wwPDB EM Validation Summary Report (i)

Aug 22, 2026 – 06:12 am BST

PDB ID	:	5LC5 / pdb_00005lc5
EMDB ID	:	EMD-4032
Title	:	Structure of mammalian respiratory Complex I, class2
Authors	:	Vinothkumar, K.R.; Zhu, J.; Hirst, J.
Deposited on	:	2016-06-19
Resolution	:	4.35 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:

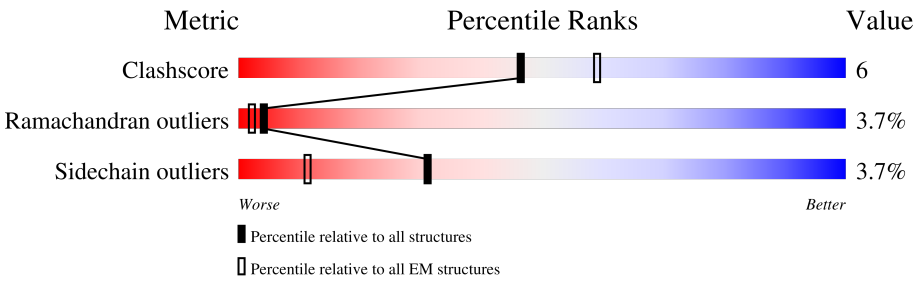
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

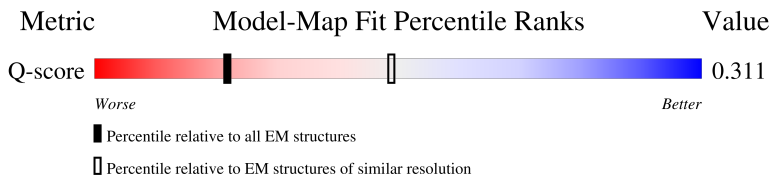
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.35 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	3796 (3.85 - 4.85)

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	111	29% 83% 16% •
2	B	147	10% 77% 20% •
3	C	206	18% 76% 21% • •
4	D	426	14% 76% 21% •

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Mol	Chain	Length	Quality of chain
5	E	249	9% 59% 9% 5% 25%
6	F	464	17% 87% 5% 8%
7	G	715	18% 93%
8	H	313	25% 74% 23%
9	I	176	16% 80% 19%
10	J	171	40% 87% 12%
11	K	95	26% 79% 20%
12	L	604	27% 84% 15%
13	M	457	20% 82% 17%
14	N	344	13% 79% 19%
15	O	314	21% 96%
16	P	335	20% 100%
17	Q	113	8% 97%
18	R	89	16% 94% 6%
19	S	80	29% 98%
20	T	75	43% 99%
21	U	85	14% 98%
22	V	116	30% 77% 11% 9%
23	W	128	20% 73% 10% 13%
24	X	169	39% 92% 5%
25	Y	138	40% 90% 9%
26	Z	138	31% 93% 7%
27	a	70	31% 83% 7% 9%
28	b	80	42% 95% 5%
29	c	76	17% 57% 39%

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Mol	Chain	Length	Quality of chain
30	d	114	14% 96%
31	e	106	21% 72% 10% 16%
32	f	57	33% 82% 9% 5%
33	g	154	20% 49% 8% 37%
34	h	186	10% 66% 6% 28%
35	i	121	30% 81% 12%
36	j	52	12% 100%
37	k	74	39% 100%
38	l	118	18% 100%
39	m	118	32% 92% 7%
40	n	166	27% 98%
41	o	58	9% 98%
42	p	169	15% 95% 5%
43	q	138	7% 88% 12%
44	r	87	18% 98%
45	s	35	100%

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 51718 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	111	806	545	122	136	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	426	3301	2102	575	600	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
			Total	C	N	O	S		
5	E	186	959	583	186	186	4	0	0

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

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

- Molecule 7 is a protein called 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, NDUFS1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	313	2389	1600	374	393	22	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, NDUFA10,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
			Total	C	N	O	S		
15	O	314	1854	1151	347	353	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	P	335	1675	1005	335	335	0	0

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

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

- 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,NADH dehydrogenase [ubiquinone]

iron-sulfur protein 6, mitochondrial.

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

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

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

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

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

- Molecule 21 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	85	432	262	85	85	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 24 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,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 26 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
			Total	C	N	O	S		
26	Z	138	921	573	172	170	6	0	0

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

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

- Molecule 28 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
			Total	C	N	O	S		
28	b	80	519	336	89	93	1	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 30 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
			Total	C	N	O	S		
30	d	114	790	504	146	137	3	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

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

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 34 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,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 35 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,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUFB2.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUFB3.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUFB8.

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

- Molecule 39 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,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 40 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,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

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

7.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10.

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

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

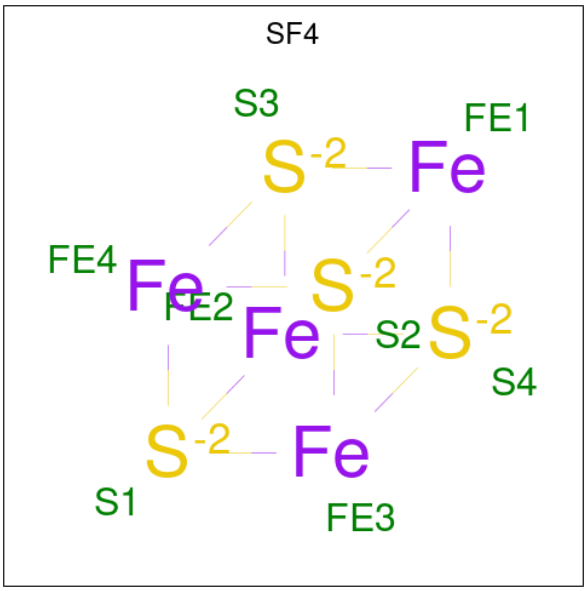
- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUFA7.

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

- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUFV3.

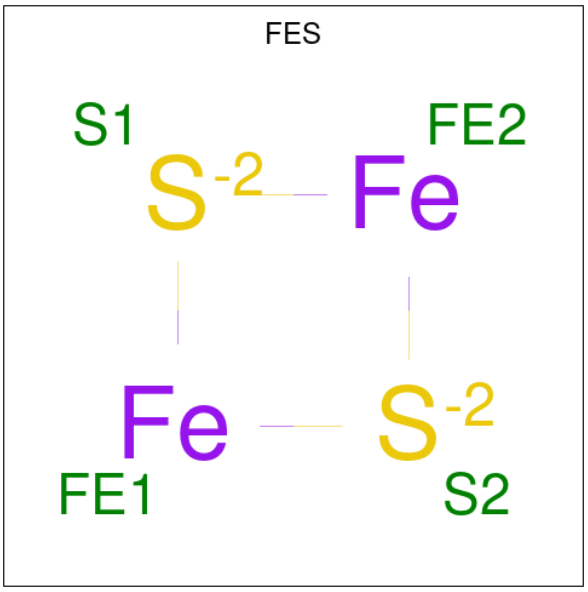
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	s	35	175	105	35	35	0	0

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



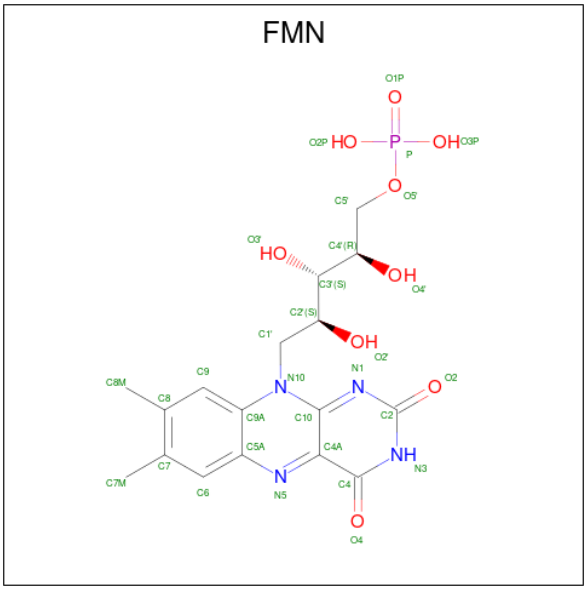
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
46	B	1	8	4	4	0
46	F	1	8	4	4	0
46	G	1	8	4	4	0
46	G	1	8	4	4	0
46	I	1	8	4	4	0
46	I	1	8	4	4	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

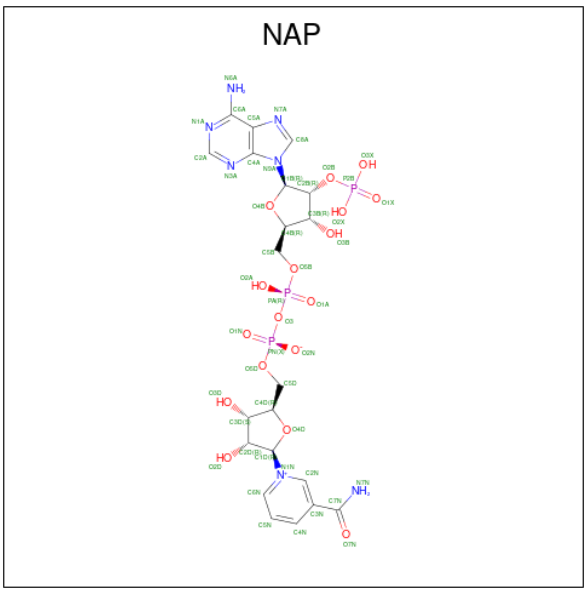
- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 49 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE

(CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

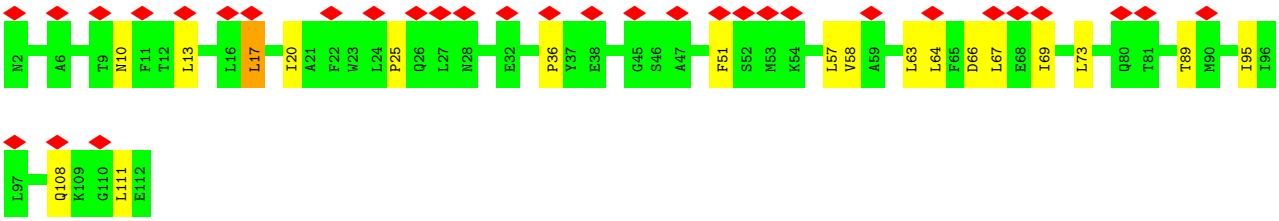
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
50	R	1	1	1	0

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.

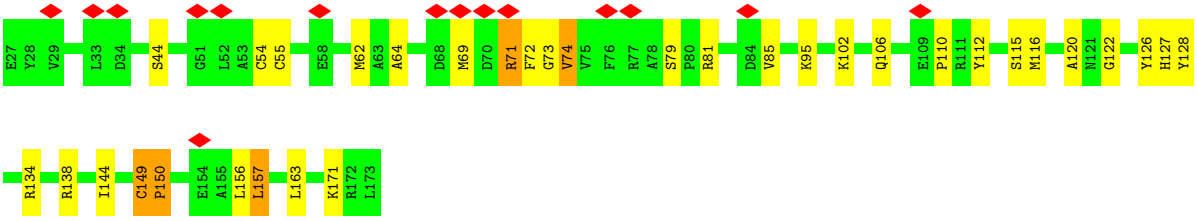
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 29% 83% 16%



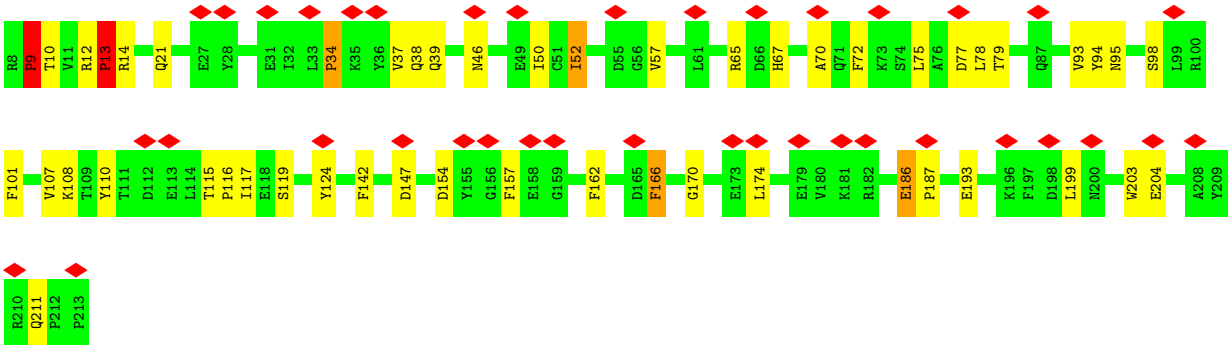
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 10% 77% 20%



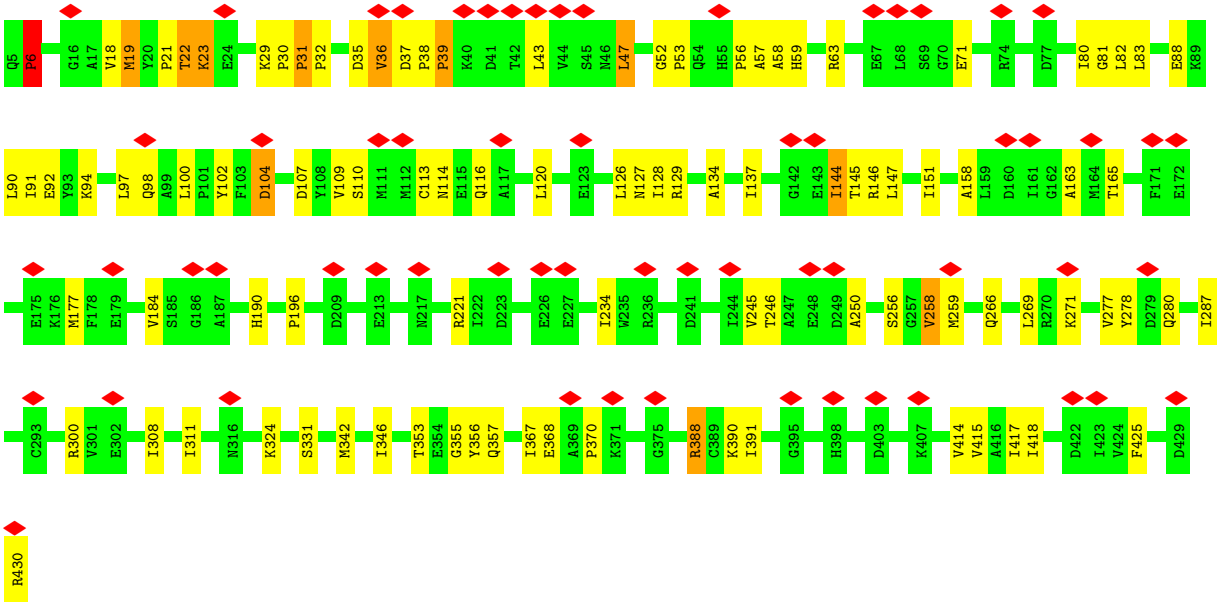
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 18% 76% 21%



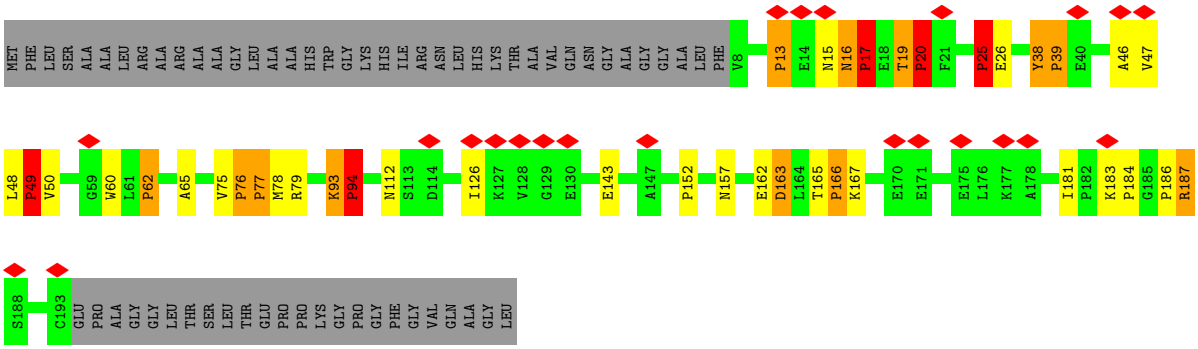
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



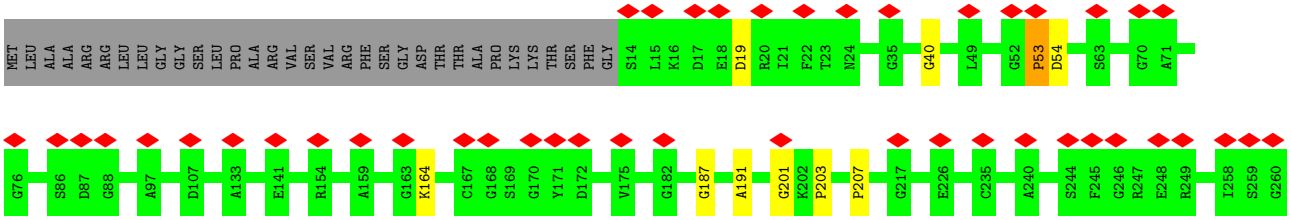
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

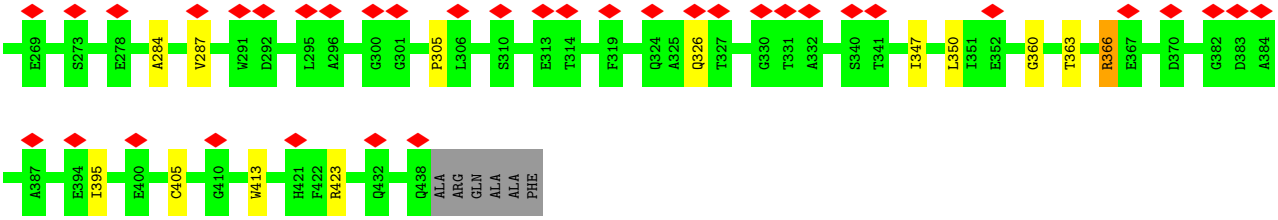
Chain E:



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

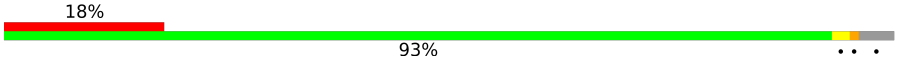
Chain F:

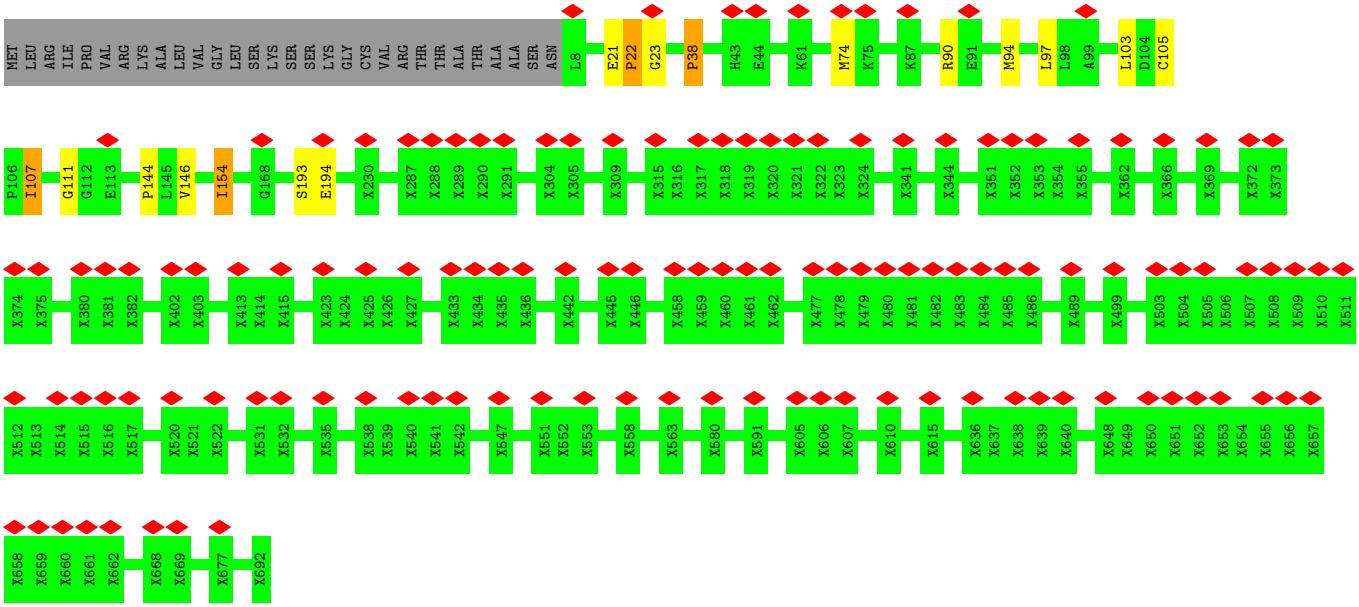




• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, NDUFS1

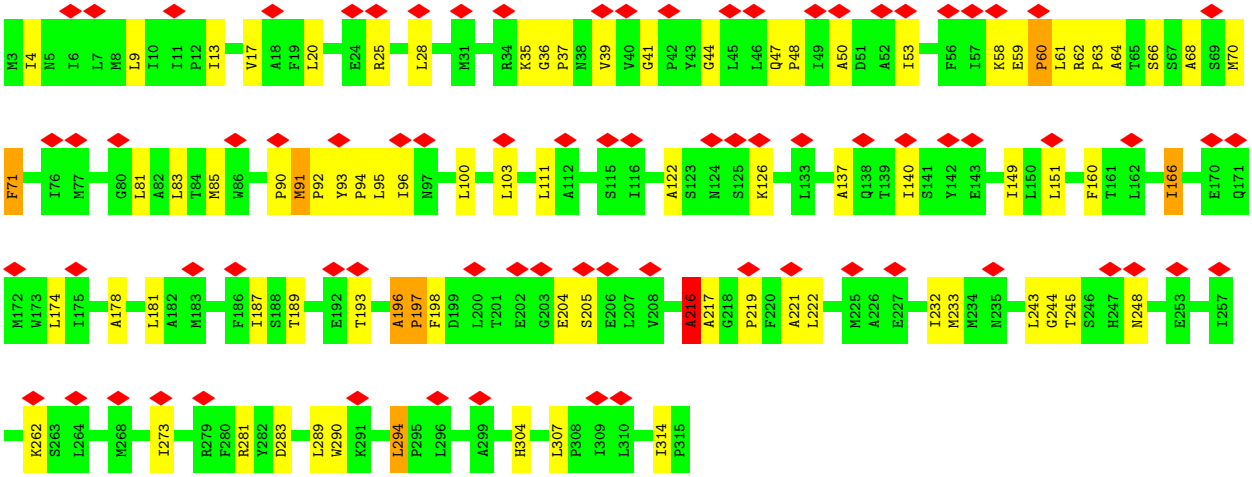
Chain G:





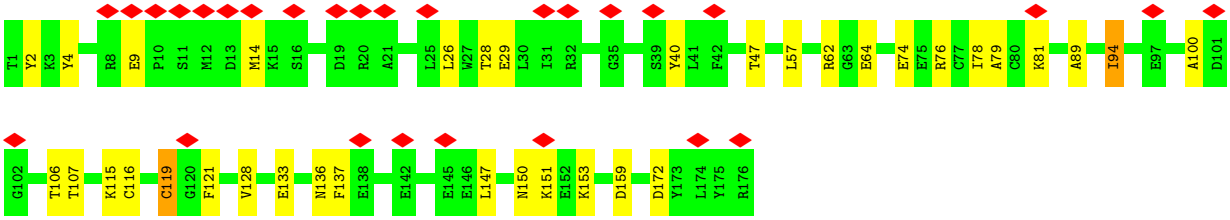
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



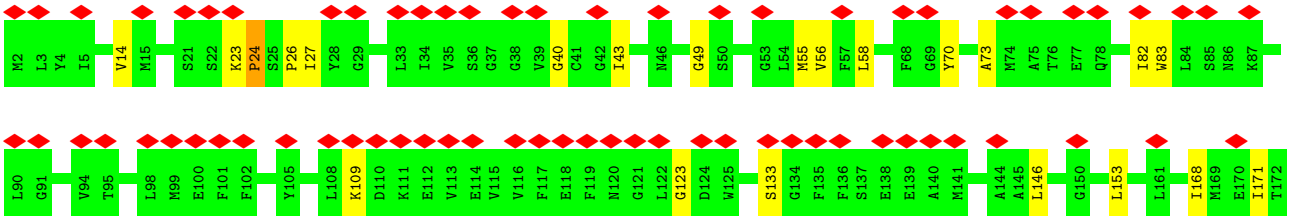
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



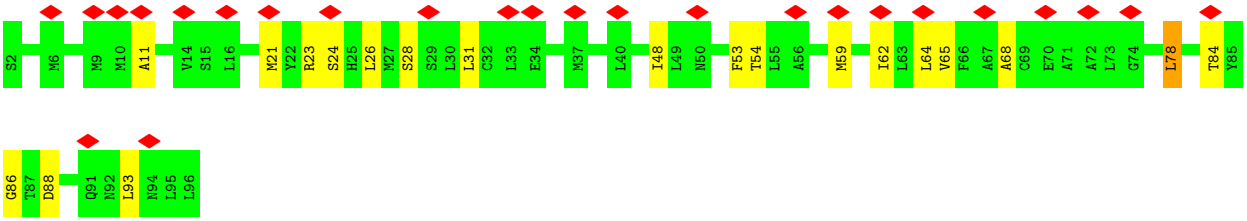
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



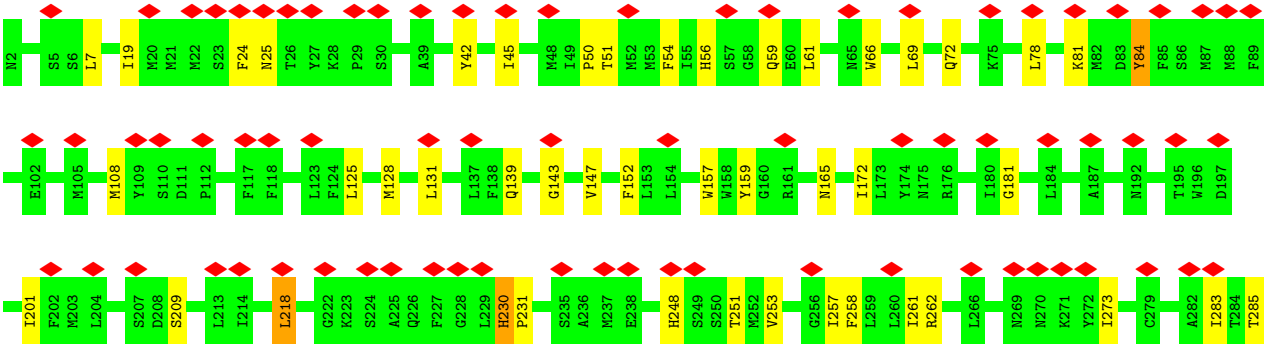
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

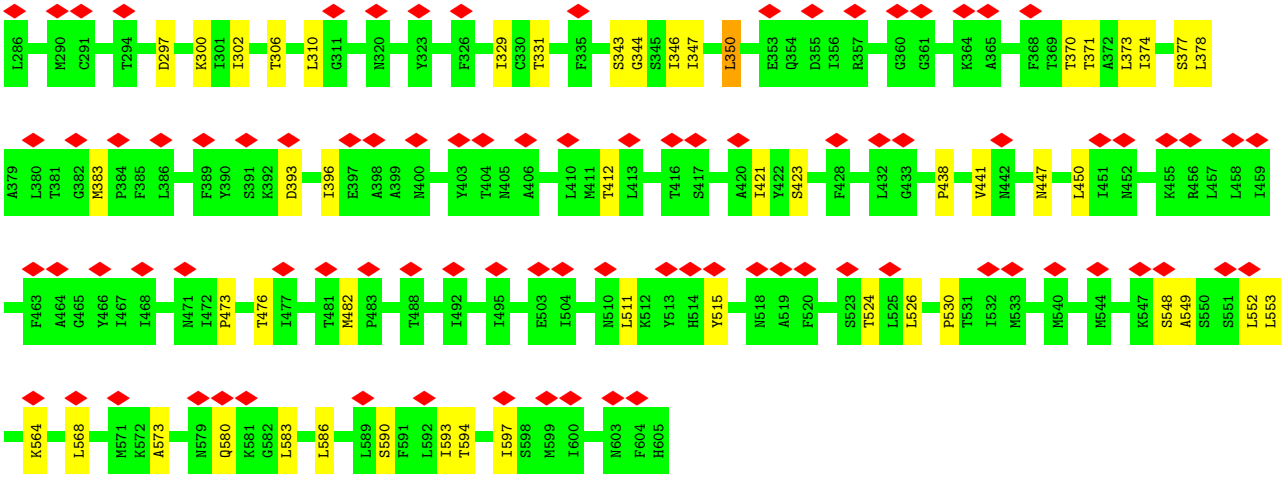
Chain K:



• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

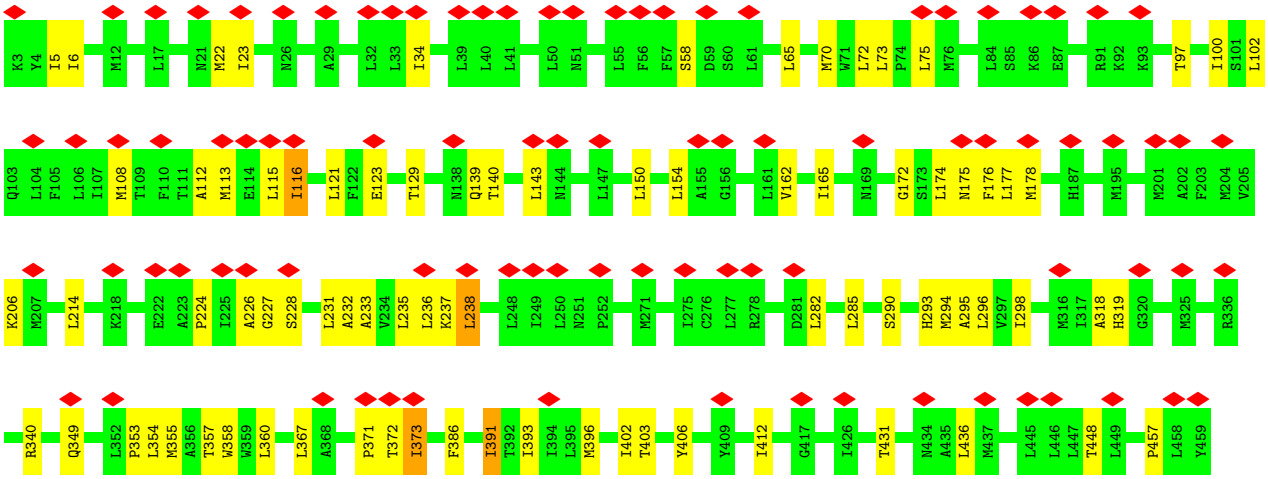
Chain L:





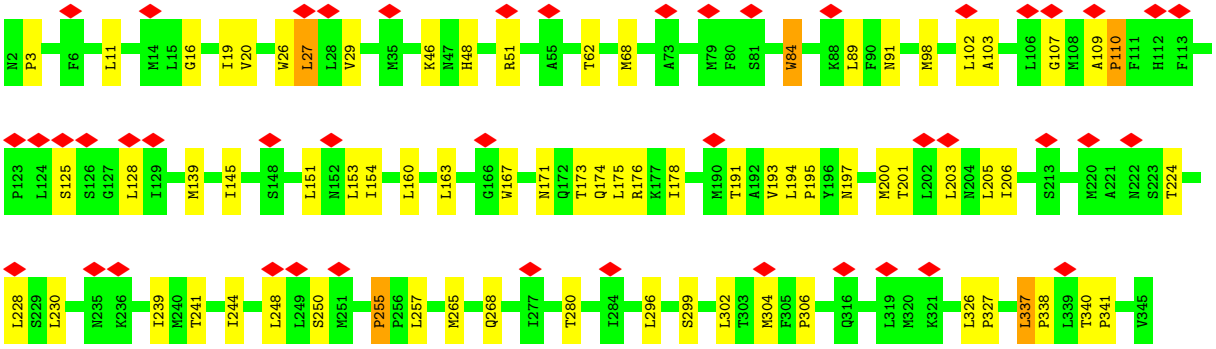
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

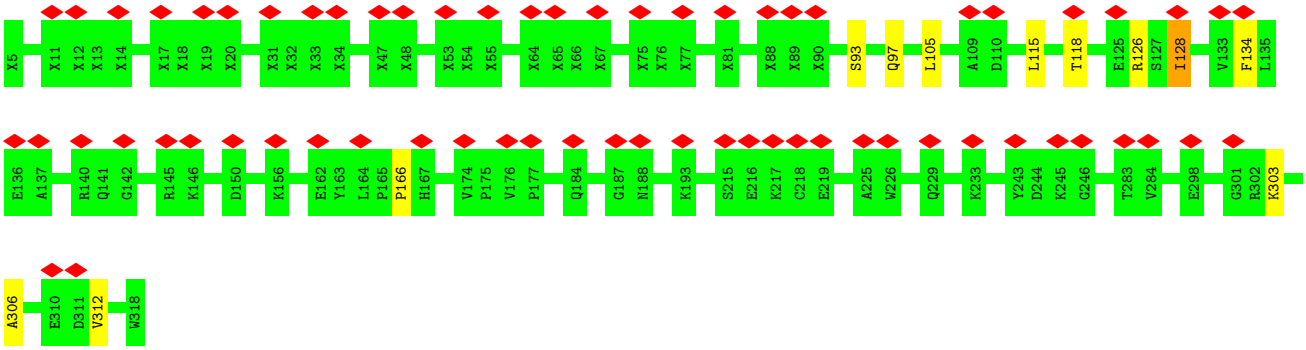
Chain N:



• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, NDUFA10,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase

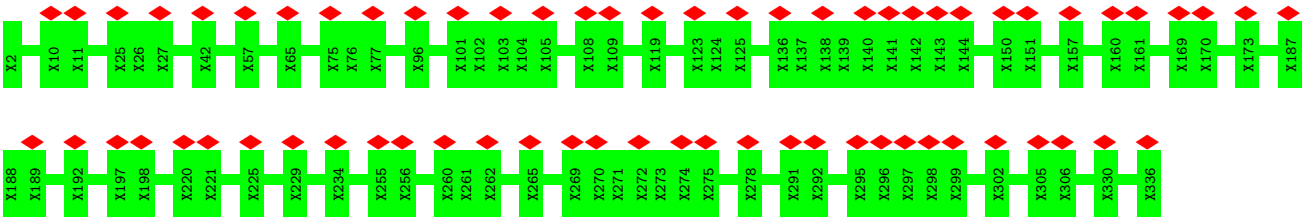
[ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 21% 96%



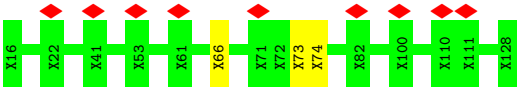
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 20% 100%



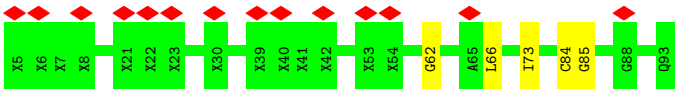
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 8% 97%



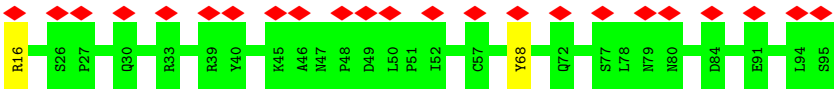
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 16% 94% 6%



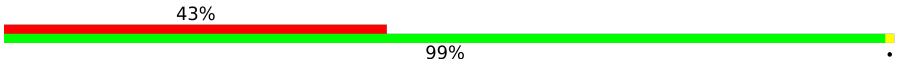
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

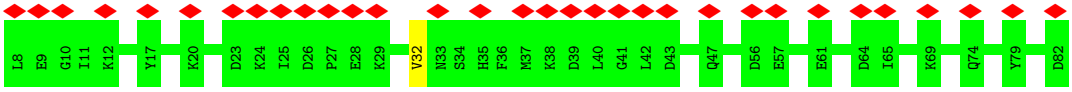
Chain S: 29% 98%



• Molecule 20: Acyl carrier protein, mitochondrial

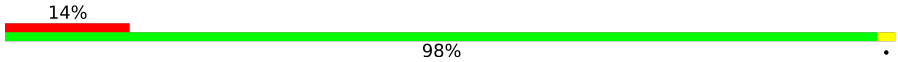
Chain T:

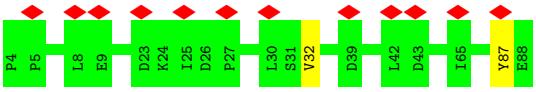




• Molecule 21: Acyl carrier protein, mitochondrial

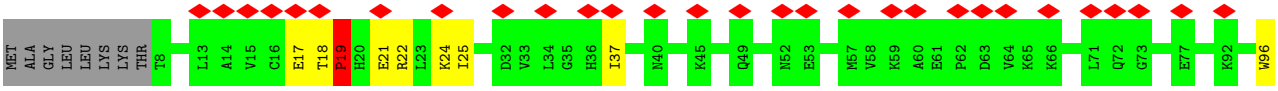
Chain U:

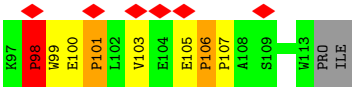




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

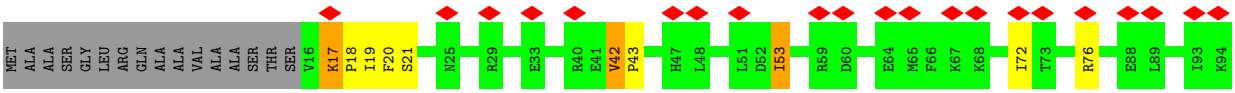
Chain V:

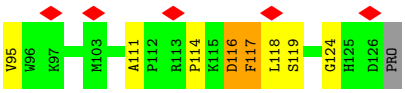




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

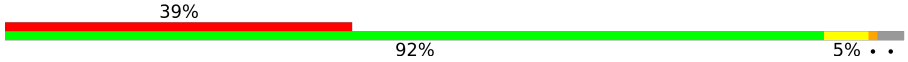
Chain W:

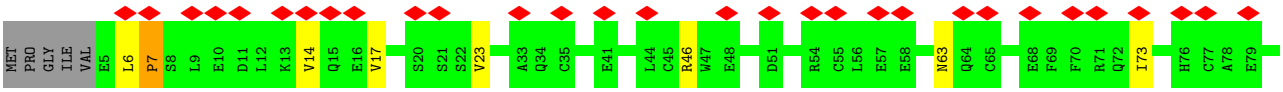


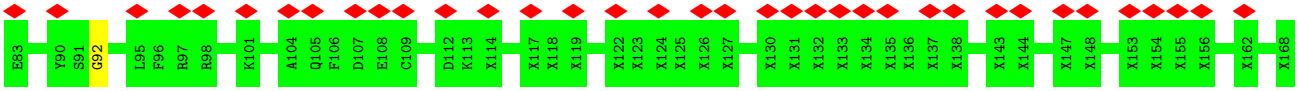


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:

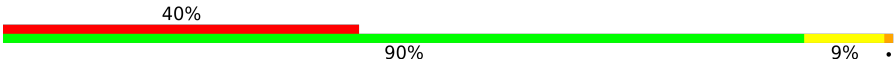


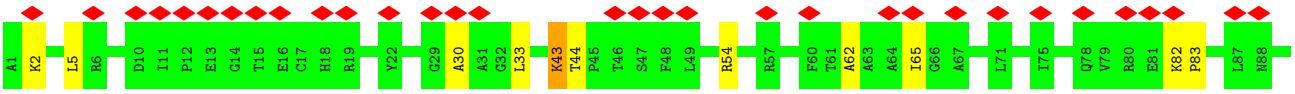


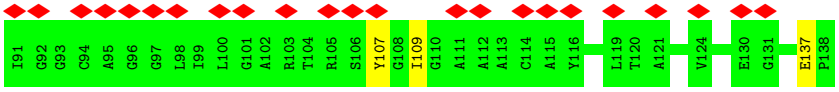


• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:

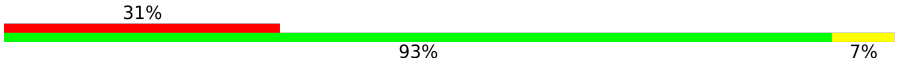


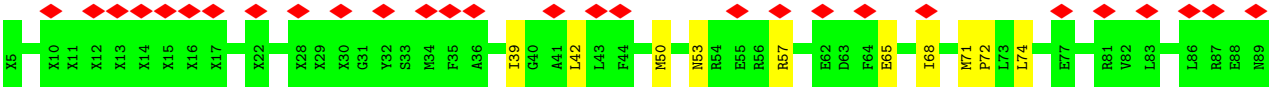


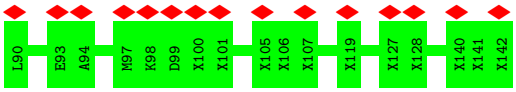


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:

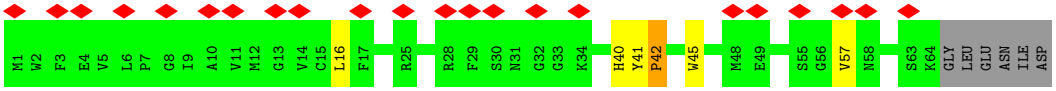






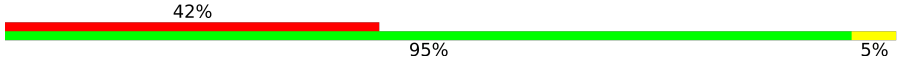
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

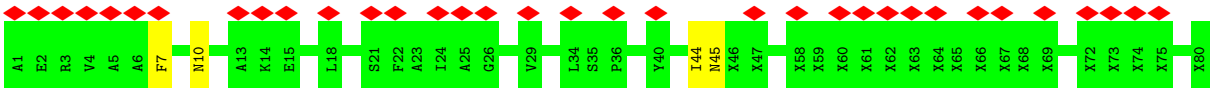
Chain a:



• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

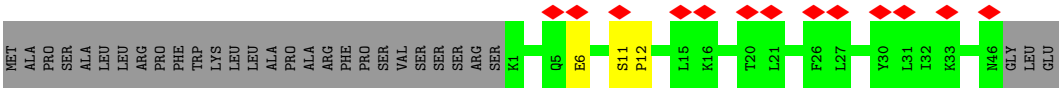
Chain b:





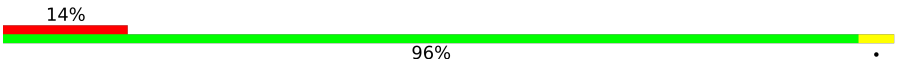
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

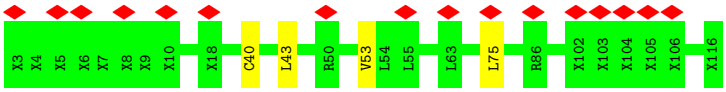
Chain c:



• Molecule 30: 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,NADH dehydrogenase [ubiquinone] 1 subunit C2

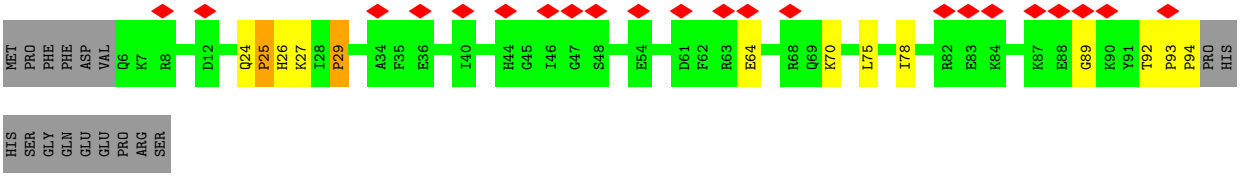
Chain d:





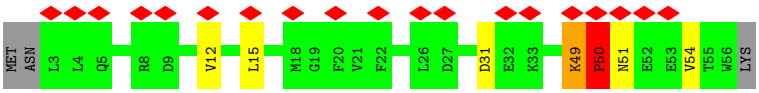
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



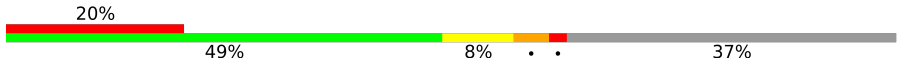
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

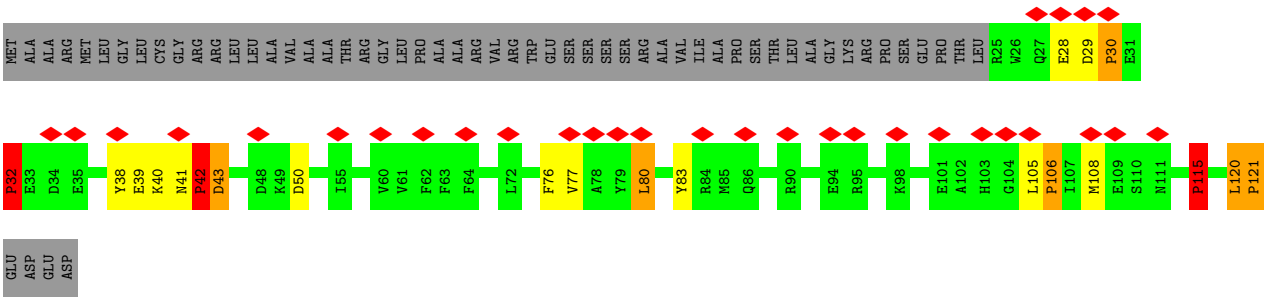
Chain f:



• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

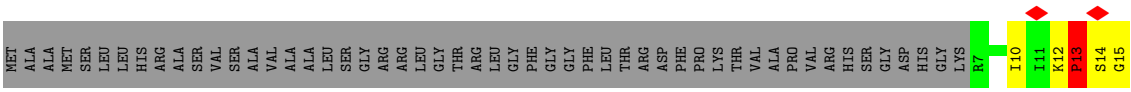
Chain g:

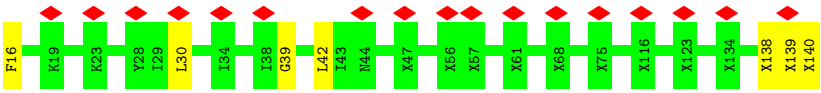




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

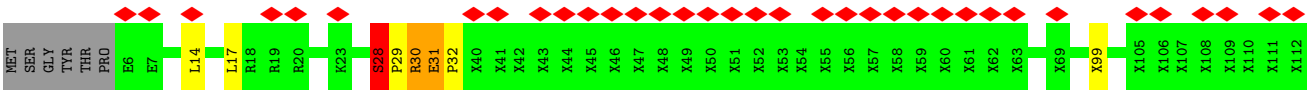
Chain h:





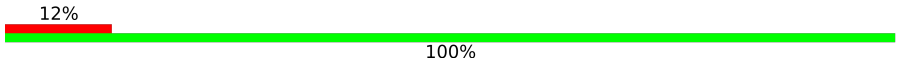
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

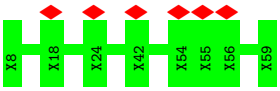
Chain i:



• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUFB2

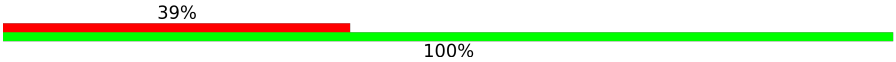
Chain j:

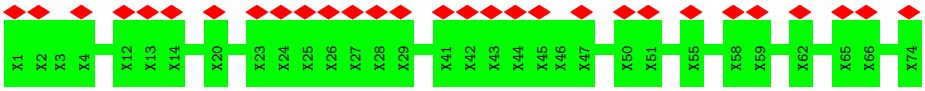




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUFB3

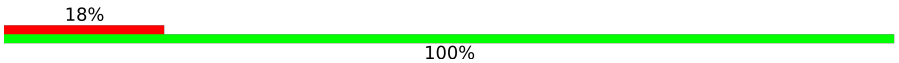
Chain k:

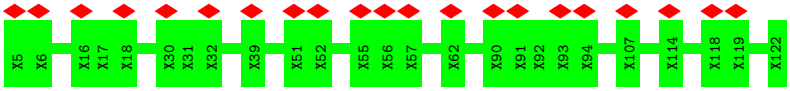




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUFB8

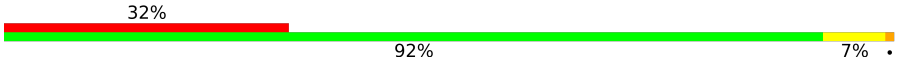
Chain l:

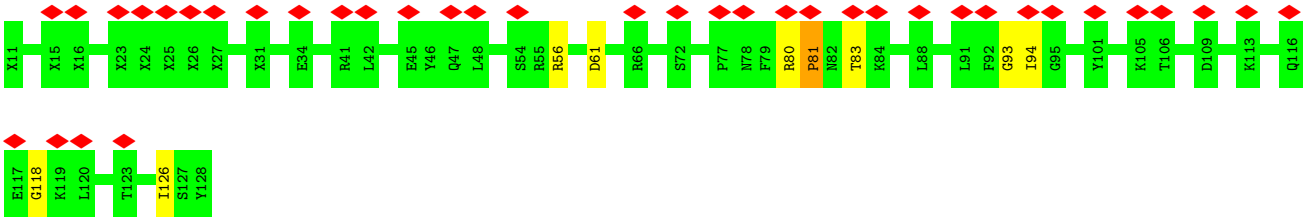




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

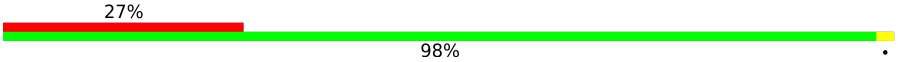
Chain m:

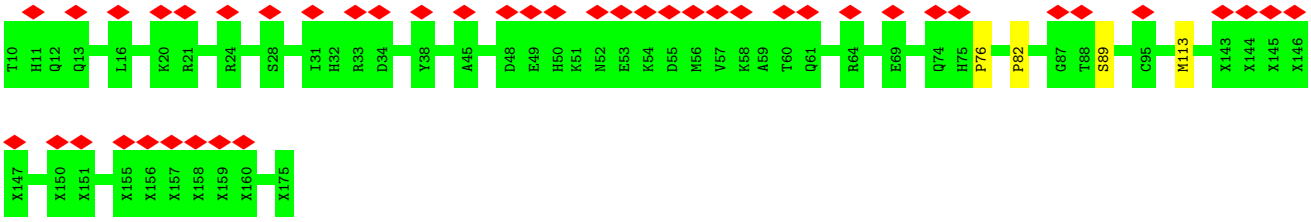




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

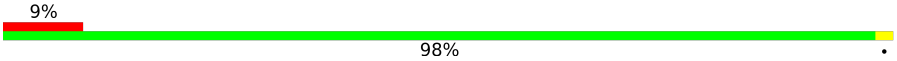
Chain n:

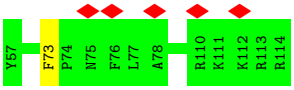




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

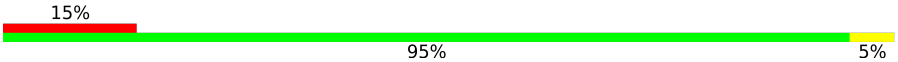
Chain o:

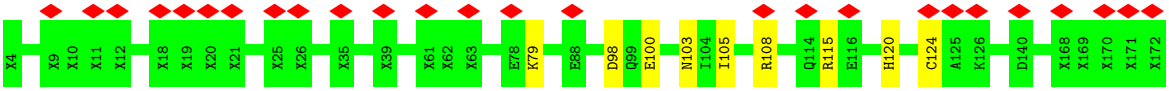




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10

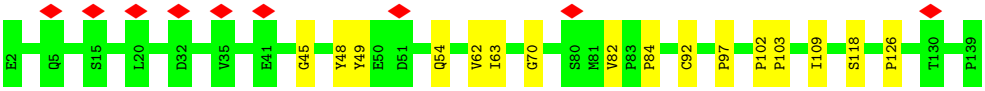
Chain p:





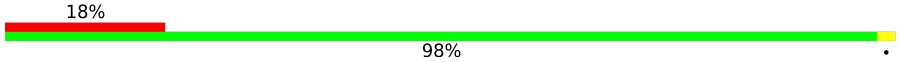
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

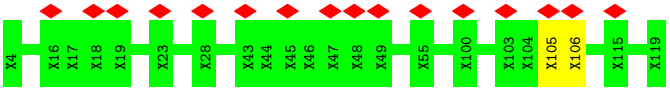
Chain q:



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUFA7

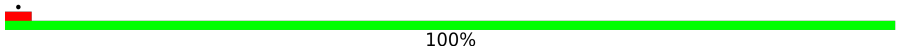
Chain r:

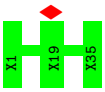




• Molecule 45: NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUFV3

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33301	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Ctf was estimated from the whole micrograph. Ctf was corrected per particle.	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	1.103	Depositor
Minimum map value	-0.273	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.165	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, FES, ZN, FMN, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.59	0/825	1.04	0/1137
2	B	0.53	0/1187	0.95	2/1607 (0.1%)
3	C	0.59	0/1735	0.97	4/2365 (0.2%)
4	D	0.61	1/3382 (0.0%)	1.07	19/4587 (0.4%)
5	E	0.81	0/975	1.46	14/1370 (1.0%)
6	F	0.59	0/2389	1.06	2/3299 (0.1%)
7	G	0.57	0/1213	1.04	2/1658 (0.1%)
8	H	0.57	0/2455	1.07	6/3359 (0.2%)
9	I	0.53	0/1395	0.93	0/1893
10	J	0.58	0/1239	1.05	0/1688
11	K	0.49	0/730	1.03	0/988
12	L	0.55	0/4653	0.99	0/6350
13	M	0.54	0/3624	0.98	0/4949
14	N	0.57	0/2656	1.05	1/3630 (0.0%)
15	O	0.52	0/1449	1.01	0/2001
18	R	0.49	0/235	0.81	0/316
19	S	0.50	0/408	1.06	0/571
20	T	0.50	0/380	1.15	0/531
21	U	0.49	0/436	1.13	0/610
22	V	0.74	1/696 (0.1%)	1.23	4/954 (0.4%)
23	W	0.64	0/831	1.13	4/1128 (0.4%)
24	X	0.55	0/877	1.00	1/1181 (0.1%)
25	Y	0.58	0/1031	1.01	0/1400
26	Z	0.46	0/585	1.01	0/781
27	a	0.61	0/494	1.00	2/669 (0.3%)
28	b	0.58	0/352	0.97	0/481
29	c	0.64	0/330	1.14	0/455
30	d	0.48	0/581	0.95	0/782
31	e	0.70	1/627 (0.2%)	1.13	4/848 (0.5%)
32	f	0.66	0/356	1.04	1/488 (0.2%)
33	g	0.71	0/696	1.26	8/957 (0.8%)
34	h	0.68	0/301	1.15	2/409 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	i	0.72	0/224	2.57	4/300 (1.3%)
39	m	0.55	0/801	0.94	0/1085
40	n	0.51	0/914	0.97	0/1247
41	o	0.51	0/296	1.20	0/412
42	p	0.48	0/535	1.02	0/718
43	q	0.61	0/704	1.11	1/984 (0.1%)
All	All	0.58	3/42597 (0.0%)	1.06	81/58188 (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
35	i	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	29	LYS	C-N	6.71	1.39	1.33
22	V	105	GLU	C-N	5.37	1.39	1.33
31	e	92	THR	C-N	5.11	1.39	1.33

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	i	30	ARG	O-C-N	-38.45	60.90	122.41
35	i	30	ARG	N-CA-C	-11.66	99.32	113.19
8	H	216	ALA	O-C-N	10.44	136.47	122.59
4	D	36	VAL	N-CA-C	9.87	121.36	110.21
5	E	166	PRO	CA-N-CD	-9.55	98.63	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	149	CYS	Peptide
35	i	30	ARG	Mainchain

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	806	0	789	8	0
2	B	1159	0	1166	15	0
3	C	1684	0	1610	65	0
4	D	3301	0	3185	78	0
5	E	959	0	509	76	0
6	F	2356	0	1535	9	0
7	G	3614	0	1337	14	0
8	H	2389	0	2462	60	0
9	I	1366	0	1286	11	0
10	J	1211	0	1165	10	0
11	K	720	0	761	19	0
12	L	4538	0	4480	37	0
13	M	3536	0	3652	39	0
14	N	2592	0	2631	47	0
15	O	1854	0	1139	3	0
16	P	1675	0	354	0	0
17	Q	565	0	122	2	0
18	R	501	0	246	3	0
19	S	405	0	197	1	0
20	T	378	0	176	0	0
21	U	432	0	207	0	0
22	V	685	0	563	28	0
23	W	817	0	743	25	0
24	X	1133	0	838	3	0
25	Y	1011	0	1018	5	0
26	Z	921	0	656	6	0
27	a	480	0	440	1	0
28	b	519	0	407	2	0
29	c	320	0	277	0	0
30	d	790	0	598	1	0
31	e	616	0	506	29	0
32	f	350	0	260	6	0
33	g	677	0	559	33	0
34	h	770	0	402	15	0
35	i	616	0	298	7	0
36	j	260	0	55	0	0
37	k	370	0	77	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	l	590	0	121	0	0
39	m	887	0	781	2	0
40	n	1088	0	768	1	0
41	o	296	0	134	0	0
42	p	1039	0	583	3	0
43	q	696	0	338	4	0
44	r	435	0	95	2	0
45	s	175	0	39	0	0
46	B	8	0	0	0	0
46	F	8	0	0	0	0
46	G	16	0	0	0	0
46	I	16	0	0	0	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	0	0
49	P	48	0	25	0	0
50	R	1	0	0	0	0
All	All	51718	0	39609	558	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 6.

The worst 5 of 558 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)
4:D:31:PRO:HG3	14:N:174:GLN:NE2	1.12	1.45
3:C:39:GLN:NE2	22:V:107:PRO:HD3	1.32	1.44
4:D:31:PRO:CG	14:N:174:GLN:NE2	1.75	1.43
4:D:31:PRO:CG	14:N:174:GLN:HE22	1.26	1.41
5:E:15:ASN:C	5:E:17:PRO:HD3	1.49	1.35

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	109/111 (98%)	89 (82%)	17 (16%)	3 (3%)	4	24
2	B	145/147 (99%)	125 (86%)	14 (10%)	6 (4%)	2	18
3	C	204/206 (99%)	174 (85%)	23 (11%)	7 (3%)	3	21
4	D	424/426 (100%)	367 (87%)	40 (9%)	17 (4%)	2	18
5	E	184/249 (74%)	158 (86%)	11 (6%)	15 (8%)	0	9
6	F	423/464 (91%)	374 (88%)	40 (10%)	9 (2%)	5	30
7	G	201/715 (28%)	168 (84%)	26 (13%)	7 (4%)	3	20
8	H	311/313 (99%)	277 (89%)	21 (7%)	13 (4%)	2	17
9	I	174/176 (99%)	144 (83%)	18 (10%)	12 (7%)	1	11
10	J	169/171 (99%)	147 (87%)	17 (10%)	5 (3%)	3	23
11	K	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	5	29
12	L	602/604 (100%)	537 (89%)	50 (8%)	15 (2%)	4	26
13	M	455/457 (100%)	413 (91%)	29 (6%)	13 (3%)	3	23
14	N	342/344 (99%)	305 (89%)	30 (9%)	7 (2%)	6	31
15	O	227/314 (72%)	201 (88%)	19 (8%)	7 (3%)	3	22
18	R	34/89 (38%)	28 (82%)	6 (18%)	0	100	100
19	S	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
20	T	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	9	39
21	U	83/85 (98%)	74 (89%)	7 (8%)	2 (2%)	4	27
22	V	104/116 (90%)	88 (85%)	10 (10%)	6 (6%)	1	14
23	W	109/128 (85%)	90 (83%)	12 (11%)	7 (6%)	1	13
24	X	108/169 (64%)	96 (89%)	8 (7%)	4 (4%)	2	20
25	Y	136/138 (99%)	122 (90%)	8 (6%)	6 (4%)	2	17
26	Z	69/138 (50%)	65 (94%)	4 (6%)	0	100	100
27	a	62/70 (89%)	55 (89%)	4 (6%)	3 (5%)	2	16
28	b	44/80 (55%)	41 (93%)	3 (7%)	0	100	100
29	c	44/76 (58%)	39 (89%)	2 (4%)	3 (7%)	1	12
30	d	69/114 (60%)	65 (94%)	3 (4%)	1 (1%)	9	39
31	e	87/106 (82%)	76 (87%)	9 (10%)	2 (2%)	5	28
32	f	52/57 (91%)	44 (85%)	5 (10%)	3 (6%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	g	95/154 (62%)	64 (67%)	19 (20%)	12 (13%)	0	4
34	h	38/186 (20%)	35 (92%)	0	3 (8%)	1	10
35	i	25/121 (21%)	23 (92%)	0	2 (8%)	1	9
39	m	96/118 (81%)	83 (86%)	7 (7%)	6 (6%)	1	13
40	n	126/166 (76%)	113 (90%)	10 (8%)	3 (2%)	4	27
41	o	56/58 (97%)	55 (98%)	0	1 (2%)	6	33
42	p	67/169 (40%)	60 (90%)	4 (6%)	3 (4%)	2	17
43	q	136/138 (99%)	109 (80%)	18 (13%)	9 (7%)	1	12
All	All	5854/7423 (79%)	5134 (88%)	505 (9%)	215 (4%)	4	20

5 of 215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	150	PRO
3	C	9	PRO
4	D	35	ASP
4	D	53	PRO
4	D	258	VAL

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	75/97 (77%)	66 (88%)	9 (12%)	5	19
2	B	124/124 (100%)	118 (95%)	6 (5%)	23	45
3	C	179/187 (96%)	169 (94%)	10 (6%)	19	41
4	D	338/368 (92%)	324 (96%)	14 (4%)	27	49
5	E	21/205 (10%)	21 (100%)	0	100	100
6	F	84/368 (23%)	81 (96%)	3 (4%)	31	52
7	G	64/196 (33%)	61 (95%)	3 (5%)	23	45
8	H	249/270 (92%)	234 (94%)	15 (6%)	17	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	138/151 (91%)	129 (94%)	9 (6%)	15	38
10	J	112/139 (81%)	109 (97%)	3 (3%)	39	59
11	K	83/83 (100%)	79 (95%)	4 (5%)	23	45
12	L	463/532 (87%)	445 (96%)	18 (4%)	28	50
13	M	384/411 (93%)	373 (97%)	11 (3%)	37	58
14	N	277/313 (88%)	265 (96%)	12 (4%)	26	48
15	O	84/205 (41%)	82 (98%)	2 (2%)	43	63
18	R	17/26 (65%)	15 (88%)	2 (12%)	5	19
19	S	4/72 (6%)	4 (100%)	0	100	100
20	T	3/69 (4%)	3 (100%)	0	100	100
21	U	5/79 (6%)	5 (100%)	0	100	100
22	V	47/102 (46%)	47 (100%)	0	100	100
23	W	71/114 (62%)	69 (97%)	2 (3%)	38	59
24	X	83/103 (81%)	82 (99%)	1 (1%)	63	73
25	Y	99/99 (100%)	99 (100%)	0	100	100
26	Z	59/59 (100%)	58 (98%)	1 (2%)	53	67
27	a	41/59 (70%)	40 (98%)	1 (2%)	43	63
28	b	36/36 (100%)	35 (97%)	1 (3%)	38	59
29	c	26/68 (38%)	26 (100%)	0	100	100
30	d	56/60 (93%)	55 (98%)	1 (2%)	51	66
31	e	45/96 (47%)	45 (100%)	0	100	100
32	f	22/54 (41%)	21 (96%)	1 (4%)	24	46
33	g	51/131 (39%)	51 (100%)	0	100	100
34	h	28/73 (38%)	27 (96%)	1 (4%)	31	52
35	i	20/32 (62%)	20 (100%)	0	100	100
39	m	75/86 (87%)	74 (99%)	1 (1%)	61	72
40	n	65/117 (56%)	65 (100%)	0	100	100
41	o	5/56 (9%)	5 (100%)	0	100	100
42	p	50/62 (81%)	49 (98%)	1 (2%)	48	65
43	q	9/124 (7%)	9 (100%)	0	100	100
All	All	3592/5426 (66%)	3460 (96%)	132 (4%)	31	51

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

Mol	Chain	Res	Type
14	N	201	THR
18	R	73	ILE
39	m	94	ILE
8	H	28	LEU
8	H	13	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	97	GLN
27	a	31	ASN
15	O	120	GLN
24	X	94	GLN
30	d	59	HIS

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	$\#\|Z\| > 2$
46	SF4	G	801	7	0,12,12	-	-	-		
46	SF4	B	201	2	0,12,12	-	-	-		
47	FES	G	803	7	0,4,4	-	-	-		
46	SF4	F	502	6	0,12,12	-	-	-		
46	SF4	I	201	9	0,12,12	-	-	-		
46	SF4	G	802	7	0,12,12	-	-	-		
46	SF4	I	202	9	0,12,12	-	-	-		
47	FES	E	301	5	0,4,4	-	-	-		
48	FMN	F	501	-	33,33,33	1.64	5 (15%)	48,50,50	1.40	7 (14%)
49	NAP	P	501	-	49,52,52	1.17	5 (10%)	69,80,80	1.69	12 (17%)

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
46	SF4	G	801	7	-	-	0/6/5/5
46	SF4	B	201	2	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
46	SF4	F	502	6	-	-	0/6/5/5
46	SF4	I	201	9	-	-	0/6/5/5
46	SF4	G	802	7	-	-	0/6/5/5
46	SF4	I	202	9	-	-	0/6/5/5
47	FES	E	301	5	-	-	0/1/1/1
48	FMN	F	501	-	-	10/18/18/18	0/3/3/3
49	NAP	P	501	-	-	6/35/67/67	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	F	501	FMN	C9A-C5A	5.77	1.50	1.41
49	P	501	NAP	C5A-C4A	4.83	1.48	1.39
48	F	501	FMN	C8-C7	3.93	1.50	1.40
49	P	501	NAP	C5A-C6A	2.96	1.49	1.41
48	F	501	FMN	C4A-N5	2.57	1.35	1.30

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	501	NAP	C5A-C4A-N3A	-6.16	118.71	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	501	NAP	N3A-C4A-N9A	4.82	135.03	127.08
49	P	501	NAP	C2A-N3A-C4A	4.06	121.35	111.75
49	P	501	NAP	N3A-C2A-N1A	-3.55	123.05	128.60
49	P	501	NAP	PN-O3-PA	-3.47	120.93	132.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

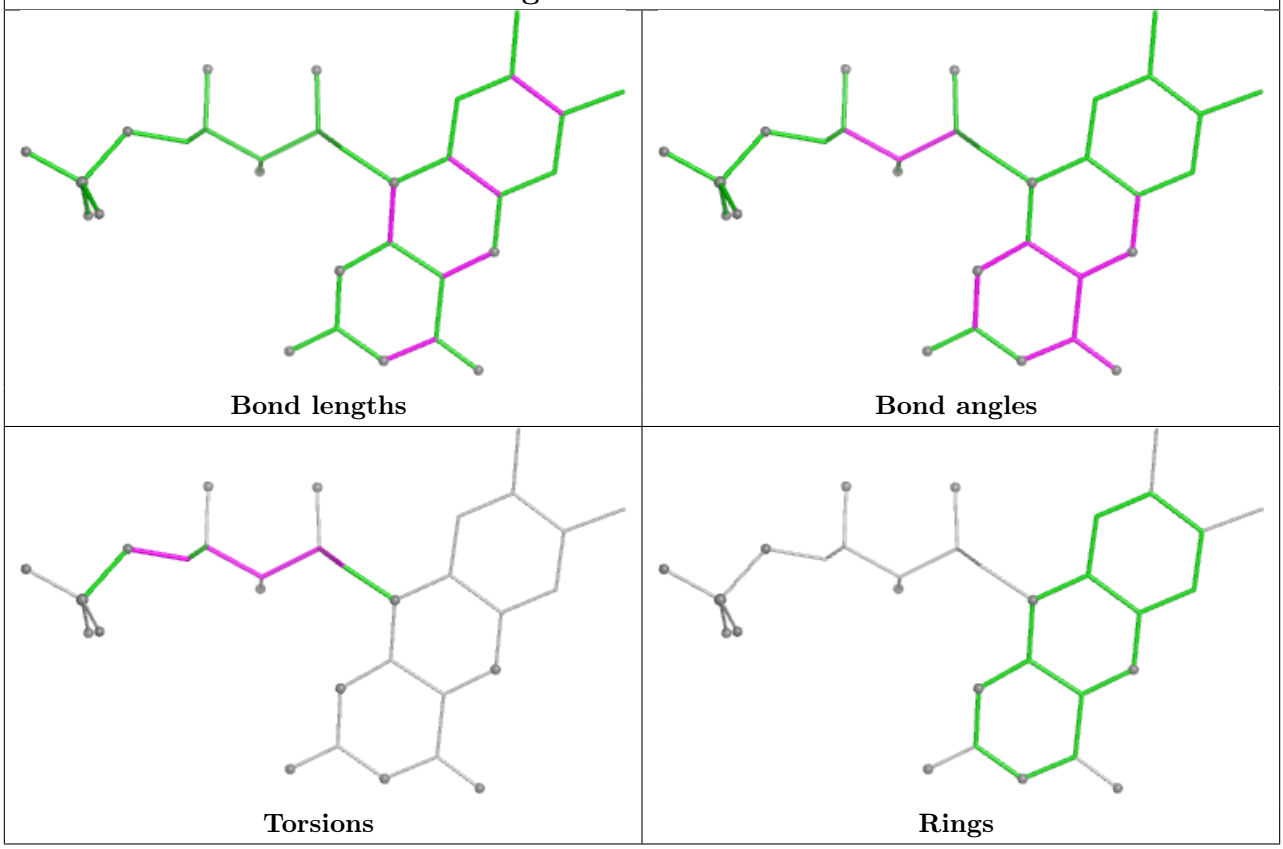
Mol	Chain	Res	Type	Atoms
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C1'-C2'-C3'-O3'
48	F	501	FMN	C1'-C2'-C3'-C4'
49	P	501	NAP	C2N-C3N-C7N-O7N

There are no ring outliers.

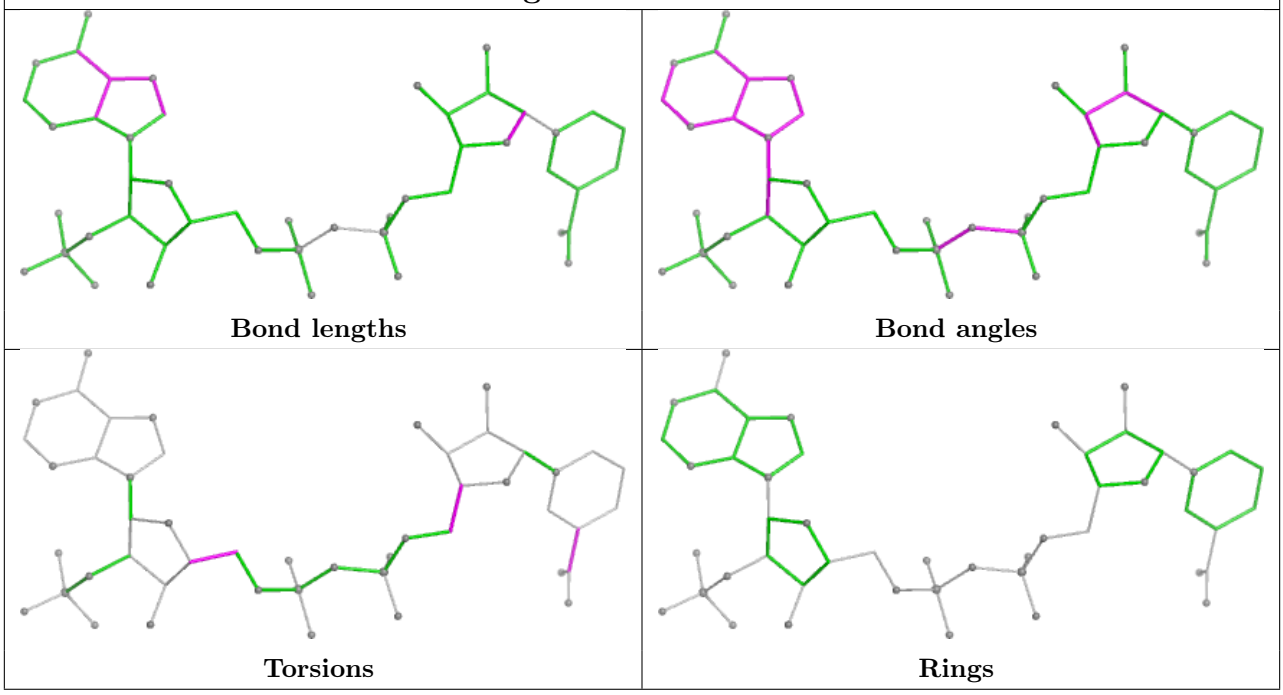
No monomer is involved in short contacts.

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 FMN F 501



Ligand NAP P 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
44	r	1
35	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	23.03
1	i	32:PRO	C	40:UNK	N	15.86

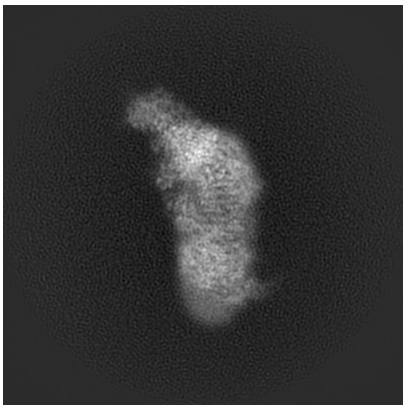
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4032. These allow visual inspection of the internal detail of the map and identification of artifacts.

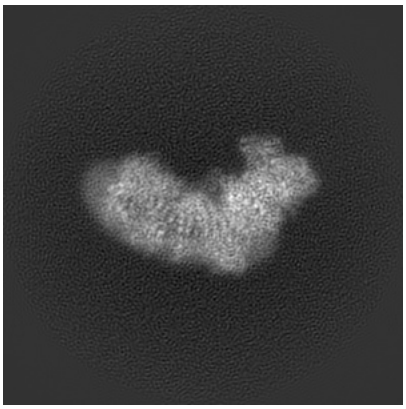
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

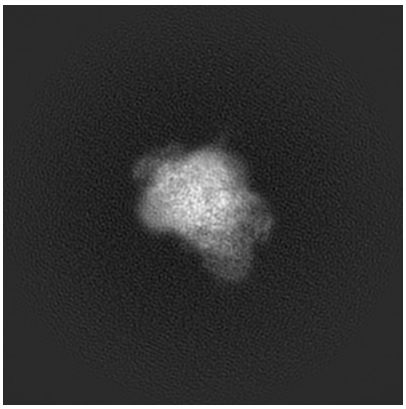
6.1.1 Primary map



X

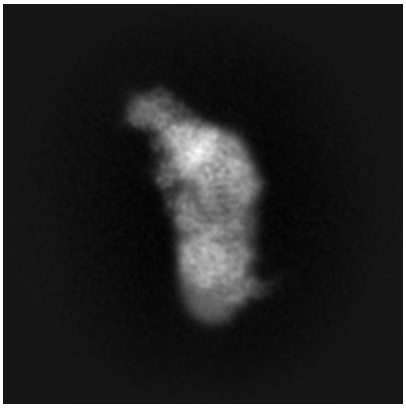


Y

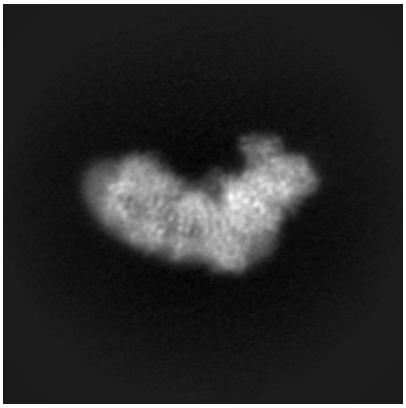


Z

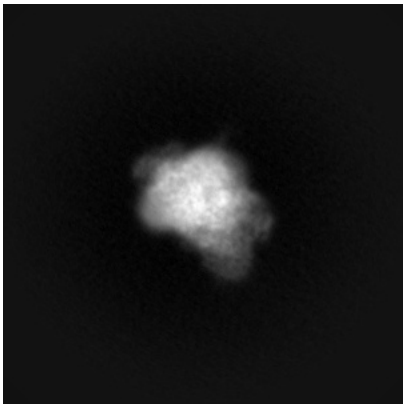
6.1.2 Raw map



X



Y

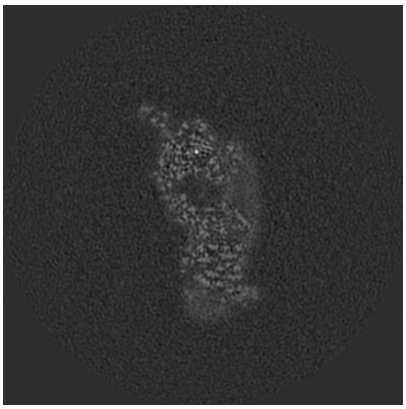


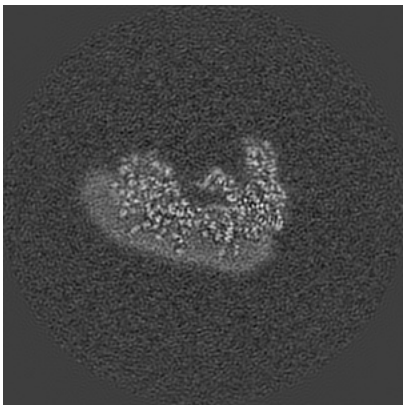
Z

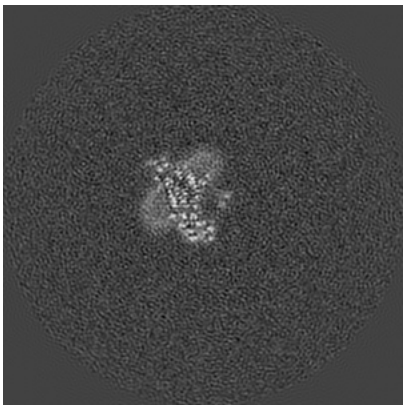
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

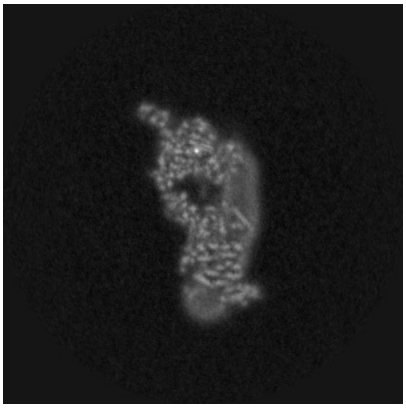
6.2.1 Primary map

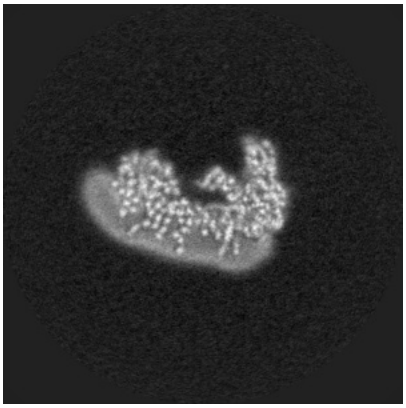

X Index: 180

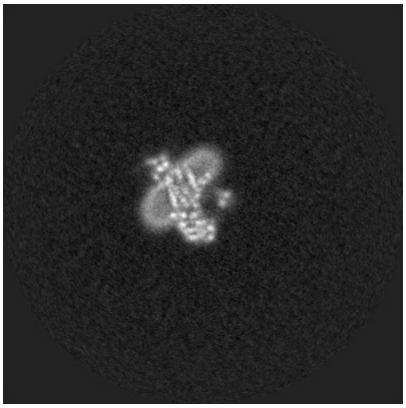

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180


Y Index: 180

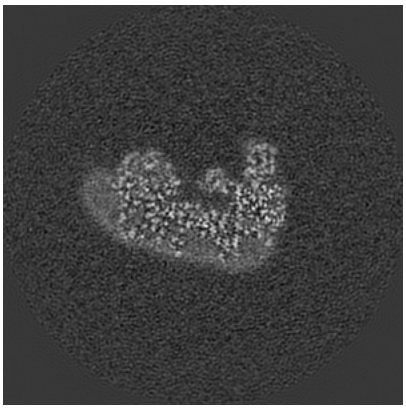

Z Index: 180

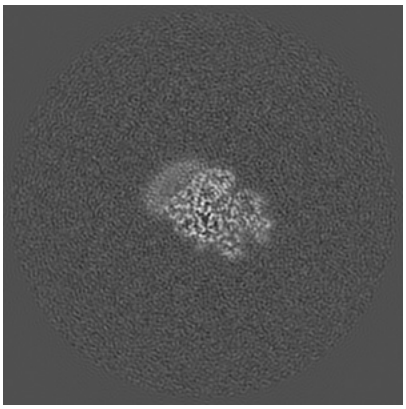
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

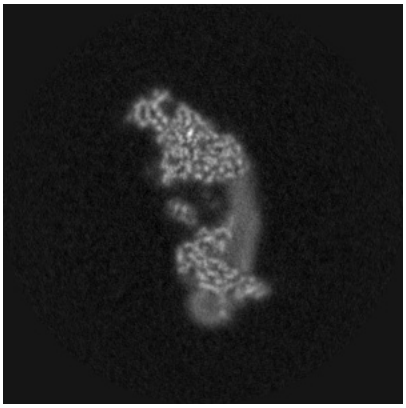
6.3.1 Primary map

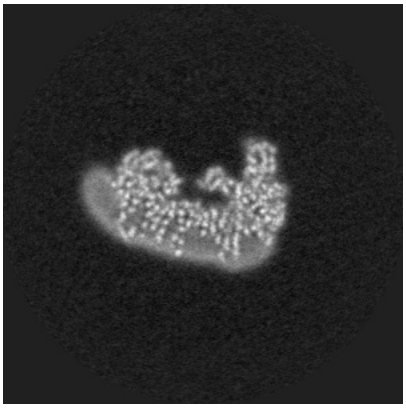
X Index: 189

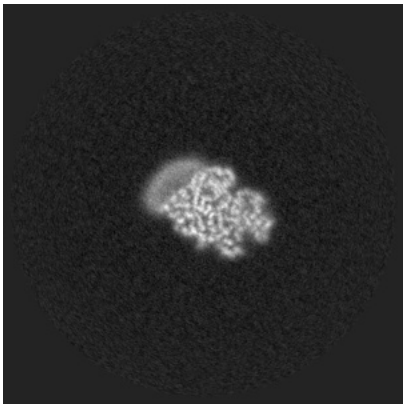

Y Index: 183


Z Index: 232

6.3.2 Raw map


X Index: 190

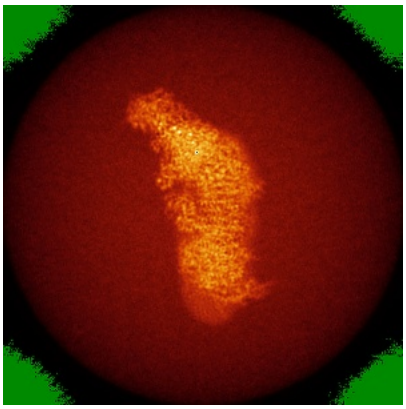

Y Index: 183

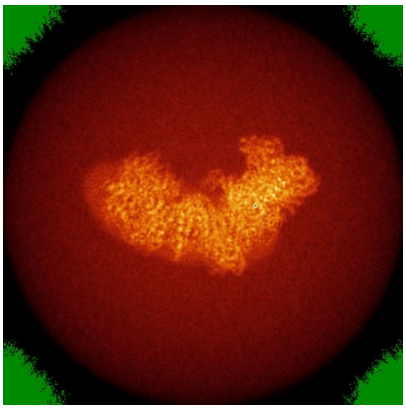

Z Index: 232

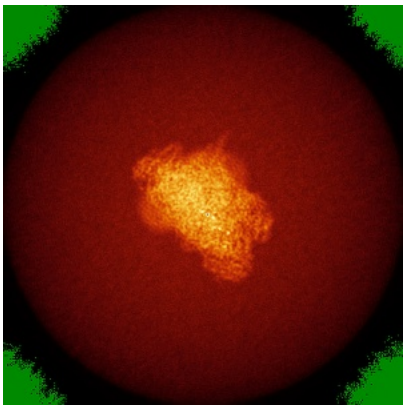
The images above show the largest variance slices of the map in three orthogonal directions.

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

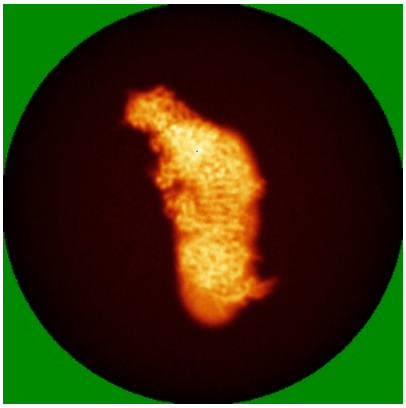
6.4.1 Primary map

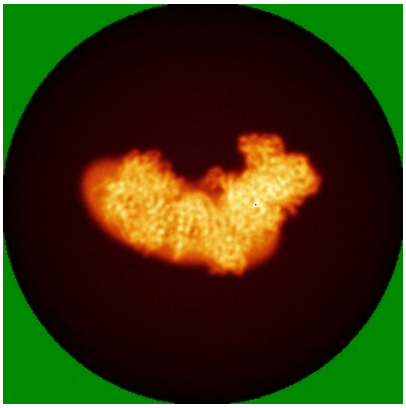

X

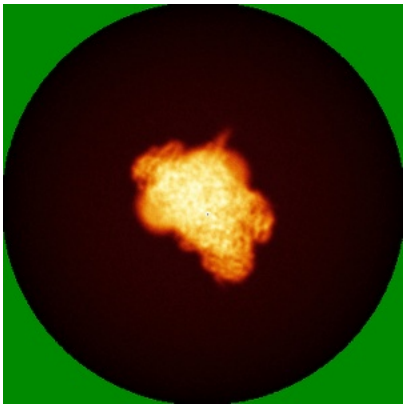

Y


Z

6.4.2 Raw map


X

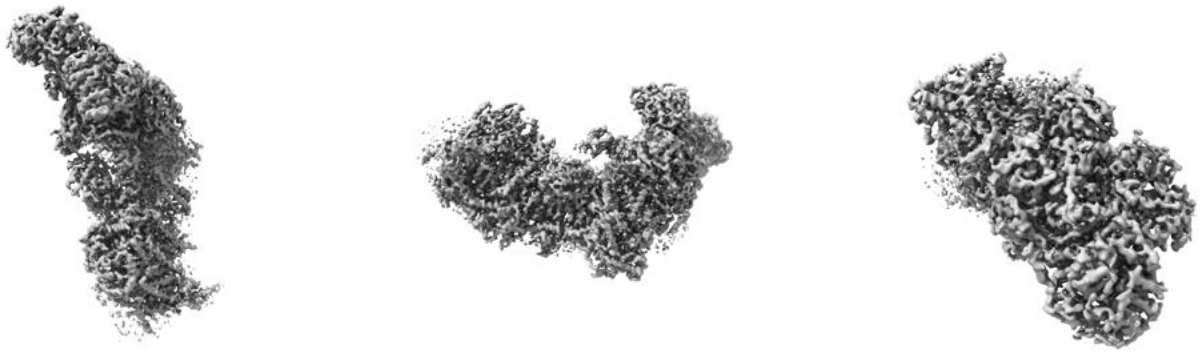

Y


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 0.165. 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.

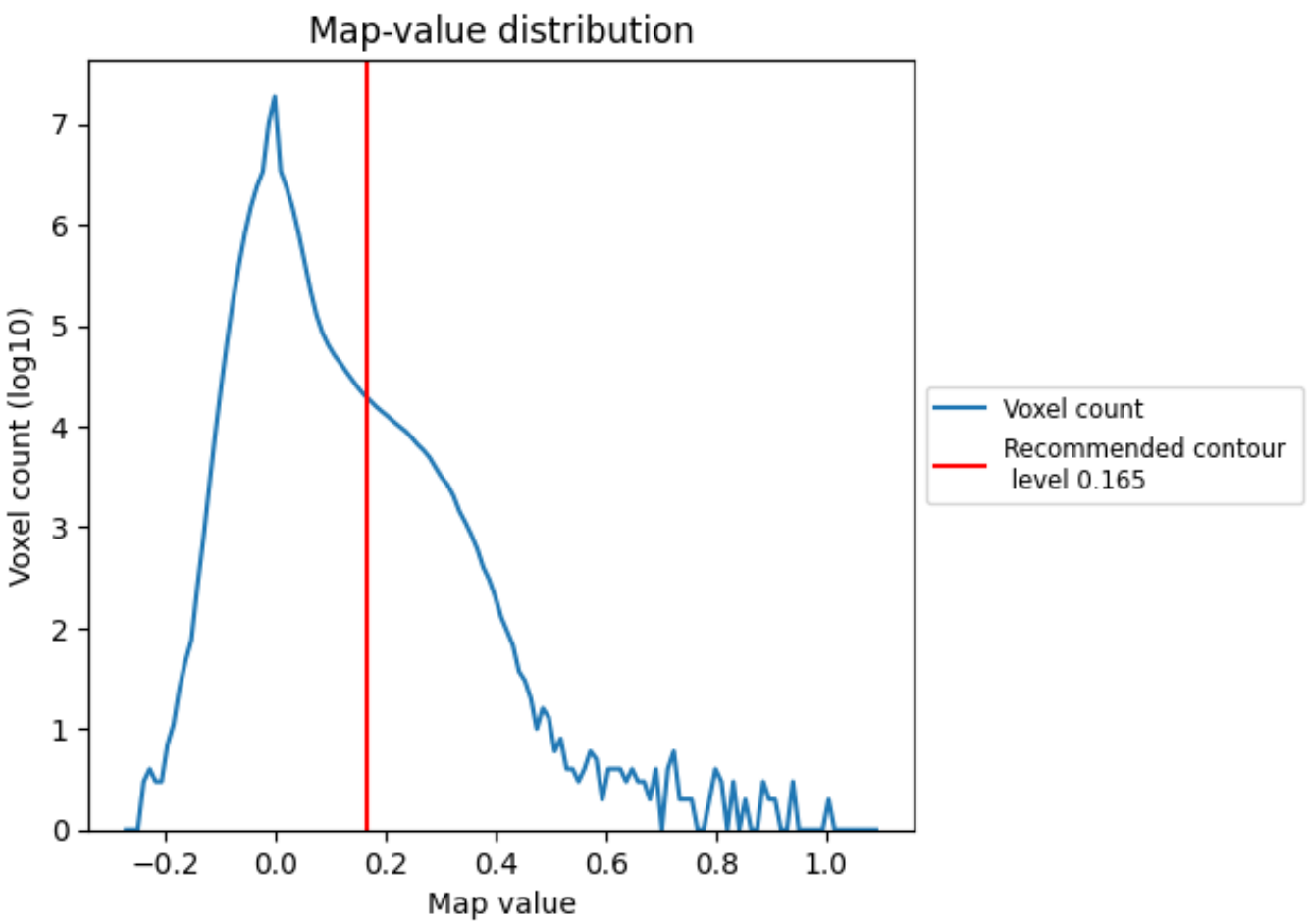
6.6 Mask visualisation (i)

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

7 Map analysis (i)

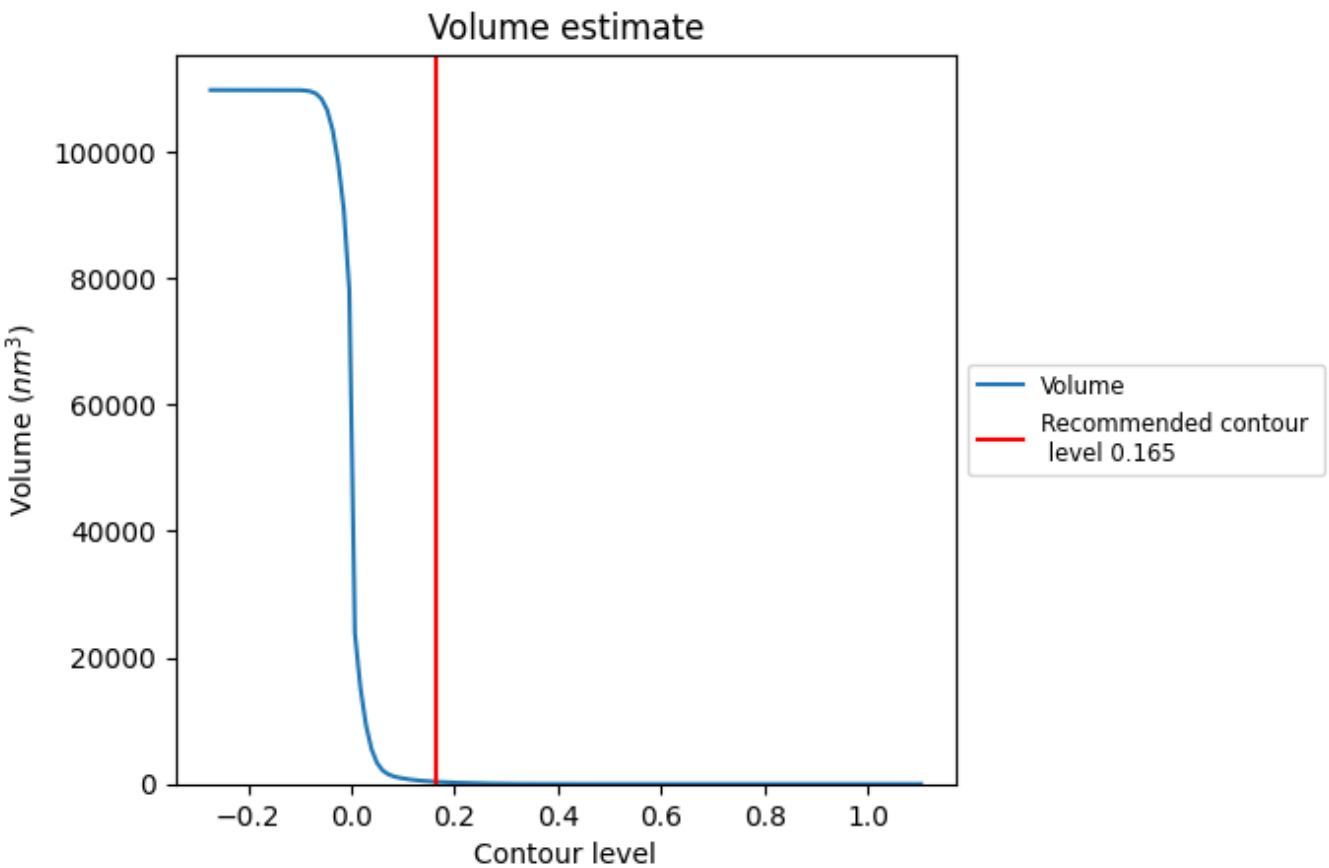
This section contains the results of statistical analysis of the map.

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.

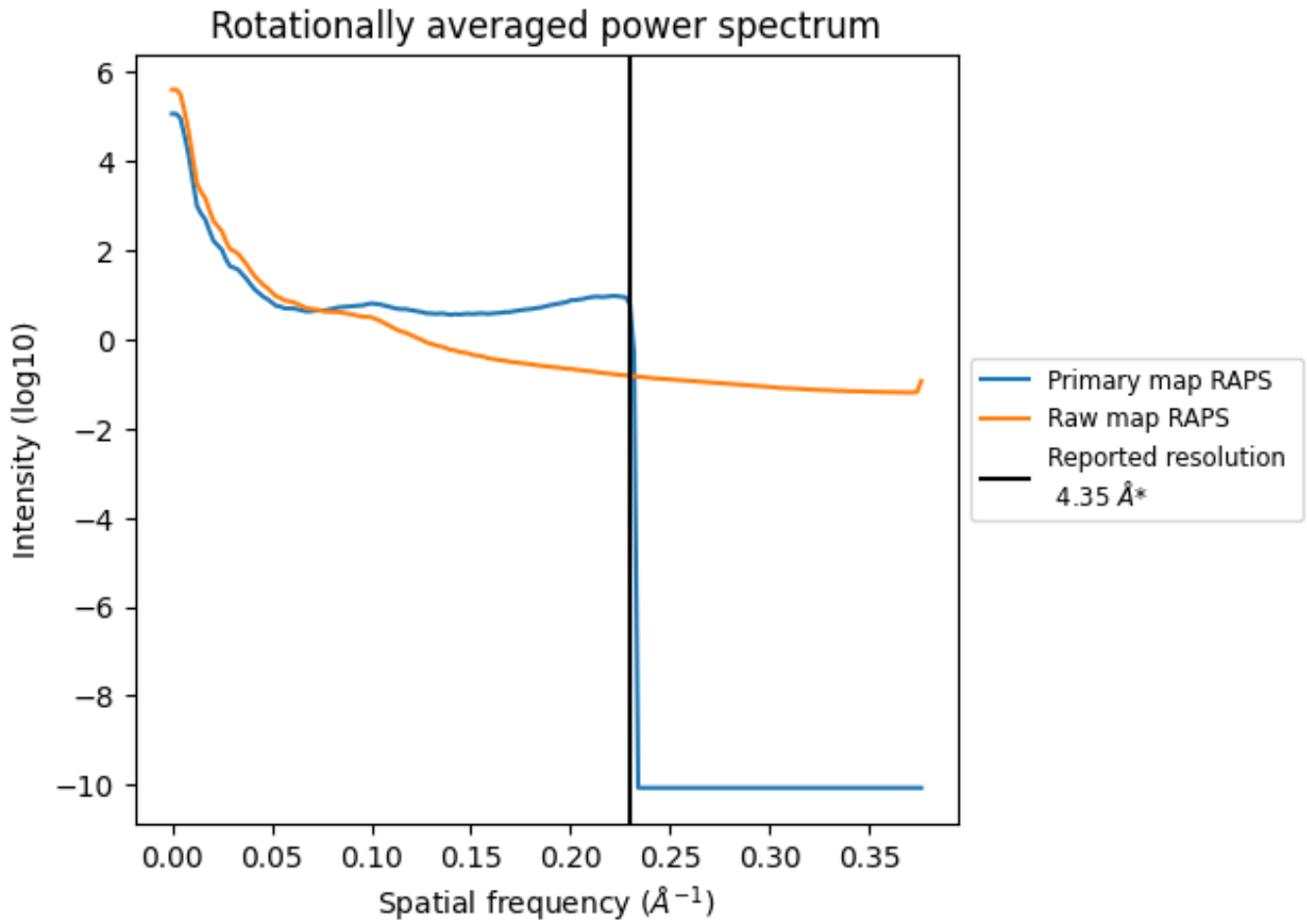
7.2 Volume estimate (i)



The volume at the recommended contour level is 339 nm^3; this corresponds to an approximate mass of 306 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)

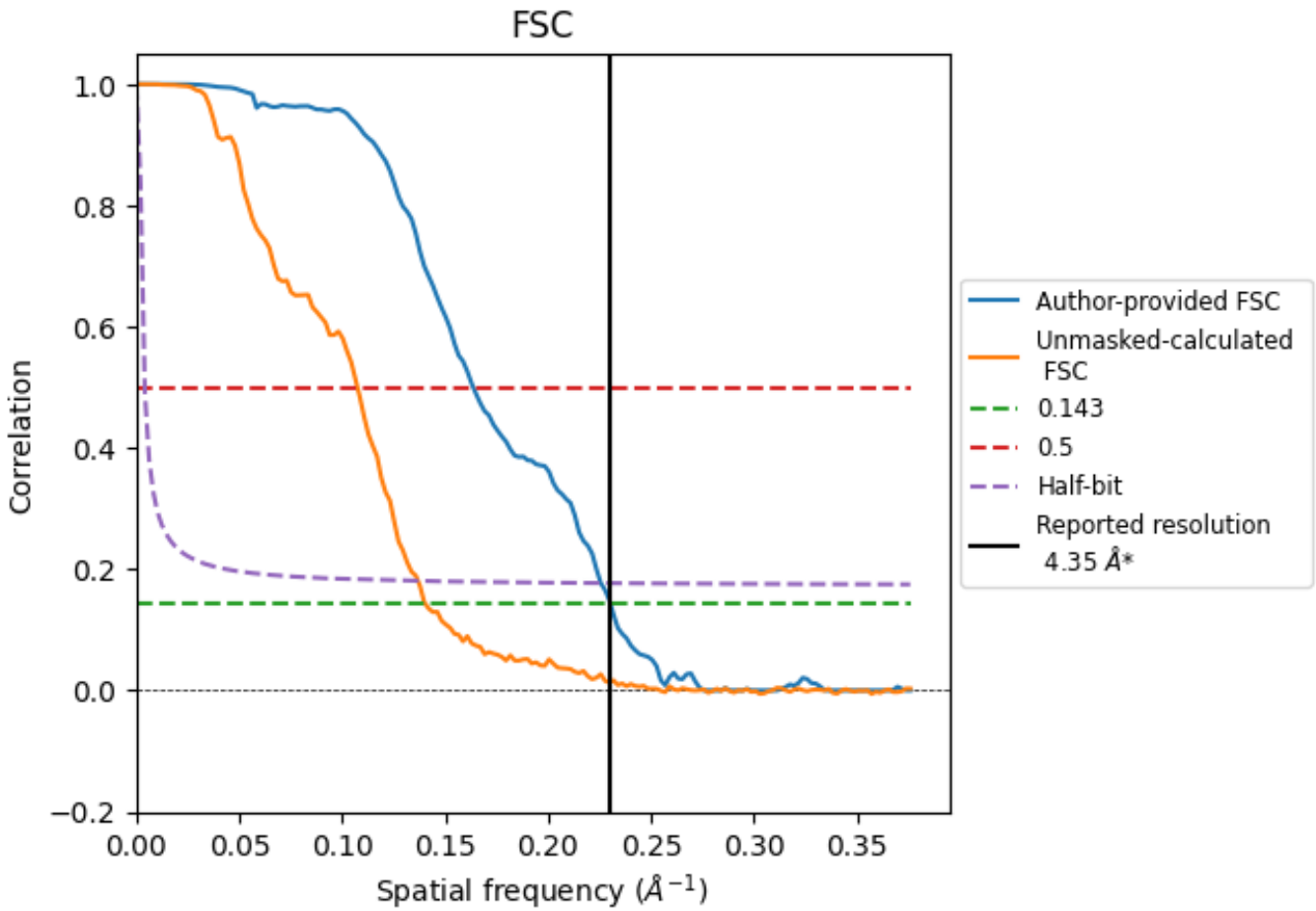


*Reported resolution corresponds to spatial frequency of 0.230 Å^{-1}

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 0.230 Å^{-1}

8.2 Resolution estimates (i)

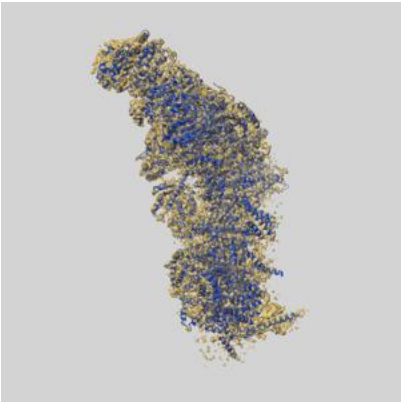
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.35	-	-
Author-provided FSC curve	4.34	6.11	4.43
Unmasked-calculated*	7.12	9.31	7.31

*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 7.12 differs from the reported value 4.35 by more than 10 %

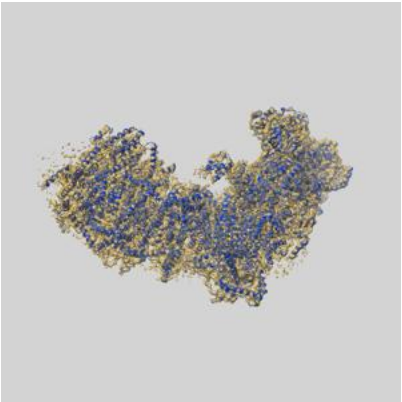
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4032 and PDB model 5LC5. Per-residue inclusion information can be found in section 3 on page 16.

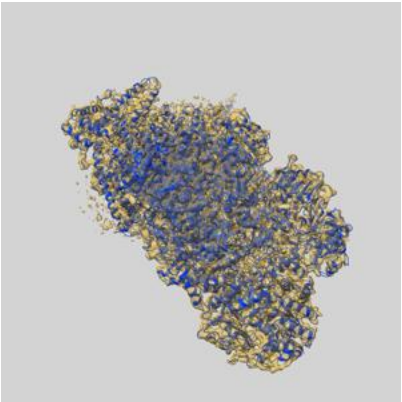
9.1 Map-model overlay (i)



X



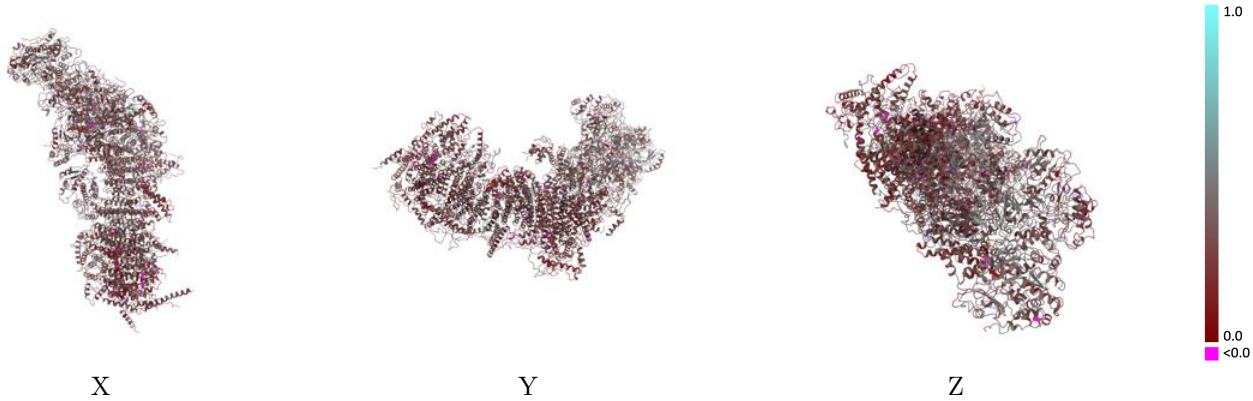
Y



Z

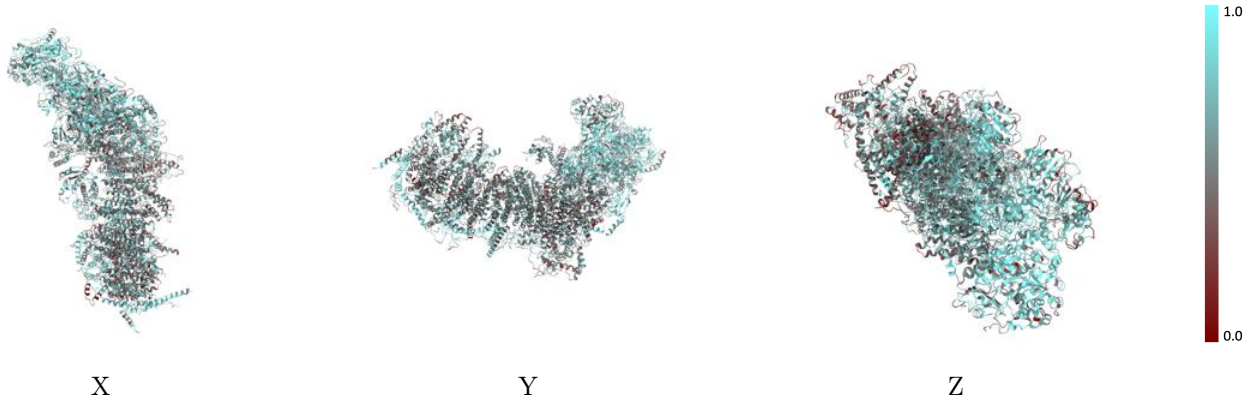
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



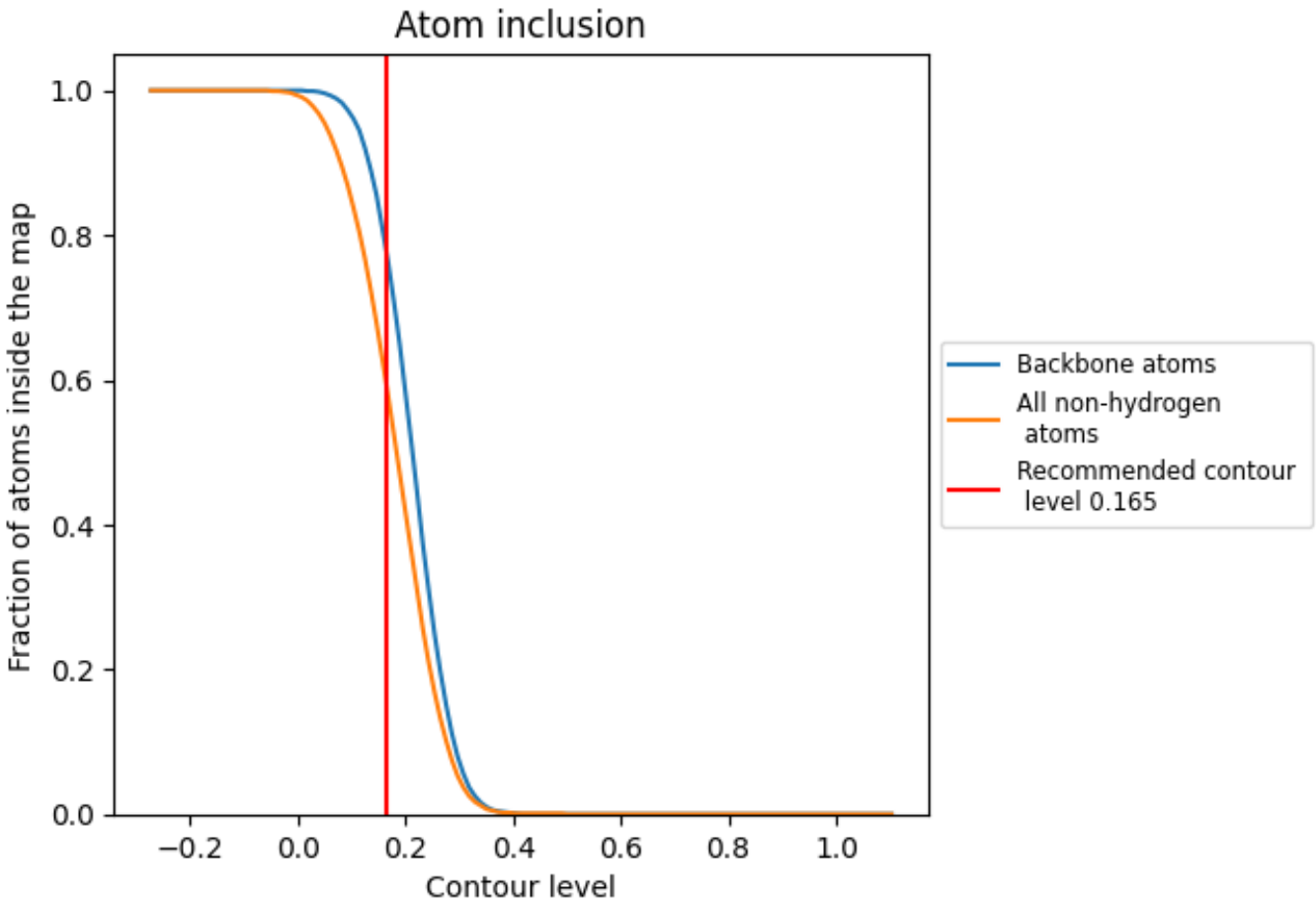
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.165).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 59% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5920	0.3110
A	0.5310	0.2970
B	0.6130	0.3240
C	0.5710	0.2990
D	0.6010	0.3280
E	0.7370	0.3690
F	0.6420	0.3220
G	0.6820	0.3610
H	0.5330	0.2910
I	0.5970	0.3030
J	0.4810	0.2690
K	0.5240	0.2960
L	0.5120	0.2700
M	0.5520	0.3010
N	0.5850	0.3200
O	0.6410	0.3340
P	0.6960	0.3680
Q	0.7770	0.3960
R	0.7100	0.3880
S	0.5930	0.2880
T	0.5420	0.3040
U	0.6690	0.3450
V	0.5530	0.2990
W	0.5570	0.3100
X	0.4960	0.2690
Y	0.4550	0.2540
Z	0.5380	0.2580
a	0.5250	0.2540
b	0.4710	0.2790
c	0.5330	0.2630
d	0.6060	0.3260
e	0.5850	0.3260
f	0.4650	0.2800
g	0.5230	0.2670
h	0.6900	0.3310

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Chain	Atom inclusion	Q-score
i	0.5490	0.2820
j	0.7120	0.3590
k	0.5350	0.3100
l	0.7150	0.3460
m	0.5370	0.2890
n	0.5770	0.2810
o	0.7400	0.2700
p	0.6510	0.3100
q	0.7500	0.3680
r	0.7200	0.3790
s	0.7890	0.3870