wwPDB EM Validation Summary Report

Sep 9, 2026 – 12:19 am BST

PDB ID	:	6QC9 / pdb_00006qc9
EMDB ID	:	EMD-4501
Title	:	Ovine respiratory complex I FRC open class 4
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-27
Resolution	:	5.70 Å(reported)
Based on initial model	:	5LNK

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

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

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

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

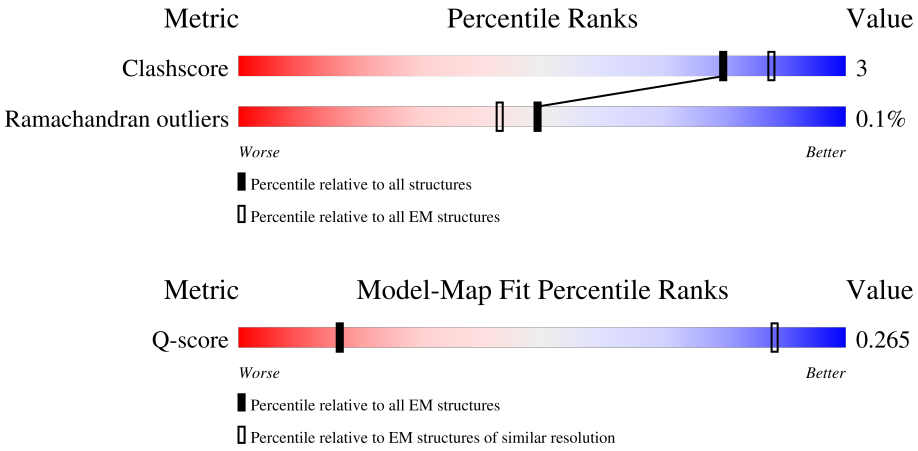
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 5.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	503 (5.20 - 6.20)

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

Mol	Chain	Length	Quality of chain
1	V1	445	16% 93%
2	V2	217	19% 92% 5%
3	S1	704	24% 93% 5%
4	S2	430	35% 96%
5	S3	228	20% 87% 9%

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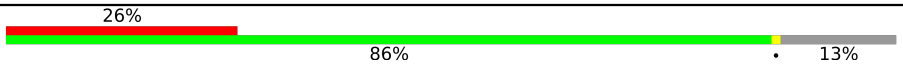
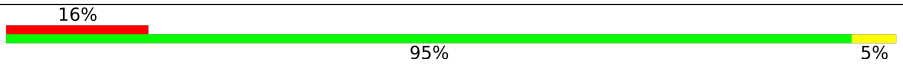
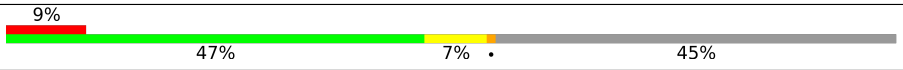
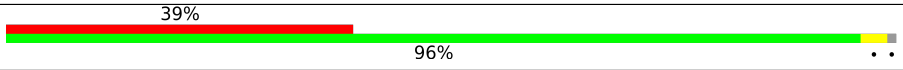
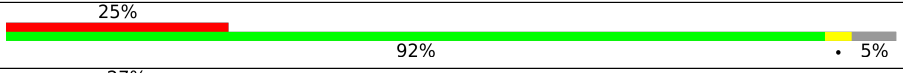
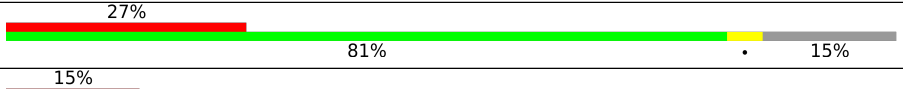
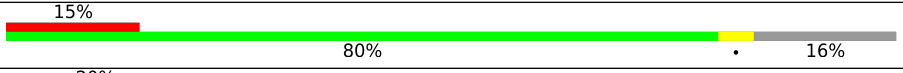
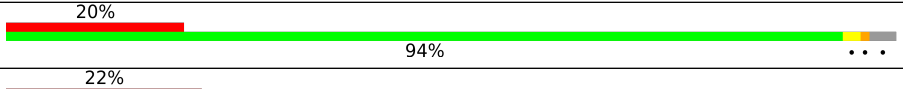
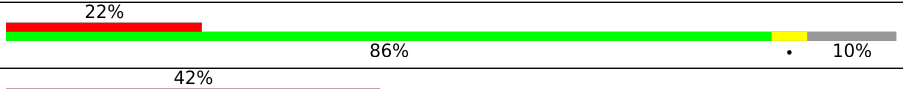
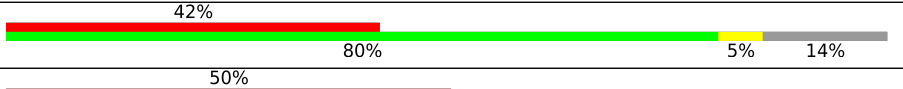
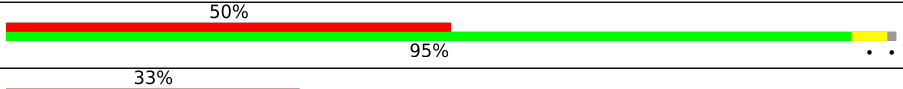
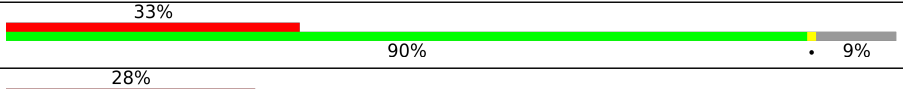
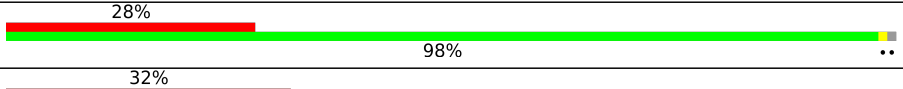
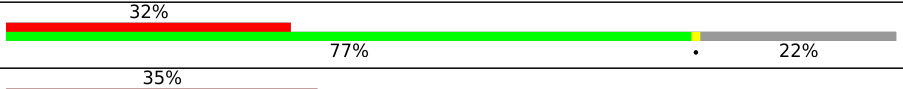
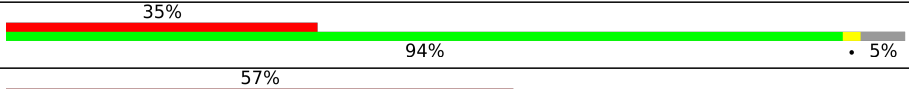
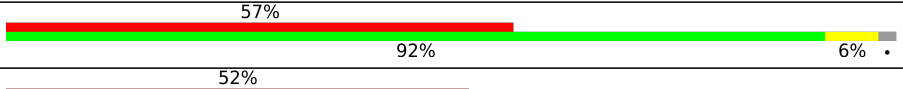
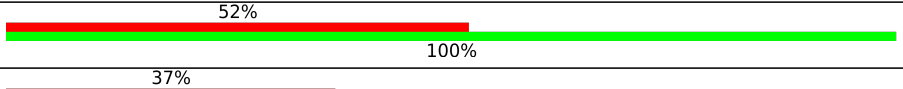
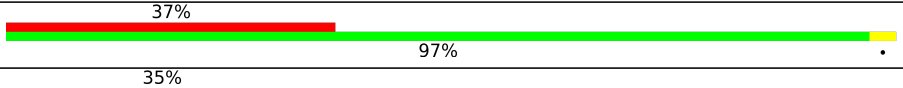
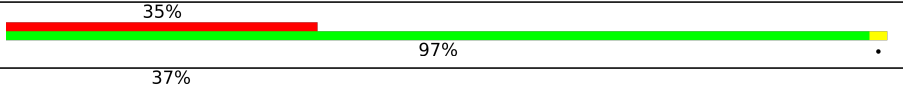
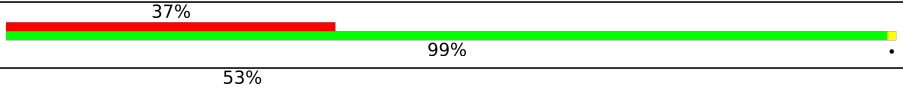
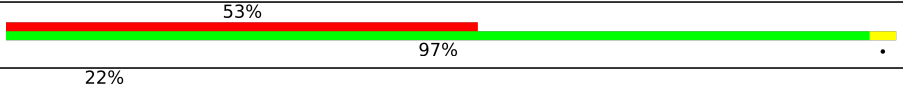
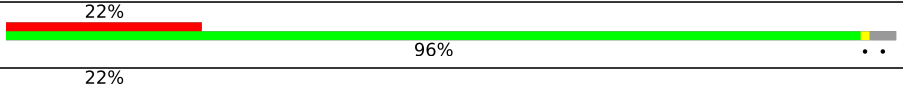
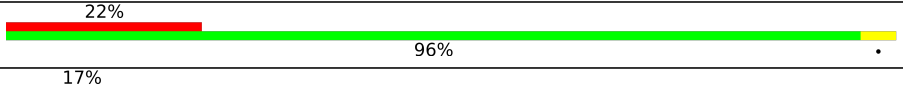
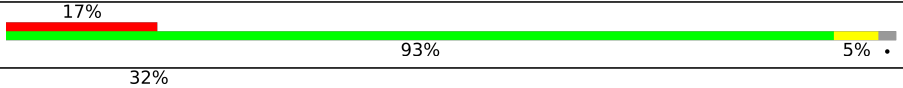
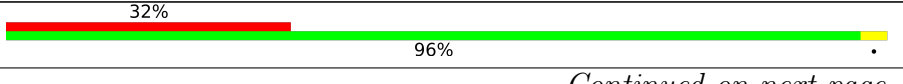
Mol	Chain	Length	Quality of chain
6	S7	179	
7	S8	176	
8	V3	75	
9	S6	96	
10	S4	133	
11	A9	338	
12	A2	98	
13	A5	115	
14	A6	127	
15	A7	112	
16	AL	145	
17	AA	88	
17	AB	88	
18	D3	115	
19	D1	318	
20	D6	175	
21	4L	98	
22	D5	606	
23	D4	459	
24	D2	347	
25	AK	140	
26	B5	143	
27	A8	171	
28	BJ	175	
29	AJ	320	

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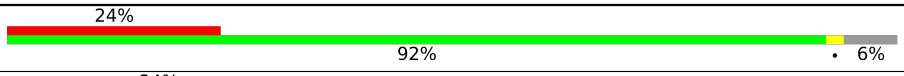
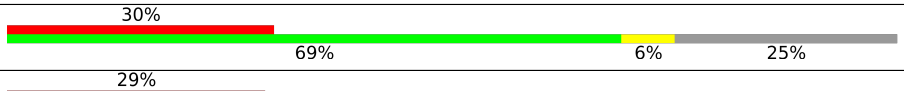
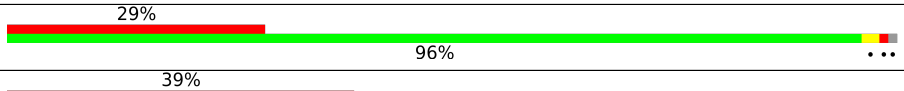
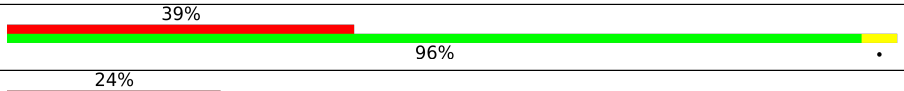
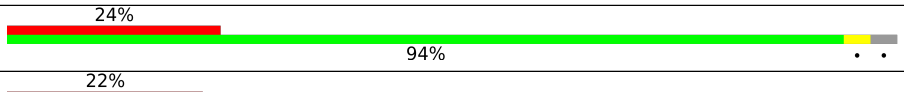
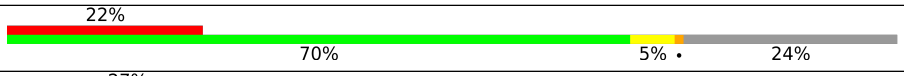
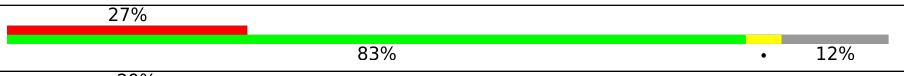
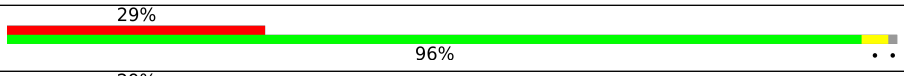
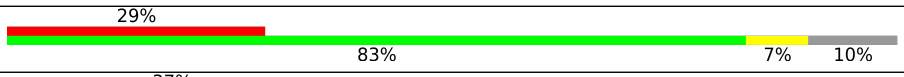
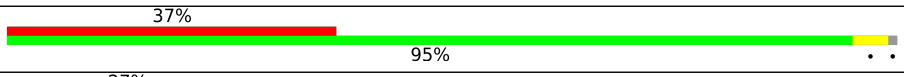
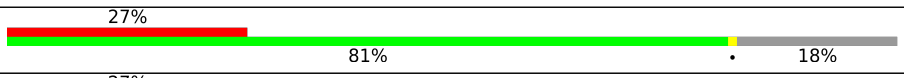
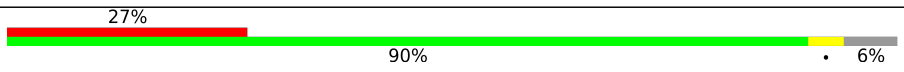
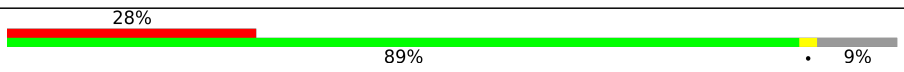
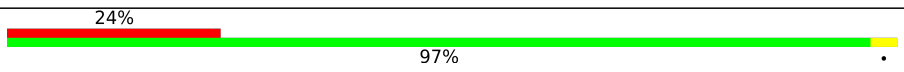
Mol	Chain	Length	Quality of chain
30	S5	105	
31	A3	83	
32	B3	97	
33	C2	120	
34	B4	128	
35	AM	143	
36	B6	127	
37	B7	136	
38	B9	178	
39	B2	72	
40	B8	158	
41	BK	125	
42	C1	49	
43	B1	57	
44	A1	70	

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 40144 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	V1	430	Total 2099	C 1239	N 430	O 430	0	0

- Molecule 2 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	V2	212	Total 1045	C 621	N 212	O 212	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	S1	688	Total 3390	C 2014	N 688	O 688	0	0

- Molecule 4 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	S2	424	Total 2090	C 1242	N 424	O 424	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	S3	208	Total 1034	C 618	N 208	O 208	0	0

- Molecule 6 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	S7	156	Total 769	C 457	N 156	O 156	0	0

- Molecule 7 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	S8	176	Total 871	C 519	N 176	O 176	0	0

- Molecule 8 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	V3	41	Total 204	C 122	N 41	O 41	0	0

- Molecule 9 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	S6	95	Total 462	C 272	N 95	O 95	0	0

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	S4	126	Total 625	C 373	N 126	O 126	0	0

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	A9	287	Total 1413	C 839	N 287	O 287	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	A2	82	Total 406	C 242	N 82	O 82	0	0

- Molecule 13 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	A5	111	Total 550	C 328	N 111	O 111	0	0

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	A6	114	Total 567	C 339	N 114	O 114	0	0

- Molecule 15 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	A7	96	Total 476	C 284	N 96	O 96	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	AL	144	Total 708	C 420	N 144	O 144	0	0

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AA	80	Total 397	C 237	N 80	O 80	0	0
17	AB	87	Total 432	C 258	N 87	O 87	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	D3	90	Total 449	C 269	N 90	O 90	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	D1	303	Total 1505	C 899	N 303	O 303	0	0

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	D6	171	Total 829	C 487	N 171	O 171	0	0

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	4L	98	Total	C	N	O	0	0
			486	290	98	98		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	D5	606	Total	C	N	O	0	0
			3001	1789	606	606		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	D4	459	Total	C	N	O	0	0
			2277	1359	459	459		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	D2	347	Total	C	N	O	0	0
			1721	1027	347	347		

- Molecule 25 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	AK	140	Total	C	N	O	0	0
			682	402	140	140		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	B5	139	Total	C	N	O	0	0
			687	409	139	139		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	A8	171	Total	C	N	O	0	0
			847	505	171	171		

- Molecule 28 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BJ	171	Total 853	C 511	N 171	O 171	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	AJ	319	Total 1575	C 937	N 319	O 319	0	0

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	S5	99	Total 490	C 292	N 99	O 99	0	0

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	A3	74	Total 367	C 219	N 74	O 74	0	0

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	B3	73	Total 356	C 210	N 73	O 73	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	C2	119	Total 589	C 351	N 119	O 119	0	0

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	B4	128	Total 635	C 379	N 128	O 128	0	0

- Molecule 35 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	AM	139	Total 681	C 403	N 139	O 139	0	0

- Molecule 36 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	B6	96	Total 477	C 285	N 96	O 96	0	0

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	B7	119	Total 592	C 354	N 119	O 119	0	0

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	B9	176	Total 874	C 522	N 176	O 176	0	0

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	B2	65	Total 323	C 193	N 65	O 65	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	B8	157	Total 775	C 461	N 157	O 157	0	0

- Molecule 41 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	BK	102	Total 506	C 302	N 102	O 102	0	0

- Molecule 42 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	C1	46	Total	C	N	O	0	0
			227	135	46	46		

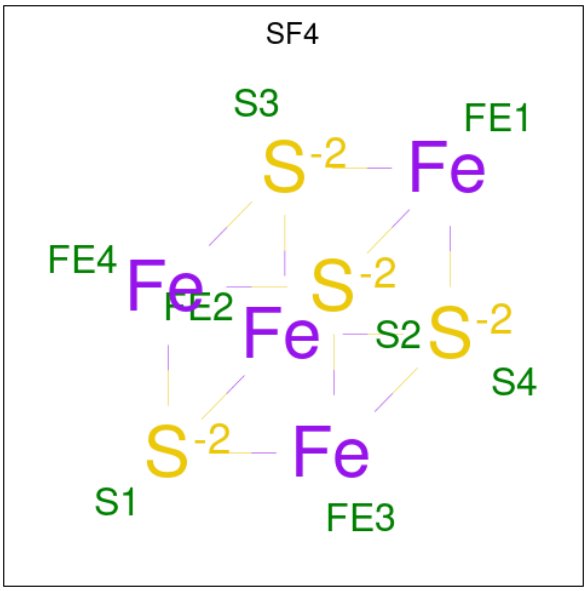
- Molecule 43 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	B1	52	Total	C	N	O	0	0
			258	154	52	52		

- Molecule 44 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	A1	70	Total	C	N	O	0	0
			343	203	70	70		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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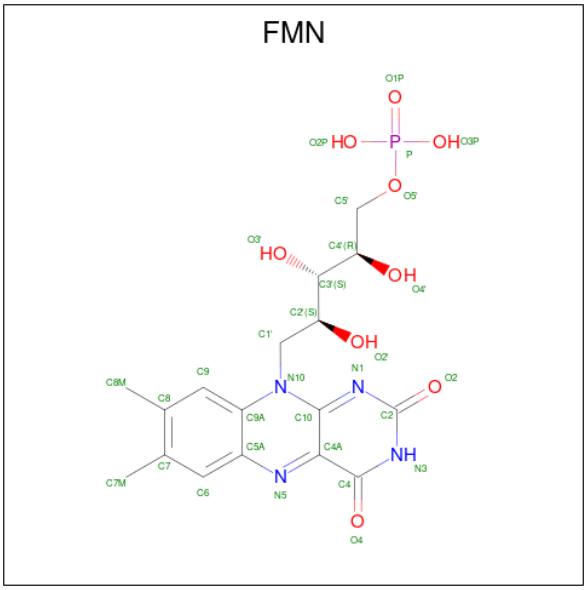
Continued from previous page...

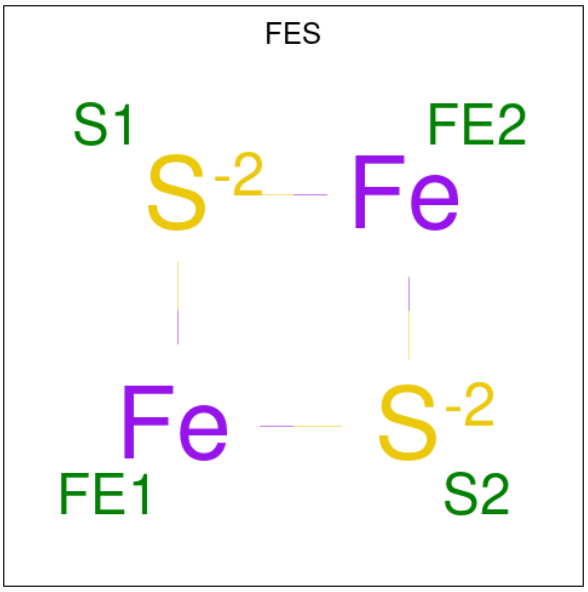
Mol	Chain	Residues	Atoms	AltConf
45	S8	1	Total Fe S 8 4 4	0
45	S8	1	Total Fe S 8 4 4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

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

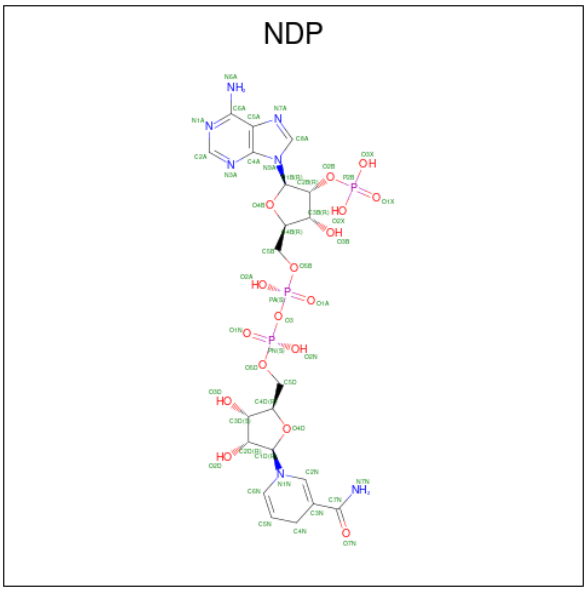


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total 4	Fe 2	S 2	0
47	S1	1	Total 4	Fe 2	S 2	0

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

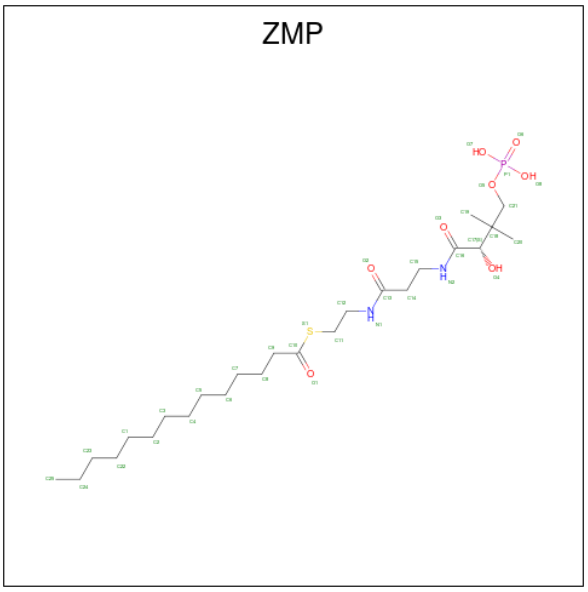
Mol	Chain	Residues	Atoms		AltConf
48	S6	1	Total 1	Zn 1	0

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



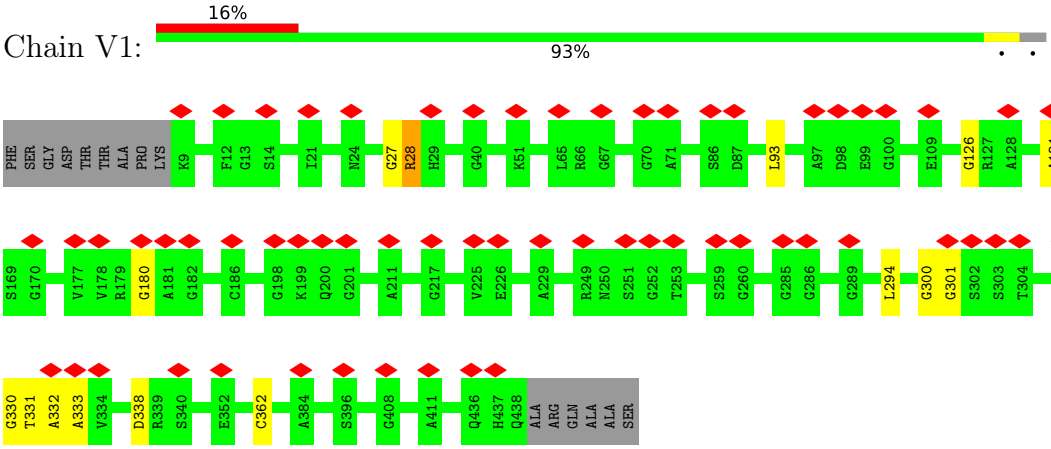
Mol	Chain	Residues	Atoms						AltConf
50	A6	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
50	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

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.

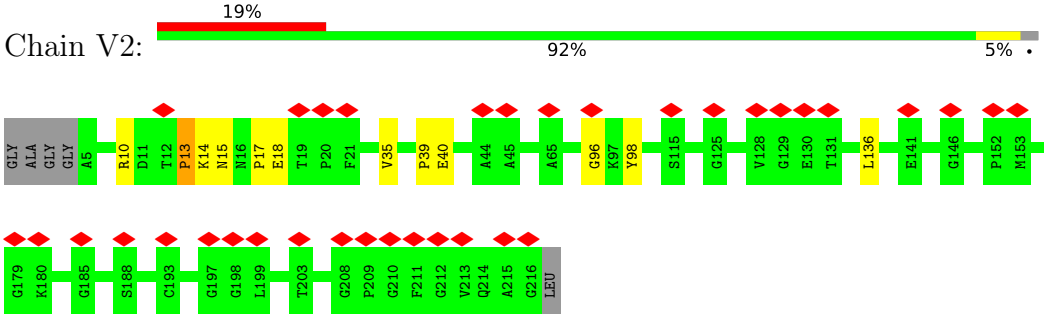
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:



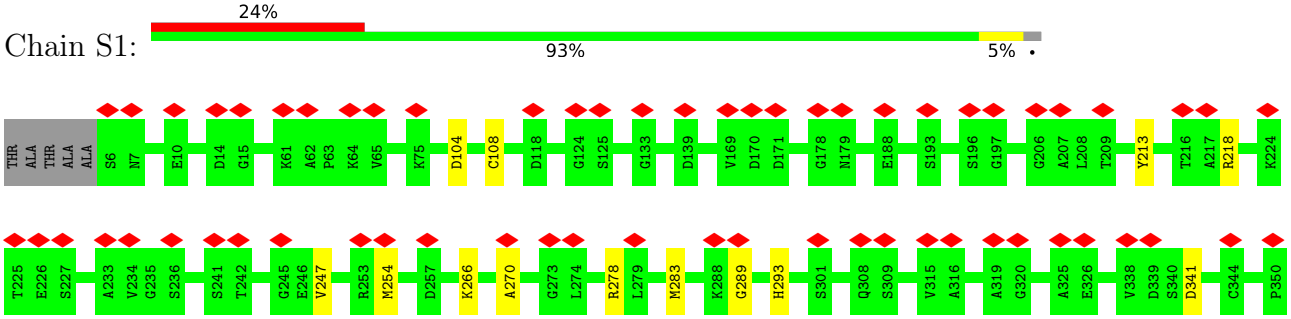
• Molecule 2: NDUFV2

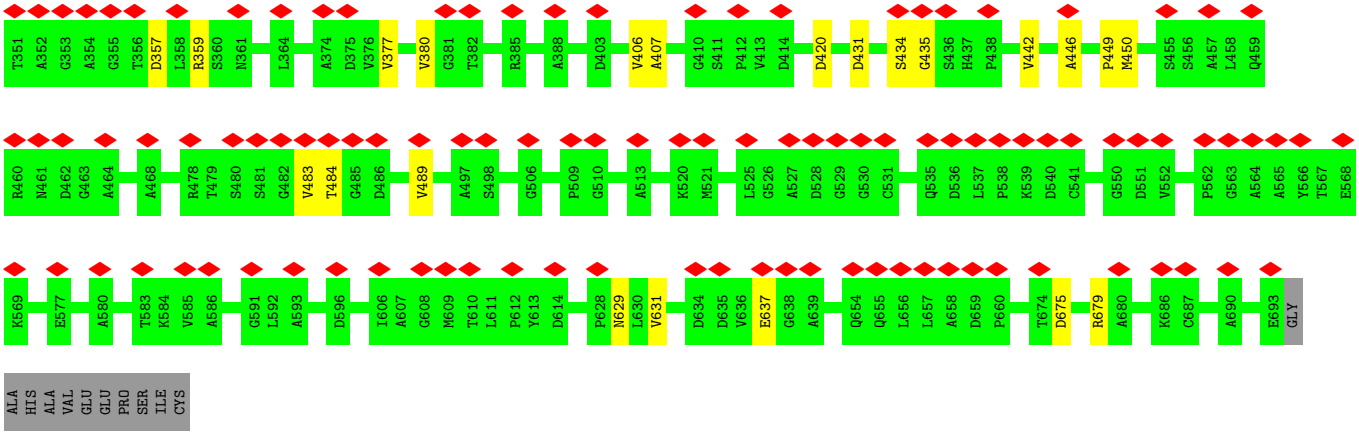
Chain V2:



• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

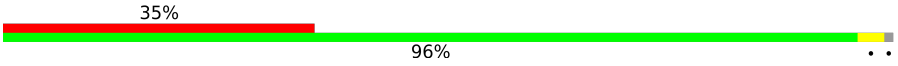
Chain S1:

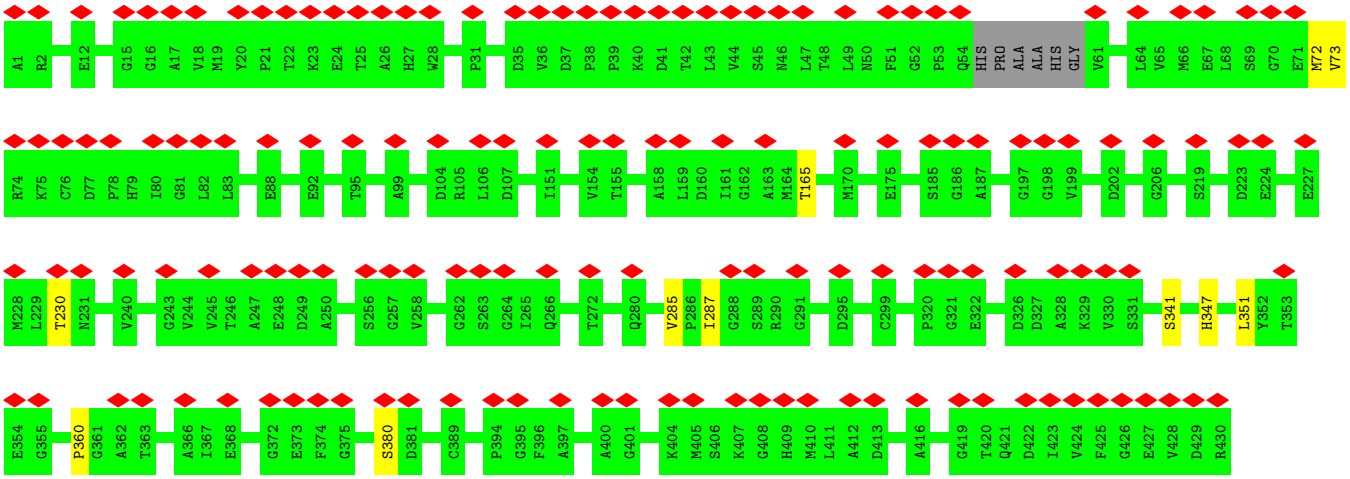




• Molecule 4: NDUFS2

Chain S2:

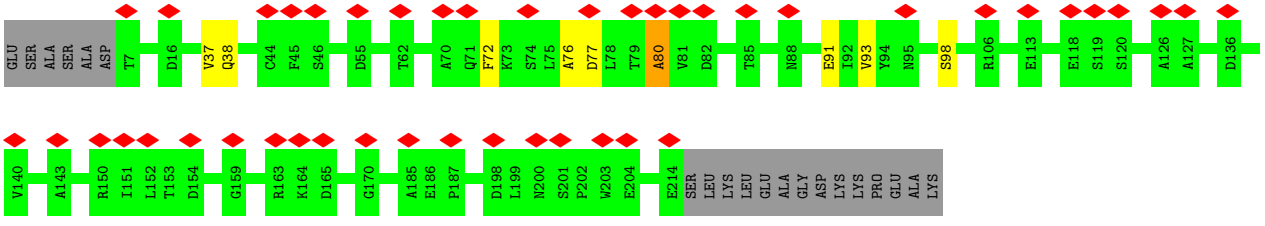




• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:

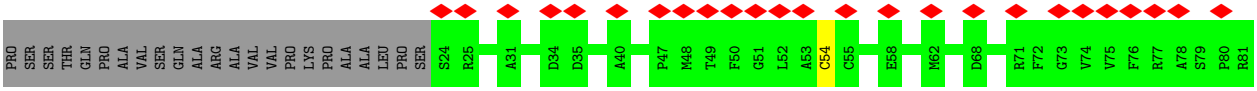


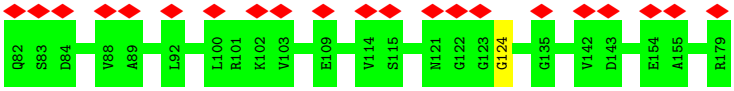


• Molecule 6: NDUFS7

Chain S7:

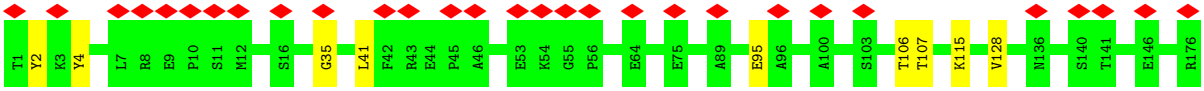






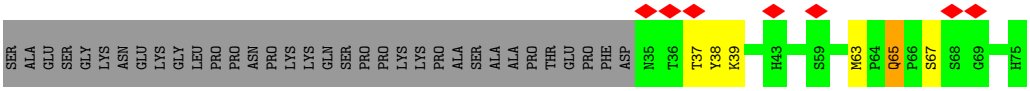
• Molecule 7: NDUFS8





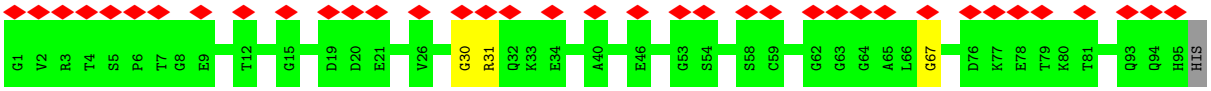
• Molecule 8: NDUFV3



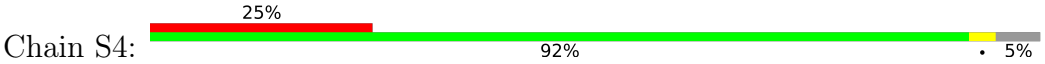


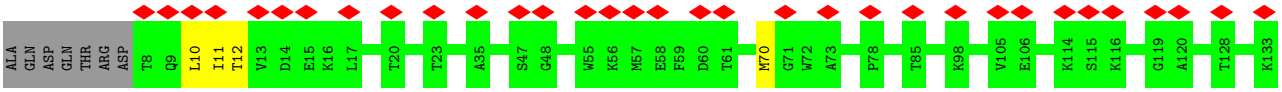
• Molecule 9: NDUFS6



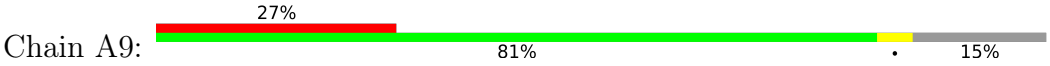


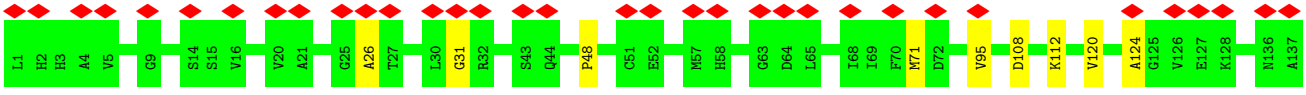
• Molecule 10: NADH:ubiquinone oxidoreductase subunit S4

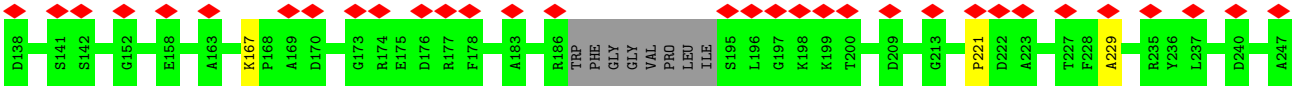


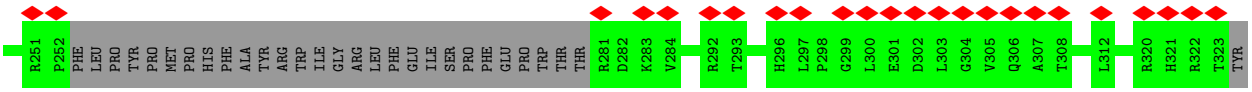


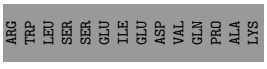
• Molecule 11: NADH:ubiquinone oxidoreductase subunit A9





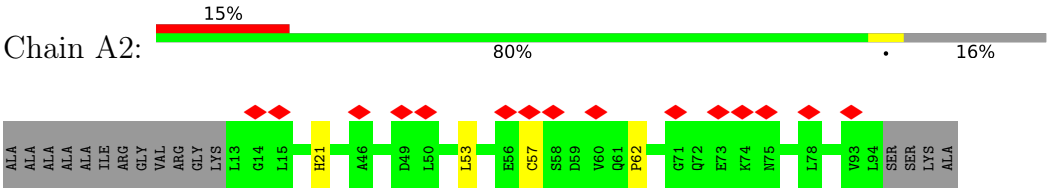






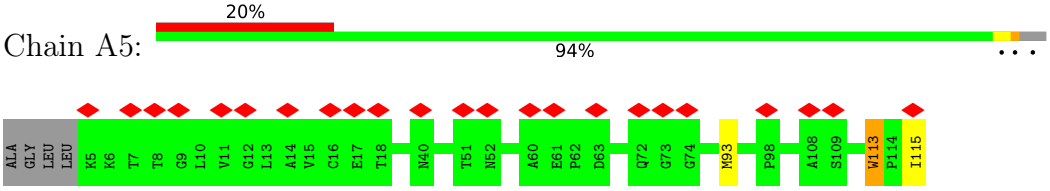
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:



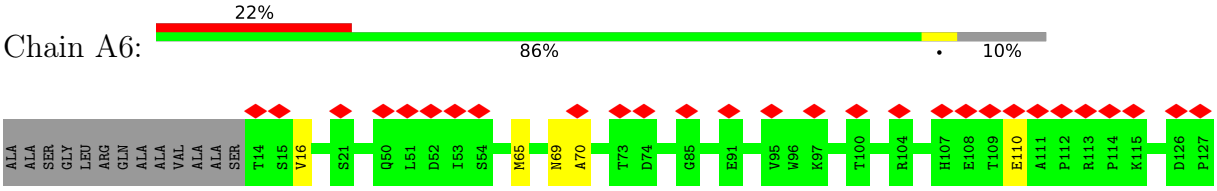
• Molecule 13: NDUFA5

Chain A5:



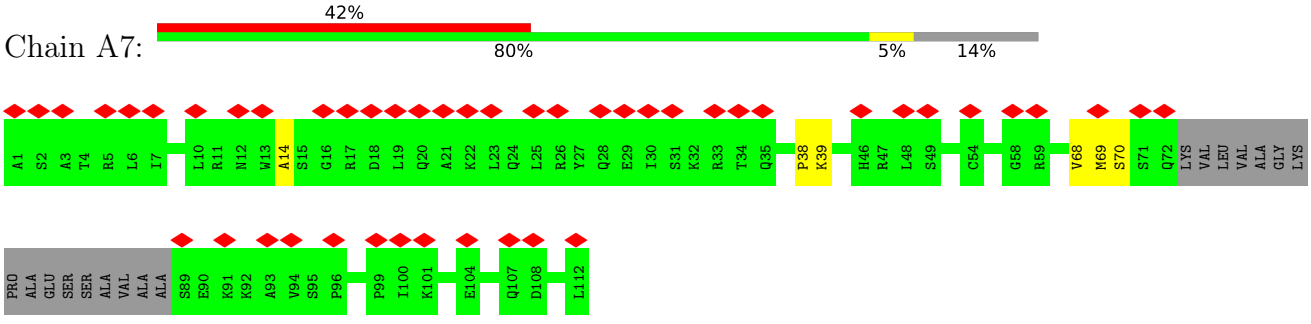
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



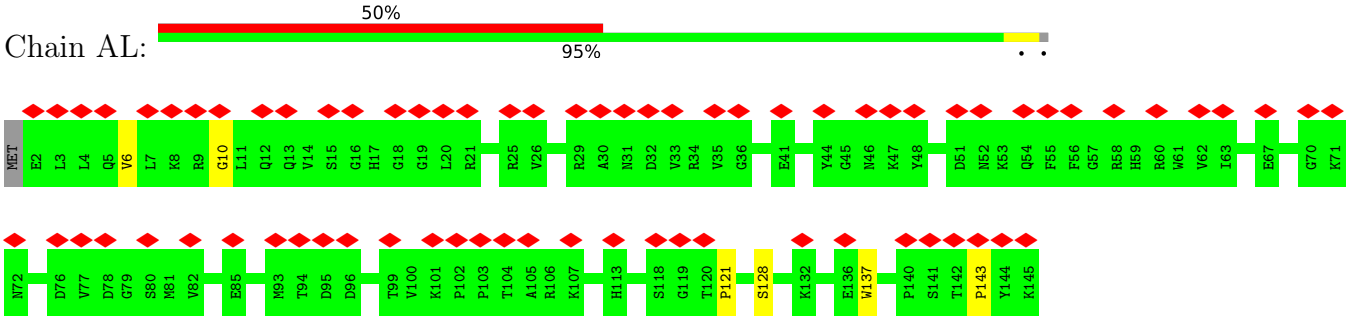
• Molecule 15: NDUFA7

Chain A7:



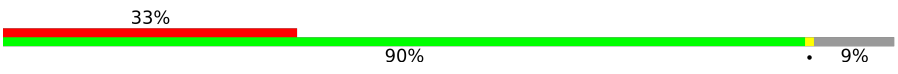
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

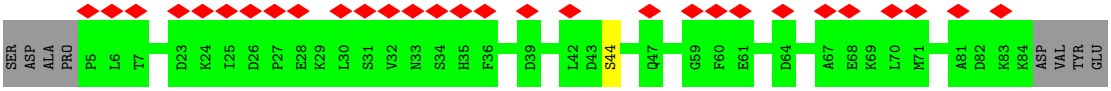
Chain AL:



• Molecule 17: Acyl carrier protein

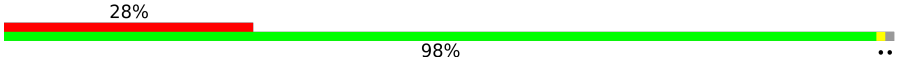
Chain AA:

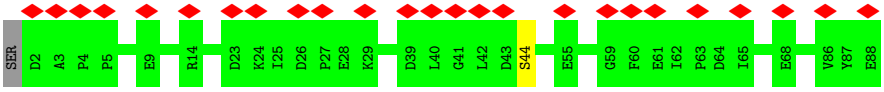




• Molecule 17: Acyl carrier protein

Chain AB:

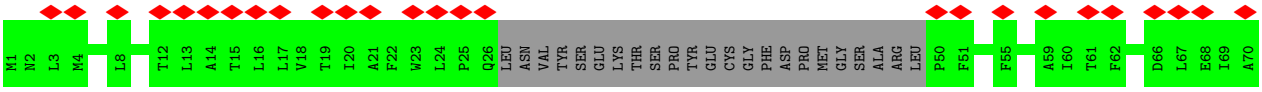


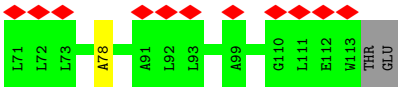


• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain D3:

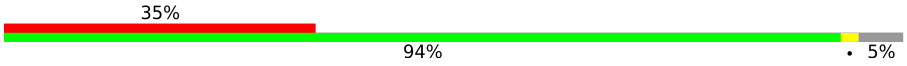


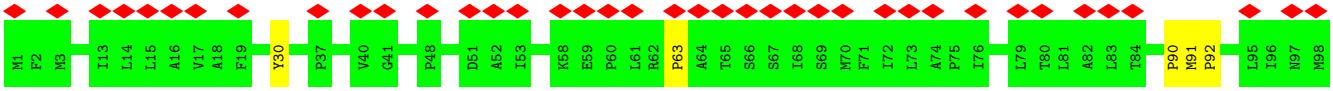


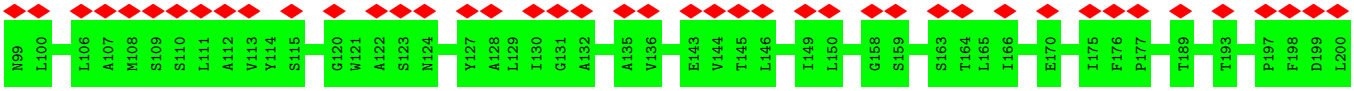


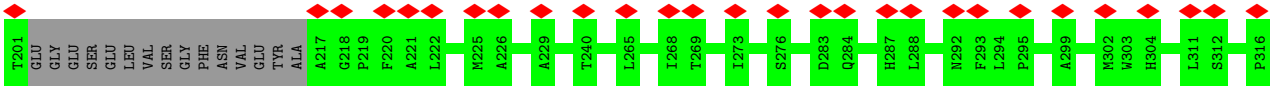
• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

Chain D1:





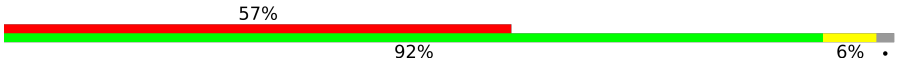


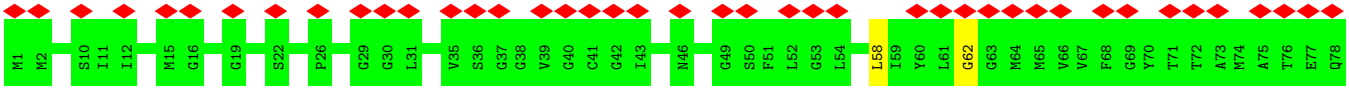


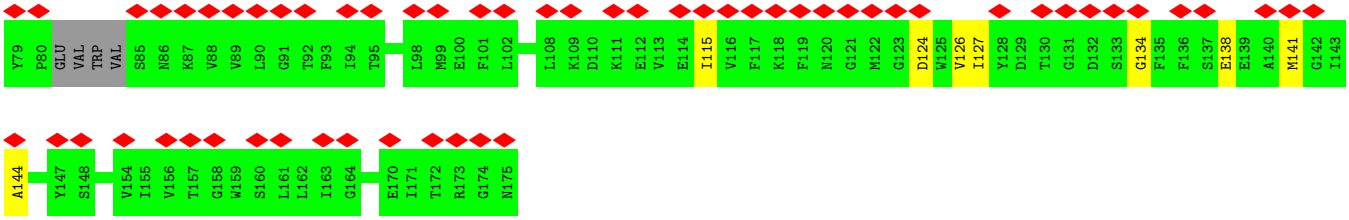


• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain D6:

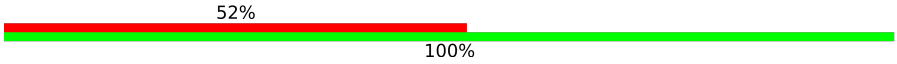


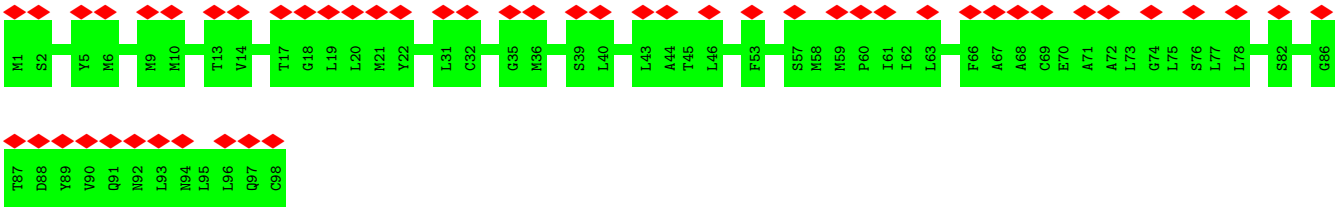




• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

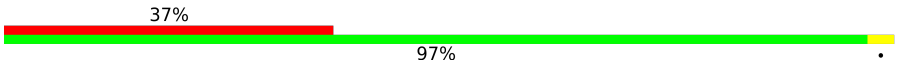
Chain 4L:

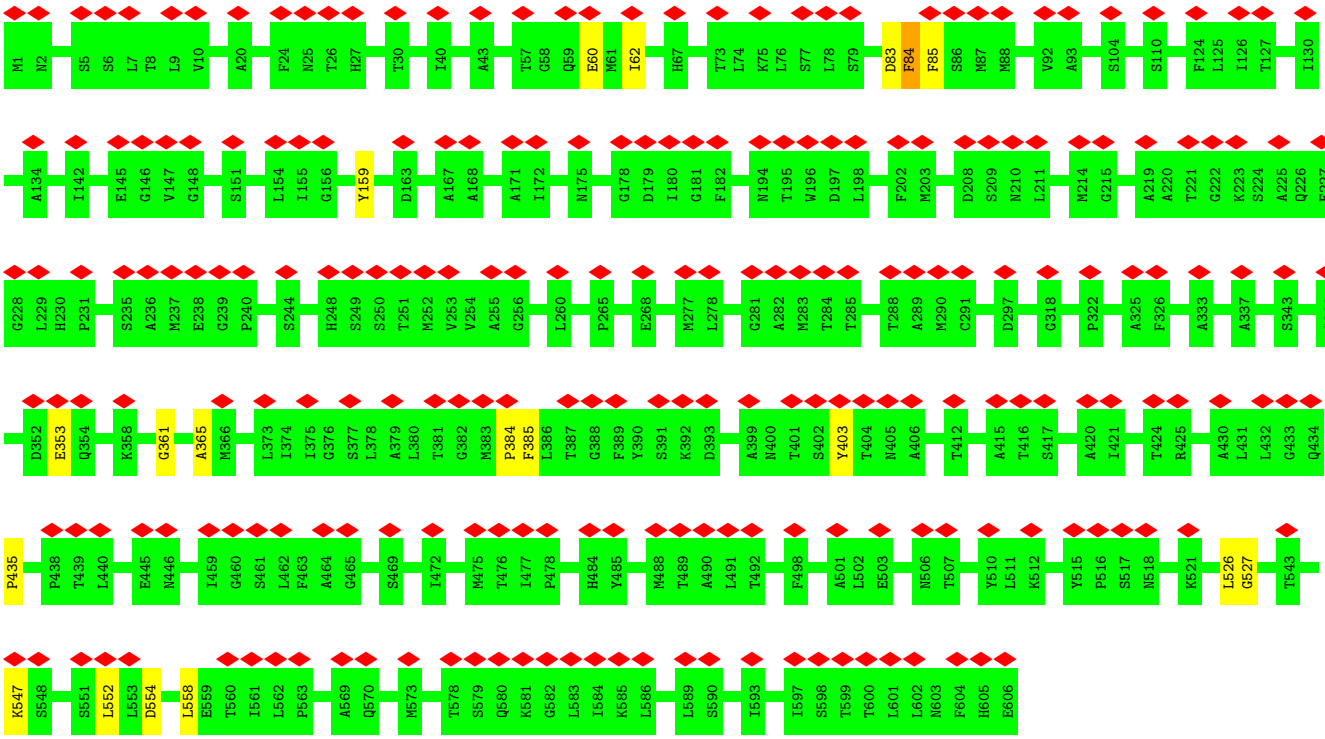




• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

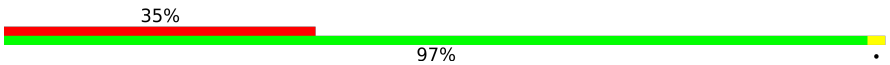
Chain D5:

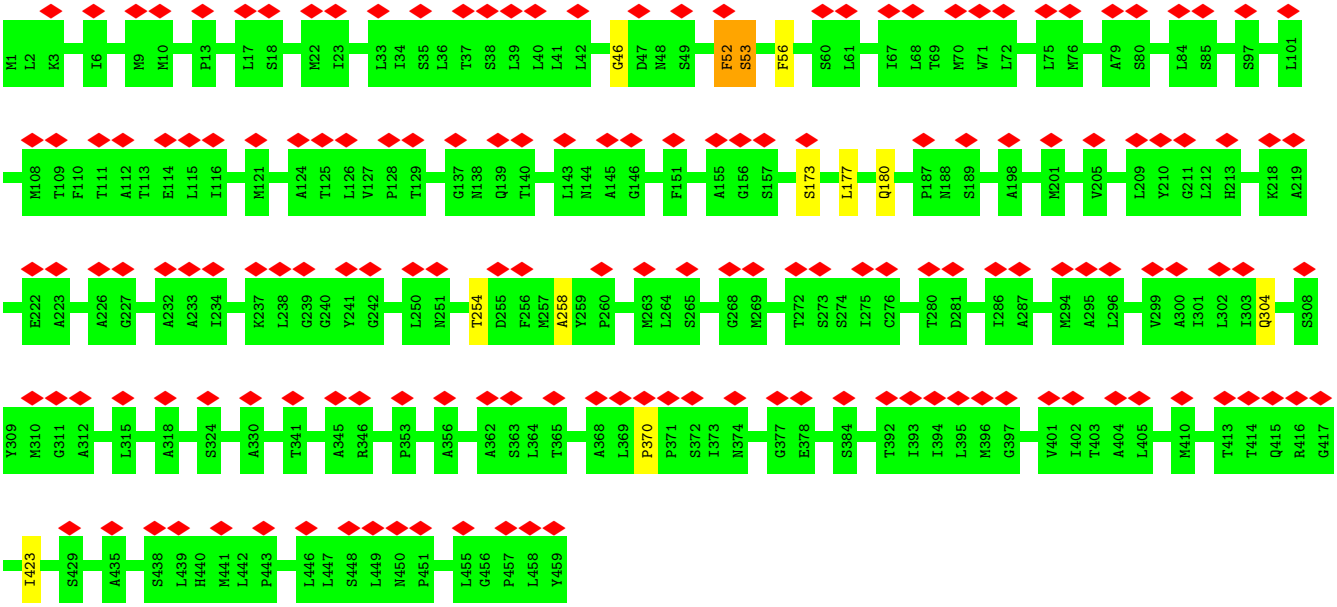




• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

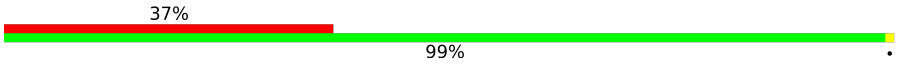
Chain D4:

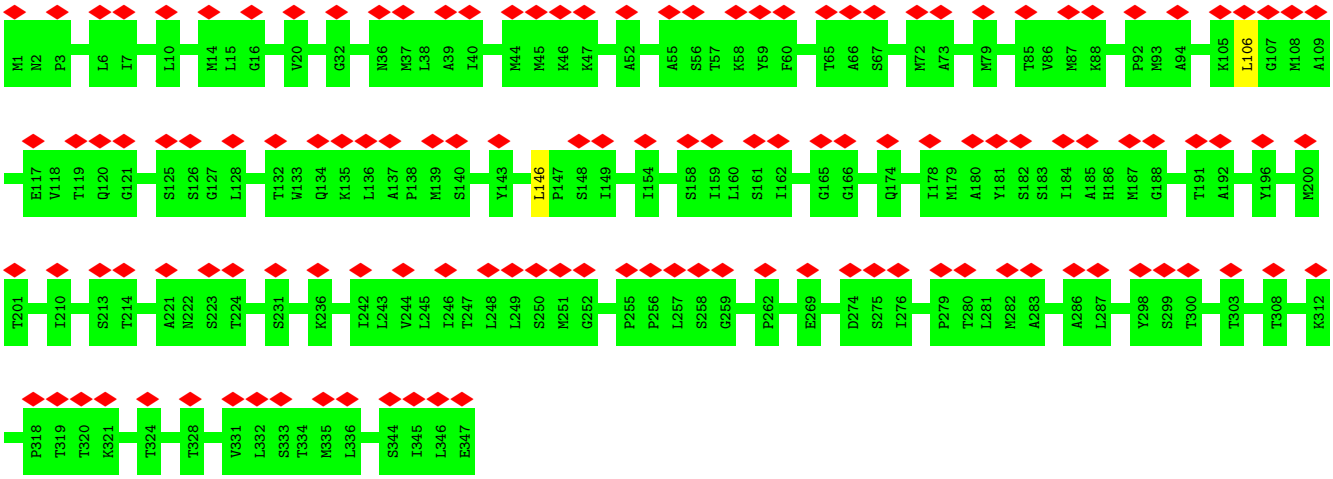




• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

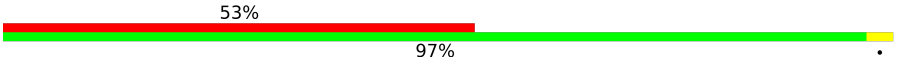
Chain D2:

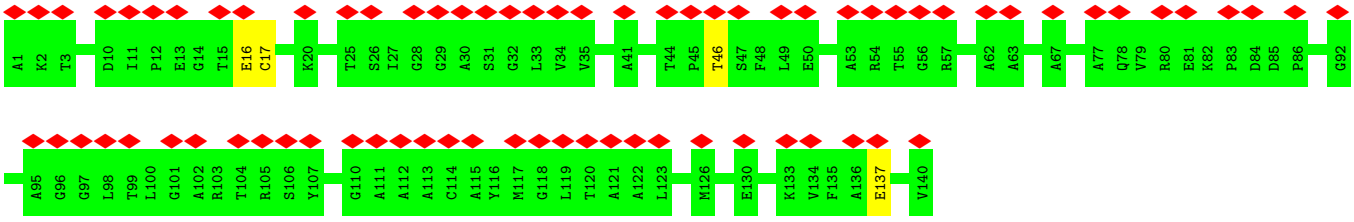




• Molecule 25: NDUFA11

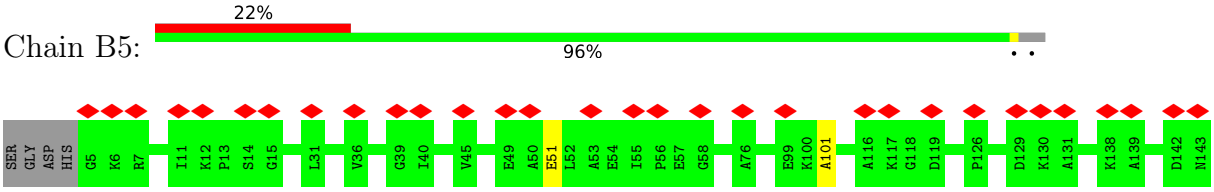
Chain AK:





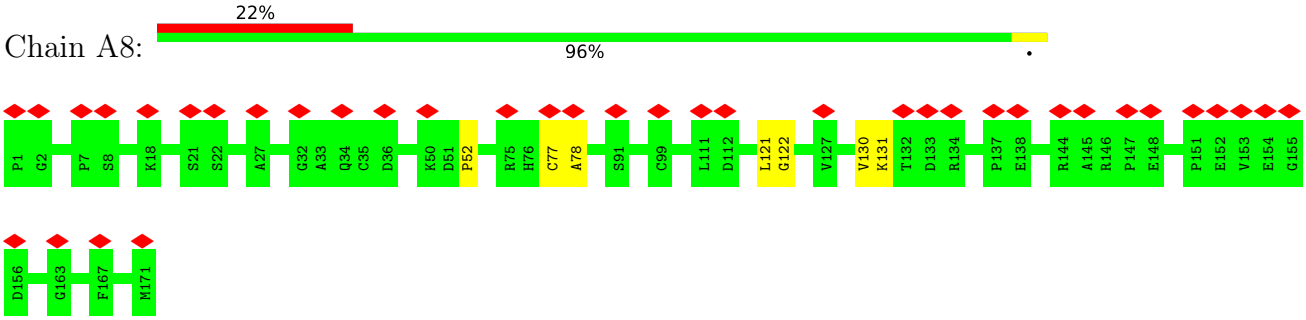
• Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

Chain B5:



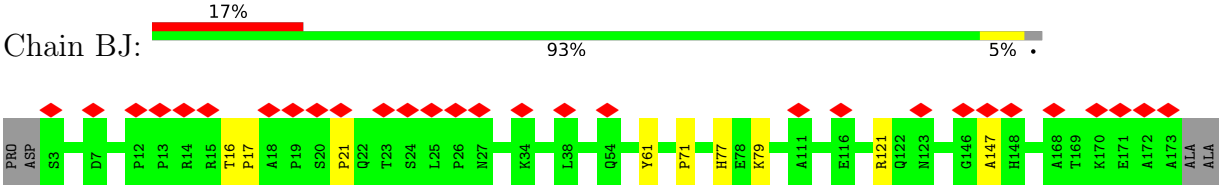
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:



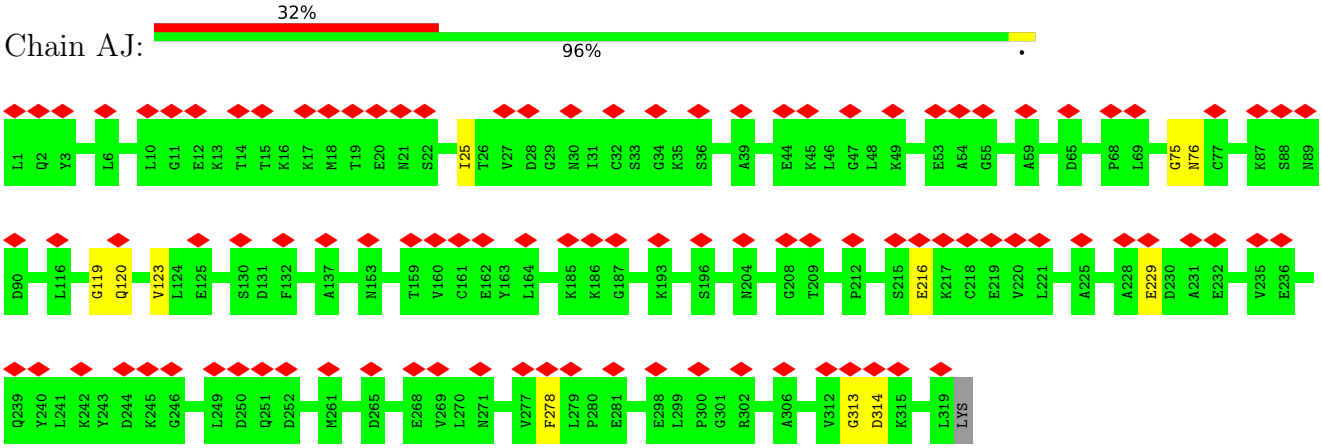
• Molecule 28: NDUFB10

Chain BJ:



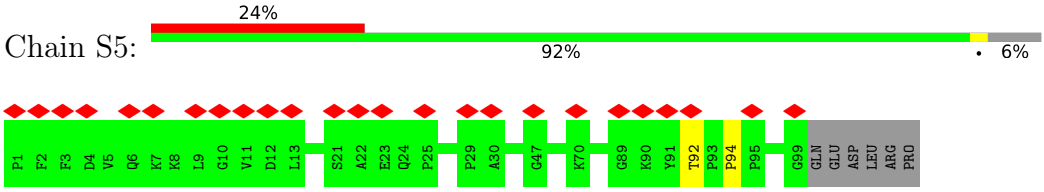
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AJ:



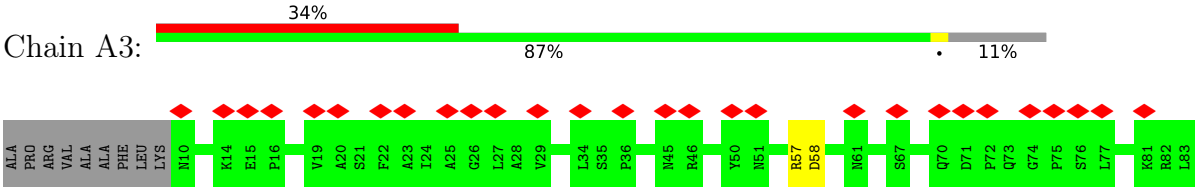
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

Chain S5:



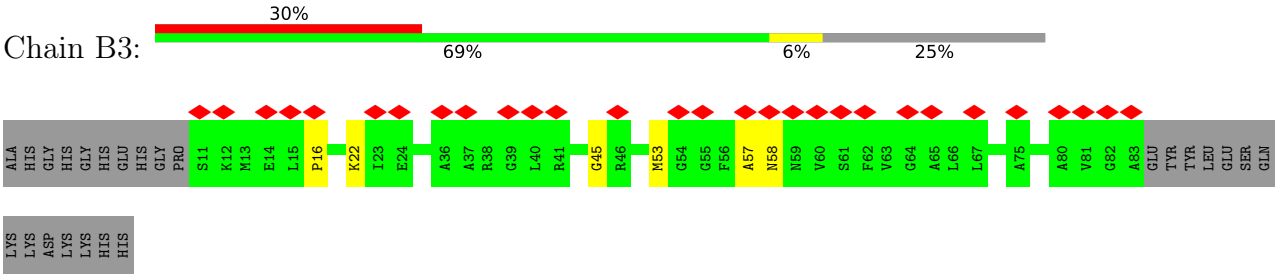
• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain A3:



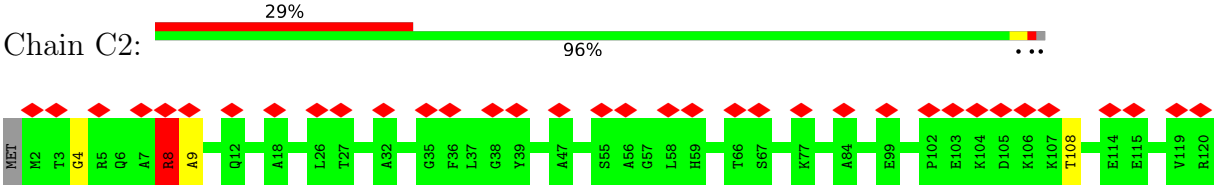
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain B3:



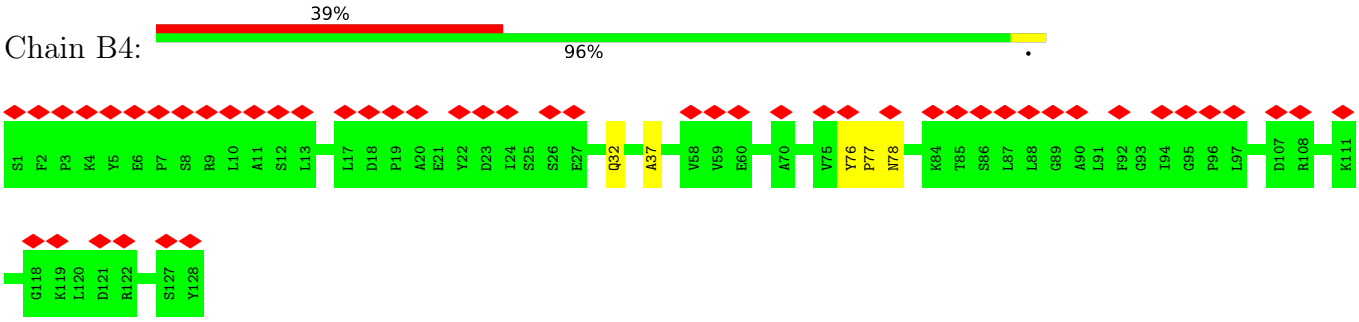
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain C2:



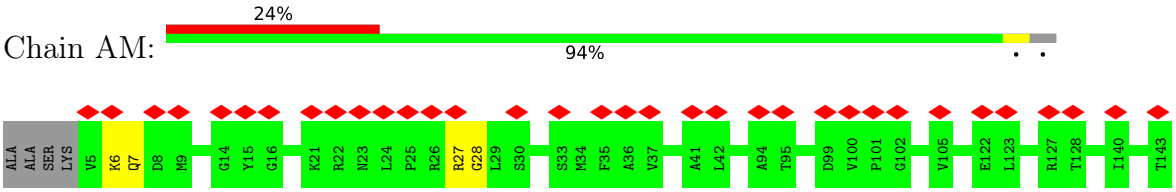
• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain B4:



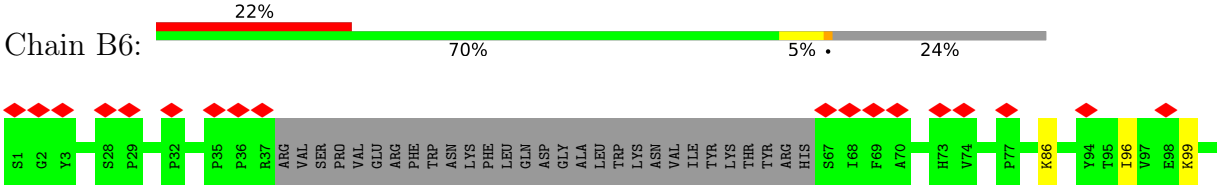
• Molecule 35: NDUFA13

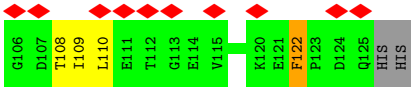
Chain AM:



• Molecule 36: NDUFB6

Chain B6:

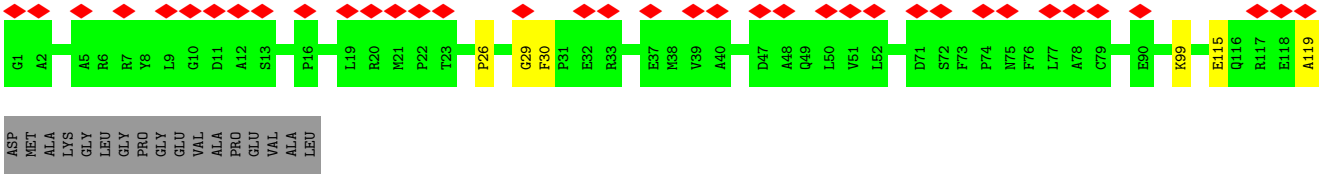




• Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

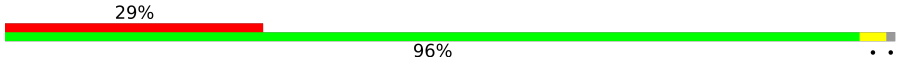
Chain B7:

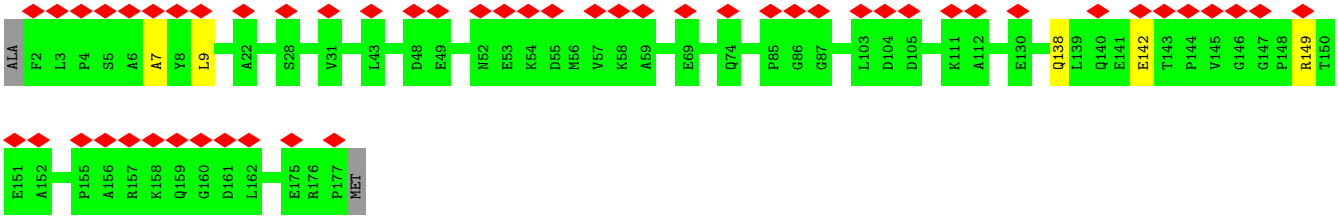




• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain B9:

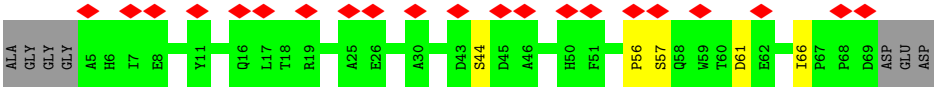




• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

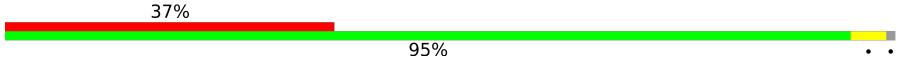
Chain B2:

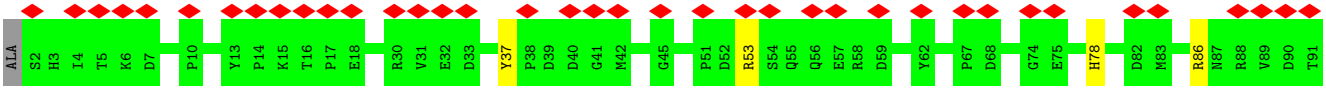


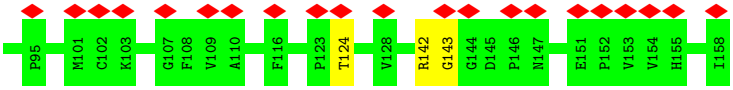


• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



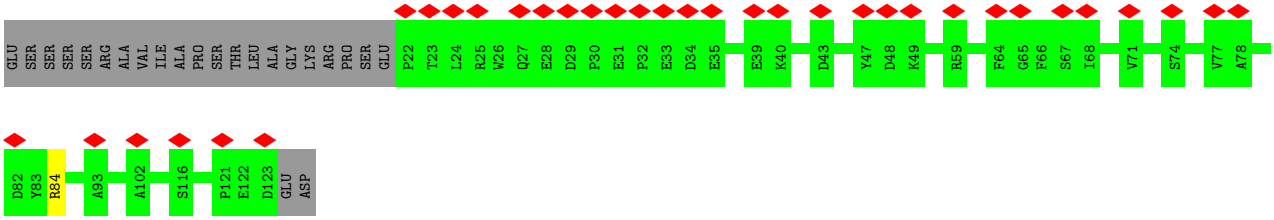




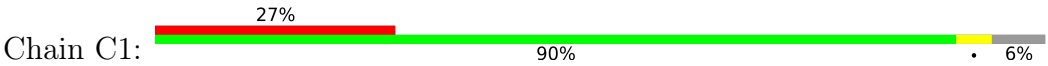
• Molecule 41: NDUFB11

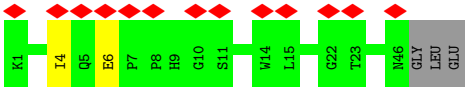
Chain BK:



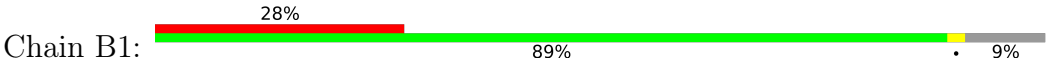


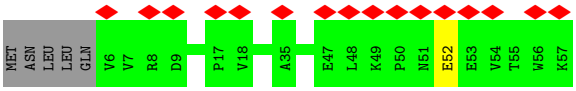
• Molecule 42: NDUFC1





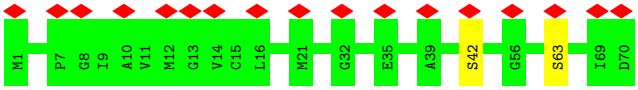
• Molecule 43: NDUFB1





• Molecule 44: NDUFA1





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.616	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	V1	0.27	0/2098	0.69	1/2905 (0.0%)
2	V2	0.32	0/1044	0.88	2/1451 (0.1%)
3	S1	0.27	0/3389	0.69	3/4713 (0.1%)
4	S2	0.32	0/2088	0.69	4/2902 (0.1%)
5	S3	0.31	0/1033	0.79	2/1441 (0.1%)
6	S7	0.32	0/768	0.71	0/1067
7	S8	0.34	0/870	0.68	0/1211
8	V3	0.30	0/203	0.76	0/282
9	S6	0.22	0/461	0.53	0/636
10	S4	0.24	0/624	0.68	2/869 (0.2%)
11	A9	0.27	0/1410	0.69	2/1956 (0.1%)
12	A2	0.25	0/405	0.66	0/563
13	A5	0.26	0/549	0.72	0/764
14	A6	0.27	0/566	0.73	2/789 (0.3%)
15	A7	0.28	0/474	0.74	0/658
16	AL	0.26	0/707	0.71	0/981
17	AA	0.26	0/396	0.74	0/551
17	AB	0.24	0/431	0.59	0/600
18	D3	0.28	0/447	0.63	0/622
19	D1	0.33	0/1503	0.79	2/2095 (0.1%)
20	D6	0.27	0/827	0.74	0/1139
21	4L	0.34	0/485	0.70	0/675
22	D5	0.32	0/3000	0.79	0/4181
23	D4	0.34	0/2276	0.80	3/3174 (0.1%)
24	D2	0.34	1/1720 (0.1%)	0.97	2/2398 (0.1%)
25	AK	0.28	0/681	0.76	4/941 (0.4%)
26	B5	0.26	0/686	0.57	0/954
27	A8	0.27	0/846	0.71	0/1178
28	BJ	0.29	0/852	0.72	2/1190 (0.2%)
29	AJ	0.29	0/1574	0.76	2/2190 (0.1%)
30	S5	0.40	1/489 (0.2%)	0.75	0/680
31	A3	0.27	0/366	0.75	0/509

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	B3	0.33	0/355	0.93	1/490 (0.2%)
33	C2	0.32	0/588	0.81	4/818 (0.5%)
34	B4	0.25	0/634	0.62	0/883
35	AM	0.28	0/680	0.68	0/942
36	B6	0.30	0/475	0.83	1/660 (0.2%)
37	B7	0.28	0/591	0.74	2/824 (0.2%)
38	B9	0.27	0/873	0.70	2/1217 (0.2%)
39	B2	0.33	0/322	0.93	4/448 (0.9%)
40	B8	0.30	0/774	0.95	4/1076 (0.4%)
41	BK	0.26	0/505	0.74	0/703
42	C1	0.27	0/226	0.76	2/313 (0.6%)
43	B1	0.24	0/257	0.68	0/357
44	A1	0.27	0/342	0.63	0/473
All	All	0.30	2/39890 (0.0%)	0.75	53/55469 (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
1	V1	0	2
2	V2	0	3
3	S1	0	6
4	S2	0	2
5	S3	0	2
7	S8	0	1
8	V3	0	2
10	S4	0	1
13	A5	0	2
15	A7	0	2
19	D1	0	2
20	D6	0	2
22	D5	0	5
23	D4	0	2
25	AK	0	2
27	A8	0	1
28	BJ	0	1
29	AJ	0	2
30	S5	0	1
31	A3	0	1
32	B3	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	C2	0	1
34	B4	0	1
36	B6	0	2
37	B7	0	1
39	B2	0	1
40	B8	0	2
42	C1	0	1
43	B1	0	1
44	A1	0	1
All	All	0	56

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S5	94	PRO	C-N	6.64	1.39	1.33
24	D2	146	LEU	C-N	5.85	1.38	1.33

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D2	106	LEU	N-CA-C	29.15	145.95	112.72
24	D2	106	LEU	CB-CA-C	-15.76	84.94	110.94
28	BJ	21	PRO	CA-C-N	7.63	135.43	121.70
28	BJ	21	PRO	C-N-CA	7.63	135.43	121.70
29	AJ	229	GLU	CA-C-N	7.62	135.42	121.70

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V1	28	ARG	Peptide
1	V1	331	THR	Peptide
2	V2	10	ARG	Peptide
2	V2	13	PRO	Peptide
2	V2	35	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V1	2099	0	994	19	0
2	V2	1045	0	462	10	0
3	S1	3390	0	1573	26	0
4	S2	2090	0	930	6	0
5	S3	1034	0	445	8	0
6	S7	769	0	351	1	0
7	S8	871	0	401	9	0
8	V3	204	0	79	18	0
9	S6	462	0	211	3	0
10	S4	625	0	274	3	0
11	A9	1413	0	639	6	0
12	A2	406	0	178	4	0
13	A5	550	0	239	1	0
14	A6	567	0	236	8	0
15	A7	476	0	210	6	0
16	AL	708	0	294	11	0
17	AA	397	0	168	2	0
17	AB	432	0	183	2	0
18	D3	449	0	203	1	0
19	D1	1505	0	676	1	0
20	D6	829	0	381	6	0
21	4L	486	0	222	0	0
22	D5	3001	0	1331	8	0
23	D4	2277	0	1004	9	0
24	D2	1721	0	744	0	0
25	AK	682	0	358	0	0
26	B5	687	0	302	2	0
27	A8	847	0	364	10	0
28	BJ	853	0	375	8	0
29	AJ	1575	0	694	4	0
30	S5	490	0	215	0	0
31	A3	367	0	157	8	0
32	B3	356	0	178	1	0
33	C2	589	0	254	2	0
34	B4	635	0	281	3	0
35	AM	681	0	302	3	0
36	B6	477	0	187	5	0
37	B7	592	0	260	4	0
38	B9	874	0	374	3	0
39	B2	323	0	136	3	0
40	B8	775	0	318	2	0
41	BK	506	0	214	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	C1	227	0	97	0	0
43	B1	258	0	109	0	0
44	A1	343	0	159	1	0
45	S1	16	0	0	0	0
45	S7	8	0	0	0	0
45	S8	16	0	0	0	0
45	V1	8	0	0	1	0
46	V1	31	0	19	1	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	1	0
50	A6	34	0	40	8	0
50	AB	31	0	34	3	0
All	All	40144	0	17881	156	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 3.

The worst 5 of 156 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)
5:S3:80:ALA:HA	5:S3:91:GLU:O	1.17	1.32
3:S1:431:ASP:O	3:S1:435:GLY:HA2	1.31	1.29
3:S1:431:ASP:O	3:S1:435:GLY:CA	1.81	1.29
1:V1:27:GLY:CA	8:V3:39:LYS:H	1.45	1.27
2:V2:39:PRO:HA	8:V3:65:GLN:CB	1.71	1.19

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	V1	428/445 (96%)	381 (89%)	47 (11%)	0	100	100
2	V2	210/217 (97%)	167 (80%)	43 (20%)	0	100	100
3	S1	686/704 (97%)	613 (89%)	72 (10%)	1 (0%)	48	83
4	S2	420/430 (98%)	379 (90%)	41 (10%)	0	100	100
5	S3	206/228 (90%)	180 (87%)	26 (13%)	0	100	100
6	S7	154/179 (86%)	136 (88%)	17 (11%)	1 (1%)	21	59
7	S8	174/176 (99%)	157 (90%)	17 (10%)	0	100	100
8	V3	39/75 (52%)	32 (82%)	7 (18%)	0	100	100
9	S6	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
10	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
11	A9	281/338 (83%)	244 (87%)	37 (13%)	0	100	100
12	A2	80/98 (82%)	72 (90%)	8 (10%)	0	100	100
13	A5	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
14	A6	112/127 (88%)	105 (94%)	7 (6%)	0	100	100
15	A7	92/112 (82%)	77 (84%)	15 (16%)	0	100	100
16	AL	142/145 (98%)	119 (84%)	23 (16%)	0	100	100
17	AA	78/88 (89%)	67 (86%)	11 (14%)	0	100	100
17	AB	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
18	D3	86/115 (75%)	81 (94%)	5 (6%)	0	100	100
19	D1	299/318 (94%)	273 (91%)	25 (8%)	1 (0%)	36	72
20	D6	167/175 (95%)	145 (87%)	21 (13%)	1 (1%)	21	59
21	4L	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
22	D5	604/606 (100%)	532 (88%)	70 (12%)	2 (0%)	36	72
23	D4	457/459 (100%)	412 (90%)	44 (10%)	1 (0%)	43	77
24	D2	345/347 (99%)	318 (92%)	27 (8%)	0	100	100
25	AK	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
26	B5	137/143 (96%)	124 (90%)	13 (10%)	0	100	100
27	A8	169/171 (99%)	137 (81%)	32 (19%)	0	100	100
28	BJ	169/175 (97%)	151 (89%)	17 (10%)	1 (1%)	21	59
29	AJ	317/320 (99%)	277 (87%)	40 (13%)	0	100	100
30	S5	97/105 (92%)	80 (82%)	17 (18%)	0	100	100
31	A3	72/83 (87%)	60 (83%)	12 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B3	71/97 (73%)	57 (80%)	14 (20%)	0	100	100
33	C2	117/120 (98%)	104 (89%)	13 (11%)	0	100	100
34	B4	126/128 (98%)	111 (88%)	15 (12%)	0	100	100
35	AM	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
36	B6	92/127 (72%)	79 (86%)	13 (14%)	0	100	100
37	B7	117/136 (86%)	100 (86%)	17 (14%)	0	100	100
38	B9	174/178 (98%)	148 (85%)	26 (15%)	0	100	100
39	B2	63/72 (88%)	54 (86%)	9 (14%)	0	100	100
40	B8	155/158 (98%)	117 (76%)	37 (24%)	1 (1%)	21	59
41	BK	100/125 (80%)	81 (81%)	19 (19%)	0	100	100
42	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
43	B1	50/57 (88%)	46 (92%)	4 (8%)	0	100	100
44	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	7980/8509 (94%)	7031 (88%)	940 (12%)	9 (0%)	49	83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	D5	84	PHE
23	D4	53	SER
3	S1	359	ARG
6	S7	54	CYS
22	D5	527	GLY

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\#\|Z\| > 2$
49	NDP	A9	401	-	49,52,52	0.43	1 (2%)	66,80,80	0.44	0
50	ZMP	A6	201	-	27,33,36	0.64	0	32,40,45	0.99	1 (3%)
50	ZMP	AB	101	-	24,30,36	0.77	1 (4%)	29,37,45	1.30	3 (10%)
45	SF4	S7	300	-	0,12,12	-	-	-		
45	SF4	S8	201	-	0,12,12	-	-	-		
45	SF4	S1	801	-	0,12,12	-	-	-		
46	FMN	V1	501	-	33,33,33	0.27	0	48,50,50	0.42	0
47	FES	V2	300	-	0,4,4	-	-	-		
47	FES	S1	803	-	0,4,4	-	-	-		
45	SF4	S8	202	-	0,12,12	-	-	-		
45	SF4	V1	500	-	0,12,12	-	-	-		
45	SF4	S1	802	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	NDP	A9	401	-	-	13/34/77/77	0/5/5/5
50	ZMP	A6	201	-	-	15/38/40/43	-
50	ZMP	AB	101	-	-	16/35/37/43	-
45	SF4	S7	300	-	-	-	0/6/5/5
45	SF4	S8	201	-	-	-	0/6/5/5
45	SF4	S1	801	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FMN	V1	501	-	-	7/18/18/18	0/3/3/3
47	FES	V2	300	-	-	-	0/1/1/1
47	FES	S1	803	-	-	-	0/1/1/1
45	SF4	S8	202	-	-	-	0/6/5/5
45	SF4	V1	500	-	-	-	0/6/5/5
45	SF4	S1	802	-	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AB	101	ZMP	C9-C10	2.33	1.53	1.50
49	A9	401	NDP	P2B-O2B	2.25	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	AB	101	ZMP	O1-C10-C9	-3.40	119.97	123.99
50	A6	201	ZMP	O1-C10-C9	-2.53	121.00	123.99
50	AB	101	ZMP	C11-C12-N1	-2.50	107.17	112.42
50	AB	101	ZMP	C15-C14-C13	-2.48	108.23	112.36

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C2'-C3'-C4'-O4'
46	V1	501	FMN	C2'-C3'-C4'-C5'
46	V1	501	FMN	O3'-C3'-C4'-C5'
46	V1	501	FMN	C5'-O5'-P-O2P
46	V1	501	FMN	C5'-O5'-P-O3P

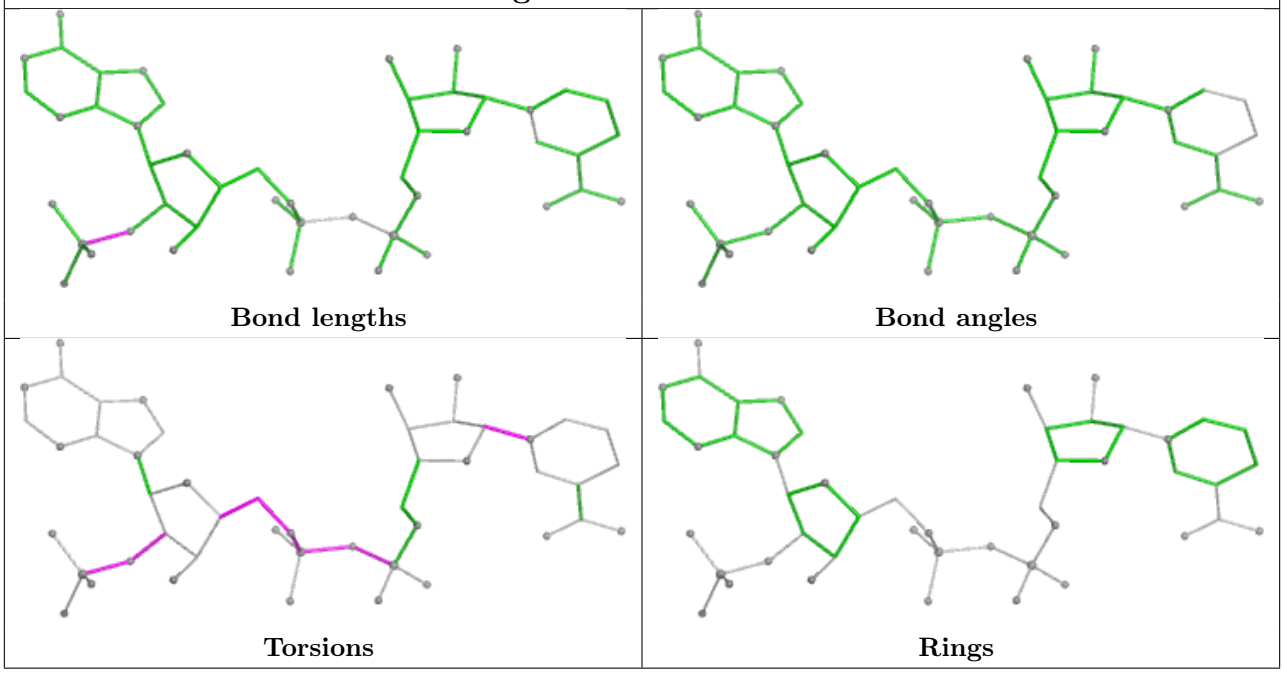
There are no ring outliers.

5 monomers are involved in 14 short contacts:

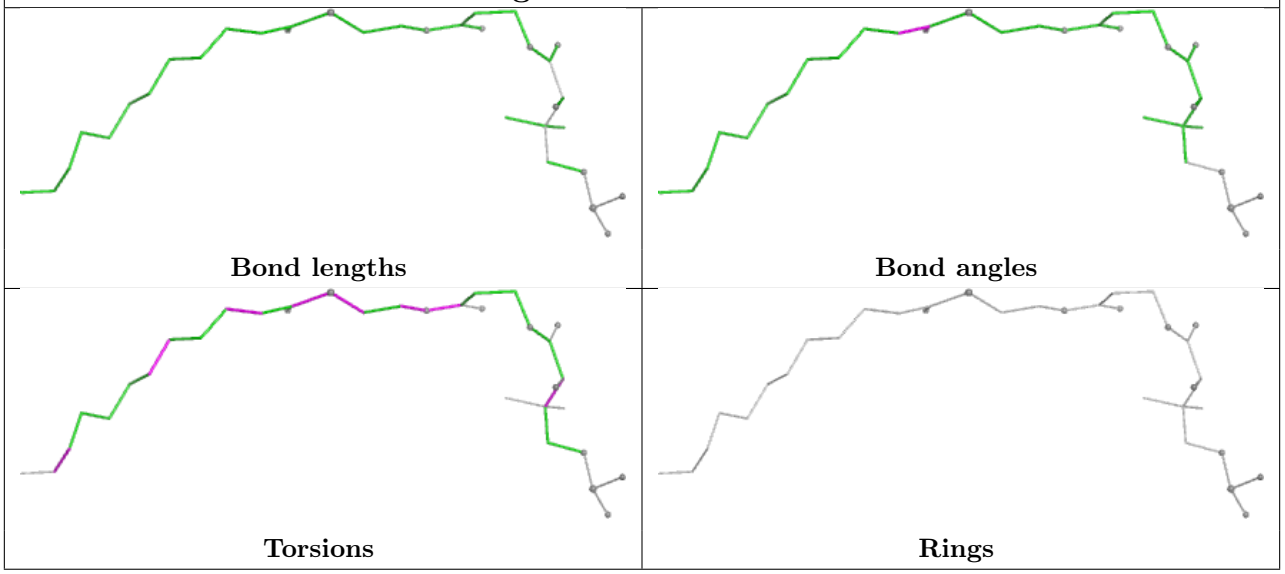
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	A9	401	NDP	1	0
50	A6	201	ZMP	8	0
50	AB	101	ZMP	3	0
46	V1	501	FMN	1	0
45	V1	500	SF4	1	0

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

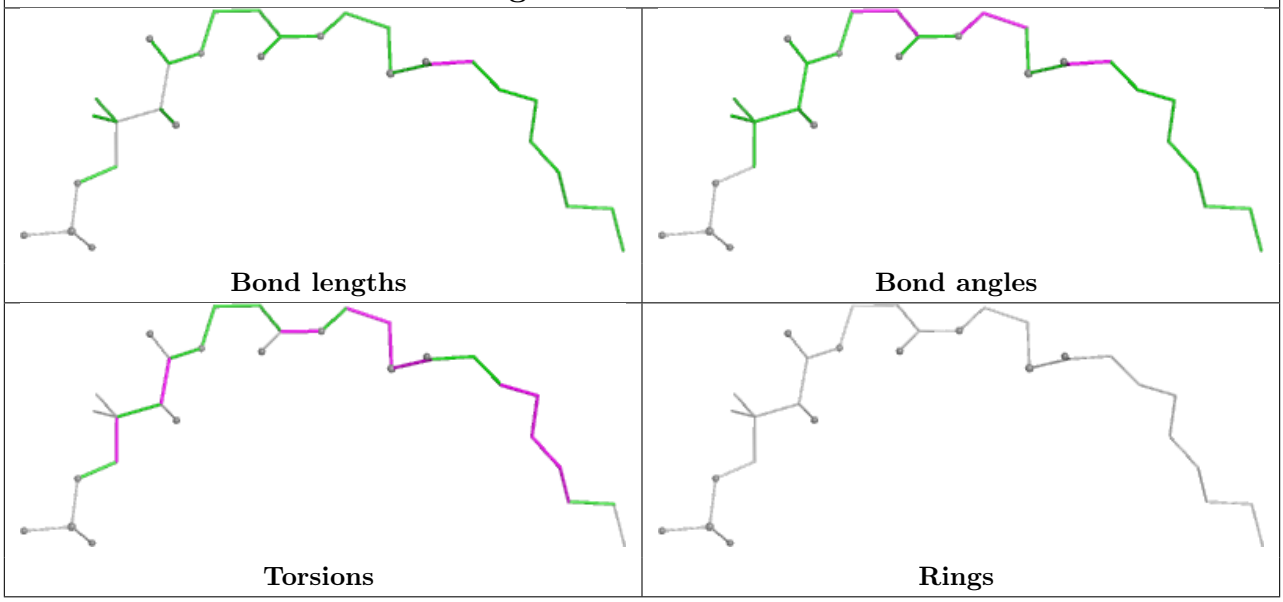
Ligand NDP A9 401



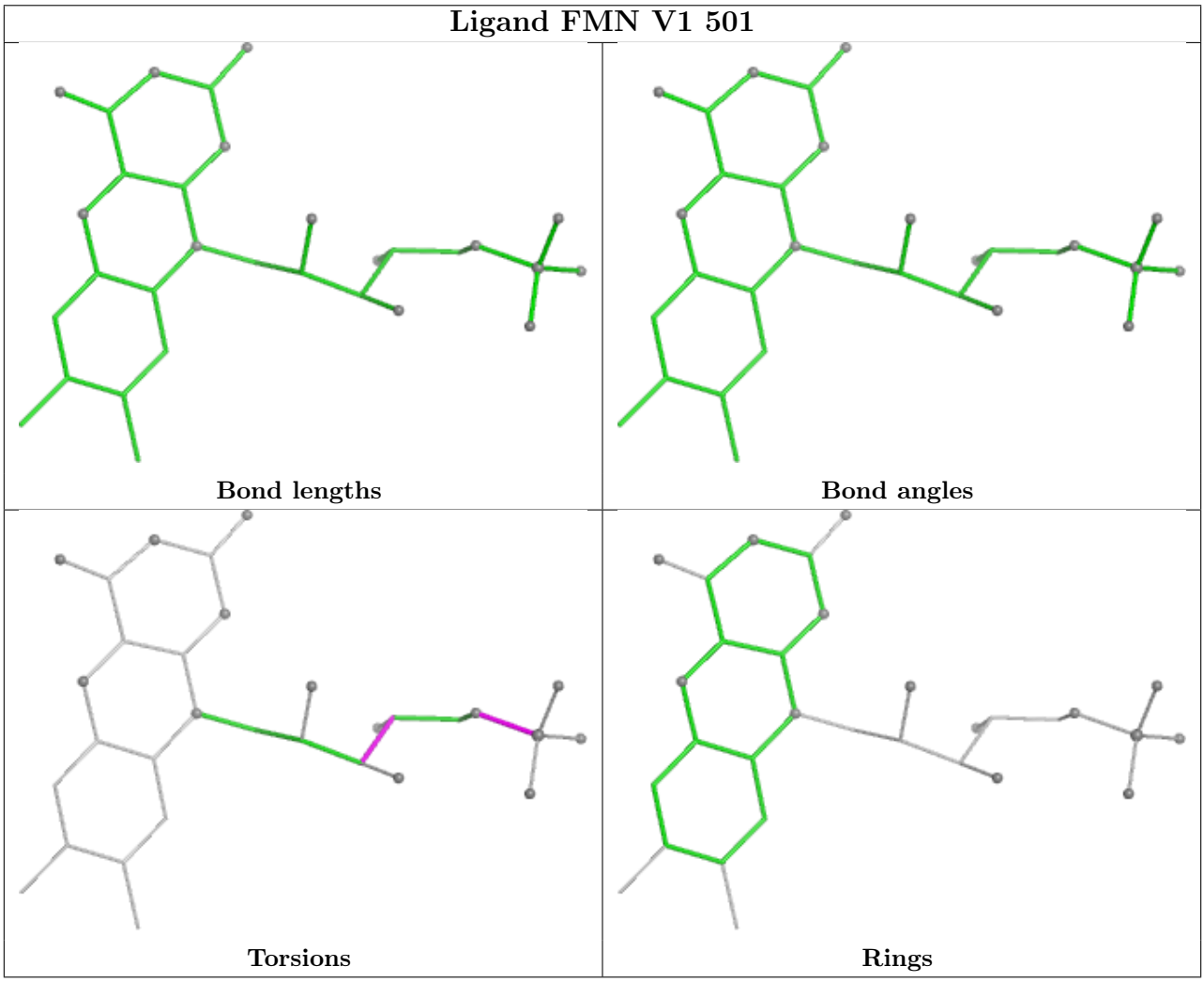
Ligand ZMP A6 201



Ligand ZMP AB 101



Ligand FMN V1 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

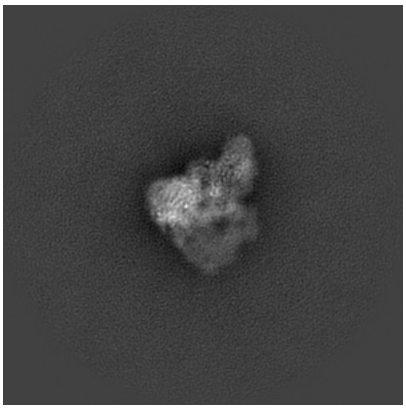
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4501. These allow visual inspection of the internal detail of the map and identification of artifacts.

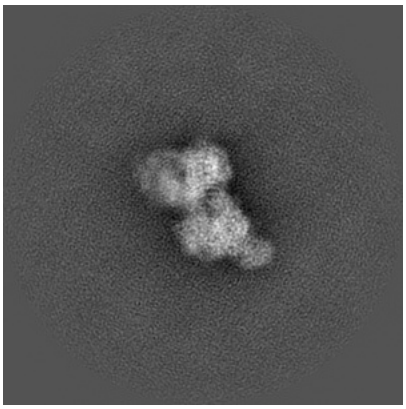
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

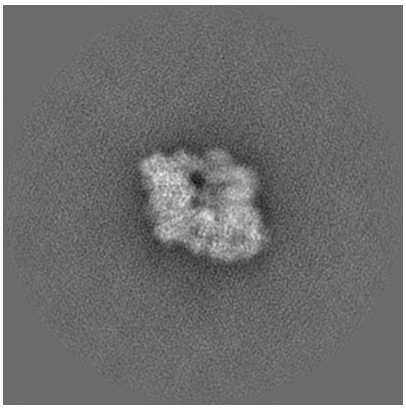
6.1.1 Primary map



X

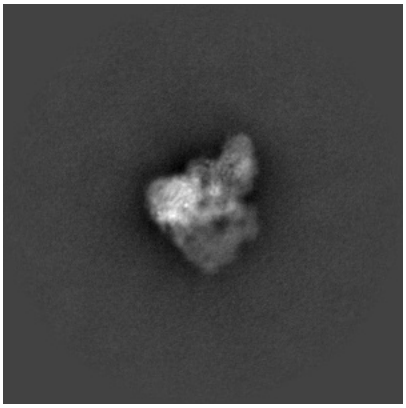


Y

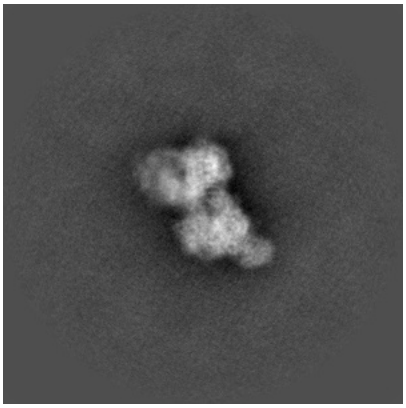


Z

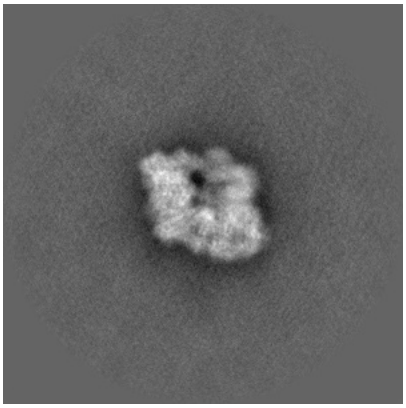
6.1.2 Raw map



X



Y

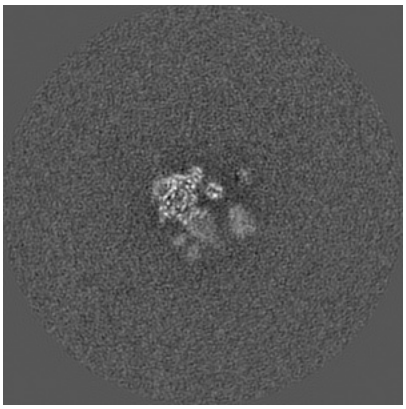


Z

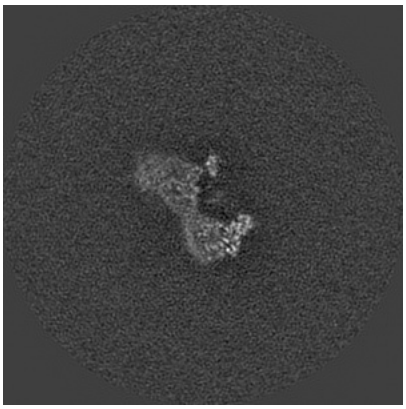
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

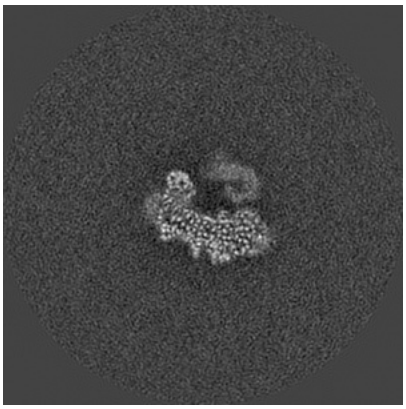
6.2.1 Primary map



X Index: 256

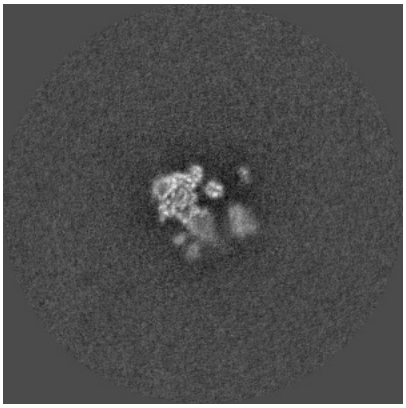


Y Index: 256

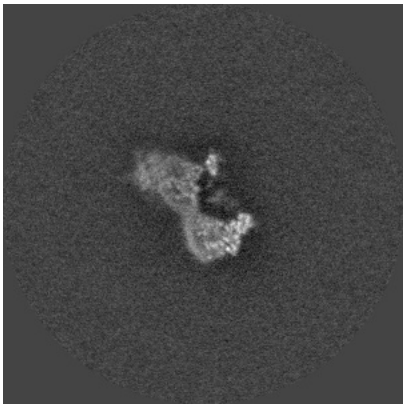


Z Index: 256

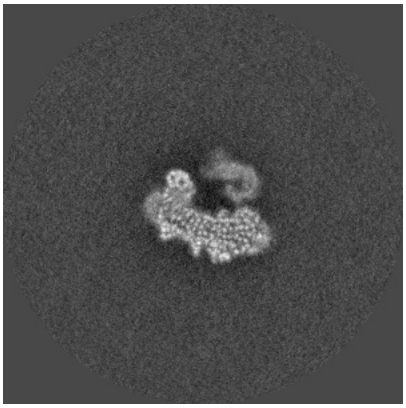
6.2.2 Raw map



X Index: 256



Y Index: 256

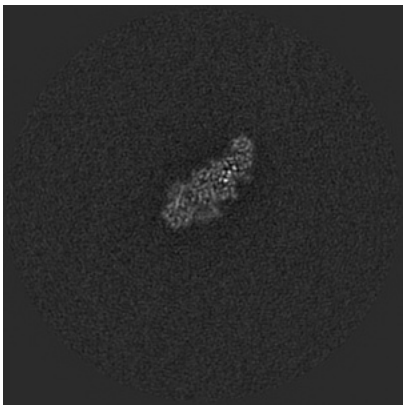


Z Index: 256

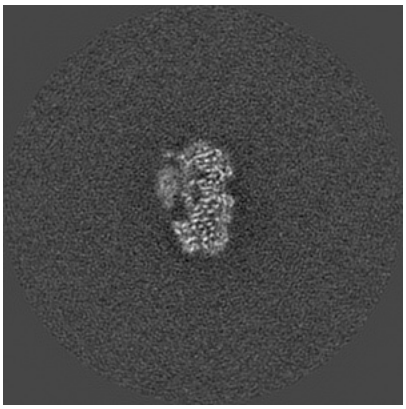
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

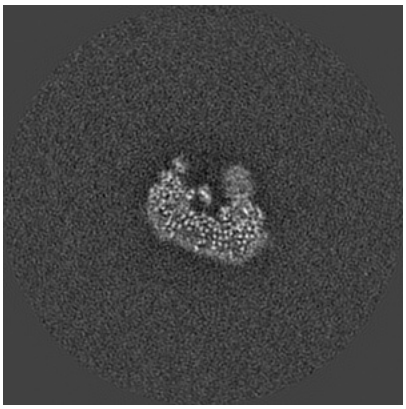
6.3.1 Primary map



X Index: 205

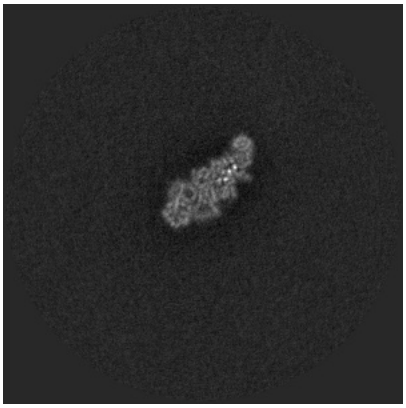


Y Index: 228

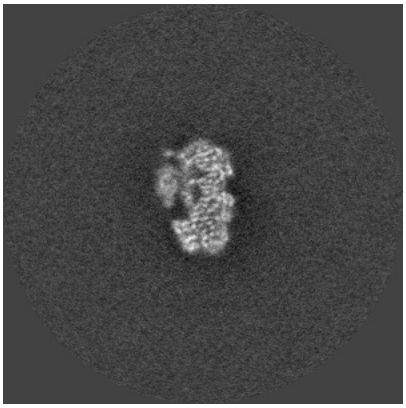


Z Index: 268

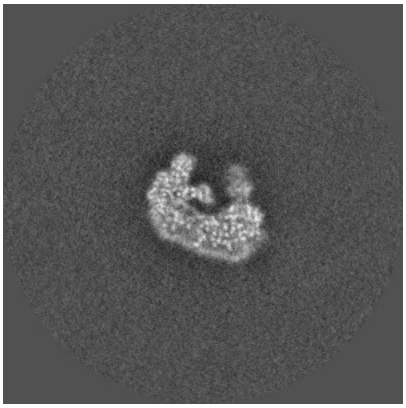
6.3.2 Raw map



X Index: 206



Y Index: 228

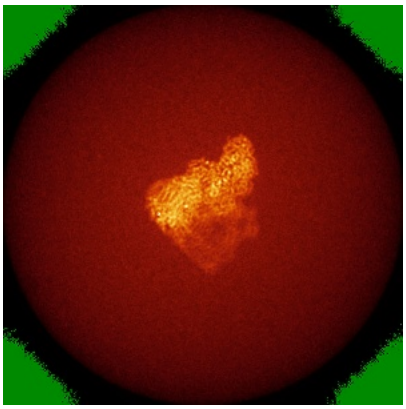


Z Index: 273

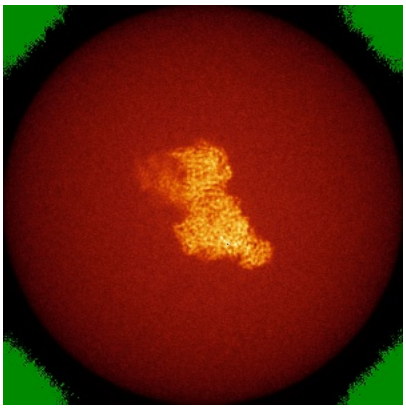
The images above show the largest variance slices of the map in three orthogonal directions.

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

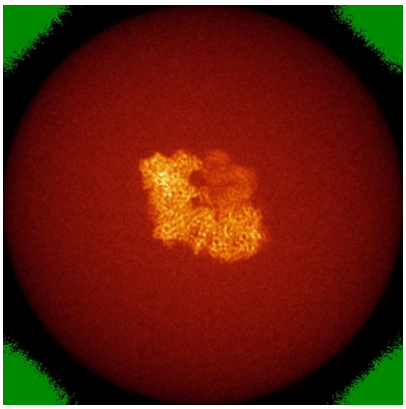
6.4.1 Primary map



X

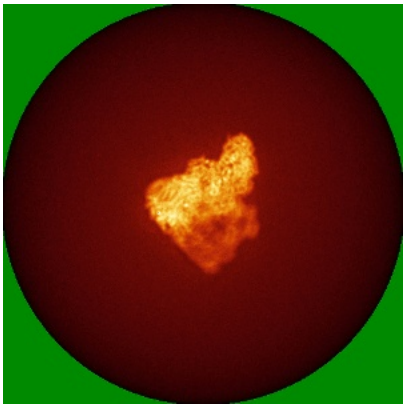


Y

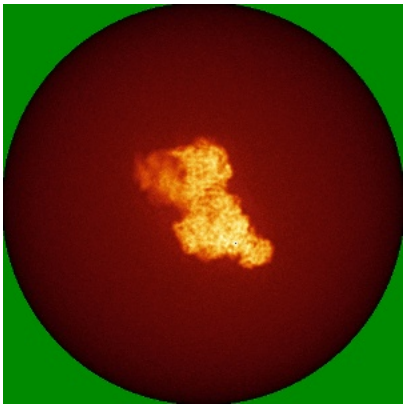


Z

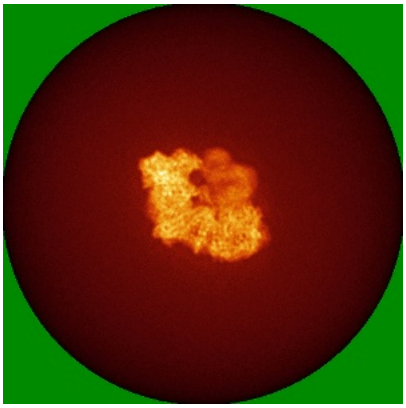
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

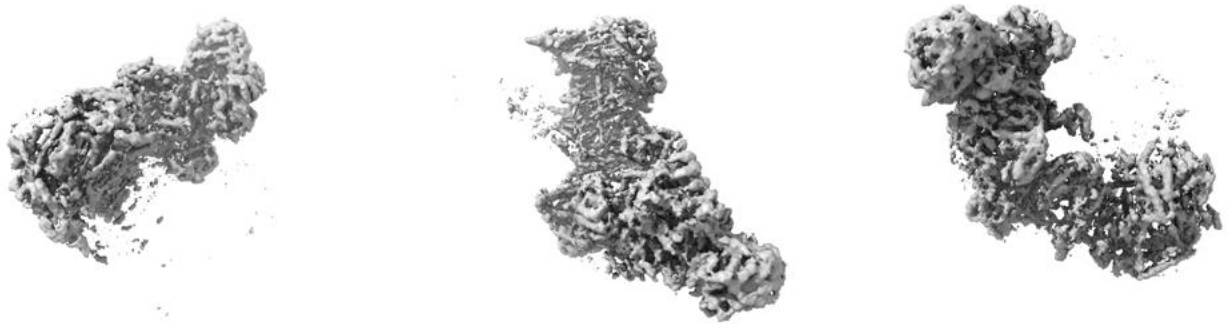
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

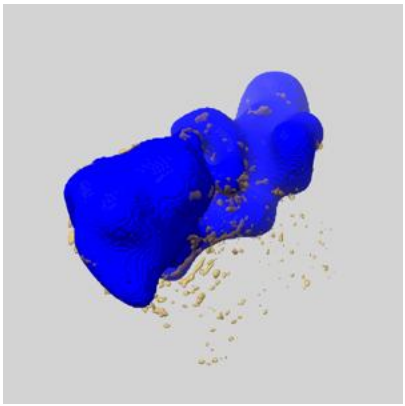
6.6 Mask visualisation (i)

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

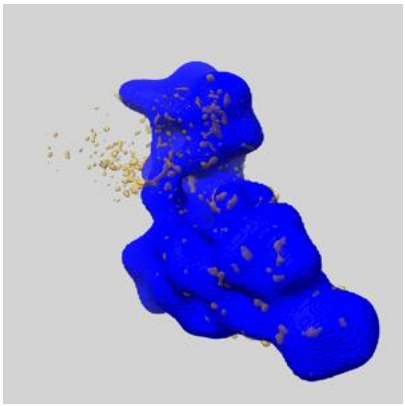
A mask typically either:

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

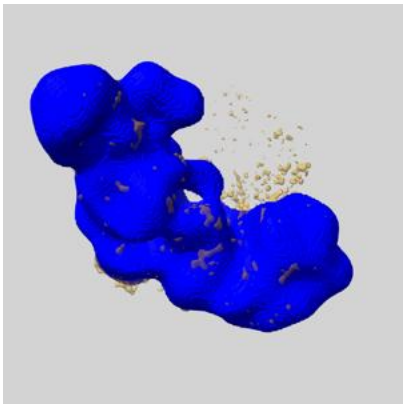
6.6.1 emd_4501_msk_1.map (i)



X



Y

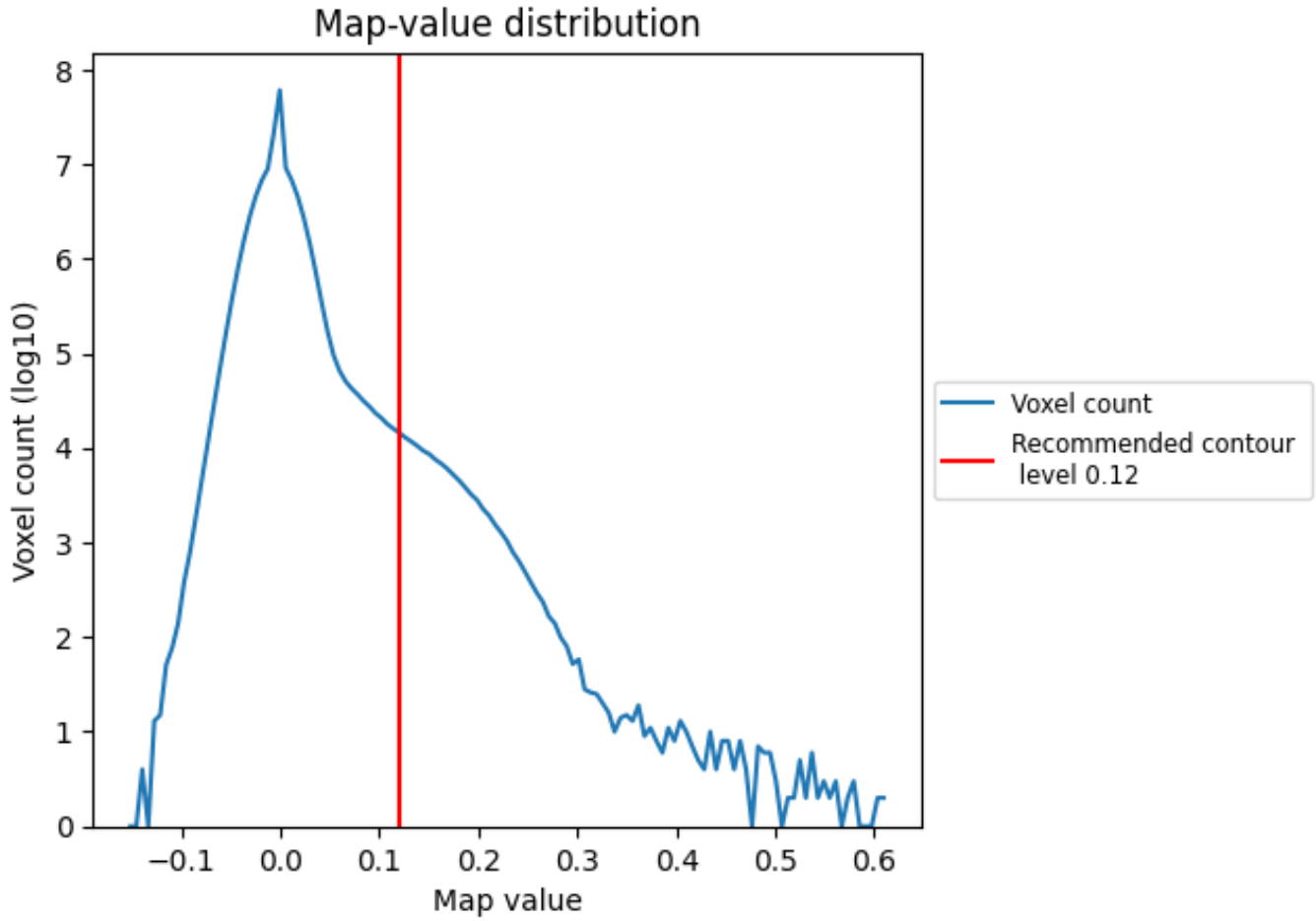


Z

7 Map analysis

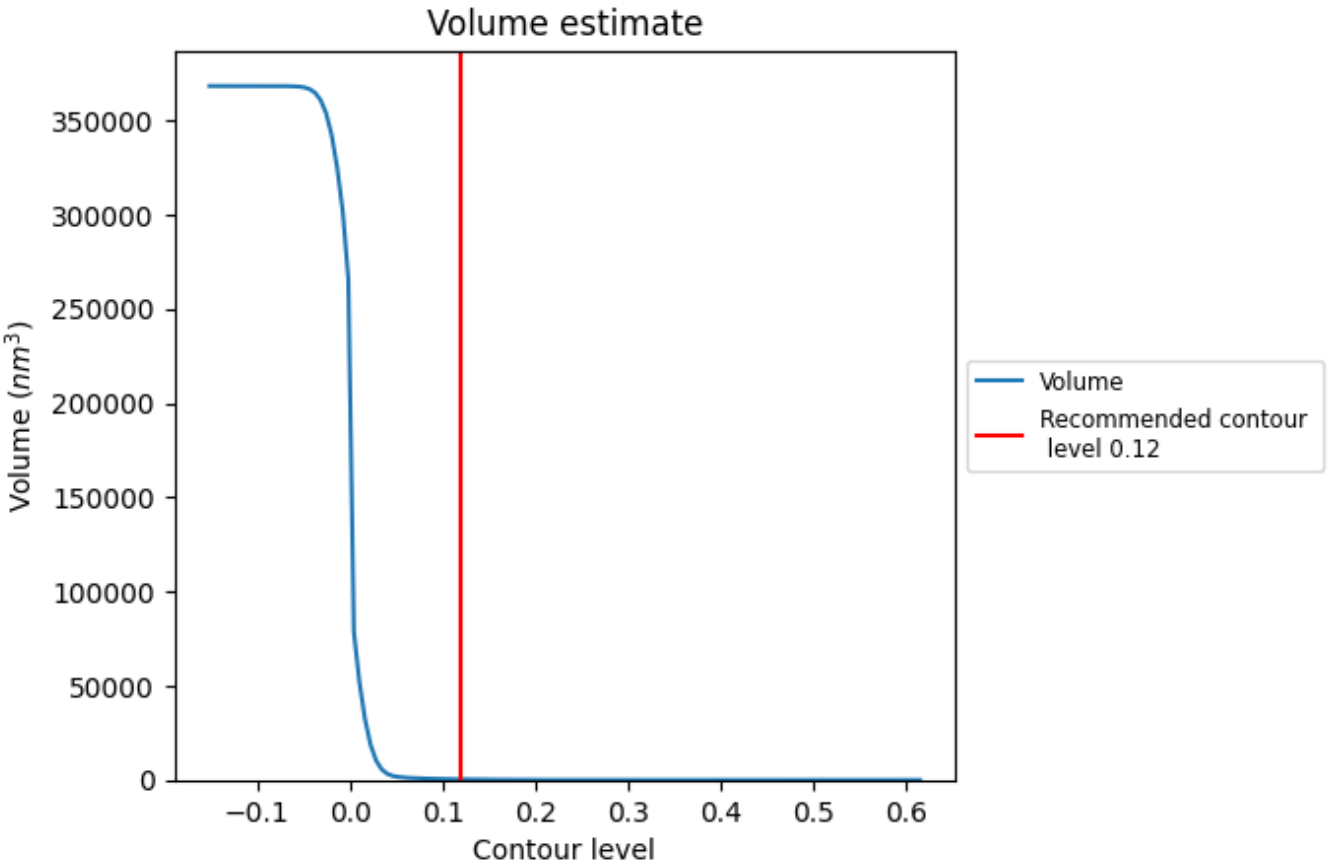
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

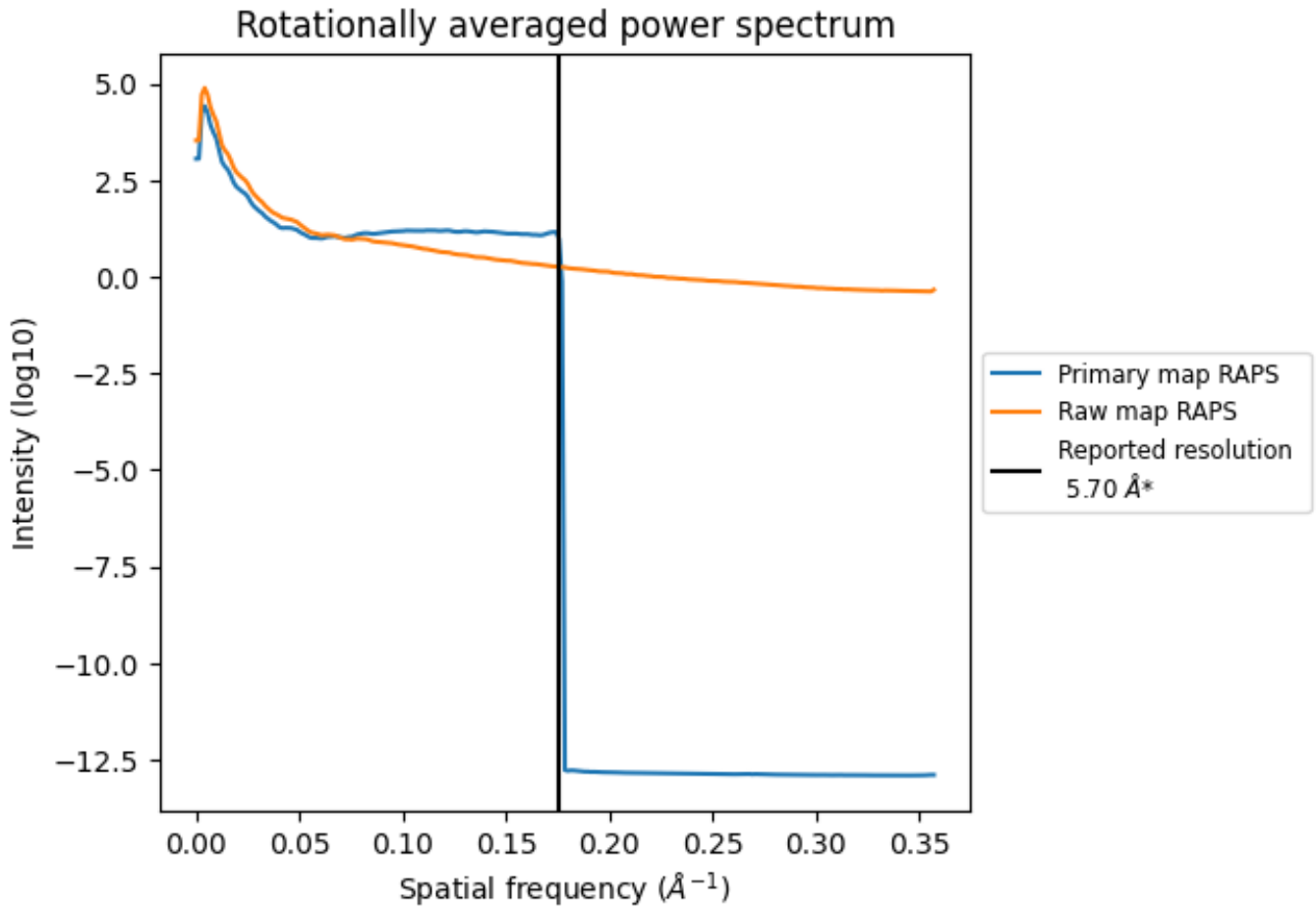
7.2 Volume estimate (i)



The volume at the recommended contour level is 329 nm^3; this corresponds to an approximate mass of 297 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)

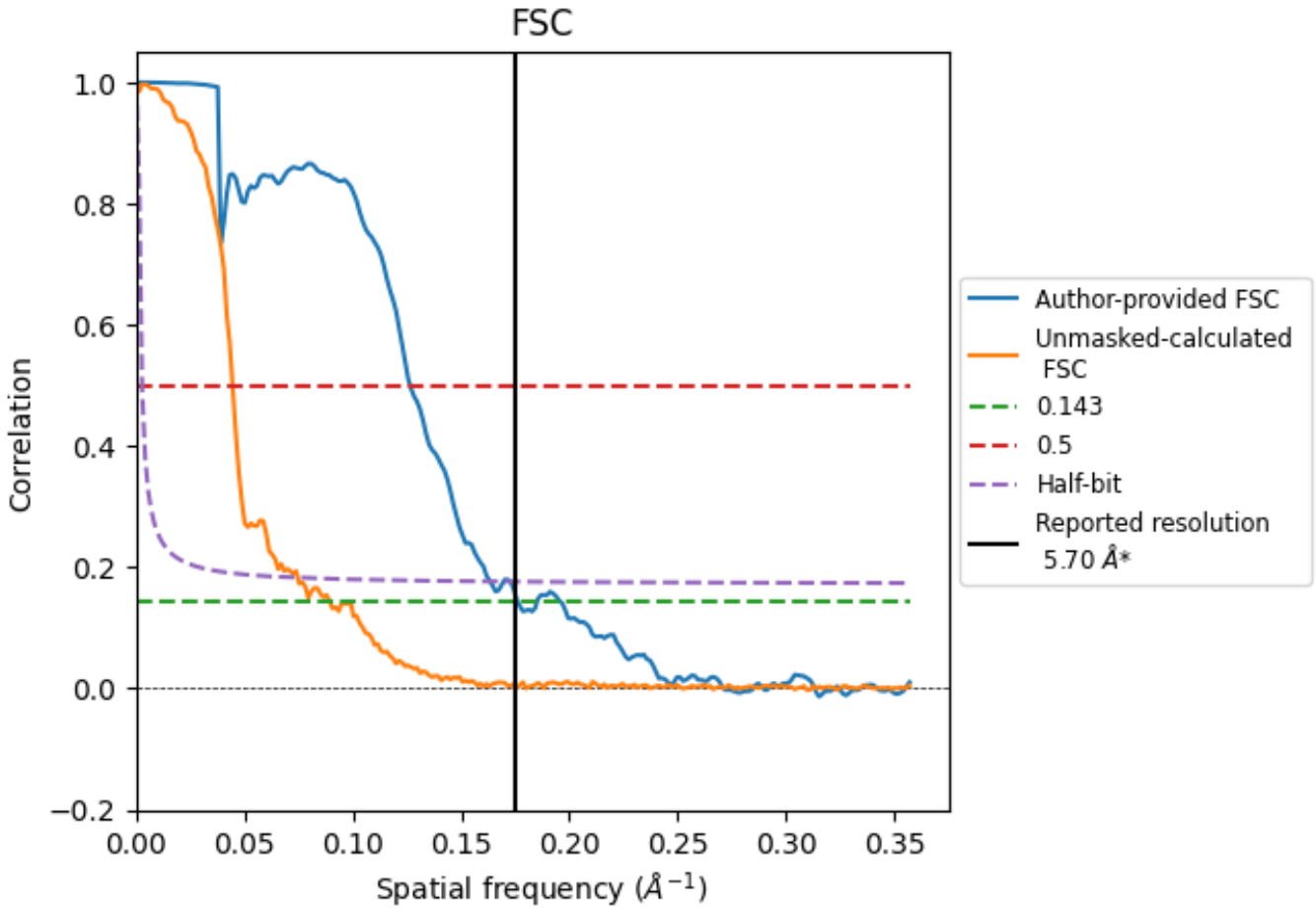


*Reported resolution corresponds to spatial frequency of 0.175 $Å^{-1}$

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 0.175 Å^{-1}

8.2 Resolution estimates (i)

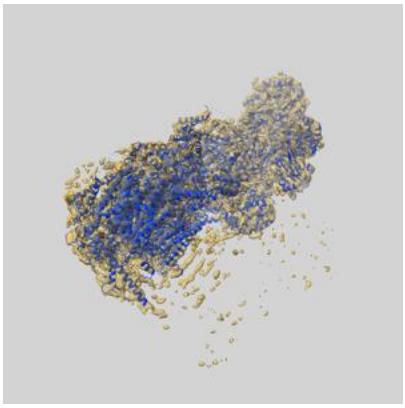
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.68	7.91	6.12
Unmasked-calculated*	11.19	22.47	13.39

*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 11.19 differs from the reported value 5.7 by more than 10 %

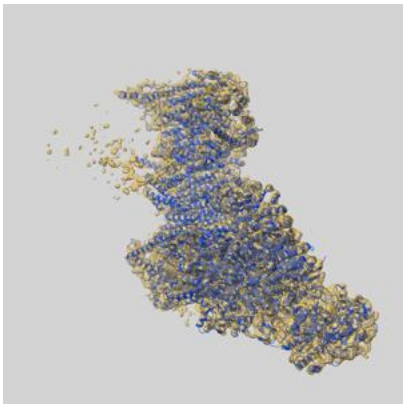
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4501 and PDB model 6QC9. Per-residue inclusion information can be found in section 3 on page 15.

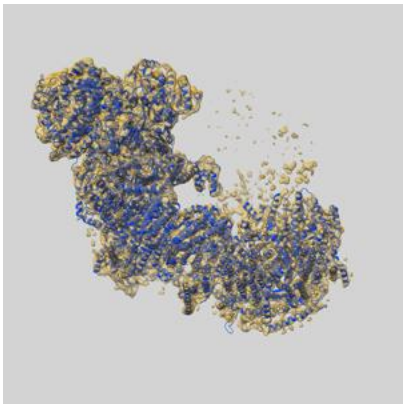
9.1 Map-model overlay



X



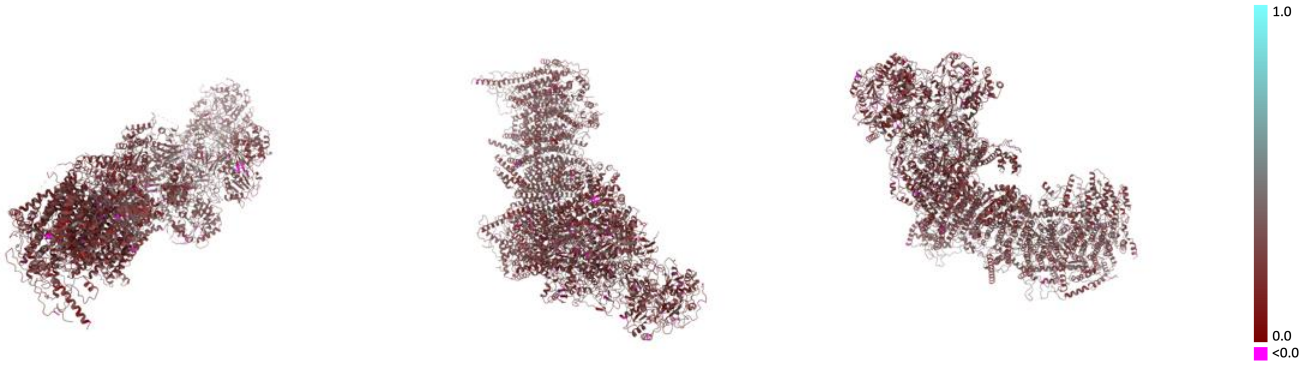
Y



Z

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

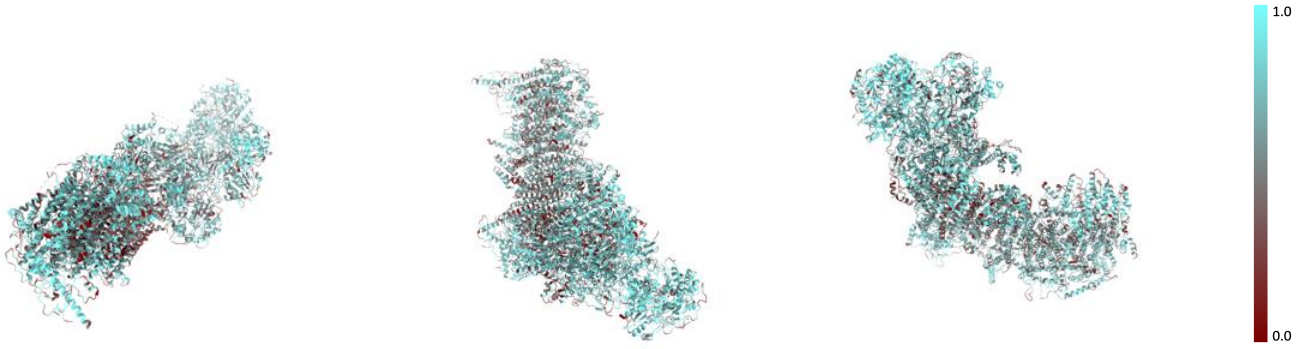
9.2 Q-score mapped to coordinate model



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.

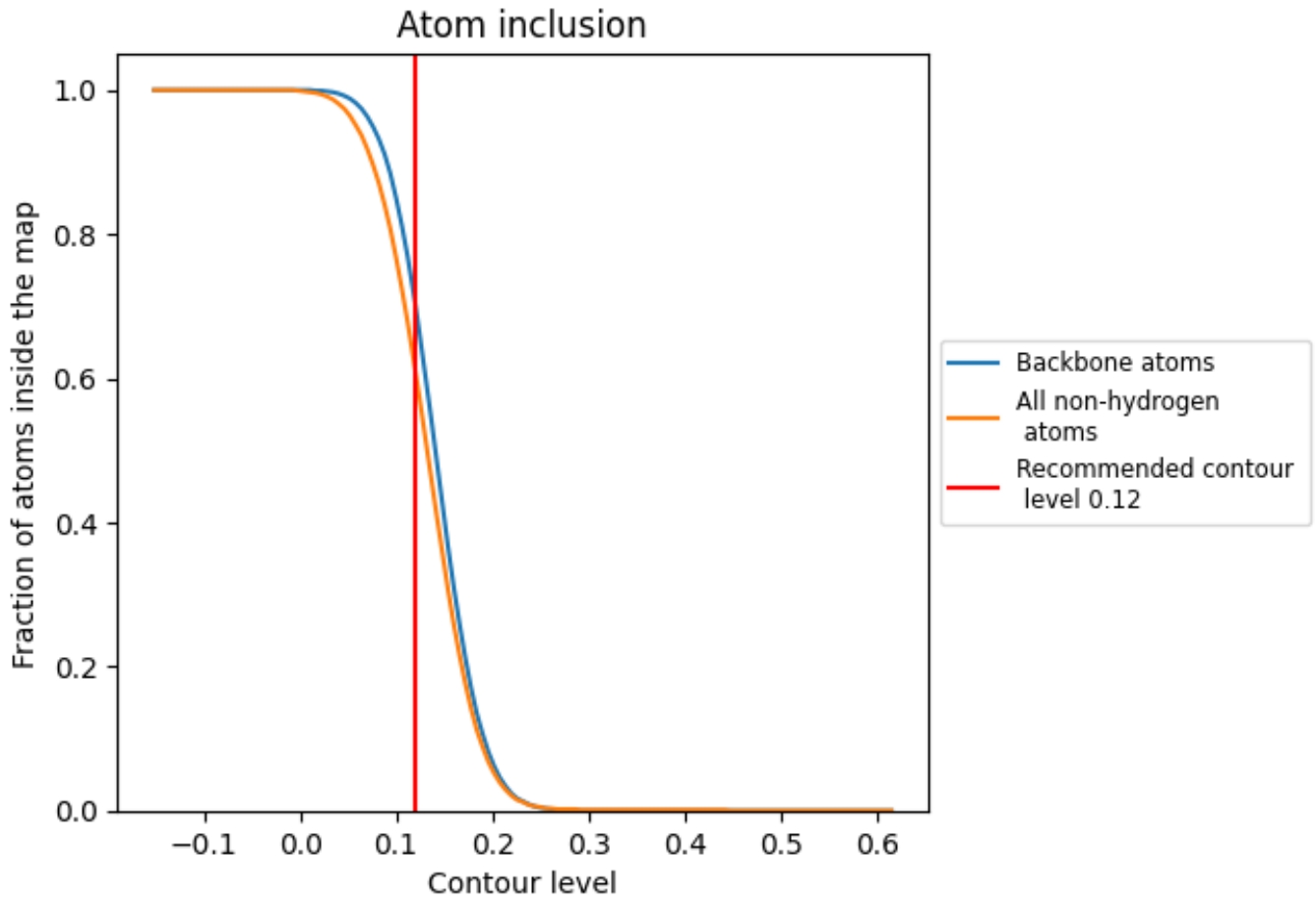
9.3 Atom inclusion mapped to coordinate model



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.2650
4L	0.4550	0.2580
A1	0.6620	0.2610
A2	0.7560	0.2360
A3	0.5940	0.2540
A5	0.7000	0.2790
A6	0.6260	0.2590
A7	0.4540	0.2830
A8	0.7030	0.2820
A9	0.6150	0.2710
AA	0.5640	0.2450
AB	0.5920	0.2610
AJ	0.5900	0.2670
AK	0.4400	0.2510
AL	0.4680	0.2580
AM	0.6680	0.2690
B1	0.5700	0.2690
B2	0.6280	0.2590
B3	0.5590	0.2660
B4	0.5620	0.2630
B5	0.6970	0.2700
B6	0.6330	0.2690
B7	0.6720	0.2400
B8	0.5730	0.2940
B9	0.6450	0.2790
BJ	0.7080	0.2640
BK	0.5870	0.2790
C1	0.6430	0.2510
C2	0.6200	0.2760
D1	0.5690	0.2610
D2	0.5510	0.2610
D3	0.5210	0.2630
D4	0.5770	0.2660
D5	0.5670	0.2530
D6	0.4080	0.2490



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Chain	Atom inclusion	Q-score
S1	0.6690	0.2690
S2	0.5850	0.2730
S3	0.6690	0.2930
S4	0.6290	0.3040
S5	0.6390	0.2460
S6	0.5770	0.2830
S7	0.6090	0.2630
S8	0.6970	0.2620
V1	0.7290	0.2540
V2	0.7250	0.2600
V3	0.7450	0.2600