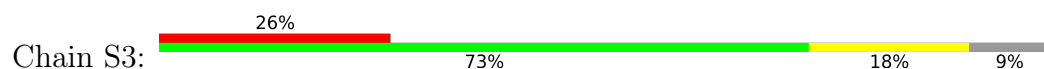




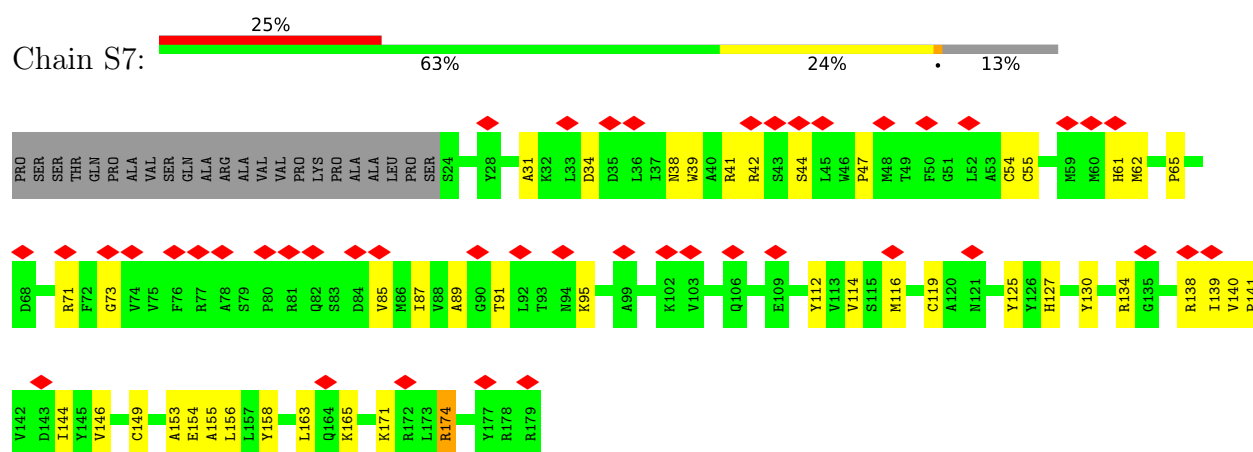
• Molecule 42: NDUFS2



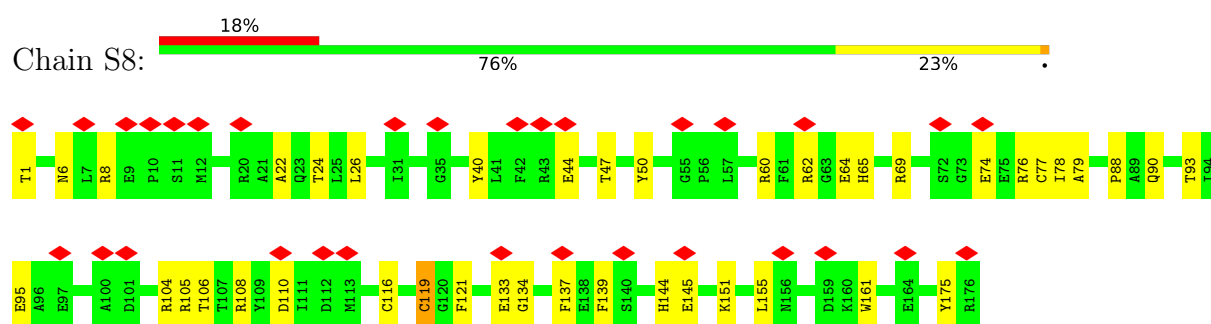
• Molecule 43: NADH:ubiquinone oxidoreductase core subunit S3



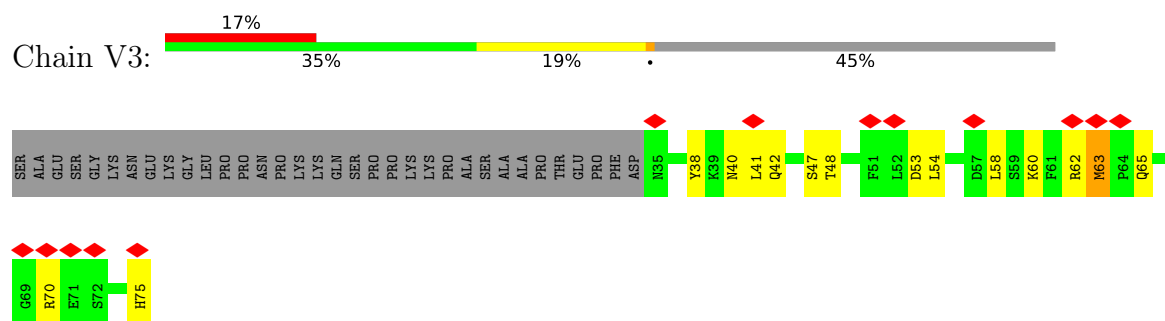
• Molecule 44: NDUFS7



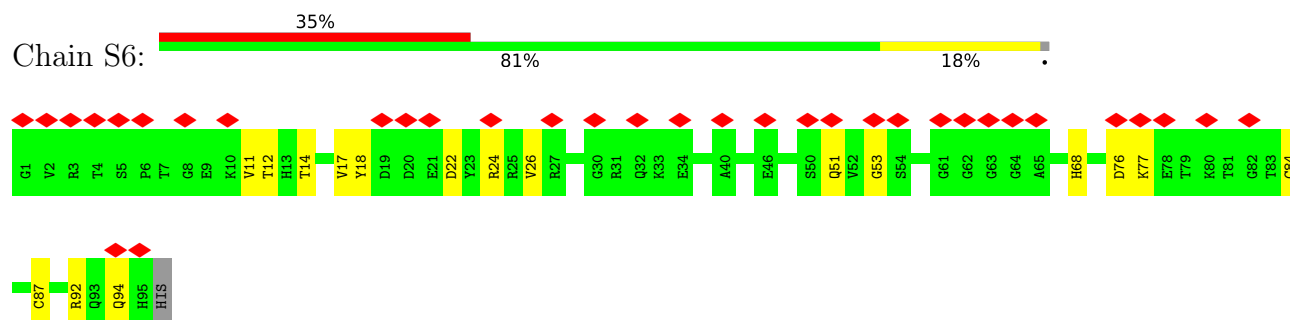
• Molecule 45: NDUFS8



• Molecule 46: NDUFV3

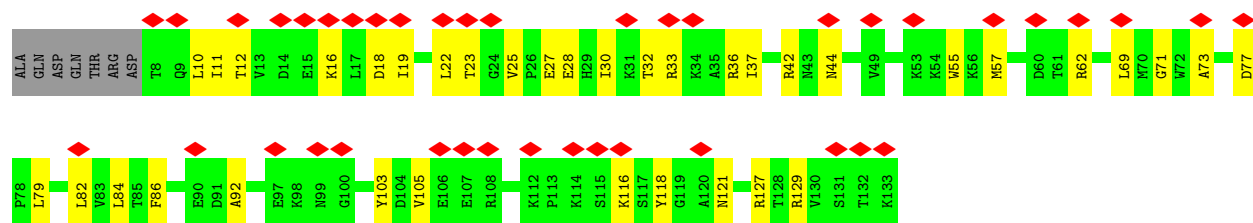


• Molecule 47: NDUFS6

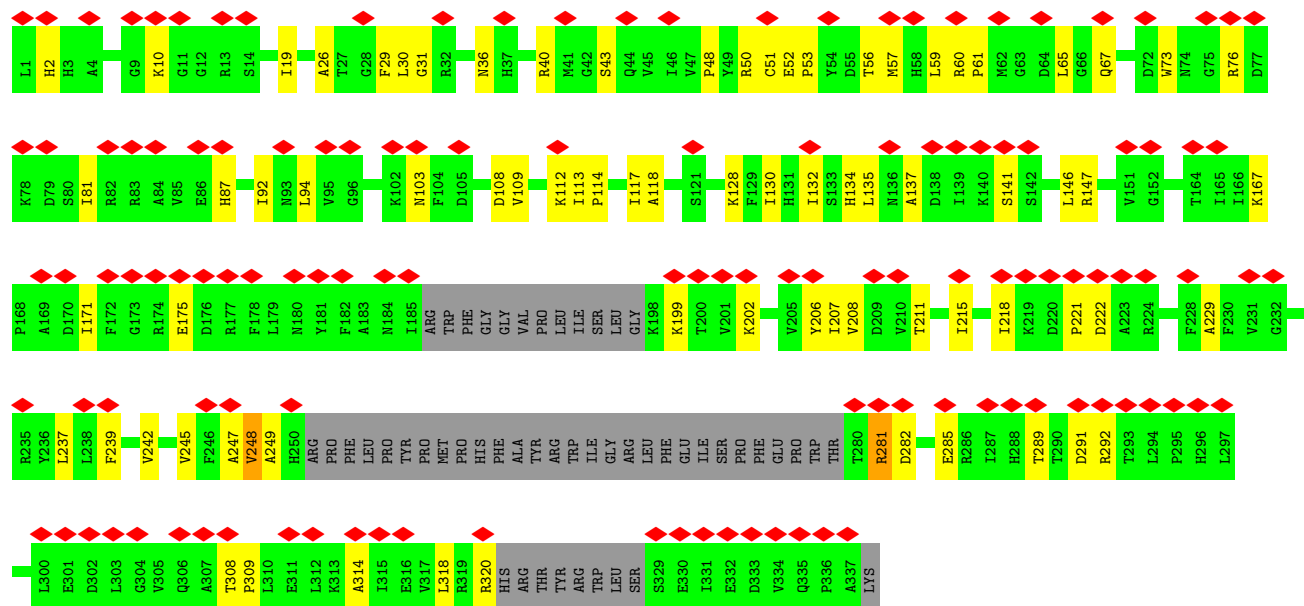
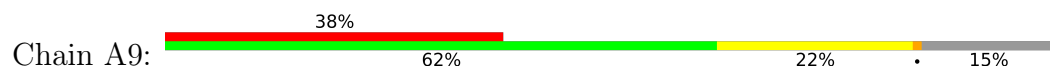


• Molecule 48: NADH:ubiquinone oxidoreductase subunit S4

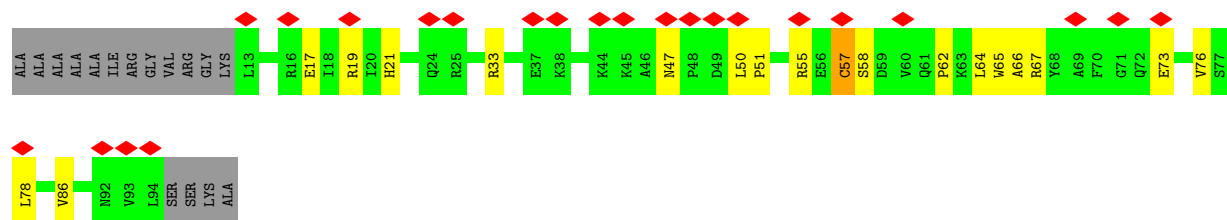




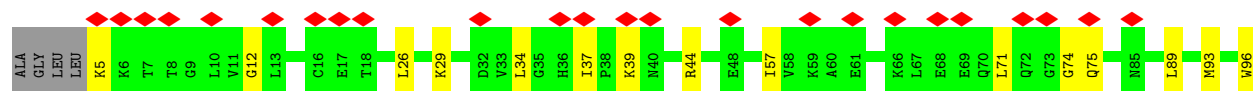
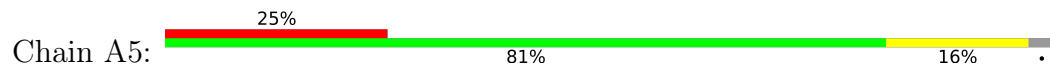
• Molecule 49: NADH:ubiquinone oxidoreductase subunit A9

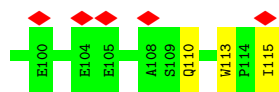


• Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



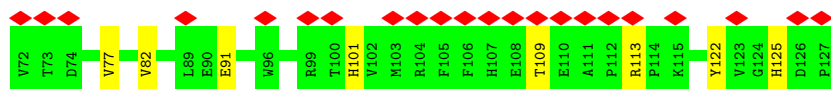
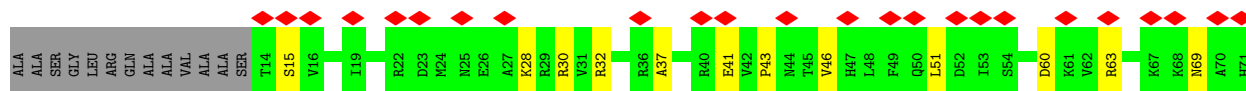
• Molecule 51: NDUFA5





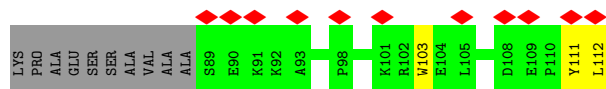
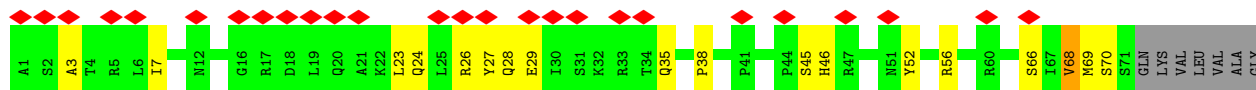
- Molecule 52: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



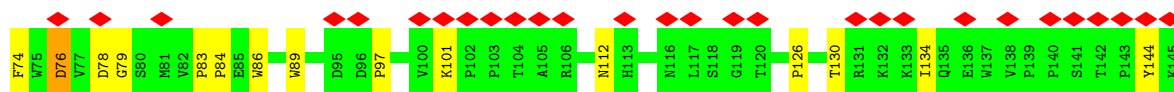
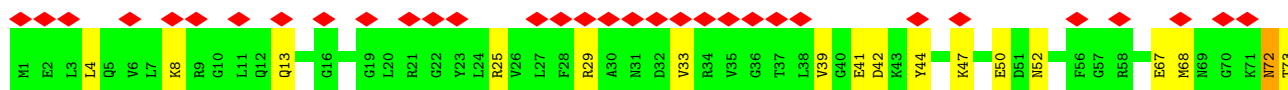
- Molecule 53: NDUFA7

Chain A7:



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

Chain AL:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14230	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 ($e^-/\text{\AA}^2$)	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	0.776	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.12	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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.55	0/4719
1	a3	0.31	0/3518	0.54	0/4776
2	a2	0.30	0/3183	0.53	1/4313 (0.0%)
2	a4	0.31	0/3179	0.52	0/4308
3	b1	0.33	0/3119	0.56	0/4268
3	b2	0.34	0/3119	0.55	0/4268
4	c1	0.32	0/1960	0.54	0/2660
4	c2	0.32	0/1962	0.55	0/2664
5	f1	0.28	0/1554	0.49	0/2101
5	f2	0.28	0/1548	0.52	0/2093
6	d1	0.30	0/906	0.52	0/1213
6	d2	0.31	0/908	0.52	0/1218
7	q1	0.31	0/638	0.51	0/862
7	q2	0.37	0/652	0.56	0/883
8	h1	0.28	0/538	0.61	0/723
8	h2	0.30	0/538	0.68	1/723 (0.1%)
10	i1	0.31	0/471	0.53	0/634
10	i2	0.30	0/486	0.50	0/655
11	D3	0.31	0/738	0.64	0/1010
12	D1	0.36	0/2442	0.69	3/3337 (0.1%)
13	D6	0.34	0/1339	0.65	0/1810
14	4L	0.32	0/758	0.69	0/1024
15	D5	0.35	0/4933	0.69	5/6710 (0.1%)
16	D4	0.36	0/3740	0.68	3/5095 (0.1%)
17	D2	0.36	0/2788	0.64	1/3795 (0.0%)
18	AK	0.33	0/1046	0.64	1/1419 (0.1%)
19	B5	0.32	0/1189	0.54	1/1607 (0.1%)
20	AA	0.30	0/655	0.65	0/881
20	AB	0.33	0/714	0.58	0/963
21	A8	0.34	0/1441	0.65	0/1942
22	BJ	0.32	0/1475	0.58	2/1989 (0.1%)
23	AJ	0.34	0/2644	0.62	3/3579 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
24	S5	0.32	0/843	0.60	1/1128 (0.1%)
25	A3	0.32	0/602	0.67	1/828 (0.1%)
26	B3	0.33	0/595	0.68	0/803
27	C2	0.33	0/1028	0.63	1/1388 (0.1%)
28	B4	0.33	0/1085	0.63	2/1467 (0.1%)
29	AM	0.33	0/1172	0.60	2/1579 (0.1%)
30	B6	0.36	0/835	0.69	0/1137
31	B7	0.33	0/1051	0.64	2/1408 (0.1%)
32	B9	0.34	0/1568	0.59	0/2123
33	B2	0.33	0/587	0.65	0/806
34	B8	0.37	0/1379	0.67	0/1884
35	BK	0.34	0/880	0.61	0/1196
36	C1	0.31	0/404	0.55	0/548
37	B1	0.31	0/462	0.62	1/624 (0.2%)
38	A1	0.32	0/592	0.63	0/795
39	V1	0.33	0/3386	0.58	0/4575
40	V2	0.33	0/1687	0.67	2/2295 (0.1%)
41	S1	0.32	0/5362	0.60	1/7266 (0.0%)
42	S2	0.36	0/3525	0.60	1/4776 (0.0%)
43	S3	0.35	0/1776	0.59	0/2417
44	S7	0.36	0/1278	0.58	0/1728
45	S8	0.40	1/1445 (0.1%)	0.59	0/1956
46	V3	0.33	0/355	0.72	1/480 (0.2%)
47	S6	0.34	0/749	0.54	0/1009
48	S4	0.31	0/1047	0.57	0/1415
49	A9	0.32	0/2317	0.64	1/3131 (0.0%)
50	A2	0.29	0/676	0.60	0/911
51	A5	0.31	0/921	0.60	1/1249 (0.1%)
52	A6	0.30	0/993	0.52	0/1336
53	A7	0.29	0/775	0.64	0/1048
54	AL	0.34	0/1250	0.60	1/1698 (0.1%)
All	All	0.33	1/98285 (0.0%)	0.60	39/133246 (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	2
1	a3	0	1
2	a4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	f2	0	1
12	D1	0	2
13	D6	0	1
15	D5	0	3
16	D4	0	2
18	AK	0	1
20	AA	0	1
21	A8	0	1
23	AJ	0	2
24	S5	0	1
25	A3	0	1
26	B3	0	2
27	C2	0	2
30	B6	0	2
31	B7	0	1
33	B2	0	2
34	B8	0	2
35	BK	0	1
36	C1	0	1
37	B1	0	1
39	V1	0	1
40	V2	0	4
41	S1	0	7
42	S2	0	2
45	S8	0	1
49	A9	0	3
50	A2	0	1
51	A5	0	1
53	A7	0	2
All	All	0	56

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S8	119	CYS	CB-SG	-5.88	1.72	1.81

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D5	69	LEU	CA-CB-CG	7.46	132.46	115.30
16	D4	367	LEU	CA-CB-CG	7.36	132.23	115.30
2	a2	41	TYR	C-N-CA	7.07	139.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	A9	222	ASP	CB-CG-OD1	7.02	124.61	118.30
31	B7	19	LEU	CA-CB-CG	6.76	130.85	115.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a1	190	TYR	Peptide
1	a1	309	THR	Peptide
1	a3	309	THR	Peptide
2	a4	30	PRO	Peptide
5	f2	188	THR	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	1902	0	1851	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	164	0	39	0	0
9	x2	150	0	43	0	0
10	i1	459	0	462	0	0
10	i2	473	0	477	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D3	719	0	765	6	0
12	D1	2372	0	2484	41	0
13	D6	1308	0	1329	22	0
14	4L	748	0	794	16	0
15	D5	4805	0	4950	92	0
16	D4	3646	0	3850	77	0
17	D2	2724	0	2930	47	0
18	AK	1025	0	1033	14	0
19	B5	1156	0	1177	17	0
20	AA	645	0	649	7	0
20	AB	702	0	692	12	0
21	A8	1404	0	1384	19	0
22	BJ	1441	0	1417	22	0
23	AJ	2583	0	2547	48	0
24	S5	822	0	820	16	0
25	A3	582	0	583	9	0
26	B3	578	0	570	8	0
27	C2	997	0	983	22	0
28	B4	1059	0	1062	23	0
29	AM	1143	0	1137	21	0
30	B6	809	0	826	18	0
31	B7	1026	0	995	18	0
32	B9	1515	0	1469	30	0
33	B2	560	0	507	12	0
34	B8	1324	0	1219	22	0
35	BK	853	0	800	14	0
36	C1	391	0	391	5	0
37	B1	449	0	453	3	0
38	A1	577	0	570	6	0
39	V1	3312	0	3266	68	0
40	V2	1647	0	1657	31	0
41	S1	5275	0	5300	116	0
42	S2	3435	0	3377	72	0
43	S3	1726	0	1676	41	0
44	S7	1247	0	1256	35	0
45	S8	1414	0	1370	39	0
46	V3	345	0	323	10	0
47	S6	737	0	710	11	0
48	S4	1024	0	1023	29	0
49	A9	2270	0	2273	52	0
50	A2	665	0	678	12	0
51	A5	901	0	936	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	A6	969	0	980	20	0
53	A7	757	0	771	20	0
54	AL	1209	0	1182	22	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	0	0
57	f1	4	0	0	0	0
57	f2	4	0	0	0	0
58	D2	28	0	30	0	0
59	AA	34	0	40	5	0
59	AB	31	0	34	2	0
60	S1	16	0	0	1	0
60	S7	8	0	0	1	0
60	S8	16	0	0	1	0
60	V1	8	0	0	1	0
61	V1	31	0	19	3	0
62	S6	1	0	0	0	0
63	A9	48	0	26	3	0
All	All	96705	0	96284	1009	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 1009 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S3:80:ALA:HA	43:S3:91:GLU:O	1.15	1.31
43:S3:78:LEU:HA	43:S3:93:VAL:O	1.43	1.14
43:S3:38:GLN:HA	53:A7:70:SER:O	1.50	1.10
15:D5:547:LYS:O	15:D5:552:LEU:HB2	1.60	1.01
43:S3:80:ALA:CA	43:S3:91:GLU:O	2.12	0.96

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a1	435/446 (98%)	399 (92%)	36 (8%)	0	100	100
1	a3	442/446 (99%)	403 (91%)	39 (9%)	0	100	100
2	a2	410/439 (93%)	381 (93%)	29 (7%)	0	100	100
2	a4	409/439 (93%)	375 (92%)	34 (8%)	0	100	100
3	b1	376/379 (99%)	360 (96%)	16 (4%)	0	100	100
3	b2	376/379 (99%)	353 (94%)	23 (6%)	0	100	100
4	c1	236/240 (98%)	200 (85%)	36 (15%)	0	100	100
4	c2	236/240 (98%)	199 (84%)	37 (16%)	0	100	100
5	f1	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
5	f2	193/196 (98%)	173 (90%)	20 (10%)	0	100	100
6	d1	98/110 (89%)	90 (92%)	8 (8%)	0	100	100
6	d2	99/110 (90%)	92 (93%)	7 (7%)	0	100	100
7	q1	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
7	q2	73/81 (90%)	66 (90%)	7 (10%)	0	100	100
8	h1	63/78 (81%)	59 (94%)	4 (6%)	0	100	100
8	h2	63/78 (81%)	57 (90%)	6 (10%)	0	100	100
10	i1	53/63 (84%)	49 (92%)	4 (8%)	0	100	100
10	i2	55/63 (87%)	49 (89%)	6 (11%)	0	100	100
11	D3	85/115 (74%)	80 (94%)	5 (6%)	0	100	100
12	D1	292/318 (92%)	266 (91%)	25 (9%)	1 (0%)	37	72
13	D6	167/175 (95%)	142 (85%)	24 (14%)	1 (1%)	22	59
14	4L	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
15	D5	604/606 (100%)	538 (89%)	63 (10%)	3 (0%)	25	64
16	D4	457/459 (100%)	415 (91%)	41 (9%)	1 (0%)	44	78
17	D2	345/347 (99%)	318 (92%)	27 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AK	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
19	B5	137/143 (96%)	124 (90%)	13 (10%)	0	100	100
20	AA	78/88 (89%)	65 (83%)	13 (17%)	0	100	100
20	AB	85/88 (97%)	78 (92%)	7 (8%)	0	100	100
21	A8	169/171 (99%)	140 (83%)	29 (17%)	0	100	100
22	BJ	169/175 (97%)	148 (88%)	20 (12%)	1 (1%)	22	59
23	AJ	317/320 (99%)	280 (88%)	36 (11%)	1 (0%)	37	72
24	S5	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
25	A3	72/83 (87%)	60 (83%)	12 (17%)	0	100	100
26	B3	71/97 (73%)	54 (76%)	16 (22%)	1 (1%)	9	40
27	C2	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
28	B4	126/128 (98%)	109 (86%)	17 (14%)	0	100	100
29	AM	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
30	B6	92/127 (72%)	78 (85%)	14 (15%)	0	100	100
31	B7	117/119 (98%)	93 (80%)	24 (20%)	0	100	100
32	B9	174/178 (98%)	144 (83%)	29 (17%)	1 (1%)	22	59
33	B2	63/72 (88%)	56 (89%)	7 (11%)	0	100	100
34	B8	155/158 (98%)	121 (78%)	33 (21%)	1 (1%)	22	59
35	BK	100/125 (80%)	84 (84%)	16 (16%)	0	100	100
36	C1	44/49 (90%)	37 (84%)	7 (16%)	0	100	100
37	B1	50/57 (88%)	45 (90%)	5 (10%)	0	100	100
38	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
39	V1	428/445 (96%)	386 (90%)	42 (10%)	0	100	100
40	V2	210/217 (97%)	172 (82%)	38 (18%)	0	100	100
41	S1	686/704 (97%)	616 (90%)	69 (10%)	1 (0%)	48	83
42	S2	423/430 (98%)	377 (89%)	43 (10%)	3 (1%)	19	56
43	S3	206/228 (90%)	174 (84%)	32 (16%)	0	100	100
44	S7	154/179 (86%)	133 (86%)	20 (13%)	1 (1%)	22	59
45	S8	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
46	V3	39/75 (52%)	29 (74%)	10 (26%)	0	100	100
47	S6	93/96 (97%)	87 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	S4	124/133 (93%)	107 (86%)	17 (14%)	0	100	100
49	A9	280/338 (83%)	241 (86%)	39 (14%)	0	100	100
50	A2	80/98 (82%)	67 (84%)	13 (16%)	0	100	100
51	A5	109/115 (95%)	93 (85%)	16 (15%)	0	100	100
52	A6	112/127 (88%)	102 (91%)	10 (9%)	0	100	100
53	A7	91/112 (81%)	76 (84%)	15 (16%)	0	100	100
54	AL	143/145 (99%)	121 (85%)	22 (15%)	0	100	100
All	All	11856/12556 (94%)	10556 (89%)	1284 (11%)	16 (0%)	50	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	D5	84	PHE
16	D4	53	SER
42	S2	293	CYS
42	S2	340	THR
44	S7	130	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a1	366/372 (98%)	361 (99%)	5 (1%)	62	75
1	a3	370/372 (100%)	363 (98%)	7 (2%)	52	69
2	a2	326/341 (96%)	322 (99%)	4 (1%)	67	79
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	91
4	c1	204/206 (99%)	201 (98%)	3 (2%)	60	75
4	c2	204/206 (99%)	201 (98%)	3 (2%)	60	75
5	f1	168/168 (100%)	167 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	f2	167/168 (99%)	166 (99%)	1 (1%)	84	88
6	d1	93/99 (94%)	93 (100%)	0	100	100
6	d2	94/99 (95%)	91 (97%)	3 (3%)	34	54
7	q1	66/72 (92%)	66 (100%)	0	100	100
7	q2	67/72 (93%)	66 (98%)	1 (2%)	60	75
8	h1	62/74 (84%)	62 (100%)	0	100	100
8	h2	62/74 (84%)	62 (100%)	0	100	100
10	i1	46/52 (88%)	45 (98%)	1 (2%)	47	65
10	i2	48/52 (92%)	48 (100%)	0	100	100
11	D3	80/103 (78%)	78 (98%)	2 (2%)	42	62
12	D1	260/278 (94%)	257 (99%)	3 (1%)	67	79
13	D6	140/144 (97%)	140 (100%)	0	100	100
14	4L	87/87 (100%)	85 (98%)	2 (2%)	45	64
15	D5	539/539 (100%)	535 (99%)	4 (1%)	81	87
16	D4	412/412 (100%)	407 (99%)	5 (1%)	67	79
17	D2	315/315 (100%)	311 (99%)	4 (1%)	65	77
18	AK	101/101 (100%)	100 (99%)	1 (1%)	73	81
19	B5	122/125 (98%)	121 (99%)	1 (1%)	79	84
20	AA	74/81 (91%)	74 (100%)	0	100	100
20	AB	80/81 (99%)	78 (98%)	2 (2%)	42	62
21	A8	154/154 (100%)	150 (97%)	4 (3%)	41	60
22	BJ	155/157 (99%)	154 (99%)	1 (1%)	84	88
23	AJ	283/284 (100%)	282 (100%)	1 (0%)	89	90
24	S5	88/94 (94%)	88 (100%)	0	100	100
25	A3	65/71 (92%)	65 (100%)	0	100	100
26	B3	55/75 (73%)	53 (96%)	2 (4%)	30	51
27	C2	106/107 (99%)	106 (100%)	0	100	100
28	B4	114/114 (100%)	113 (99%)	1 (1%)	75	83
29	AM	119/121 (98%)	115 (97%)	4 (3%)	32	53
30	B6	91/121 (75%)	88 (97%)	3 (3%)	33	54
31	B7	108/108 (100%)	104 (96%)	4 (4%)	29	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	B9	159/160 (99%)	157 (99%)	2 (1%)	65	77
33	B2	58/62 (94%)	58 (100%)	0	100	100
34	B8	142/142 (100%)	140 (99%)	2 (1%)	62	75
35	BK	93/112 (83%)	92 (99%)	1 (1%)	70	80
36	C1	42/44 (96%)	42 (100%)	0	100	100
37	B1	48/53 (91%)	48 (100%)	0	100	100
38	A1	59/59 (100%)	56 (95%)	3 (5%)	20	41
39	V1	344/354 (97%)	340 (99%)	4 (1%)	67	79
40	V2	182/183 (100%)	181 (100%)	1 (0%)	86	89
41	S1	578/588 (98%)	573 (99%)	5 (1%)	75	83
42	S2	370/371 (100%)	367 (99%)	3 (1%)	79	84
43	S3	189/204 (93%)	189 (100%)	0	100	100
44	S7	132/150 (88%)	130 (98%)	2 (2%)	60	75
45	S8	151/151 (100%)	150 (99%)	1 (1%)	81	87
46	V3	40/68 (59%)	37 (92%)	3 (8%)	11	31
47	S6	79/80 (99%)	79 (100%)	0	100	100
48	S4	113/119 (95%)	112 (99%)	1 (1%)	75	83
49	A9	239/292 (82%)	235 (98%)	4 (2%)	56	72
50	A2	73/81 (90%)	72 (99%)	1 (1%)	62	75
51	A5	99/101 (98%)	99 (100%)	0	100	100
52	A6	107/113 (95%)	107 (100%)	0	100	100
53	A7	83/94 (88%)	83 (100%)	0	100	100
54	AL	131/131 (100%)	128 (98%)	3 (2%)	45	64
All	All	10388/10814 (96%)	10273 (99%)	115 (1%)	69	80

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	AB	33	ASN
49	A9	320	ARG
29	AM	89	ASN
49	A9	292	ARG
42	S2	388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
41	S1	430	GLN
41	S1	682	GLN
49	A9	67	GLN
15	D5	113	ASN
14	4L	83	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	f2	501	5	0,4,4	-	-	-		
60	SF4	S8	202	45	0,12,12	-	-	-		
56	HEC	c1	501	4	32,50,50	2.07	4 (12%)	24,82,82	2.44	14 (58%)
59	ZMP	AB	101	20	24,30,36	0.92	1 (4%)	29,37,45	1.12	2 (6%)
57	FES	S1	803	41	0,4,4	-	-	-		
63	NDP	A9	401	-	45,52,52	0.61	1 (2%)	53,80,80	0.68	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PC1	D2	401	-	27,27,53	0.40	0	33,35,61	0.35	0
55	HEM	b2	401	3	41,50,50	1.32	4 (9%)	45,82,82	1.76	7 (15%)
60	SF4	S1	801	41	0,12,12	-	-	-	-	-
60	SF4	S7	300	44	0,12,12	-	-	-	-	-
57	FES	f1	501	5	0,4,4	-	-	-	-	-
55	HEM	b2	402	3	41,50,50	1.35	4 (9%)	45,82,82	1.78	9 (20%)
61	FMN	V1	501	-	33,33,33	0.20	0	48,50,50	0.42	0
55	HEM	b1	402	3	41,50,50	1.35	5 (12%)	45,82,82	1.82	9 (20%)
59	ZMP	AA	101	20	27,33,36	0.69	1 (3%)	32,40,45	1.00	2 (6%)
55	HEM	b1	401	3	41,50,50	1.33	4 (9%)	45,82,82	1.88	10 (22%)
60	SF4	S1	802	41	0,12,12	-	-	-	-	-
60	SF4	S8	201	45	0,12,12	-	-	-	-	-
56	HEC	c2	501	4	32,50,50	2.08	4 (12%)	24,82,82	2.13	11 (45%)
57	FES	V2	300	40	0,4,4	-	-	-	-	-
60	SF4	V1	500	39	0,12,12	-	-	-	-	-

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	f2	501	5	-	-	0/1/1/1
60	SF4	S8	202	45	-	-	0/6/5/5
56	HEC	c1	501	4	-	4/10/54/54	-
59	ZMP	AB	101	20	-	13/35/37/43	-
57	FES	S1	803	41	-	-	0/1/1/1
63	NDP	A9	401	-	-	8/30/77/77	0/5/5/5
58	PC1	D2	401	-	-	12/31/31/57	-
55	HEM	b2	401	3	-	2/12/54/54	-
60	SF4	S1	801	41	-	-	0/6/5/5
60	SF4	S7	300	44	-	-	0/6/5/5
57	FES	f1	501	5	-	-	0/1/1/1
55	HEM	b2	402	3	-	6/12/54/54	-
61	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
55	HEM	b1	402	3	-	6/12/54/54	-
59	ZMP	AA	101	20	-	13/38/40/43	-
55	HEM	b1	401	3	-	3/12/54/54	-
60	SF4	S1	802	41	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	S8	201	45	-	-	0/6/5/5
56	HEC	c2	501	4	-	2/10/54/54	-
57	FES	V2	300	40	-	-	0/1/1/1
60	SF4	V1	500	39	-	-	0/6/5/5

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	c1	501	HEC	C3C-C2C	-6.73	1.33	1.40
56	c2	501	HEC	C3C-C2C	-6.69	1.33	1.40
56	c2	501	HEC	C2B-C3B	-6.52	1.33	1.40
56	c1	501	HEC	C2B-C3B	-6.40	1.34	1.40
55	b1	402	HEM	C4D-ND	-4.15	1.33	1.40

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	b1	401	HEM	CHC-C4B-NB	5.14	130.02	124.43
55	b1	402	HEM	CHC-C4B-NB	5.13	130.00	124.43
55	b2	401	HEM	CHC-C4B-NB	5.01	129.87	124.43
56	c1	501	HEC	CBD-CAD-C3D	4.74	120.71	112.62
55	b2	402	HEM	CHC-C4B-NB	4.66	129.50	124.43

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

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

There are no ring outliers.

8 monomers are involved in 17 short contacts:

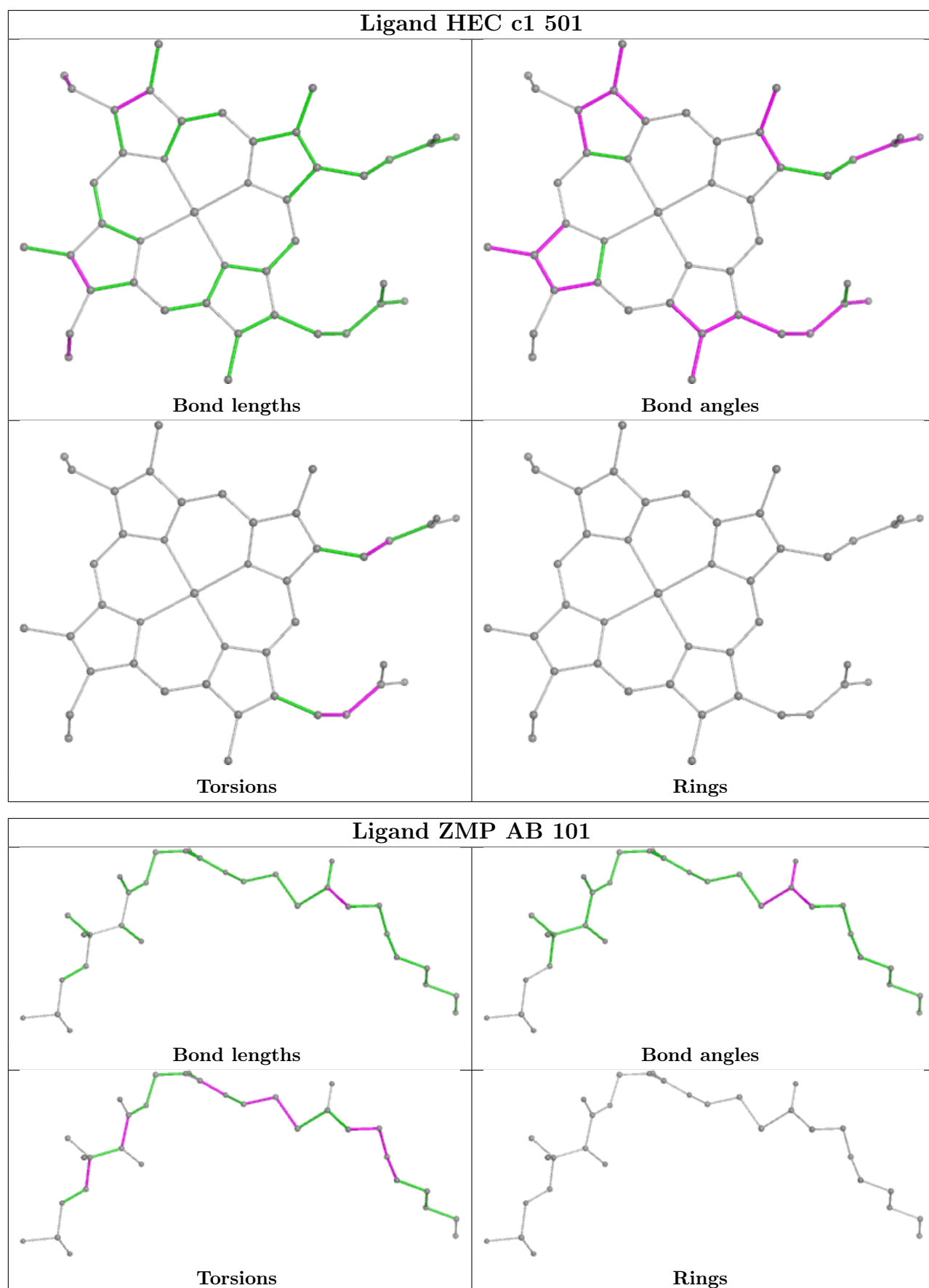
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AB	101	ZMP	2	0
63	A9	401	NDP	3	0
60	S1	801	SF4	1	0
60	S7	300	SF4	1	0

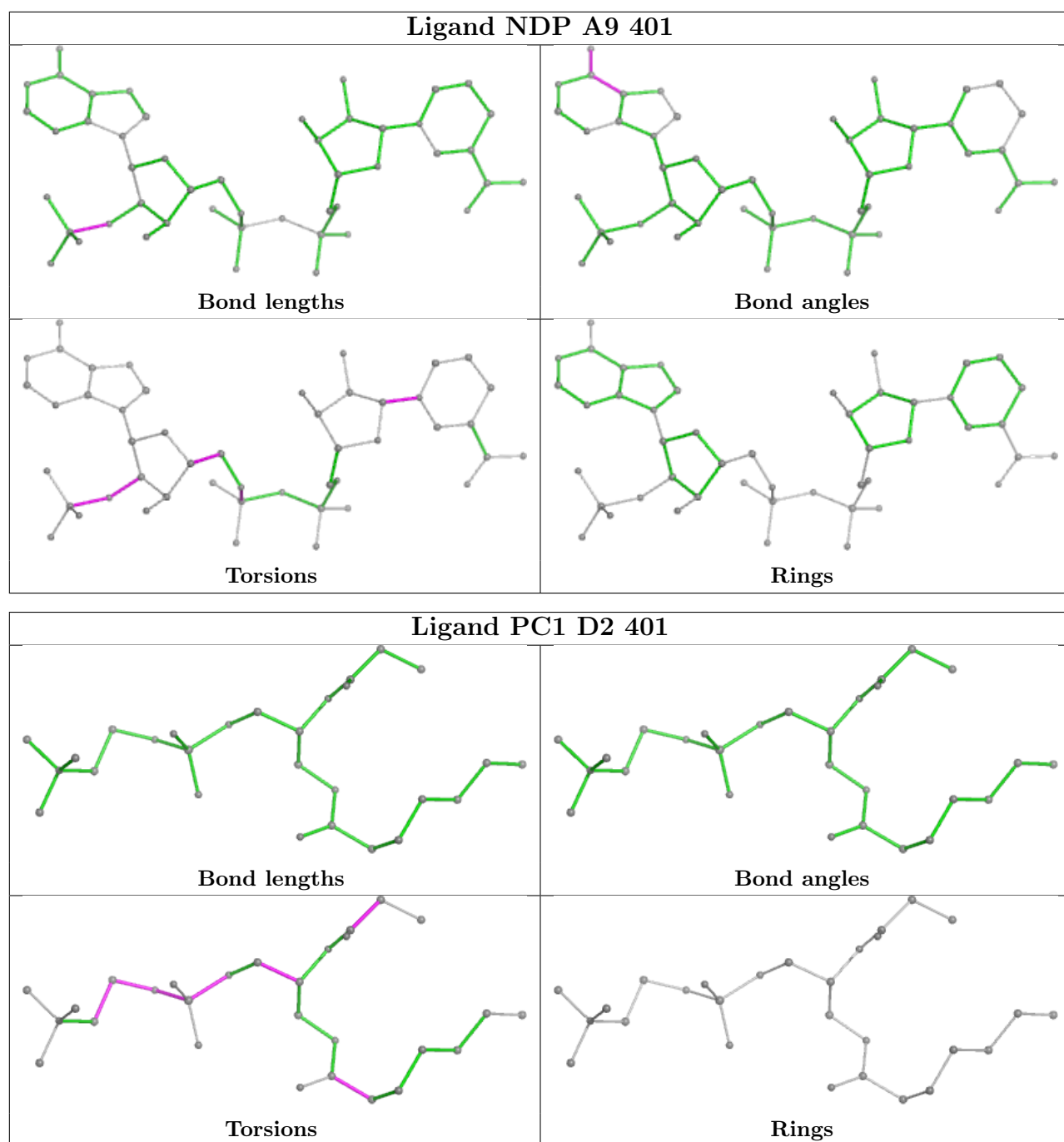
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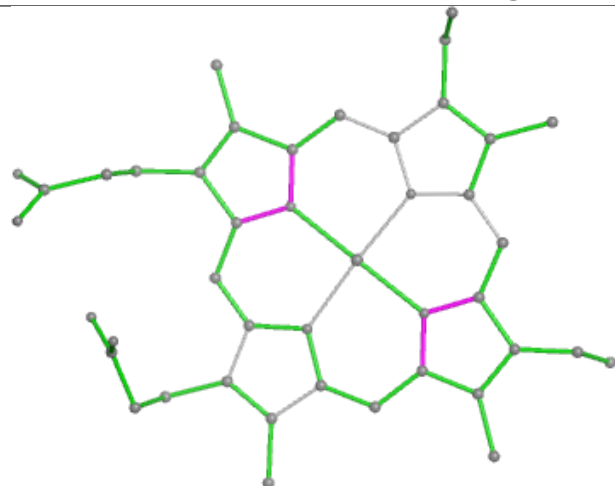
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	V1	501	FMN	3	0
59	AA	101	ZMP	5	0
60	S8	201	SF4	1	0
60	V1	500	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

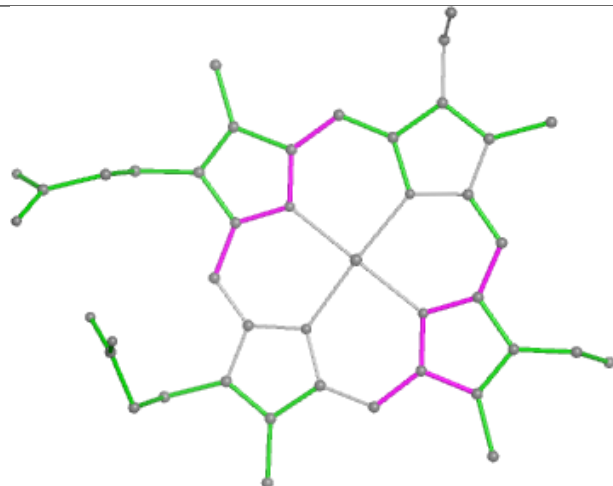




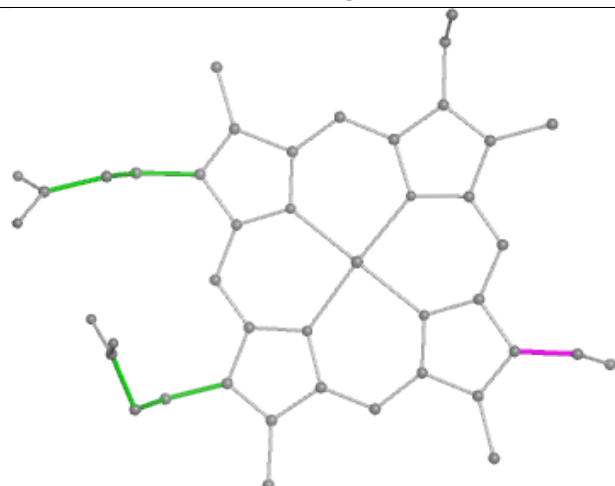
Ligand HEM b2 401



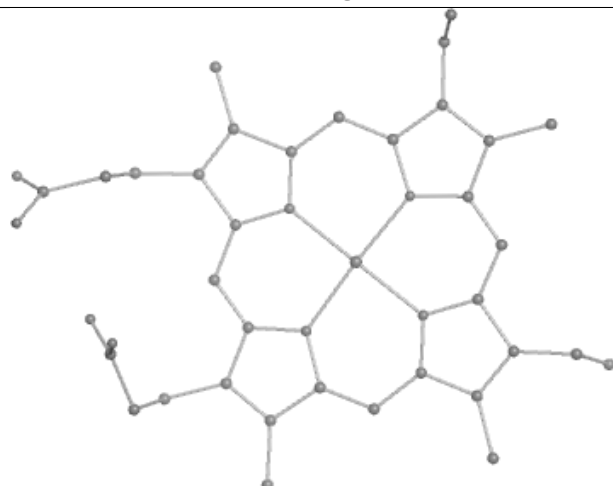
Bond lengths



Bond angles

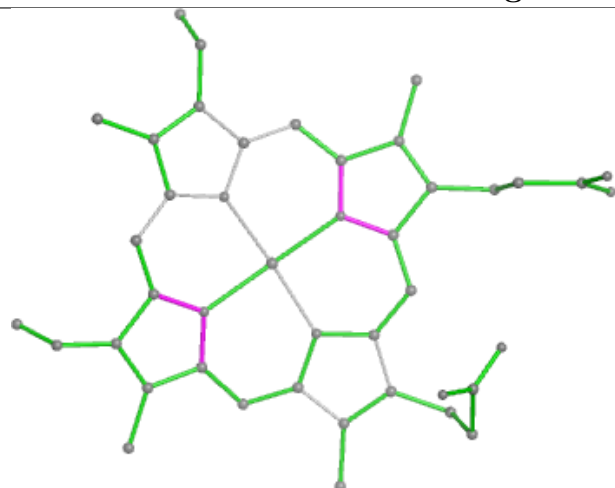


Torsions

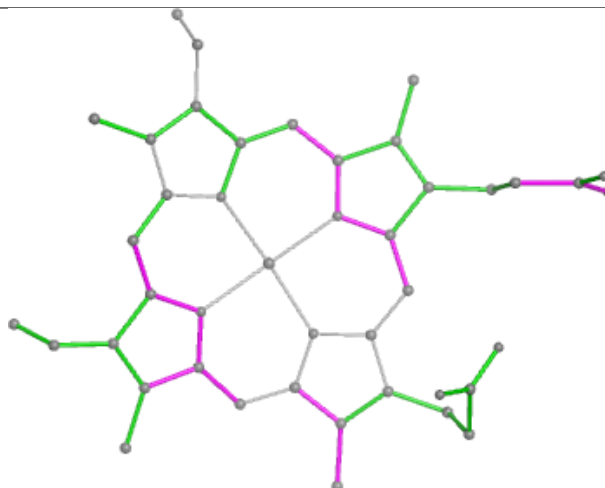


Rings

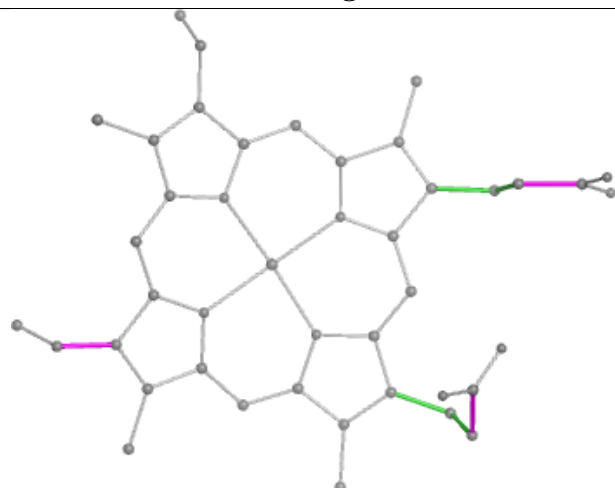
Ligand HEM b2 402



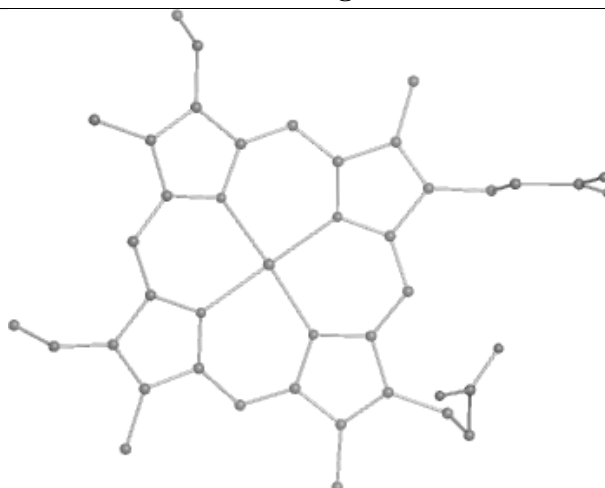
Bond lengths



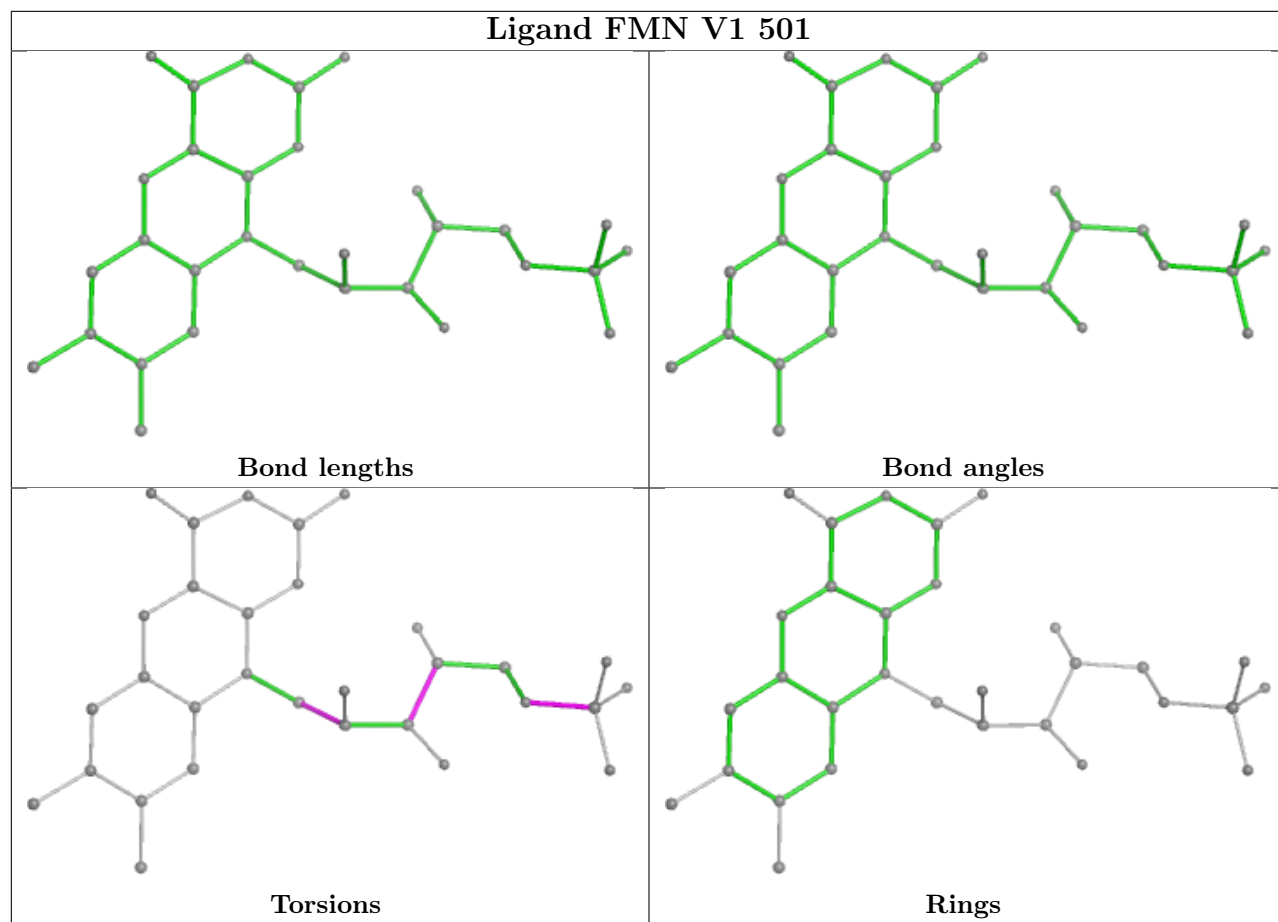
Bond angles



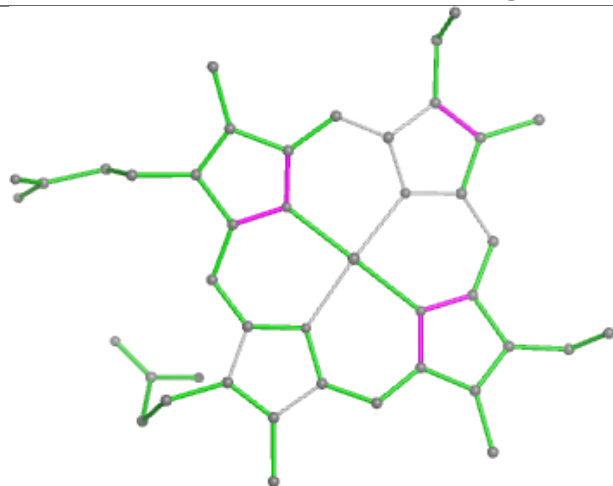
Torsions



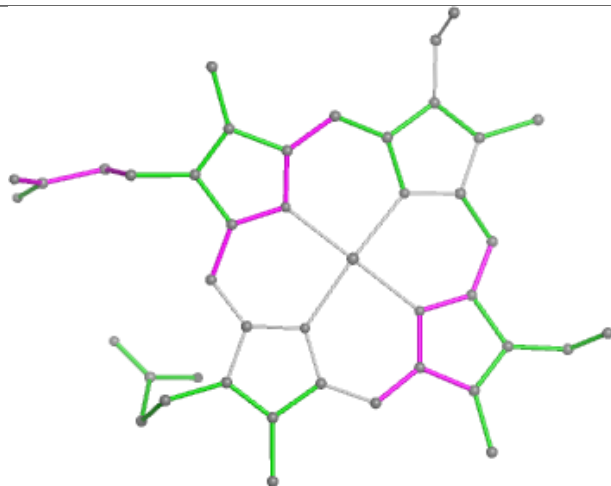
Rings



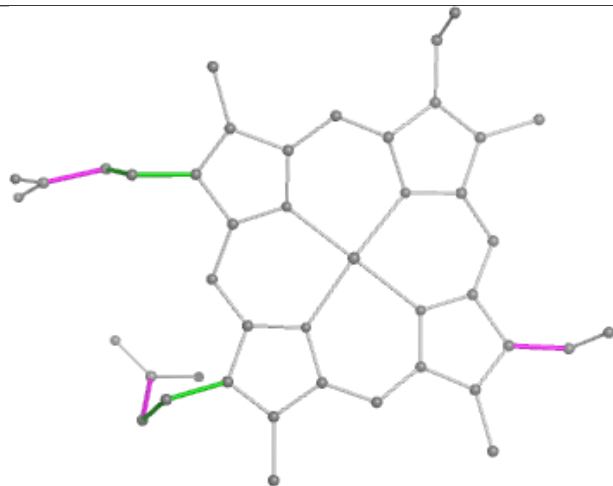
Ligand HEM b1 402



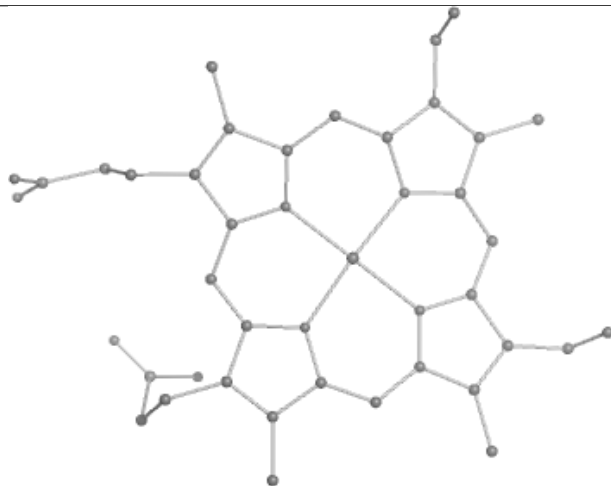
Bond lengths



Bond angles

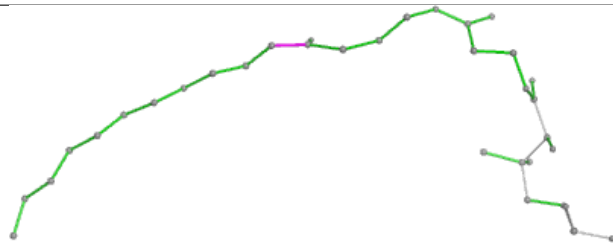


Torsions

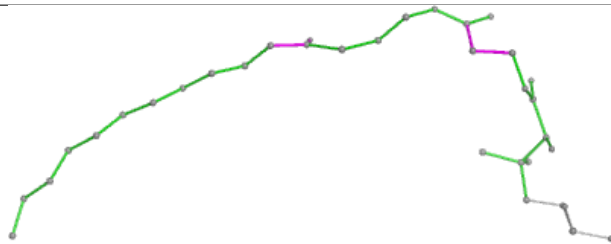


Rings

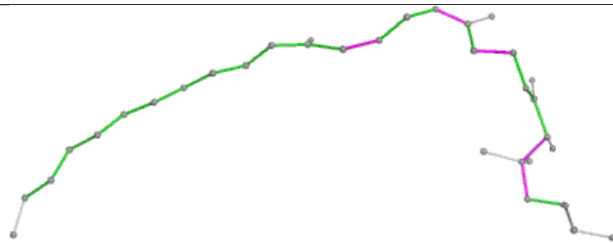
Ligand ZMP AA 101



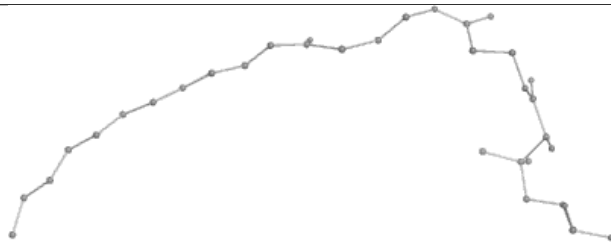
Bond lengths



Bond angles

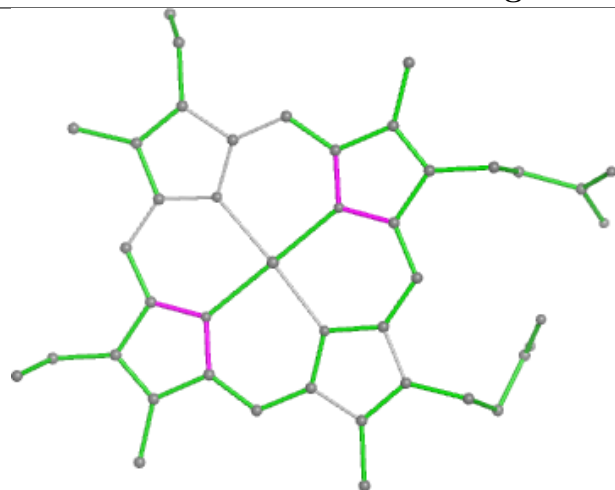


Torsions

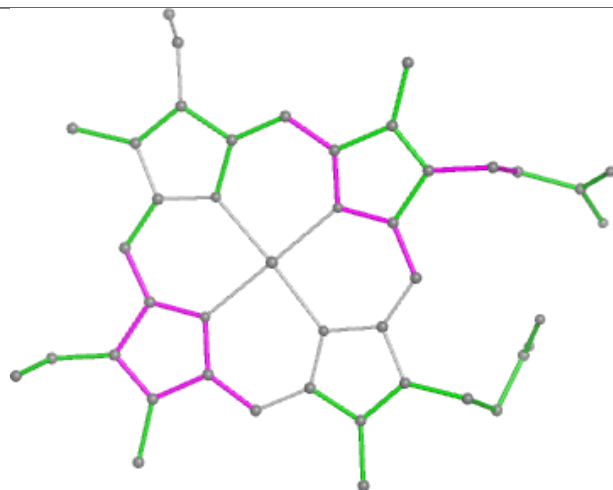


Rings

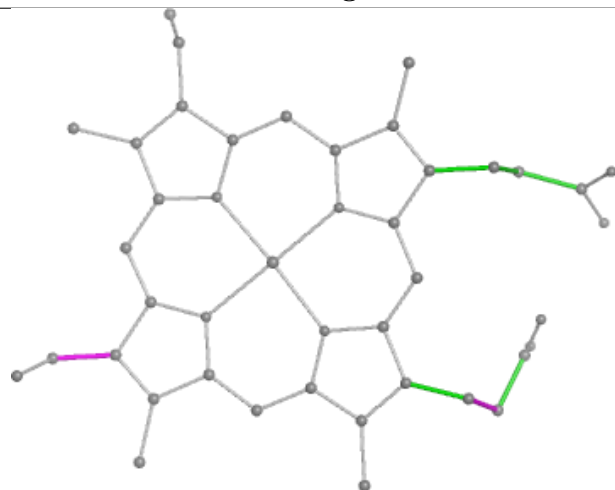
Ligand HEM b1 401



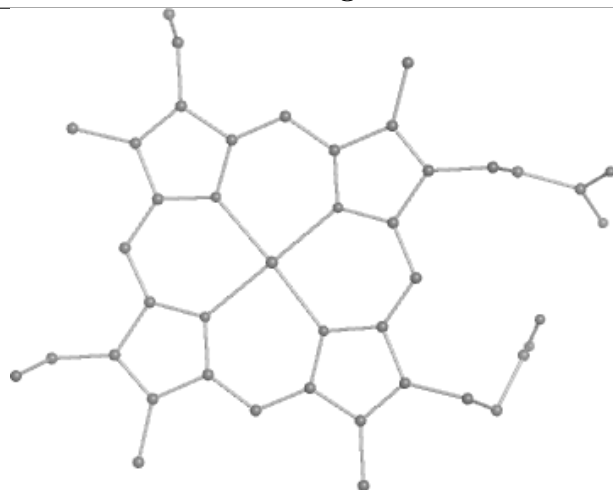
Bond lengths



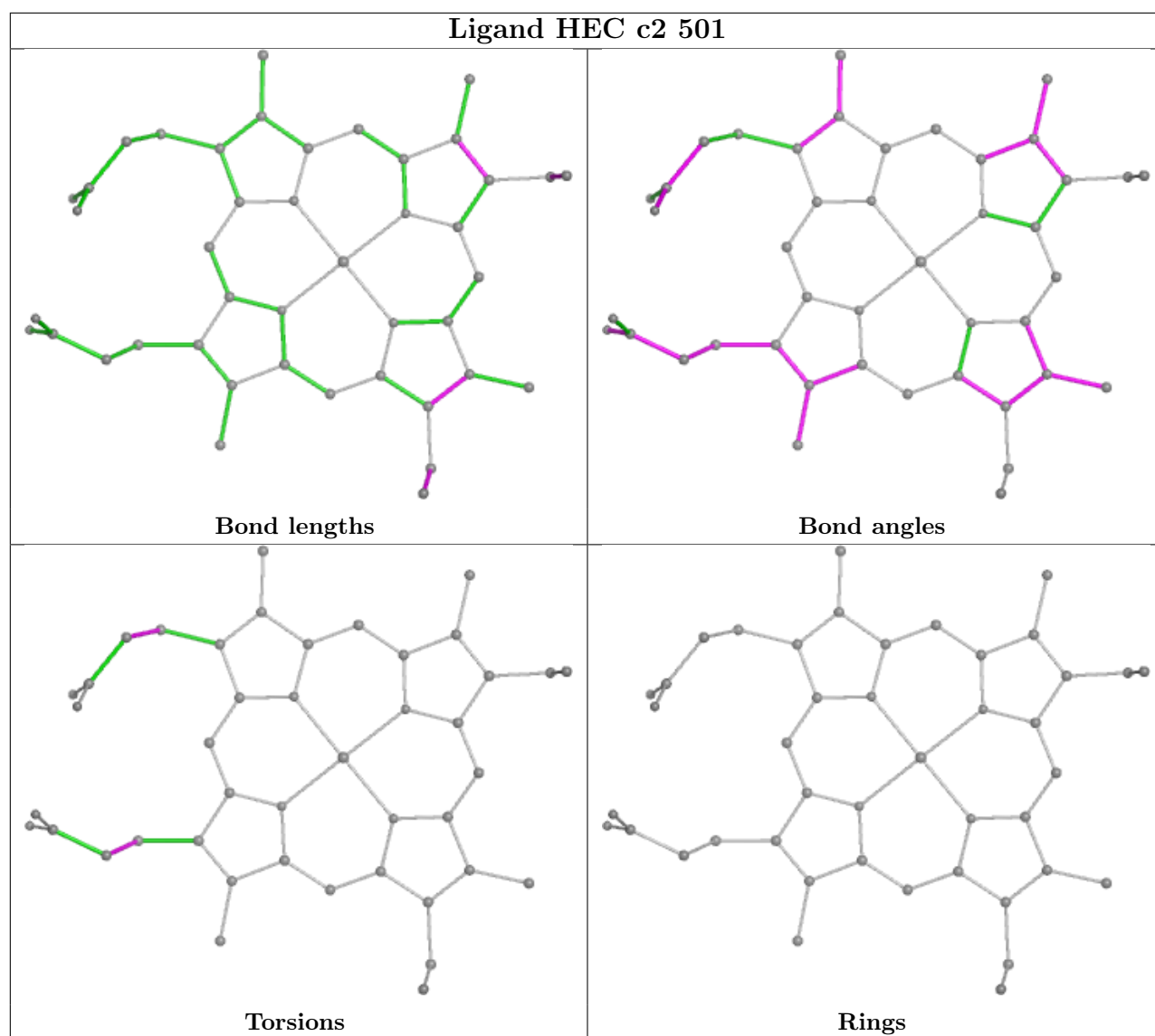
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	x2	1
9	x1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x2	26:UNK	C	45:UNK	N	26.45
1	x1	27:UNK	C	29:UNK	N	5.41

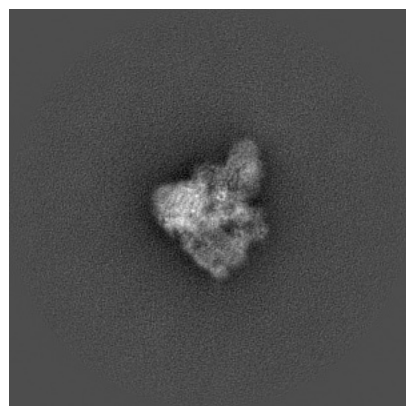
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4496. These allow visual inspection of the internal detail of the map and identification of artifacts.

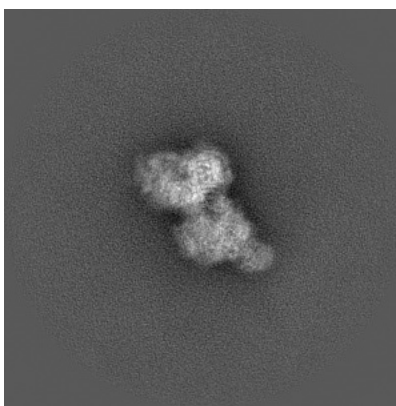
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

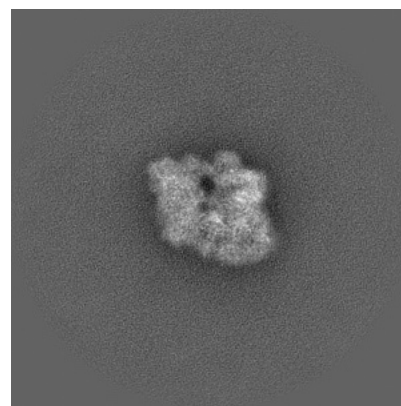
6.1.1 Primary map



X

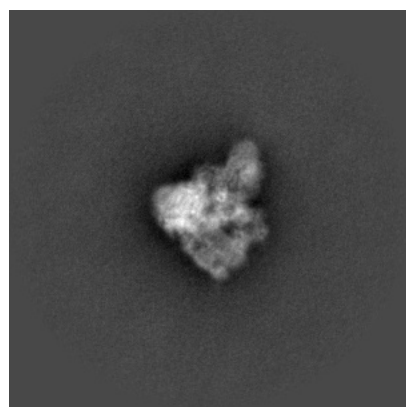


Y

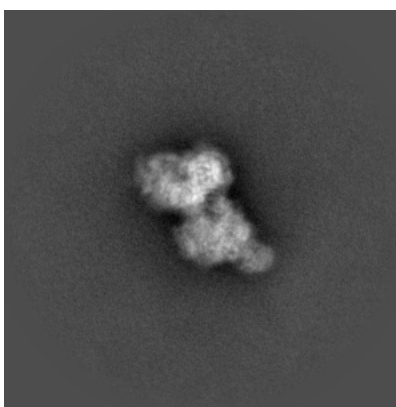


Z

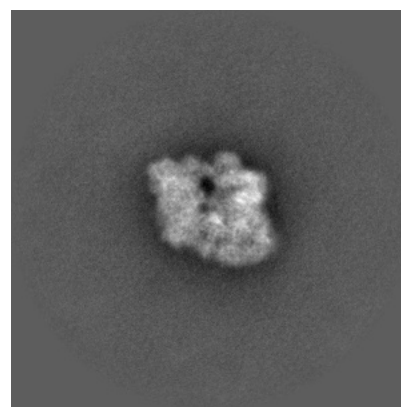
6.1.2 Raw map



X



Y

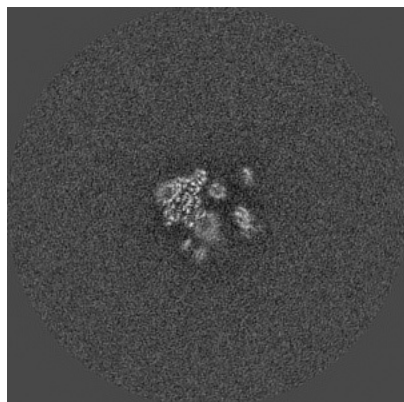


Z

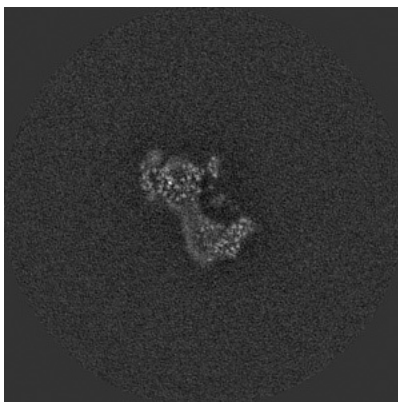
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

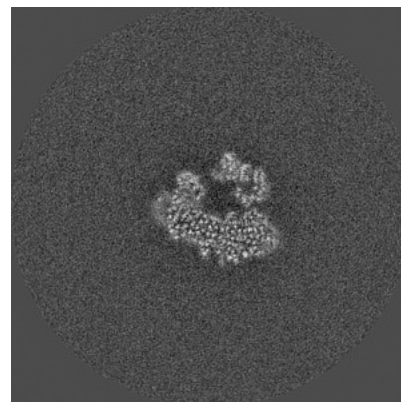
6.2.1 Primary map



X Index: 256

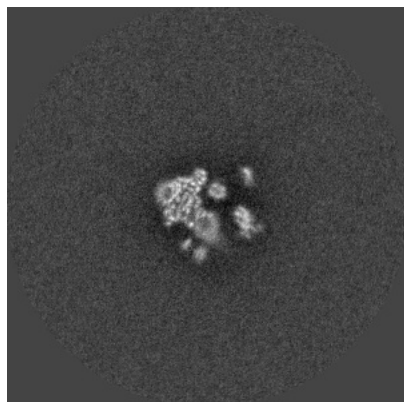


Y Index: 256

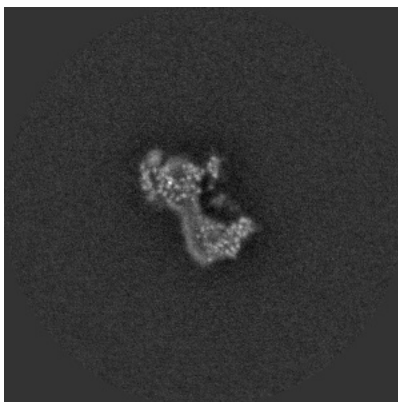


Z Index: 256

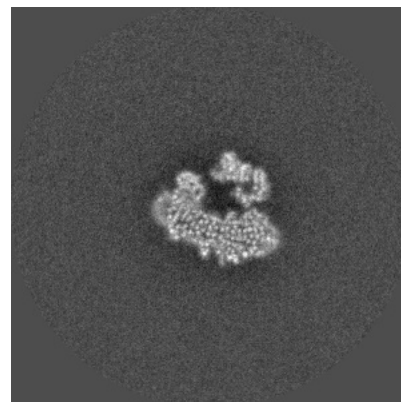
6.2.2 Raw map



X Index: 256



Y Index: 256

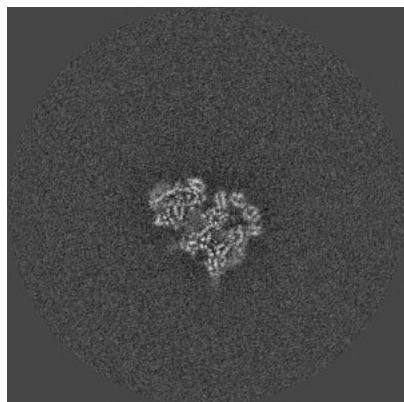


Z Index: 256

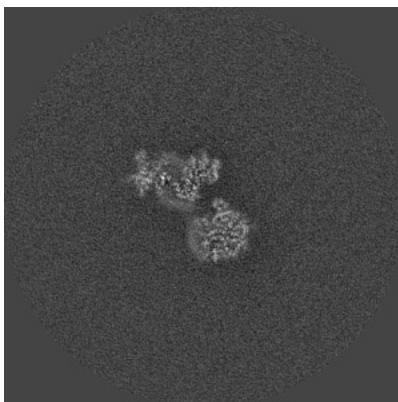
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

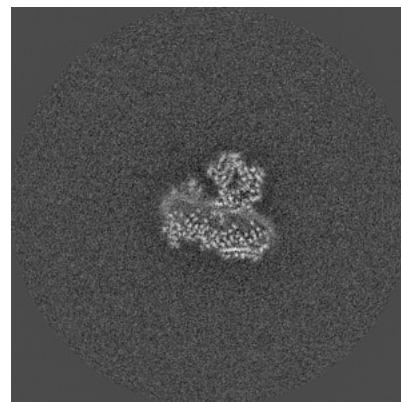
6.3.1 Primary map



X Index: 290

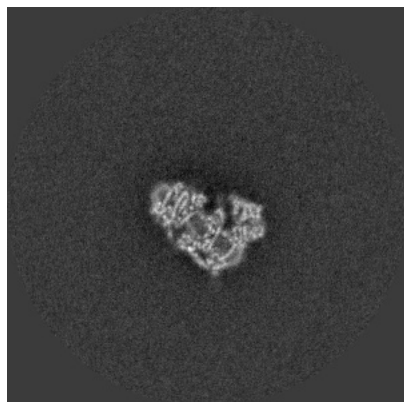


Y Index: 267

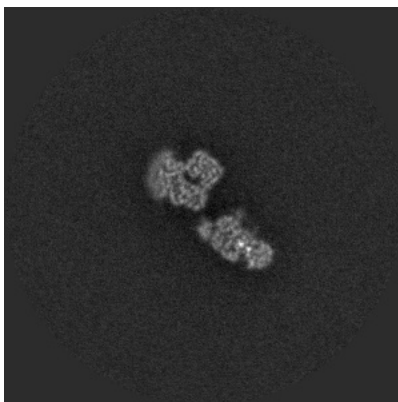


Z Index: 243

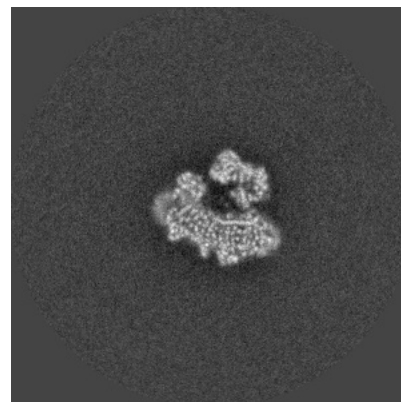
6.3.2 Raw map



X Index: 284



Y Index: 296

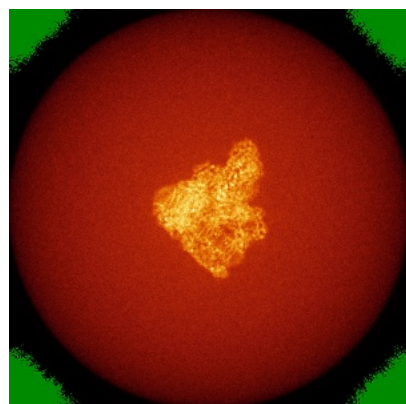


Z Index: 253

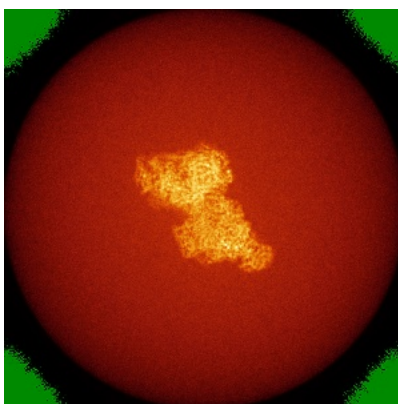
The images above show the largest variance slices of the map in three orthogonal directions.

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

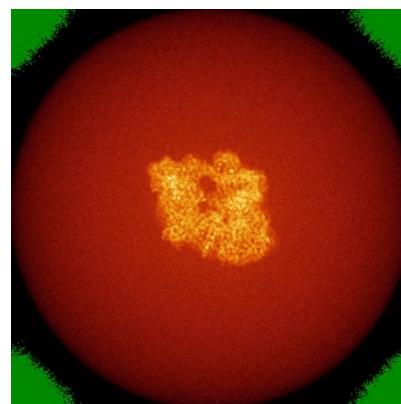
6.4.1 Primary map



X

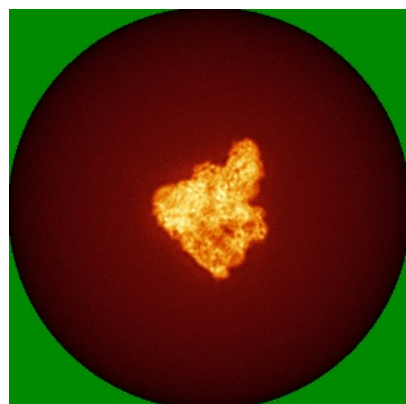


Y

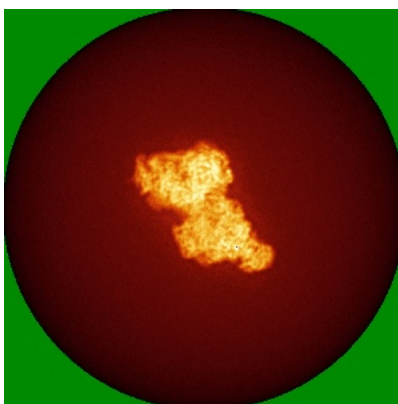


Z

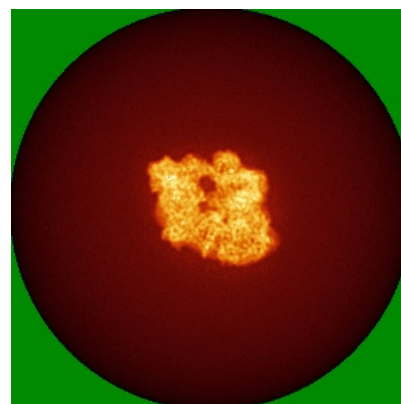
6.4.2 Raw map



X



Y

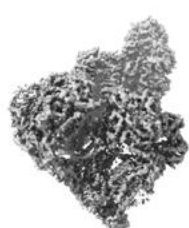


Z

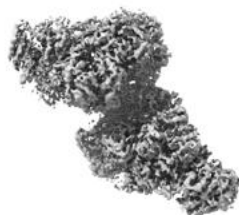
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

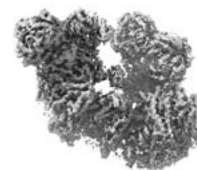
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

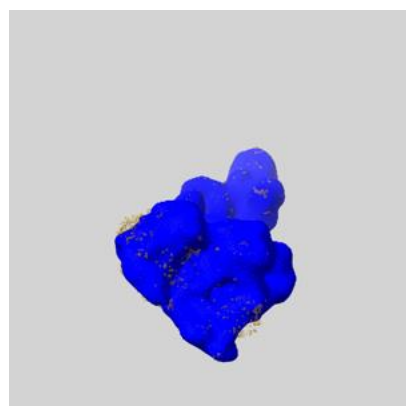
6.6 Mask visualisation [i](#)

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

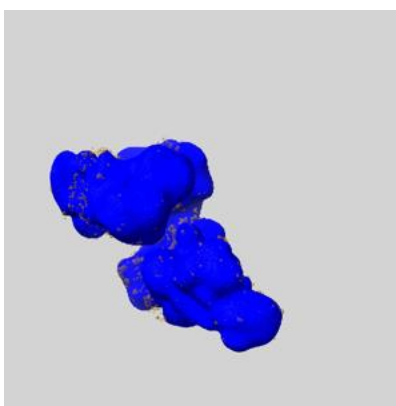
A mask typically either:

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

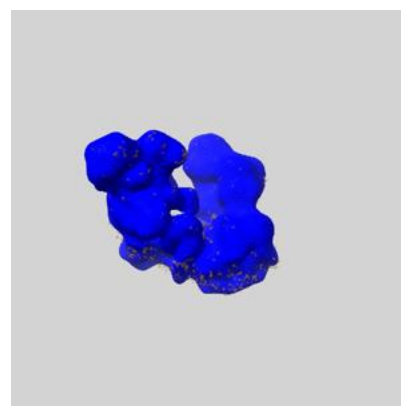
6.6.1 emd_4496_msk_1.map [i](#)



X



Y

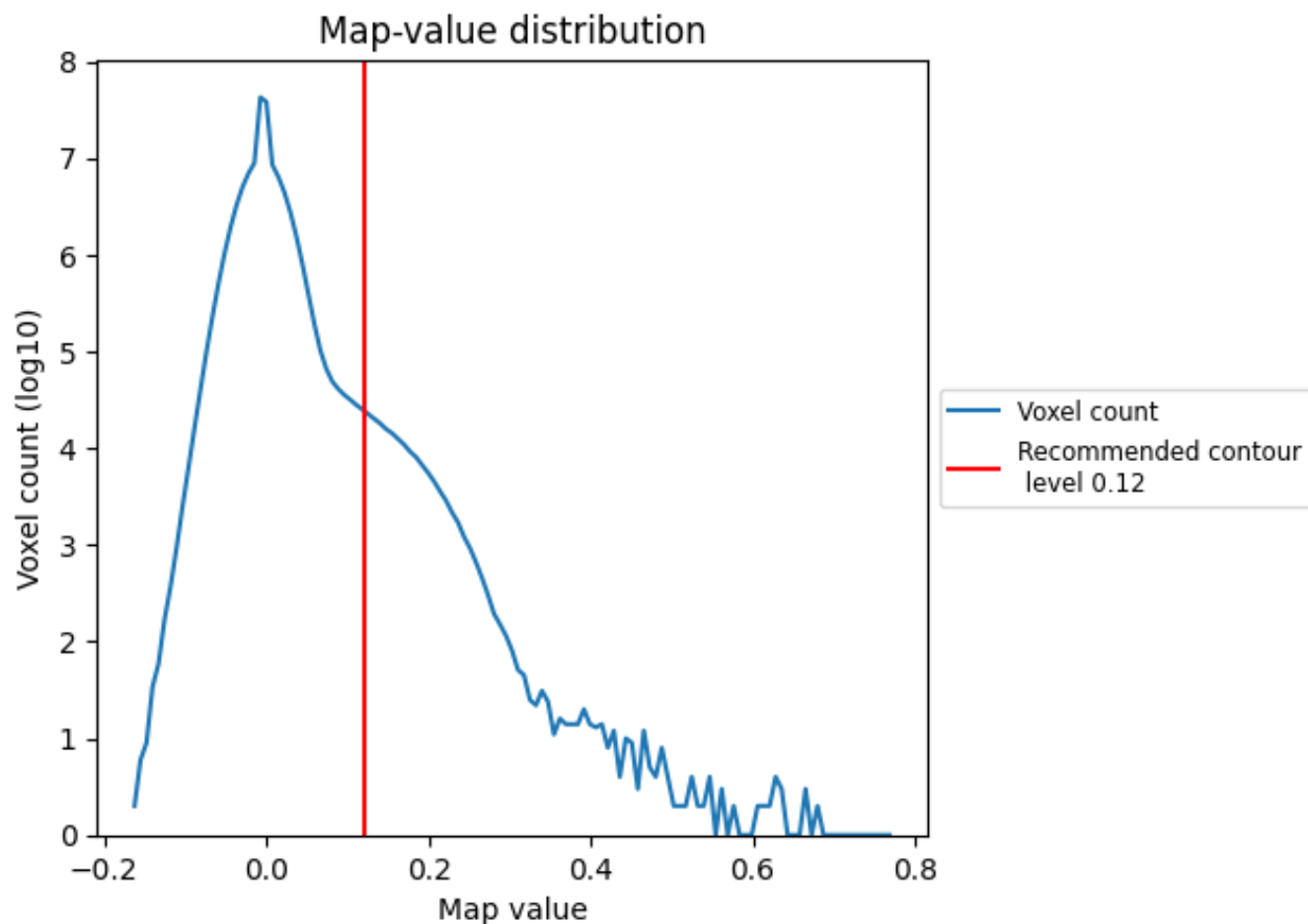


Z

7 Map analysis [i](#)

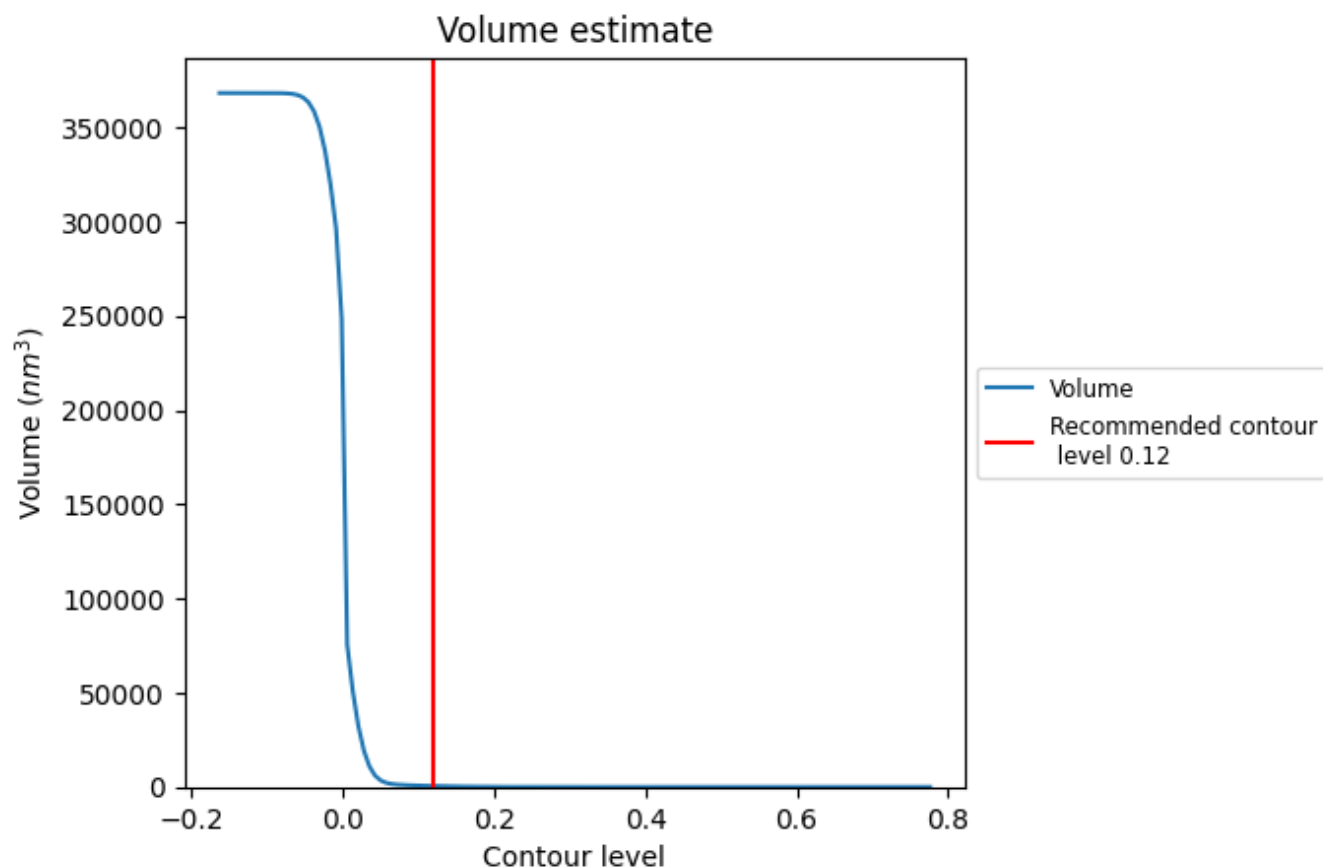
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

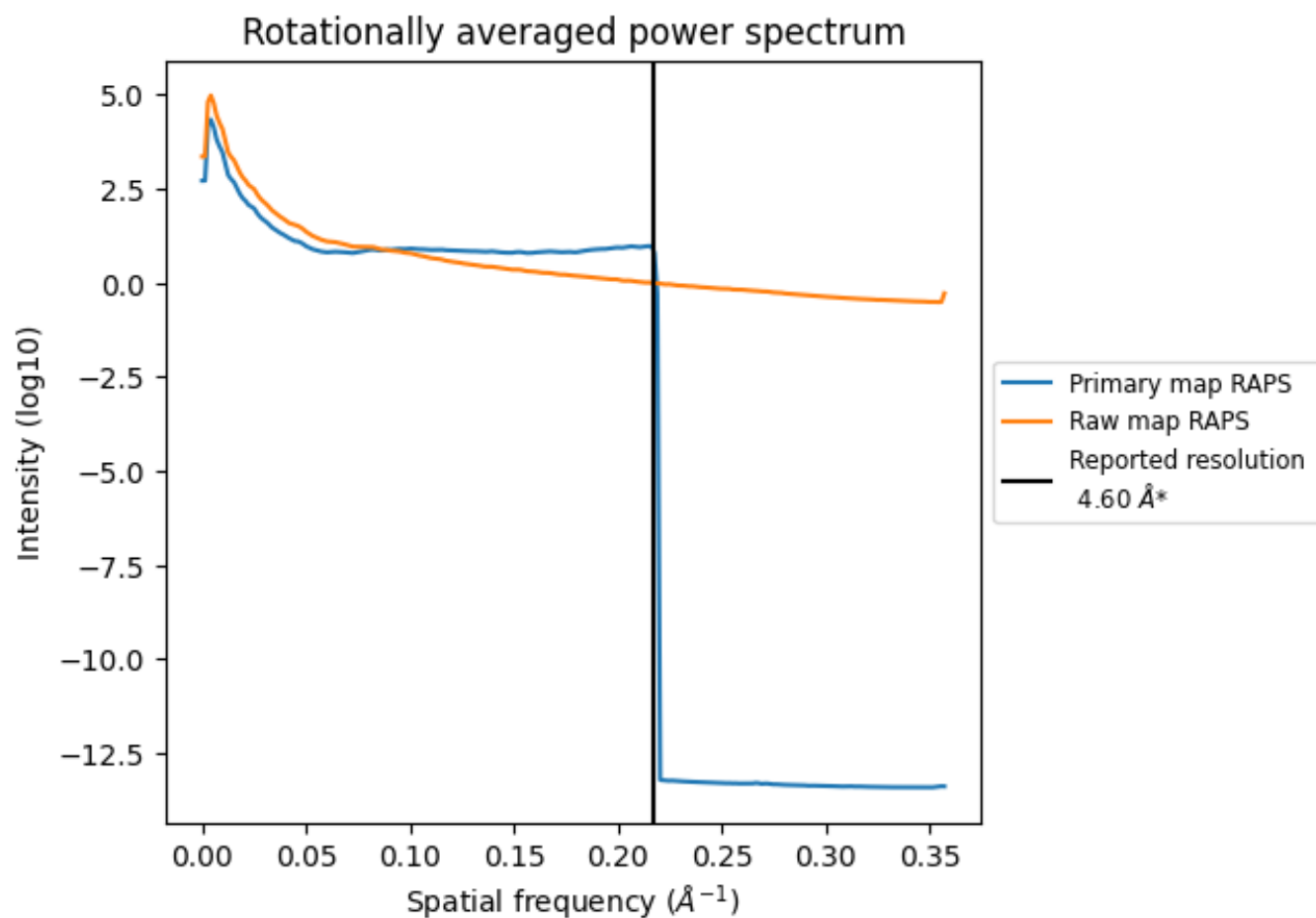
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 502 nm^3 ; this corresponds to an approximate mass of 454 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

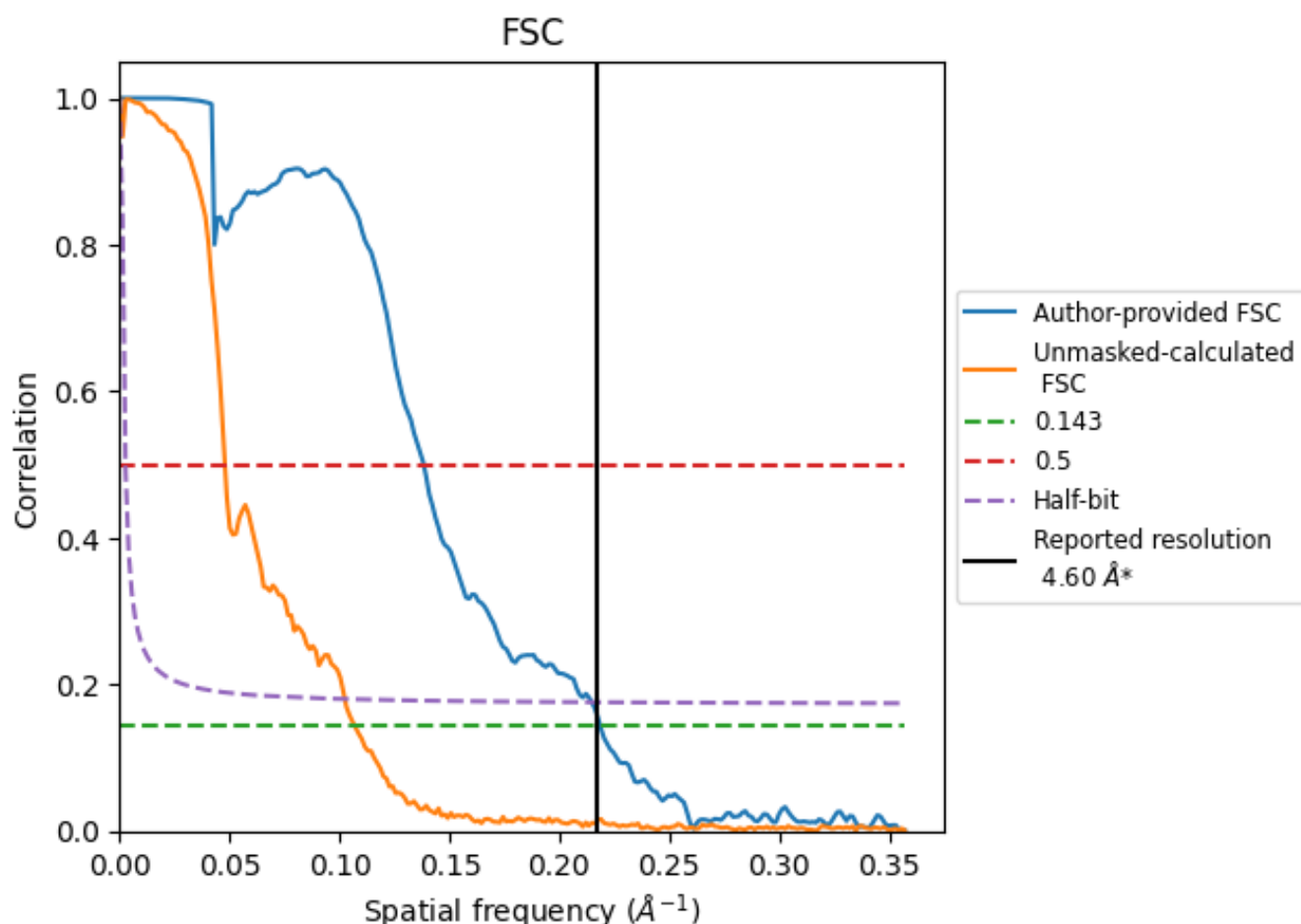


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

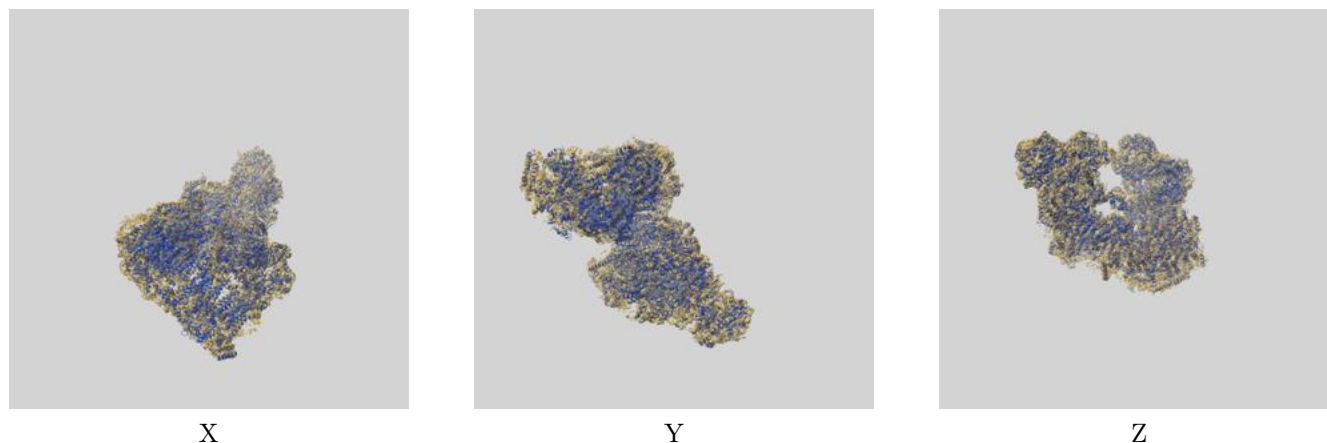
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.57	7.23	4.65
Unmasked-calculated*	9.35	20.83	9.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.35 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

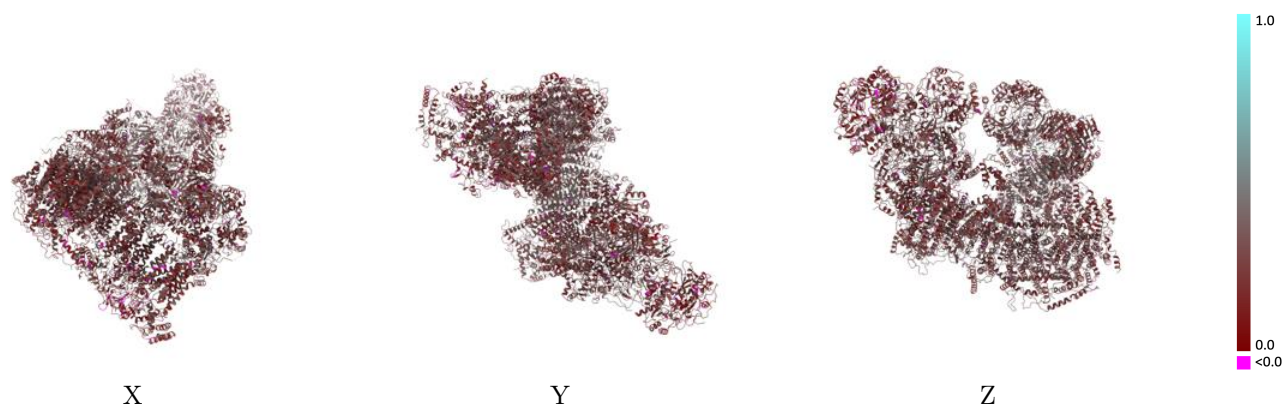
This section contains information regarding the fit between EMDB map EMD-4496 and PDB model 6QC4. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



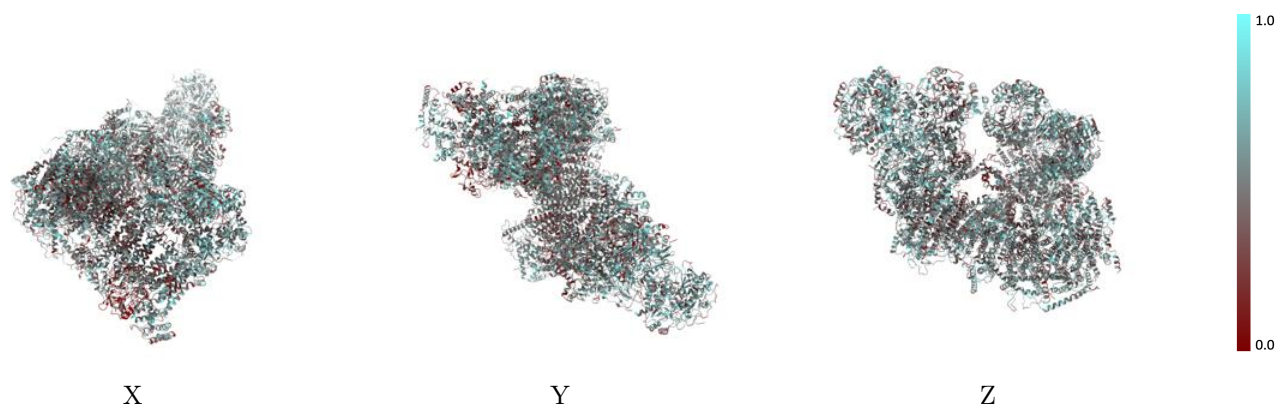
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



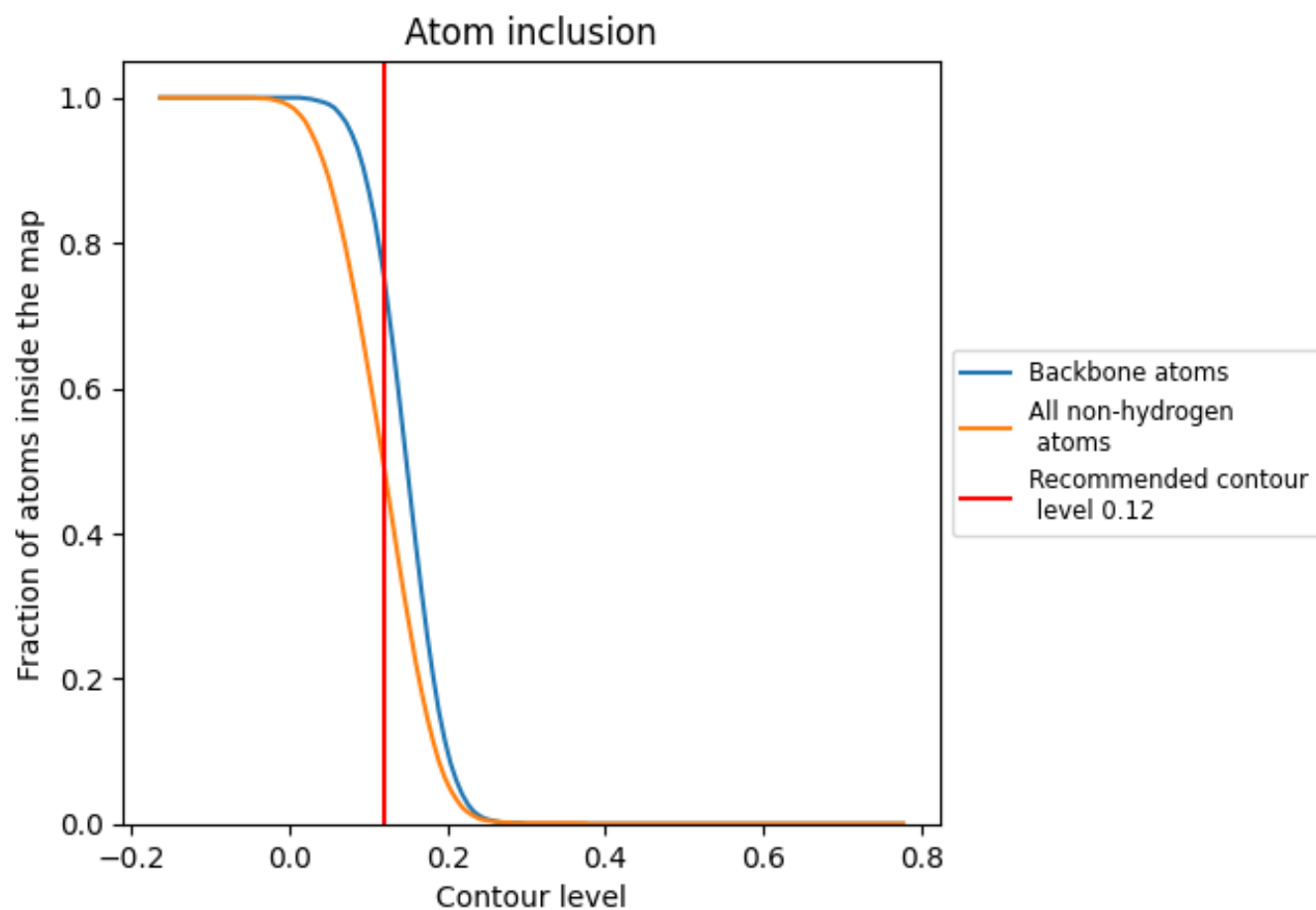
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 49% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4940	0.2820
4L	0.4080	0.2740
A1	0.5410	0.2920
A2	0.5420	0.2540
A3	0.5210	0.2880
A5	0.5030	0.2650
A6	0.4470	0.2750
A7	0.4580	0.2930
A8	0.5470	0.2970
A9	0.4350	0.2810
AA	0.3160	0.2390
AB	0.5170	0.2800
AJ	0.5280	0.2970
AK	0.4210	0.2800
AL	0.4820	0.2900
AM	0.5370	0.2720
B1	0.5270	0.3100
B2	0.5430	0.2610
B3	0.4730	0.2680
B4	0.5200	0.3010
B5	0.5400	0.2890
B6	0.5300	0.2850
B7	0.5410	0.2390
B8	0.5150	0.3120
B9	0.5570	0.2990
BJ	0.5560	0.2800
BK	0.4960	0.2990
C1	0.5520	0.3040
C2	0.5300	0.2950
D1	0.4500	0.2810
D2	0.4860	0.2950
D3	0.4010	0.2850
D4	0.4620	0.2970
D5	0.4720	0.2830
D6	0.3870	0.2760



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Chain	Atom inclusion	Q-score
S1	 0.4970	 0.2820
S2	 0.5010	 0.2940
S3	 0.5240	 0.3090
S4	 0.5110	 0.3050
S5	 0.5320	 0.2820
S6	 0.5240	 0.3320
S7	 0.5150	 0.2890
S8	 0.5700	 0.3030
V1	 0.5450	 0.2390
V2	 0.5210	 0.2530
V3	 0.5180	 0.2180
a1	 0.5300	 0.2740
a2	 0.5170	 0.2750
a3	 0.5400	 0.3170
a4	 0.5400	 0.2870
b1	 0.4910	 0.2760
b2	 0.4810	 0.2940
c1	 0.5460	 0.2870
c2	 0.5260	 0.3030
d1	 0.5490	 0.2860
d2	 0.5120	 0.2900
f1	 0.2340	 0.2070
f2	 0.2260	 0.2210
h1	 0.5100	 0.2350
h2	 0.4170	 0.2310
i1	 0.5030	 0.2500
i2	 0.4510	 0.2660
q1	 0.5090	 0.2820
q2	 0.4950	 0.3190
x1	 0.2010	 0.2850
x2	 0.3400	 0.3460