wwPDB EM Validation Summary Report (i)

Nov 3, 2024 – 08:19 am GMT

PDB ID	:	5LDX
EMDB ID	:	EMD-4041
Title	:	Structure of mammalian respiratory Complex I, class3.
Authors	:	Vinothkumar, K.R.; Zhu, J.; Hirst, J.
Deposited on	:	2016-06-28
Resolution	:	5.60 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 (i)) were used in the production of this report:

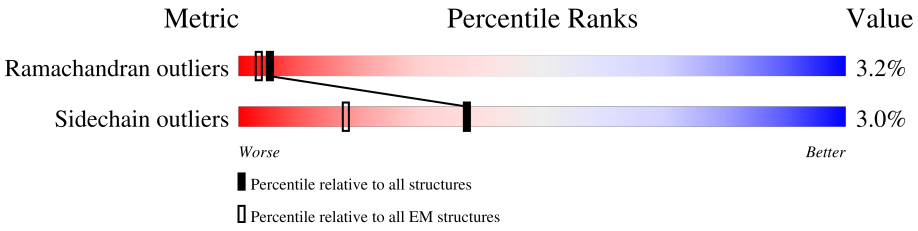
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.60 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	115	17% 73% · 23%
2	B	179	9% 74% 7% · 18%
3	C	228	12% 85% 5% · 10%
4	D	429	19% 90% 6% · ·
5	E	217	· 75% 9% · 14%
6	F	444	10% 92% · ·
7	G	700	11% 96% · ·
8	H	318	13% 89% · 7%
9	I	176	10% 88% 12%

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Mol	Chain	Length	Quality of chain
10	J	175	38% 93% 5%
11	K	98	17% 95%
12	L	606	26% 95%
13	M	459	16% 96%
14	N	347	17% 93% 6%
15	O	314	23% 97%
16	P	283	12% 100%
17	Q	113	5% 100%
18	R	89	10% 98%
19	S	99	11% 80% 19%
20	T	88	11% 84% 15%
20	U	88	26% 94%
21	V	115	11% 86% 8%
22	W	127	11% 82% 6% 13%
23	X	164	20% 98%
24	Y	140	71% 94%
25	Z	138	18% 100%
26	a	70	19% 84% 7% 9%
27	b	80	8% 99%
28	c	49	6% 88% 6% 6%
29	d	114	23% 98%
30	e	106	12% 80% 16%
31	f	57	16% 88% 5% 5%
32	g	125	16% 63% 13% 22%
33	h	134	22% 99%

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Mol	Chain	Length	Quality of chain
34	i	106	23% 99%
35	j	52	100%
36	k	74	26% 100%
37	l	118	19% 100%
38	m	118	41% 95% 5%
39	n	166	24% 98%
40	o	58	12% 98%
41	p	169	11% 97%
42	q	138	96%
43	r	87	9% 100%
44	s	35	100%

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 51181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	88	687	472	99	113	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	147	1159	740	203	202	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1684	1091	285	305	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	416	3229	2056	560	589	24	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	conflict	UNP P17694

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	186	Total	C	N	O	S	0	0
			959	583	186	186	4		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	425	Total	C	N	O	S	0	0
			2356	1432	463	455	6		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochon drial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinon e oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	685	Total	C	N	O	S	0	0
			3614	2172	715	712	15		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	296	Total	C	N	O	S	0	0
			2306	1551	357	376	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1366	857	238	261	10		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1211	814	179	207	11		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total	C	N	O	S	0	0
			720	472	108	126	14		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	604	Total	C	N	O	S	0	0
			4538	3005	708	787	38		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	457	Total	C	N	O	S	0	0
			3536	2352	555	591	38		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2592	1713	405	440	34		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	314	Total	C	N	O	S	0	0
			1851	1148	347	353	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, NDUFA9.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	283	Total	C	N	O	0	0
			1415	849	283	283		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, NDUFS4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	113	Total	C	N	O	0	0
			565	339	113	113		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			501	304	99	95	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	80	Total	C	N	O	0	0
			405	245	80	80		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	75	Total	C	N	O	0	0
			378	228	75	75		
20	U	85	Total	C	N	O	0	0
			432	262	85	85		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	106	Total	C	N	O	S	0	0
			685	430	126	128	1		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	111	Total	C	N	O	S	0	0
			817	516	154	144	3		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	164	Total	C	N	O	S	0	0
			1133	703	213	208	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	138	Total	C	N	O	S	0	0
			1011	644	173	188	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	138	Total	C	N	O	S	0	0
			921	573	172	170	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	64	Total	C	N	O	S	0	0
			480	312	86	77	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	80	Total	C	N	O	S	0	0
			519	336	89	93	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	46	Total	C	N	O	0	0
			320	211	56	53		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	114	Total	C	N	O	S	0	0
			790	504	146	137	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	89	Total	C	N	O	S	0	0
			616	382	121	108	5		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	54	Total	C	N	O	S	0	0
			350	223	62	64	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	97	Total	C	N	O	S	0	0
			677	438	120	117	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	h	134	Total	C	N	O	0	0
			770	486	143	141		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	i	106	Total	C	N	O	0	0
			616	376	126	114		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUFB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	j	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUFB3.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	k	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUFB8.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	l	118	Total	C	N	O	0	0
			590	354	118	118		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	118	Total	C	N	O	0	0
			887	566	165	156		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	166	Total	C	N	O	S	0	0
			1088	677	212	196	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	58	Total	C	N	O	S	0	0
			296	176	58	58	4		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1

beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	169	Total	C	N	O	S	0	0
			1039	633	198	202	6		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	q	138	Total	C	N	O	0	0
			696	420	138	138		

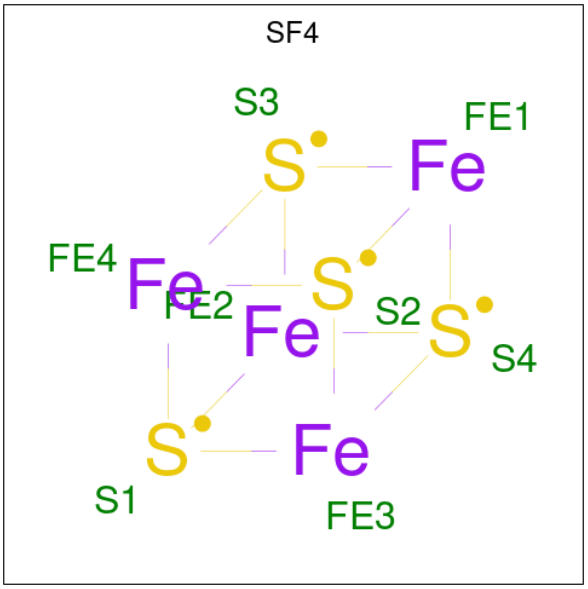
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUFA7.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	r	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUFV3.

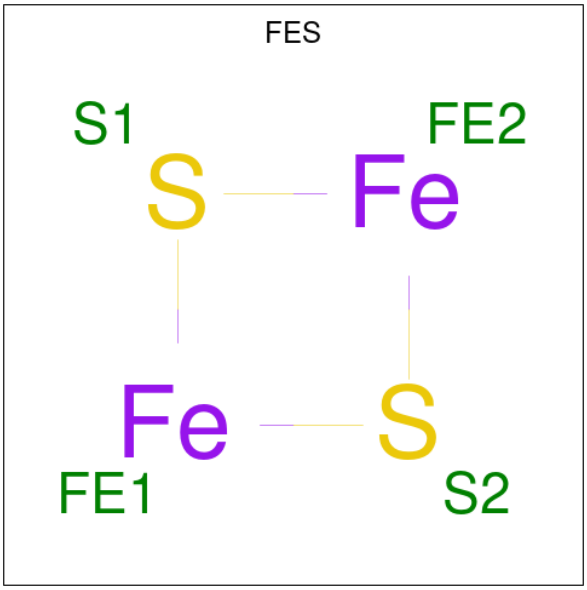
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



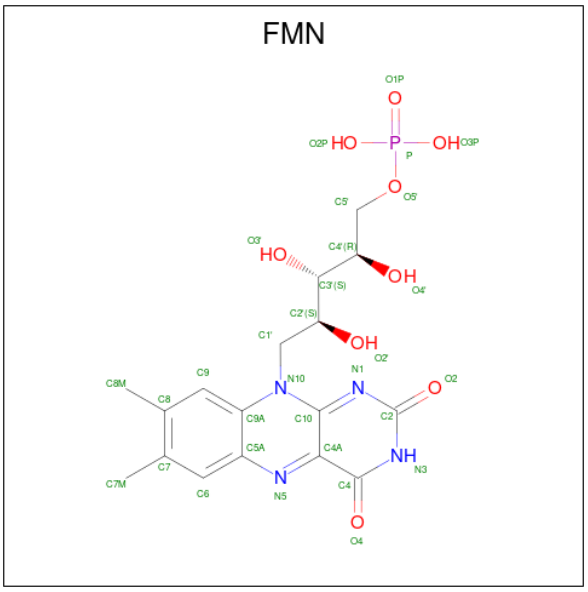
Mol	Chain	Residues	Atoms	AltConf
45	B	1	Total Fe S 8 4 4	0
45	F	1	Total Fe S 8 4 4	0
45	G	1	Total Fe S 8 4 4	0
45	G	1	Total Fe S 8 4 4	0
45	I	1	Total Fe S 8 4 4	0
45	I	1	Total Fe S 8 4 4	0

- Molecule 46 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



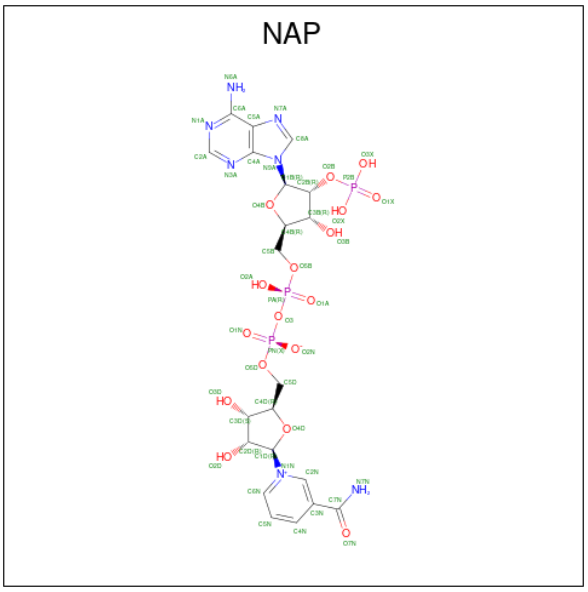
Mol	Chain	Residues	Atoms	AltConf
46	E	1	Total Fe S 4 2 2	0
46	G	1	Total Fe S 4 2 2	0

- Molecule 47 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 48 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

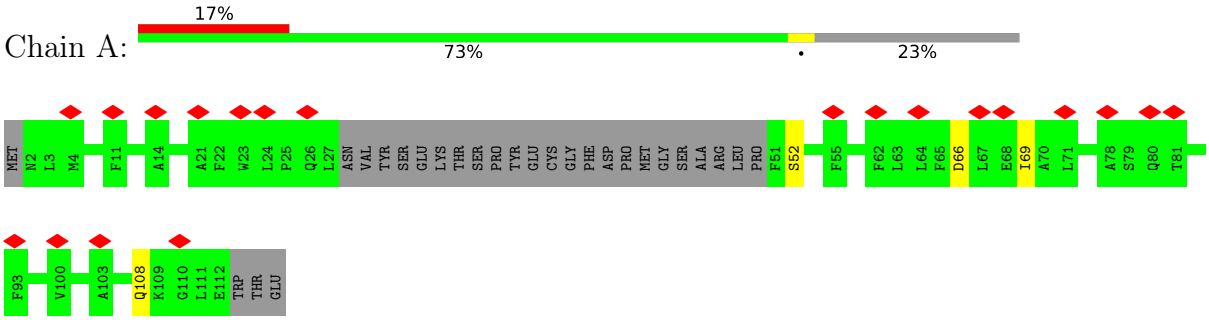
- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

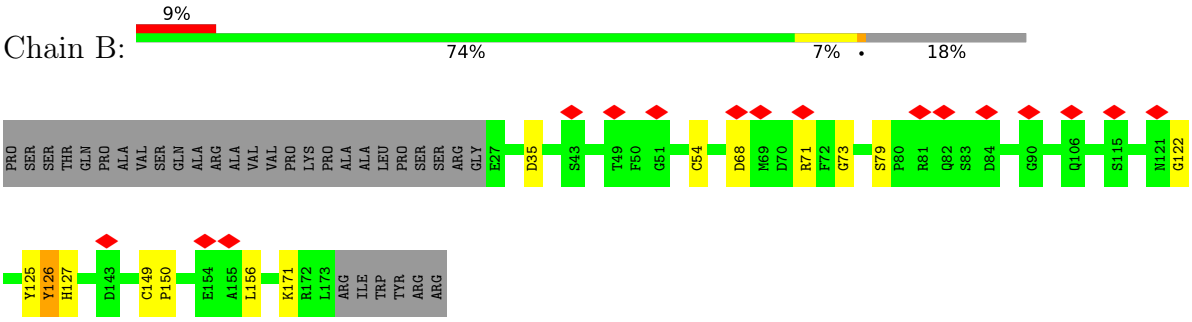
3 Residue-property plots (i)

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

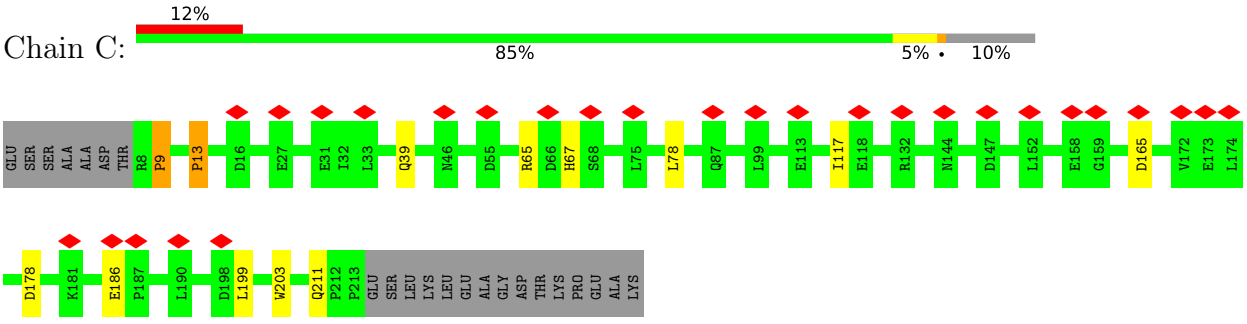
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



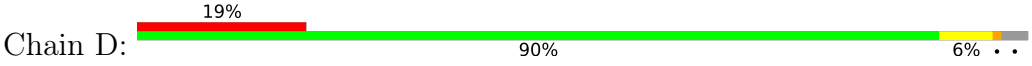
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

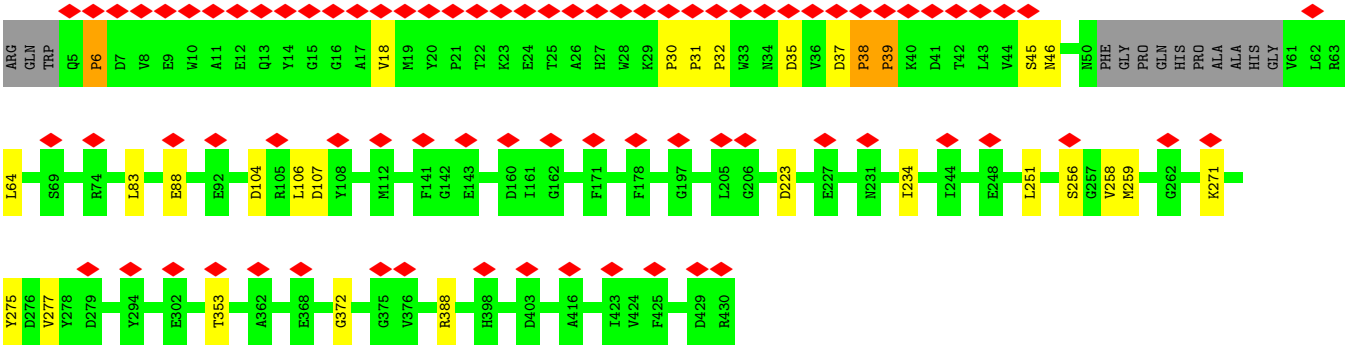


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



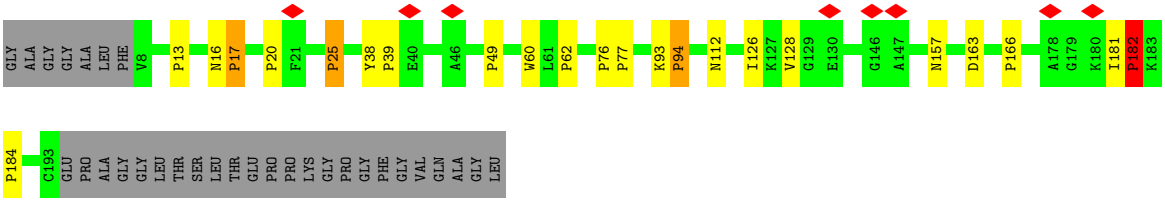
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





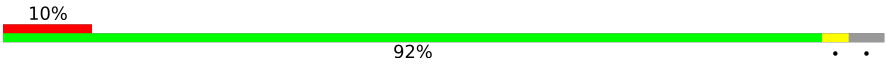
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

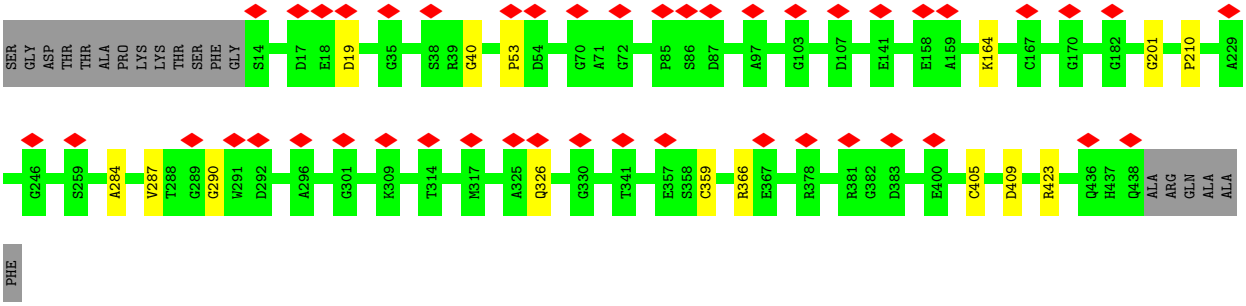
Chain E:



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

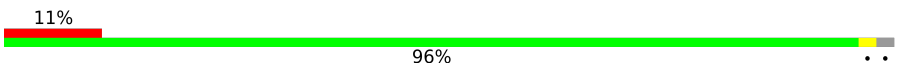
Chain F:

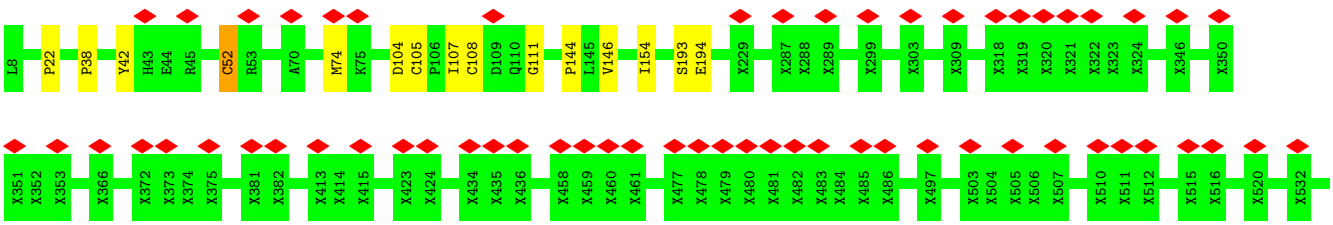


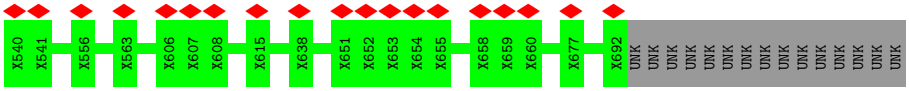


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

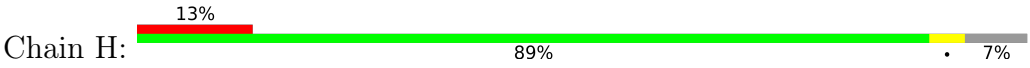
Chain G:

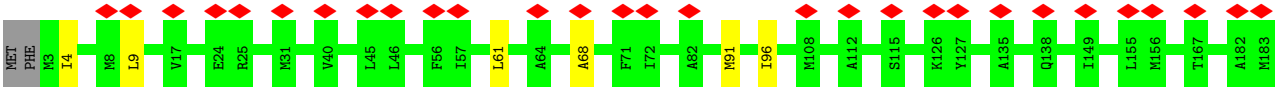


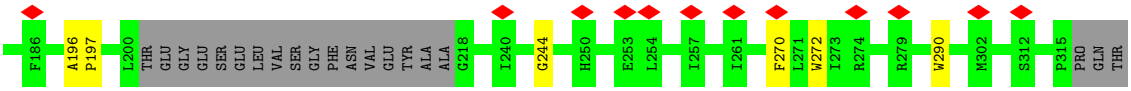




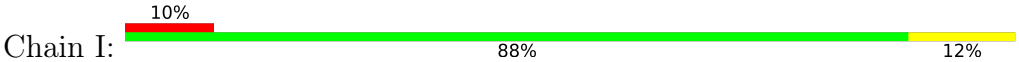
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

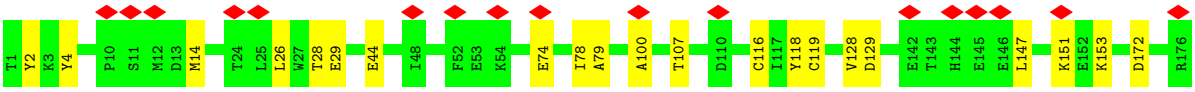




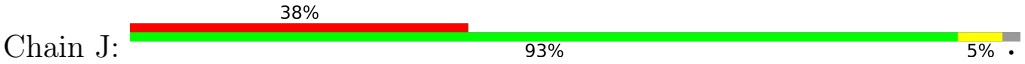


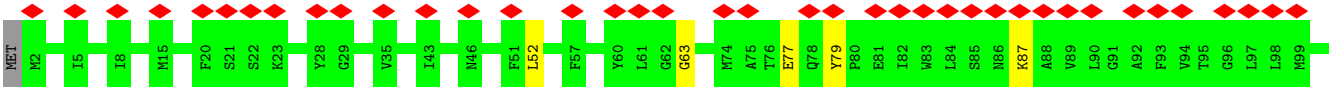
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



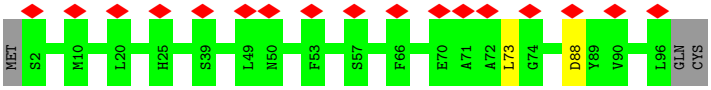


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

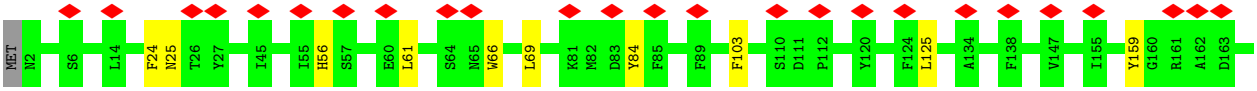


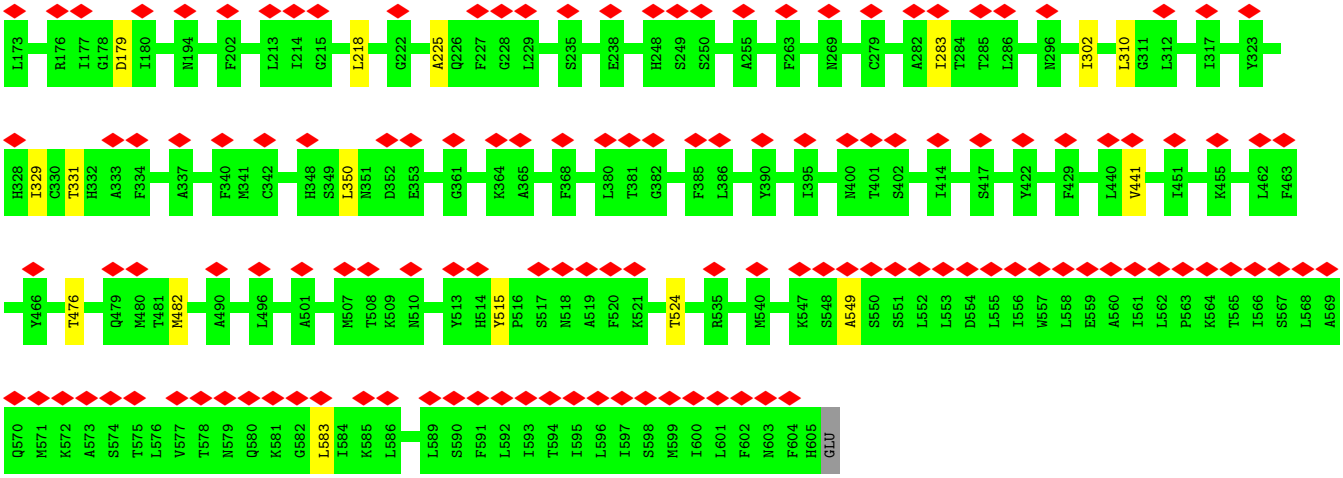


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

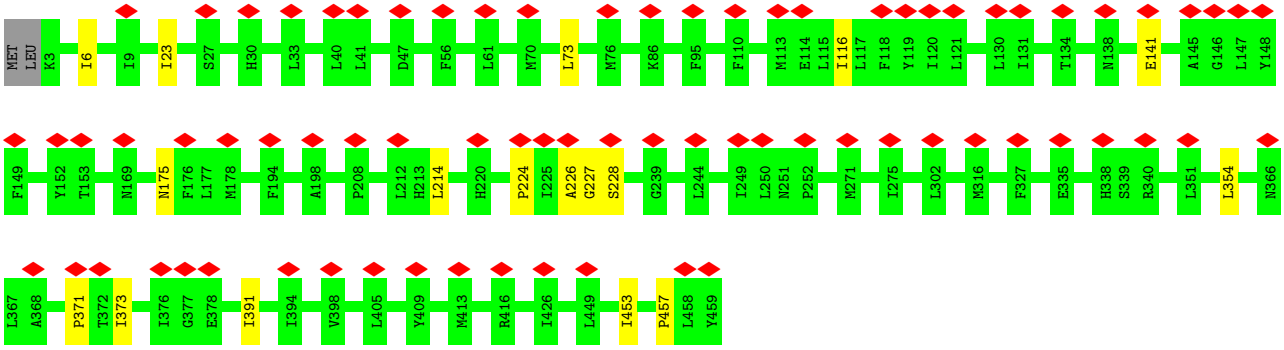


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

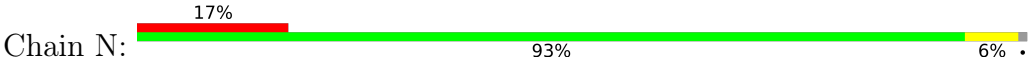


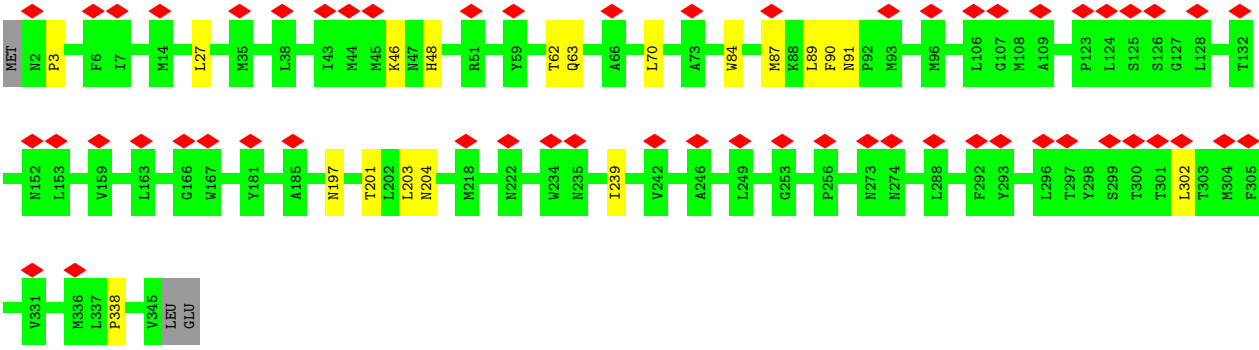


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

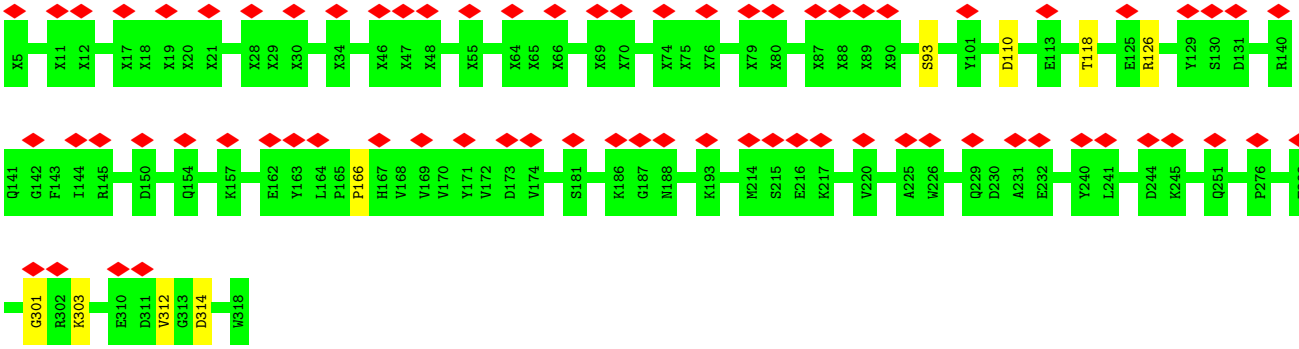


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

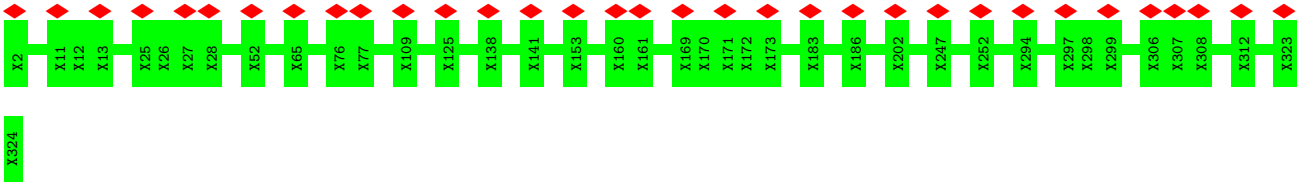




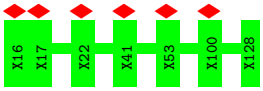
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



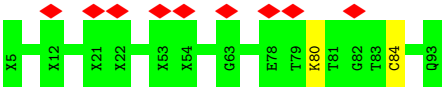
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, NDUFA9



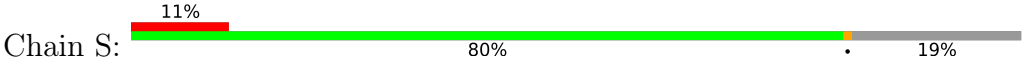
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, NDUFS4

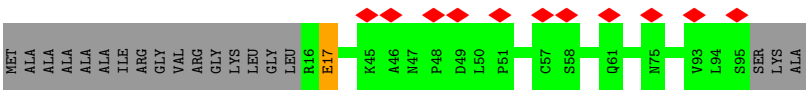


• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

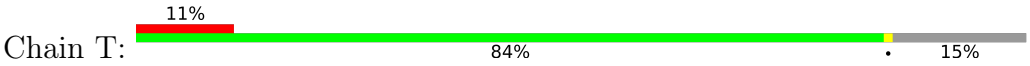


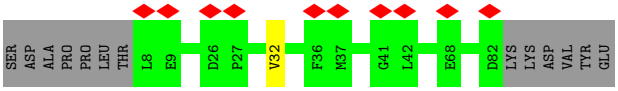
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



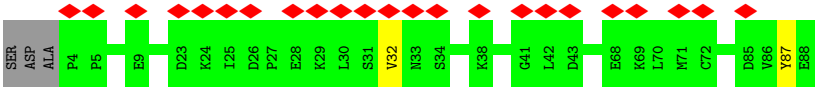


• Molecule 20: Acyl carrier protein, mitochondrial

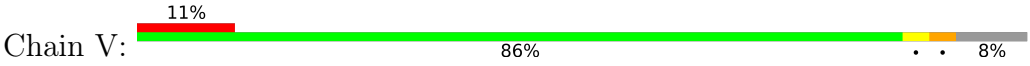


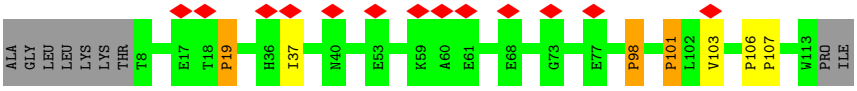


• Molecule 20: Acyl carrier protein, mitochondrial

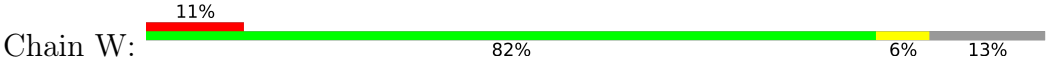


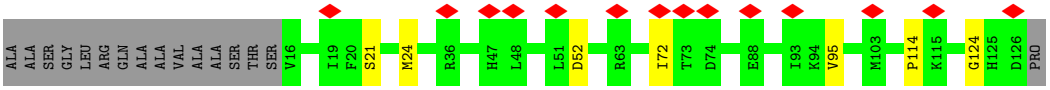
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



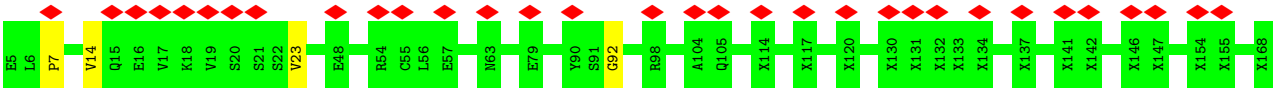


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

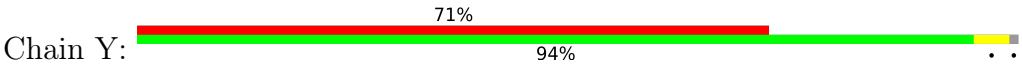


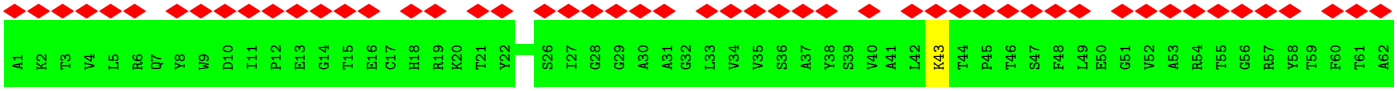


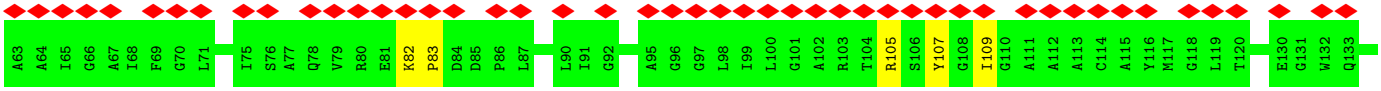
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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

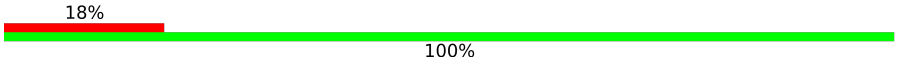


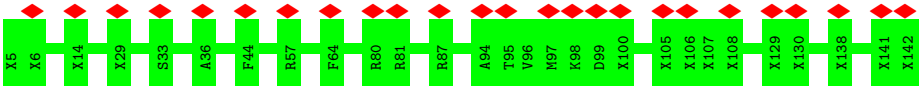




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha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

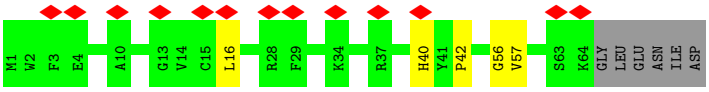
Chain Z:





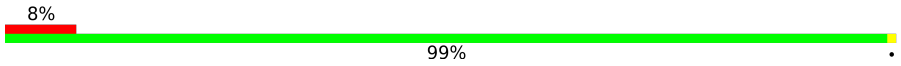
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

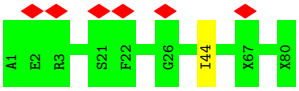
Chain a:



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

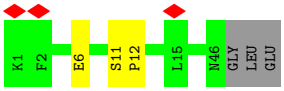
Chain b:





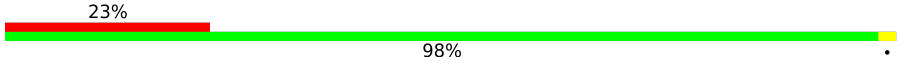
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

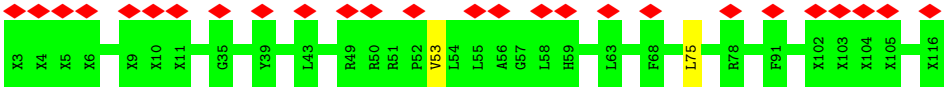
Chain c:



• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2

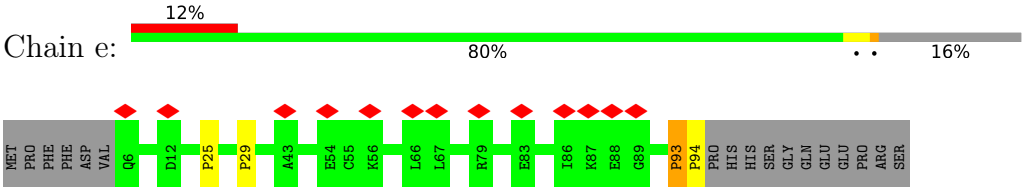
Chain d:





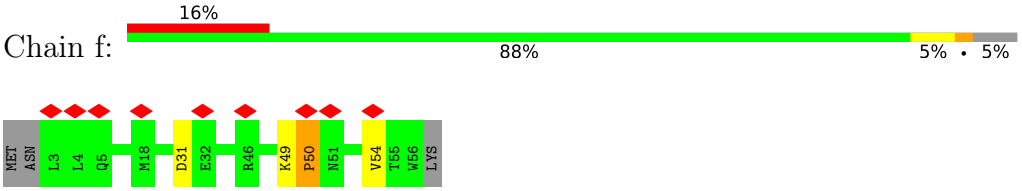
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



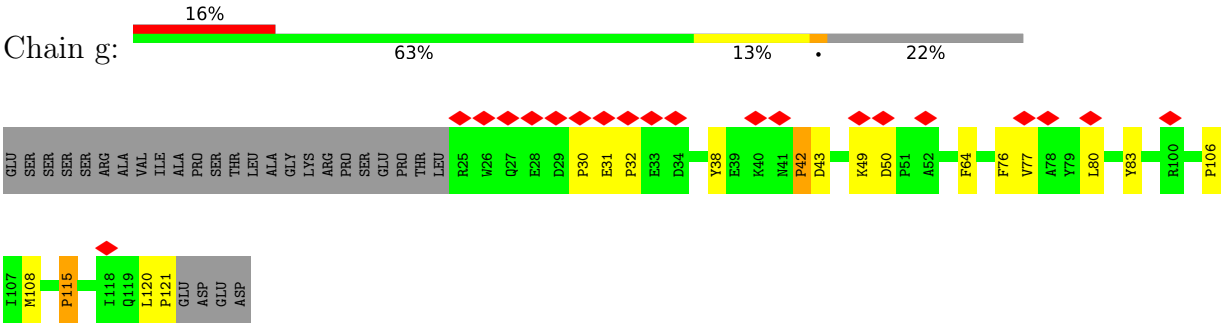
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



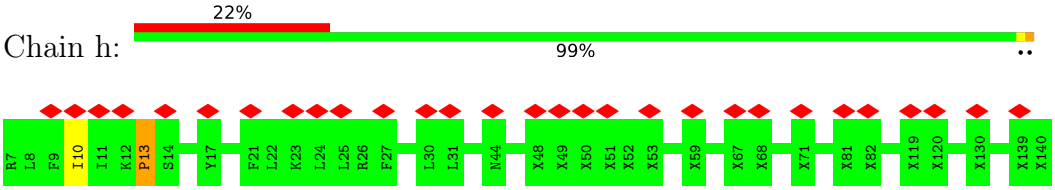
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



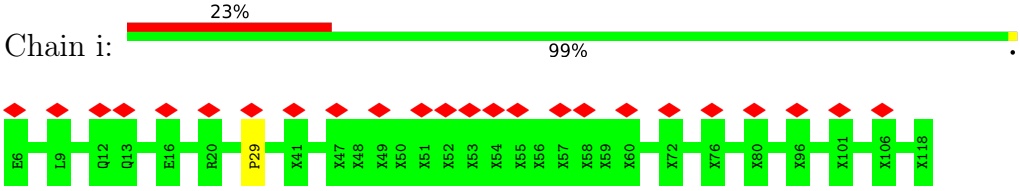
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



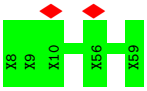
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



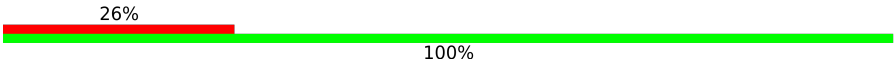
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUFB2

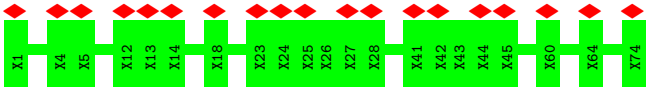
Chain j:



• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUFB3

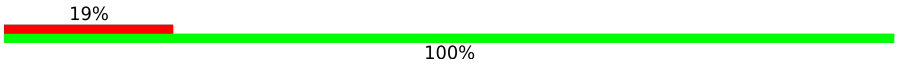
Chain k:

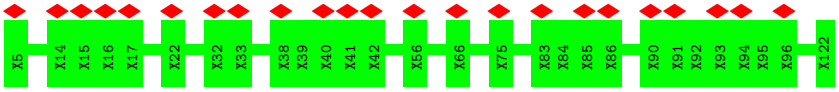




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUFB8

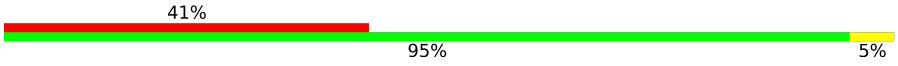
Chain l:

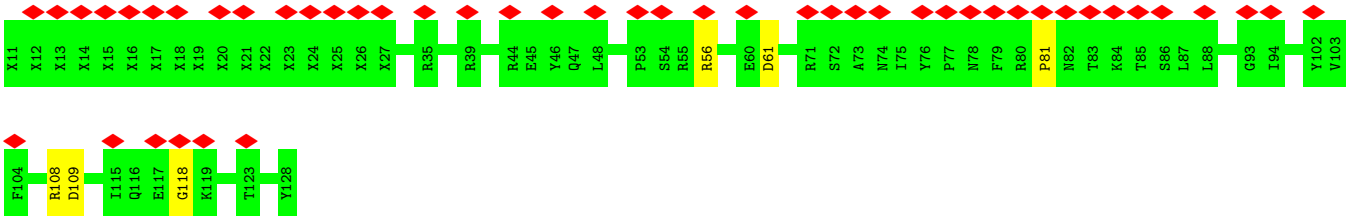




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

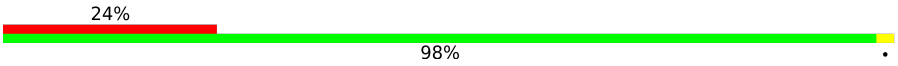
Chain m:

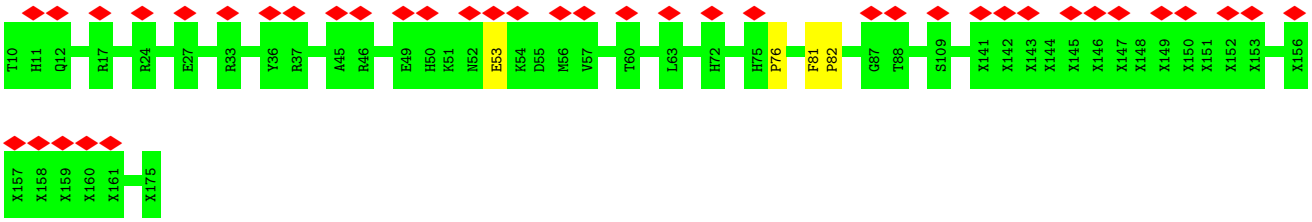




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

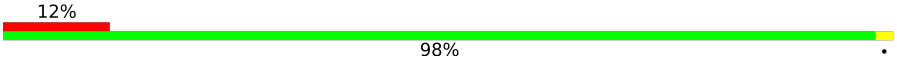
Chain n:

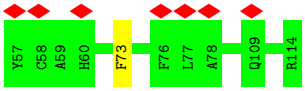




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

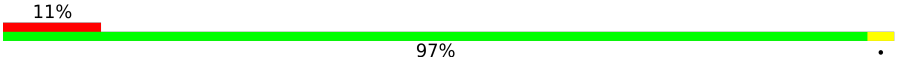
Chain o:

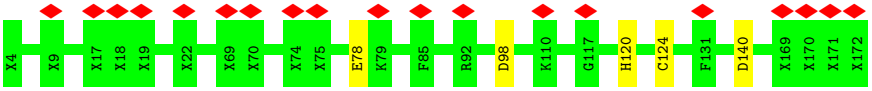




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex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

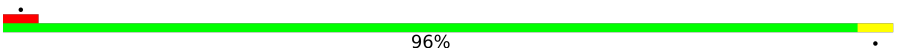
Chain p:

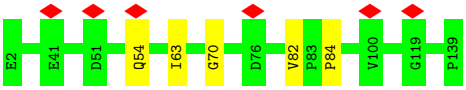




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

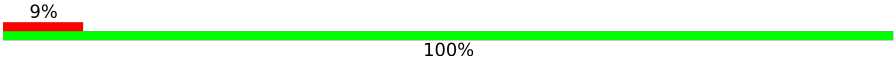
Chain q:

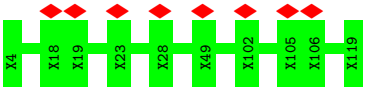




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUFA7

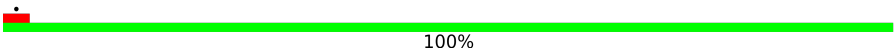
Chain r:

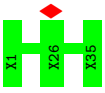




• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUFV3

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19306	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Ctf was corrected per particle. Ctf was estimated on the whole micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	105263	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.679	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	478.80002, 478.80002, 478.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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, FES, ZN, FMN, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/702	0.63	0/962
2	B	0.39	0/1187	0.62	0/1607
3	C	0.43	0/1735	0.66	2/2365 (0.1%)
4	D	0.42	0/3304	0.67	6/4478 (0.1%)
5	E	0.63	0/975	1.06	12/1370 (0.9%)
6	F	0.37	0/2389	0.55	1/3299 (0.0%)
7	G	0.40	0/1213	0.66	2/1658 (0.1%)
8	H	0.40	0/2371	0.58	0/3241
9	I	0.38	0/1395	0.62	0/1893
10	J	0.45	0/1239	0.55	0/1688
11	K	0.38	0/730	0.63	0/988
12	L	0.41	0/4653	0.57	0/6350
13	M	0.40	0/3624	0.60	0/4949
14	N	0.41	0/2656	0.61	0/3630
15	O	0.36	0/1446	0.53	0/1997
18	R	0.37	0/235	0.52	0/316
19	S	0.44	0/408	0.84	1/571 (0.2%)
20	T	0.31	0/380	0.52	0/531
20	U	0.30	0/436	0.50	0/610
21	V	0.51	0/696	0.86	5/954 (0.5%)
22	W	0.50	0/831	0.70	0/1128
23	X	0.43	0/877	0.63	1/1181 (0.1%)
24	Y	0.41	0/1031	0.55	0/1400
25	Z	0.37	0/585	0.54	0/781
26	a	0.45	0/494	0.57	0/669
27	b	0.42	0/352	0.53	0/481
28	c	0.46	0/330	0.61	0/455
29	d	0.40	0/581	0.50	0/782
30	e	0.49	0/627	0.84	4/848 (0.5%)
31	f	0.50	0/356	0.70	1/488 (0.2%)
32	g	0.55	0/696	0.94	6/957 (0.6%)
33	h	0.49	0/301	0.71	1/409 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
34	i	0.54	0/224	0.87	1/300 (0.3%)
38	m	0.42	0/801	0.56	0/1085
39	n	0.37	0/914	0.55	0/1247
40	o	0.32	0/296	0.50	0/412
41	p	0.37	0/535	0.53	0/718
42	q	0.36	0/704	0.56	0/984
All	All	0.42	0/42309	0.63	43/57782 (0.1%)

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	1
19	S	1	0
All	All	1	1

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	S	17	GLU	N-CA-C	14.07	148.98	111.00
7	G	22	PRO	CA-N-CD	-9.25	98.55	111.50
5	E	77	PRO	CA-N-CD	-9.12	98.73	111.50
6	F	53	PRO	CA-N-CD	-9.12	98.73	111.50
4	D	32	PRO	CA-N-CD	-9.06	98.81	111.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	S	17	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	149	CYS	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	84/115 (73%)	79 (94%)	3 (4%)	2 (2%)	5 27
2	B	145/179 (81%)	128 (88%)	10 (7%)	7 (5%)	2 16
3	C	204/228 (90%)	174 (85%)	23 (11%)	7 (3%)	3 20
4	D	412/429 (96%)	360 (87%)	37 (9%)	15 (4%)	3 20
5	E	184/217 (85%)	151 (82%)	18 (10%)	15 (8%)	1 9
6	F	423/444 (95%)	375 (89%)	38 (9%)	10 (2%)	5 27
7	G	201/700 (29%)	168 (84%)	26 (13%)	7 (4%)	3 20
8	H	292/318 (92%)	270 (92%)	16 (6%)	6 (2%)	5 29
9	I	174/176 (99%)	144 (83%)	19 (11%)	11 (6%)	1 12
10	J	169/175 (97%)	150 (89%)	14 (8%)	5 (3%)	3 22
11	K	93/98 (95%)	88 (95%)	5 (5%)	0	100 100
12	L	602/606 (99%)	539 (90%)	52 (9%)	11 (2%)	7 34
13	M	455/459 (99%)	411 (90%)	34 (8%)	10 (2%)	5 29
14	N	342/347 (99%)	309 (90%)	26 (8%)	7 (2%)	6 31
15	O	227/314 (72%)	199 (88%)	20 (9%)	8 (4%)	3 20
18	R	34/89 (38%)	30 (88%)	3 (9%)	1 (3%)	3 23
19	S	78/99 (79%)	72 (92%)	5 (6%)	1 (1%)	10 41
20	T	73/88 (83%)	69 (94%)	3 (4%)	1 (1%)	9 40
20	U	83/88 (94%)	74 (89%)	7 (8%)	2 (2%)	5 27
21	V	104/115 (90%)	91 (88%)	8 (8%)	5 (5%)	2 16
22	W	109/127 (86%)	90 (83%)	12 (11%)	7 (6%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	X	108/164 (66%)	94 (87%)	11 (10%)	3 (3%)	4 24
24	Y	136/140 (97%)	124 (91%)	8 (6%)	4 (3%)	3 23
25	Z	69/138 (50%)	65 (94%)	4 (6%)	0	100 100
26	a	62/70 (89%)	54 (87%)	4 (6%)	4 (6%)	1 12
27	b	44/80 (55%)	40 (91%)	4 (9%)	0	100 100
28	c	44/49 (90%)	39 (89%)	2 (4%)	3 (7%)	1 11
29	d	69/114 (60%)	64 (93%)	4 (6%)	1 (1%)	9 40
30	e	87/106 (82%)	76 (87%)	10 (12%)	1 (1%)	12 46
31	f	52/57 (91%)	44 (85%)	5 (10%)	3 (6%)	1 13
32	g	95/125 (76%)	67 (70%)	15 (16%)	13 (14%)	0 4
33	h	38/134 (28%)	35 (92%)	1 (3%)	2 (5%)	1 14
34	i	25/106 (24%)	24 (96%)	1 (4%)	0	100 100
38	m	96/118 (81%)	84 (88%)	8 (8%)	4 (4%)	2 17
39	n	126/166 (76%)	113 (90%)	10 (8%)	3 (2%)	5 27
40	o	56/58 (97%)	52 (93%)	3 (5%)	1 (2%)	7 34
41	p	67/169 (40%)	60 (90%)	4 (6%)	3 (4%)	2 17
42	q	136/138 (99%)	110 (81%)	21 (15%)	5 (4%)	2 19
All	All	5798/7343 (79%)	5116 (88%)	494 (8%)	188 (3%)	5 21

5 of 188 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	HIS
2	B	150	PRO
3	C	9	PRO
4	D	38	PRO
5	E	16	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	72/101 (71%)	70 (97%)	2 (3%)	38 57
2	B	124/150 (83%)	117 (94%)	7 (6%)	17 38
3	C	179/204 (88%)	173 (97%)	6 (3%)	32 51
4	D	332/371 (90%)	321 (97%)	11 (3%)	33 52
5	E	21/183 (12%)	20 (95%)	1 (5%)	21 43
6	F	84/353 (24%)	80 (95%)	4 (5%)	21 43
7	G	64/172 (37%)	57 (89%)	7 (11%)	5 18
8	H	249/275 (90%)	243 (98%)	6 (2%)	44 62
9	I	138/151 (91%)	128 (93%)	10 (7%)	12 32
10	J	112/142 (79%)	109 (97%)	3 (3%)	40 58
11	K	83/86 (96%)	81 (98%)	2 (2%)	44 62
12	L	463/534 (87%)	448 (97%)	15 (3%)	34 53
13	M	384/413 (93%)	377 (98%)	7 (2%)	54 71
14	N	277/316 (88%)	264 (95%)	13 (5%)	22 44
15	O	83/205 (40%)	82 (99%)	1 (1%)	67 78
18	R	17/26 (65%)	16 (94%)	1 (6%)	16 38
19	S	4/82 (5%)	4 (100%)	0	100 100
20	T	3/81 (4%)	3 (100%)	0	100 100
20	U	5/81 (6%)	5 (100%)	0	100 100
21	V	47/101 (46%)	47 (100%)	0	100 100
22	W	71/113 (63%)	71 (100%)	0	100 100
23	X	83/99 (84%)	83 (100%)	0	100 100
24	Y	99/101 (98%)	97 (98%)	2 (2%)	50 67
25	Z	59/59 (100%)	59 (100%)	0	100 100
26	a	41/59 (70%)	40 (98%)	1 (2%)	44 62
27	b	36/36 (100%)	35 (97%)	1 (3%)	38 57
28	c	26/45 (58%)	26 (100%)	0	100 100
29	d	56/60 (93%)	55 (98%)	1 (2%)	54 71
30	e	45/96 (47%)	45 (100%)	0	100 100
31	f	22/54 (41%)	21 (96%)	1 (4%)	23 45
32	g	51/112 (46%)	50 (98%)	1 (2%)	50 67
33	h	28/35 (80%)	28 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	i	20/27 (74%)	20 (100%)	0	100 100
38	m	75/86 (87%)	73 (97%)	2 (3%)	40 58
39	n	65/117 (56%)	64 (98%)	1 (2%)	60 74
40	o	5/56 (9%)	5 (100%)	0	100 100
41	p	50/62 (81%)	48 (96%)	2 (4%)	27 47
42	q	9/124 (7%)	9 (100%)	0	100 100
All	All	3582/5368 (67%)	3474 (97%)	108 (3%)	37 55

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	73	LEU
12	L	331	THR
27	b	44	ILE
12	L	61	LEU
12	L	179	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
28	c	34	GLN
29	d	59	HIS
39	n	13	GLN
8	H	5	ASN
7	G	100	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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#\|Z\| > 2$
45	SF4	F	502	6	0,12,12	-	-	-		
45	SF4	I	201	9	0,12,12	-	-	-		
45	SF4	G	801	7	0,12,12	-	-	-		
45	SF4	G	802	7	0,12,12	-	-	-		
48	NAP	P	501	-	45,52,52	0.92	3 (6%)	56,80,80	1.24	4 (7%)
45	SF4	B	201	2	0,12,12	-	-	-		
45	SF4	I	202	9	0,12,12	-	-	-		
46	FES	G	803	7	0,4,4	-	-	-		
47	FMN	F	501	-	33,33,33	1.64	5 (15%)	48,50,50	1.40	8 (16%)
46	FES	E	301	5	0,4,4	-	-	-		

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
45	SF4	F	502	6	-	-	0/6/5/5
45	SF4	I	201	9	-	-	0/6/5/5
45	SF4	G	801	7	-	-	0/6/5/5
45	SF4	G	802	7	-	-	0/6/5/5
48	NAP	P	501	-	-	6/31/67/67	0/5/5/5
45	SF4	B	201	2	-	-	0/6/5/5
45	SF4	I	202	9	-	-	0/6/5/5
46	FES	G	803	7	-	-	0/1/1/1
47	FMN	F	501	-	-	12/18/18/18	0/3/3/3
46	FES	E	301	5	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	F	501	FMN	C9A-C5A	5.78	1.50	1.41
47	F	501	FMN	C8-C7	3.99	1.50	1.40
48	P	501	NAP	C5A-C4A	2.67	1.48	1.40
47	F	501	FMN	C10-N10	2.58	1.43	1.37
47	F	501	FMN	C4A-N5	2.57	1.35	1.30

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	P	501	NAP	N3A-C2A-N1A	-3.61	123.03	128.68
48	P	501	NAP	C3D-C2D-C1D	3.45	106.17	100.98
48	P	501	NAP	PN-O3-PA	-3.36	121.29	132.83
47	F	501	FMN	C4A-C10-N1	-3.19	117.32	124.73
47	F	501	FMN	C4'-C3'-C2'	2.86	119.30	113.36

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

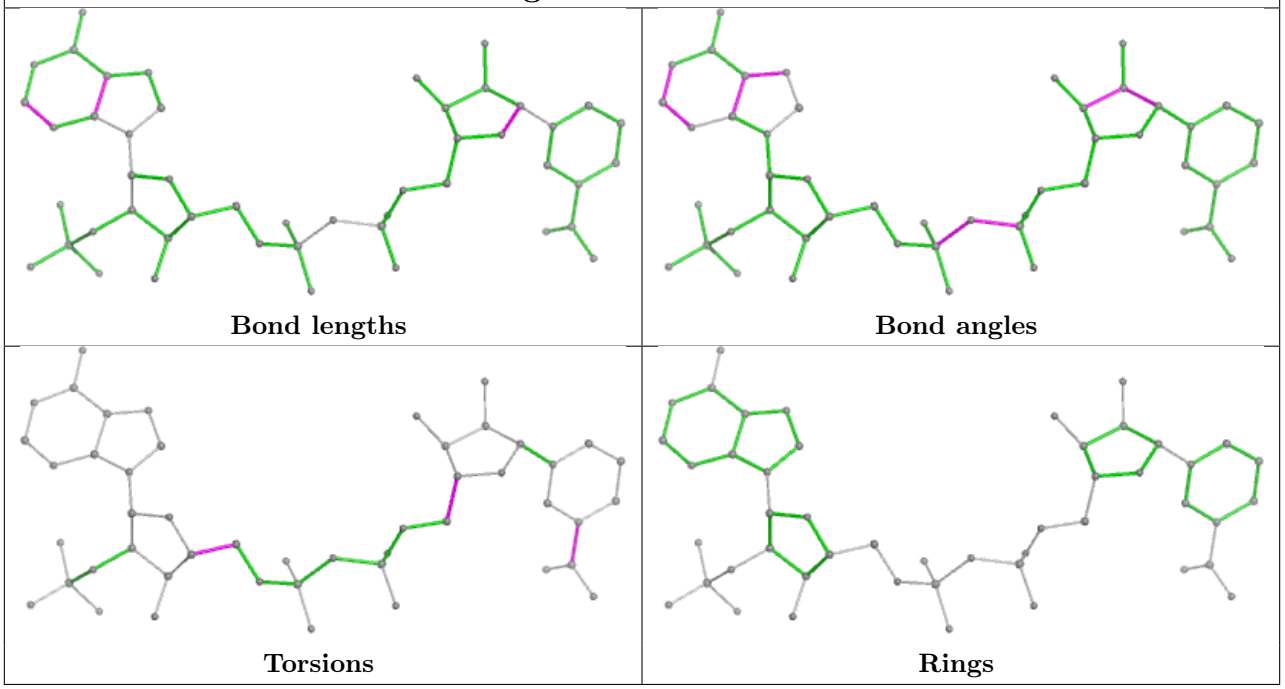
Mol	Chain	Res	Type	Atoms
47	F	501	FMN	N10-C1'-C2'-O2'
47	F	501	FMN	N10-C1'-C2'-C3'
47	F	501	FMN	C1'-C2'-C3'-O3'
47	F	501	FMN	C1'-C2'-C3'-C4'
47	F	501	FMN	C3'-C4'-C5'-O5'

There are no ring outliers.

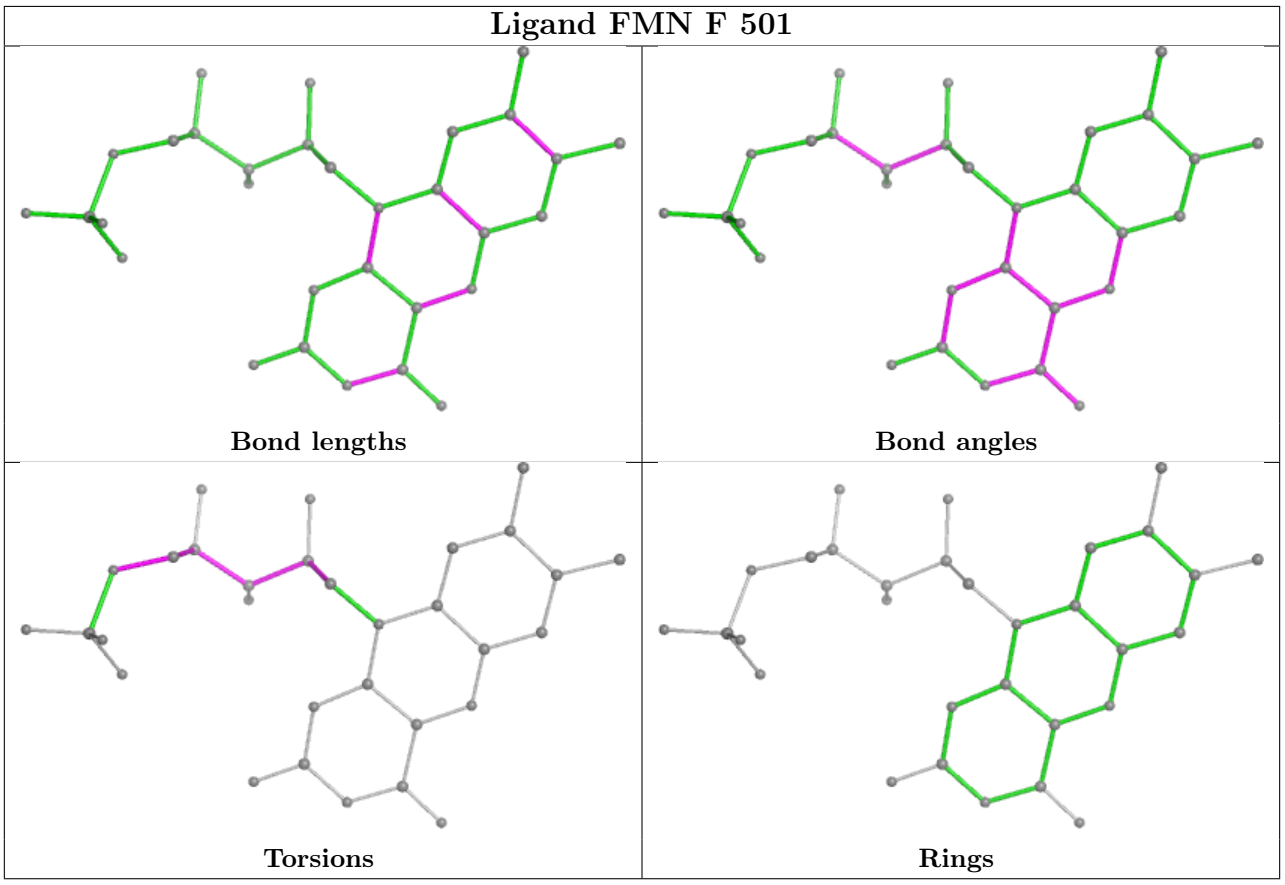
No monomer is involved in short contacts.

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

Ligand NAP P 501



Ligand FMN F 501



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
16	P	2
43	r	1
34	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	70:UNK	C	100:UNK	N	22.99
1	P	252:UNK	C	280:UNK	N	21.70
1	P	186:UNK	C	200:UNK	N	21.19
1	i	32:PRO	C	40:UNK	N	15.55

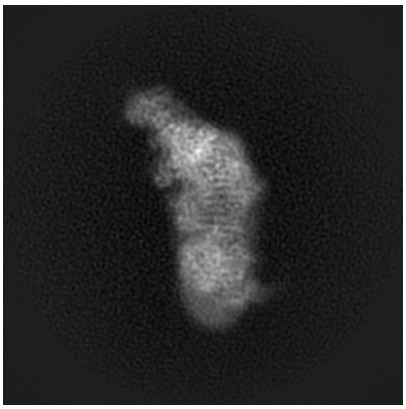
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4041. These allow visual inspection of the internal detail of the map and identification of artifacts.

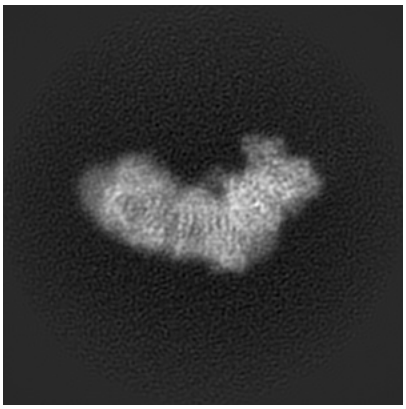
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

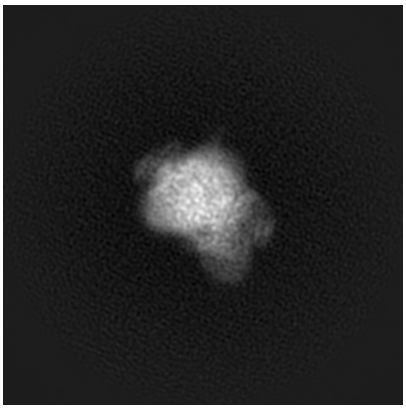
6.1.1 Primary map



X

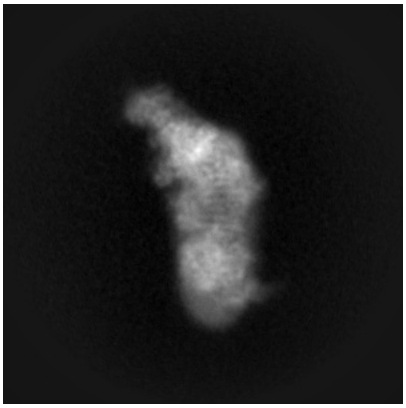


Y

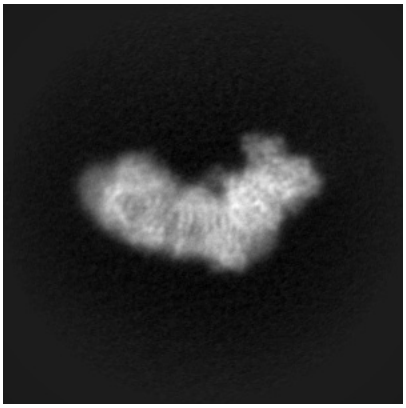


Z

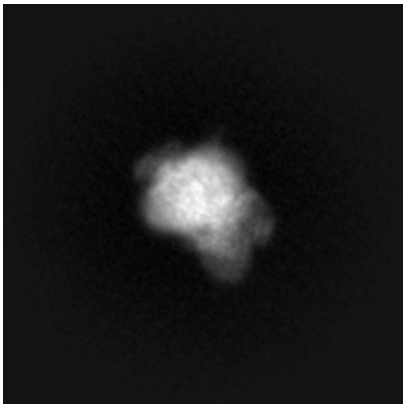
6.1.2 Raw map



X



Y

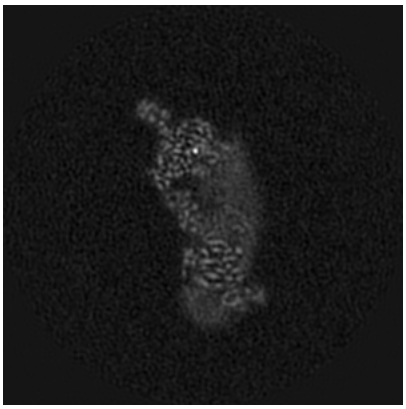


Z

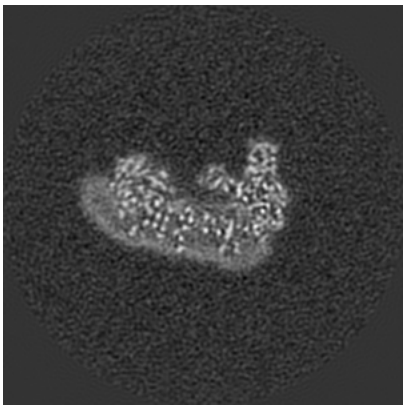
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

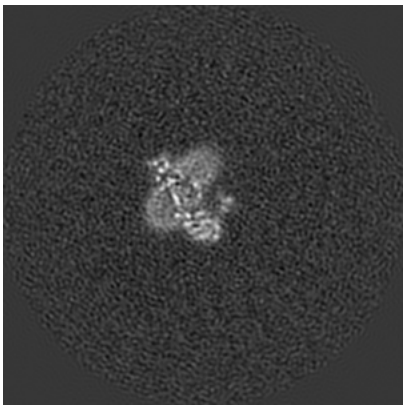
6.2.1 Primary map



X Index: 180

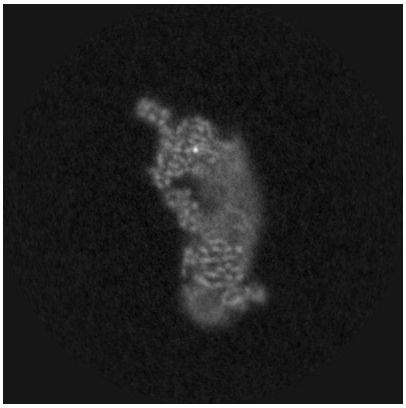


Y Index: 180

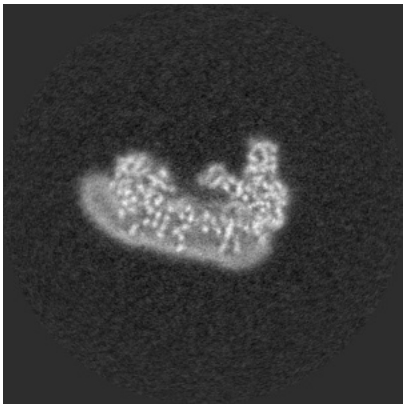


Z Index: 180

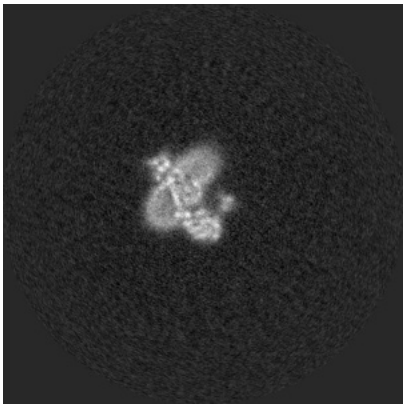
6.2.2 Raw map



X Index: 180



Y Index: 180

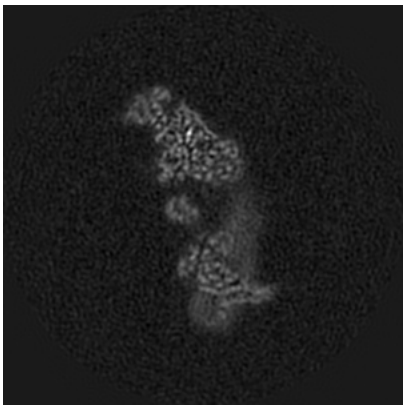


Z Index: 180

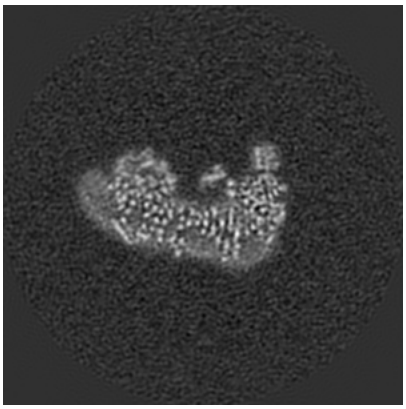
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

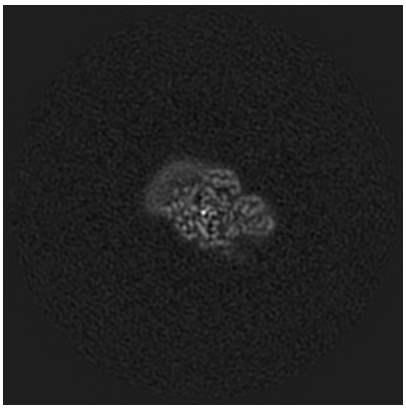
6.3.1 Primary map



X Index: 190

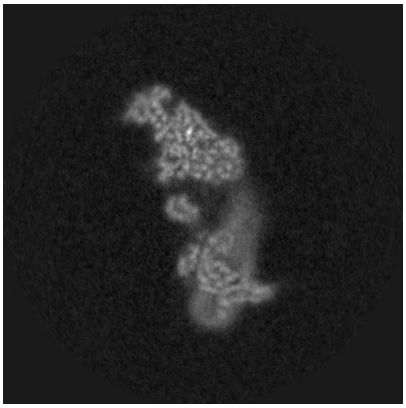


Y Index: 185

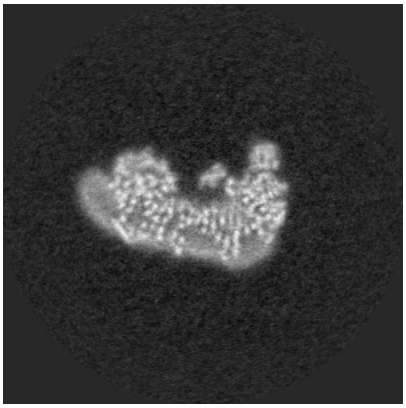


Z Index: 228

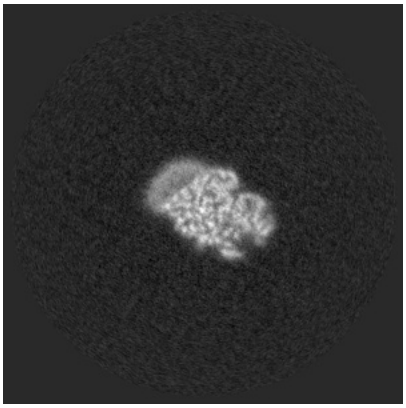
6.3.2 Raw map



X Index: 190



Y Index: 184

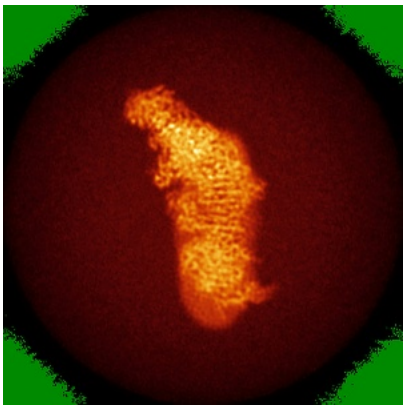


Z Index: 232

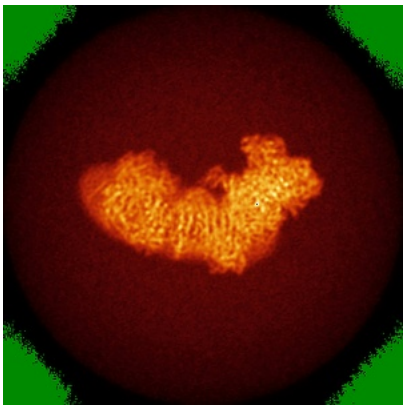
The images above show the largest variance slices of the map in three orthogonal directions.

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

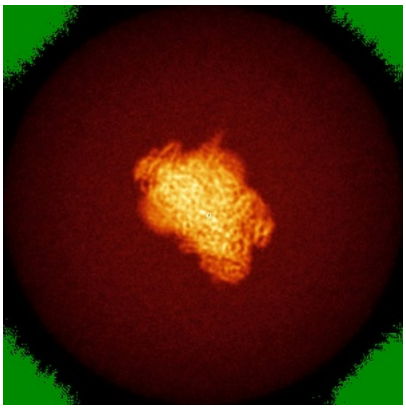
6.4.1 Primary map



X

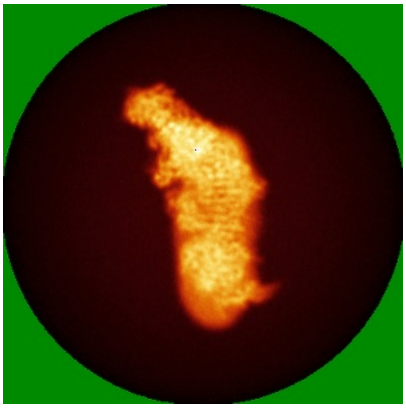


Y

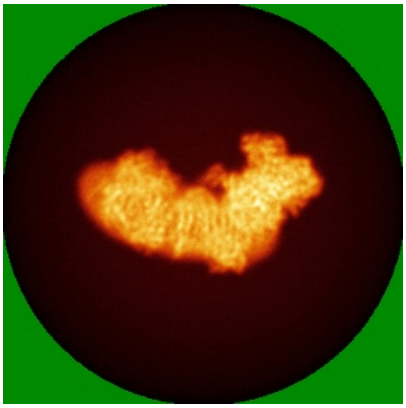


Z

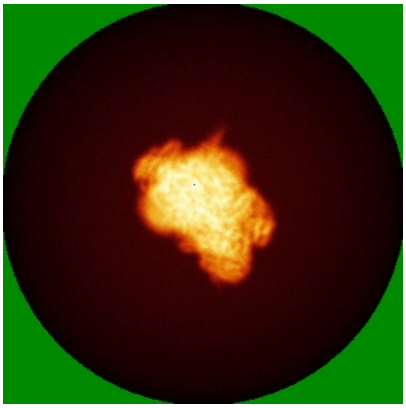
6.4.2 Raw map



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 0.125. 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.

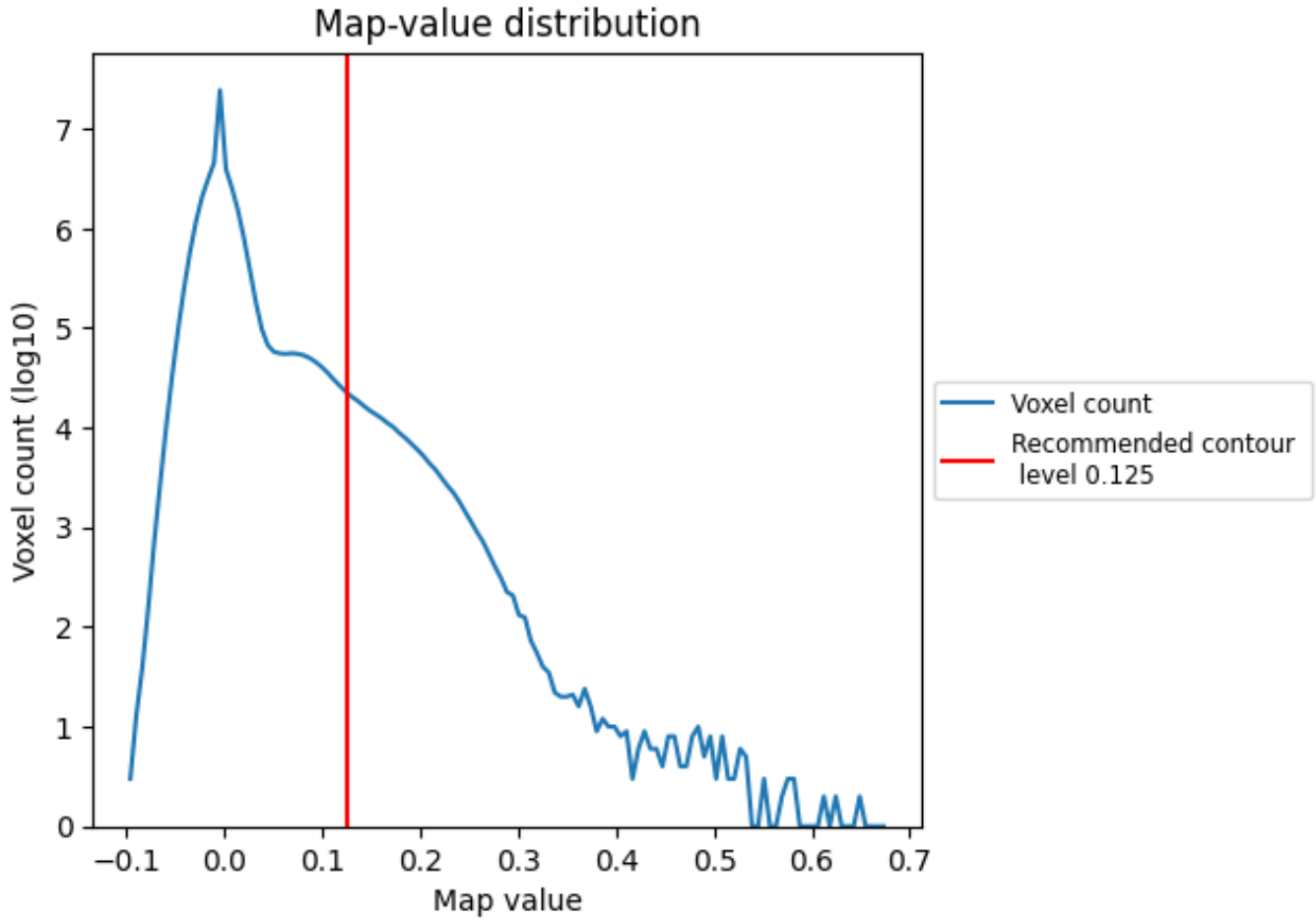
6.6 Mask visualisation (i)

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

7 Map analysis

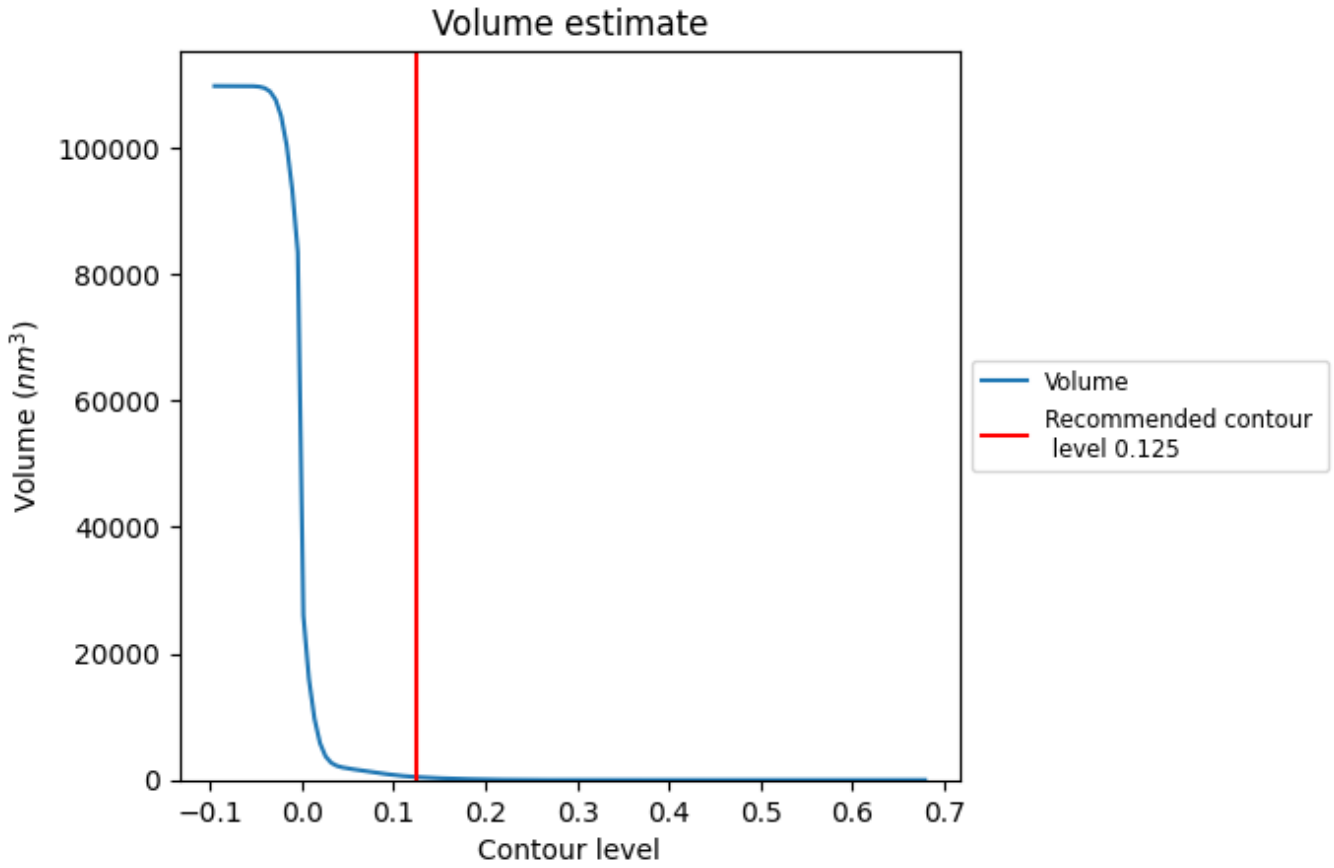
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

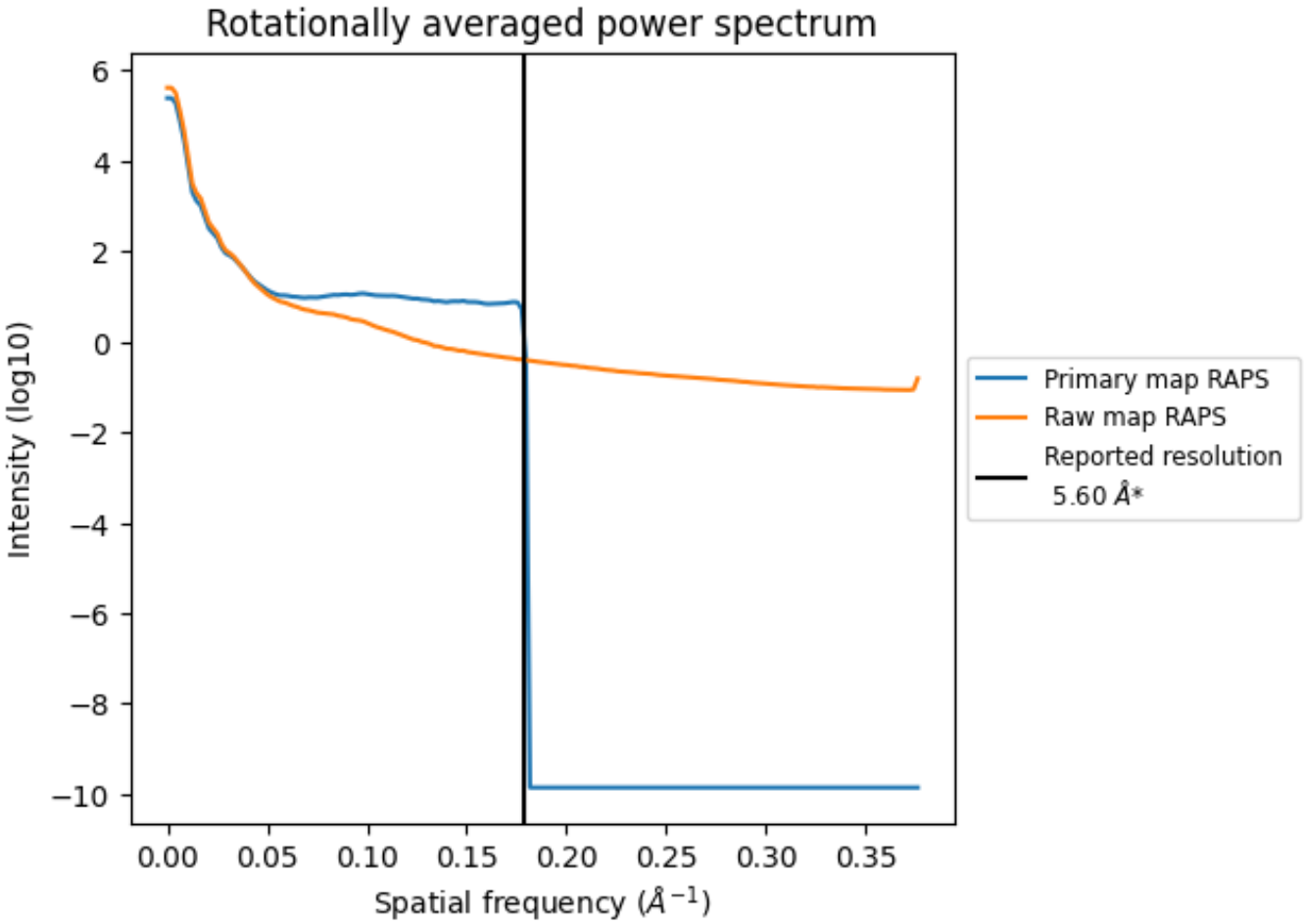
7.2 Volume estimate (i)



The volume at the recommended contour level is 469 nm^3; this corresponds to an approximate mass of 423 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)

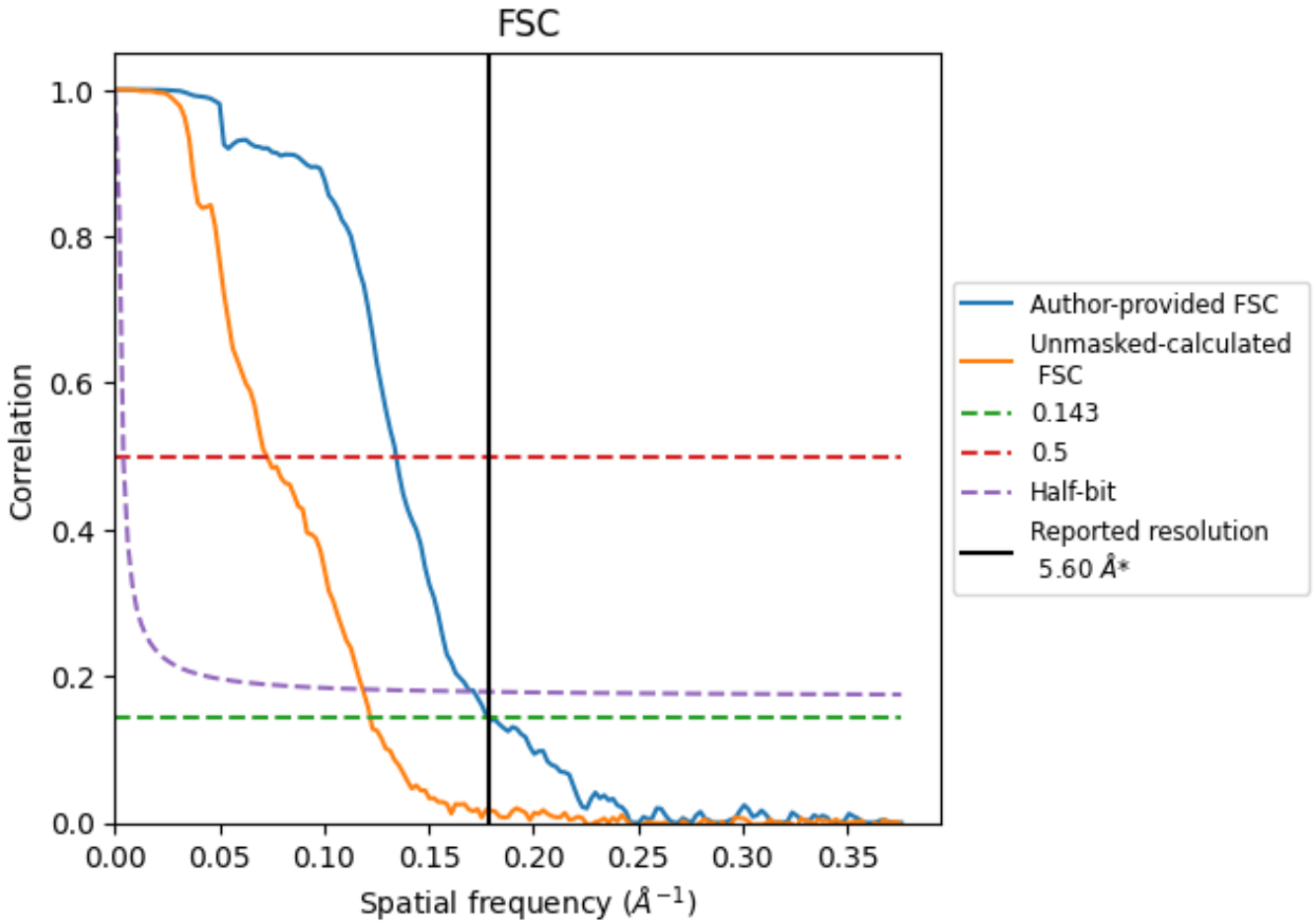


*Reported resolution corresponds to spatial frequency of 0.179 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.179 Å^{-1}

8.2 Resolution estimates (i)

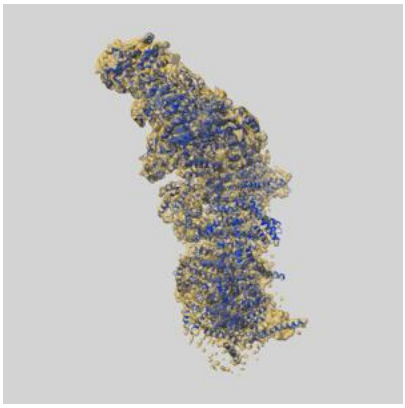
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.60	-	-
Author-provided FSC curve	5.60	7.44	5.83
Unmasked-calculated*	8.18	13.77	8.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.18 differs from the reported value 5.6 by more than 10 %

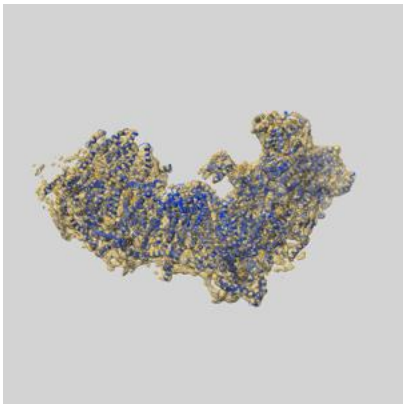
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4041 and PDB model 5LDX. Per-residue inclusion information can be found in section 3 on page 16.

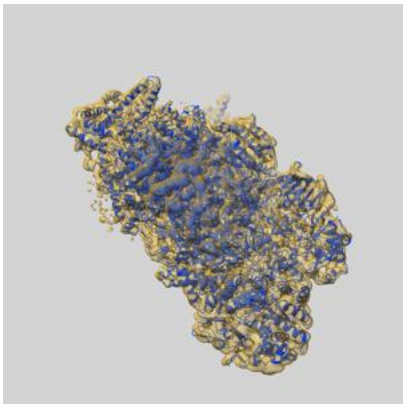
9.1 Map-model overlay



X



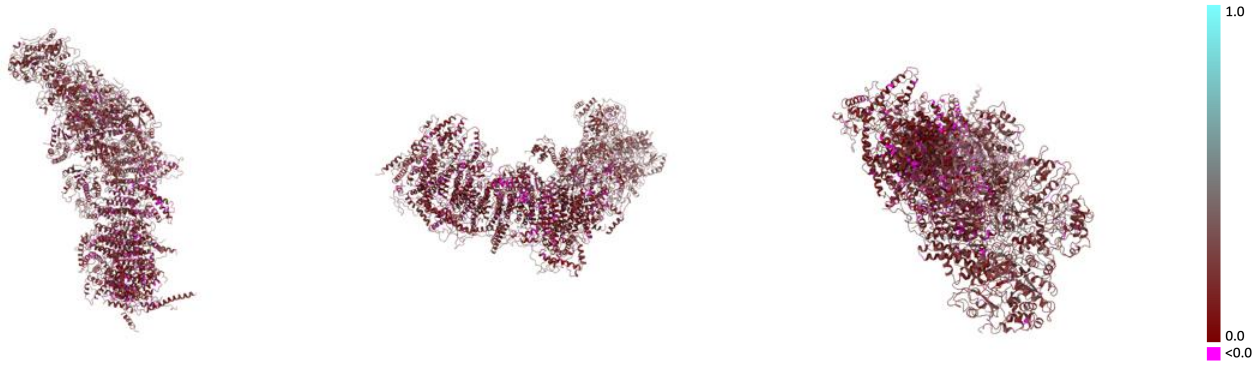
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

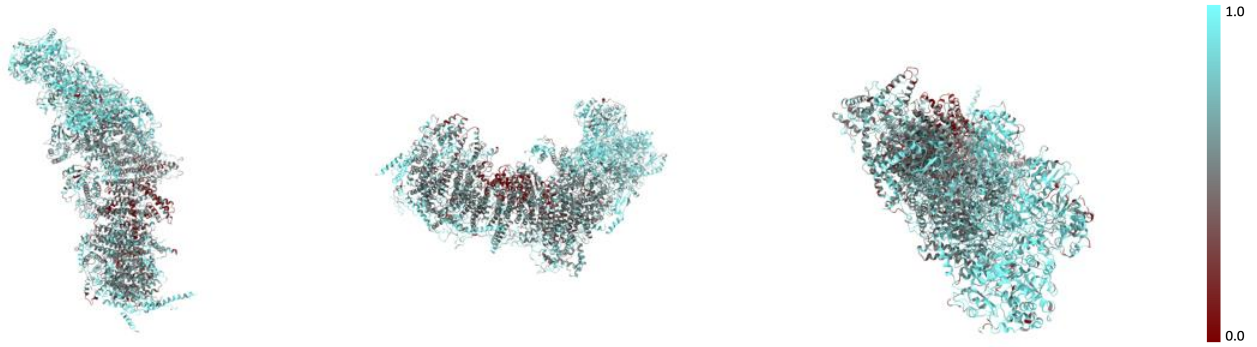
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

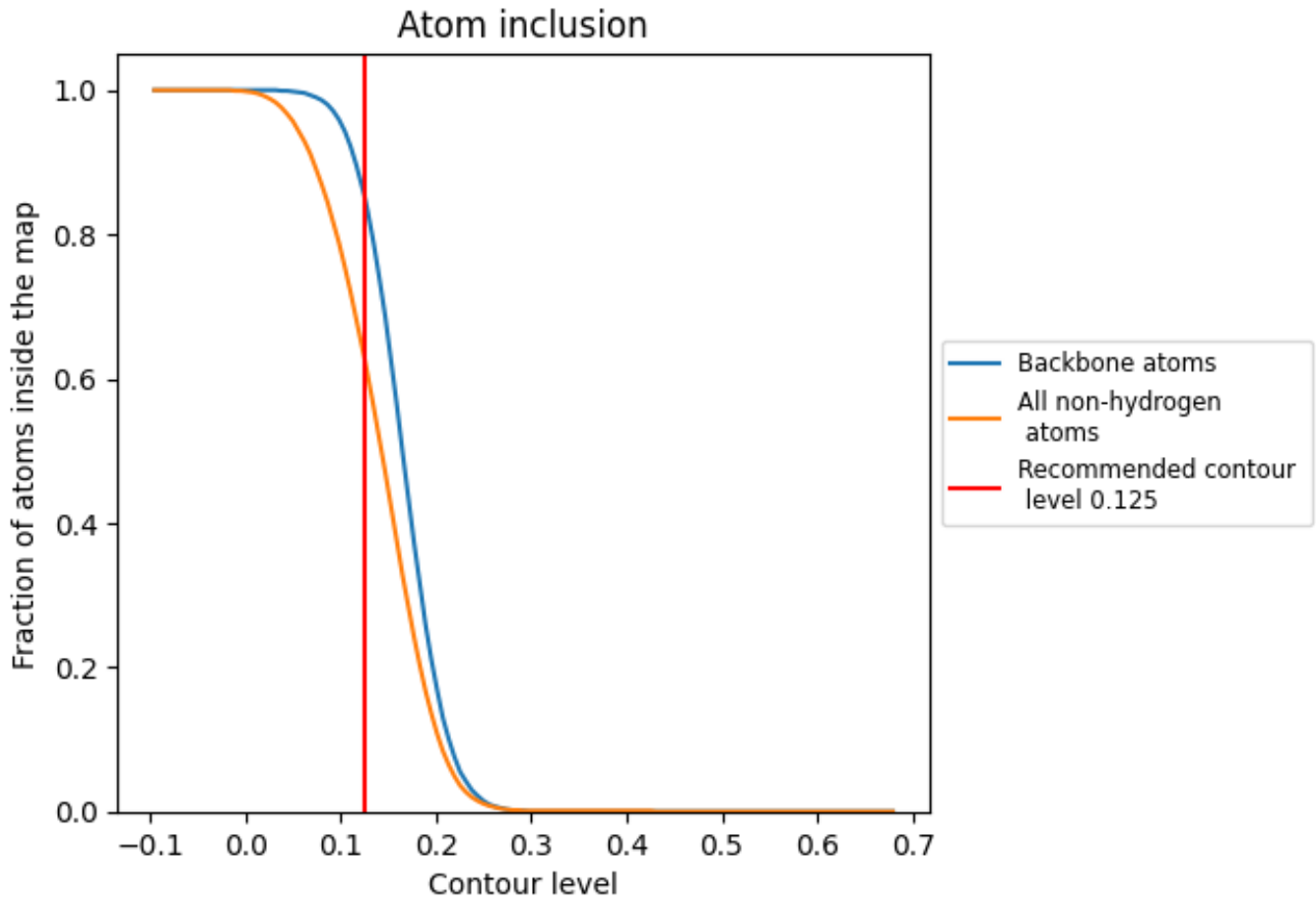
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.125).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 63% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6290	0.1910
A	0.5080	0.1470
B	0.6230	0.1700
C	0.6150	0.1820
D	0.5560	0.1590
E	0.8510	0.2770
F	0.7550	0.2280
G	0.7650	0.2480
H	0.5780	0.1590
I	0.6370	0.1560
J	0.4450	0.1510
K	0.5530	0.1480
L	0.5200	0.1330
M	0.5590	0.1460
N	0.5670	0.1550
O	0.6150	0.2200
P	0.7960	0.2530
Q	0.8530	0.3160
R	0.7840	0.2750
S	0.7800	0.2540
T	0.7330	0.2500
U	0.6530	0.2330
V	0.6330	0.2110
W	0.6170	0.1890
X	0.6240	0.2200
Y	0.2620	0.1310
Z	0.6330	0.1820
a	0.6040	0.1670
b	0.6540	0.2080
c	0.6620	0.2160
d	0.6090	0.1960
e	0.6350	0.1940
f	0.6330	0.2110
g	0.5700	0.1710
h	0.6910	0.1870

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.6610	0.2020
j	0.8620	0.2700
k	0.6970	0.2470
l	0.7360	0.2620
m	0.5060	0.1430
n	0.6140	0.2020
o	0.7970	0.1940
p	0.6920	0.1960
q	0.8430	0.2860
r	0.8390	0.3180
s	0.8570	0.2860