



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 03:15 AM EDT

PDB ID : 9CWT / pdb_00009cwt
EMDB ID : EMD-45974
Title : Human kidney respiratory complex I
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2024-07-30
Resolution : 3.44 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.dev133
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) : 2.50

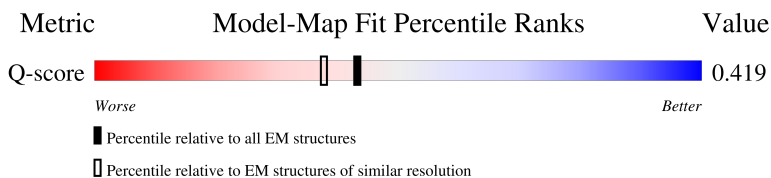
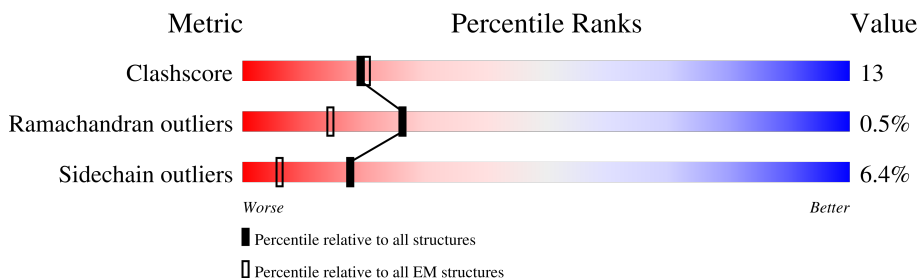
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

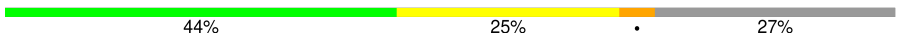
The reported resolution of this entry is 3.44 Å.

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.



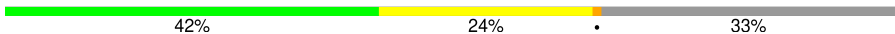
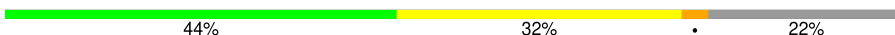
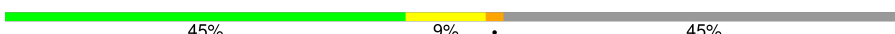
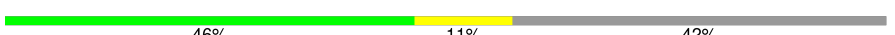
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13877 (2.94 - 3.94)

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	A	464	 66% 25% 7%
2	B	210	 54% 28% 16%
3	C	213	 44% 25% 27%
4	E	128	 57% 30% 12%

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Mol	Chain	Length	Quality of chain
5	F	99	
6	G	156	
6	X	156	
7	H	116	
8	I	113	
9	J	377	
10	K	108	
11	L	175	
12	M	727	
13	N	145	
14	O	249	
15	P	264	
16	Q	463	
17	S	70	
18	T	124	
19	U	84	
20	V	141	
21	W	144	
22	Y	105	
23	Z	98	
24	a	189	
25	b	128	
26	c	186	
27	d	172	
28	e	153	

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Mol	Chain	Length	Quality of chain
29	f	76	
30	g	119	
31	h	106	
32	j	115	
33	k	98	
34	l	603	
35	m	174	
36	n	58	
37	o	129	
38	p	179	
39	r	459	
40	s	318	
41	u	172	
42	v	137	
43	D	22	
44	i	347	

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
45	SF4	A	501	-	-	X	-
45	SF4	B	302	-	-	X	-
45	SF4	C	301	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 60914 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	A	431	Total	C	N	O	S	0	0
			3316	2093	591	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	83	Total	C	N	O	S	0	0
			647	416	96	130	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	313	Total	C	N	O	S	0	0
			2486	1598	447	433	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	30	Total	C	N	O	S	0	0
			247	157	42	47	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	117	Total	C	N	O	S	0	0
			955	602	171	178	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	686	Total	C	N	O	S	0	0
			5261	3302	915	1006	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1188	764	210	211	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1637	1044	273	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	207	Total	C	N	O	S	0	0
			1721	1112	296	310	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	384	Total	C	N	O	S	0	0
			3073	1961	534	556	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1116	715	195	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	58	Total	C	N	O	S	0	0
			510	338	83	88	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	72	Total	C	N	O	S	0	0
			582	382	102	96	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	120	Total	C	N	O	S	0	0
			1022	674	175	169	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	138	Total	C	N	O	S	0	0
			1094	708	178	197	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	166	Total	C	N	O	S	0	0
			1393	870	257	254	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	88	Total	C	N	O	S	0	0
			731	472	121	134	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			840	531	154	149	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	92	Total	C	N	O	S	0	0
			732	507	103	116	6		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	84	Total	C	N	O	S	0	0
			627	413	95	107	12		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	565	Total	C	N	O	S	0	0
			4383	2882	697	774	30		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	m	166	Total	C	N	O	S	0	0
			1239	830	184	215	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	102	Total	C	N	O	S	0	0
			841	538	156	145	2		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	p	171	Total	C	N	O	S	0	0
			1480	950	264	259	7		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	r	459	Total	C	N	O	S	0	0
			3623	2404	569	620	30		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	s	318	Total	C	N	O	S	0	0
			2494	1667	375	436	16		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	v	112	Total	C	N	O	S	0	0
			887	546	178	154	9		

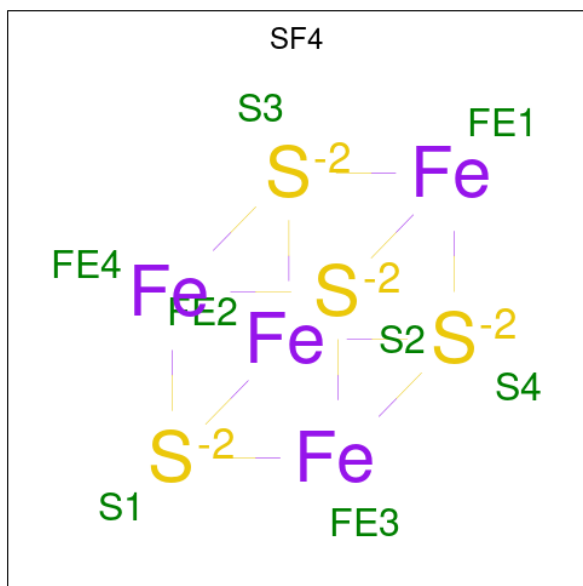
- Molecule 43 is a protein called Unknow peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	D	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 2.

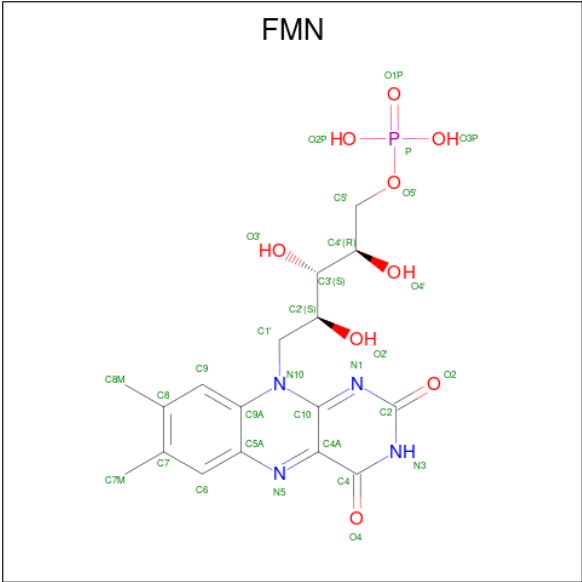
Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	306	Total	C	N	O	S	0	0
			2385	1595	359	409	22		

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



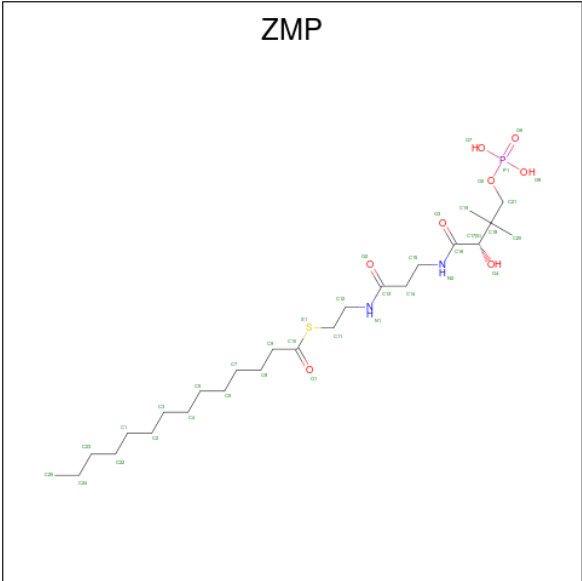
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



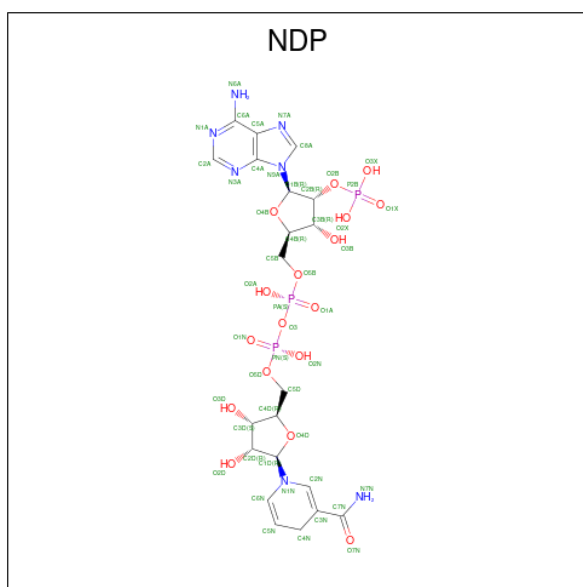
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



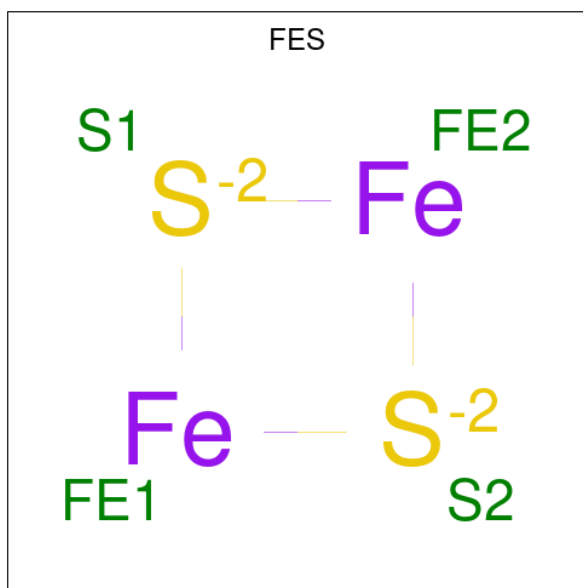
Mol	Chain	Residues	Atoms					AltConf	
47	E	1	Total	C	N	O	P	S	0
			30	18	2	8	1	1	

- Molecule 48 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

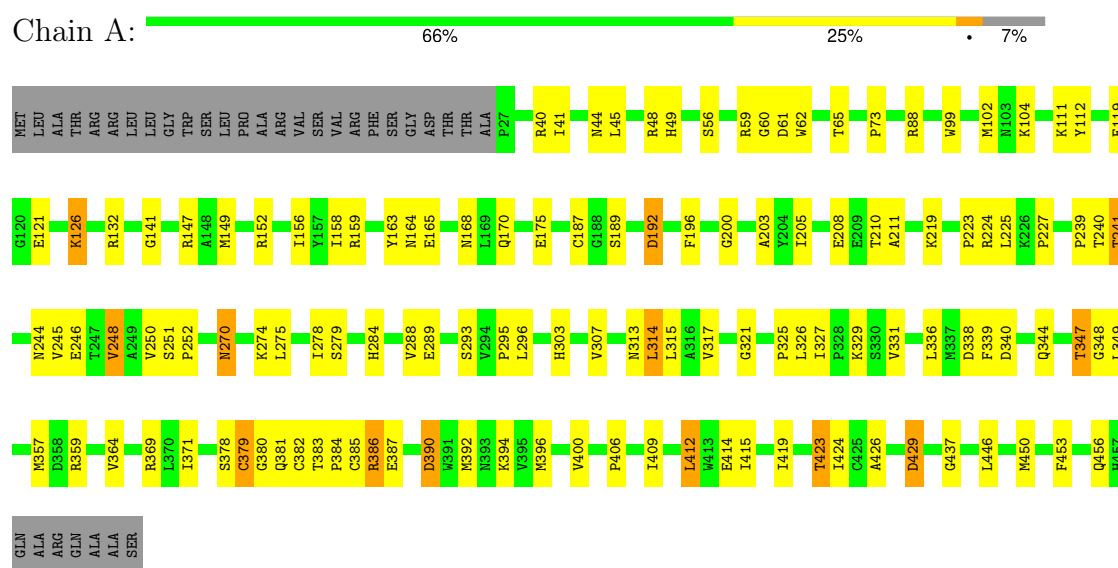


Mol	Chain	Residues	Atoms			AltConf
49	M	1	Total 4	Fe 2	S 2	0
49	O	1	Total 4	Fe 2	S 2	0

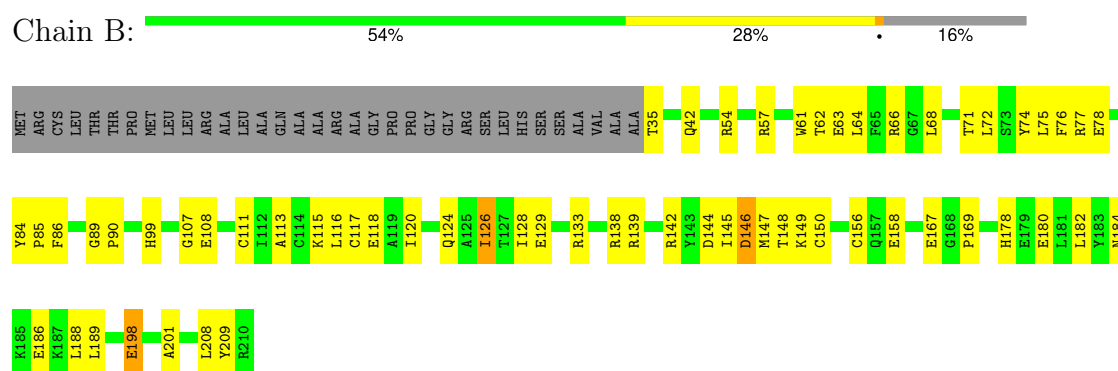
3 Residue-property plots [i](#)

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

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

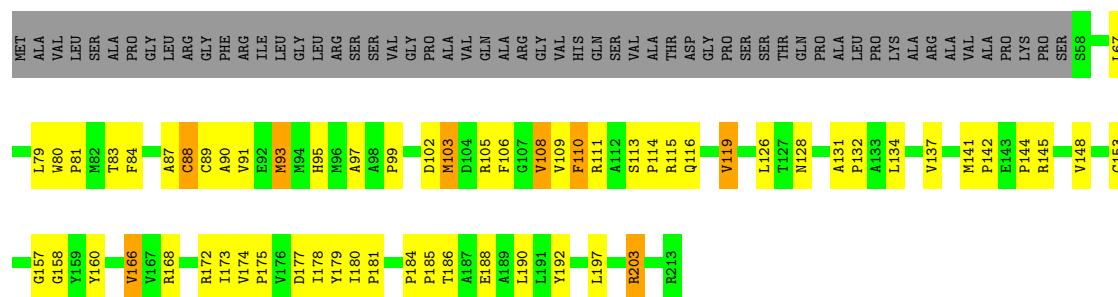


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



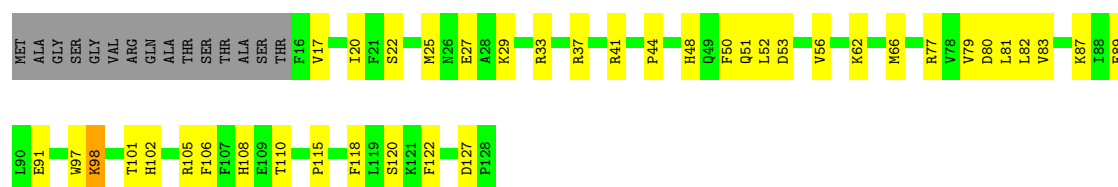
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial





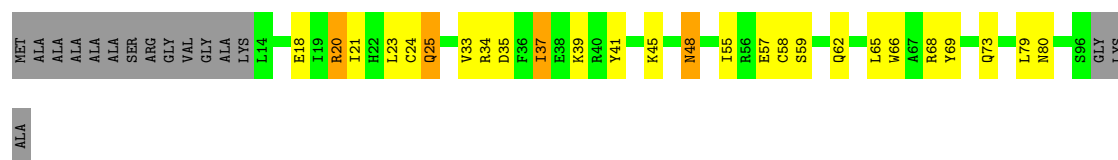
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 57% 30% 12%



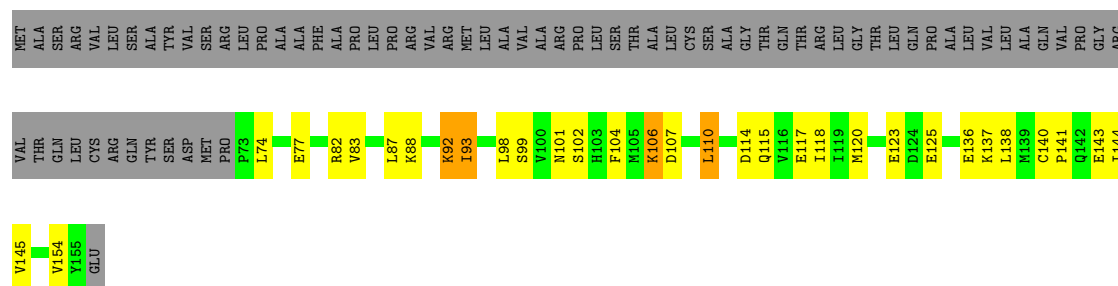
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F: 58% 22% 16%



- Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 33% 18% 47%



- Molecule 6: Acyl carrier protein, mitochondrial

Chain X: 39% 15% 46%





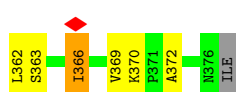
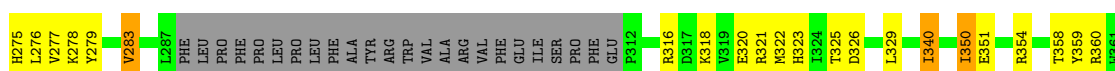
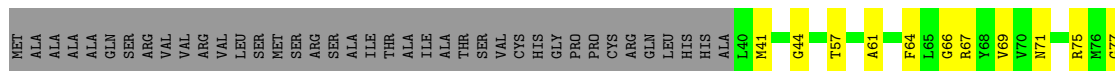
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



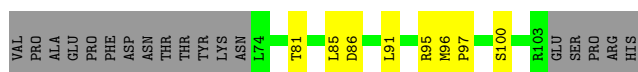
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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

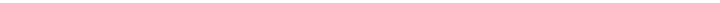


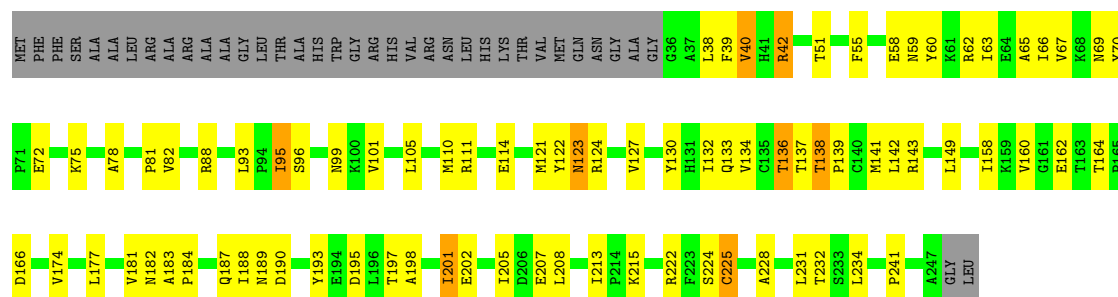
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



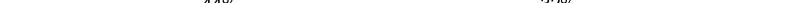
- [illegible]

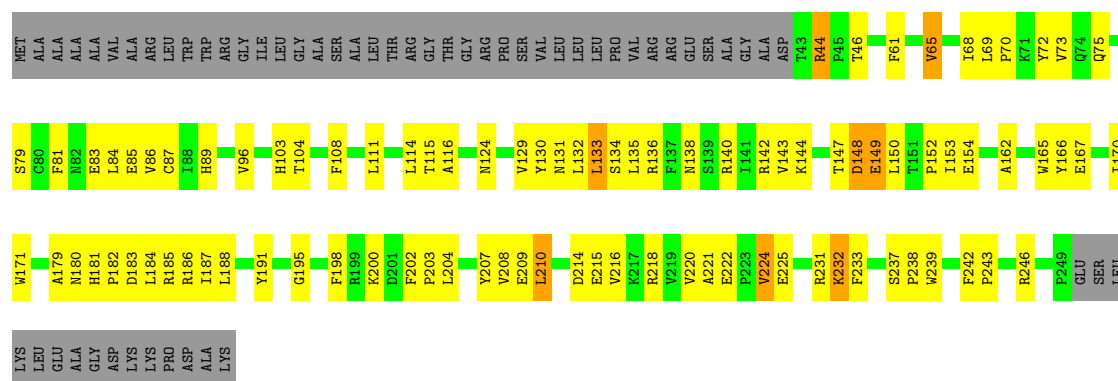
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 0:  52% 30% 2% 15%



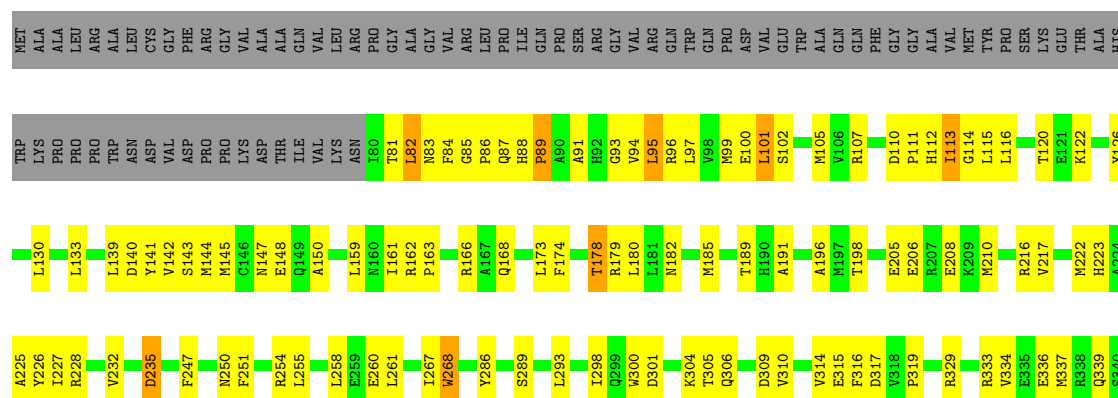
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

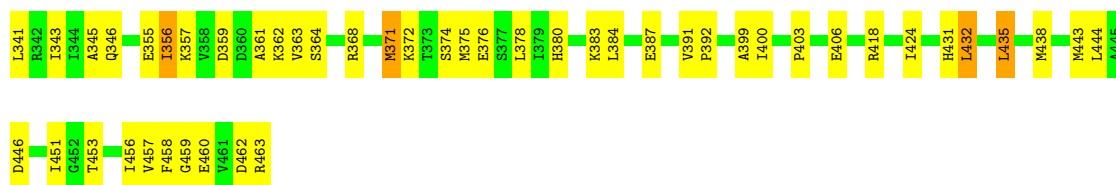
Chain P:  44% 32% 2% 22%



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

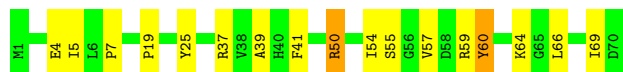
Chain Q: 50% 30% 1% 17%





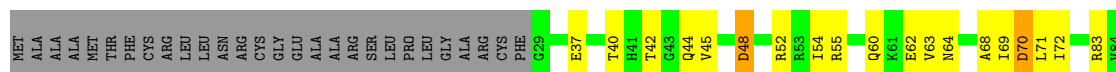
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 76% 21% .



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

Chain T: 50% 23% . 23%



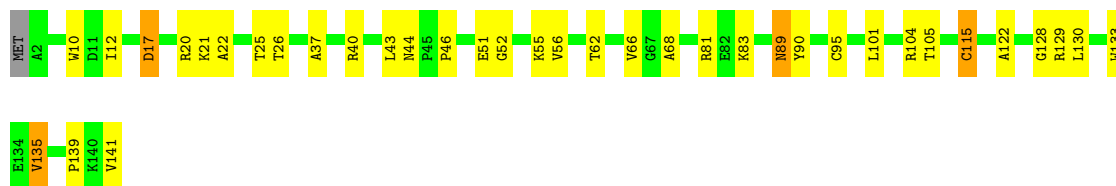
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U: 79% 18% ..



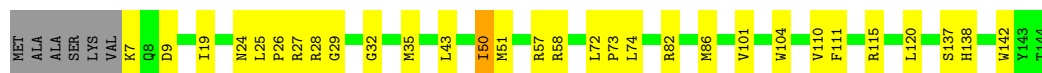
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 73% 23% ..

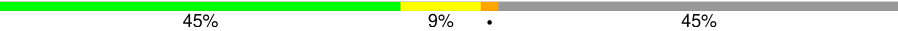


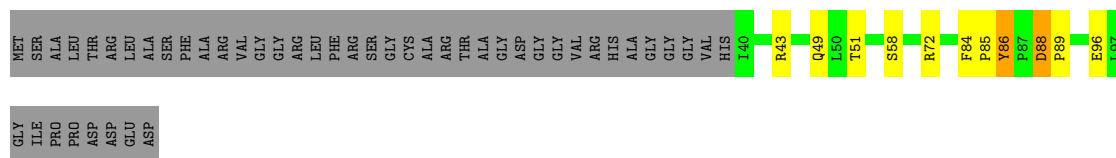
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W: 75% 20% . .



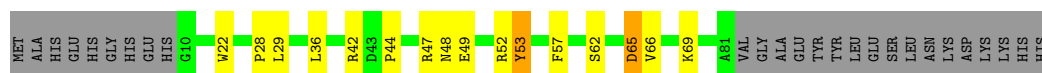
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y: 



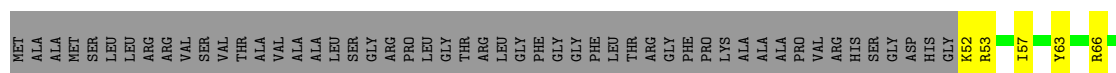
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z: 



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a: 



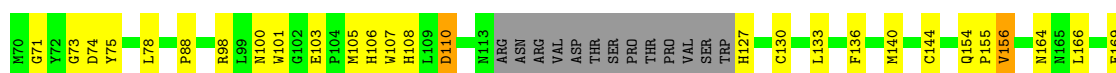
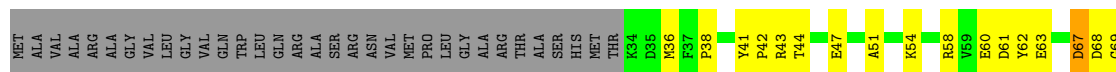
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 



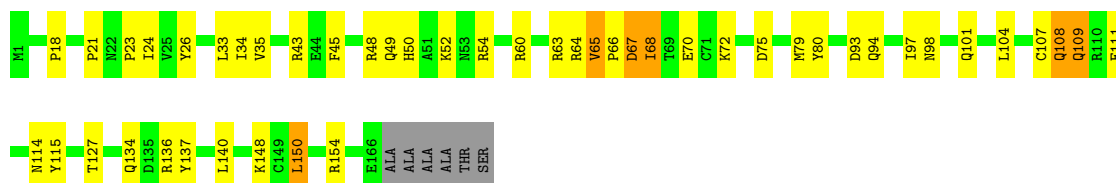
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 

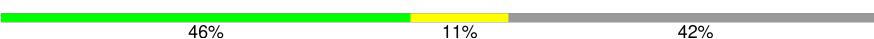


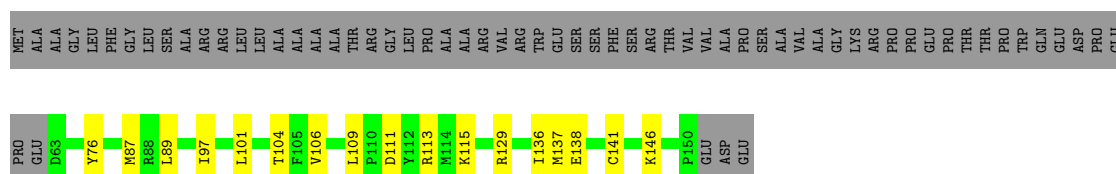
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 



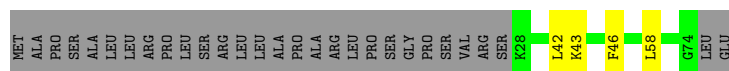
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 



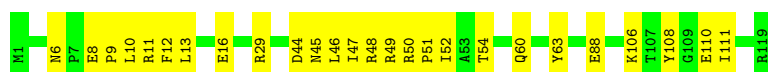
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 



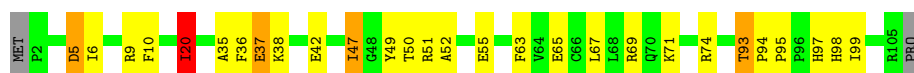
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



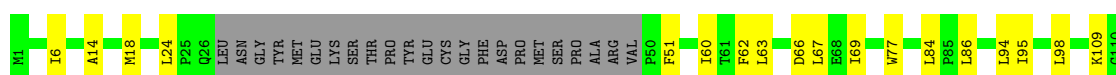
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



- Molecule 32: NADH-ubiquinone oxidoreductase chain 3

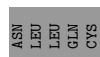
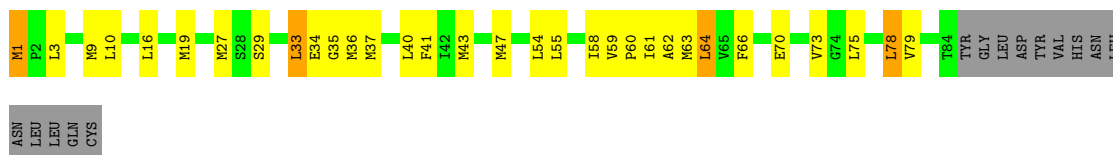
Chain j: 





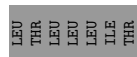
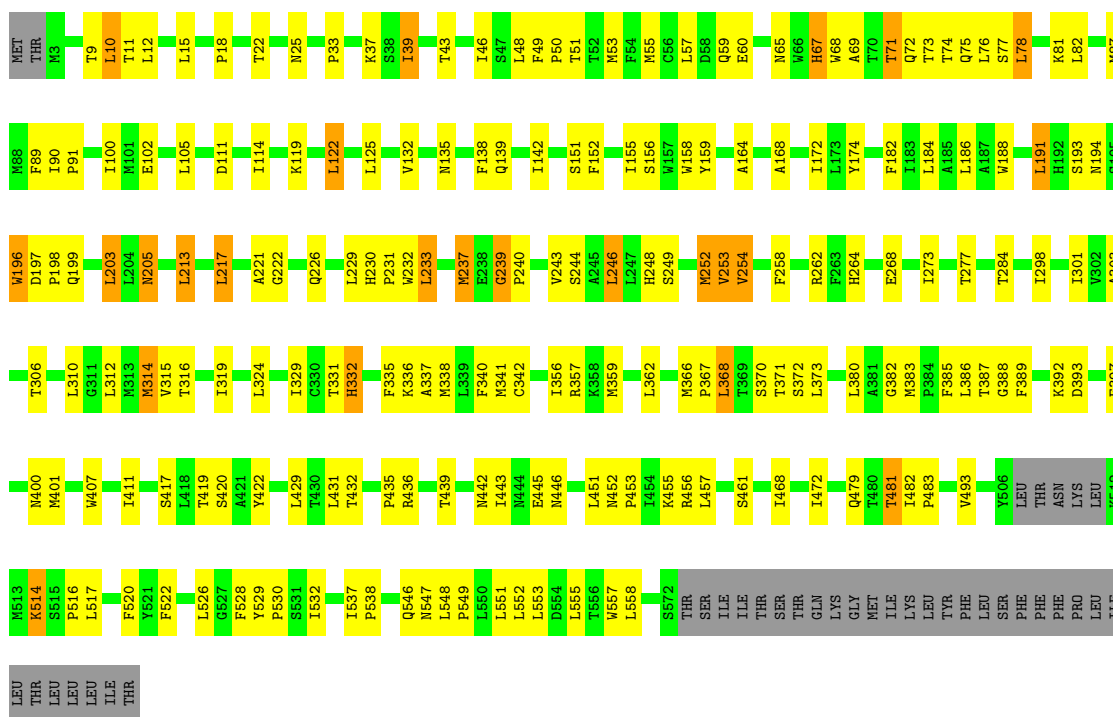
- Molecule 33: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 53% 29% 14%



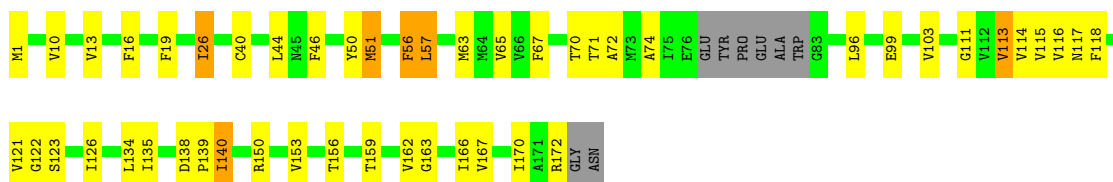
- Molecule 34: NADH-ubiquinone oxidoreductase chain 5

Chain l: 60% 29% 6%



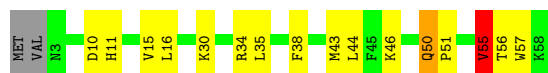
- Molecule 35: NADH-ubiquinone oxidoreductase chain 6

Chain m: 67% 25% 5%



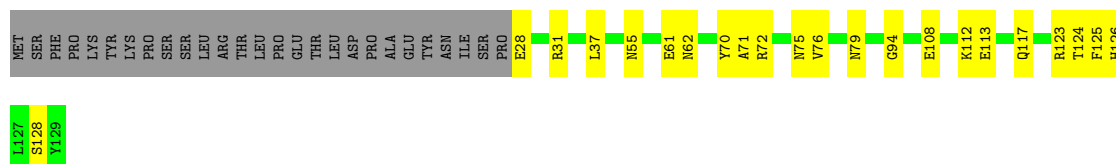
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  69% 24% . . .



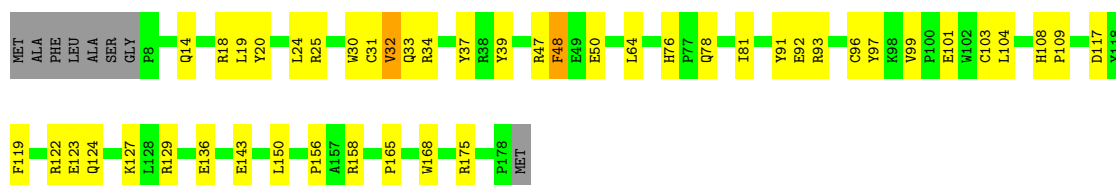
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  62% 17% 21%



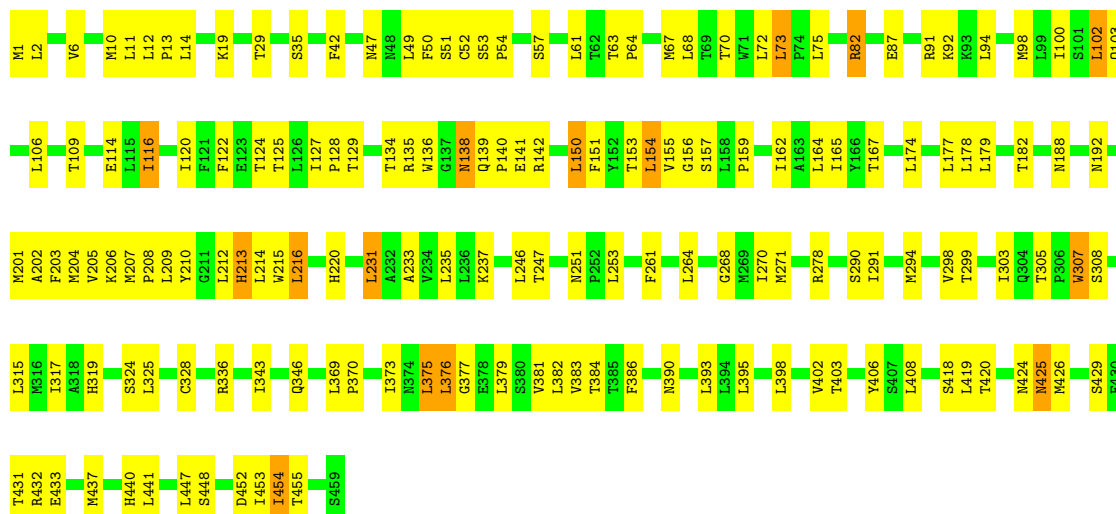
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:  70% 25% . . .



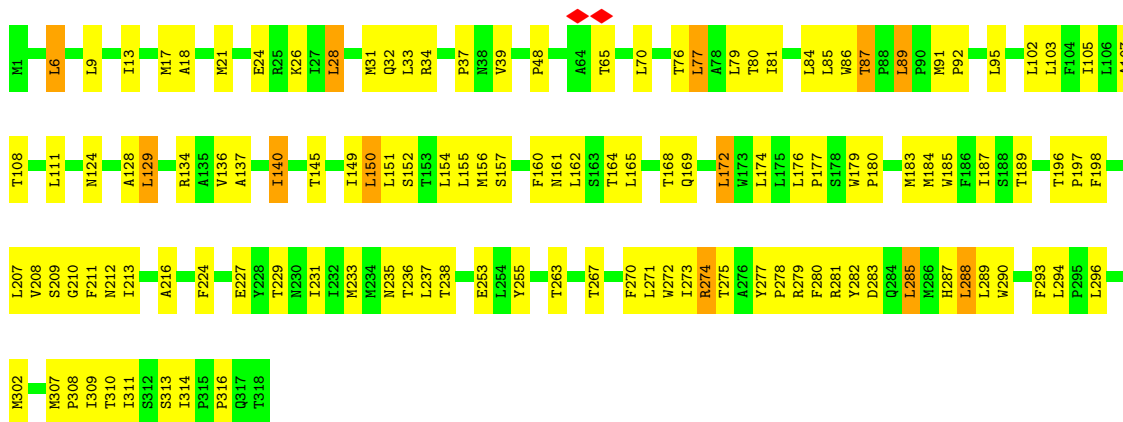
- Molecule 39: NADH-ubiquinone oxidoreductase chain 4

Chain r:  64% 32% .



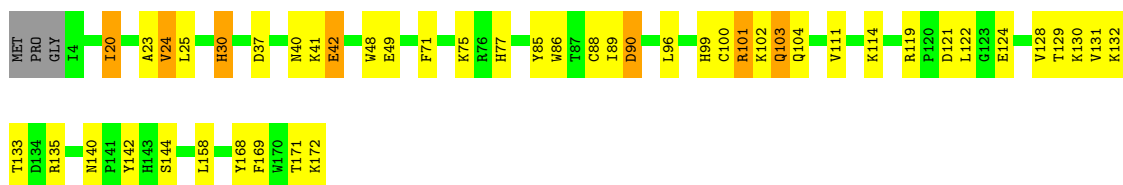
- Molecule 40: NADH-ubiquinone oxidoreductase chain 1

Chain s:  61% 36% .



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 71% 23%



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 61% 20% 18%



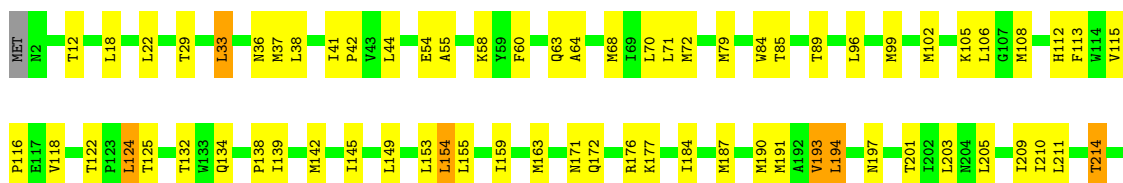
- Molecule 43: Unknow peptide

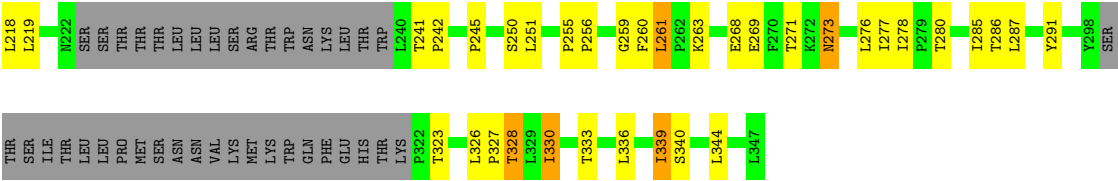
Chain D: 100%

There are no outlier residues recorded for this chain.

- Molecule 44: NADH-ubiquinone oxidoreductase chain 2

Chain i: 58% 27% 12%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16097	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 ($e^-/\text{\AA}^2$)	38	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	2.246	Depositor
Minimum map value	-0.386	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.135	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZMP, FES, NDP, 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	A	0.25	0/3392	0.44	0/4583
2	B	0.37	0/1452	0.58	0/1964
3	C	0.57	0/1280	0.76	0/1732
4	E	0.18	0/993	0.36	0/1335
5	F	0.20	0/682	0.33	0/922
6	G	0.08	0/657	0.27	0/890
6	X	0.23	0/698	0.39	0/942
7	H	0.12	0/941	0.34	0/1275
8	I	0.20	0/788	0.44	0/1066
9	J	0.21	0/2544	0.35	1/3437 (0.0%)
10	K	0.11	0/253	0.24	0/341
11	L	0.28	0/978	0.43	0/1320
12	M	0.35	0/5349	0.50	0/7250
13	N	0.12	0/1228	0.35	0/1670
14	O	0.17	0/1676	0.34	0/2282
15	P	0.17	0/1771	0.39	0/2412
16	Q	0.51	0/3146	0.70	0/4255
17	S	0.27	0/583	0.47	0/785
18	T	0.37	0/755	0.47	0/1017
19	U	0.42	0/670	0.58	0/920
20	V	0.19	0/1065	0.32	0/1450
21	W	0.44	0/1147	0.61	0/1557
22	Y	0.13	0/533	0.39	0/727
23	Z	0.09	0/601	0.25	0/806
24	a	0.21	0/1209	0.36	0/1639
25	b	0.12	0/1056	0.33	0/1427
26	c	0.17	0/1139	0.32	0/1558
27	d	0.15	0/1420	0.31	0/1910
28	e	0.12	0/751	0.31	0/1017
29	f	0.16	0/418	0.26	0/566
30	g	0.11	0/1035	0.27	0/1398
31	h	0.22	0/860	0.43	0/1153

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	j	0.45	0/749	0.72	0/1022
33	k	0.49	0/635	0.71	0/861
34	l	0.42	0/4495	0.58	1/6146 (0.0%)
35	m	0.49	0/1266	0.69	0/1721
36	n	0.22	0/484	0.36	0/652
37	o	0.10	0/859	0.29	0/1160
38	p	0.25	0/1533	0.38	0/2077
39	r	0.35	0/3717	0.50	0/5082
40	s	0.60	0/2563	0.81	0/3518
41	u	0.18	0/1433	0.34	0/1937
42	v	0.10	0/898	0.48	2/1198 (0.2%)
44	i	0.25	0/2447	0.42	1/3350 (0.0%)
All	All	0.33	0/62149	0.49	5/84330 (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
1	A	0	2
2	B	0	2
12	M	0	1
14	O	0	1
16	Q	0	1
40	s	0	3
All	All	0	10

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	v	27	PRO	N-CA-CB	11.54	110.55	102.35
42	v	26	PRO	N-CA-CB	7.25	110.11	103.08
9	J	44	GLY	CA-C-O	-6.10	118.02	122.23
44	i	84	TRP	N-CA-C	-5.66	106.18	114.39
34	l	237	MET	N-CA-C	-5.12	107.41	113.97

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	ARG	Sidechain
1	A	59	ARG	Sidechain
2	B	54	ARG	Sidechain
2	B	66	ARG	Sidechain
12	M	158	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	A	3316	0	3274	85	0
2	B	1420	0	1365	61	0
3	C	1249	0	1253	51	0
4	E	968	0	982	37	0
5	F	670	0	679	22	0
6	G	647	0	623	23	0
6	X	686	0	676	18	0
7	H	922	0	950	22	0
8	I	769	0	788	27	0
9	J	2486	0	2531	74	0
10	K	247	0	234	8	0
11	L	955	0	949	33	0
12	M	5261	0	5292	194	0
13	N	1188	0	1148	29	0
14	O	1637	0	1633	60	0
15	P	1721	0	1679	72	0
16	Q	3073	0	3056	127	0
17	S	568	0	567	13	0
18	T	742	0	721	22	0
19	U	647	0	653	16	0
20	V	1038	0	1027	24	0
21	W	1116	0	1087	27	0
22	Y	510	0	456	11	0
23	Z	582	0	569	12	0
24	a	1174	0	1177	29	0
25	b	1022	0	1037	34	0
26	c	1094	0	946	39	0
27	d	1393	0	1353	36	0
28	e	731	0	710	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	f	405	0	407	2	0
30	g	1004	0	1008	16	0
31	h	840	0	821	29	0
32	j	732	0	794	17	0
33	k	627	0	684	31	0
34	l	4383	0	4510	159	0
35	m	1239	0	1272	39	0
36	n	473	0	480	9	0
37	o	841	0	851	20	0
38	p	1480	0	1424	32	0
39	r	3623	0	3817	111	0
40	s	2494	0	2596	102	0
41	u	1394	0	1367	39	0
42	v	887	0	817	21	0
43	D	110	0	24	0	0
44	i	2385	0	2517	72	0
45	A	8	0	0	2	0
45	B	16	0	0	4	0
45	C	8	0	0	4	0
45	M	16	0	0	1	0
46	A	31	0	19	2	0
47	E	30	0	30	1	0
48	J	48	0	26	1	0
49	M	4	0	0	0	0
49	O	4	0	0	0	0
All	All	60914	0	60879	1536	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 13.

The worst 5 of 1536 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)
34:l:246:LEU:HD11	34:l:337:ALA:HA	1.20	1.10
2:B:99:HIS:CD2	45:B:302:SF4:S4	2.61	0.93
40:s:28:LEU:O	40:s:32:GLN:HB2	1.69	0.92
2:B:111:CYS:HG	45:B:301:SF4:FE1	0.73	0.91
14:O:183:ALA:HB3	14:O:195:ASP:HA	1.57	0.84

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	A	429/464 (92%)	413 (96%)	16 (4%)	0	100	100
2	B	174/210 (83%)	168 (97%)	6 (3%)	0	100	100
3	C	154/213 (72%)	141 (92%)	12 (8%)	1 (1%)	21	52
4	E	111/128 (87%)	103 (93%)	7 (6%)	1 (1%)	14	45
5	F	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
6	G	81/156 (52%)	77 (95%)	4 (5%)	0	100	100
6	X	83/156 (53%)	76 (92%)	7 (8%)	0	100	100
7	H	110/116 (95%)	102 (93%)	8 (7%)	0	100	100
8	I	91/113 (80%)	82 (90%)	7 (8%)	2 (2%)	5	28
9	J	309/377 (82%)	288 (93%)	20 (6%)	1 (0%)	36	66
10	K	28/108 (26%)	27 (96%)	1 (4%)	0	100	100
11	L	115/175 (66%)	105 (91%)	9 (8%)	1 (1%)	14	45
12	M	684/727 (94%)	630 (92%)	47 (7%)	7 (1%)	12	42
13	N	141/145 (97%)	126 (89%)	13 (9%)	2 (1%)	9	35
14	O	210/249 (84%)	198 (94%)	11 (5%)	1 (0%)	24	56
15	P	205/264 (78%)	179 (87%)	24 (12%)	2 (1%)	12	42
16	Q	382/463 (82%)	354 (93%)	26 (7%)	2 (0%)	24	56
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
19	U	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
20	V	138/141 (98%)	131 (95%)	6 (4%)	1 (1%)	18	50
21	W	136/144 (94%)	132 (97%)	3 (2%)	1 (1%)	18	50
22	Y	56/105 (53%)	46 (82%)	9 (16%)	1 (2%)	6	31
23	Z	70/98 (71%)	69 (99%)	1 (1%)	0	100	100
24	a	136/189 (72%)	132 (97%)	3 (2%)	1 (1%)	18	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	b	116/128 (91%)	108 (93%)	8 (7%)	0	100	100
26	c	134/186 (72%)	123 (92%)	11 (8%)	0	100	100
27	d	164/172 (95%)	161 (98%)	3 (2%)	0	100	100
28	e	86/153 (56%)	77 (90%)	9 (10%)	0	100	100
29	f	45/76 (59%)	43 (96%)	2 (4%)	0	100	100
30	g	117/119 (98%)	108 (92%)	6 (5%)	3 (3%)	4	25
31	h	102/106 (96%)	94 (92%)	6 (6%)	2 (2%)	6	29
32	j	88/115 (76%)	85 (97%)	3 (3%)	0	100	100
33	k	82/98 (84%)	76 (93%)	6 (7%)	0	100	100
34	l	561/603 (93%)	528 (94%)	32 (6%)	1 (0%)	43	73
35	m	162/174 (93%)	151 (93%)	11 (7%)	0	100	100
36	n	54/58 (93%)	53 (98%)	0	1 (2%)	6	30
37	o	100/129 (78%)	98 (98%)	2 (2%)	0	100	100
38	p	169/179 (94%)	163 (96%)	5 (3%)	1 (1%)	21	52
39	r	457/459 (100%)	439 (96%)	17 (4%)	1 (0%)	43	73
40	s	316/318 (99%)	298 (94%)	17 (5%)	1 (0%)	36	66
41	u	167/172 (97%)	158 (95%)	8 (5%)	1 (1%)	21	52
42	v	108/137 (79%)	101 (94%)	6 (6%)	1 (1%)	14	45
44	i	300/347 (86%)	289 (96%)	11 (4%)	0	100	100
All	All	7494/8847 (85%)	7040 (94%)	418 (6%)	36 (0%)	26	56

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	98	LYS
12	M	210	ILE
13	N	115	PHE
31	h	20	ILE
36	n	55	VAL

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	A	345/371 (93%)	322 (93%)	23 (7%)	15	41
2	B	151/174 (87%)	145 (96%)	6 (4%)	28	54
3	C	132/174 (76%)	121 (92%)	11 (8%)	10	35
4	E	106/116 (91%)	104 (98%)	2 (2%)	50	67
5	F	74/80 (92%)	69 (93%)	5 (7%)	14	41
6	G	71/136 (52%)	67 (94%)	4 (6%)	19	46
6	X	78/136 (57%)	76 (97%)	2 (3%)	40	63
7	H	100/102 (98%)	99 (99%)	1 (1%)	68	75
8	I	87/98 (89%)	83 (95%)	4 (5%)	24	51
9	J	268/323 (83%)	251 (94%)	17 (6%)	16	43
10	K	28/93 (30%)	28 (100%)	0	100	100
11	L	106/157 (68%)	99 (93%)	7 (7%)	15	42
12	M	574/608 (94%)	525 (92%)	49 (8%)	10	34
13	N	128/131 (98%)	115 (90%)	13 (10%)	7	27
14	O	180/206 (87%)	166 (92%)	14 (8%)	11	37
15	P	189/229 (82%)	174 (92%)	15 (8%)	11	37
16	Q	329/393 (84%)	308 (94%)	21 (6%)	16	43
17	S	59/59 (100%)	56 (95%)	3 (5%)	21	49
18	T	79/100 (79%)	72 (91%)	7 (9%)	9	32
19	U	72/73 (99%)	66 (92%)	6 (8%)	10	35
20	V	102/103 (99%)	97 (95%)	5 (5%)	22	49
21	W	115/123 (94%)	112 (97%)	3 (3%)	40	63
22	Y	54/87 (62%)	52 (96%)	2 (4%)	30	56
23	Z	56/79 (71%)	52 (93%)	4 (7%)	13	39
24	a	124/159 (78%)	122 (98%)	2 (2%)	55	70
25	b	113/122 (93%)	109 (96%)	4 (4%)	32	57
26	c	106/161 (66%)	100 (94%)	6 (6%)	18	46
27	d	145/155 (94%)	132 (91%)	13 (9%)	9	32
28	e	81/130 (62%)	79 (98%)	2 (2%)	42	63
29	f	43/67 (64%)	42 (98%)	1 (2%)	44	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	g	105/105 (100%)	102 (97%)	3 (3%)	37	61
31	h	86/92 (94%)	80 (93%)	6 (7%)	14	40
32	j	81/104 (78%)	76 (94%)	5 (6%)	16	43
33	k	72/85 (85%)	65 (90%)	7 (10%)	8	30
34	l	491/533 (92%)	458 (93%)	33 (7%)	15	41
35	m	130/137 (95%)	118 (91%)	12 (9%)	8	31
36	n	53/55 (96%)	47 (89%)	6 (11%)	5	24
37	o	86/115 (75%)	83 (96%)	3 (4%)	32	57
38	p	155/161 (96%)	151 (97%)	4 (3%)	40	63
39	r	416/416 (100%)	385 (92%)	31 (8%)	12	38
40	s	276/279 (99%)	254 (92%)	22 (8%)	11	36
41	u	153/155 (99%)	140 (92%)	13 (8%)	10	34
42	v	81/121 (67%)	79 (98%)	2 (2%)	42	63
44	i	271/314 (86%)	253 (93%)	18 (7%)	15	42
All	All	6551/7617 (86%)	6134 (94%)	417 (6%)	18	43

5 of 417 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	c	67	ASP
34	l	203	LEU
44	i	29	THR
27	d	49	GLN
31	h	99	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
17	S	68	ASN
41	u	95	GLN
26	c	164	ASN
40	s	235	ASN
44	i	36	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
49	FES	O	301	14	0,4,4	-	-	-		
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	7 (14%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
47	ZMP	E	201	-	27,29,36	1.76	6 (22%)	34,38,45	1.66	6 (17%)
49	FES	M	803	12	0,4,4	-	-	-		
48	NDP	J	401	-	51,52,52	0.50	0	71,80,80	0.68	2 (2%)
45	SF4	C	301	3	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
45	SF4	M	802	12	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	FES	O	301	14	-	-	0/1/1/1
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
47	ZMP	E	201	-	-	13/36/36/43	-
49	FES	M	803	12	-	-	0/1/1/1
48	NDP	J	401	-	-	2/34/77/77	0/5/5/5
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	E	201	ZMP	C16-N2	5.22	1.45	1.33
47	E	201	ZMP	C13-N1	5.11	1.45	1.33
46	A	502	FMN	C4A-N5	3.46	1.38	1.30
46	A	502	FMN	C10-N1	2.53	1.38	1.33
47	E	201	ZMP	C10-S1	2.44	1.82	1.76

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	E	201	ZMP	C9-C10-S1	5.82	120.34	113.40
48	J	401	NDP	P2B-O2B-C2B	-3.66	113.66	123.43
47	E	201	ZMP	O1-C10-C9	-3.61	119.81	123.98
46	A	502	FMN	C4-N3-C2	-3.18	120.00	125.64
46	A	502	FMN	C5A-C9A-N10	2.85	120.55	117.97

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

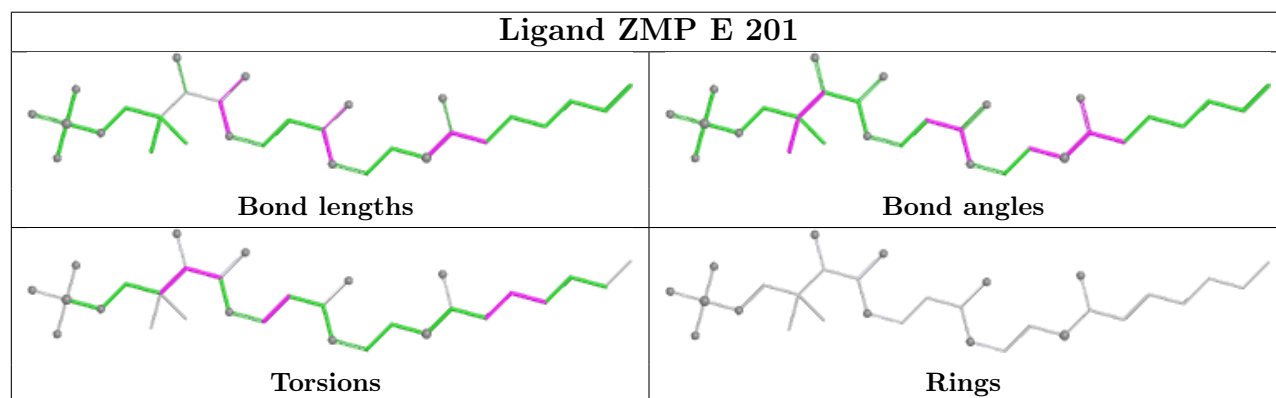
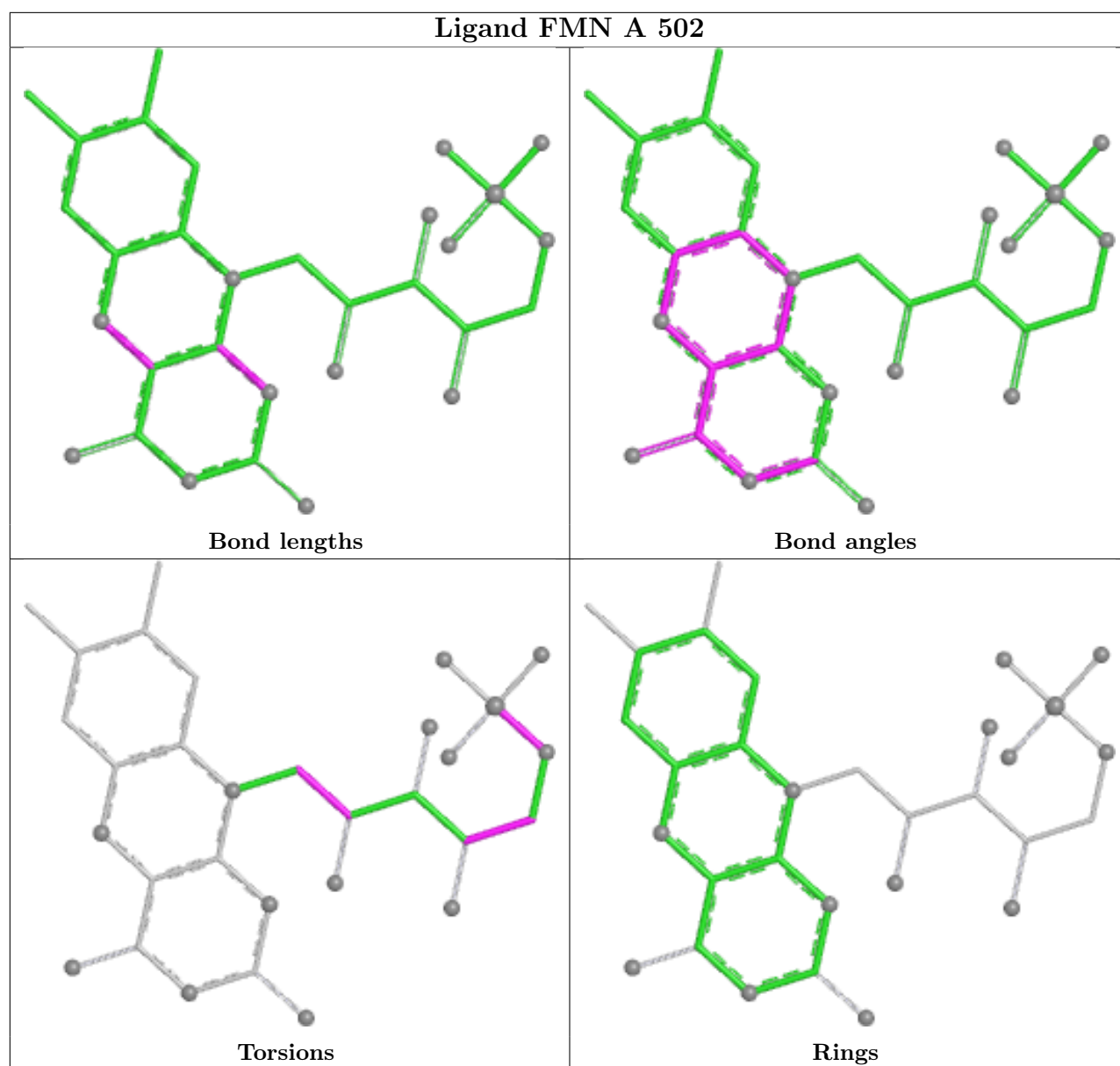
Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O2P
46	A	502	FMN	C5'-O5'-P-O3P
47	E	201	ZMP	O4-C17-C18-C21
47	E	201	ZMP	C16-C17-C18-C21

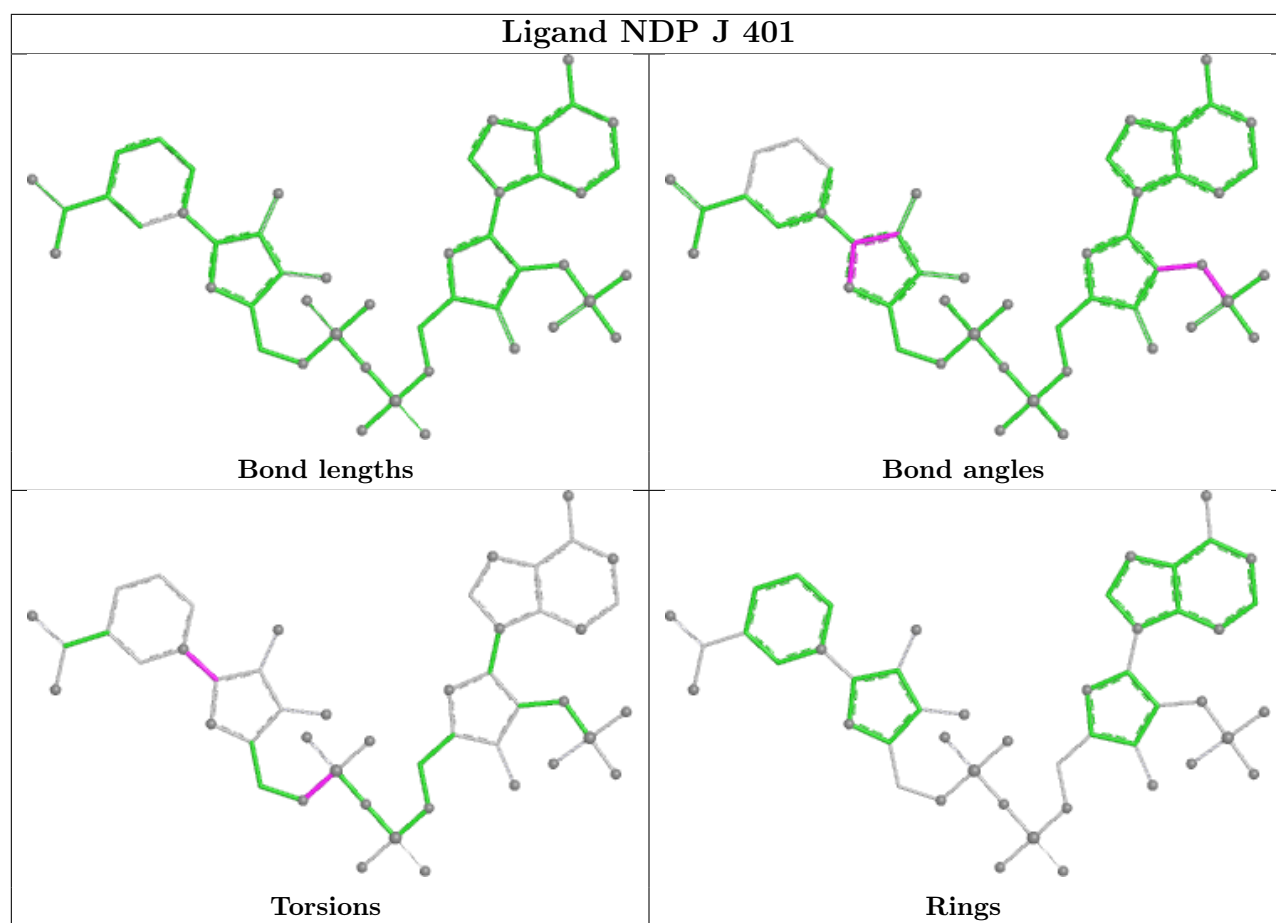
There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	502	FMN	2	0
45	B	302	SF4	3	0
45	M	801	SF4	1	0
45	A	501	SF4	2	0
47	E	201	ZMP	1	0
48	J	401	NDP	1	0
45	C	301	SF4	4	0
45	B	301	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 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

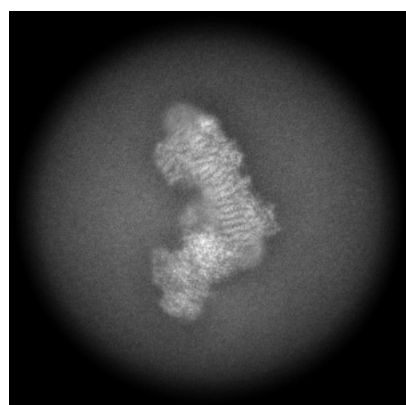
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45974. These allow visual inspection of the internal detail of the map and identification of artifacts.

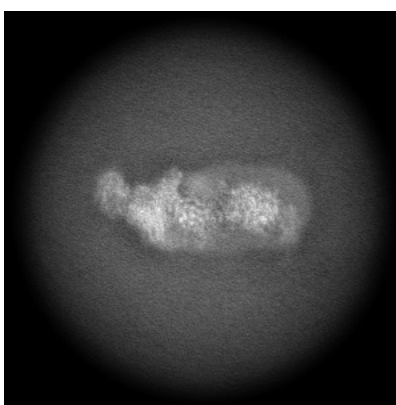
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

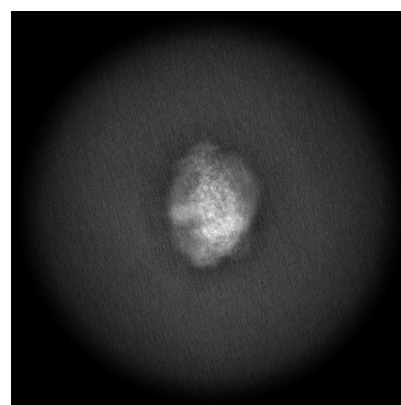
6.1.1 Primary map



X



Y

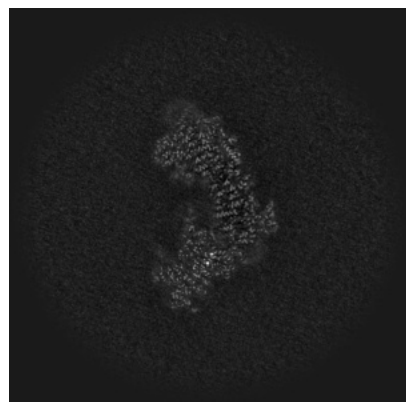


Z

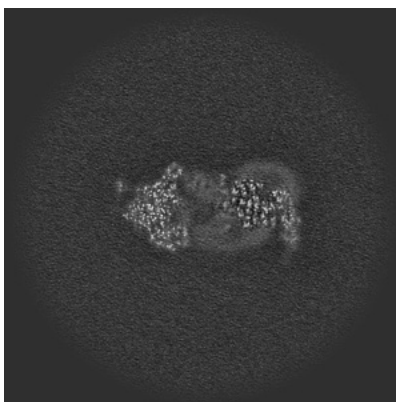
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

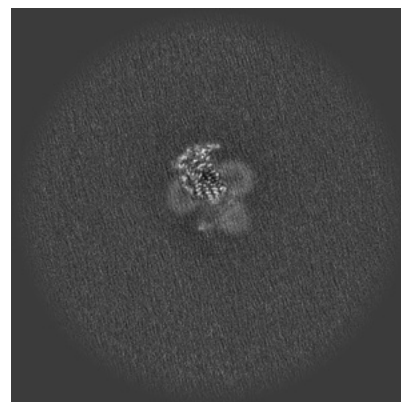
6.2.1 Primary map



X Index: 256



Y Index: 256

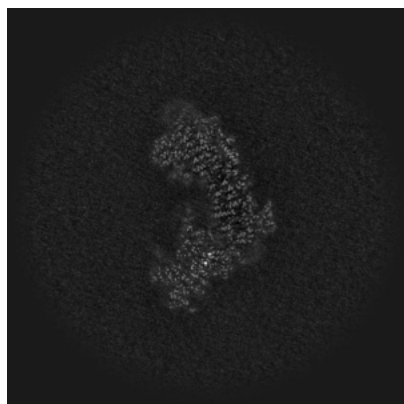


Z Index: 256

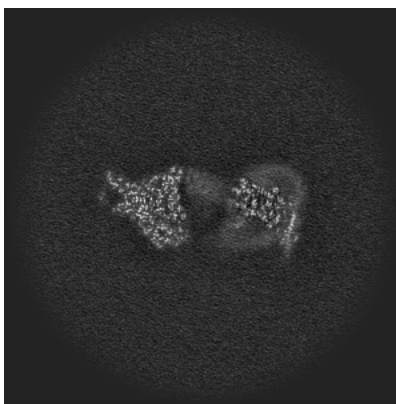
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

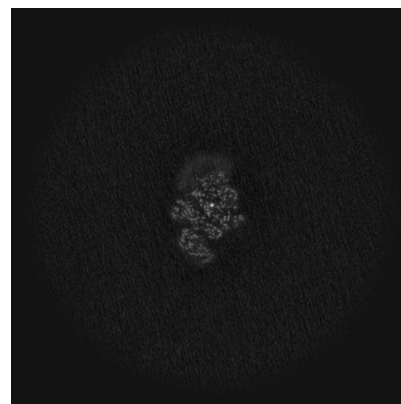
6.3.1 Primary map



X Index: 256



Y Index: 246

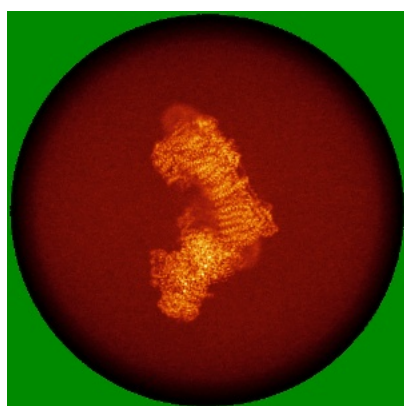


Z Index: 196

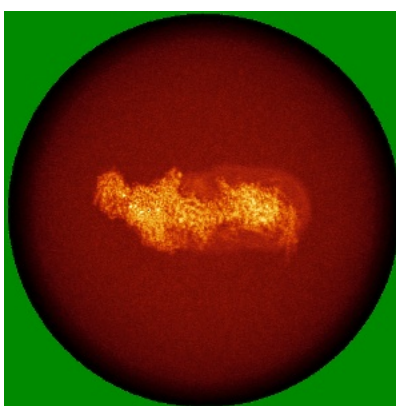
The images above show the largest variance slices of the map in three orthogonal directions.

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

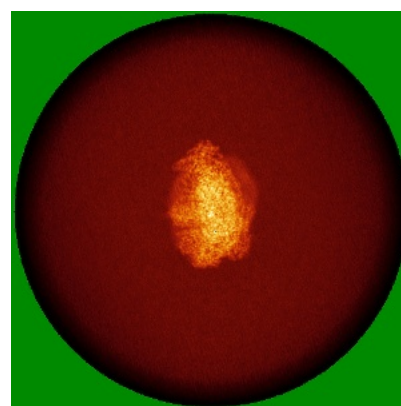
6.4.1 Primary map



X



Y



Z

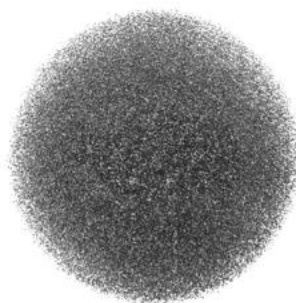
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

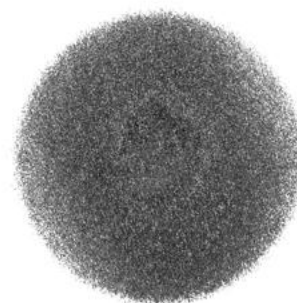
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

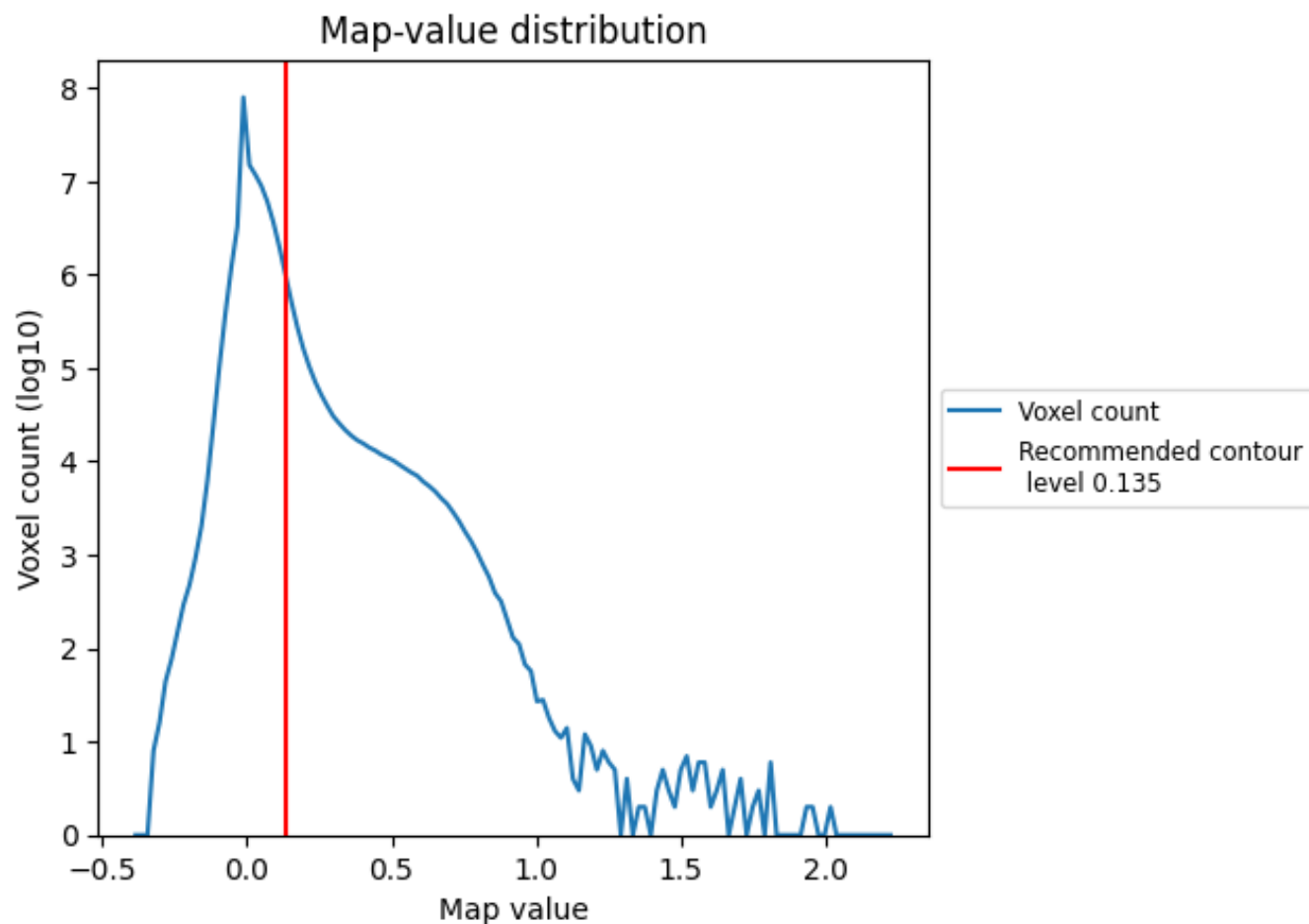
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

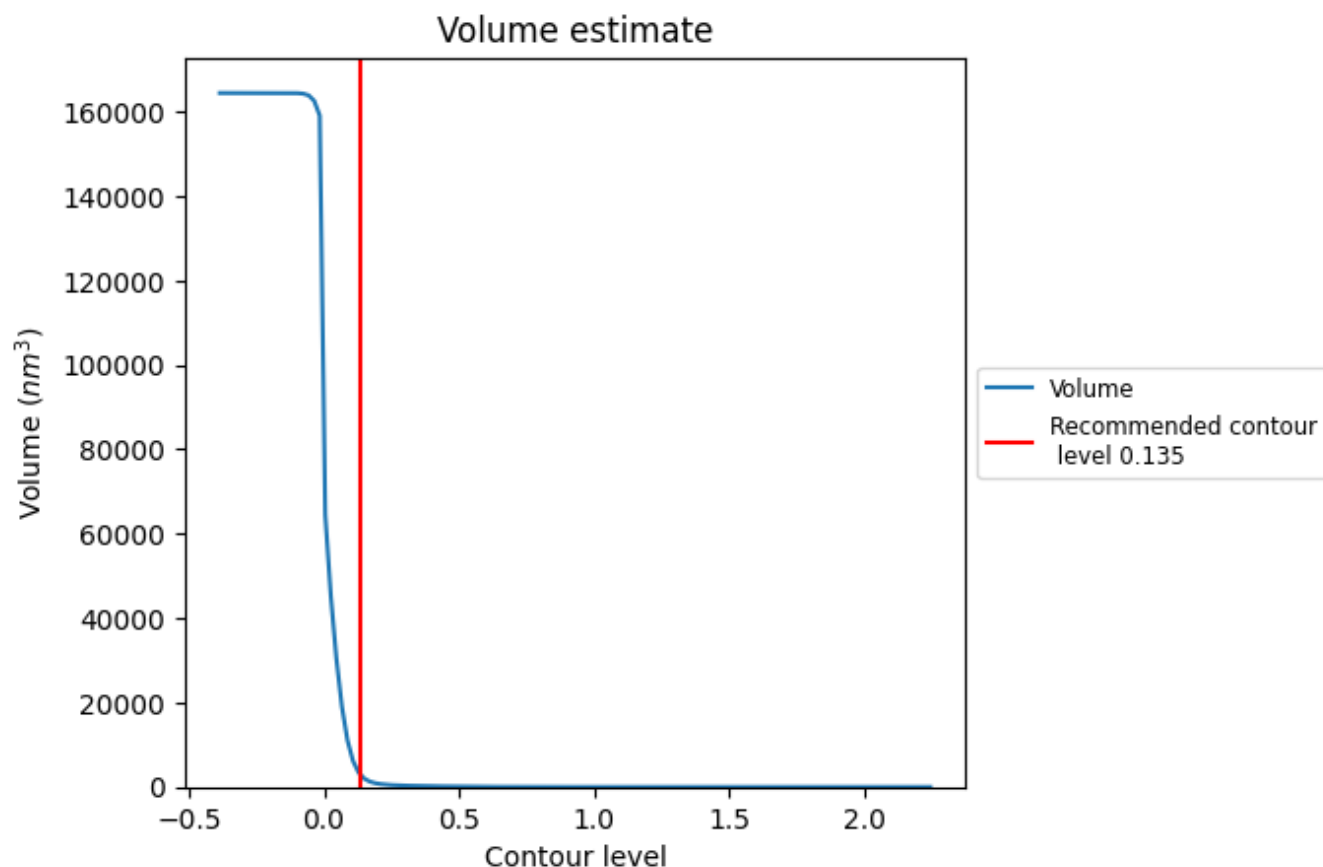
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

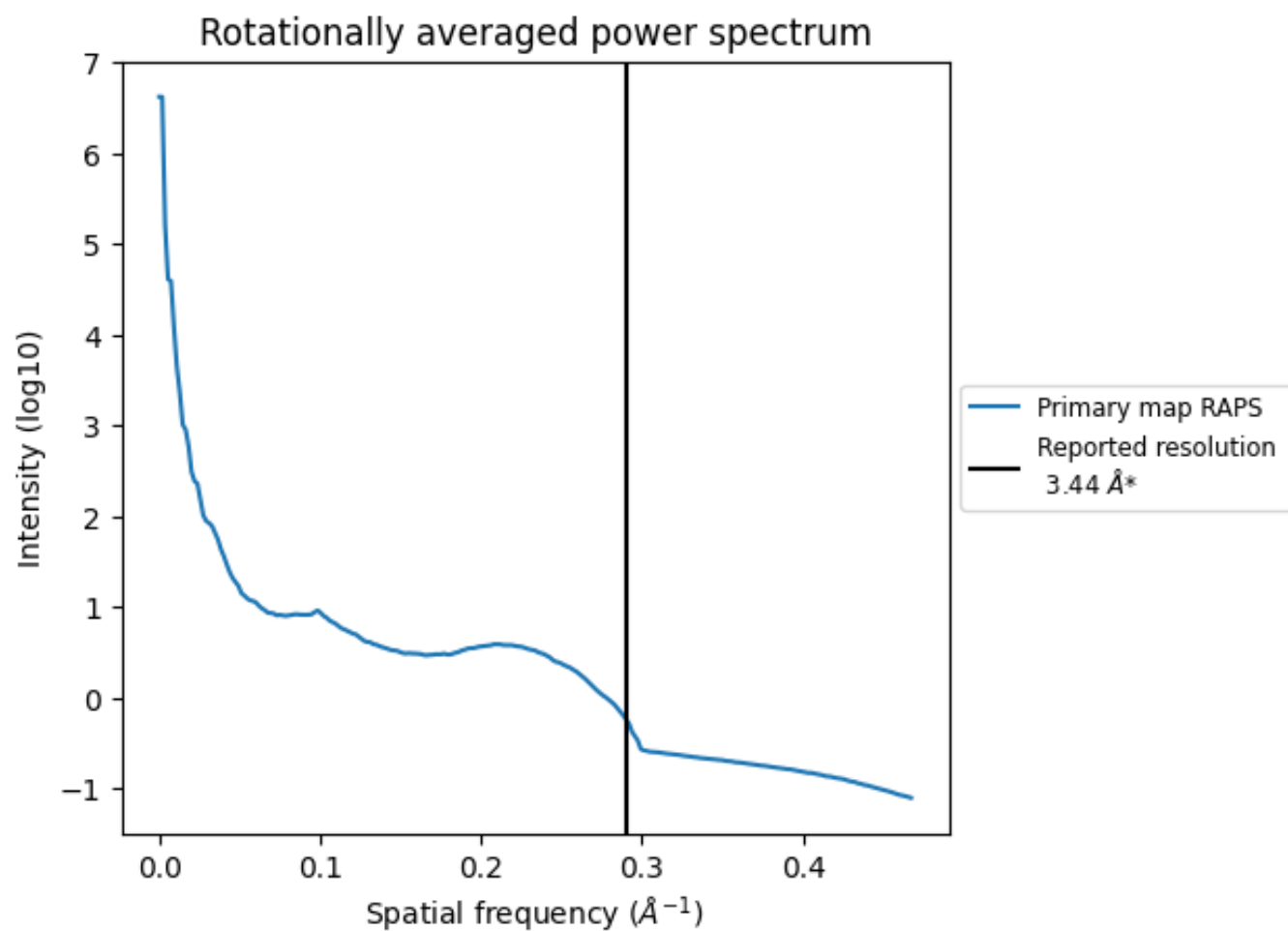
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2955 nm^3 ; this corresponds to an approximate mass of 2670 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 0.291 Å⁻¹

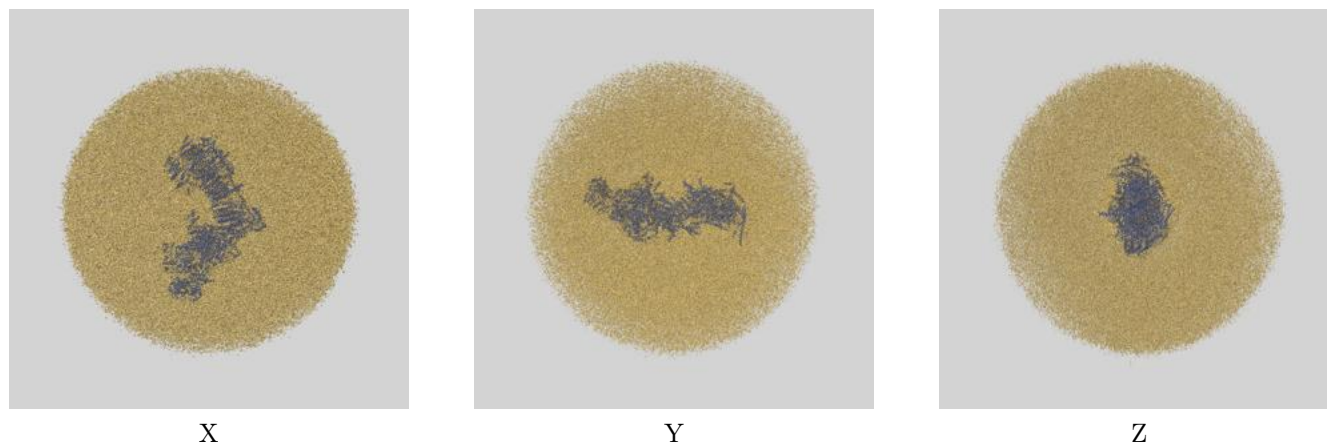
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45974 and PDB model 9CWT. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



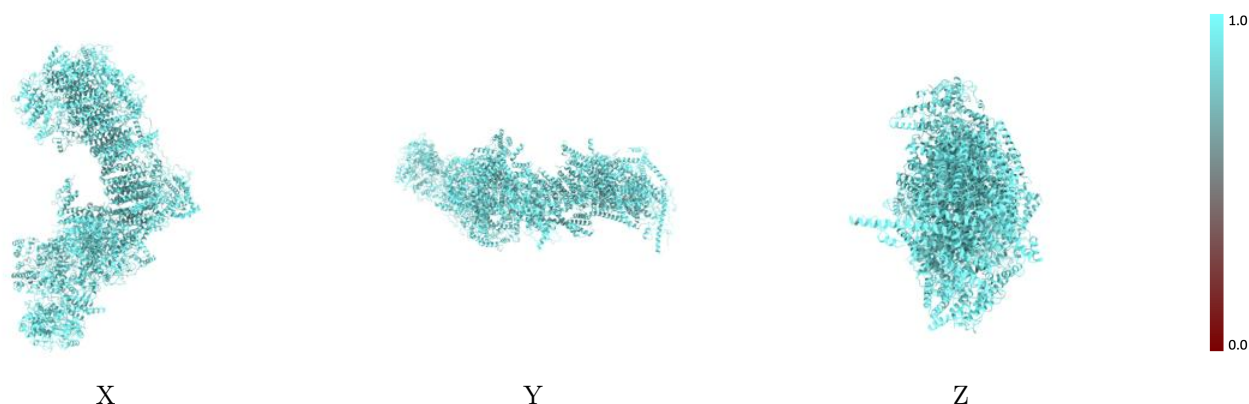
The images above show the 3D surface view of the map at the recommended contour level 0.135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



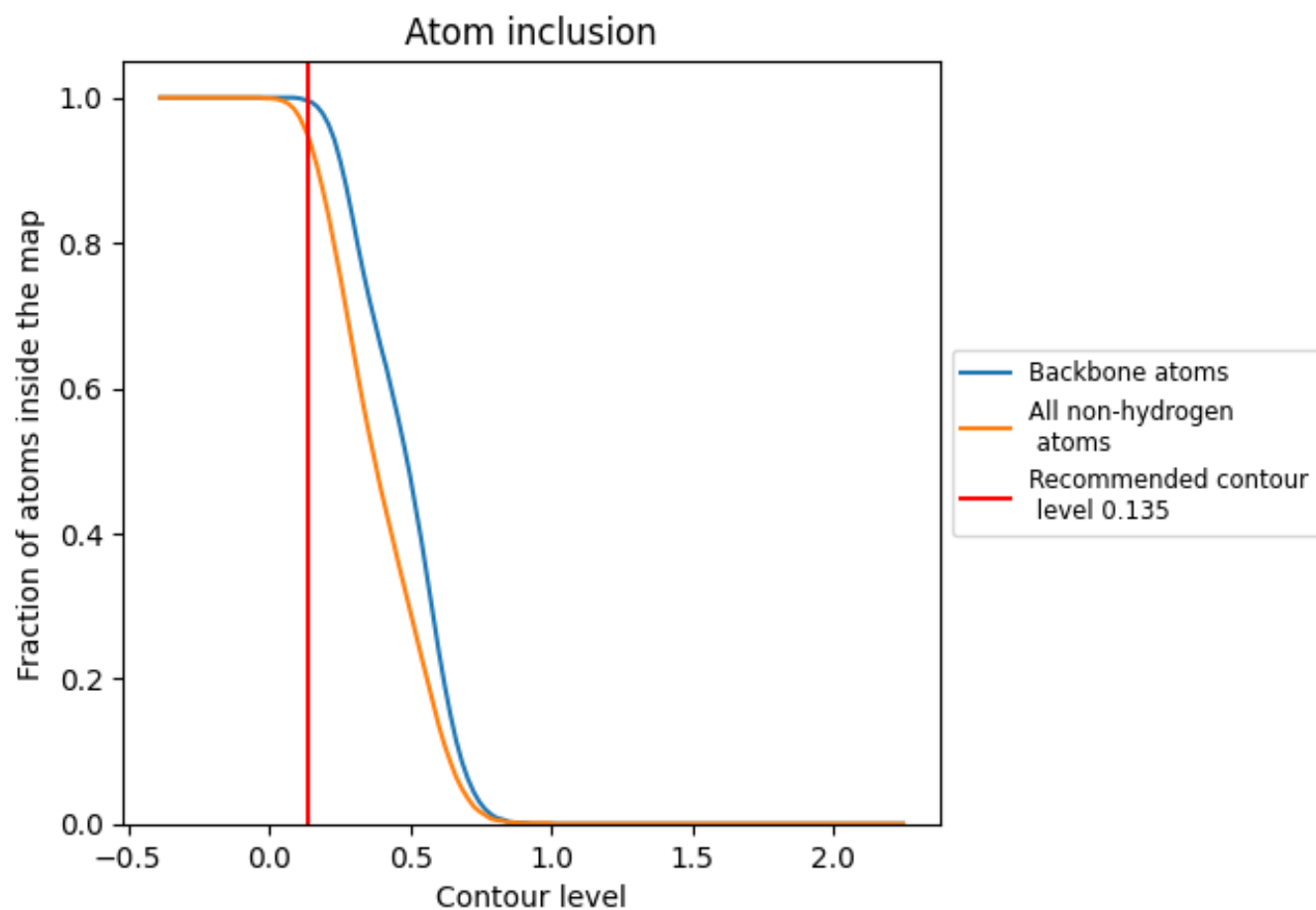
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 95% 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 (0.135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.4190
A	 0.9710	 0.4220
B	 0.9700	 0.4590
C	 0.9570	 0.4600
D	 0.9910	 0.4220
E	 0.9390	 0.4200
F	 0.9290	 0.3780
G	 0.9170	 0.3100
H	 0.9390	 0.3980
I	 0.9300	 0.4290
J	 0.9480	 0.3920
K	 0.9500	 0.4140
L	 0.9540	 0.4610
M	 0.9560	 0.4230
N	 0.9460	 0.4350
O	 0.9590	 0.4160
P	 0.9730	 0.4580
Q	 0.9590	 0.4460
S	 0.9580	 0.4500
T	 0.9570	 0.4510
U	 0.9550	 0.4240
V	 0.9150	 0.2990
W	 0.9620	 0.4340
X	 0.9620	 0.4040
Y	 0.9820	 0.3810
Z	 0.9680	 0.4220
a	 0.9580	 0.4550
b	 0.9650	 0.3730
c	 0.9500	 0.3490
d	 0.9690	 0.4370
e	 0.9590	 0.4380
f	 0.9210	 0.3270
g	 0.9510	 0.4400
h	 0.9440	 0.4350
i	 0.9330	 0.4560



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Chain	Atom inclusion	Q-score
j	 0.9020	 0.4140
k	 0.9310	 0.4430
l	 0.9400	 0.3910
m	 0.9350	 0.4160
n	 0.9410	 0.3930
o	 0.9470	 0.3650
p	 0.9520	 0.4040
r	 0.9470	 0.4430
s	 0.9240	 0.4310
u	 0.9430	 0.4210
v	 0.9660	 0.3720