wwPDB EM Validation Summary Report (i)

Sep 9, 2026 – 09:41 am BST

PDB ID	:	5J7Y / pdb_00005j7y
EMDB ID	:	EMD-8128
Title	:	Architecture of loose respirasome
Authors	:	Letts, J.A.; Fiedorczuk, F.; Sazanov, L.A.
Deposited on	:	2016-04-07
Resolution	:	6.70 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

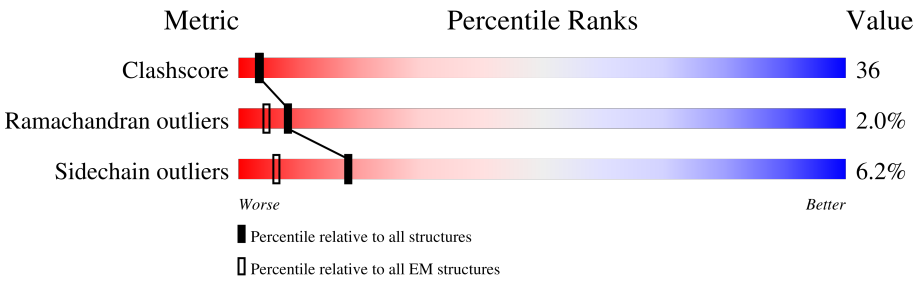
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

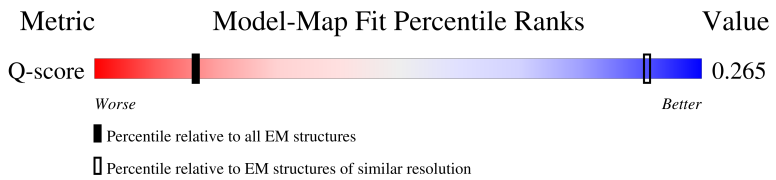
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.70 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	523 (6.20 - 7.20)

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

Mol	Chain	Length	Quality of chain
1	A	102	88% 12%
2	B	154	7% 61% 38%
3	C	194	67% 32%
4	D	384	68% 32%

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Mol	Chain	Length	Quality of chain
5	E	189	77% 23%
6	F	429	6% 66% 33%
7	G	652	7% 68% 31%
8	H	297	78% 22%
9	I	171	60% 37%
10	J	171	54% 27% 19%
11	K	93	78% 22%
12	L	575	72% 27%
13	M	455	67% 33%
14	N	345	64% 35%
15	O	104	5% 70% 30%
16	P	85	6% 72% 28%
17	Q	66	64% 36%
18	R	29	10% 83% 17%
19	S	80	5% 54% 46%
19	d	80	71% 29%
20	T	53	6% 83% 17%
21	U	96	92% 8%
22	V	112	12% 75% 24%
23	W	103	81% 19%
24	X	309	5% 62% 21% 17%
25	Y	322	59% 39%
26	Z	119	7% 84% 16%
27	a	111	5% 80% 20%
28	b	92	85% 15%

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Mol	Chain	Length	Quality of chain
29	c	79	61% 29% 10%
30	e	55	64% 36%
31	f	59	71% 27%
32	g	130	73% 27%
33	9	63	86% 14%
33	h	63	37% 63%
33	z	63	19% 22% 59%
34	i	70	90% 10%
35	j	44	89% 11%
36	k	83	84% 12%
37	0	36	6% 83% 17%
38	1	30	83% 17%
39	2	38	74% 26%
40	3	28	86% 14%
40	4	28	18% 79% 21%
41	5	34	82% 18%
42	6	21	33% 67%
43	7	39	5% 82% 18%
44	8	27	67% 33%
45	y	46	83% 17%
46	x	13	100%
47	w	24	75% 25%
48	v	18	89% 11%
49	u	16	88% 12%
50	t	12	67% 33%

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Mol	Chain	Length	Quality of chain
51	AA	446	47% 49%
51	AL	446	7% 48% 48%
52	AB	423	6% 49% 48%
52	AM	423	12% 49% 47%
53	AC	378	55% 43%
53	AN	378	6% 55% 42%
54	AD	241	54% 41% 5%
54	AO	241	7% 55% 40% 5%
55	AE	196	36% 67% 30%
55	AP	196	28% 67% 29%
56	AF	105	7% 52% 43%
56	AQ	105	10% 53% 42%
57	AG	75	59% 37%
57	AR	75	9% 59% 37%
58	AH	67	6% 67% 31%
58	AS	67	16% 63% 37%
59	AI	57	67% 33% 49% 16%
59	AT	57	67% 35% 47% 16%
60	AJ	60	5% 47% 52%
60	AU	60	7% 47% 52%
61	AK	51	6% 84% 16%
61	AV	51	22% 88% 12%
62	BN	514	33% 78% 22%
63	BO	227	41% 72% 28%
64	BC	259	24% 90% 10%

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Mol	Chain	Length	Quality of chain
65	BD	144	51% 93% 7%
66	BE	105	53% 72% 28%
67	BP	98	30% 95% 5%
68	BG	84	60% 75% 23%
69	BH	79	44% 70% 30%
70	BI	73	52% 84% 16%
71	BJ	58	26% 81% 19%
72	BK	49	39% 88% 12%
73	BL	46	28% 91% 9%
74	BM	43	56% 91% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
75	SF4	F	500	-	-	X	-
75	SF4	G	802	-	-	X	-
75	SF4	I	201	-	-	X	-
75	SF4	I	202	-	-	X	-
76	FES	E	201	-	-	X	-

2 Entry composition (i)

There are 80 unique types of molecules in this entry. The entry contains 64743 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 COMPLEX I ND3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	102	510	306	102	102	0	0

- Molecule 2 is a protein called COMPLEX I PSST/NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	154	774	462	154	154	4	0	0

- Molecule 3 is a protein called COMPLEX I 30KDA/NDUFS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	194	970	582	194	194	0	0

- Molecule 4 is a protein called COMPLEX I 49KDA/NDUFS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	384	1920	1152	384	384	0	0

- Molecule 5 is a protein called COMPLEX I 24KDA/NDUFV2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	189	949	567	189	189	4	0	0

- Molecule 6 is a protein called COMPLEX I 51KDA/NDUFV1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	429	2149	1287	429	429	4	0	0

- Molecule 7 is a protein called COMPLEX I 75KDA/NDUFS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	652	3276	1959	654	652	11	0	0

- Molecule 8 is a protein called COMPLEX I ND1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	297	1485	891	297	297	0	0

- Molecule 9 is a protein called COMPLEX I TYKY/NDUFS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	171	863	513	171	171	8	0	0

- Molecule 10 is a protein called COMPLEX I ND6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	139	695	417	139	139	0	0

- Molecule 11 is a protein called COMPLEX I ND4L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	93	465	279	93	93	0	0

- Molecule 12 is a protein called COMPLEX I ND5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	575	2875	1725	575	575	0	0

- Molecule 13 is a protein called COMPLEX I ND4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	455	2275	1365	455	455	0	0

- Molecule 14 is a protein called COMPLEX I ND2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	N	345	1725	1035	345	345	0	0

- Molecule 15 is a protein called COMPLEX I 18KDA/NDUFS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	104	520	312	104	104	0	0

- Molecule 16 is a protein called COMPLEX I 13KDA/NDUFS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	P	85	425	255	85	85	0	0

- Molecule 17 is a protein called COMPLEX I 15KDA/NDUFS5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	66	330	198	66	66	0	0

- Molecule 18 is a protein called COMPLEX I MWFE/NDUFA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	R	29	145	87	29	29	0	0

- Molecule 19 is a protein called COMPLEX I B8/NDUFA2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	S	80	400	240	80	80	0	0
19	d	80	400	240	80	80	0	0

- Molecule 20 is a protein called COMPLEX I B9/NDUFA3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	T	53	265	159	53	53	0	0

- Molecule 21 is a protein called COMPLEX I B13/NDUFA5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	96	480	288	96	96	0	0

- Molecule 22 is a protein called COMPLEX I B14/NDUFA6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	V	112	560	336	112	112	0	0

- Molecule 23 is a protein called COMPLEX I PGIV/NDUFA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	W	103	515	309	103	103	0	0

- Molecule 24 is a protein called COMPLEX I 39KDA/NDUFA9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	X	258	1290	774	258	258	0	0

- Molecule 25 is a protein called COMPLEX I 42KDA/NDUFA10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	Y	322	1595	951	322	322	0	0

- Molecule 26 is a protein called COMPLEX I B14.7/NDUFA11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	Z	119	595	357	119	119	0	0

- Molecule 27 is a protein called COMPLEX I B17.2/NDUFA12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	a	111	555	333	111	111	0	0

- Molecule 28 is a protein called COMPLEX I B16.6/NDUFA13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	b	92	460	276	92	92	0	0

- Molecule 29 is a protein called COMPLEX I SDAP/NDUFAB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	c	71	355	213	71	71	0	0

- Molecule 30 is a protein called COMPLEX I SDAP/NDUFAB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	e	55	275	165	55	55	0	0

- Molecule 31 is a protein called COMPLEX I SDAP/NDUFAB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	f	58	290	174	58	58	0	0

- Molecule 32 is a protein called COMPLEX I B15/NDUFB4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	g	130	650	390	130	130	0	0

- Molecule 33 is a protein called COMPLEX I B18/NDUFB7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	h	63	315	189	63	63	0	0
33	9	63	315	189	63	63	0	0
33	z	26	130	78	26	26	0	0

- Molecule 34 is a protein called COMPLEX I B22/NDUFB9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	i	70	350	210	70	70	0	0

- Molecule 35 is a protein called COMPLEX I PDSW/NDUFB10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	j	44	220	132	44	44	0	0

- Molecule 36 is a protein called COMPLEX I ESSS/NDUFB11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	k	80	400	240	80	80	0	0

- Molecule 37 is a protein called COMPLEX I KFYI/NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	0	36	180	108	36	36	0	0

- Molecule 38 is a protein called COMPLEX I B14.5B/NDUFC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	1	30	150	90	30	30	0	0

- Molecule 39 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	2	38	190	114	38	38	0	0

- Molecule 40 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	3	28	140	84	28	28	0	0
40	4	28	140	84	28	28	0	0

- Molecule 41 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	5	34	170	102	34	34	0	0

- Molecule 42 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	6	21	105	63	21	21	0	0

- Molecule 43 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	7	39	195	117	39	39	0	0

- Molecule 44 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	8	27	135	81	27	27	0	0

- Molecule 45 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	y	46	230	138	46	46	0	0

- Molecule 46 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	x	13	65	39	13	13	0	0

- Molecule 47 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	w	24	120	72	24	24	0	0

- Molecule 48 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	v	18	90	54	18	18	0	0

- Molecule 49 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	u	16	80	48	16	16	0	0

- Molecule 50 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	t	12	60	36	12	12	0	0

- Molecule 51 is a protein called COMPLEX III SUBUNIT 1 / CORE 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	AA	446	2198	1306	446	446	0	0
51	AL	446	2198	1306	446	446	0	0

There are 32 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
AL	?	-	PRO	deletion	UNP W5Q5G6
AL	249	PRO	GLN	conflict	UNP W5Q5G6
AL	251	ALA	TRP	conflict	UNP W5Q5G6
AL	254	ALA	PRO	conflict	UNP W5Q5G6
AL	255	ILE	PHE	conflict	UNP W5Q5G6
AL	256	ALA	GLN	conflict	UNP W5Q5G6
AL	257	VAL	ILE	conflict	UNP W5Q5G6
AL	258	GLU	ARG	conflict	UNP W5Q5G6
AL	259	GLY	HIS	conflict	UNP W5Q5G6

- Molecule 52 is a protein called COMPLEX III SUBUNIT 2 / CORE 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	AB	423	2081	1235	423	423	0	0
52	AM	423	2081	1235	423	423	0	0

- Molecule 53 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	AC	378	1866	1110	378	378	0	0
53	AN	378	1866	1110	378	378	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	185	SER	PHE	conflict	UNP P24959
AC	295	ILE	VAL	conflict	UNP P24959
AC	303	LEU	ILE	conflict	UNP P24959
AC	359	ILE	PHE	conflict	UNP P24959
AC	361	LEU	ILE	conflict	UNP P24959
AC	363	MET	LEU	conflict	UNP P24959
AN	185	SER	PHE	conflict	UNP P24959
AN	295	ILE	VAL	conflict	UNP P24959
AN	303	LEU	ILE	conflict	UNP P24959
AN	359	ILE	PHE	conflict	UNP P24959
AN	361	LEU	ILE	conflict	UNP P24959
AN	363	MET	LEU	conflict	UNP P24959

- Molecule 54 is a protein called COMPLEX III SUBUNIT 4 / CYTOCHROME C1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	AD	241	1188	706	241	241	0	0
54	AO	241	1188	706	241	241	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AD	139	THR	-	insertion	UNP W5Q0A9
AD	140	GLY	ARG	conflict	UNP W5Q0A9
AO	139	THR	-	insertion	UNP W5Q0A9
AO	140	GLY	ARG	conflict	UNP W5Q0A9

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	AE	196	967	575	196	196	0	0
55	AP	196	967	575	196	196	0	0

- Molecule 56 is a protein called COMPLEX III SUBUNIT 7 / 14KDA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
56	AF	105	522	312	105	105	0	0
56	AQ	105	522	312	105	105	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	56	ASP	ASN	conflict	UNP W5P642
AF	108	ALA	THR	conflict	UNP W5P642
AQ	56	ASP	ASN	conflict	UNP W5P642
AQ	108	ALA	THR	conflict	UNP W5P642

- Molecule 57 is a protein called COMPLEX III SUBUNIT 8 / QP-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
57	AG	75	371	221	75	75	0	0
57	AR	75	371	221	75	75	0	0

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	AH	67	335	201	67	67	0	0
58	AS	67	335	201	67	67	0	0

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
59	AI	57	281	167	57	57	0	0
59	AT	57	281	167	57	57	0	0

- Molecule 60 is a protein called COMPLEX III SUBUNIT 9 / 7.2KDA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
60	AJ	60	297	177	60	60	0	0
60	AU	60	297	177	60	60	0	0

- Molecule 61 is a protein called COMPLEX III SUBUNIT 10 / 6.4KDA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
61	AK	51	250	148	51	51	0	0
61	AV	51	250	148	51	51	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	22	GLN	SER	conflict	UNP W5PSD1
AV	22	GLN	SER	conflict	UNP W5PSD1

- Molecule 62 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	BN	514	2523	1495	514	514	0	0

- Molecule 63 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
63	BO	227	1127	673	227	227	0	0

- Molecule 64 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
64	BC	259	1275	757	259	259	0	0

- Molecule 65 is a protein called COMPLEX IV COX4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
65	BD	144	716	428	144	144	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	97	ILE	LEU	conflict	UNP W5PPE8
BD	99	GLU	GLY	conflict	UNP W5PPE8
BD	100	LYS	TRP	conflict	UNP W5PPE8
BD	101	HIS	THR	conflict	UNP W5PPE8
BD	102	TYR	ALA	conflict	UNP W5PPE8

- Molecule 66 is a protein called COMPLEX IV COX5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
66	BE	105	520	310	105	105	0	0

- Molecule 67 is a protein called COMPLEX IV COX5B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
67	BP	98	481	285	98	98	0	0

- Molecule 68 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
68	BG	84	412	244	84	84	0	0

- Molecule 69 is a protein called COMPLEX IV COX6B1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
69	BH	79	391	233	79	79	0	0

- Molecule 70 is a protein called COMPLEX IV COX6C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
70	BI	73	361	215	73	73	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	26	MET	VAL	conflict	UNP W5PXG3
BI	31	PHE	SER	conflict	UNP W5PXG3
BI	36	LYS	ASN	conflict	UNP W5PXG3

- Molecule 71 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
71	BJ	58	284	168	58	58	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BJ	1	PHE	LEU	conflict	UNP W5P5H0
BJ	36	LEU	MET	conflict	UNP W5P5H0

- Molecule 72 is a protein called COMPLEX IV COX7B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
72	BK	49	241	143	49	49	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	9	PHE	CYS	conflict	UNP W5QE72
BK	30	ILE	VAL	conflict	UNP W5QE72
BK	47	ARG	THR	conflict	UNP W5QE72

- Molecule 73 is a protein called COMPLEX IV COX7C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
73	BL	46	226	134	46	46	0	0

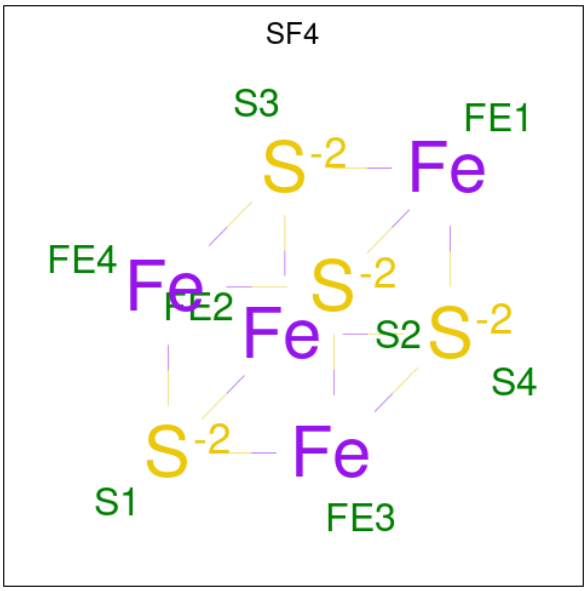
- Molecule 74 is a protein called COMPLEX IV COX8B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
74	BM	43	213	127	43	43	0	0

There are 5 discrepancies between the modelled and reference sequences:

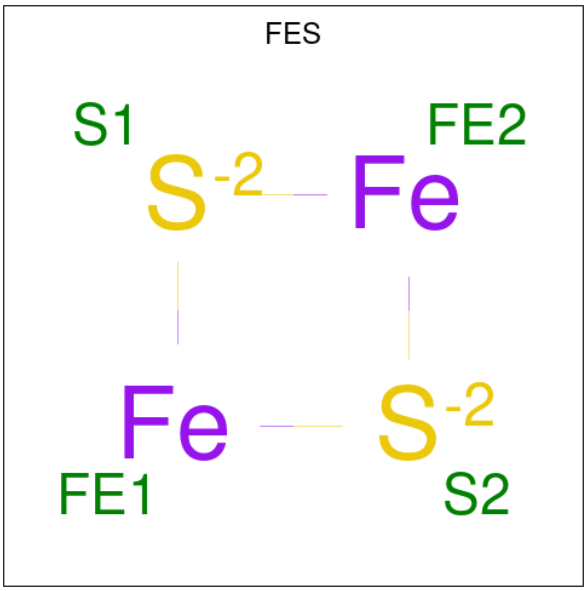
Chain	Residue	Modelled	Actual	Comment	Reference
BM	?	-	THR	deletion	UNP W5PFK9
BM	?	-	GLN	deletion	UNP W5PFK9
BM	18	GLY	ALA	conflict	UNP W5PFK9
BM	21	VAL	ALA	conflict	UNP W5PFK9
BM	39	ASN	HIS	conflict	UNP W5PFK9

- Molecule 75 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



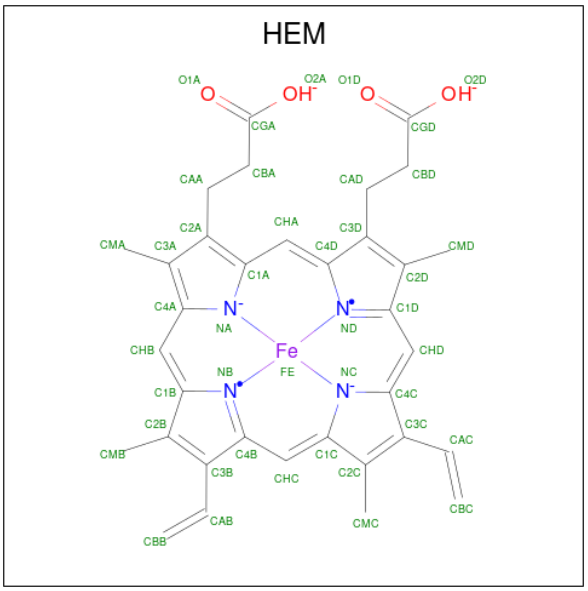
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
75	B	1	8	4	4	0
75	F	1	8	4	4	0
75	G	1	8	4	4	0
75	G	1	8	4	4	0
75	I	1	8	4	4	0
75	I	1	8	4	4	0

- Molecule 76 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
76	E	1	4	2	2	0
76	G	1	4	2	2	0
76	AE	1	4	2	2	0
76	AP	1	4	2	2	0

- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

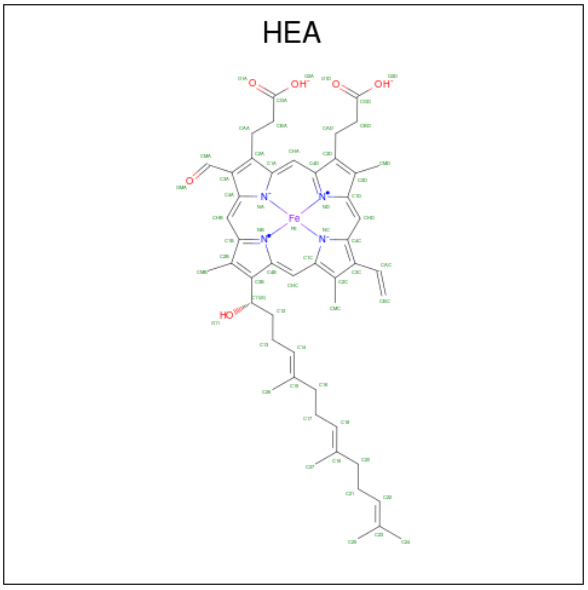


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
77	AC	1	43	34	1	4	4	0
77	AC	1	43	34	1	4	4	0
77	AD	1	43	34	1	4	4	0
77	AN	1	43	34	1	4	4	0
77	AN	1	43	34	1	4	4	0
77	AO	1	43	34	1	4	4	0

- Molecule 78 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

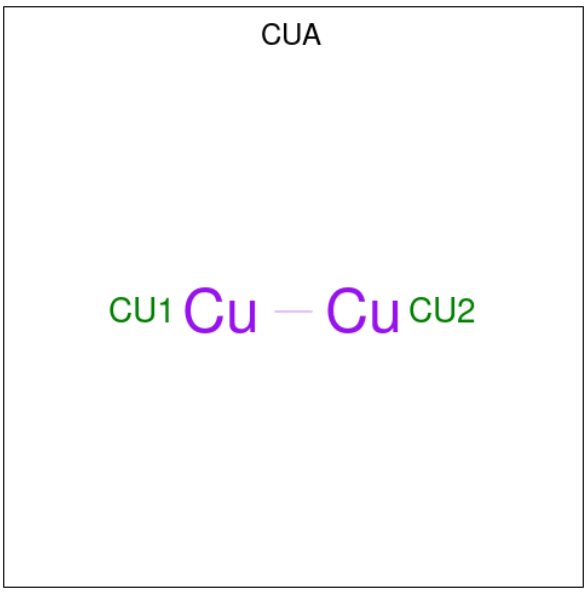
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
78	BN	1	1	1	0

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
79	BN	1	60	49	1	4	6	0
79	BN	1	60	49	1	4	6	0

- Molecule 80 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



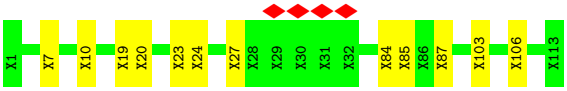
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
80	BO	1	2	2	0

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.

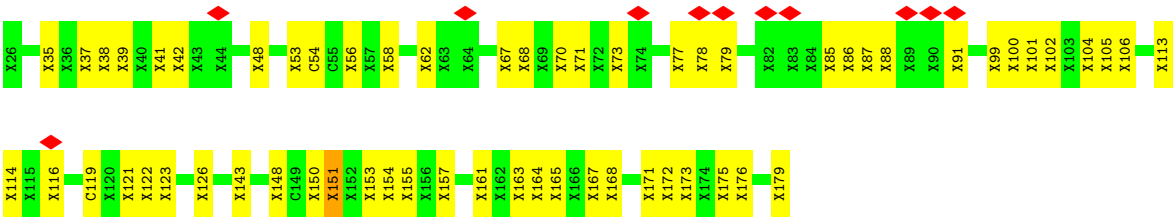
- Molecule 1: COMPLEX I ND3

Chain A:



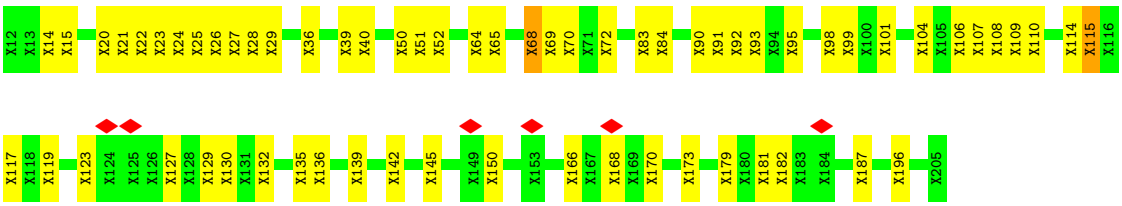
- Molecule 2: COMPLEX I PSST/NDUFS7

Chain B:



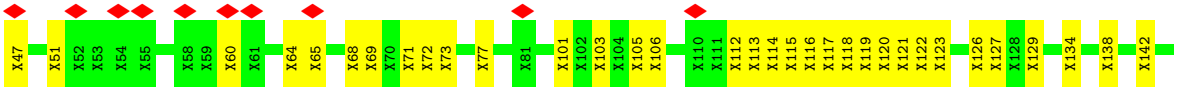
- Molecule 3: COMPLEX I 30KDA/NDUFS3

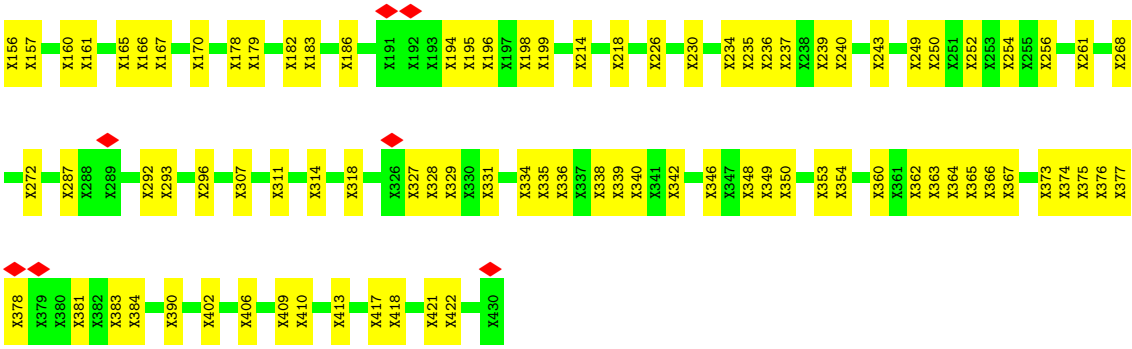
Chain C:



- Molecule 4: COMPLEX I 49KDA/NDUFS2

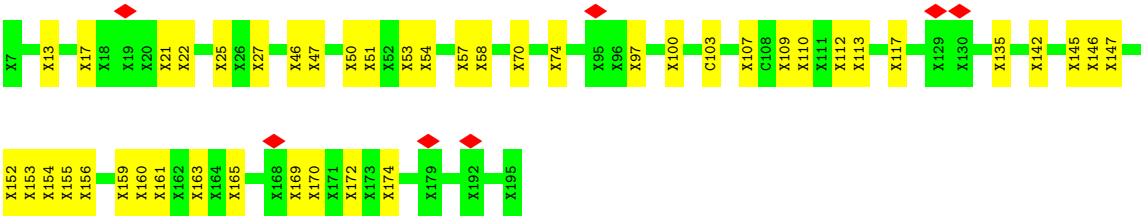
Chain D:





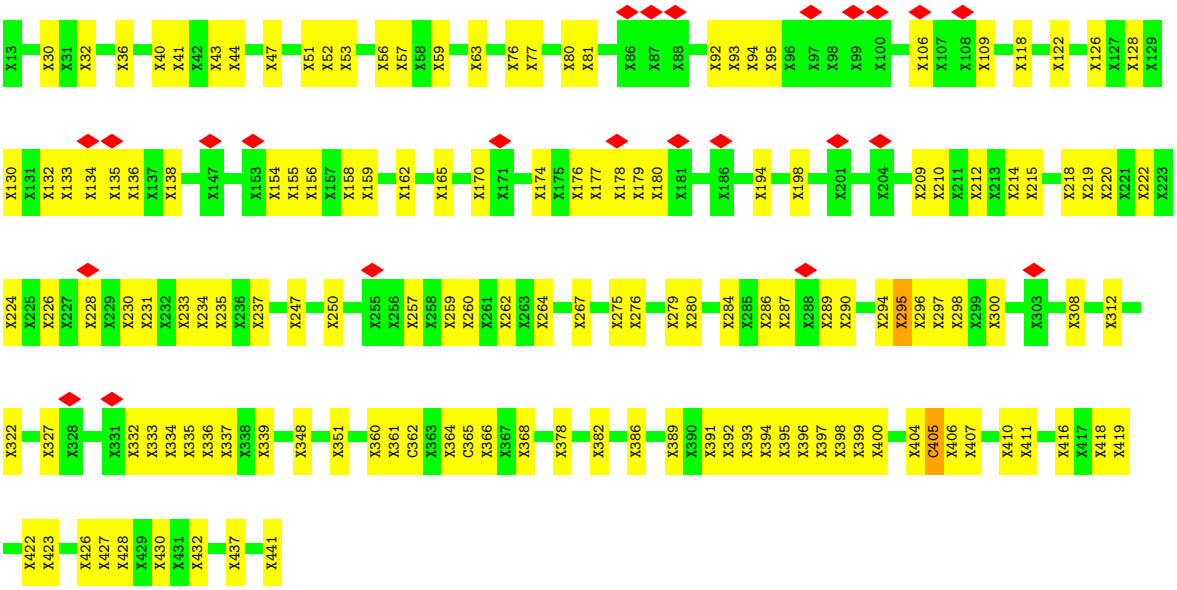
- Molecule 5: COMPLEX I 24KDA/NDUFV2

Chain E:



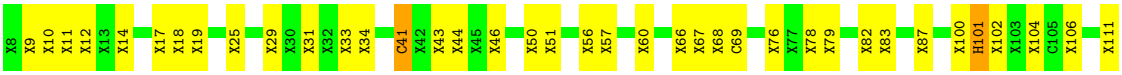
- Molecule 6: COMPLEX I 51KDA/NDUFV1

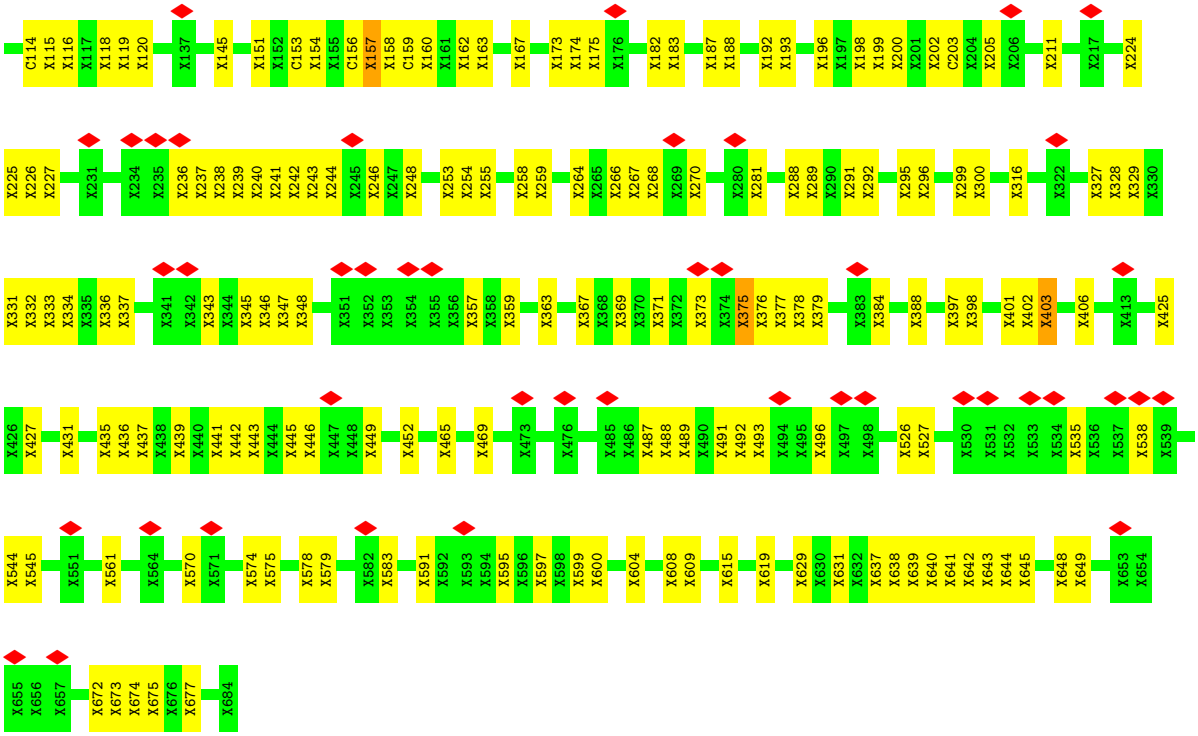
Chain F:



- Molecule 7: COMPLEX I 75KDA/NDUFS1

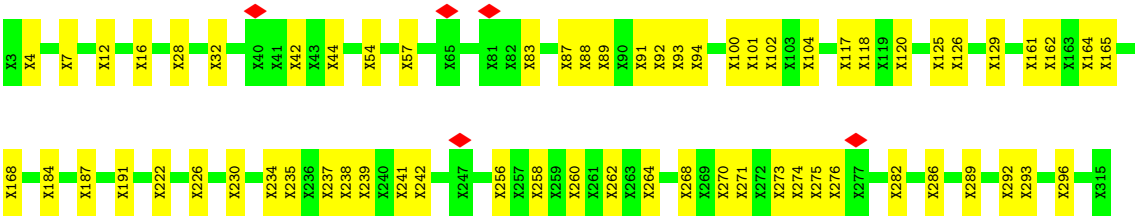
Chain G:





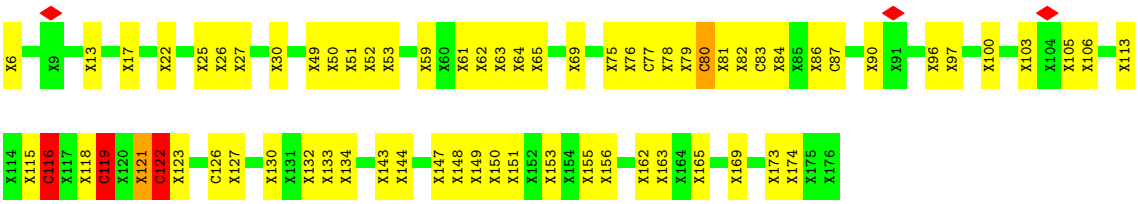
• Molecule 8: COMPLEX I ND1

Chain H:



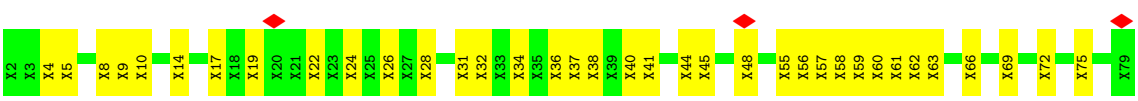
• Molecule 9: COMPLEX I TYKY/NDUFS8

Chain I:



• Molecule 10: COMPLEX I ND6

Chain J:

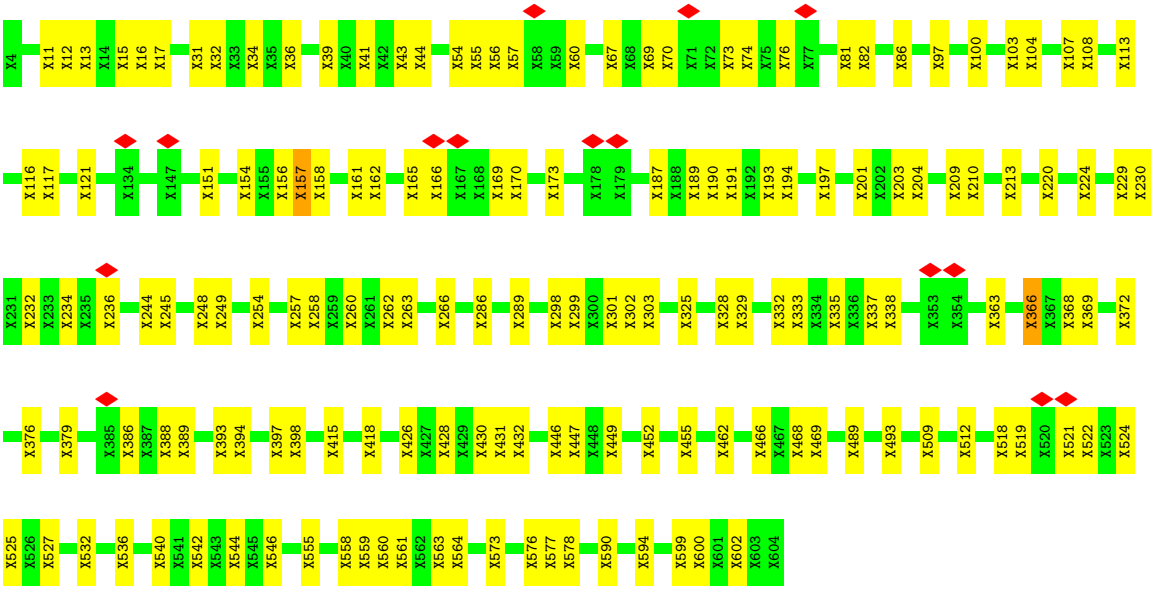


• Molecule 11: COMPLEX I ND4L

Chain K:

• Molecule 12: COMPLEX I ND5

Chain L:

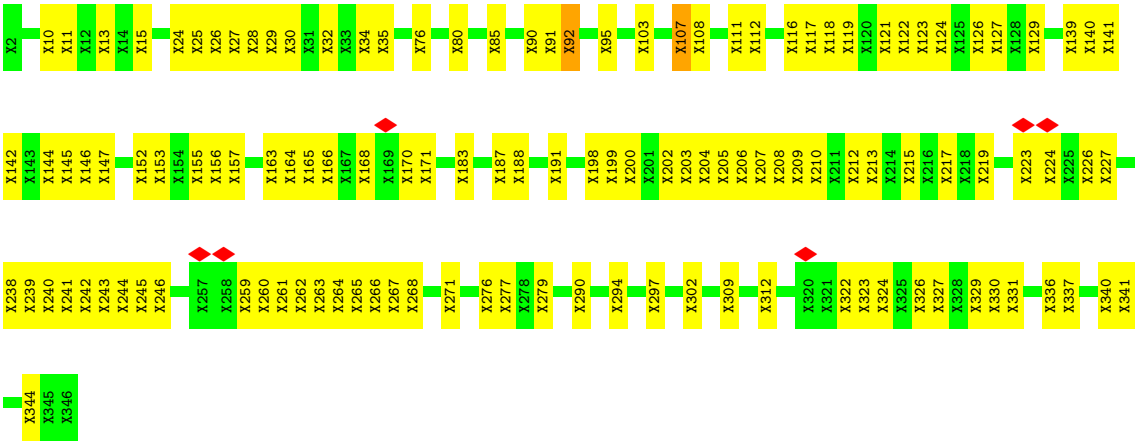


• Molecule 13: COMPLEX I ND4

Chain M:

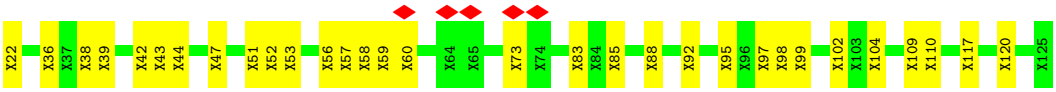
- Molecule 14: COMPLEX I ND2

Chain N:



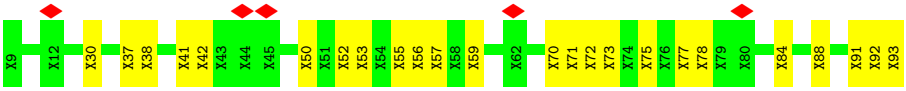
- Molecule 15: COMPLEX I 18KDA/NDUFS6

Chain O:



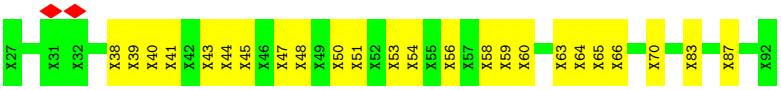
- Molecule 16: COMPLEX I 13KDA/NDUFS6

Chain P:



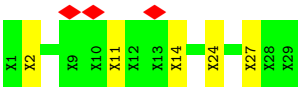
- Molecule 17: COMPLEX I 15KDA/NDUFS5

Chain Q:



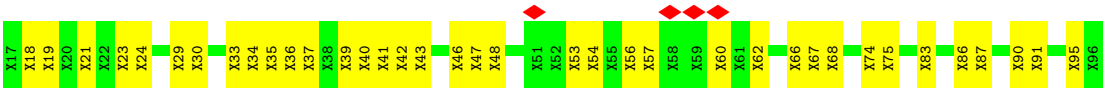
- Molecule 18: COMPLEX I MWFE/NDUFA1

Chain R:



- Molecule 19: COMPLEX I B8/NDUFA2

Chain S: 5% 54% 46%

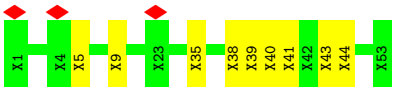


• Molecule 19: COMPLEX I B8/NDUFA2

Chain d: 71% 29%

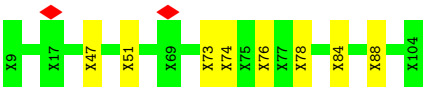
• Molecule 20: COMPLEX I B9/NDUFA3

Chain T: 6% 83% 17%



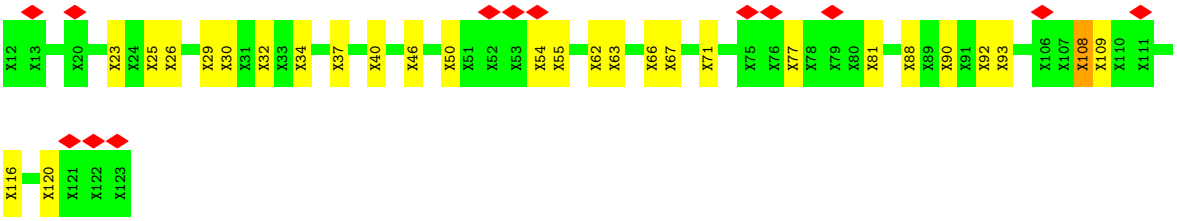
• Molecule 21: COMPLEX I B13/NDUFA5

Chain U: 92% 8%



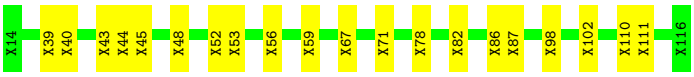
• Molecule 22: COMPLEX I B14/NDUFA6

Chain V: 12% 75% 24%



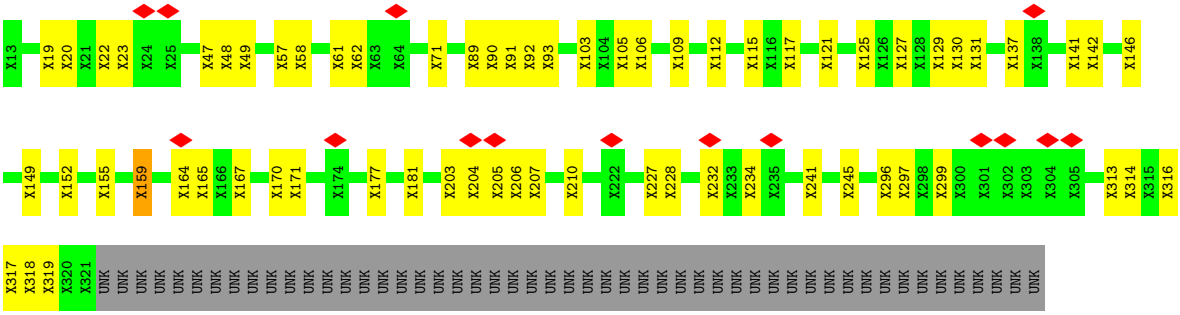
• Molecule 23: COMPLEX I PGIV/NDUFA8

Chain W: 81% 19%



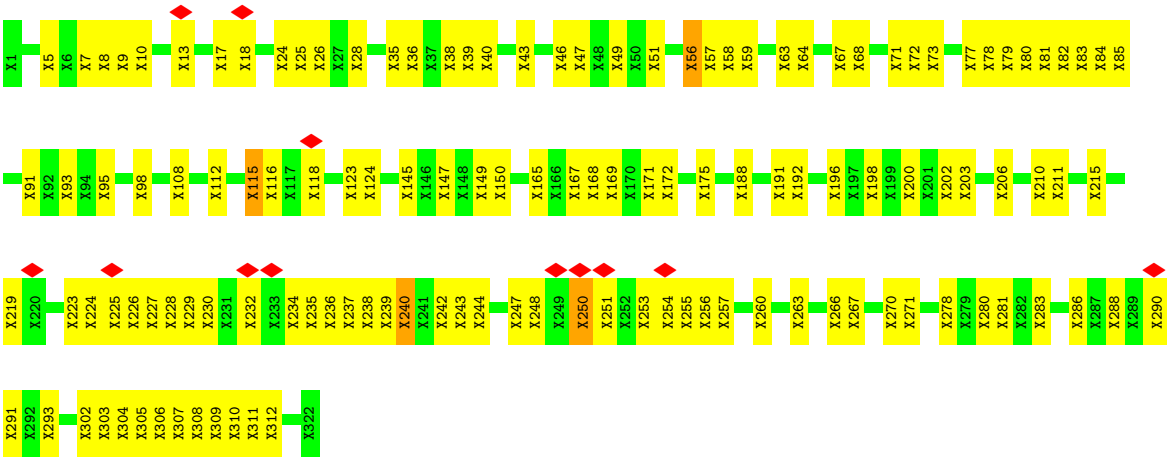
• Molecule 24: COMPLEX I 39KDA/NDUFA9

Chain X: 5% 62% 21% 17%



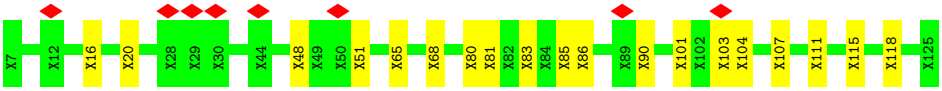
• Molecule 25: COMPLEX I 42KDA/NDUFA10

Chain Y:



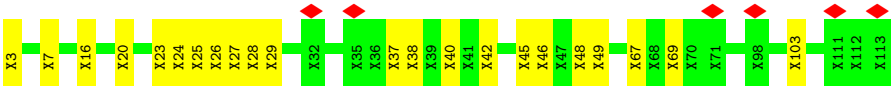
• Molecule 26: COMPLEX I B14.7/NDUFA11

Chain Z:



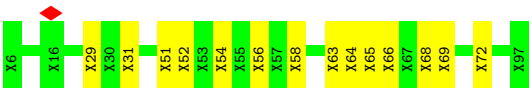
• Molecule 27: COMPLEX I B17.2/NDUFA12

Chain a:



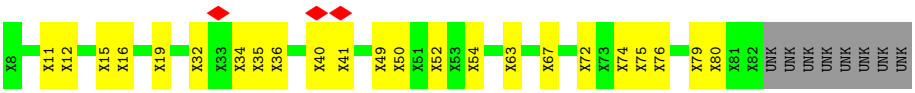
• Molecule 28: COMPLEX I B16.6/NDUFA13

Chain b:



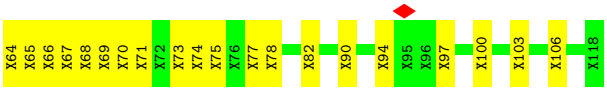
- Molecule 29: COMPLEX I SDAP/NDUFAB1

Chain c:



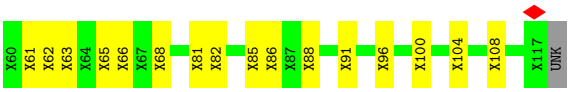
- Molecule 30: COMPLEX I SDAP/NDUFAB1

Chain e:



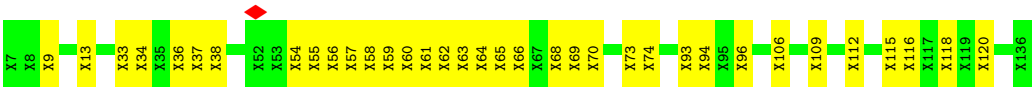
- Molecule 31: COMPLEX I SDAP/NDUFAB1

Chain f:



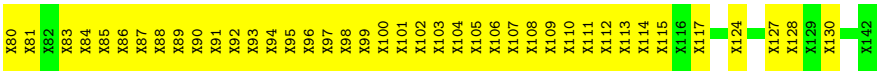
- Molecule 32: COMPLEX I B15/NDUFB4

Chain g:



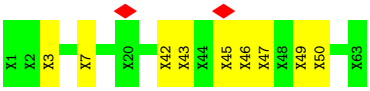
- Molecule 33: COMPLEX I B18/NDUFB7

Chain h:



- Molecule 33: COMPLEX I B18/NDUFB7

Chain 9:

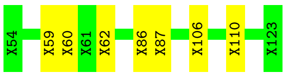


- Molecule 33: COMPLEX I B18/NDUFB7

Chain z:

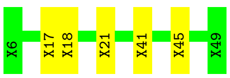
- Molecule 34: COMPLEX I B22/NDUFB9

Chain i:



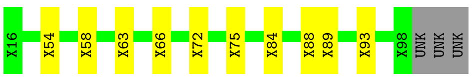
- Molecule 35: COMPLEX I PDSW/NDUFB10

Chain j:



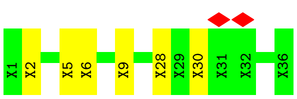
- Molecule 36: COMPLEX I ESSS/NDUFB11

Chain k:



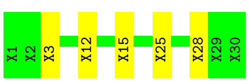
- Molecule 37: COMPLEX I KFYI/NDUFC1

Chain 0:



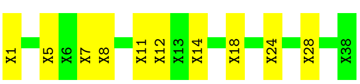
- Molecule 38: COMPLEX I B14.5B/NDUFC2

Chain 1:



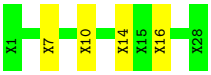
- Molecule 39: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 1

Chain 2:



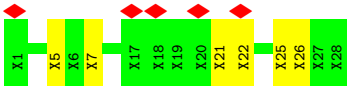
- Molecule 40: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 2

Chain 3:



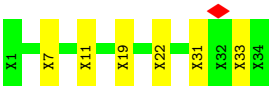
• Molecule 40: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 2

Chain 4:



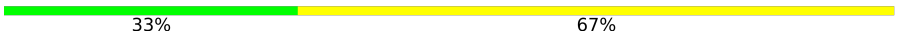
• Molecule 41: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 3

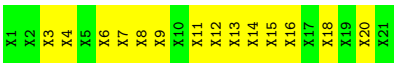
Chain 5:



• Molecule 42: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4

Chain 6:



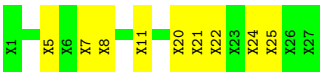


• Molecule 43: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 5

Chain 7:

• Molecule 44: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 6

Chain 8:

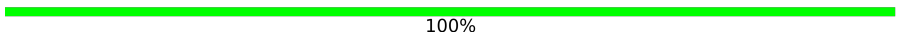


• Molecule 45: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 11

Chain y:

• Molecule 46: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 12

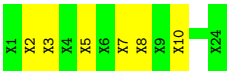
Chain x:



There are no outlier residues recorded for this chain.

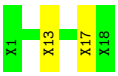
- Molecule 47: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 13

Chain w:



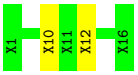
- Molecule 48: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 14

Chain v:



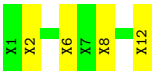
- Molecule 49: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 15

Chain u:



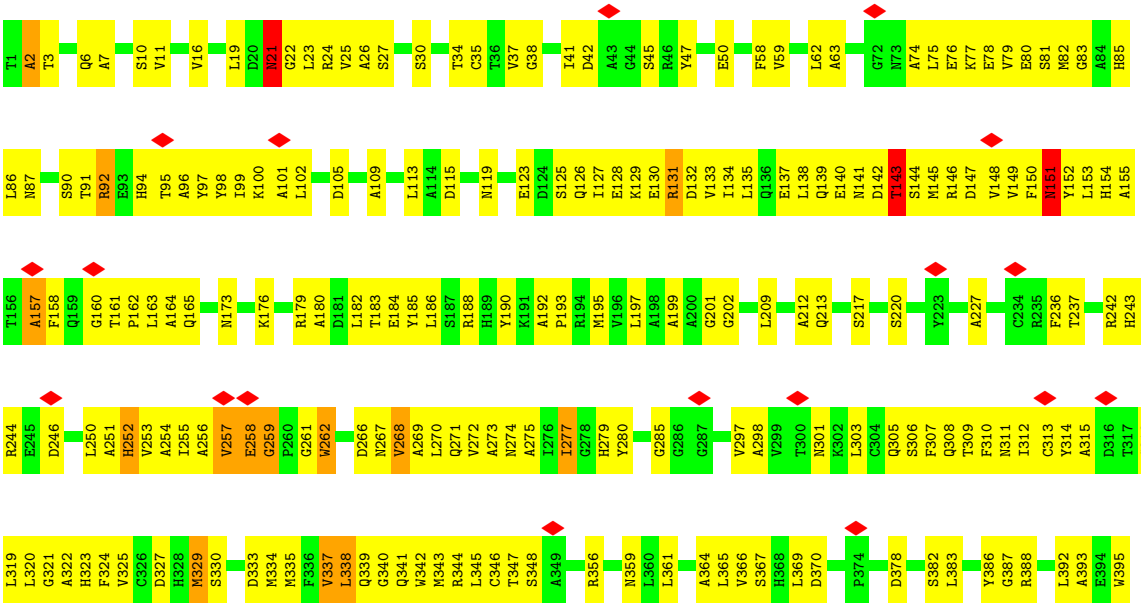
- Molecule 50: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 16

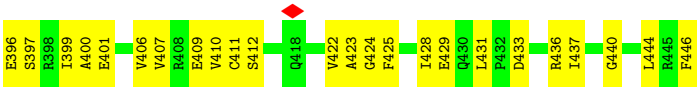
Chain t:



- Molecule 51: COMPLEX III SUBUNIT 1 / CORE 1

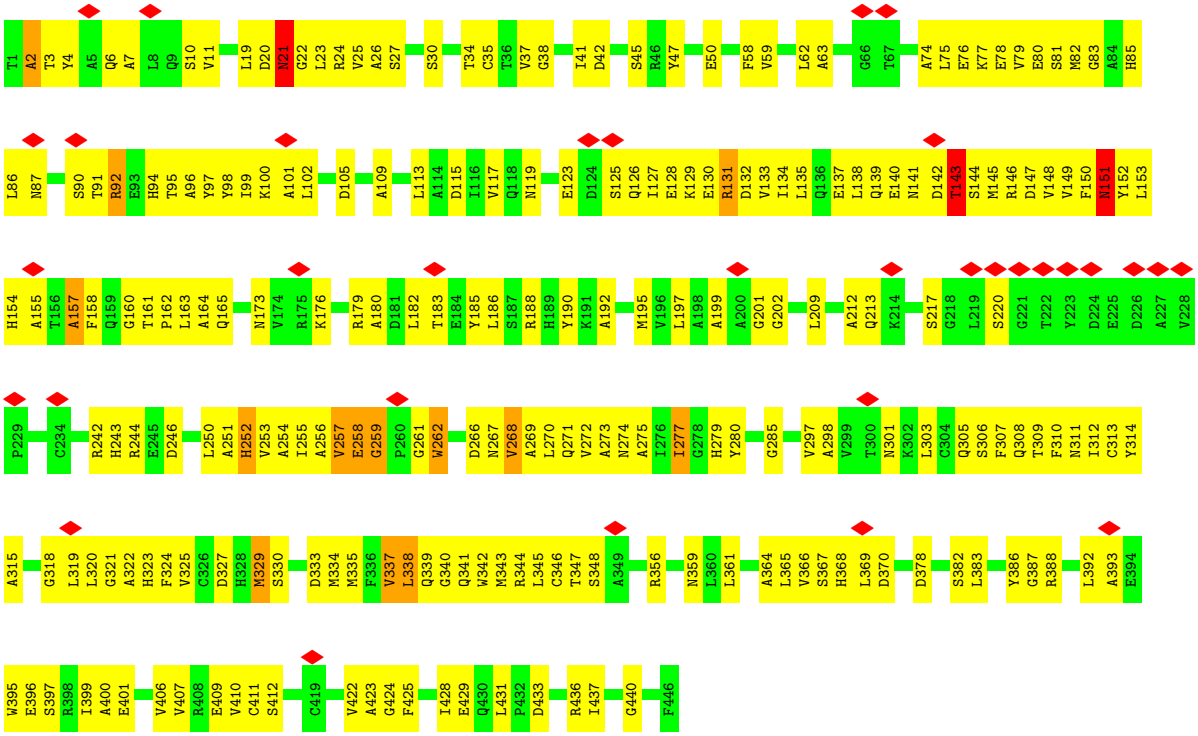
Chain AA:





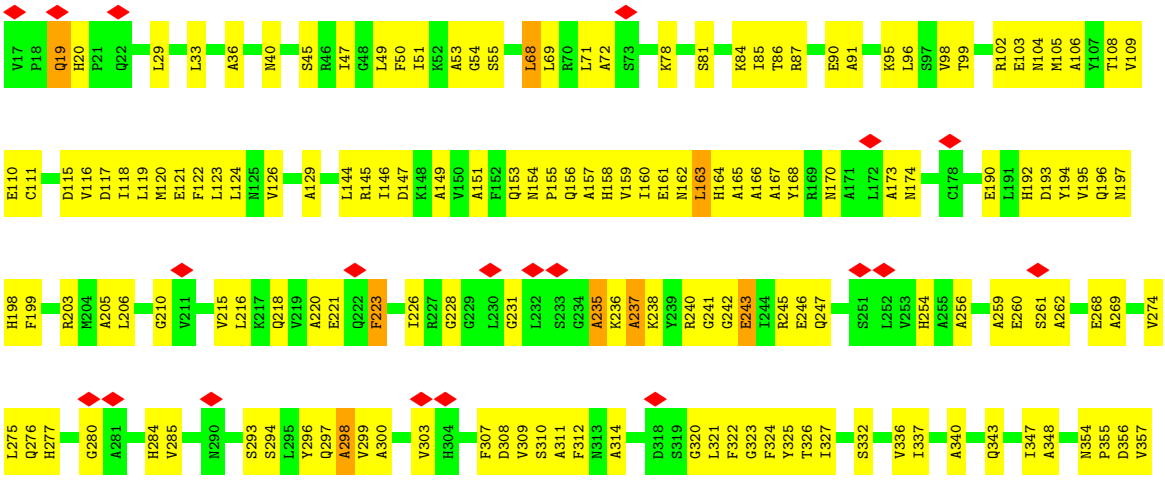
• Molecule 51: COMPLEX III SUBUNIT 1 / CORE 1

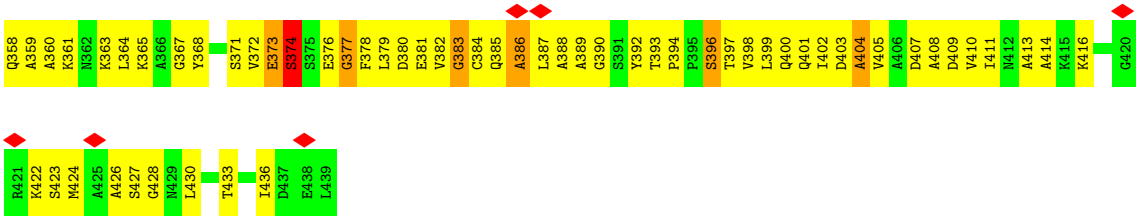
Chain AL:



• Molecule 52: COMPLEX III SUBUNIT 2 / CORE 2

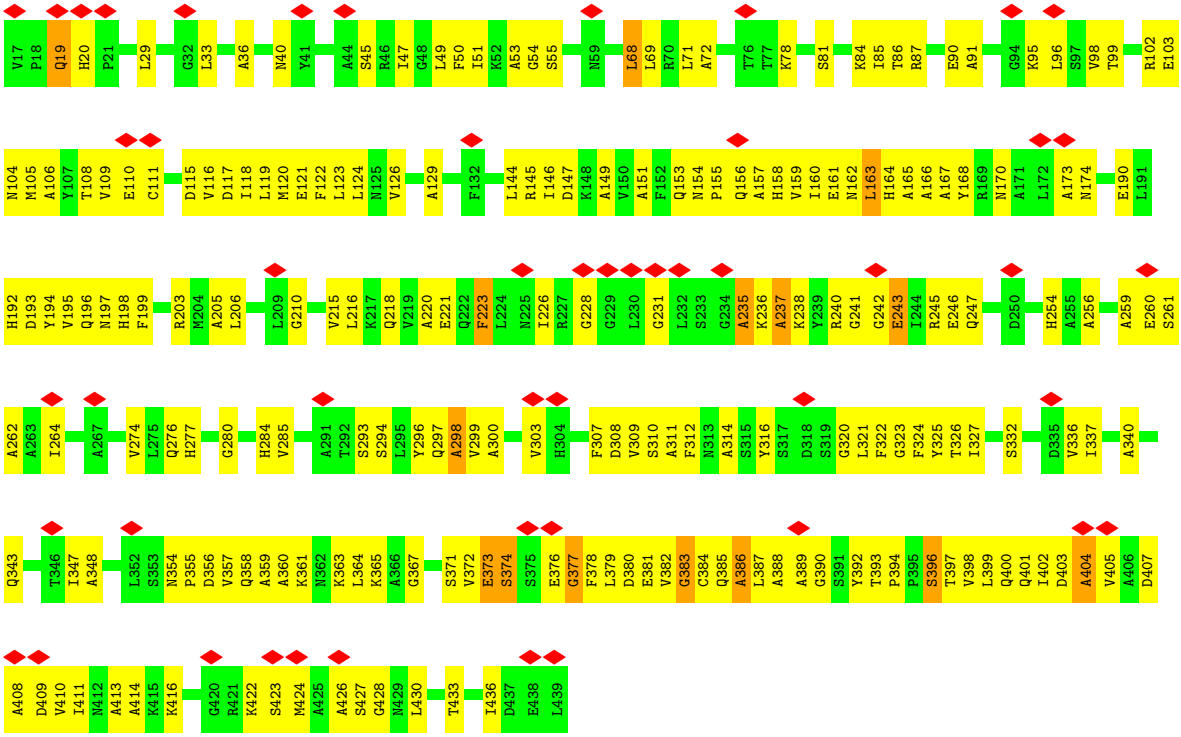
Chain AB:





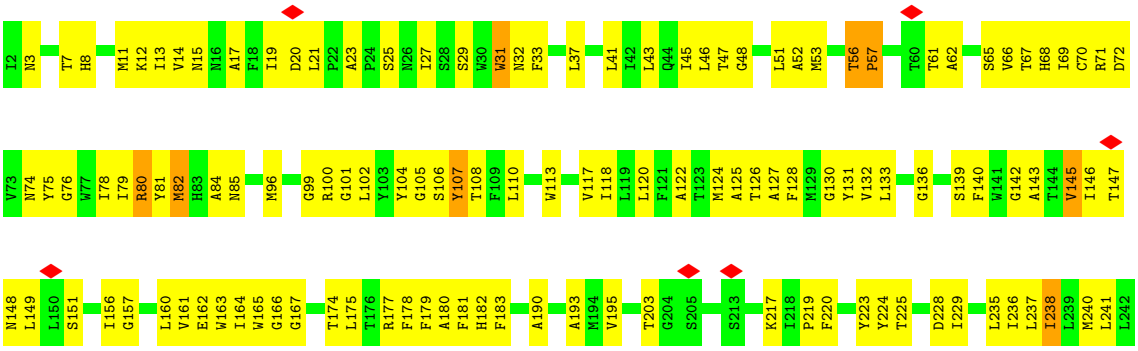
• Molecule 52: COMPLEX III SUBUNIT 2 / CORE 2

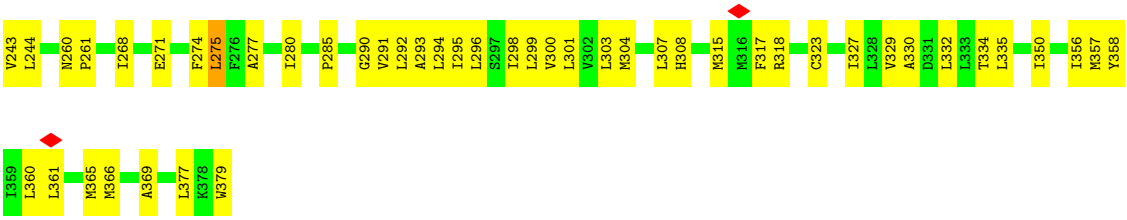
Chain AM:



• Molecule 53: Cytochrome b

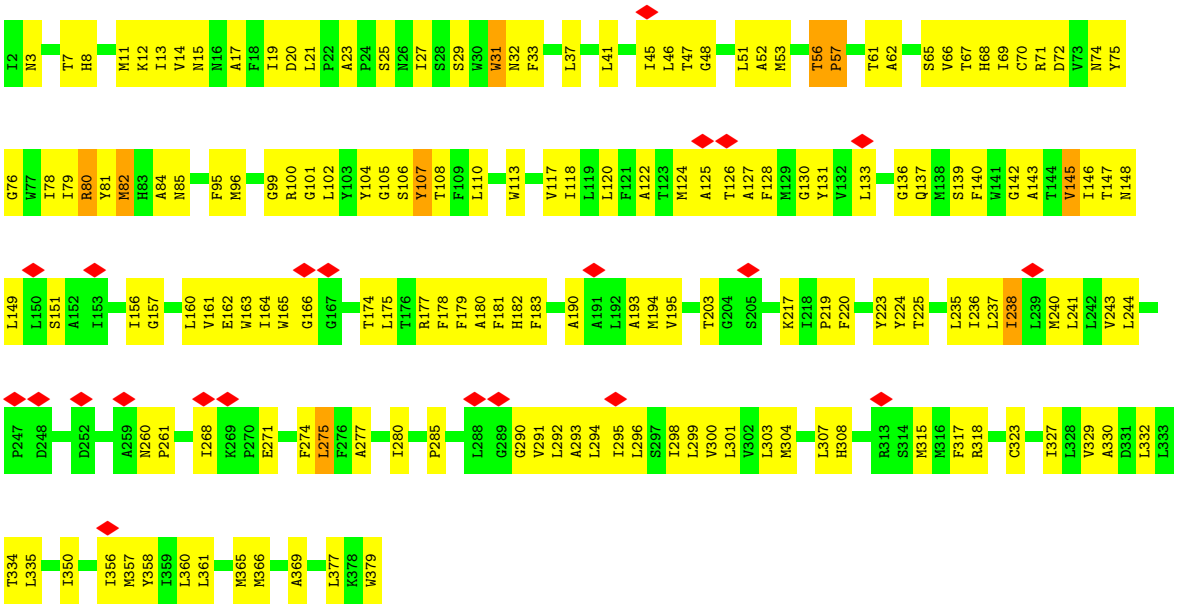
Chain AC:





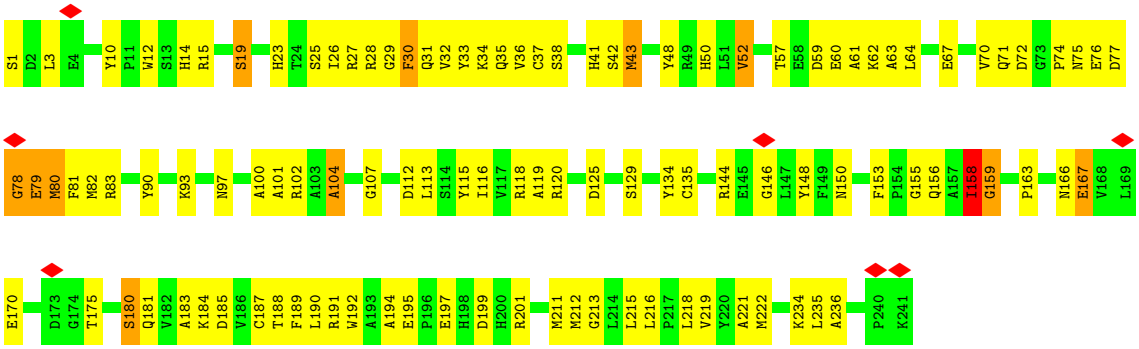
• Molecule 53: Cytochrome b

Chain AN: 6% 55% 42%



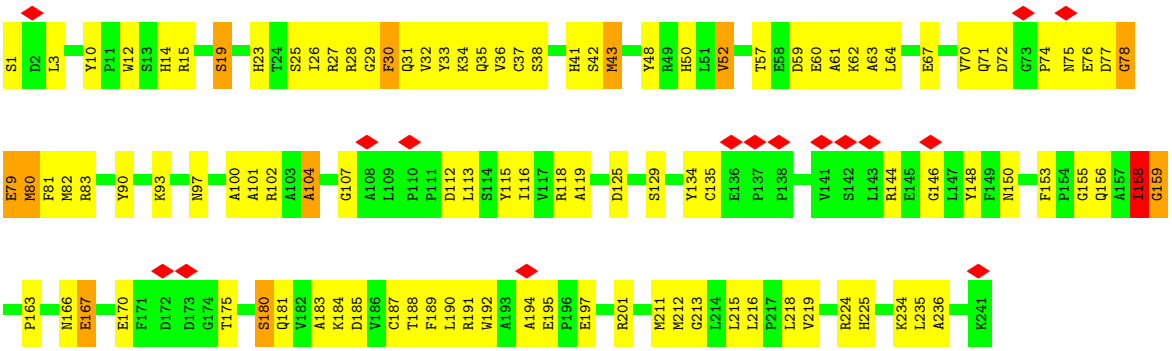
• Molecule 54: COMPLEX III SUBUNIT 4 / CYTOCHROME C1

Chain AD: 54% 41% 5%



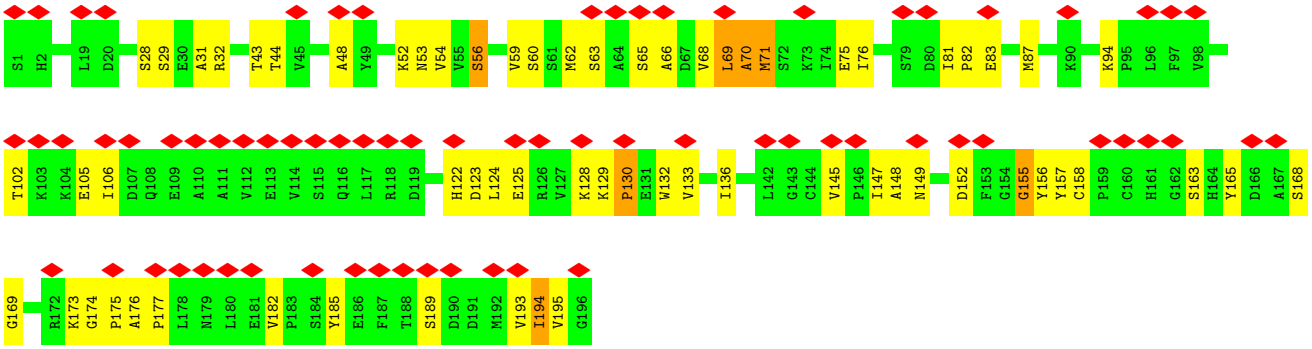
• Molecule 54: COMPLEX III SUBUNIT 4 / CYTOCHROME C1

Chain AO: 7% 55% 40% 5%



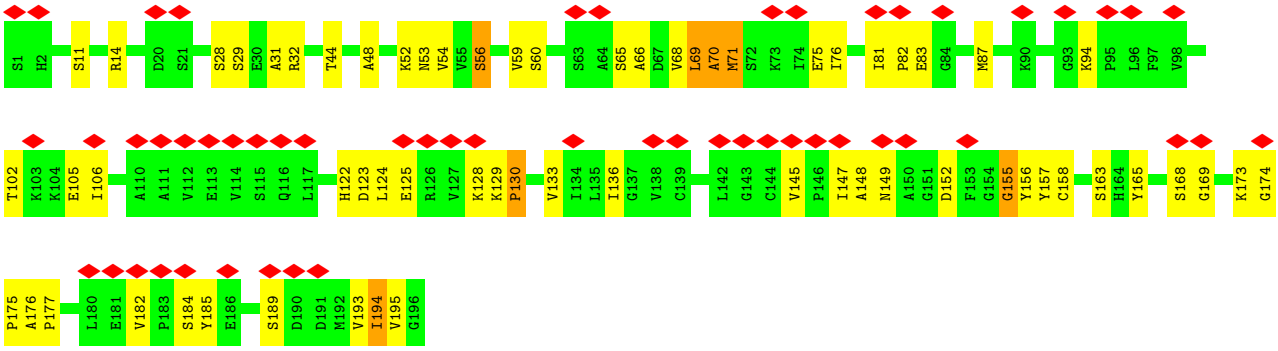
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE:



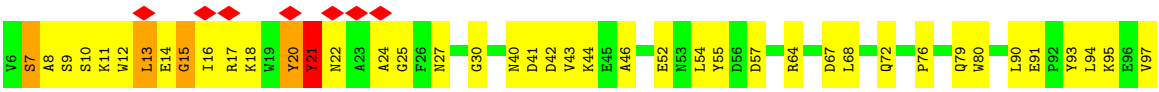
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AP:



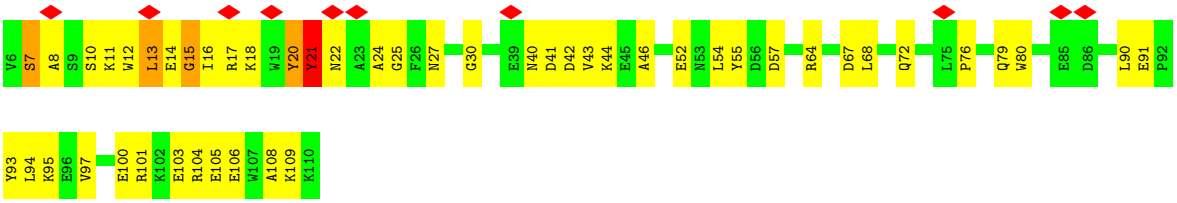
- Molecule 56: COMPLEX III SUBUNIT 7 / 14KDA

Chain AF:



• Molecule 56: COMPLEX III SUBUNIT 7 / 14KDA

Chain AQ:

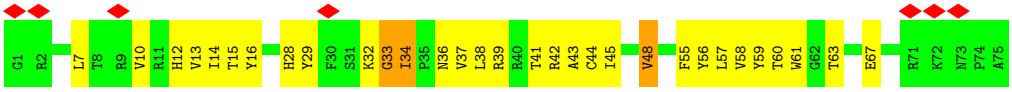


• Molecule 57: COMPLEX III SUBUNIT 8 / QP-C

Chain AG:

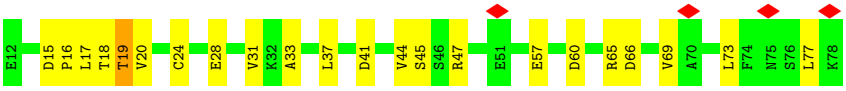
• Molecule 57: COMPLEX III SUBUNIT 8 / QP-C

Chain AR:



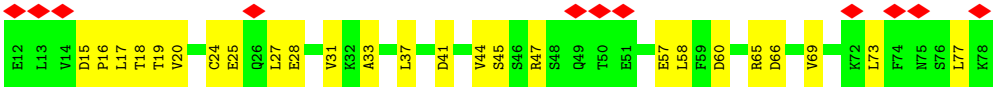
• Molecule 58: Cytochrome b-c1 complex subunit 6

Chain AH:



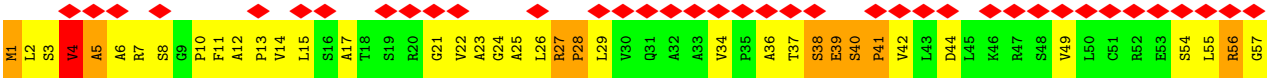
• Molecule 58: Cytochrome b-c1 complex subunit 6

Chain AS:



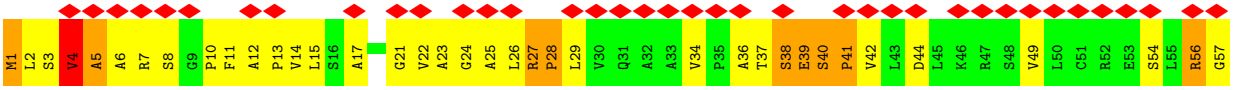
• Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:



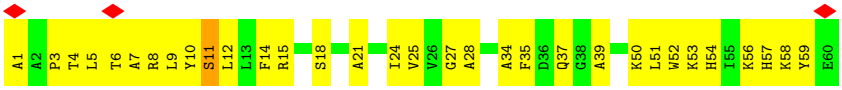
• Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AT:



• Molecule 60: COMPLEX III SUBUNIT 9 / 7.2KDA

Chain AJ:

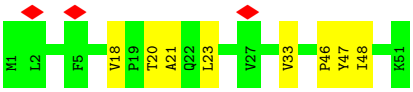


• Molecule 60: COMPLEX III SUBUNIT 9 / 7.2KDA

Chain AU:

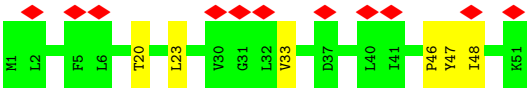
• Molecule 61: COMPLEX III SUBUNIT 10 / 6.4KDA

Chain AK:



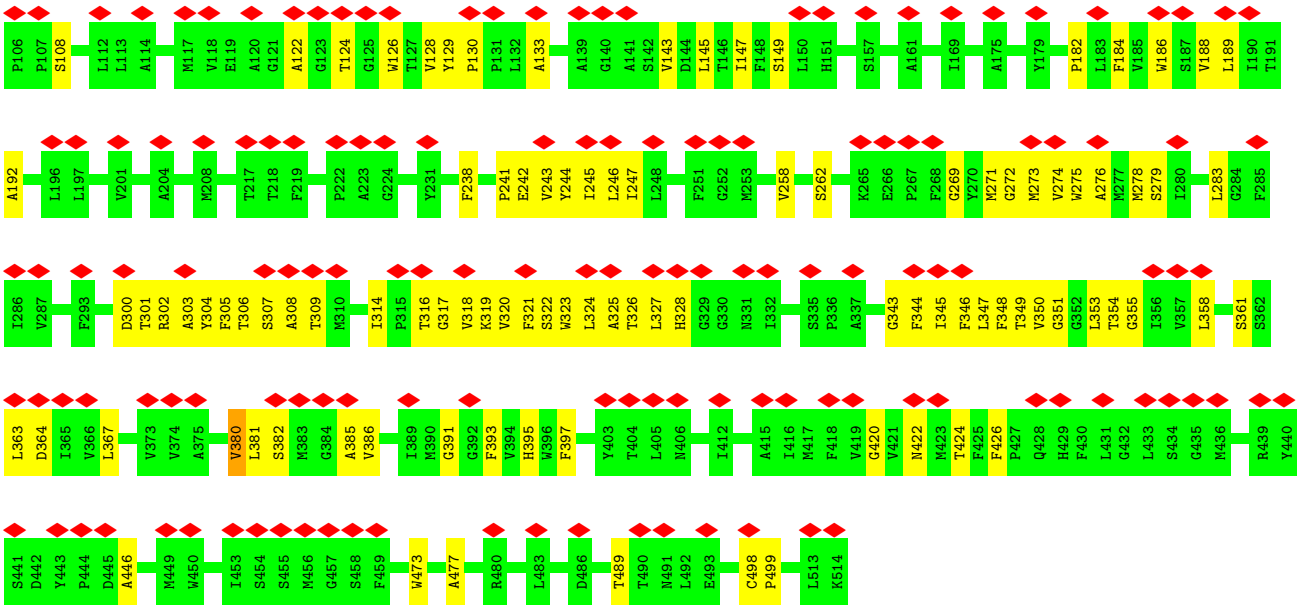
• Molecule 61: COMPLEX III SUBUNIT 10 / 6.4KDA

Chain AV:



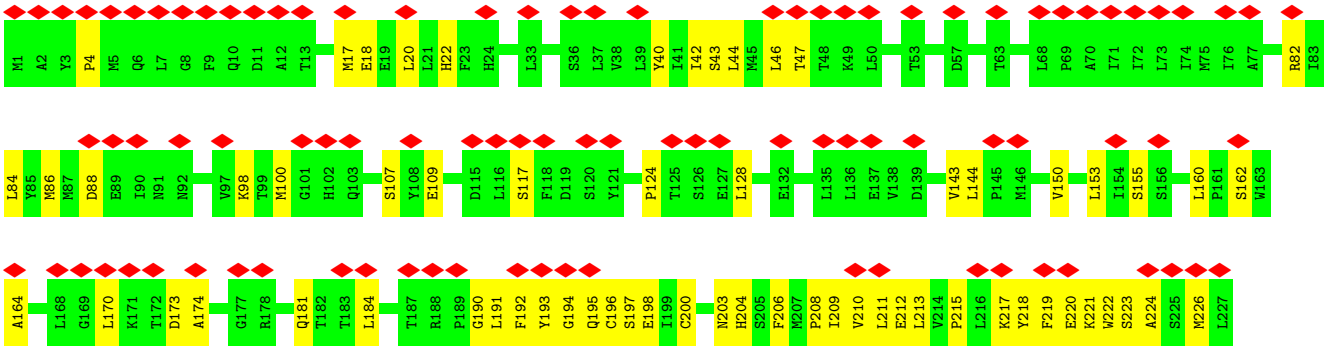
• Molecule 62: Cytochrome c oxidase subunit 1

Chain BN:



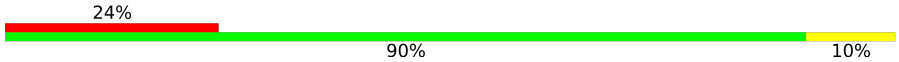
- Molecule 63: Cytochrome c oxidase subunit 2

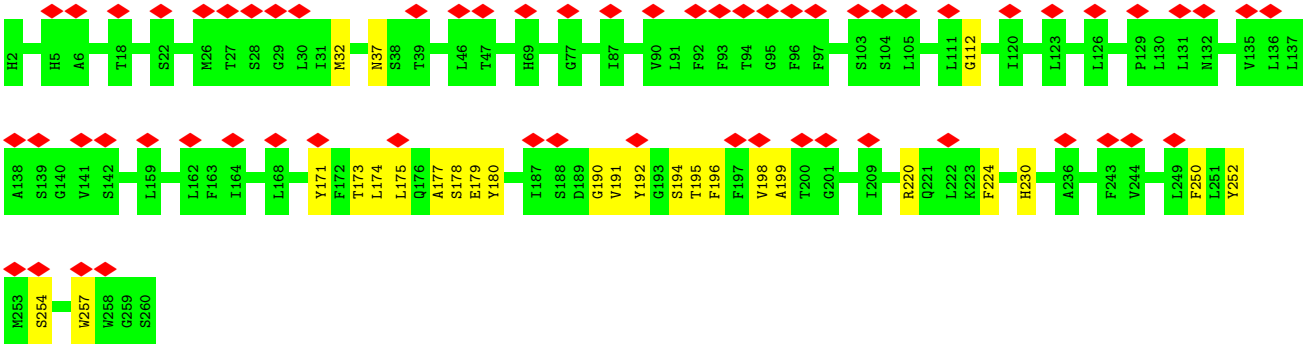
Chain BO:



- Molecule 64: Cytochrome c oxidase subunit 3

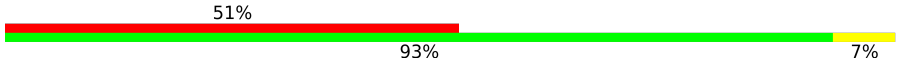
Chain BC:

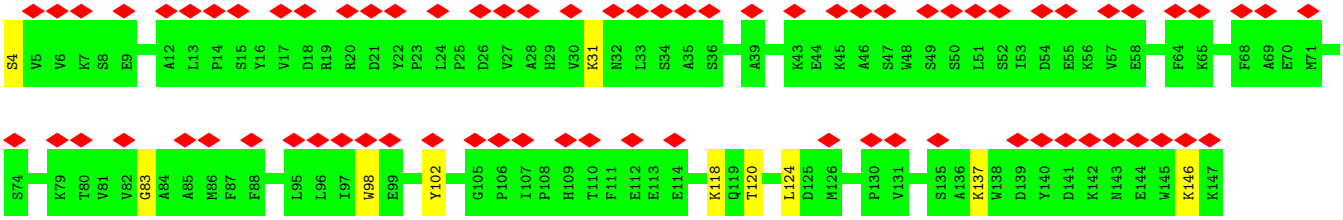




- Molecule 65: COMPLEX IV COX4

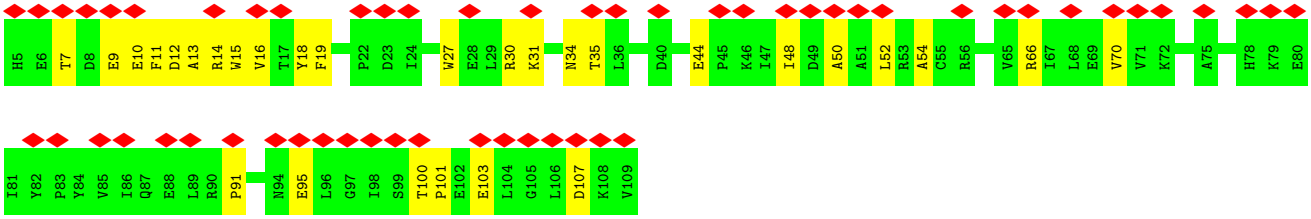
Chain BD:





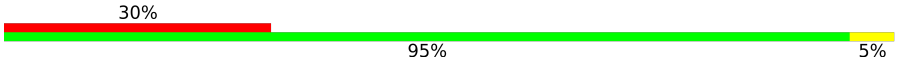
- Molecule 66: COMPLEX IV COX5A

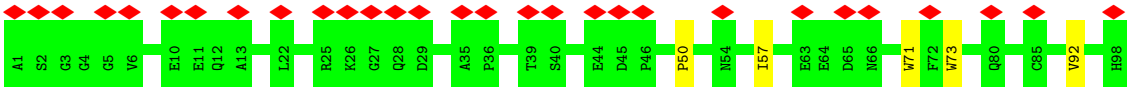
Chain BE:



- Molecule 67: COMPLEX IV COX5B

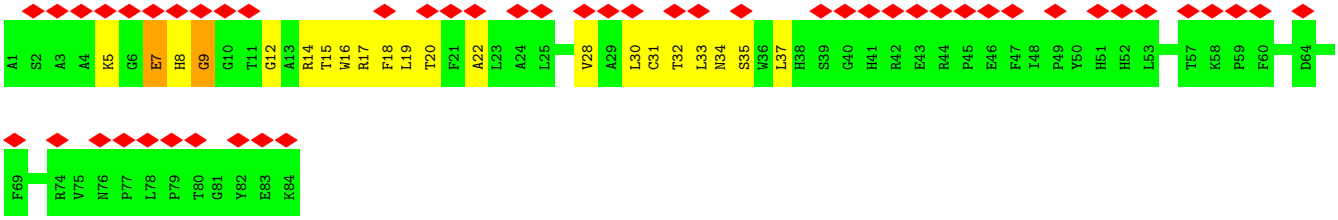
Chain BP:





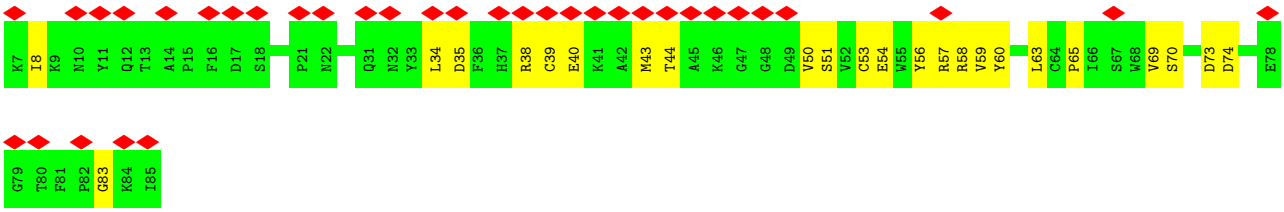
- Molecule 68: Cytochrome c oxidase subunit 6A, mitochondrial

Chain BG:



- Molecule 69: COMPLEX IV COX6B1

Chain BH:

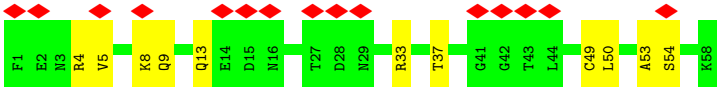


- Molecule 70: COMPLEX IV COX6C

Chain BI:

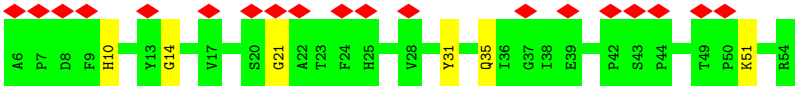
- Molecule 71: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain BJ:



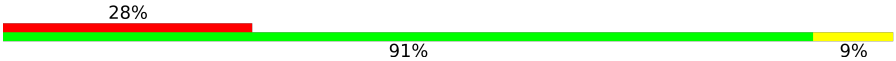
- Molecule 72: COMPLEX IV COX7B

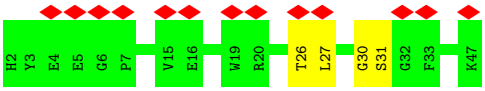
Chain BK:



- Molecule 73: COMPLEX IV COX7C

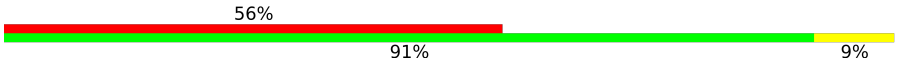
Chain BL:

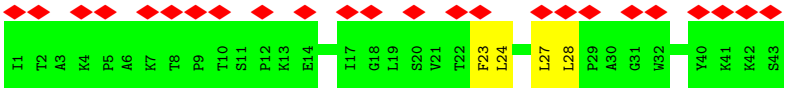




- Molecule 74: COMPLEX IV COX8B

Chain BM:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13910	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 ($e^-/Å^2$)	34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81395	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.173	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.094	Depositor
Map size (Å)	853.12, 853.12, 853.12	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	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: FES, HEM, CU, SF4, HEA, CUA

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	$\#\|Z\|>5$
2	B	0.73	0/21	0.97	0/23
5	E	0.36	0/20	0.72	0/20
6	F	0.85	0/20	1.08	0/20
7	G	0.51	0/65	1.13	1/67 (1.5%)
9	I	0.91	0/40	1.88	1/40 (2.5%)
51	AA	0.54	0/2197	0.95	9/3055 (0.3%)
51	AL	0.54	0/2197	0.95	11/3055 (0.4%)
52	AB	0.54	0/2080	0.87	6/2890 (0.2%)
52	AM	0.54	0/2080	0.87	5/2890 (0.2%)
53	AC	0.77	1/1865 (0.1%)	0.74	0/2595
53	AN	0.77	1/1865 (0.1%)	0.74	0/2595
54	AD	0.53	0/1187	1.00	3/1650 (0.2%)
54	AO	0.53	0/1187	1.00	3/1650 (0.2%)
55	AE	0.80	2/965 (0.2%)	1.85	29/1340 (2.2%)
55	AP	1.01	3/966 (0.3%)	1.87	28/1343 (2.1%)
56	AF	0.58	0/521	0.97	2/726 (0.3%)
56	AQ	0.58	0/521	0.98	2/726 (0.3%)
57	AG	0.45	0/370	0.61	0/514
57	AR	0.45	0/370	0.61	0/514
58	AH	0.49	0/334	0.61	0/466
58	AS	0.50	0/334	0.62	0/466
59	AI	0.74	0/280	1.70	6/388 (1.5%)
59	AT	0.74	0/280	1.71	6/388 (1.5%)
60	AJ	0.49	0/296	0.77	0/411
60	AU	0.48	0/296	0.77	0/411
61	AK	0.41	0/249	0.52	0/344
61	AV	0.42	0/249	0.52	0/344
62	BN	0.26	0/2522	0.72	2/3501 (0.1%)
63	BO	0.30	0/1126	0.75	0/1570
64	BC	0.18	0/1274	0.44	0/1770
65	BD	0.19	0/715	0.45	0/997
66	BE	0.26	0/519	0.68	0/722

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
67	BP	0.26	0/480	0.60	0/665
68	BG	0.32	0/411	0.82	1/569 (0.2%)
69	BH	0.26	0/390	0.66	0/542
70	BI	0.28	0/360	0.53	0/500
71	BJ	0.19	0/283	0.67	0/391
72	BK	0.28	0/240	0.57	0/332
73	BL	0.20	0/225	0.49	0/311
74	BM	0.23	0/212	0.60	0/294
All	All	0.55	7/29612 (0.0%)	0.93	115/41095 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	5
4	D	0	1
6	F	0	3
7	G	0	10
9	I	0	5
12	L	0	5
13	M	0	5
14	N	0	5
17	Q	0	1
18	R	0	1
19	d	0	2
22	V	0	1
23	W	0	1
24	X	0	3
25	Y	0	8
32	g	0	1
33	h	0	1
33	z	0	1
34	i	0	1
38	1	0	1
51	AA	0	13
51	AL	0	13
52	AB	0	17
52	AM	0	17
53	AC	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	AN	0	2
54	AD	0	8
54	AO	0	8
55	AE	0	3
55	AP	0	4
56	AF	0	5
56	AQ	0	5
57	AG	0	2
57	AR	0	2
59	AI	0	6
59	AT	0	6
60	AJ	0	1
60	AU	0	1
61	AK	0	1
61	AV	0	1
62	BN	0	1
63	BO	0	1
64	BC	0	1
68	BG	0	1
All	All	0	184

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	AC	56	THR	C-N	-21.38	0.83	1.33
53	AN	56	THR	C-N	-21.36	0.83	1.33
55	AP	44	THR	C-N	-19.48	1.09	1.33
55	AP	56	SER	C-O	7.39	1.33	1.24
55	AE	56	SER	C-O	7.28	1.33	1.24

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	AO	159	GLY	N-CA-C	16.30	137.11	115.59
54	AD	159	GLY	N-CA-C	16.21	136.98	115.59
62	BN	129	TYR	CA-C-N	13.33	134.11	120.38
62	BN	129	TYR	C-N-CA	13.33	134.11	120.38
59	AT	4	VAL	N-CA-C	12.78	127.36	113.43

There are no chirality outliers.

5 of 184 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	151	UNK	Peptide
2	B	54	CYS	Peptide
3	C	115	UNK	Peptide
3	C	150	UNK	Peptide
3	C	68	UNK	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	A	510	0	109	7	0
2	B	774	0	177	33	0
3	C	970	0	232	45	0
4	D	1920	0	409	73	0
5	E	949	0	216	26	0
6	F	2149	0	468	88	0
7	G	3276	0	762	132	0
8	H	1485	0	307	37	0
9	I	863	0	208	55	0
10	J	695	0	144	30	0
11	K	465	0	100	10	0
12	L	2875	0	596	91	0
13	M	2275	0	466	93	0
14	N	1725	0	354	81	0
15	O	520	0	119	19	0
16	P	425	0	98	16	0
17	Q	330	0	69	15	0
18	R	145	0	31	2	0
19	S	400	0	82	24	0
19	d	400	0	87	12	0
20	T	265	0	55	5	0
21	U	480	0	107	4	0
22	V	560	0	119	15	0
23	W	515	0	111	10	0
24	X	1290	0	283	42	0
25	Y	1595	0	325	89	0
26	Z	595	0	124	11	0
27	a	555	0	129	14	0
28	b	460	0	103	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c	355	0	76	13	0
30	e	275	0	58	14	0
31	f	290	0	61	8	0
32	g	650	0	136	21	0
33	9	315	0	70	5	0
33	h	315	0	65	33	0
33	z	130	0	29	8	0
34	i	350	0	81	4	0
35	j	220	0	47	3	0
36	k	400	0	86	5	0
37	0	180	0	39	3	0
38	1	150	0	32	2	0
39	2	190	0	41	5	0
40	3	140	0	33	2	0
40	4	140	0	30	3	0
41	5	170	0	37	4	0
42	6	105	0	23	9	0
43	7	195	0	42	19	0
44	8	135	0	29	5	0
45	y	230	0	48	4	0
46	x	65	0	15	0	0
47	w	120	0	27	4	0
48	v	90	0	20	1	0
49	u	80	0	18	1	0
50	t	60	0	15	2	0
51	AA	2198	0	1034	236	0
51	AL	2198	0	1034	215	0
52	AB	2081	0	1035	197	0
52	AM	2081	0	1035	197	0
53	AC	1866	0	827	145	0
53	AN	1866	0	827	141	0
54	AD	1188	0	533	109	0
54	AO	1188	0	533	109	0
55	AE	967	0	440	25	0
55	AP	967	0	440	23	0
56	AF	522	0	227	49	0
56	AQ	522	0	227	50	0
57	AG	371	0	162	25	0
57	AR	371	0	162	25	0
58	AH	335	0	141	14	0
58	AS	335	0	141	17	0
59	AI	281	0	142	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AT	281	0	142	39	0
60	AJ	297	0	148	30	0
60	AU	297	0	148	31	0
61	AK	250	0	121	5	0
61	AV	250	0	121	4	0
62	BN	2523	0	1169	82	0
63	BO	1127	0	474	39	0
64	BC	1275	0	576	18	0
65	BD	716	0	321	6	0
66	BE	520	0	231	24	0
67	BP	481	0	224	3	0
68	BG	412	0	192	12	0
69	BH	391	0	169	15	0
70	BI	361	0	184	7	0
71	BJ	284	0	131	7	0
72	BK	241	0	115	4	0
73	BL	226	0	101	3	0
74	BM	213	0	98	2	0
75	B	8	0	0	1	0
75	F	8	0	0	3	0
75	G	16	0	0	5	0
75	I	16	0	0	13	0
76	AE	4	0	0	0	0
76	AP	4	0	0	0	0
76	E	4	0	0	3	0
76	G	4	0	0	1	0
77	AC	86	0	60	7	0
77	AD	43	0	30	8	0
77	AN	86	0	60	2	0
77	AO	43	0	30	11	0
78	BN	1	0	0	0	0
79	BN	120	0	108	11	0
80	BO	2	0	0	1	0
All	All	64743	0	21441	3105	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 36.

The worst 5 of 3105 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)
54:AO:37:CYS:CA	77:AO:301:HEM:HAB	1.54	1.36
62:BN:126:TRP:N	79:BN:602:HEA:O1D	1.64	1.29
53:AN:56:THR:C	53:AN:57:PRO:CA	2.05	1.27
53:AC:56:THR:C	53:AC:57:PRO:CA	2.05	1.27
6:F:298:UNK:O	6:F:334:UNK:HA	1.35	1.26

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	
2	B	4/154 (3%)	4 (100%)	0	0	100	100
5	E	4/189 (2%)	2 (50%)	2 (50%)	0	100	100
6	F	4/429 (1%)	4 (100%)	0	0	100	100
7	G	12/652 (2%)	6 (50%)	4 (33%)	2 (17%)	0	2
9	I	8/171 (5%)	4 (50%)	3 (38%)	1 (12%)	0	4
51	AA	444/446 (100%)	369 (83%)	68 (15%)	7 (2%)	7	38
51	AL	444/446 (100%)	370 (83%)	67 (15%)	7 (2%)	7	38
52	AB	421/423 (100%)	369 (88%)	47 (11%)	5 (1%)	10	44
52	AM	421/423 (100%)	369 (88%)	47 (11%)	5 (1%)	10	44
53	AC	376/378 (100%)	288 (77%)	73 (19%)	15 (4%)	2	18
53	AN	376/378 (100%)	287 (76%)	74 (20%)	15 (4%)	2	18
54	AD	239/241 (99%)	180 (75%)	52 (22%)	7 (3%)	3	23
54	AO	239/241 (99%)	180 (75%)	52 (22%)	7 (3%)	3	23
55	AE	192/196 (98%)	148 (77%)	36 (19%)	8 (4%)	2	17
55	AP	194/196 (99%)	151 (78%)	35 (18%)	8 (4%)	2	18
56	AF	103/105 (98%)	86 (84%)	17 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	AQ	103/105 (98%)	86 (84%)	17 (16%)	0	100	100
57	AG	73/75 (97%)	59 (81%)	11 (15%)	3 (4%)	2	18
57	AR	73/75 (97%)	59 (81%)	11 (15%)	3 (4%)	2	18
58	AH	65/67 (97%)	53 (82%)	11 (17%)	1 (2%)	8	40
58	AS	65/67 (97%)	52 (80%)	13 (20%)	0	100	100
59	AI	55/57 (96%)	31 (56%)	17 (31%)	7 (13%)	0	4
59	AT	55/57 (96%)	31 (56%)	17 (31%)	7 (13%)	0	4
60	AJ	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	7	36
60	AU	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	7	36
61	AK	49/51 (96%)	44 (90%)	4 (8%)	1 (2%)	6	31
61	AV	49/51 (96%)	44 (90%)	4 (8%)	1 (2%)	6	31
62	BN	512/514 (100%)	485 (95%)	26 (5%)	1 (0%)	43	78
63	BO	225/227 (99%)	200 (89%)	24 (11%)	1 (0%)	30	67
64	BC	257/259 (99%)	249 (97%)	8 (3%)	0	100	100
65	BD	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
66	BE	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
67	BP	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
68	BG	82/84 (98%)	70 (85%)	10 (12%)	2 (2%)	4	27
69	BH	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	9	42
70	BI	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
71	BJ	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
72	BK	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
73	BL	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
74	BM	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
All	All	5937/7572 (78%)	5008 (84%)	812 (14%)	117 (2%)	8	31

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	AA	143	THR
52	AB	436	ILE
54	AD	79	GLU
55	AE	70	ALA
55	AE	177	PRO

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	
2	B	4/4 (100%)	4 (100%)	0	100	100
5	E	4/4 (100%)	4 (100%)	0	100	100
6	F	4/4 (100%)	4 (100%)	0	100	100
7	G	12/12 (100%)	12 (100%)	0	100	100
9	I	8/8 (100%)	6 (75%)	2 (25%)	0	4
All	All	32/32 (100%)	30 (94%)	2 (6%)	18	37

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

Mol	Chain	Res	Type
9	I	116	CYS
9	I	119	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\#\|Z\| > 2$
80	CUA	BO	301	63	0,1,1	-	-	-		
76	FES	AE	201	-	0,4,4	-	-	-		
75	SF4	B	201	2	0,12,12	-	-	-		
77	HEM	AD	301	-	50,50,50	3.43	24 (48%)	66,82,82	2.84	31 (46%)
77	HEM	AC	402	-	50,50,50	3.36	23 (46%)	66,82,82	2.67	27 (40%)
79	HEA	BN	603	-	66,67,67	1.17	4 (6%)	78,103,103	1.07	3 (3%)
76	FES	G	803	7	0,4,4	-	-	-		
77	HEM	AN	401	-	50,50,50	3.43	26 (52%)	66,82,82	2.93	26 (39%)
77	HEM	AO	301	-	50,50,50	3.43	24 (48%)	66,82,82	2.84	33 (50%)
76	FES	E	201	5	0,4,4	-	-	-		
75	SF4	I	201	9	0,12,12	-	-	-		
75	SF4	F	500	6	0,12,12	-	-	-		
75	SF4	G	802	7	0,12,12	-	-	-		
79	HEA	BN	602	-	66,67,67	0.98	2 (3%)	78,103,103	1.19	6 (7%)
75	SF4	I	202	9	0,12,12	-	-	-		
77	HEM	AN	402	-	50,50,50	3.36	22 (44%)	66,82,82	2.68	27 (40%)
76	FES	AP	201	-	0,4,4	-	-	-		
77	HEM	AC	401	-	50,50,50	3.44	27 (54%)	66,82,82	2.92	26 (39%)
75	SF4	G	801	7	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
79	HEA	BN	602	-	-	7/36/76/76	-
77	HEM	AO	301	-	-	4/14/54/54	-
76	FES	AE	201	-	-	-	0/1/1/1
75	SF4	F	500	6	-	-	0/6/5/5
76	FES	AP	201	-	-	-	0/1/1/1
76	FES	E	201	5	-	-	0/1/1/1
75	SF4	B	201	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	SF4	I	202	9	-	-	0/6/5/5
77	HEM	AN	402	-	-	9/14/54/54	-
75	SF4	I	201	9	-	-	0/6/5/5
77	HEM	AD	301	-	-	4/14/54/54	-
77	HEM	AC	402	-	-	9/14/54/54	-
75	SF4	G	802	7	-	-	0/6/5/5
79	HEA	BN	603	-	-	7/36/76/76	-
76	FES	G	803	7	-	-	0/1/1/1
77	HEM	AC	401	-	-	8/14/54/54	-
75	SF4	G	801	7	-	-	0/6/5/5
77	HEM	AN	401	-	-	8/14/54/54	-

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	AC	401	HEM	C4D-C3D	-7.61	1.31	1.45
77	AN	401	HEM	C4D-C3D	-7.59	1.32	1.45
77	AN	402	HEM	C3C-C4C	-7.44	1.32	1.46
77	AC	402	HEM	C3C-C4C	-7.44	1.32	1.46
77	AC	401	HEM	C3C-C4C	-7.06	1.33	1.46

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	AN	402	HEM	C4A-NA-C1A	8.19	113.37	105.35
77	AC	402	HEM	C4A-NA-C1A	8.11	113.29	105.35
77	AD	301	HEM	C4A-NA-C1A	7.10	112.30	105.35
77	AN	402	HEM	C4C-CHD-C1D	-7.08	110.78	126.06
77	AC	402	HEM	C4C-CHD-C1D	-7.07	110.80	126.06

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
77	AC	401	HEM	C2B-C3B-CAB-CBB
77	AC	401	HEM	C4B-C3B-CAB-CBB
77	AC	401	HEM	C2C-C3C-CAC-CBC
77	AC	401	HEM	C4C-C3C-CAC-CBC
77	AC	402	HEM	C1A-C2A-CAA-CBA

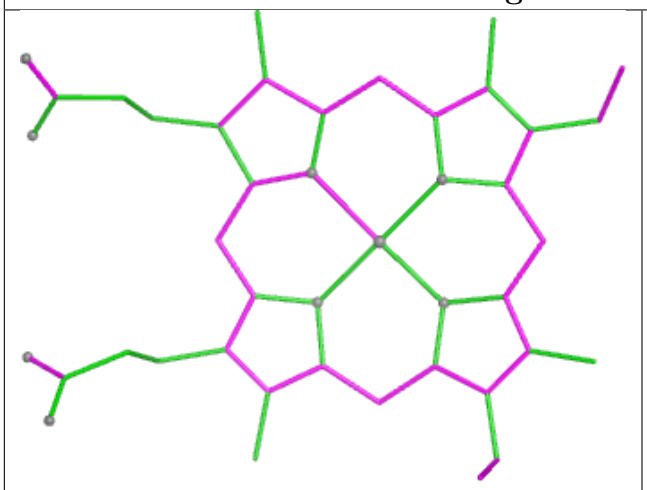
There are no ring outliers.

15 monomers are involved in 66 short contacts:

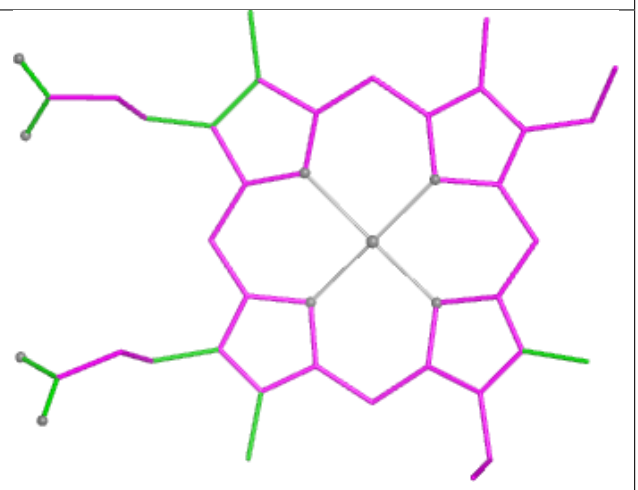
Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	BO	301	CUA	1	0
75	B	201	SF4	1	0
77	AD	301	HEM	8	0
79	BN	603	HEA	2	0
76	G	803	FES	1	0
77	AN	401	HEM	2	0
77	AO	301	HEM	11	0
76	E	201	FES	3	0
75	I	201	SF4	8	0
75	F	500	SF4	3	0
75	G	802	SF4	4	0
79	BN	602	HEA	9	0
75	I	202	SF4	5	0
77	AC	401	HEM	7	0
75	G	801	SF4	1	0

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

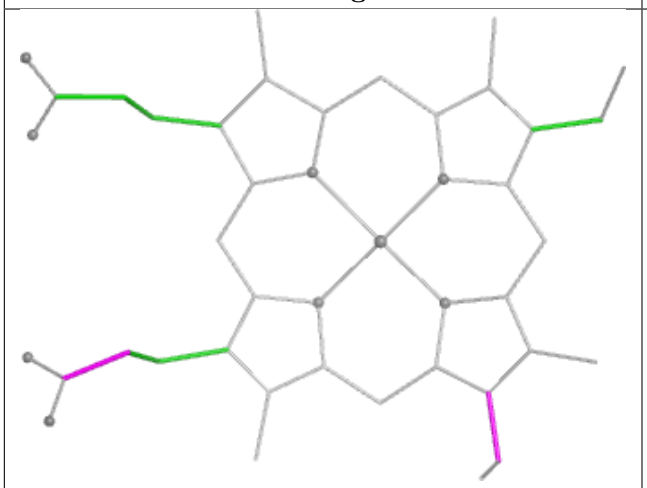
Ligand HEM AD 301



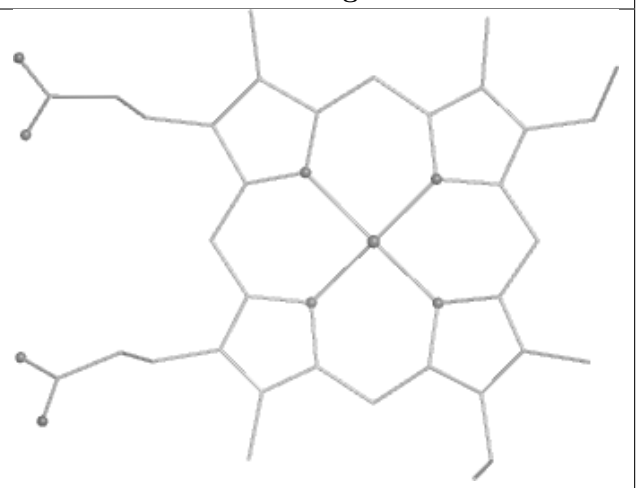
Bond lengths



Bond angles

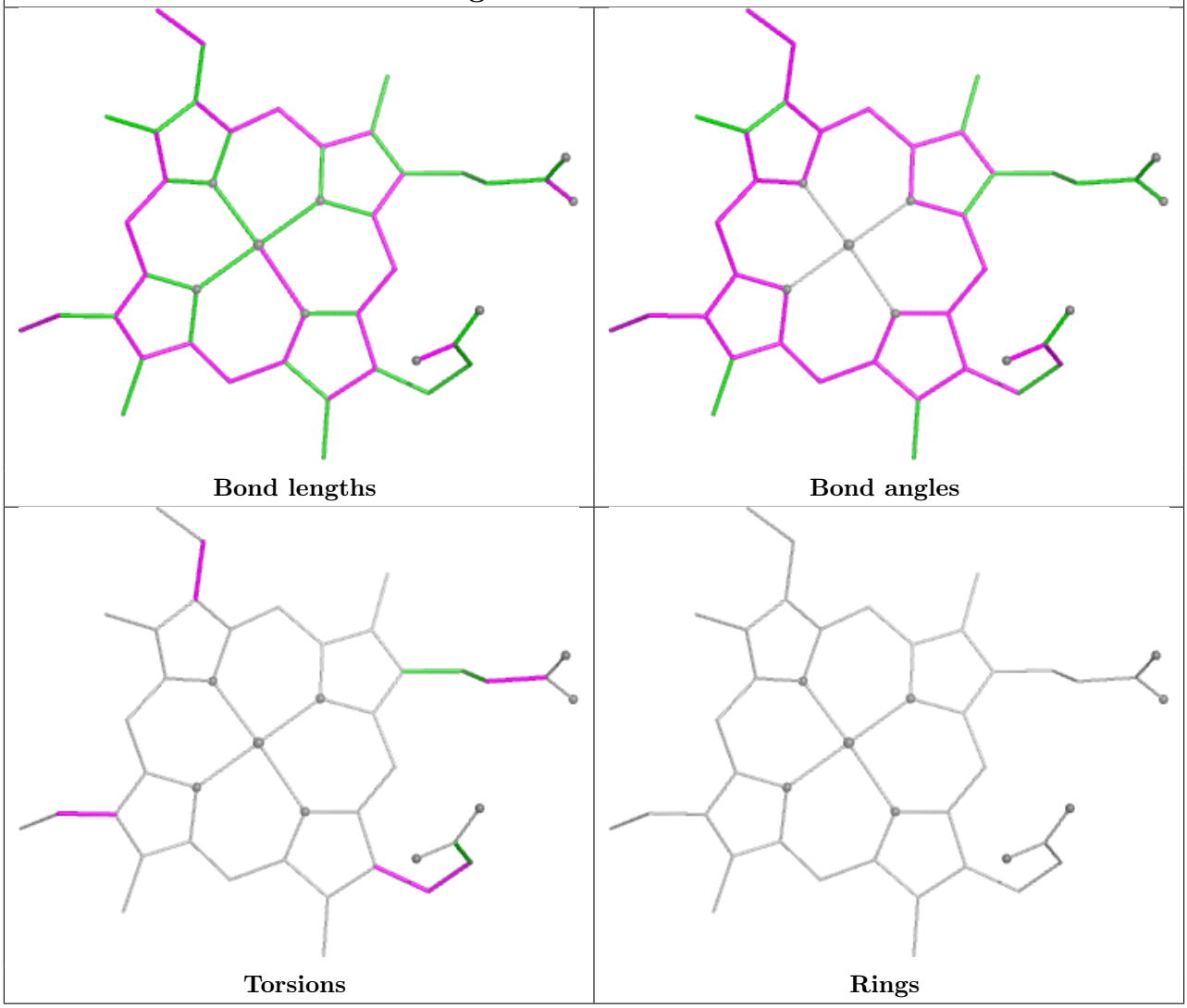


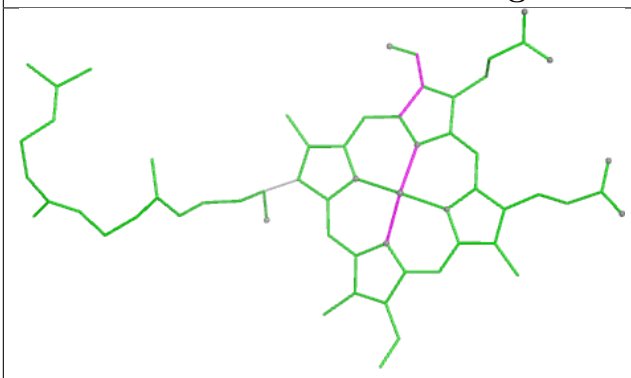
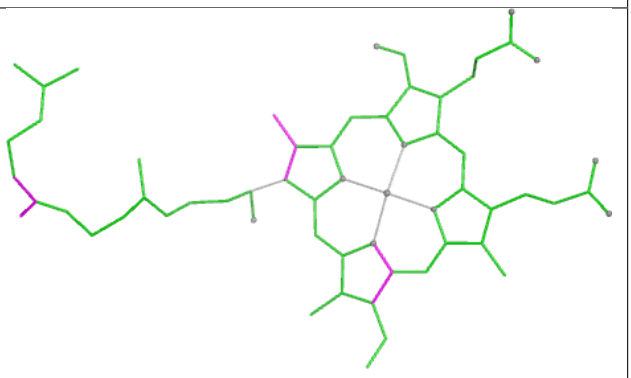
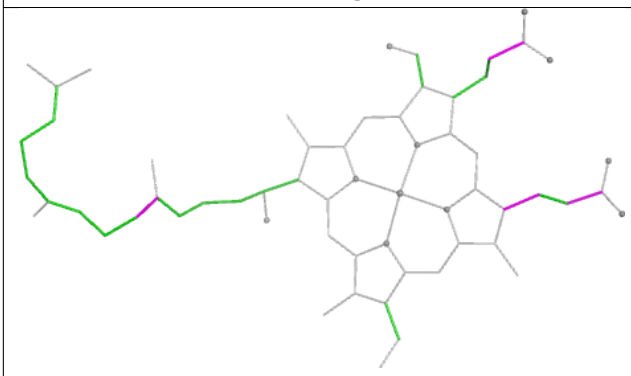
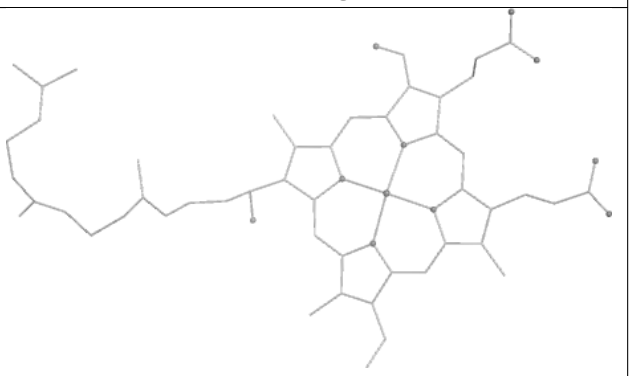
Torsions



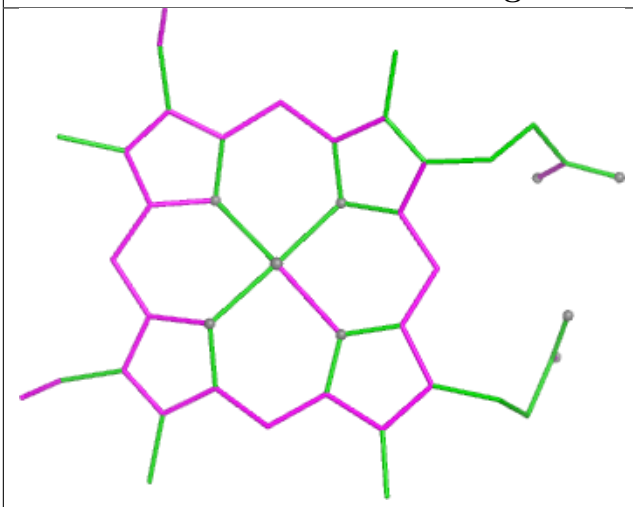
Rings

Ligand HEM AC 402

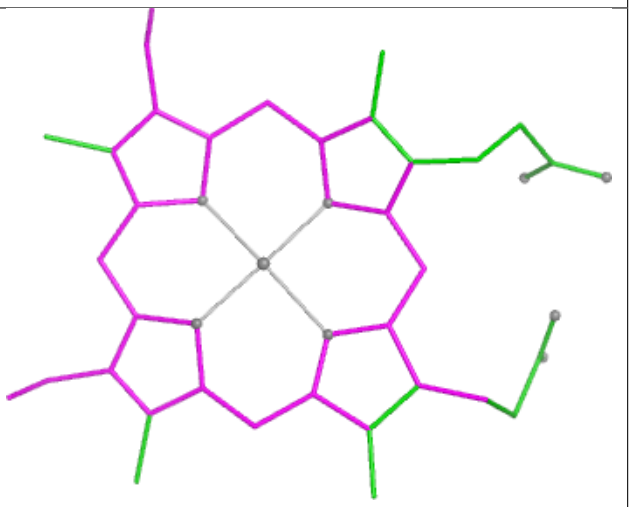


Ligand HEA BN 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

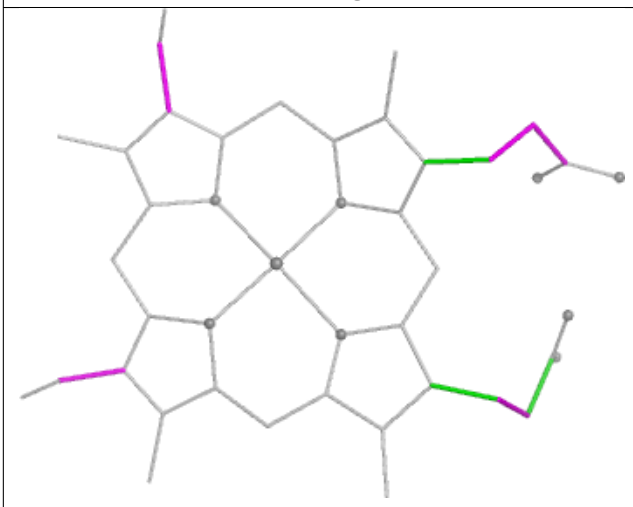
Ligand HEM AN 401



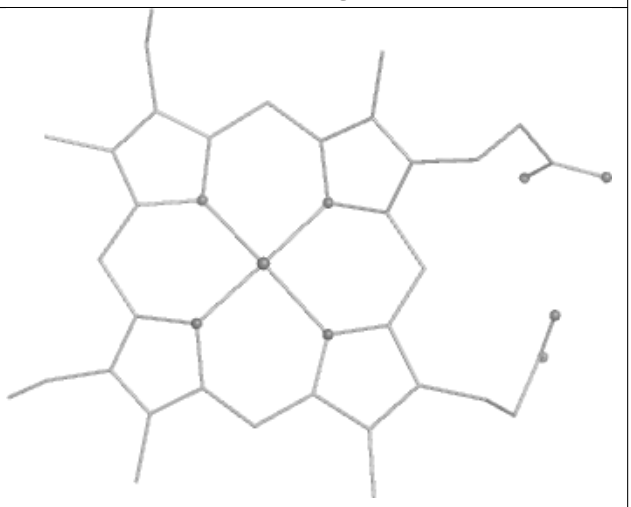
Bond lengths



Bond angles

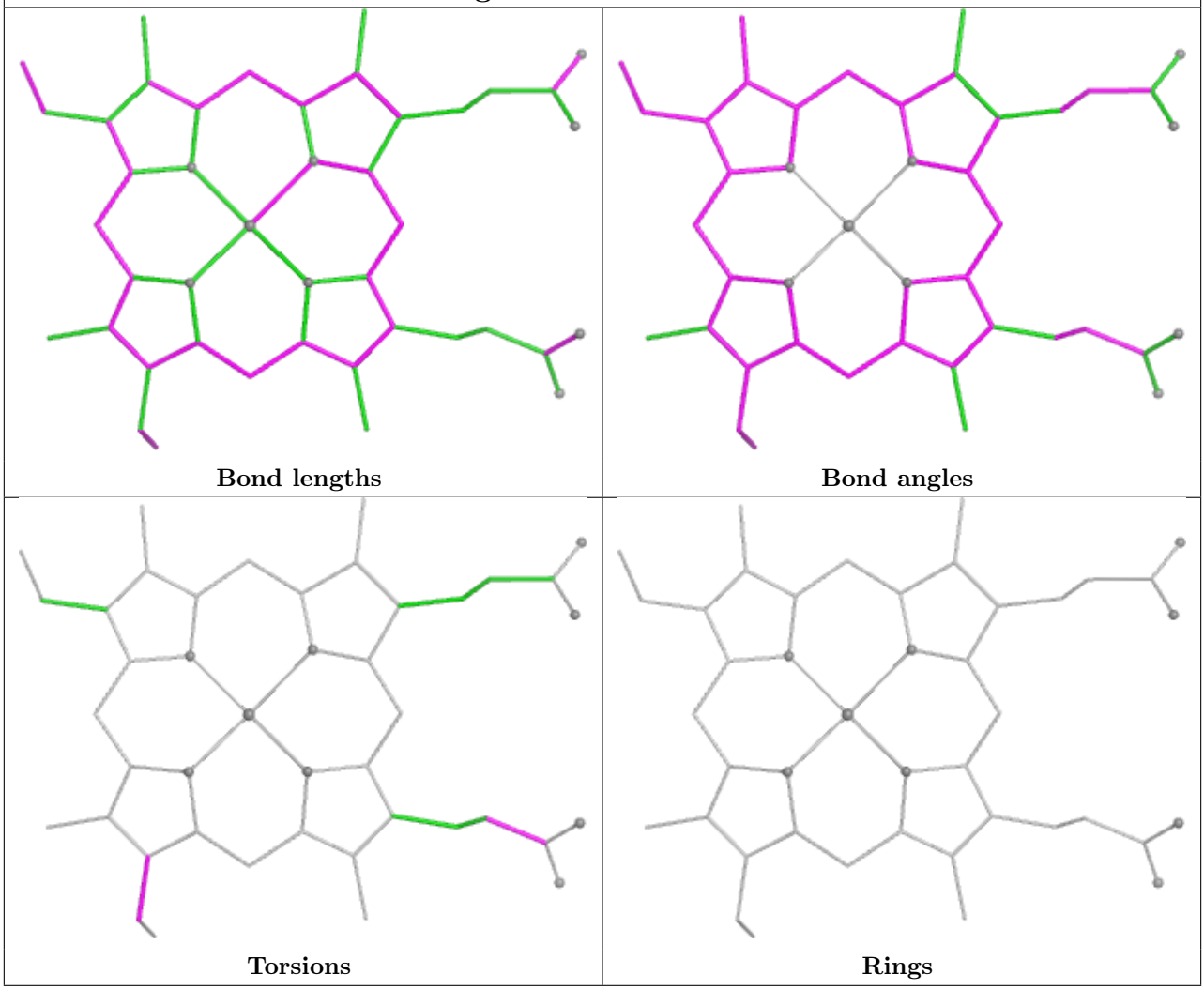


Torsions

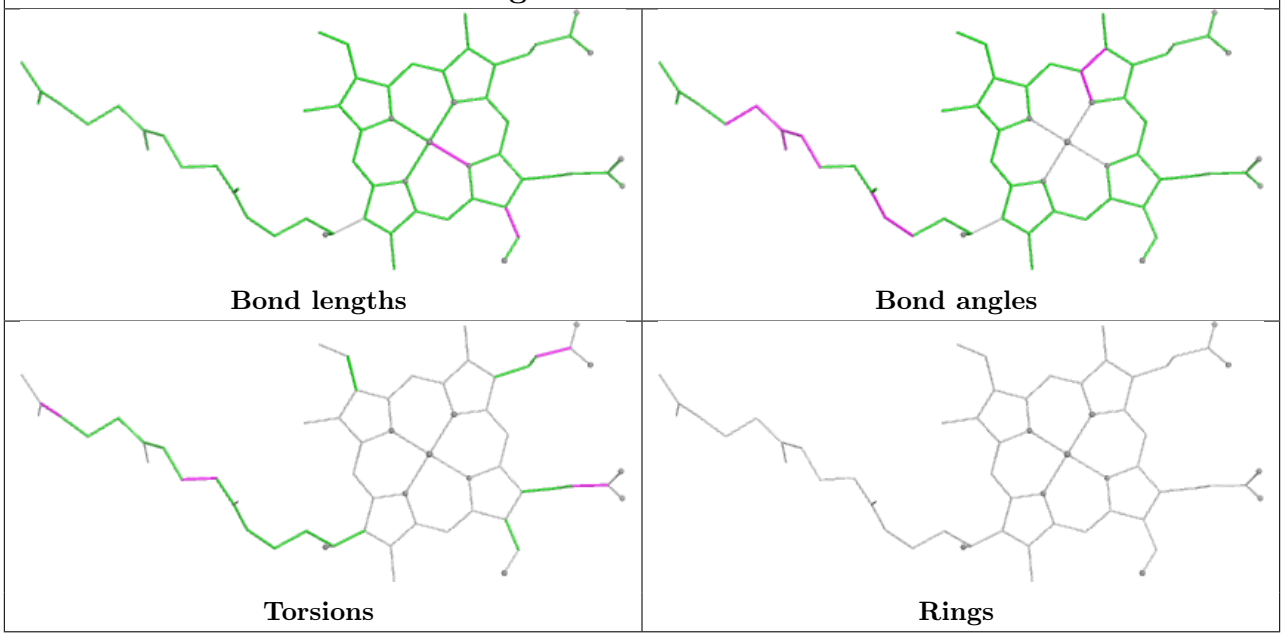


Rings

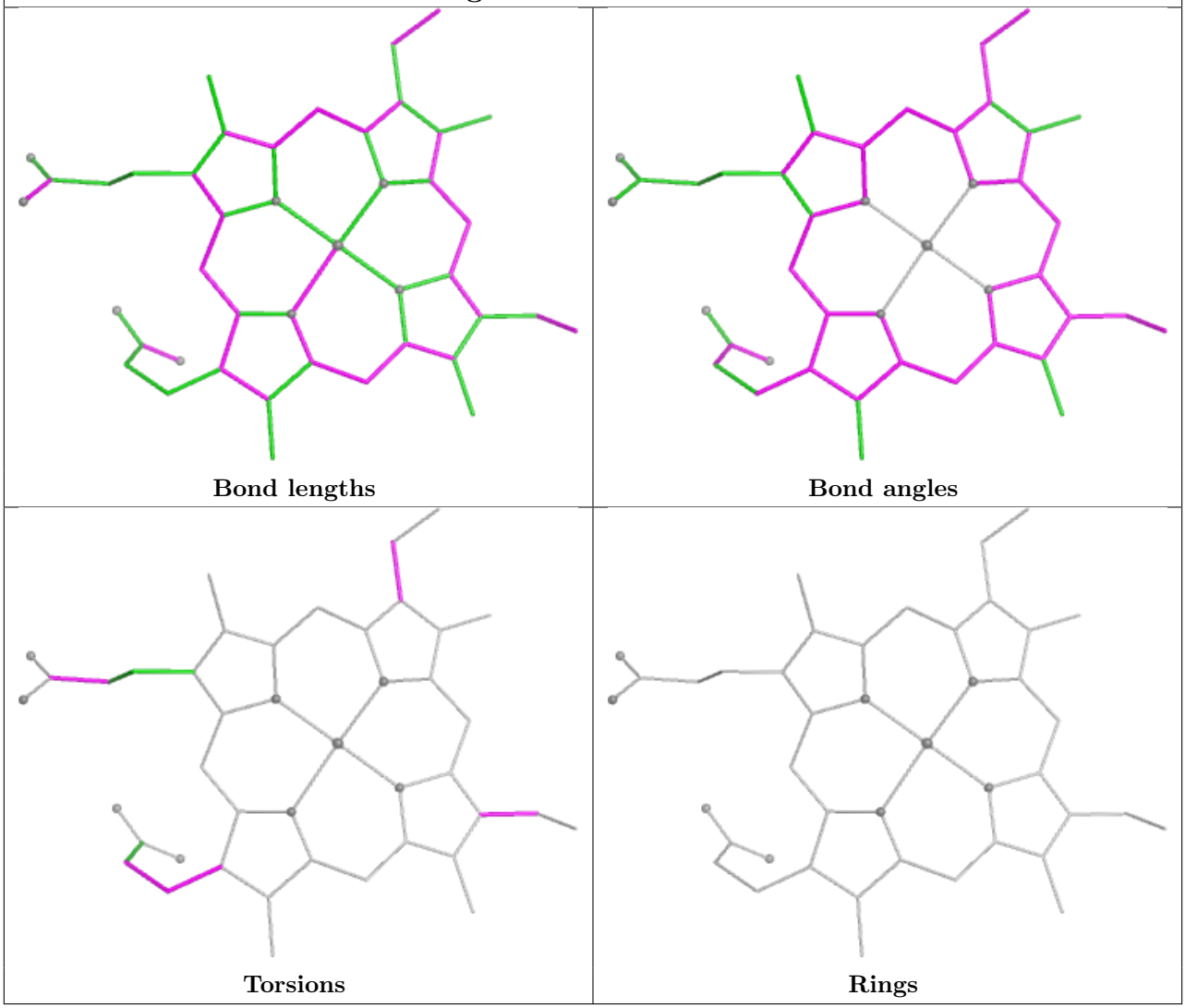
Ligand HEM AO 301



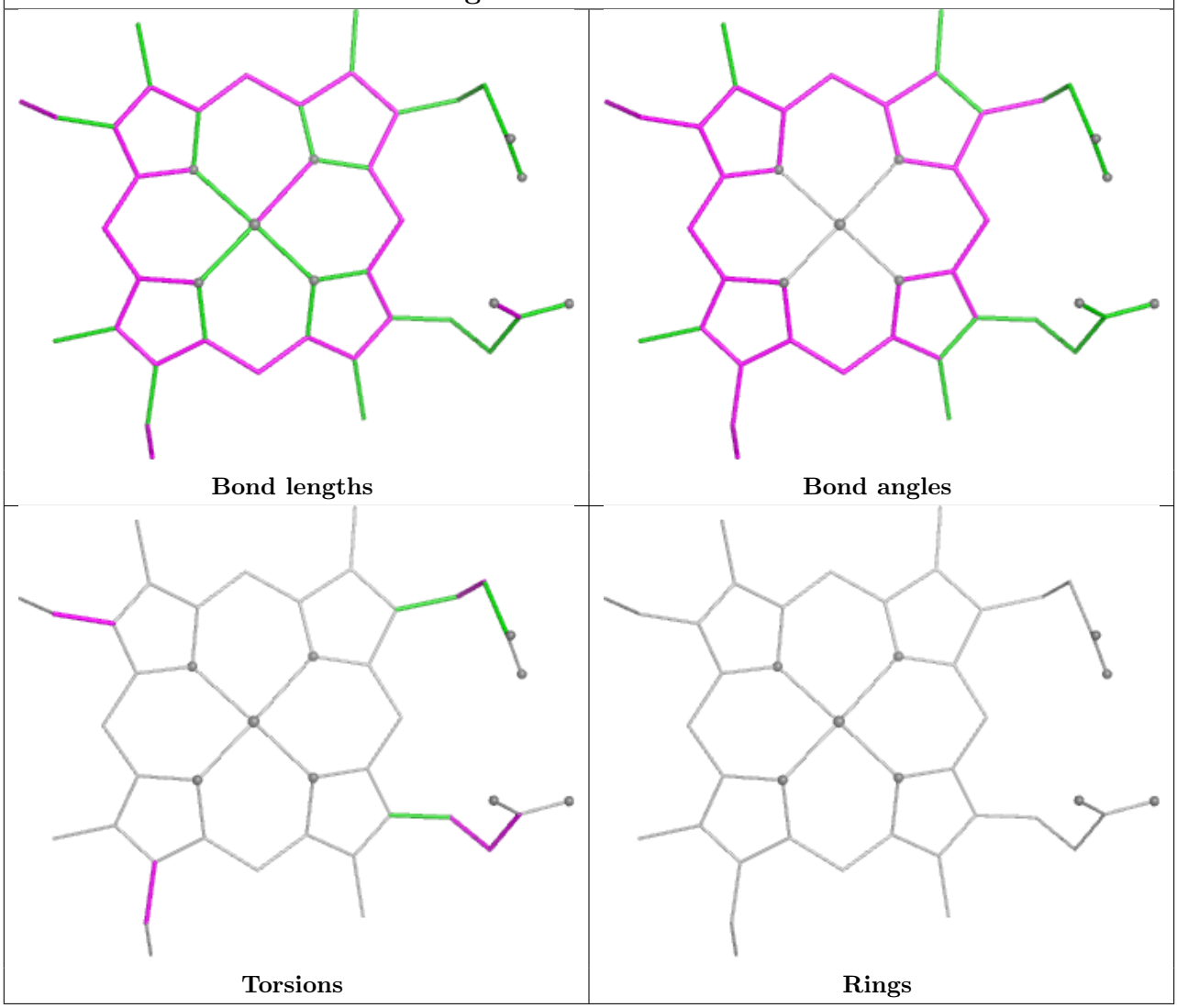
Ligand HEA BN 602



Ligand HEM AN 402



Ligand HEM AC 401



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
7	G	3
12	L	3
24	X	2
10	J	1
1	A	1

Continued on next page...

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Mol	Chain	Number of breaks
36	k	1
8	H	1
29	c	1
55	AE	1
55	AP	1
53	AC	1
53	AN	1

The worst 5 of 17 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	107:UNK	C	140:UNK	N	31.95
1	X	250:UNK	C	285:UNK	N	27.39
1	G	632:UNK	C	637:UNK	N	21.00
1	X	185:UNK	C	203:UNK	N	20.68
1	A	37:UNK	C	49:UNK	N	20.22

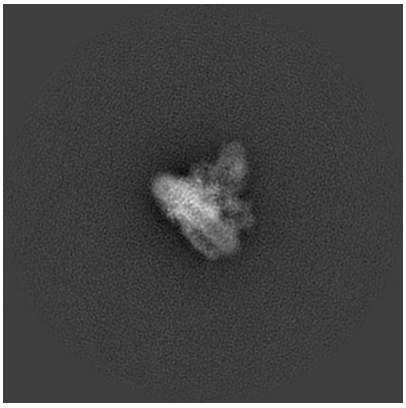
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8128. These allow visual inspection of the internal detail of the map and identification of artifacts.

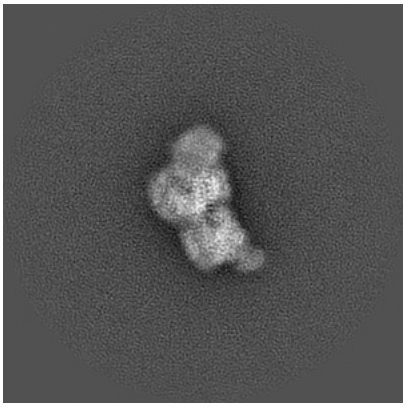
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

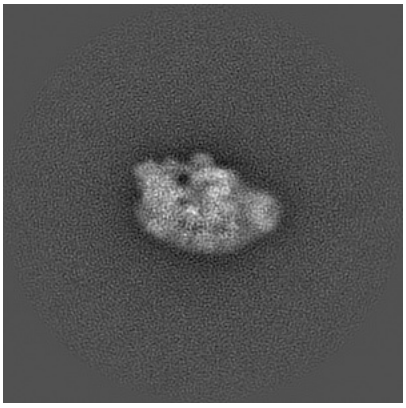
6.1.1 Primary map



X



Y

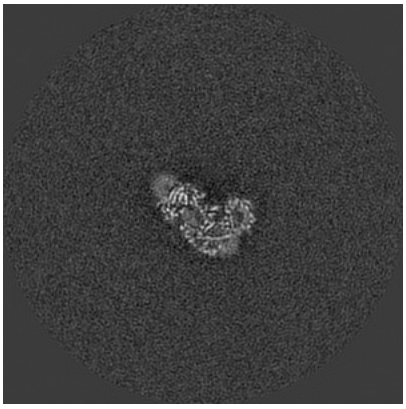


Z

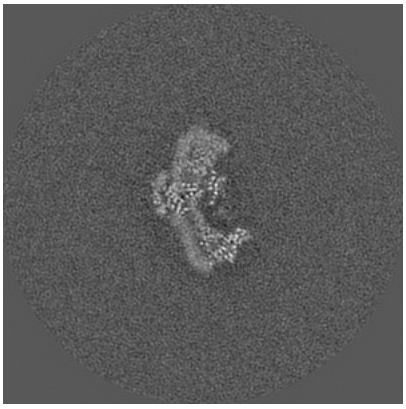
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

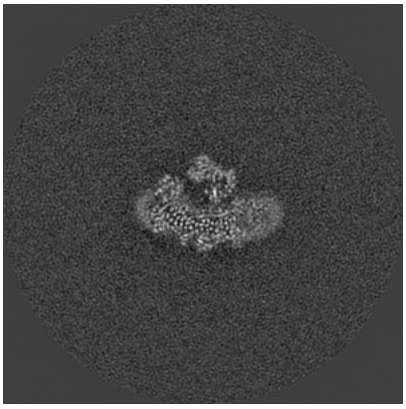
6.2.1 Primary map



X Index: 248



Y Index: 248

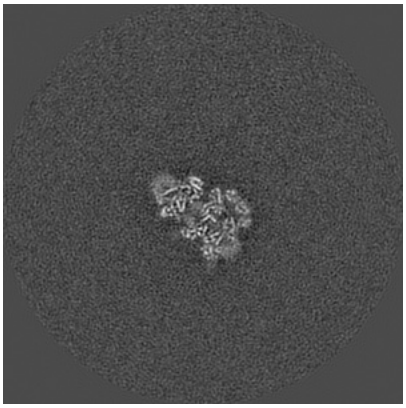


Z Index: 248

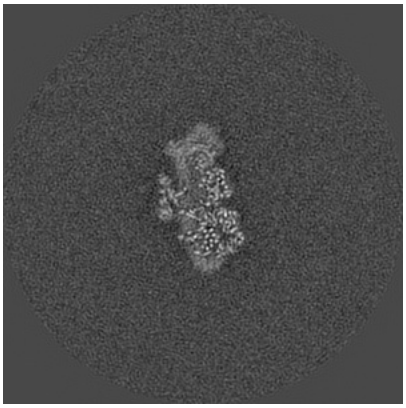
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

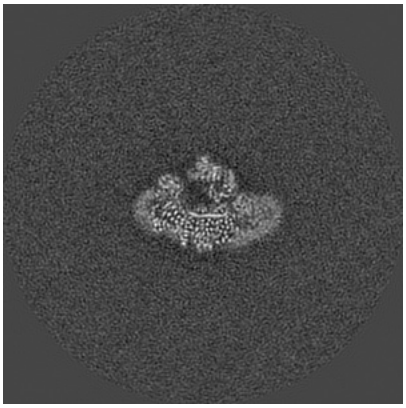
6.3.1 Primary map



X Index: 258



Y Index: 237

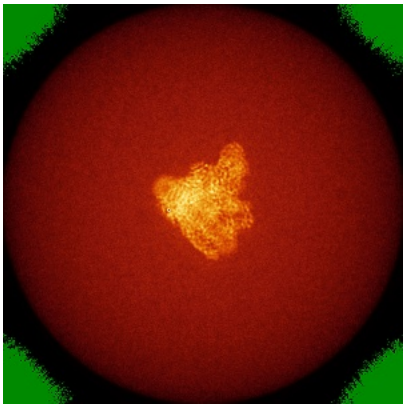


Z Index: 250

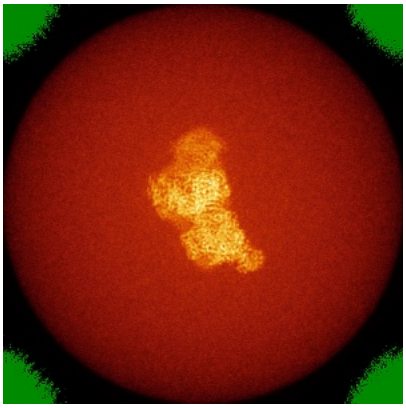
The images above show the largest variance slices of the map in three orthogonal directions.

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

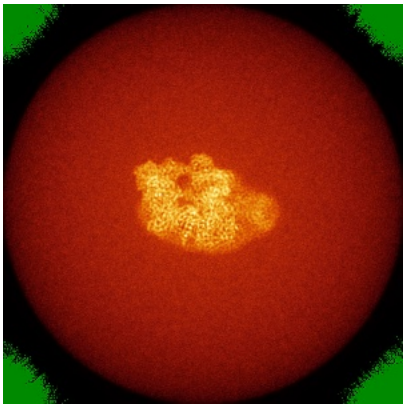
6.4.1 Primary map



X



Y

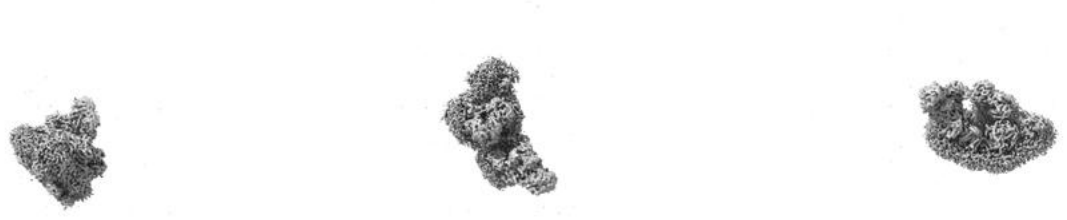


Z

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 0.094. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

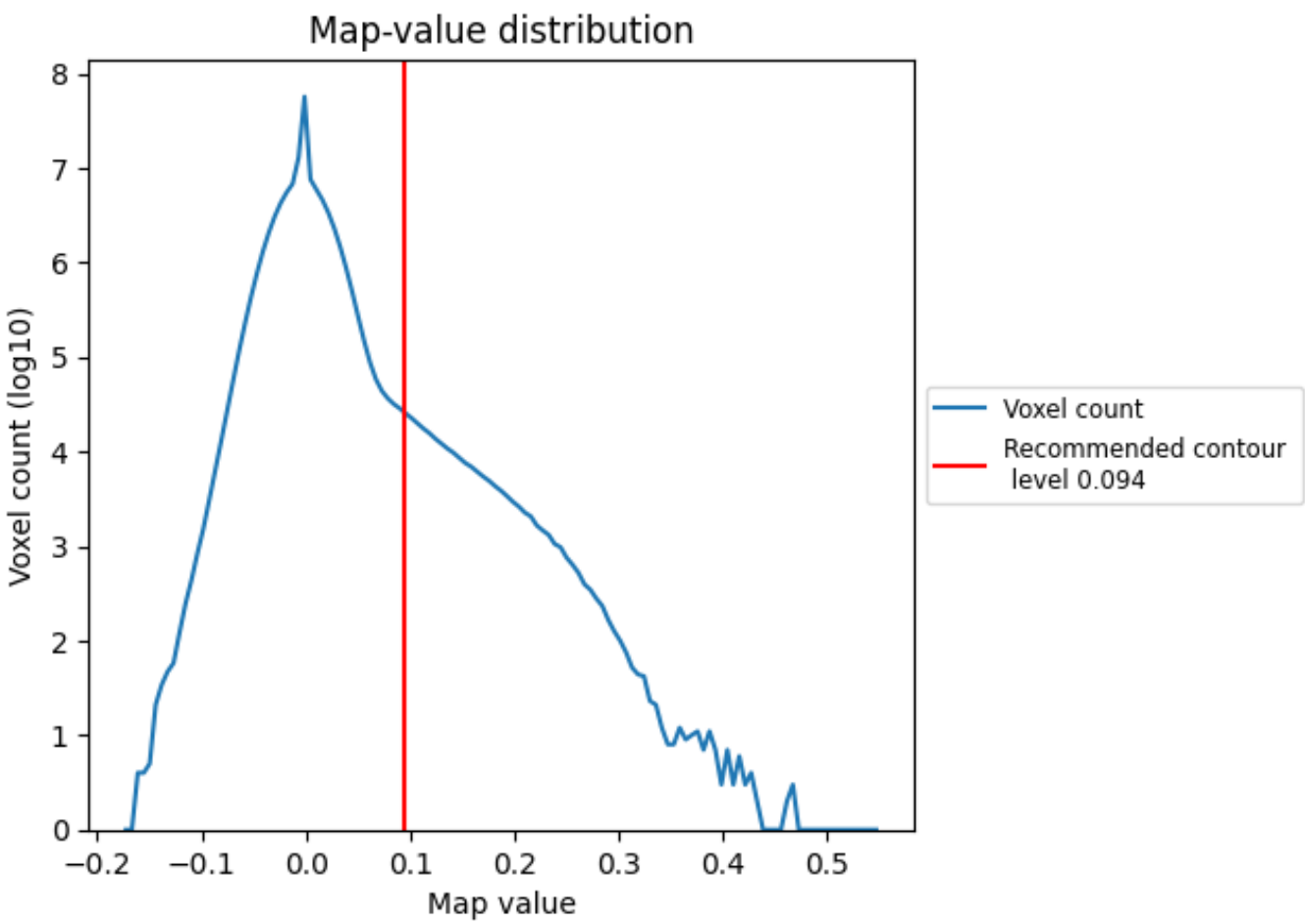
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

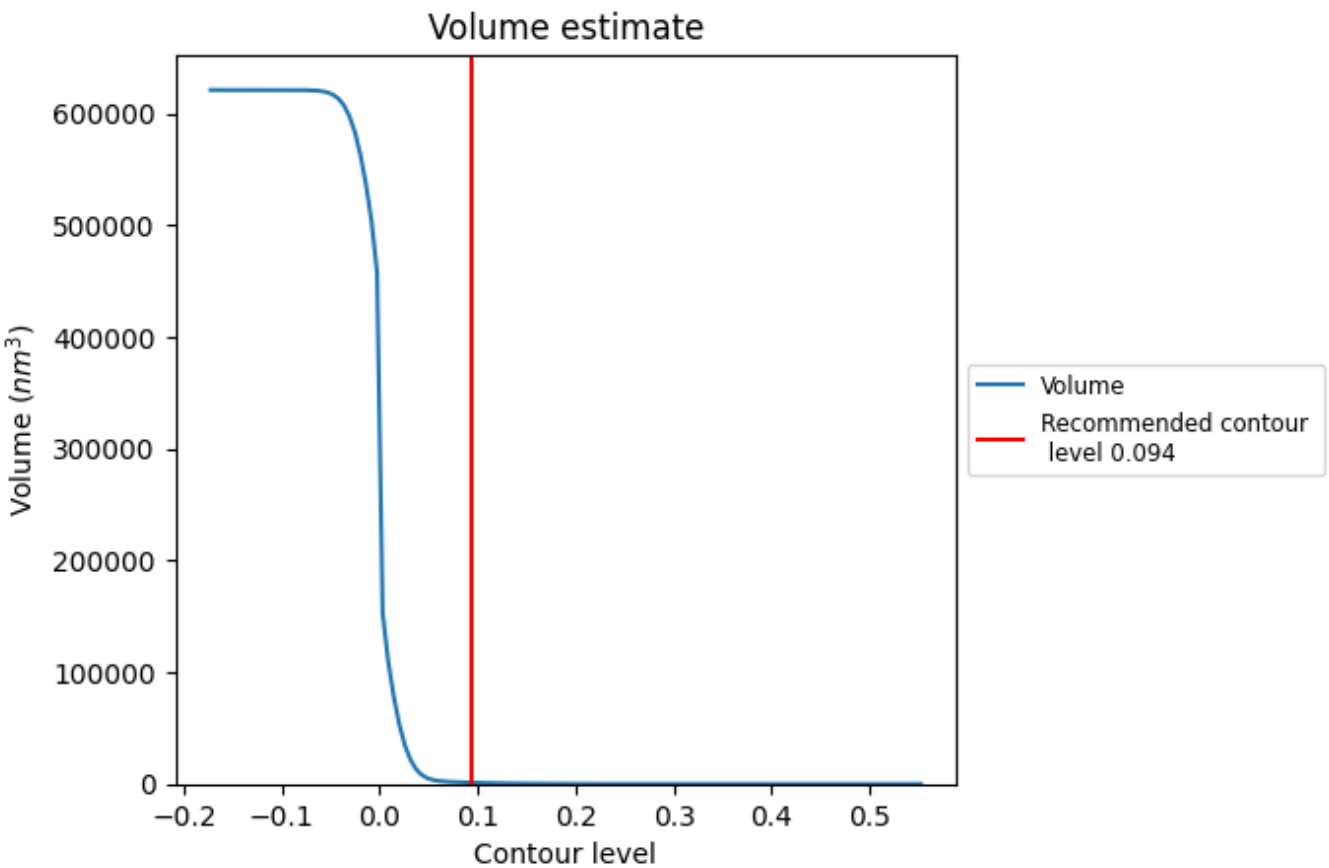
This section contains the results of statistical analysis of the map.

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.

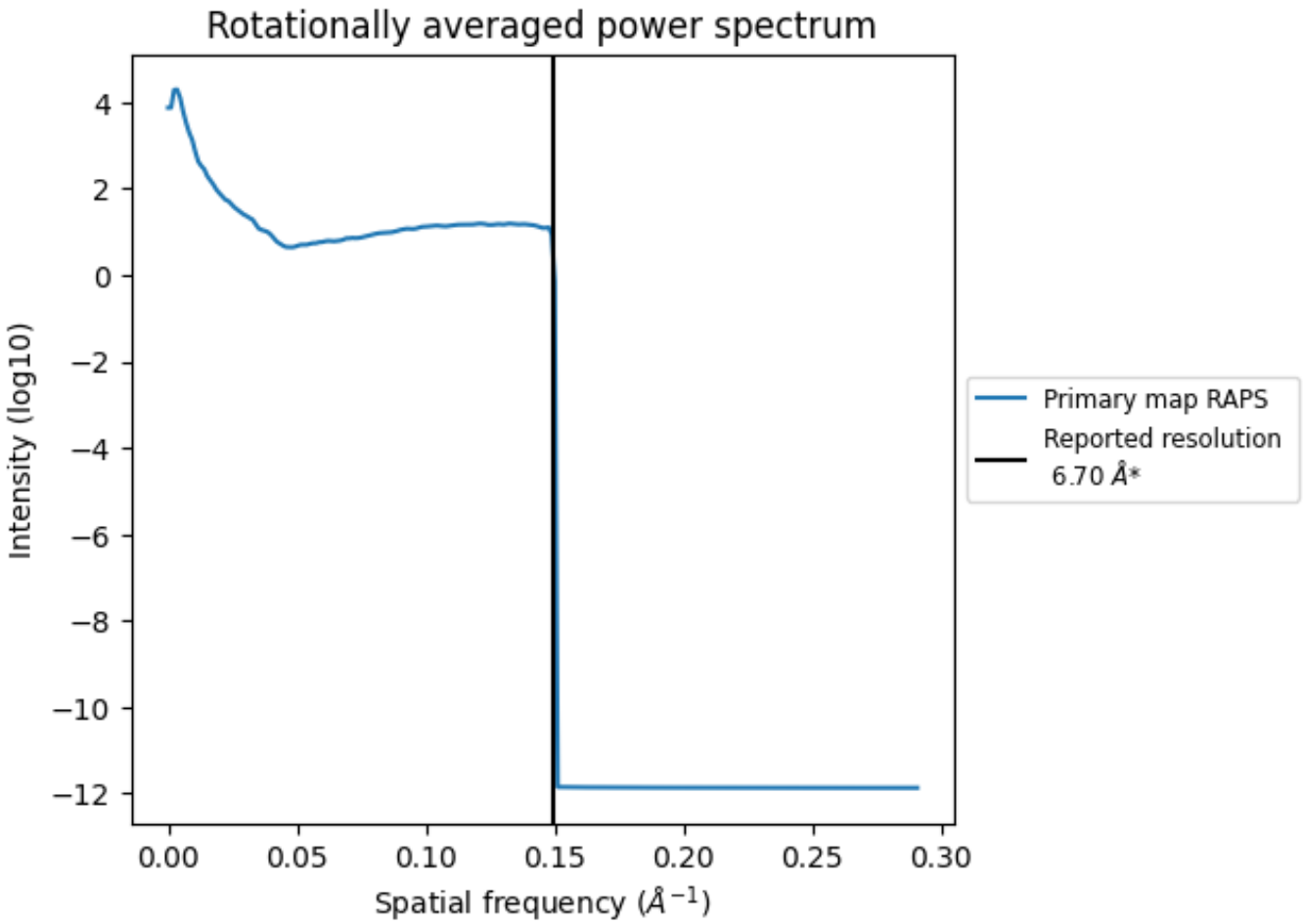
7.2 Volume estimate (i)



The volume at the recommended contour level is 1154 nm^3; this corresponds to an approximate mass of 1043 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)

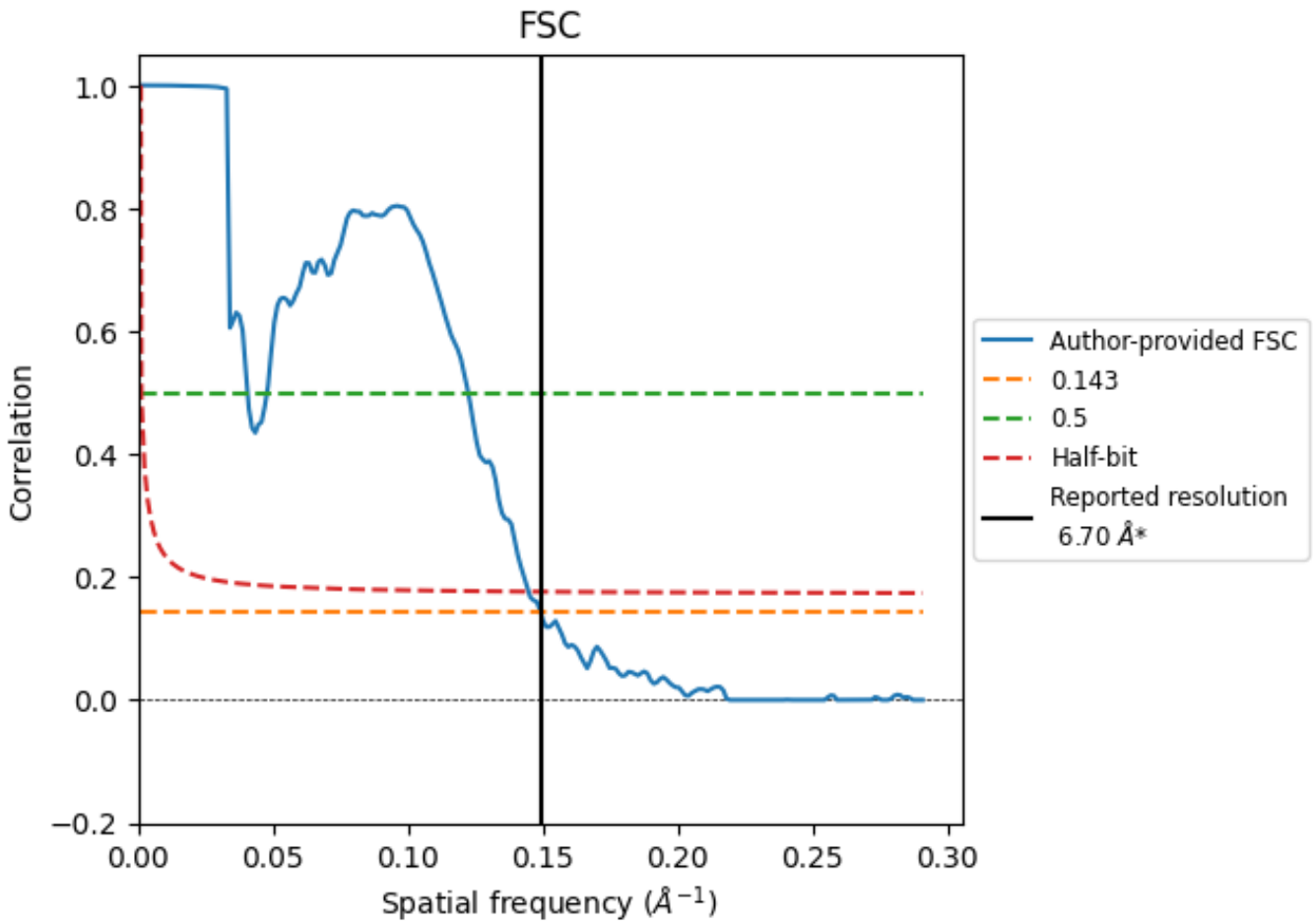


*Reported resolution corresponds to spatial frequency of 0.149 Å^{-1}

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 0.149 Å^{-1}

8.2 Resolution estimates (i)

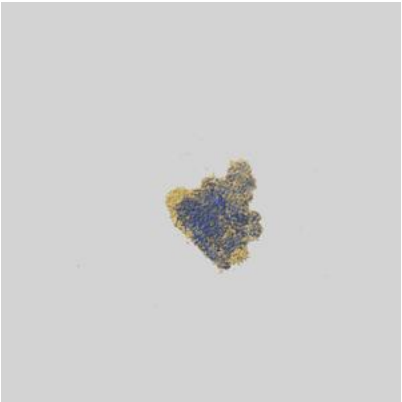
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	6.71	24.69	6.91
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

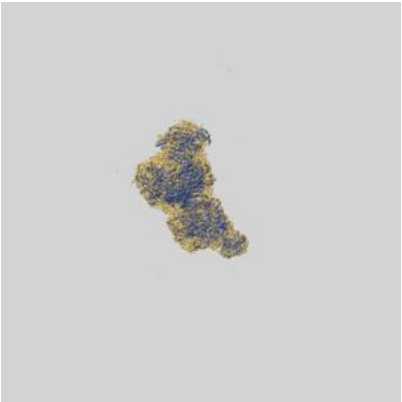
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8128 and PDB model 5J7Y. Per-residue inclusion information can be found in section 3 on page 25.

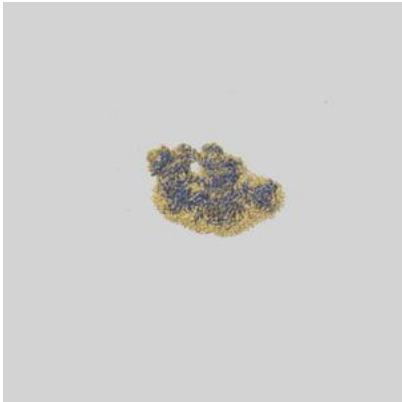
9.1 Map-model overlay (i)



X



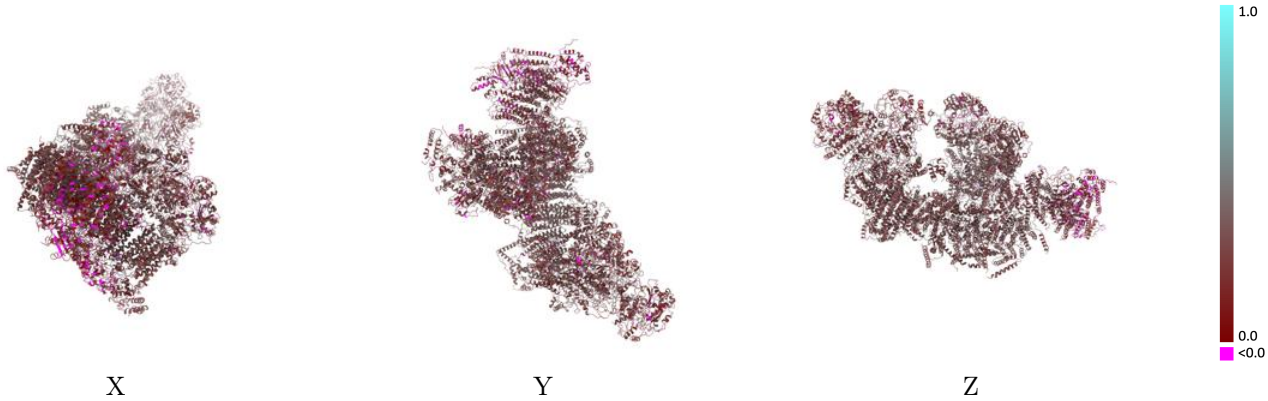
Y



Z

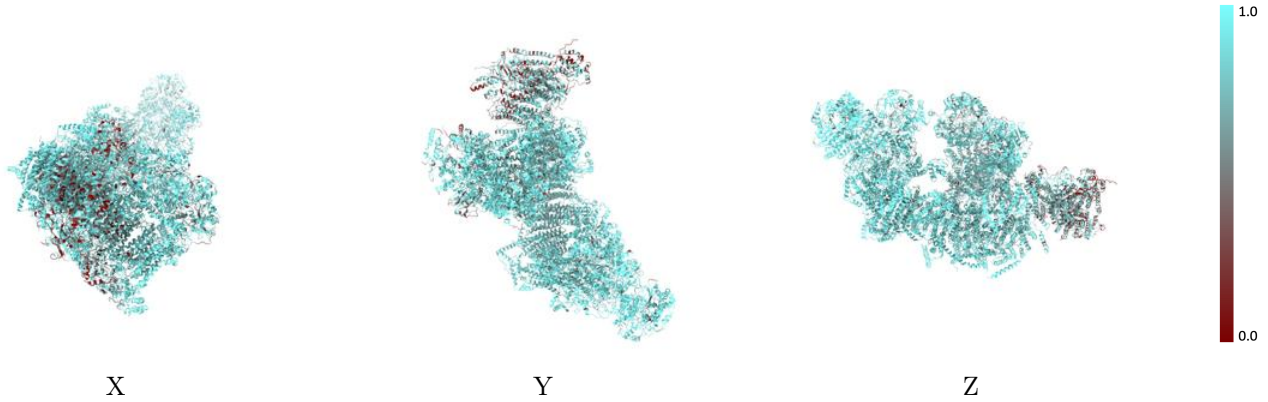
The images above show the 3D surface view of the map at the recommended contour level 0.094 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



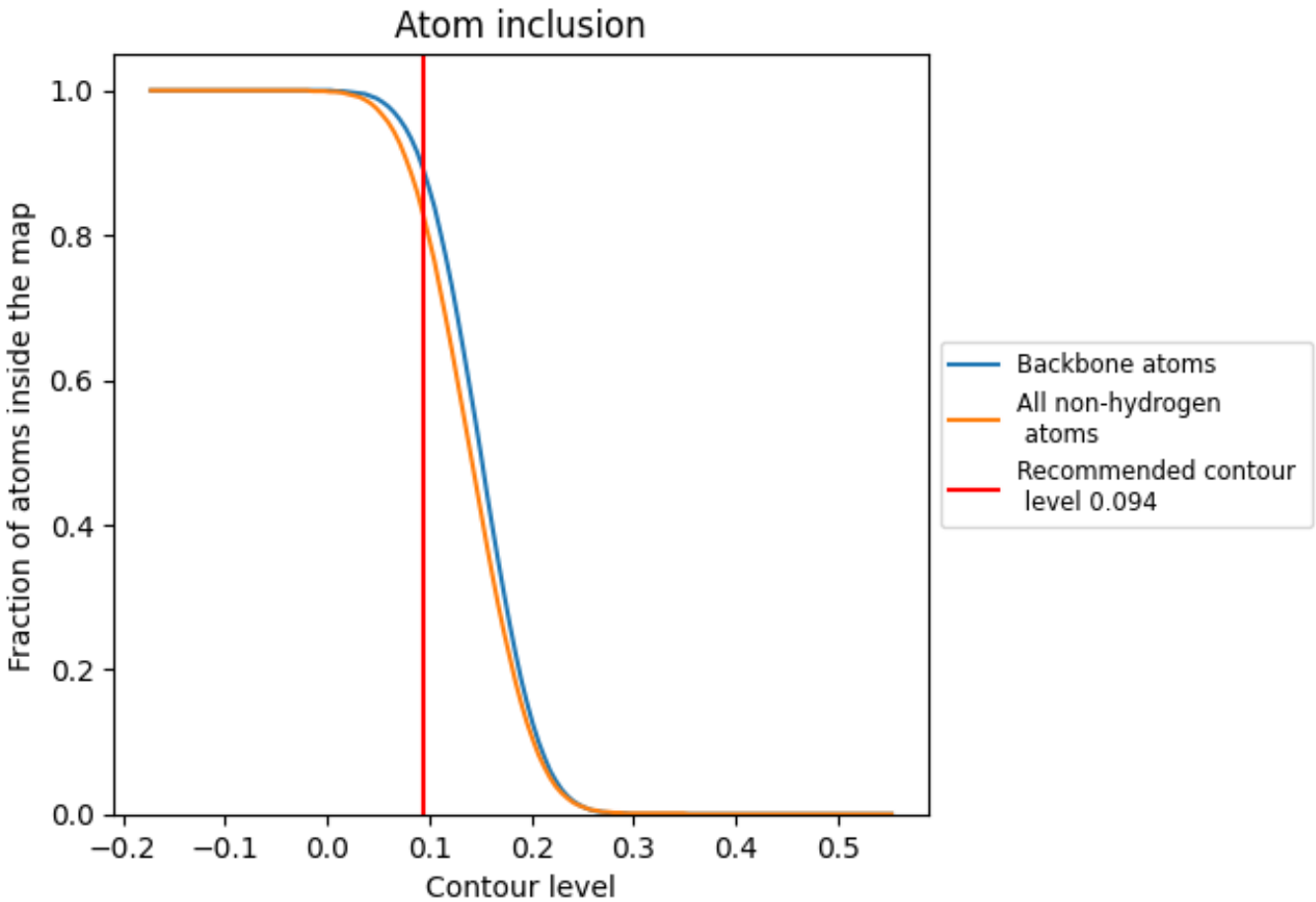
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.094).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.094) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.2650
0	0.8670	0.2770
1	0.8930	0.3010
2	0.9260	0.2940
3	0.9500	0.3360
4	0.7640	0.2660
5	0.9000	0.3060
6	0.9810	0.2890
7	0.9080	0.3100
8	0.9410	0.3000
9	0.8860	0.2980
A	0.8290	0.2950
AA	0.8860	0.2820
AB	0.8690	0.2750
AC	0.8700	0.2930
AD	0.8790	0.2870
AE	0.5980	0.1690
AF	0.8620	0.2900
AG	0.8980	0.2970
AH	0.8720	0.2890
AI	0.3810	0.1600
AJ	0.8380	0.2850
AK	0.8280	0.2820
AL	0.8590	0.2640
AM	0.8260	0.2550
AN	0.8580	0.2920
AO	0.8670	0.2650
AP	0.6950	0.2040
AQ	0.8660	0.2700
AR	0.8790	0.2970
AS	0.8240	0.2570
AT	0.4060	0.1240
AU	0.8820	0.2780
AV	0.7080	0.2490
B	0.8490	0.2780

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Chain	Atom inclusion	Q-score
BC	0.6900	0.2240
BD	0.4860	0.1170
BE	0.4650	0.1380
BG	0.4300	0.1560
BH	0.5650	0.1420
BI	0.4820	0.1260
BJ	0.6830	0.2230
BK	0.5640	0.1610
BL	0.6420	0.2070
BM	0.4650	0.1580
BN	0.6250	0.1880
BO	0.5460	0.1230
BP	0.6530	0.2060
C	0.8900	0.3000
D	0.8860	0.2990
E	0.9090	0.2540
F	0.8940	0.2440
G	0.8720	0.2550
H	0.8670	0.3010
I	0.9150	0.2870
J	0.8480	0.3000
K	0.8770	0.3110
L	0.8720	0.2970
M	0.8860	0.3030
N	0.8810	0.3000
O	0.8940	0.2940
P	0.8870	0.2840
Q	0.9180	0.2990
R	0.8140	0.2990
S	0.8920	0.2330
T	0.8750	0.2890
U	0.9540	0.3100
V	0.8480	0.2940
W	0.9590	0.2940
X	0.8850	0.2740
Y	0.8990	0.2990
Z	0.8470	0.3030
a	0.9220	0.3040
b	0.9240	0.2930
c	0.8650	0.2680
d	0.9150	0.3060
e	0.9090	0.3220

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Chain	Atom inclusion	Q-score
f	0.9480	0.2930
g	0.9510	0.3300
h	0.9560	0.3170
i	0.9460	0.3320
j	0.9270	0.2960
k	0.9250	0.3120
t	1.0000	0.3030
u	0.9250	0.3300
v	1.0000	0.3020
w	0.9500	0.3010
x	0.9390	0.3380
y	0.9610	0.3030
z	0.9080	0.3020