



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 09:40 PM UTC

PDB ID : 9BWD / pdb_00009bwd
EMDB ID : EMD-44967
Title : Cryo-EM structure of respiratory supercomplex I
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-05-21
Resolution : 2.88 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 ⓘ 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:

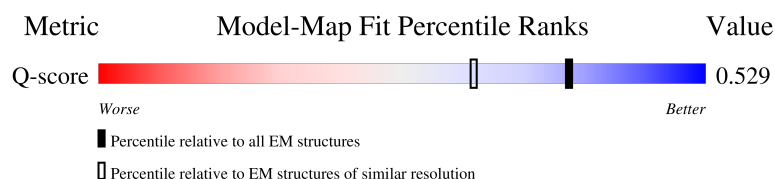
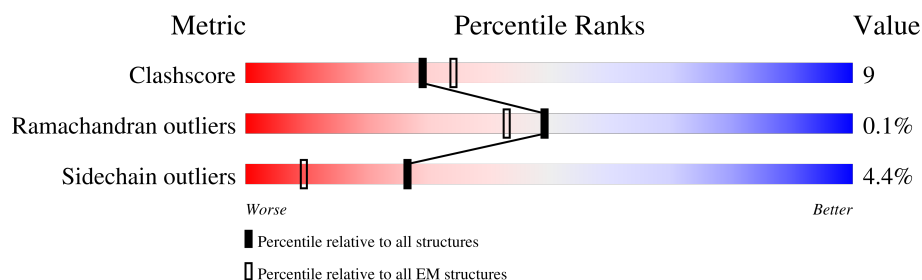
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

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

Mol	Chain	Length	Quality of chain
1	B	464	
2	C	469	
3	D	264	
4	F	123	

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Mol	Chain	Length	Quality of chain
5	G	727	
6	I	258	
7	J	175	
8	K	145	
9	M	113	
10	N	116	
11	O	156	
11	X	156	
12	P	99	
13	Q	154	
14	U	357	
15	V	141	
16	Y	105	
17	Z	114	
18	a	189	
19	c	186	
20	H	212	
21	S	70	
22	E	249	
23	L	372	
24	T	169	
25	W	144	
26	b	188	
27	d	176	
28	e	154	

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Mol	Chain	Length	Quality of chain
29	f	76	
30	g	122	
31	h	106	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	58	
38	o	129	
39	p	221	
40	q	459	
41	r	318	
42	s	249	
43	t	137	
44	R	110	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	SF4	B	502	-	-	X	-
46	SF4	H	301	-	-	X	-
47	FES	E	301	-	-	X	-

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 65929 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	B	429	Total	C	N	O	S	0	0
			3300	2084	587	609	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	430	Total	C	N	O	S	0	0
			3453	2207	592	630	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	208	Total	C	N	O	S	0	0
			1737	1123	298	314	2		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	93	Total	C	N	O	S	0	0
			720	439	135	143	3		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	684	Total	C	N	O	S	0	0
			5260	3298	917	1006	39		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	118	Total	C	N	O	S	0	0
			963	608	173	179	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	144	Total	C	N	O	S	0	0
			1203	769	217	212	5		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	96	Total	C	N	O	S	0	0
			774	487	146	138	3		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	112	Total	C	N	O	S	0	0
			911	588	154	166	3		

- Molecule 11 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	83	Total	C	N	O	S	0	0
			668	431	99	133	5		
11	X	85	Total	C	N	O	S	0	0
			689	445	101	138	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	83	Total	C	N	O	S	0	0
			669	419	125	123	2		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	112	Total	C	N	O	S	0	0
			955	610	176	164	5		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	318	Total	C	N	O	S	0	0
			2573	1638	437	488	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	66	Total	C	N	O	S	0	0
			571	378	94	98	1		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	77	Total	C	N	O	S	0	0
			620	407	104	108	1		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	153	Total	C	N	O	S	0	0
			1291	838	208	237	8		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	340	Total	C	N	O	S	0	0
			2735	1771	479	476	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	82	Total	C	N	O	S	0	0
			638	414	109	114	1		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	140	Total	C	N	O	S	0	0
			1162	749	201	203	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	111	Total	C	N	O	S	0	0
			946	623	163	159	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	169	Total	C	N	O	S	0	0
			1426	895	259	264	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	99	Total	C	N	O	S	0	0
			826	530	137	155	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	46	Total	C	N	O	0	0
			391	259	67	65		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	114	Total	C	N	O	S	0	0
			905	610	133	155	7		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4785	3174	741	819	51		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	173	Total	C	N	O	S	0	0
			1321	888	187	234	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	126	Total	C	N	O		0	0
			1041	677	179	185			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	177	Total	C	N	O	S	0	0
			1529	979	278	264	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	459	Total	C	N	O	S	0	0
			3630	2410	572	609	39		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

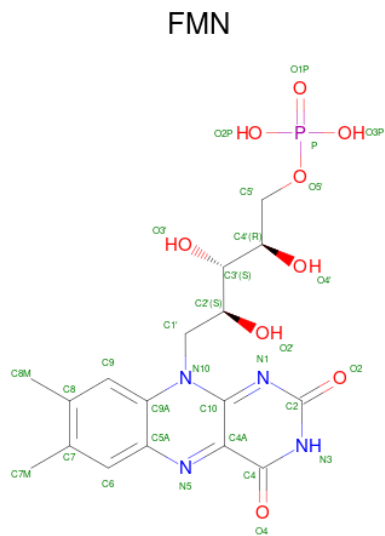
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	117	Total	C	N	O	S	0	0
			1014	632	193	180	9		

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

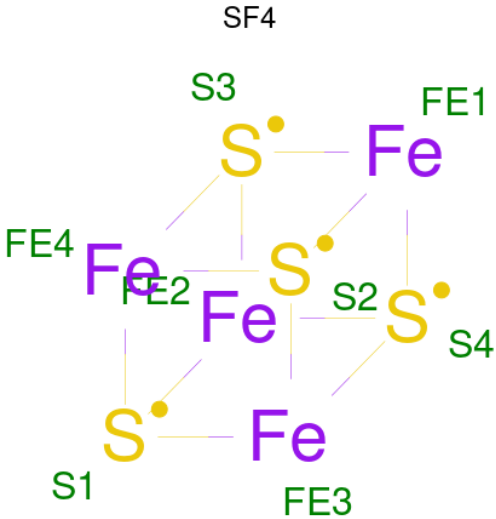
Mol	Chain	Residues	Atoms					AltConf	Trace
44	R	35	Total	C	N	O	S	0	0
			295	185	55	54	1		

- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

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



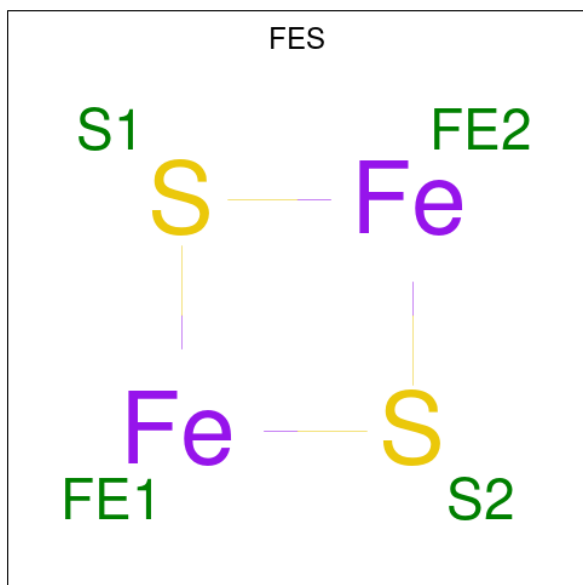
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total 8	Fe 4	S 4	0
46	G	1	Total 8	Fe 4	S 4	0
46	G	1	Total 8	Fe 4	S 4	0

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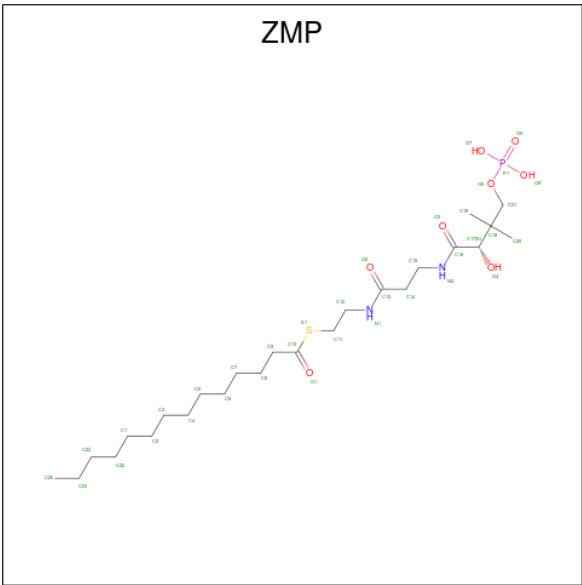
Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	Fe	S	0
			8	4	4	
46	H	1	Total	Fe	S	0
			8	4	4	
46	H	1	Total	Fe	S	0
			8	4	4	

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



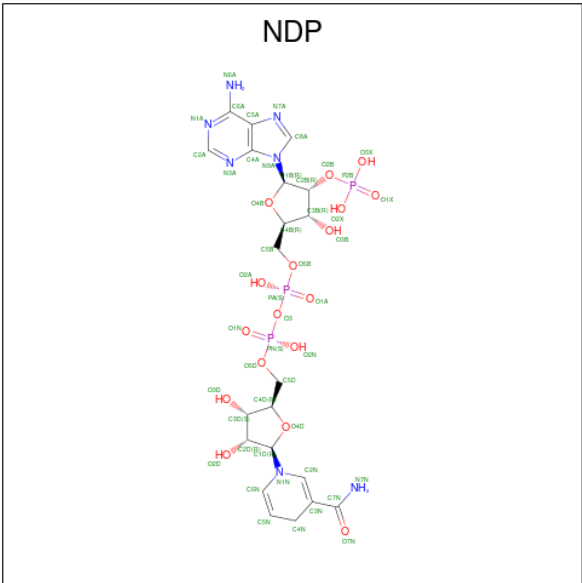
Mol	Chain	Residues	Atoms			AltConf
47	G	1	Total	Fe	S	0
			4	2	2	
47	E	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $\text{C}_{25}\text{H}_{49}\text{N}_2\text{O}_8\text{PS}$).



Mol	Chain	Residues	Atoms					AltConf	
48	Q	1	Total	C	N	O	P	S	0
			30	18	2	8	1	1	

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

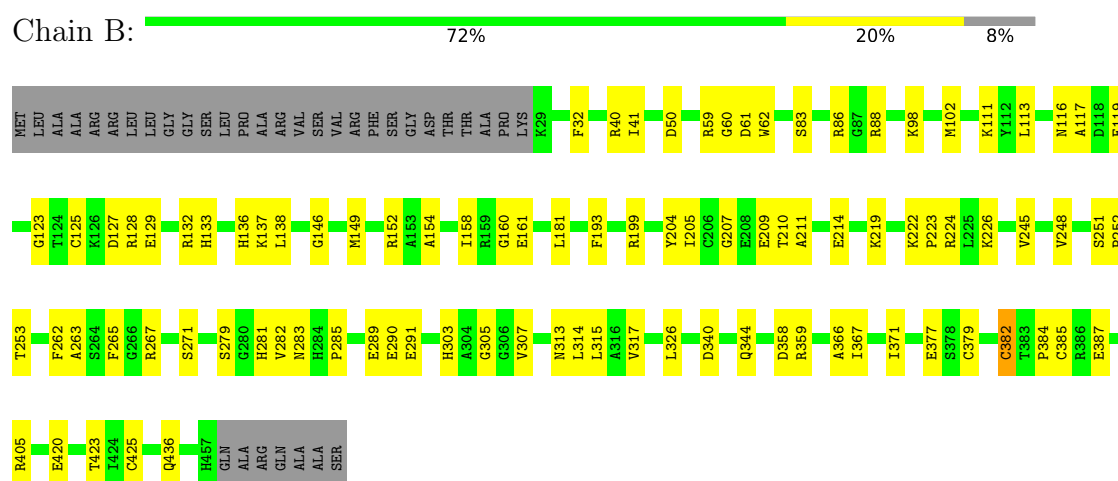


Mol	Chain	Residues	Atoms					AltConf
49	L	1	Total	C	N	O	P	0
			48	21	7	17	3	

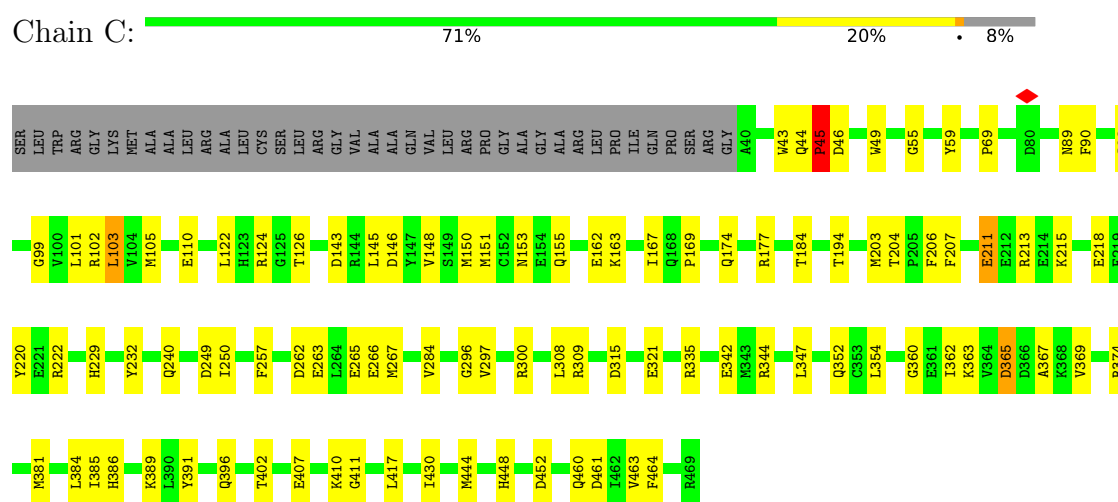
3 Residue-property plots

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

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

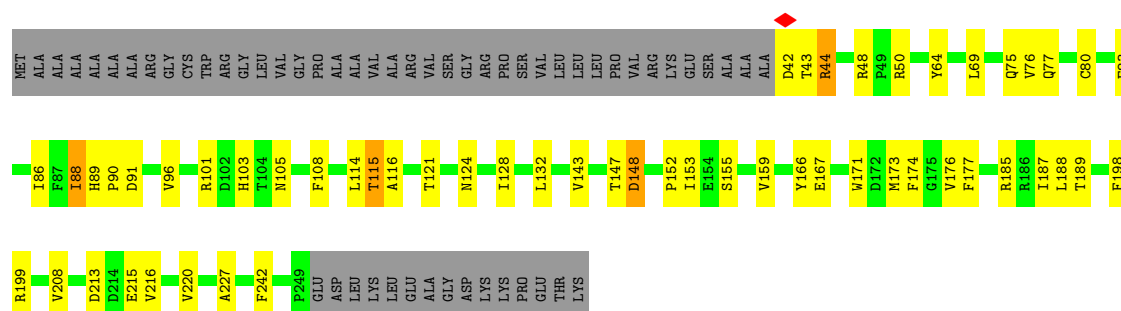


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

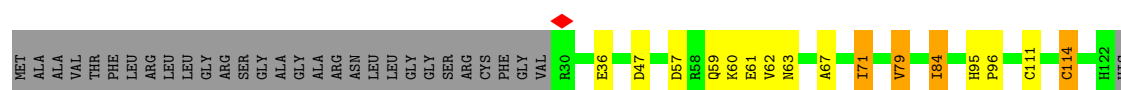


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

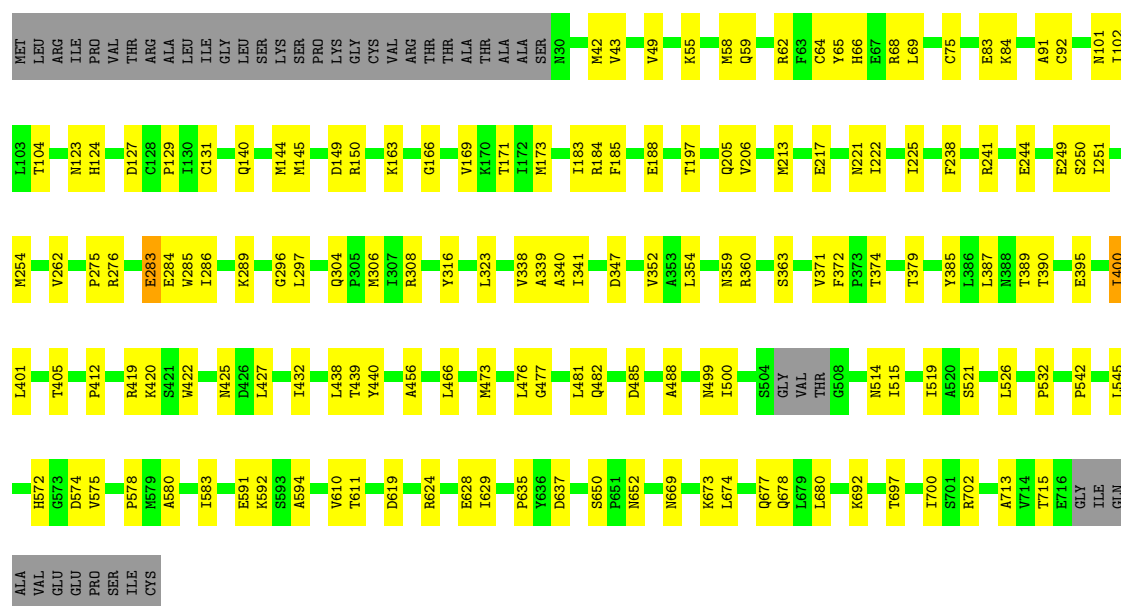




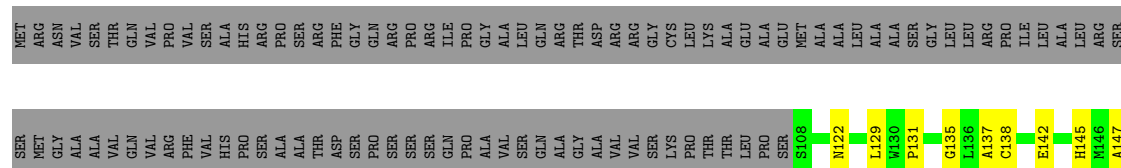
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 5: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

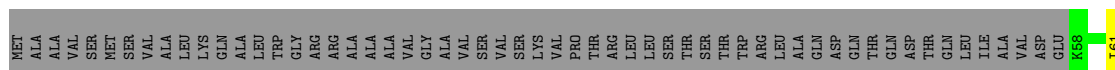


- Molecule 6: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

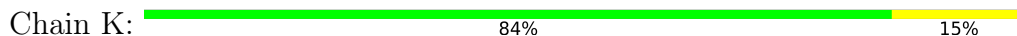




- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



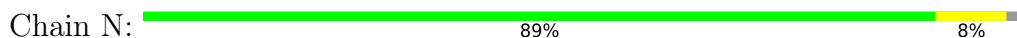
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



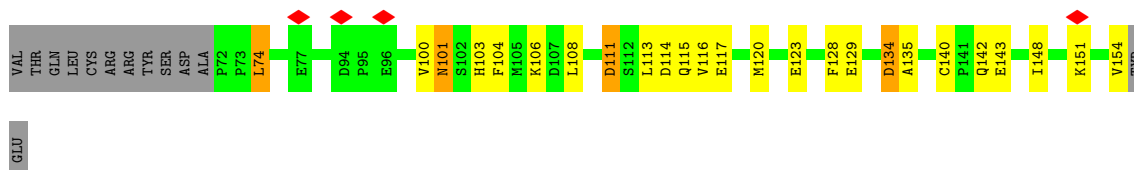
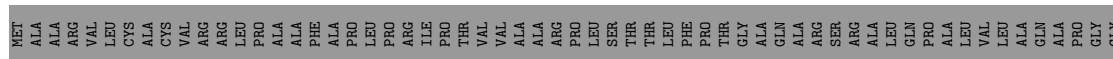
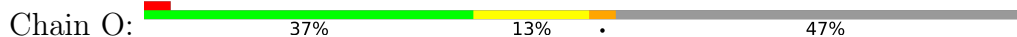
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



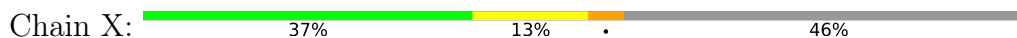
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

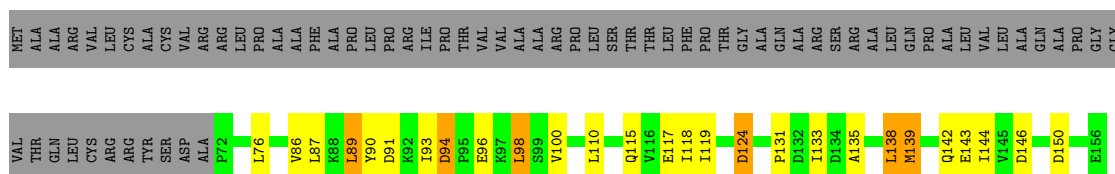


- Molecule 11: Acyl carrier protein



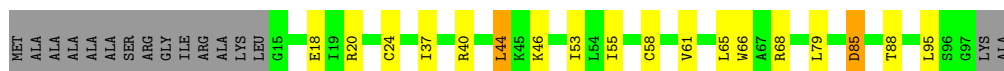
- Molecule 11: Acyl carrier protein





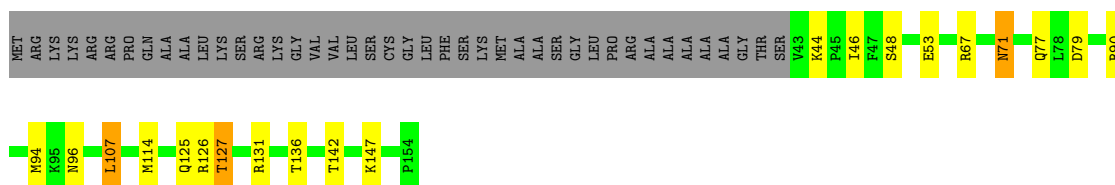
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P: 66% 16% 16%



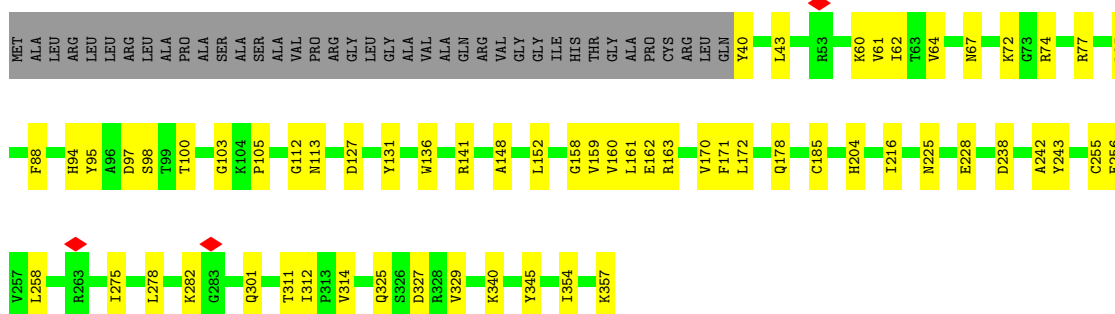
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q: 60% 11% 27%



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain U: 72% 17% 11%



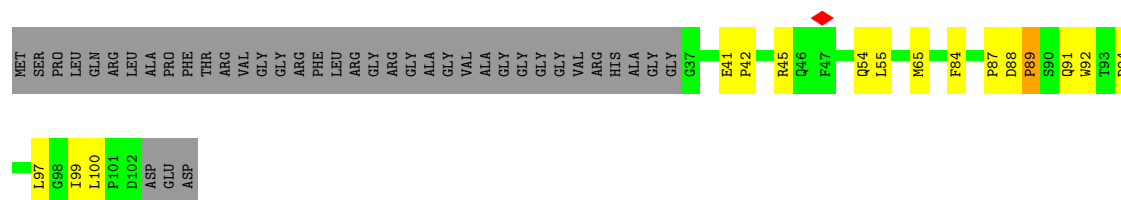
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 81% 18% ..

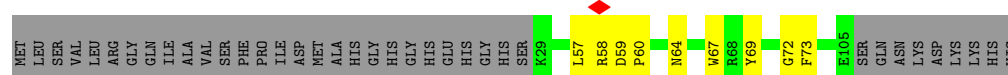


- Molecule 16: NADH:ubiquinone oxidoreductase subunit B2

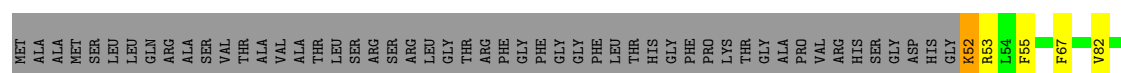
Chain Y: 48% 14% 37%



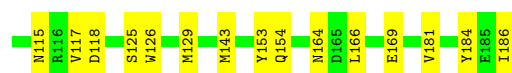
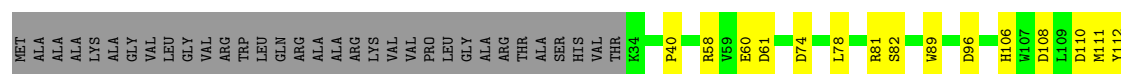
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



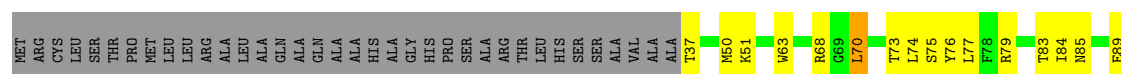
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

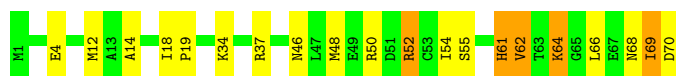


- Molecule 20: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



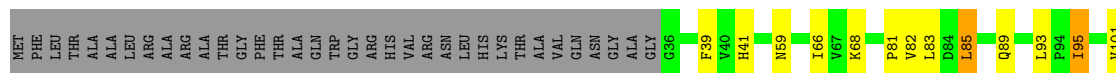
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 



- Molecule 22: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 




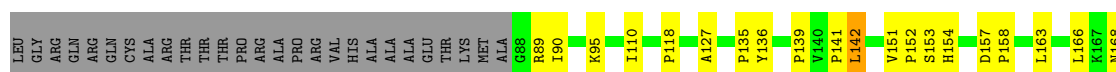
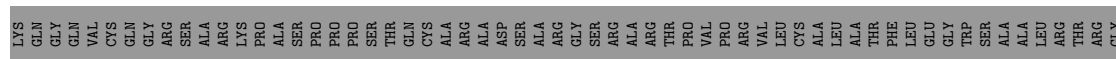
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain L: 




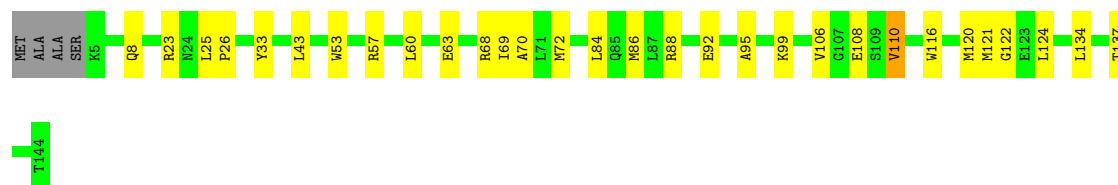
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T: 

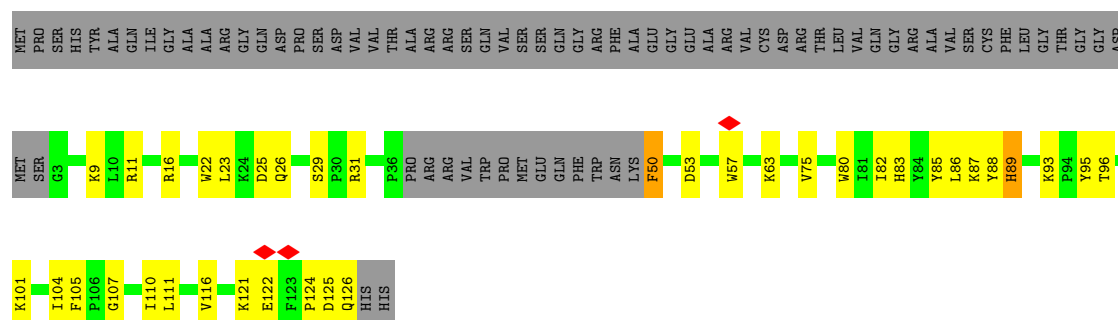


- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

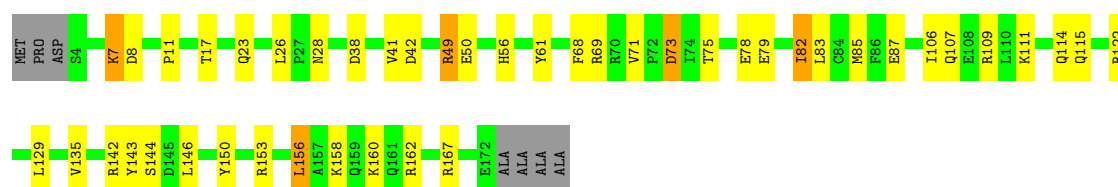
Chain W: 



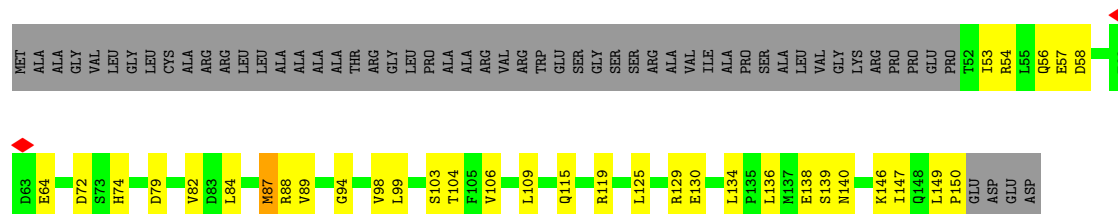
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



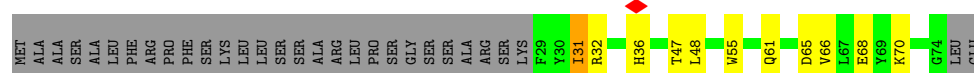
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10




- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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




- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  79% 18% ..



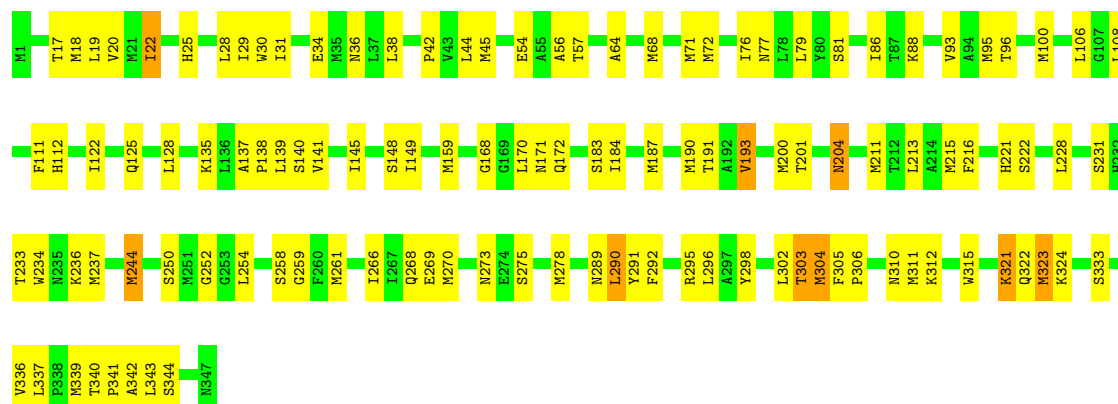
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  87% 11% ..




- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  66% 31% .



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  70% 26% ..



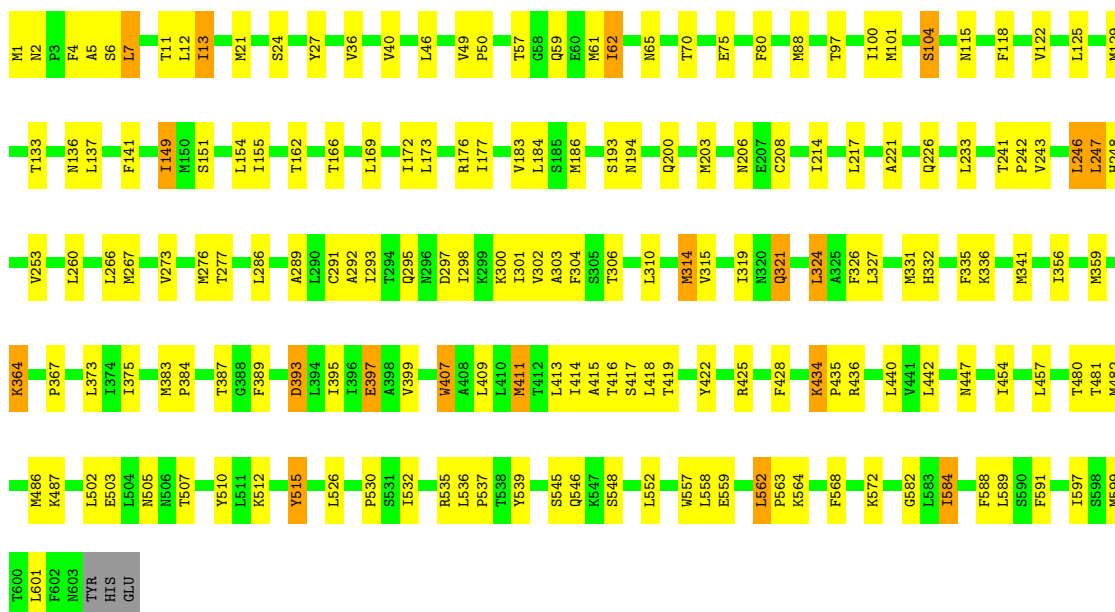
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  65% 33% .

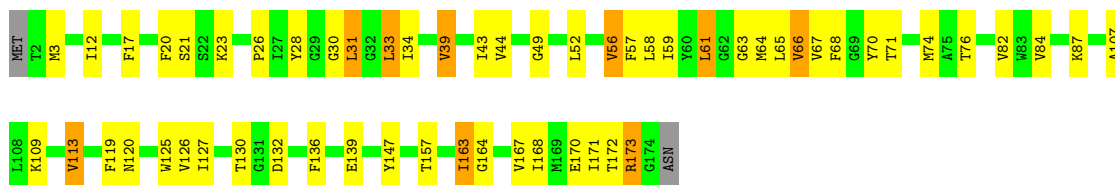


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  70% 26% .



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



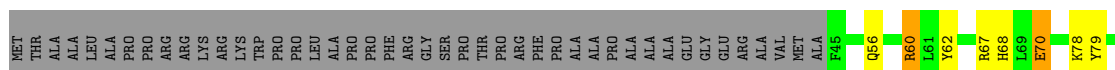
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

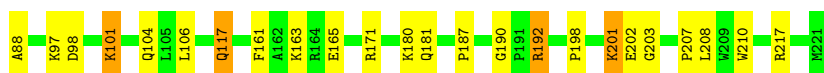


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

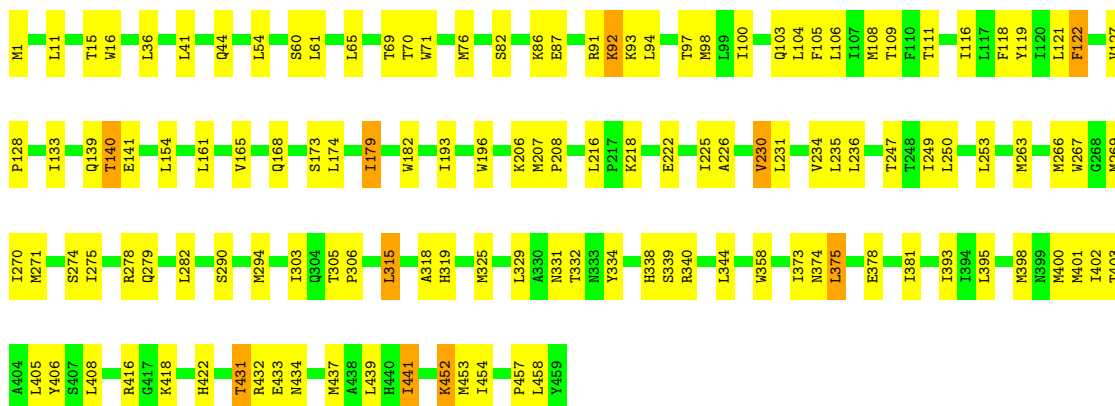


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

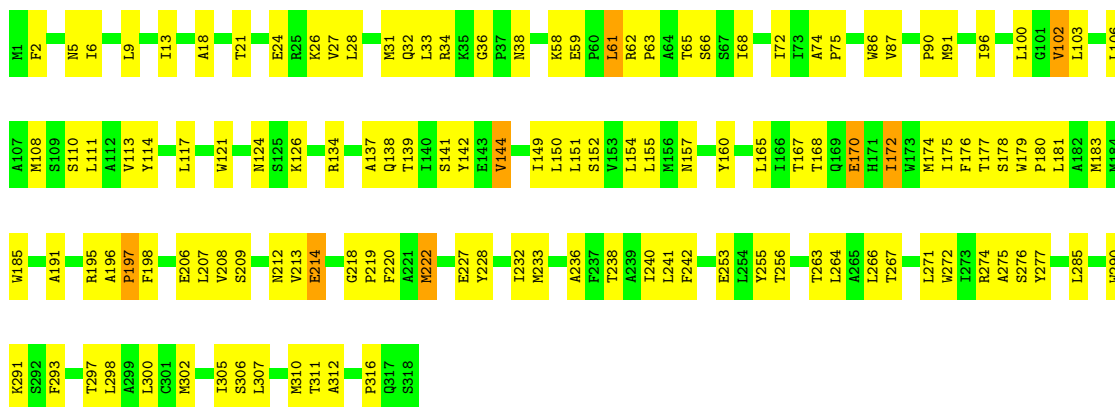




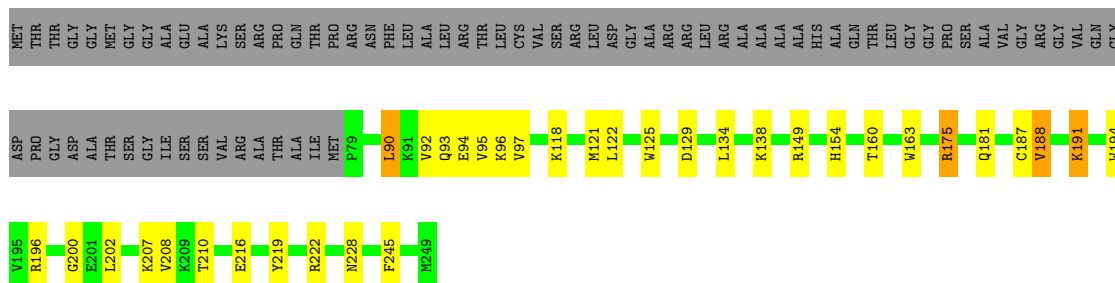
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4



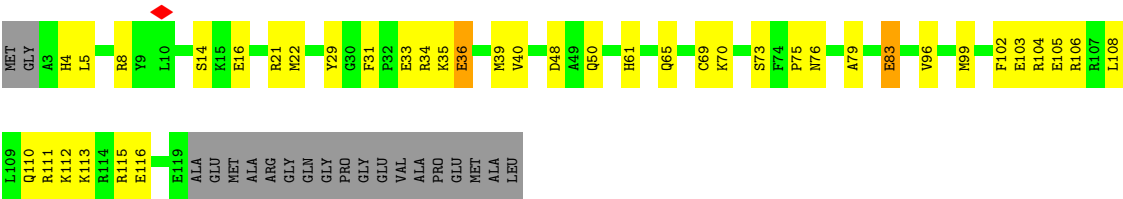
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1



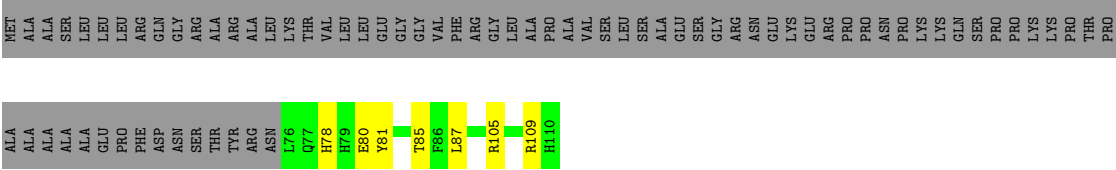
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.907	Depositor
Minimum map value	-0.559	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.13	0/3375	0.32	0/4561
2	C	0.20	0/3545	0.37	1/4805 (0.0%)
3	D	0.13	0/1788	0.31	0/2435
4	F	0.36	0/733	0.54	0/988
5	G	0.21	0/5347	0.37	0/7243
6	I	0.17	0/1280	0.34	0/1730
7	J	0.11	0/986	0.28	0/1329
8	K	0.17	0/1244	0.30	0/1693
9	M	0.12	0/792	0.34	0/1069
10	N	0.12	0/930	0.26	0/1258
11	O	0.09	0/679	0.30	0/916
11	X	0.11	0/701	0.27	0/946
12	P	0.29	0/680	0.46	0/916
13	Q	0.10	0/979	0.27	0/1317
14	U	0.35	0/2633	0.47	0/3565
15	V	0.17	0/1042	0.28	0/1411
16	Y	0.43	0/597	0.58	0/818
17	Z	0.09	0/639	0.24	0/864
18	a	0.12	0/1184	0.29	0/1603
19	c	0.29	0/1346	0.42	0/1840
20	H	0.49	0/1443	0.69	0/1952
21	S	0.38	0/577	0.55	0/777
22	E	0.24	0/1698	0.42	2/2311 (0.1%)
23	L	0.38	0/2812	0.49	0/3812
24	T	0.14	0/659	0.39	0/905
25	W	0.12	0/1193	0.28	0/1609
26	b	0.14	0/976	0.40	0/1328
27	d	0.16	0/1458	0.32	0/1965
28	e	0.24	0/849	0.38	0/1153
29	f	0.10	0/404	0.29	0/547
30	g	0.19	0/1031	0.33	0/1394
31	h	0.15	0/889	0.29	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.27	0/2773	0.43	0/3768
33	j	0.15	0/929	0.35	0/1269
34	k	0.36	0/759	0.58	0/1029
35	l	0.29	0/4914	0.50	0/6683
36	m	0.33	0/1356	0.53	0/1839
37	n	0.20	0/491	0.49	0/663
38	o	0.13	0/1070	0.36	0/1451
39	p	0.10	0/1585	0.31	0/2148
40	q	0.28	0/3721	0.47	0/5073
41	r	0.42	0/2581	0.62	0/3529
42	s	0.14	0/1436	0.31	0/1938
43	t	0.31	0/1038	0.48	0/1389
44	R	0.11	0/304	0.31	0/410
All	All	0.25	0/67446	0.42	3/91439 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	U	0	1
20	H	0	3
21	S	0	2
23	L	0	1
27	d	0	1
32	i	0	1
35	l	0	1
41	r	0	1
All	All	0	11

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	E	247	ALA	CB-CA-C	-5.71	109.97	116.54
2	C	148	VAL	N-CA-C	-5.16	107.80	112.96
22	E	179	ALA	N-CA-C	-5.00	104.44	110.44

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	H	105	ARG	Sidechain
20	H	96	ARG	Sidechain
20	H	98	ARG	Sidechain
21	S	50	ARG	Sidechain
14	U	163	ARG	Sidechain

5.2 Too-close contacts

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	B	3300	0	3263	77	0
2	C	3453	0	3389	77	0
3	D	1737	0	1691	37	0
4	F	720	0	683	16	0
5	G	5260	0	5287	99	0
6	I	1249	0	1254	34	0
7	J	963	0	962	23	0
8	K	1203	0	1161	16	0
9	M	774	0	801	13	0
10	N	911	0	950	5	0
11	O	668	0	672	17	0
11	X	689	0	687	19	0
12	P	669	0	675	12	0
13	Q	955	0	960	21	0
14	U	2573	0	2534	38	0
15	V	1021	0	1025	13	0
16	Y	571	0	522	18	0
17	Z	620	0	602	8	0
18	a	1151	0	1164	23	0
19	c	1291	0	1185	26	0
20	H	1412	0	1366	53	0
21	S	562	0	557	13	0
22	E	1658	0	1662	44	0
23	L	2735	0	2751	50	0
24	T	638	0	637	20	0
25	W	1162	0	1156	31	0
26	b	946	0	963	28	0
27	d	1426	0	1394	37	0
28	e	826	0	788	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	f	391	0	392	7	0
30	g	1000	0	994	19	0
31	h	867	0	871	14	0
32	i	2710	0	2874	84	0
33	j	905	0	945	34	0
34	k	748	0	799	39	0
35	l	4785	0	4935	121	0
36	m	1321	0	1320	58	0
37	n	479	0	486	9	0
38	o	1041	0	1053	14	0
39	p	1529	0	1465	23	0
40	q	3630	0	3837	82	0
41	r	2508	0	2607	104	0
42	s	1398	0	1374	32	0
43	t	1014	0	983	30	0
44	R	295	0	279	4	0
45	B	31	0	19	1	0
46	B	8	0	0	21	0
46	G	16	0	0	0	0
46	H	16	0	0	8	0
46	I	8	0	0	1	0
47	E	4	0	0	9	0
47	G	4	0	0	0	0
48	Q	30	0	30	1	0
49	L	48	0	26	3	0
All	All	65929	0	66030	1224	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 9.

The worst 5 of 1224 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)
1:B:425:CYS:SG	46:B:502:SF4:FE1	1.08	1.46
1:B:379:CYS:SG	46:B:502:SF4:FE3	1.10	1.41
22:E:140:CYS:SG	47:E:301:FES:FE2	1.12	1.38
1:B:382:CYS:SG	46:B:502:SF4:FE4	1.15	1.38
22:E:135:CYS:SG	47:E:301:FES:FE2	1.40	1.13

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	427/464 (92%)	423 (99%)	4 (1%)	0	100	100
2	C	428/469 (91%)	414 (97%)	13 (3%)	1 (0%)	43	70
3	D	206/264 (78%)	199 (97%)	7 (3%)	0	100	100
4	F	91/123 (74%)	89 (98%)	2 (2%)	0	100	100
5	G	680/727 (94%)	668 (98%)	11 (2%)	1 (0%)	48	74
6	I	154/258 (60%)	149 (97%)	5 (3%)	0	100	100
7	J	116/175 (66%)	113 (97%)	3 (3%)	0	100	100
8	K	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
9	M	92/113 (81%)	88 (96%)	4 (4%)	0	100	100
10	N	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
11	O	81/156 (52%)	80 (99%)	1 (1%)	0	100	100
11	X	83/156 (53%)	79 (95%)	3 (4%)	1 (1%)	10	31
12	P	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
13	Q	110/154 (71%)	106 (96%)	4 (4%)	0	100	100
14	U	316/357 (88%)	309 (98%)	7 (2%)	0	100	100
15	V	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
16	Y	64/105 (61%)	59 (92%)	4 (6%)	1 (2%)	7	24
17	Z	75/114 (66%)	75 (100%)	0	0	100	100
18	a	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
19	c	151/186 (81%)	147 (97%)	4 (3%)	0	100	100
20	H	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
21	S	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
22	E	212/249 (85%)	201 (95%)	10 (5%)	1 (0%)	24	51
23	L	338/372 (91%)	326 (96%)	11 (3%)	1 (0%)	36	62
24	T	80/169 (47%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	W	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
26	b	107/188 (57%)	93 (87%)	13 (12%)	1 (1%)	14	38
27	d	167/176 (95%)	163 (98%)	4 (2%)	0	100	100
28	e	97/154 (63%)	90 (93%)	7 (7%)	0	100	100
29	f	44/76 (58%)	44 (100%)	0	0	100	100
30	g	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
31	h	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
32	i	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
33	j	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
34	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
35	l	601/606 (99%)	571 (95%)	29 (5%)	1 (0%)	43	70
36	m	171/175 (98%)	166 (97%)	5 (3%)	0	100	100
37	n	54/58 (93%)	52 (96%)	1 (2%)	1 (2%)	6	21
38	o	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
39	p	175/221 (79%)	173 (99%)	2 (1%)	0	100	100
40	q	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
41	r	316/318 (99%)	304 (96%)	10 (3%)	2 (1%)	21	48
42	s	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
43	t	115/137 (84%)	113 (98%)	2 (2%)	0	100	100
44	R	33/110 (30%)	33 (100%)	0	0	100	100
All	All	8096/9571 (85%)	7860 (97%)	225 (3%)	11 (0%)	49	74

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	n	44	LEU
41	r	197	PRO
2	C	45	PRO
22	E	183	ALA
23	L	199	SER

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	343/368 (93%)	341 (99%)	2 (1%)	78	92
2	C	370/398 (93%)	364 (98%)	6 (2%)	55	81
3	D	190/228 (83%)	184 (97%)	6 (3%)	34	65
4	F	77/97 (79%)	73 (95%)	4 (5%)	21	50
5	G	576/610 (94%)	574 (100%)	2 (0%)	86	95
6	I	132/212 (62%)	127 (96%)	5 (4%)	29	61
7	J	107/152 (70%)	104 (97%)	3 (3%)	38	70
8	K	130/131 (99%)	129 (99%)	1 (1%)	73	89
9	M	86/98 (88%)	86 (100%)	0	100	100
10	N	99/101 (98%)	98 (99%)	1 (1%)	68	87
11	O	77/132 (58%)	73 (95%)	4 (5%)	21	50
11	X	79/132 (60%)	71 (90%)	8 (10%)	7	22
12	P	74/82 (90%)	72 (97%)	2 (3%)	39	70
13	Q	105/134 (78%)	102 (97%)	3 (3%)	37	68
14	U	281/307 (92%)	276 (98%)	5 (2%)	51	78
15	V	101/102 (99%)	98 (97%)	3 (3%)	36	67
16	Y	60/84 (71%)	60 (100%)	0	100	100
17	Z	59/90 (66%)	58 (98%)	1 (2%)	53	80
18	a	121/158 (77%)	119 (98%)	2 (2%)	53	80
19	c	138/160 (86%)	138 (100%)	0	100	100
20	H	151/176 (86%)	141 (93%)	10 (7%)	15	40
21	S	58/58 (100%)	53 (91%)	5 (9%)	10	28
22	E	183/207 (88%)	171 (93%)	12 (7%)	15	40
23	L	294/320 (92%)	276 (94%)	18 (6%)	17	43
24	T	69/134 (52%)	65 (94%)	4 (6%)	18	46
25	W	122/124 (98%)	120 (98%)	2 (2%)	55	81
26	b	104/166 (63%)	96 (92%)	8 (8%)	12	33
27	d	153/156 (98%)	141 (92%)	12 (8%)	11	32
28	e	91/129 (70%)	84 (92%)	7 (8%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	f	42/66 (64%)	40 (95%)	2 (5%)	23	53
30	g	108/109 (99%)	102 (94%)	6 (6%)	19	47
31	h	93/94 (99%)	91 (98%)	2 (2%)	45	75
32	i	311/311 (100%)	294 (94%)	17 (6%)	19	48
33	j	99/100 (99%)	93 (94%)	6 (6%)	17	43
34	k	85/85 (100%)	80 (94%)	5 (6%)	18	45
35	l	537/540 (99%)	498 (93%)	39 (7%)	13	35
36	m	139/141 (99%)	122 (88%)	17 (12%)	5	14
37	n	53/55 (96%)	48 (91%)	5 (9%)	8	24
38	o	110/114 (96%)	98 (89%)	12 (11%)	6	18
39	p	159/190 (84%)	149 (94%)	10 (6%)	16	42
40	q	409/409 (100%)	389 (95%)	20 (5%)	22	51
41	r	275/275 (100%)	255 (93%)	20 (7%)	13	35
42	s	153/206 (74%)	148 (97%)	5 (3%)	33	65
43	t	108/120 (90%)	102 (94%)	6 (6%)	19	47
44	R	34/92 (37%)	31 (91%)	3 (9%)	9	27
All	All	7145/8153 (88%)	6834 (96%)	311 (4%)	27	56

5 of 311 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	n	9	ARG
41	r	111	LEU
38	o	33	GLN
40	q	122	PHE
42	s	188	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
31	h	97	HIS
35	l	447	ASN
32	i	134	GLN
34	k	52	HIS
37	n	40	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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	802	5	0,12,12	-	-	-		
47	FES	G	803	5	0,4,4	-	-	-		
49	NDP	L	401	-	51,52,52	0.50	0	71,80,80	0.75	1 (1%)
46	SF4	I	301	6	0,12,12	-	-	-		
47	FES	E	301	-	0,4,4	-	-	-		
46	SF4	B	502	-	0,12,12	-	-	-		
46	SF4	G	801	5	0,12,12	-	-	-		
46	SF4	H	301	20	0,12,12	-	-	-		
46	SF4	H	302	20	0,12,12	-	-	-		
45	FMN	B	501	-	33,33,33	1.05	2 (6%)	48,50,50	1.20	7 (14%)
48	ZMP	Q	201	-	27,29,36	1.77	6 (22%)	34,38,45	1.66	5 (14%)

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	802	5	-	-	0/6/5/5
47	FES	G	803	5	-	-	0/1/1/1
49	NDP	L	401	-	-	7/34/77/77	0/5/5/5
46	SF4	I	301	6	-	-	0/6/5/5
47	FES	E	301	-	-	-	0/1/1/1
46	SF4	G	801	5	-	-	0/6/5/5
46	SF4	B	502	-	-	-	0/6/5/5
46	SF4	H	301	20	-	-	0/6/5/5
46	SF4	H	302	20	-	-	0/6/5/5
45	FMN	B	501	-	-	7/18/18/18	0/3/3/3
48	ZMP	Q	201	-	-	9/36/36/43	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Q	201	ZMP	C13-N1	5.17	1.45	1.33
48	Q	201	ZMP	C16-N2	5.09	1.45	1.33
45	B	501	FMN	C4A-N5	3.39	1.38	1.30
48	Q	201	ZMP	C10-S1	2.50	1.82	1.76
45	B	501	FMN	C10-N1	2.43	1.38	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	Q	201	ZMP	C9-C10-S1	5.56	120.03	113.40
49	L	401	NDP	P2B-O2B-C2B	-5.04	109.97	123.43
48	Q	201	ZMP	O1-C10-C9	-3.35	120.11	123.98
45	B	501	FMN	C4-N3-C2	-3.17	120.02	125.64
45	B	501	FMN	C4A-C10-N10	2.69	120.33	116.48

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

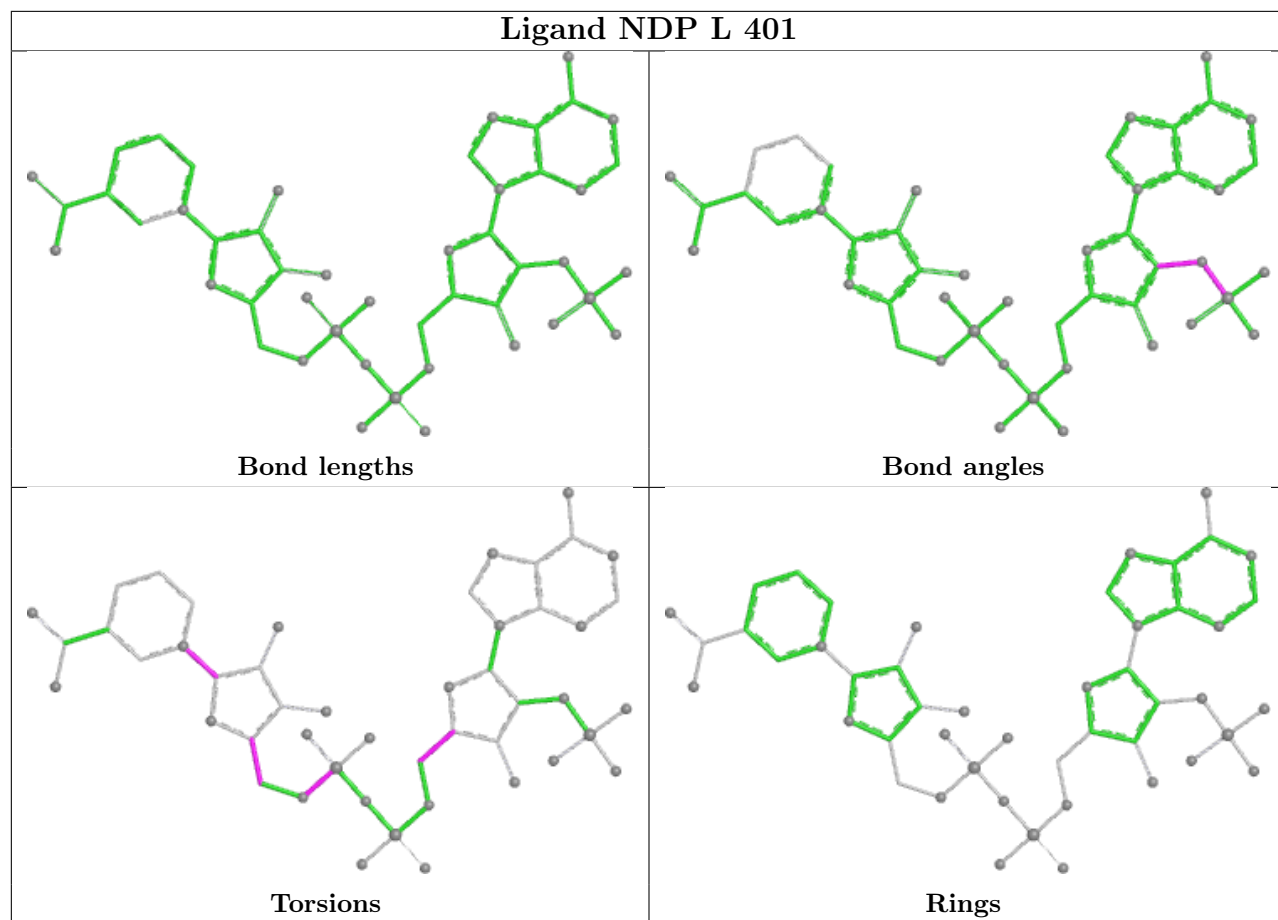
Mol	Chain	Res	Type	Atoms
45	B	501	FMN	N10-C1'-C2'-O2'
45	B	501	FMN	N10-C1'-C2'-C3'
45	B	501	FMN	C3'-C4'-C5'-O5'
45	B	501	FMN	O4'-C4'-C5'-O5'
45	B	501	FMN	C5'-O5'-P-O1P

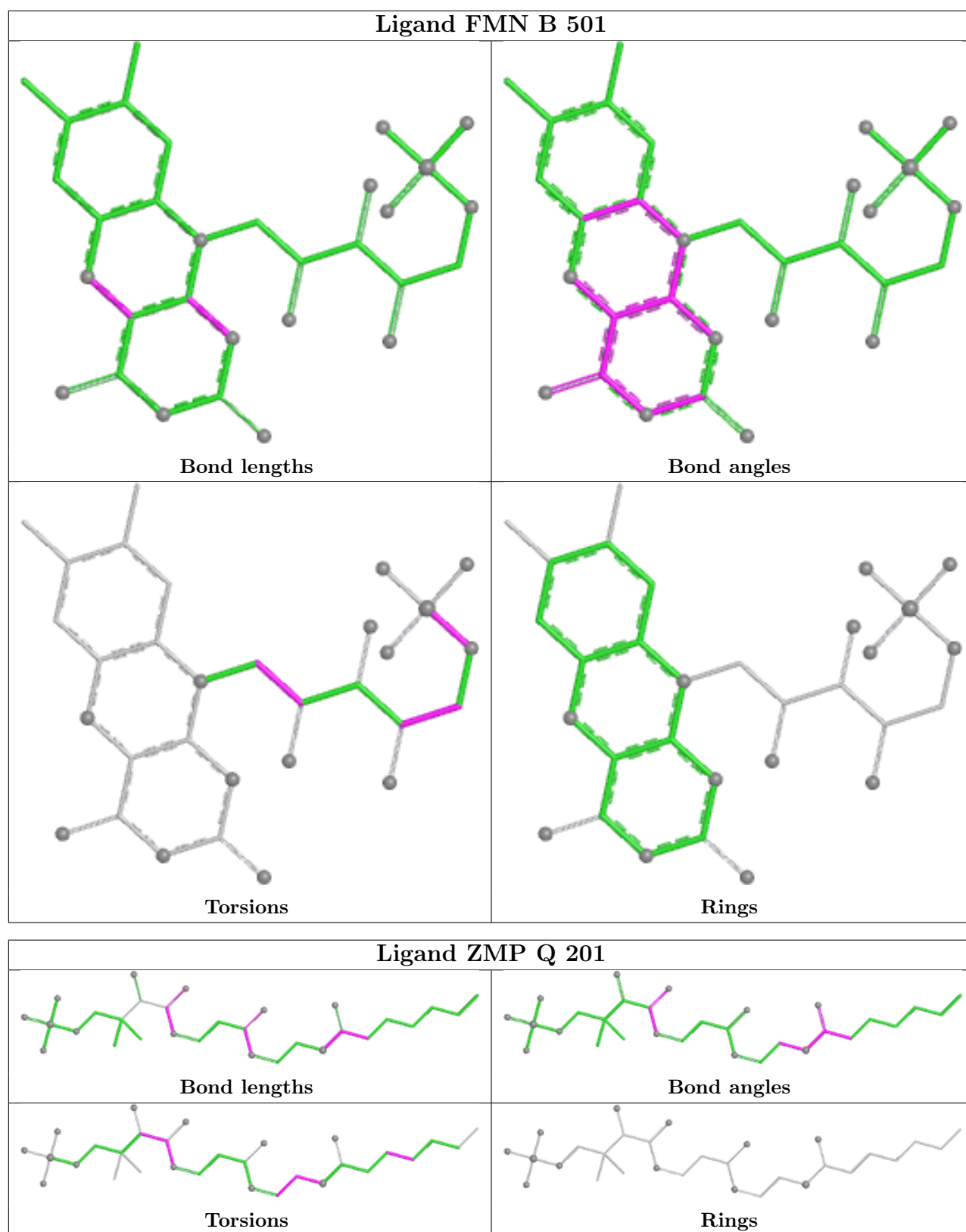
There are no ring outliers.

8 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	L	401	NDP	3	0
46	I	301	SF4	1	0
47	E	301	FES	9	0
46	B	502	SF4	21	0
46	H	301	SF4	7	0
46	H	302	SF4	1	0
45	B	501	FMN	1	0
48	Q	201	ZMP	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

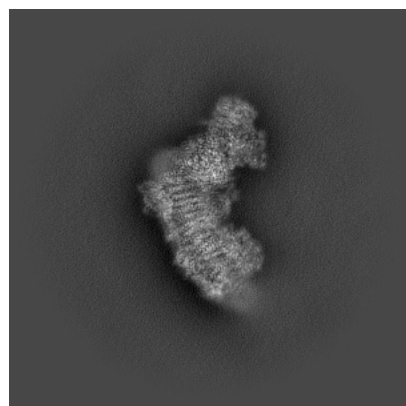
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44967. These allow visual inspection of the internal detail of the map and identification of artifacts.

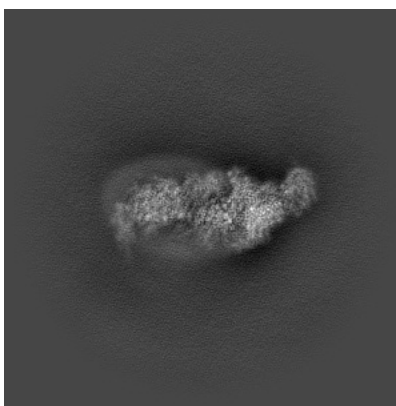
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

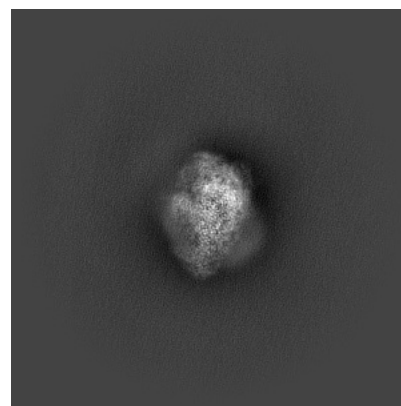
6.1.1 Primary map



X

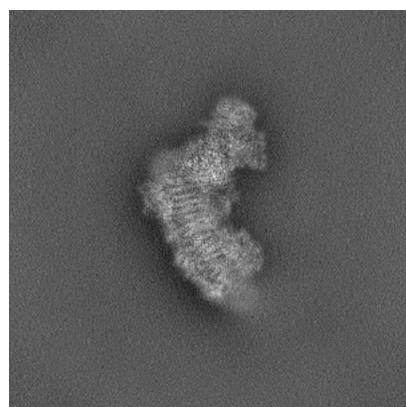


Y

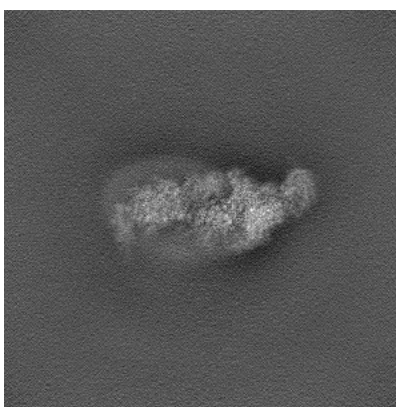


Z

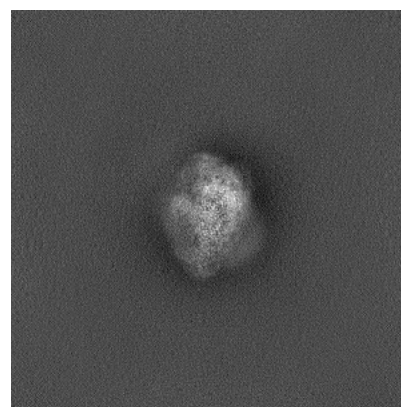
6.1.2 Raw map



X



Y

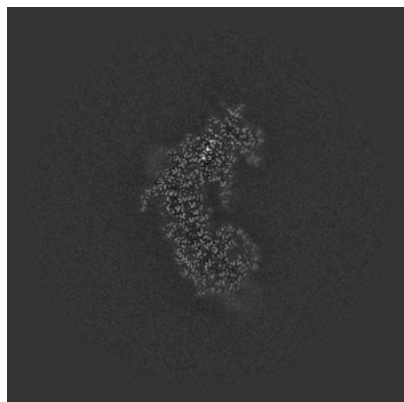


Z

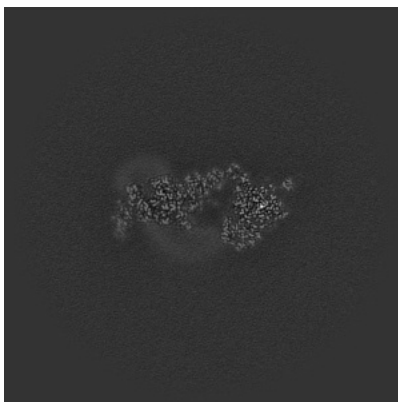
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

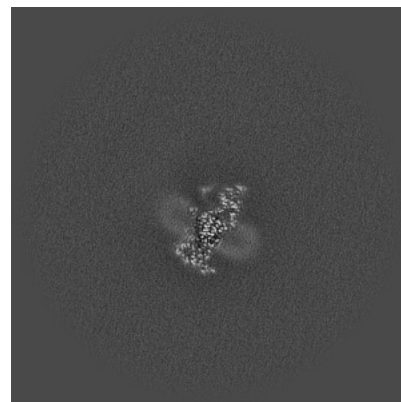
6.2.1 Primary map



X Index: 256

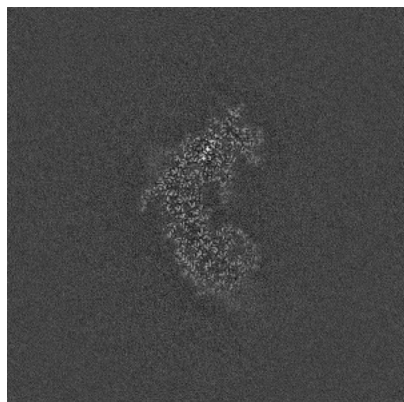


Y Index: 256

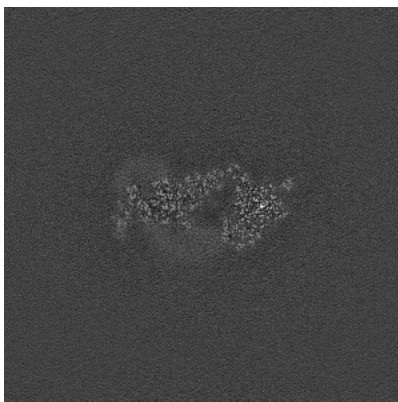


Z Index: 256

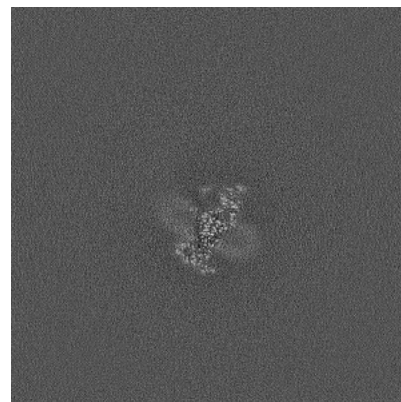
6.2.2 Raw map



X Index: 256



Y Index: 256

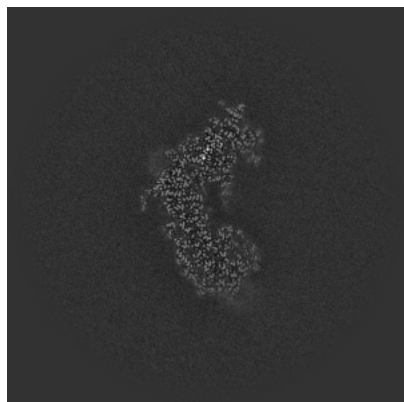


Z Index: 256

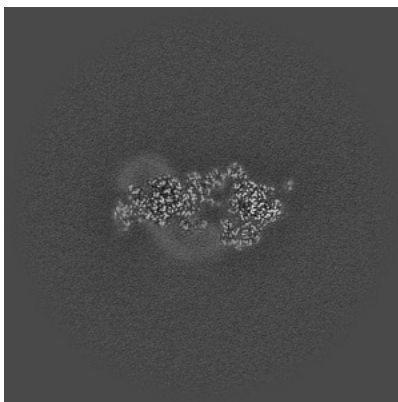
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

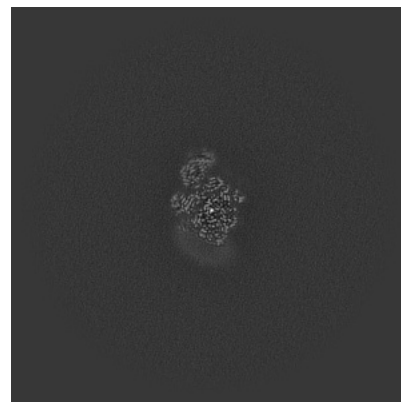
6.3.1 Primary map



X Index: 257

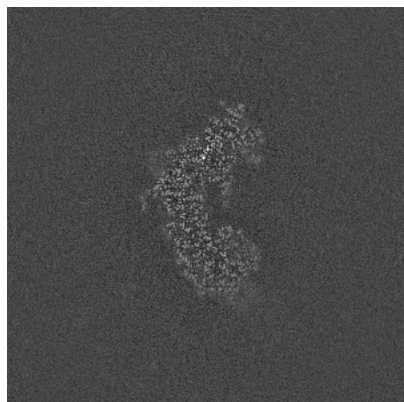


Y Index: 253

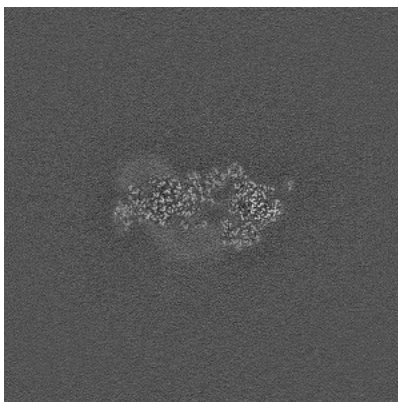


Z Index: 318

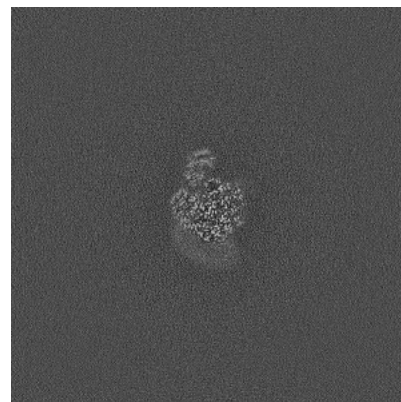
6.3.2 Raw map



X Index: 257



Y Index: 253

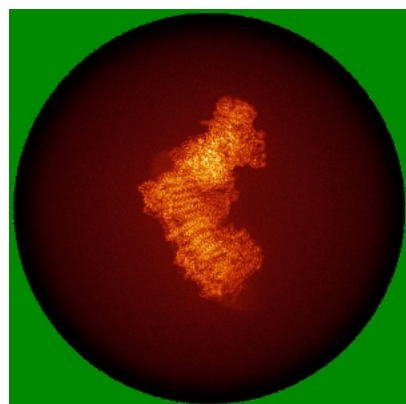


Z Index: 313

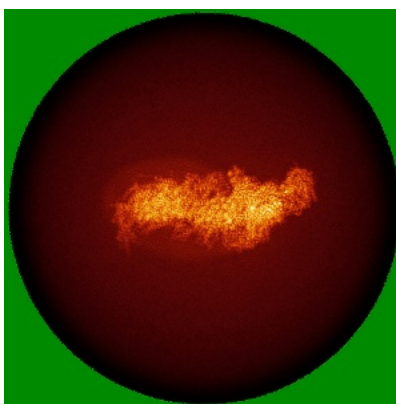
The images above show the largest variance slices of the map in three orthogonal directions.

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

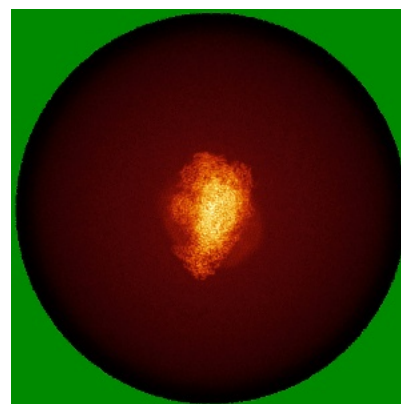
6.4.1 Primary map



X

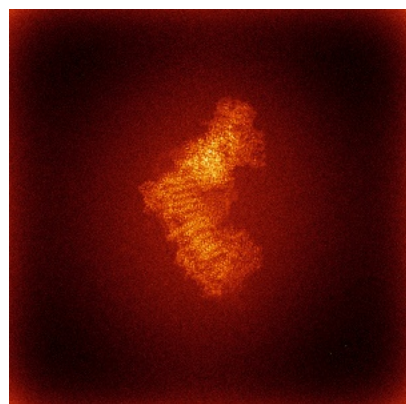


Y

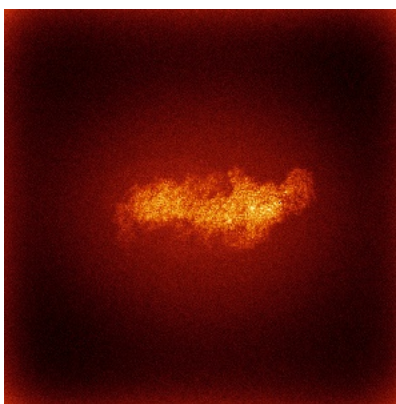


Z

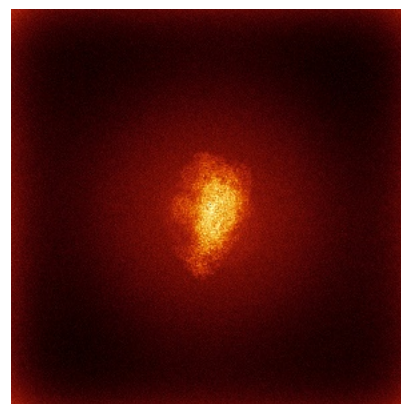
6.4.2 Raw map



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



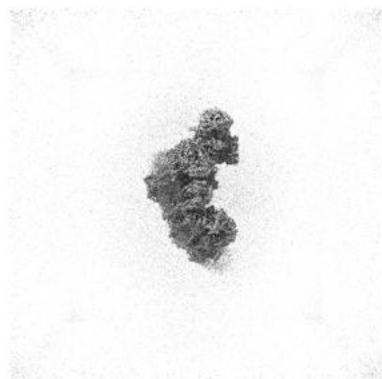
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

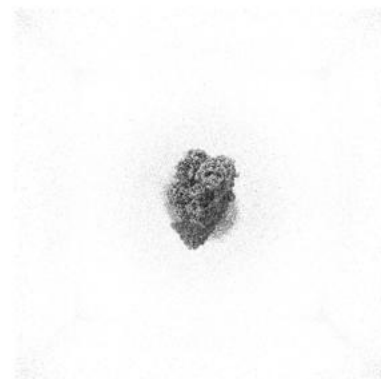
6.5.2 Raw map



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.

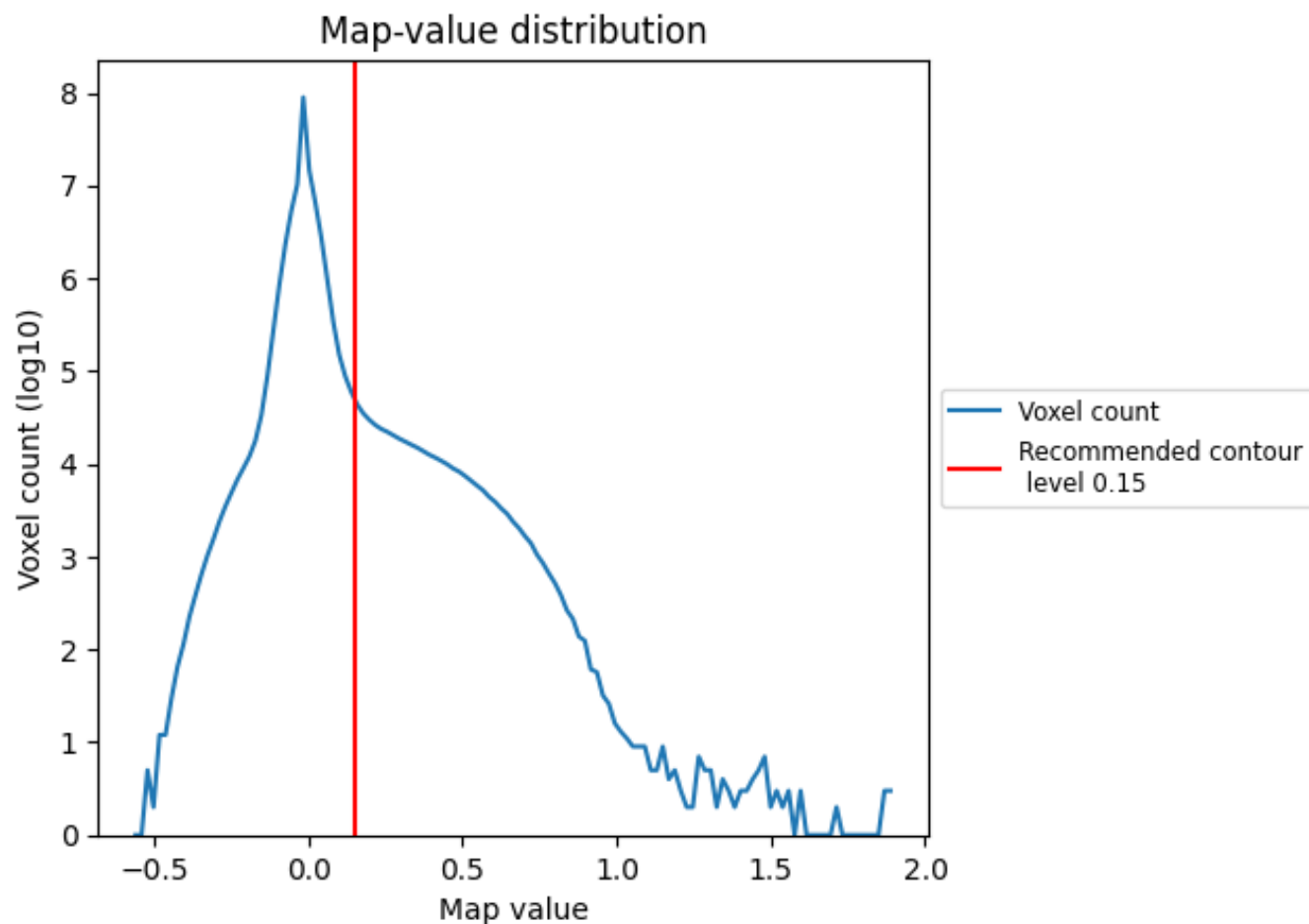
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

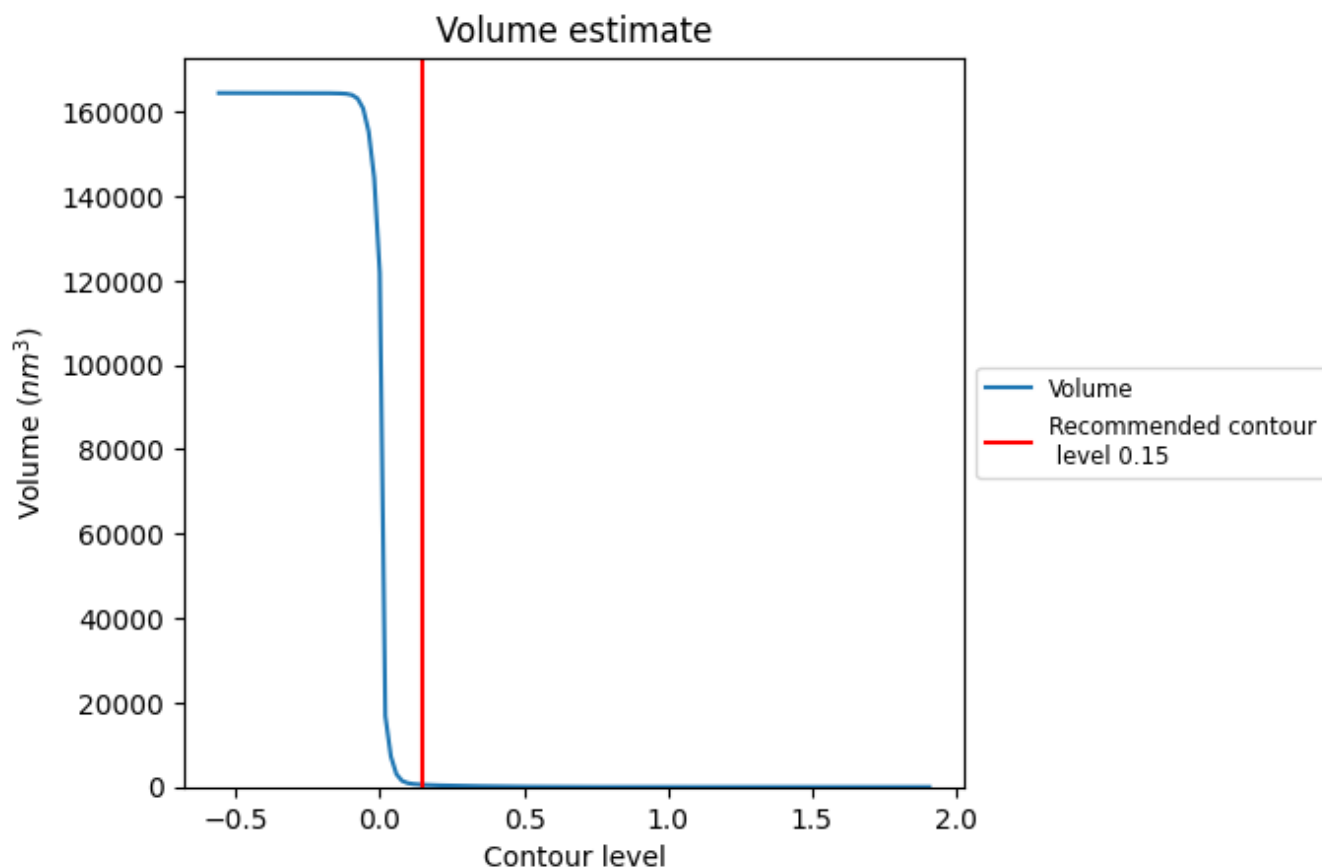
This section contains the results of statistical analysis of the map.

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.

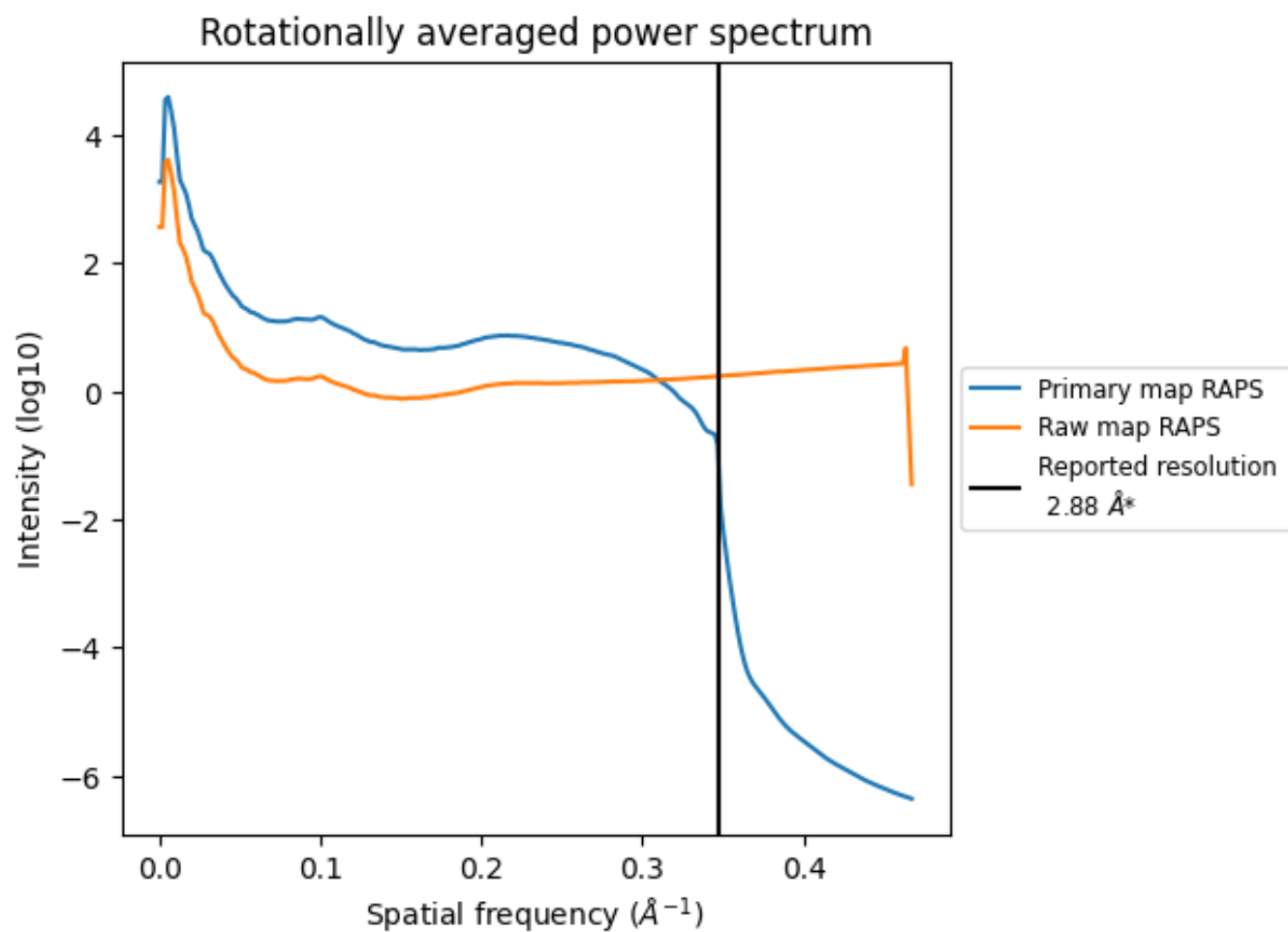
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 518 nm^3 ; this corresponds to an approximate mass of 468 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

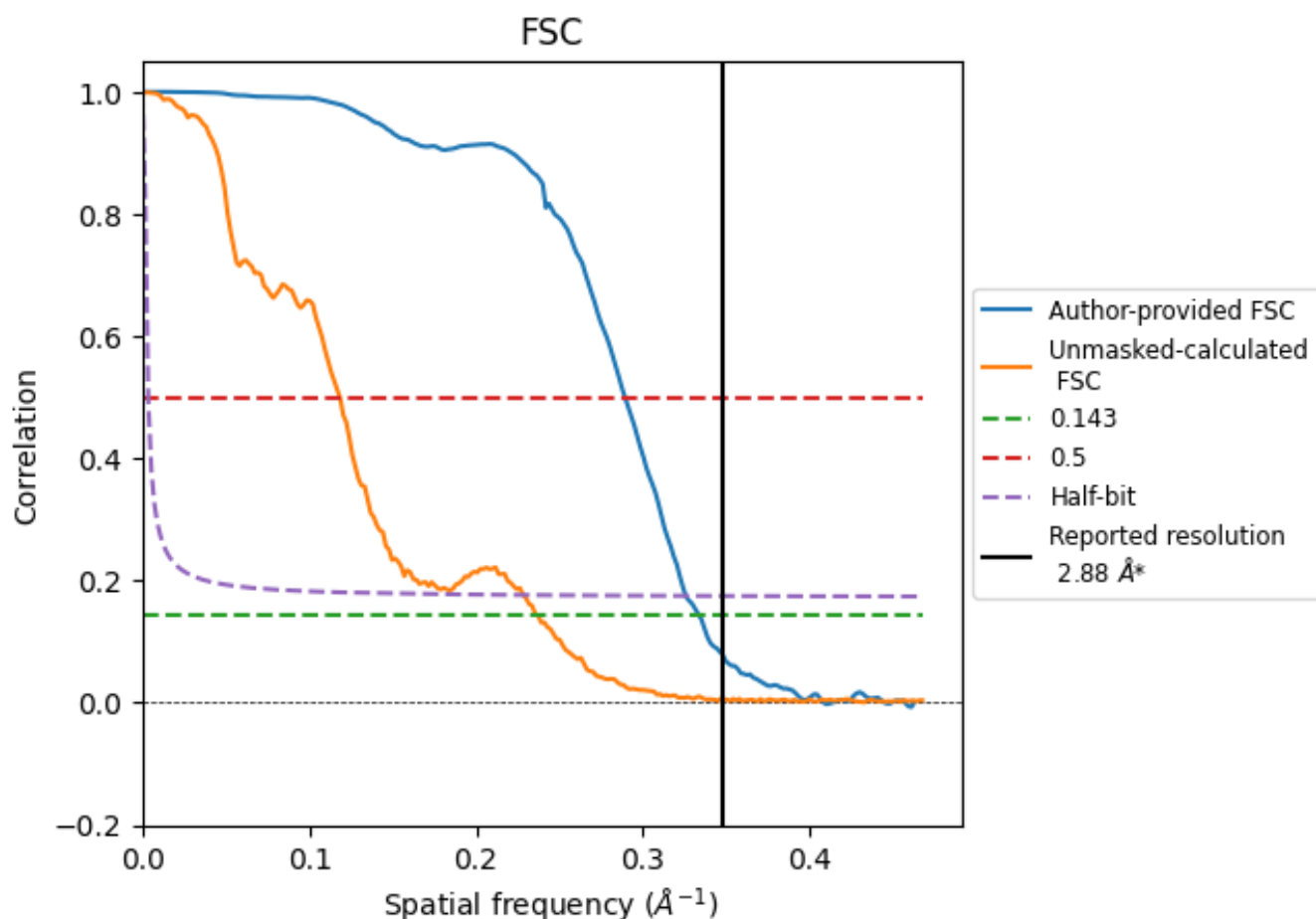


*Reported resolution corresponds to spatial frequency of 0.347 \AA^{-1}

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 0.347 Å⁻¹

8.2 Resolution estimates [i](#)

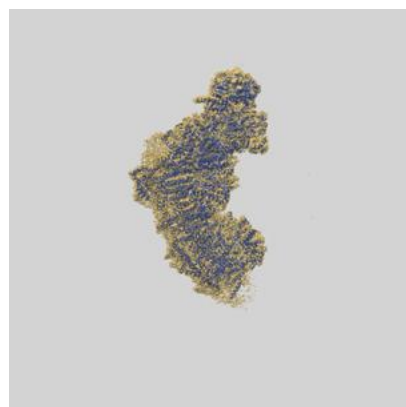
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	3.00	3.46	3.07
Unmasked-calculated*	4.22	8.45	4.38

*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 4.22 differs from the reported value 2.88 by more than 10 %

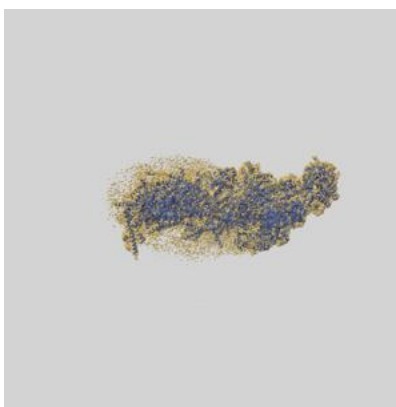
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44967 and PDB model 9BWD. Per-residue inclusion information can be found in section [3](#) on page [15](#).

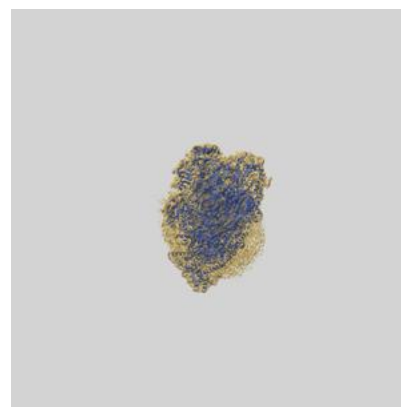
9.1 Map-model overlay [i](#)



X



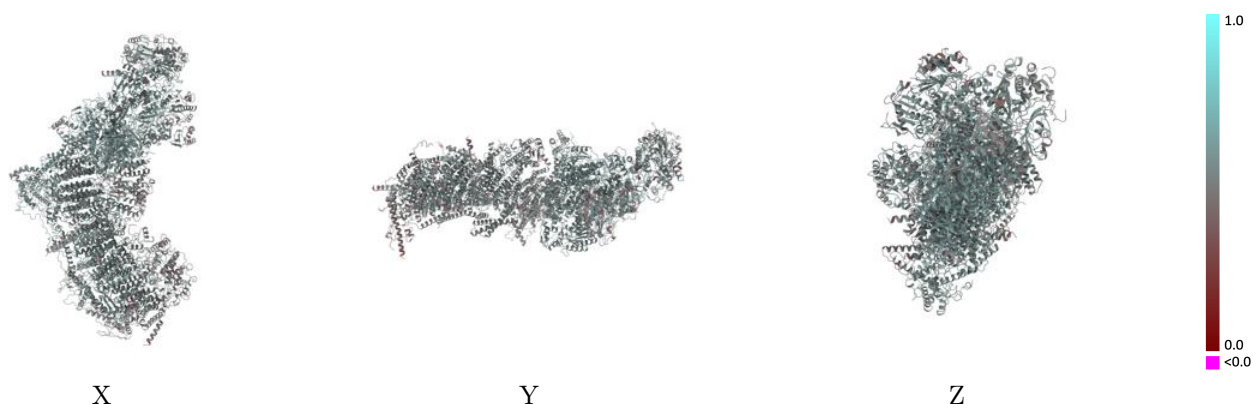
Y



Z

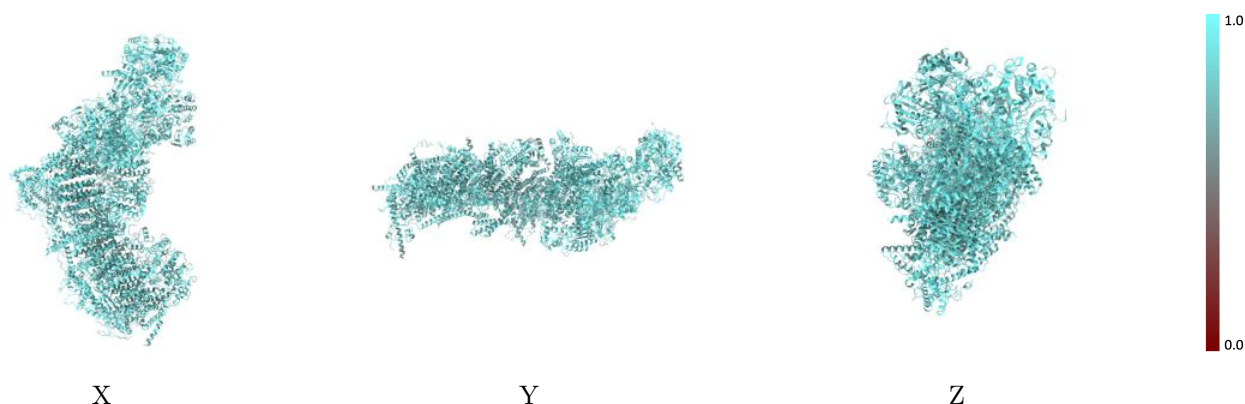
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



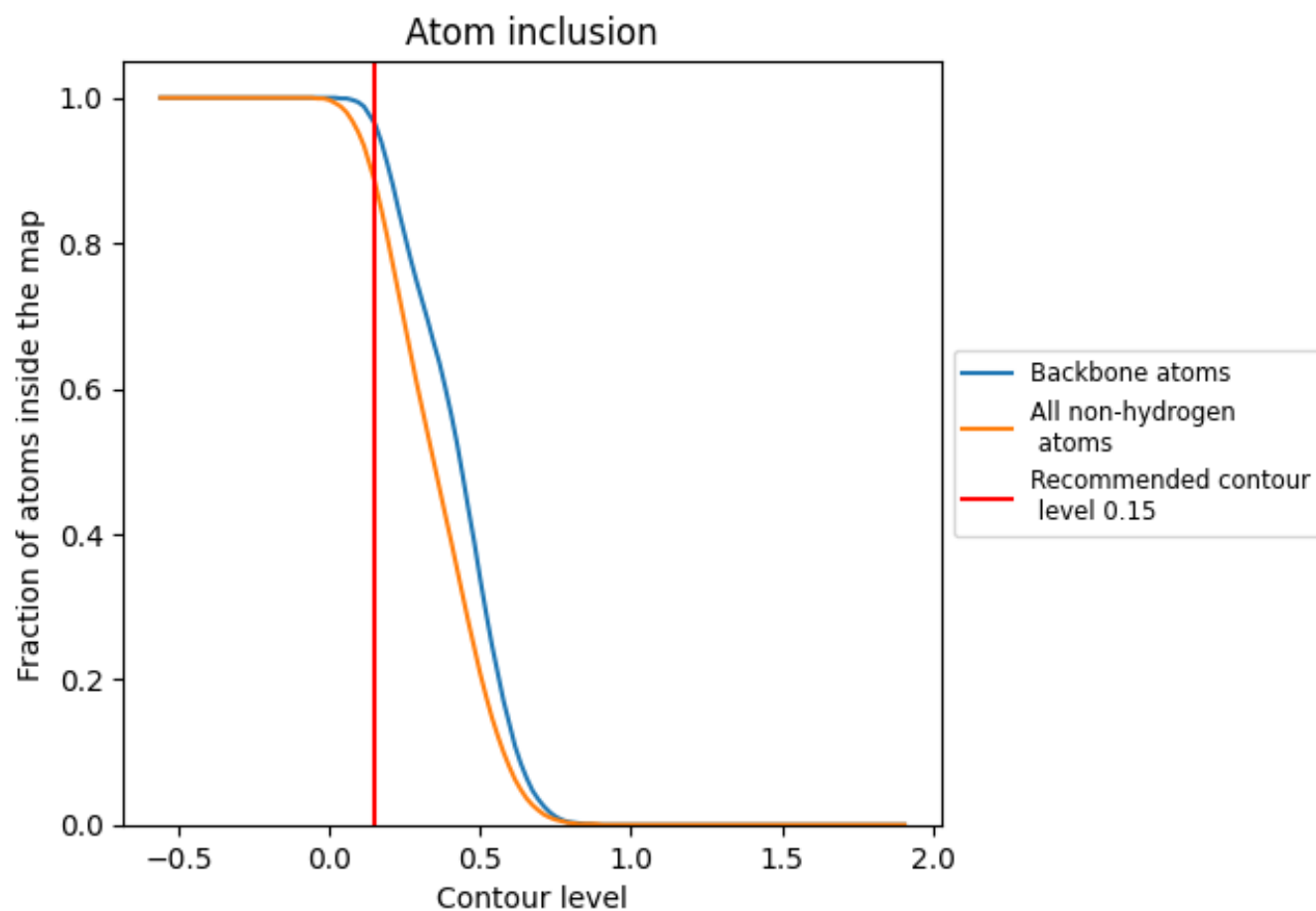
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.5290
B	 0.9110	 0.5270
C	 0.9330	 0.5710
D	 0.9370	 0.5680
E	 0.8920	 0.5130
F	 0.8730	 0.5450
G	 0.8990	 0.5390
H	 0.9350	 0.5630
I	 0.9510	 0.5690
J	 0.9060	 0.5470
K	 0.8810	 0.5500
L	 0.9040	 0.5420
M	 0.8890	 0.5510
N	 0.8880	 0.5320
O	 0.7800	 0.4520
P	 0.8400	 0.4740
Q	 0.8870	 0.5320
R	 0.8400	 0.4950
S	 0.9310	 0.5540
T	 0.8770	 0.5090
U	 0.8480	 0.4990
V	 0.8590	 0.5010
W	 0.8950	 0.5360
X	 0.8050	 0.4700
Y	 0.8330	 0.4540
Z	 0.8060	 0.4720
a	 0.9130	 0.5490
b	 0.8140	 0.4530
c	 0.8610	 0.5150
d	 0.8830	 0.5010
e	 0.8410	 0.5030
f	 0.7950	 0.4750
g	 0.9150	 0.5400
h	 0.8860	 0.5240
i	 0.9040	 0.5510



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.8810	 0.5460
k	 0.8710	 0.5410
l	 0.8620	 0.5260
m	 0.8540	 0.5220
n	 0.8380	 0.4830
o	 0.8540	 0.5060
p	 0.8570	 0.4990
q	 0.9010	 0.5510
r	 0.9050	 0.5540
s	 0.9020	 0.5360
t	 0.8180	 0.4430