



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 06:51 AM EST

PDB ID : 6U8Y
EMDB ID : EMD-20692
Title : Structure of the membrane-bound sulfane sulfur reductase (MBS), an archaeal respiratory membrane complex
Authors : Yu, H.J.; Li, H.L.
Deposited on : 2019-09-06
Resolution : 4.00 Å(reported)

This is a Full wwPDB EM Validation 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:

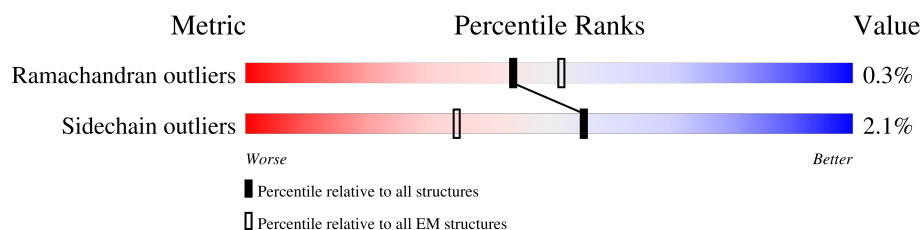
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	168	
1	a	168	
2	B	84	
2	b	84	
3	C	124	
3	c	124	
4	D	94	
4	d	94	
5	E	235	

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Mol	Chain	Length	Quality of chain
5	e	235	<div> <div>43%</div> <div>96%</div> <div>..</div> </div>
6	G	114	<div> <div>35%</div> <div>94%</div> <div>..</div> </div>
6	g	114	<div> <div>34%</div> <div>94%</div> <div>..</div> </div>
7	H	493	<div> <div>25%</div> <div>96%</div> <div>..</div> </div>
7	h	493	<div> <div>26%</div> <div>96%</div> <div>..</div> </div>
8	X	618	<div> <div>25%</div> <div>96%</div> <div>..</div> </div>
8	x	618	<div> <div>25%</div> <div>96%</div> <div>..</div> </div>
9	J	192	<div> <div>14%</div> <div>88%</div> <div>.. 8%</div> </div>
9	j	192	<div> <div>13%</div> <div>88%</div> <div>.. 8%</div> </div>
10	K	174	<div> <div>20%</div> <div>95%</div> <div>...</div> </div>
10	k	174	<div> <div>20%</div> <div>95%</div> <div>...</div> </div>
11	L	391	<div> <div>14%</div> <div>94%</div> <div>• 5%</div> </div>
11	l	391	<div> <div>14%</div> <div>95%</div> <div>• 5%</div> </div>
12	M	309	<div> <div>25%</div> <div>96%</div> <div>..</div> </div>
12	m	309	<div> <div>25%</div> <div>96%</div> <div>..</div> </div>
13	N	208	<div> <div>9%</div> <div>82%</div> <div>• 15%</div> </div>
13	n	208	<div> <div>11%</div> <div>82%</div> <div>• 15%</div> </div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 48364 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 Monovalent cation/H⁺ antiporter subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	161	Total	C	N	O	S	0	0
			1300	868	205	223	4		
1	a	161	Total	C	N	O	S	0	0
			1300	868	205	223	4		

- Molecule 2 is a protein called Monovalent cation/H⁺ antiporter subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			624	421	98	102	3		
2	b	79	Total	C	N	O	S	0	0
			624	421	98	102	3		

- Molecule 3 is a protein called Monovalent cation/H⁺ antiporter subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	112	Total	C	N	O	S	0	0
			858	567	140	149	2		
3	c	112	Total	C	N	O	S	0	0
			858	567	140	149	2		

- Molecule 4 is a protein called DUF4040 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	89	Total	C	N	O	S	0	0
			685	462	107	111	5		
4	d	89	Total	C	N	O	S	0	0
			685	462	107	111	5		

- Molecule 5 is a protein called Monovalent cation/H⁺ antiporter subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	232	Total	C	N	O	S	0	0
			1792	1192	286	308	6		
5	e	232	Total	C	N	O	S	0	0
			1792	1192	286	308	6		

- Molecule 6 is a protein called Monovalent cation/H⁺ antiporter subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	110	Total	C	N	O	S	0	0
			816	539	126	149	2		
6	g	110	Total	C	N	O	S	0	0
			816	539	126	149	2		

- Molecule 7 is a protein called NADH dehydrogenase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	487	Total	C	N	O	S	0	0
			3696	2480	575	622	19		
7	h	487	Total	C	N	O	S	0	0
			3696	2480	575	622	19		

- Molecule 8 is a protein called NADH dehydrogenase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	603	Total	C	N	O	S	0	0
			4677	3143	726	787	21		
8	x	603	Total	C	N	O	S	0	0
			4677	3143	726	787	21		

- Molecule 9 is a protein called NADH dehydrogenase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	177	Total	C	N	O	S	0	0
			1461	954	240	255	12		
9	j	177	Total	C	N	O	S	0	0
			1461	954	240	255	12		

- Molecule 10 is a protein called NADH dehydrogenase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	170	Total	C	N	O	S	0	0
			1437	925	245	260	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	170	Total	C	N	O	S	0	0
			1437	925	245	260	7		

- Molecule 11 is a protein called NADH dehydrogenase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	373	Total	C	N	O	S	0	0
			3010	1955	509	535	11		
11	l	373	Total	C	N	O	S	0	0
			3010	1955	509	535	11		

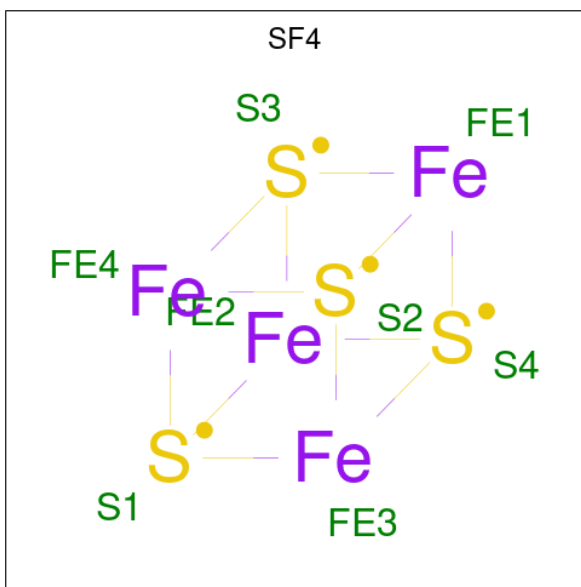
- Molecule 12 is a protein called NADH dehydrogenase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	301	Total	C	N	O	S	0	0
			2319	1567	362	376	14		
12	m	301	Total	C	N	O	S	0	0
			2319	1567	362	376	14		

- Molecule 13 is a protein called NADH dehydrogenase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	176	Total	C	N	O	S	0	0
			1483	988	233	251	11		
13	n	176	Total	C	N	O	S	0	0
			1483	988	233	251	11		

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

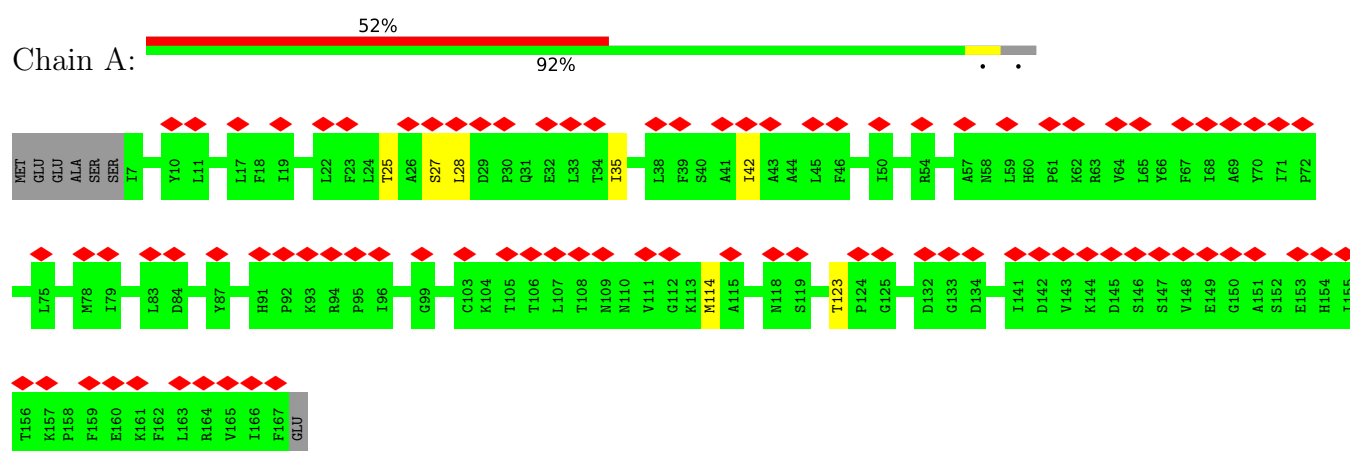


Mol	Chain	Residues	Atoms			AltConf
14	J	1	Total	Fe	S	0
			8	4	4	
14	N	1	Total	Fe	S	0
			16	8	8	
14	N	1	Total	Fe	S	0
			16	8	8	
14	j	1	Total	Fe	S	0
			8	4	4	
14	n	1	Total	Fe	S	0
			16	8	8	
14	n	1	Total	Fe	S	0
			16	8	8	

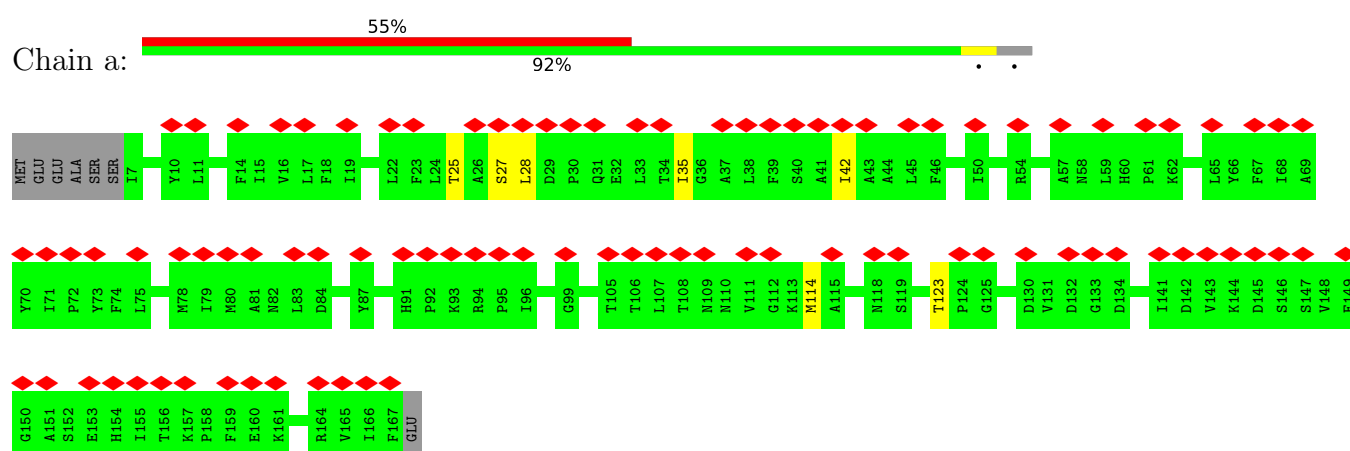
3 Residue-property plots [i](#)

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.

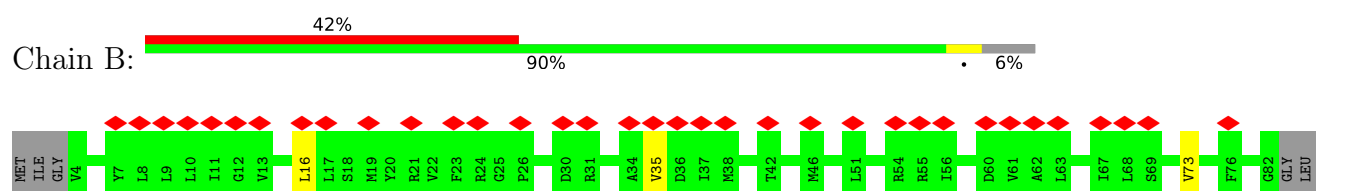
- Molecule 1: Monovalent cation/H⁺ antiporter subunit E



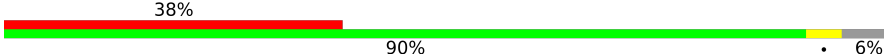
- Molecule 1: Monovalent cation/H⁺ antiporter subunit E

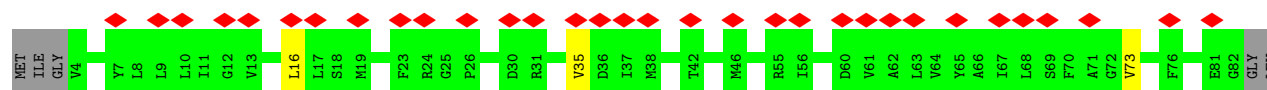


- Molecule 2: Monovalent cation/H⁺ antiporter subunit F




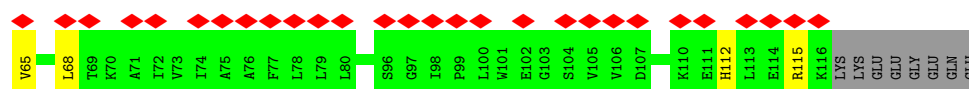
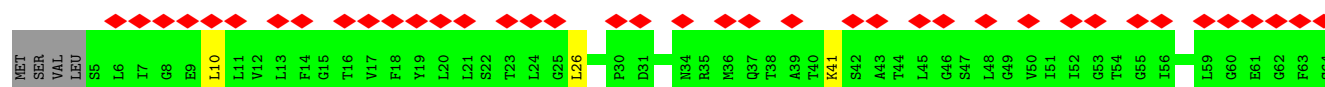
- Molecule 2: Monovalent cation/H⁺ antiporter subunit F

Chain b: 

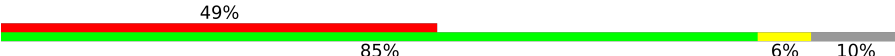


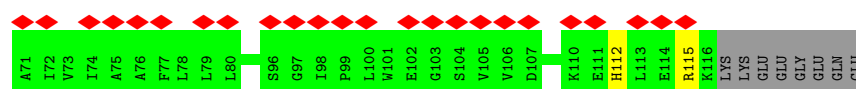
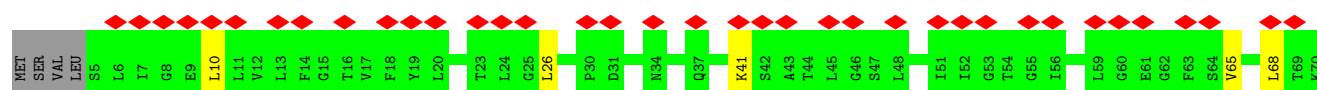
- Molecule 3: Monovalent cation/H⁺ antiporter subunit G

Chain C: 

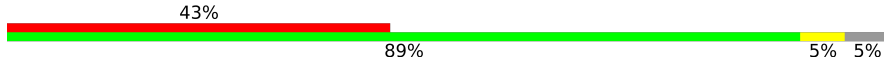


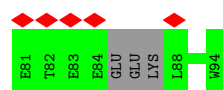
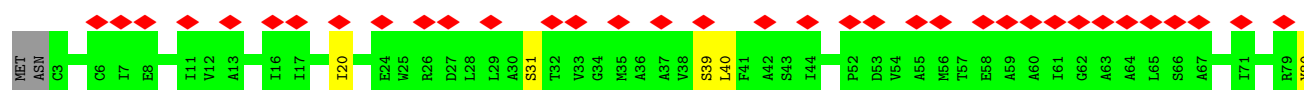
- Molecule 3: Monovalent cation/H⁺ antiporter subunit G

Chain c: 




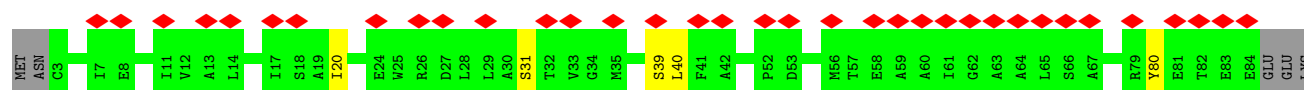
- Molecule 4: DUF4040 domain-containing protein

Chain D: 



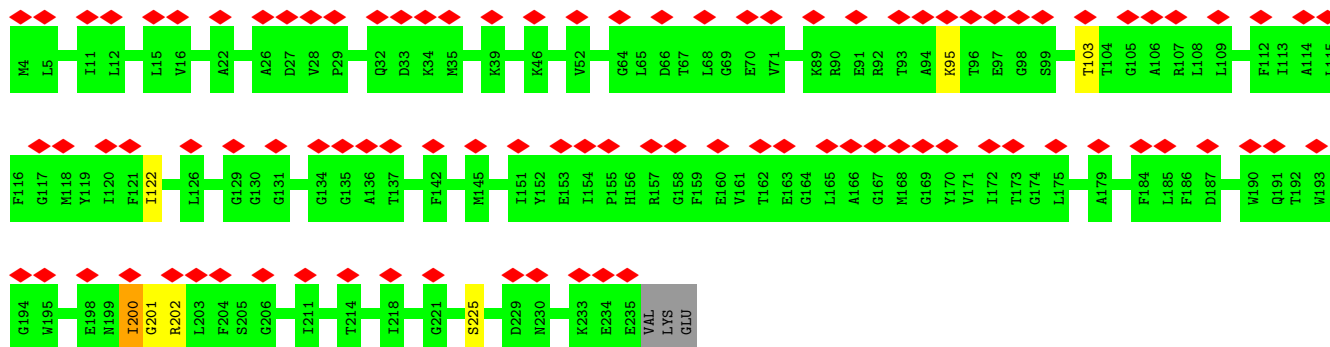
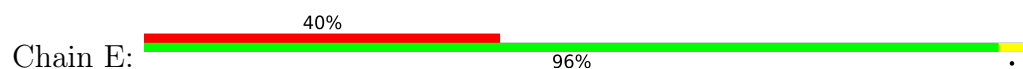
- Molecule 4: DUF4040 domain-containing protein

Chain d: 

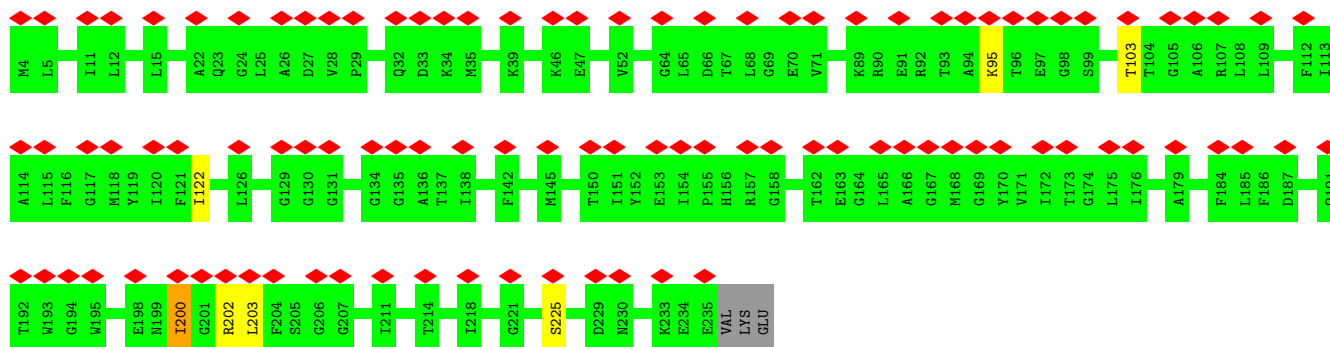
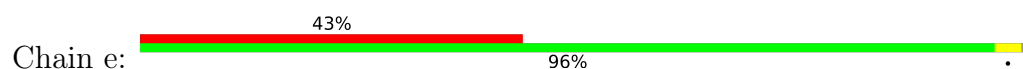




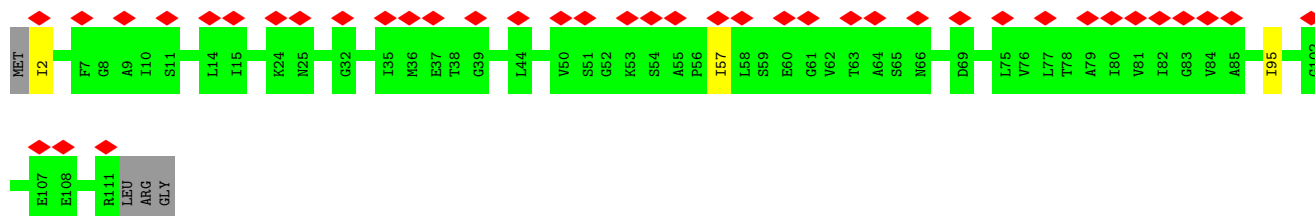
- Molecule 5: Monovalent cation/H⁺ antiporter subunit B



- Molecule 5: Monovalent cation/H⁺ antiporter subunit B

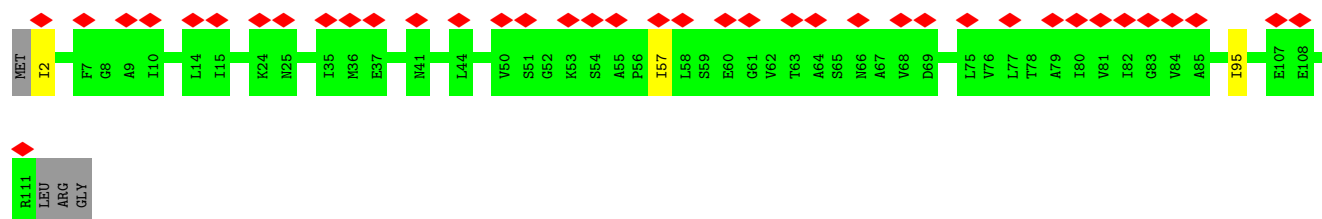


- Molecule 6: Monovalent cation/H⁺ antiporter subunit C



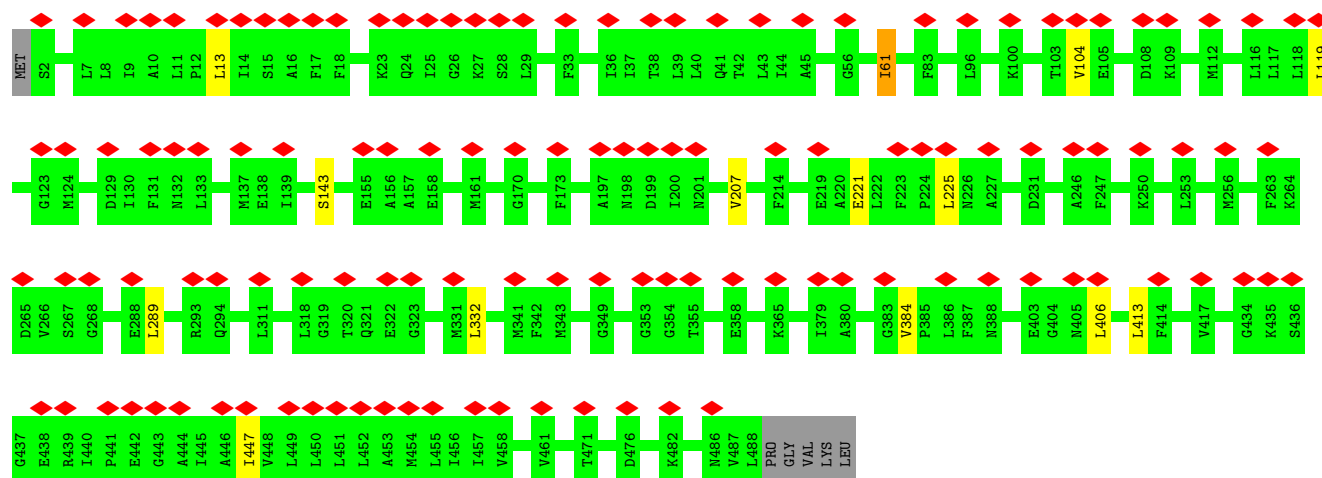
- Molecule 6: Monovalent cation/H⁺ antiporter subunit C





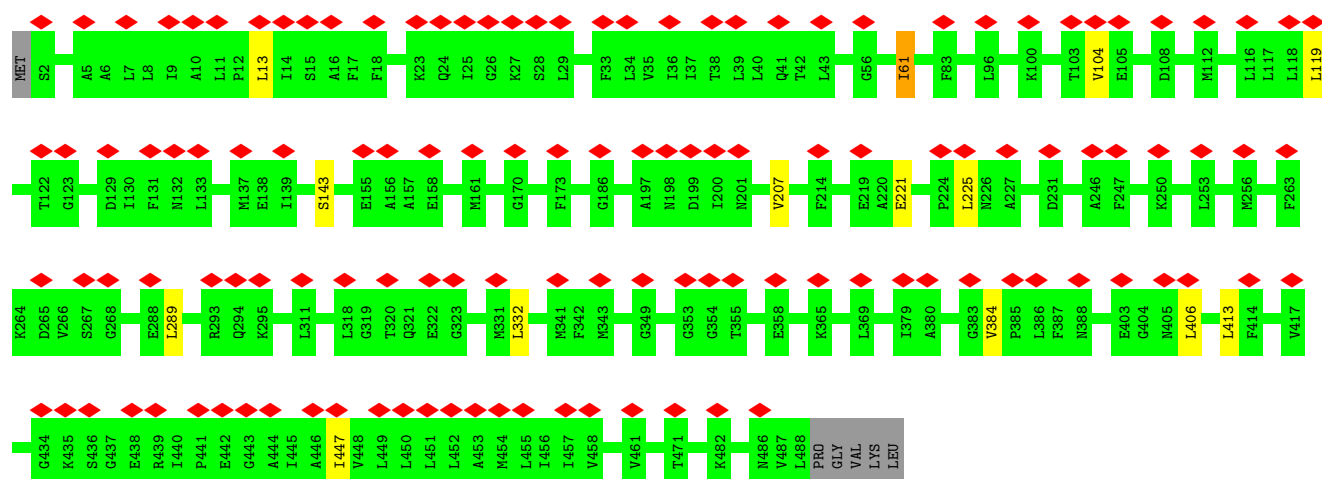
• Molecule 7: NADH dehydrogenase subunit N

Chain H: 25% 96%



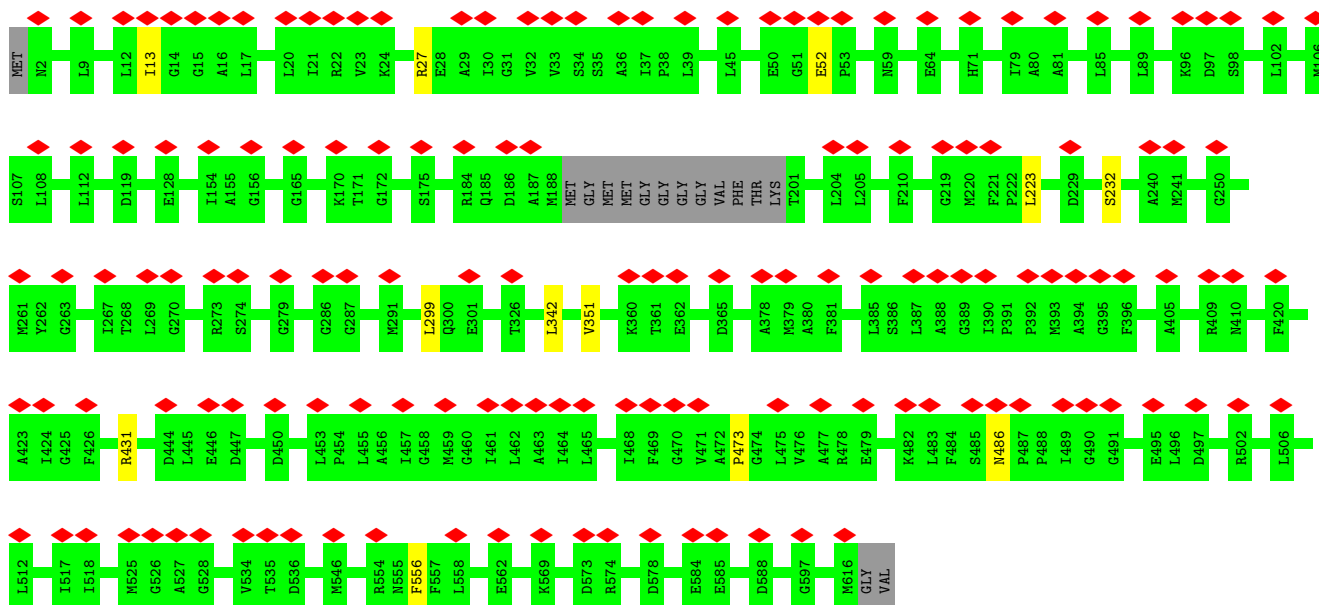
• Molecule 7: NADH dehydrogenase subunit N

Chain h: 26% 96%

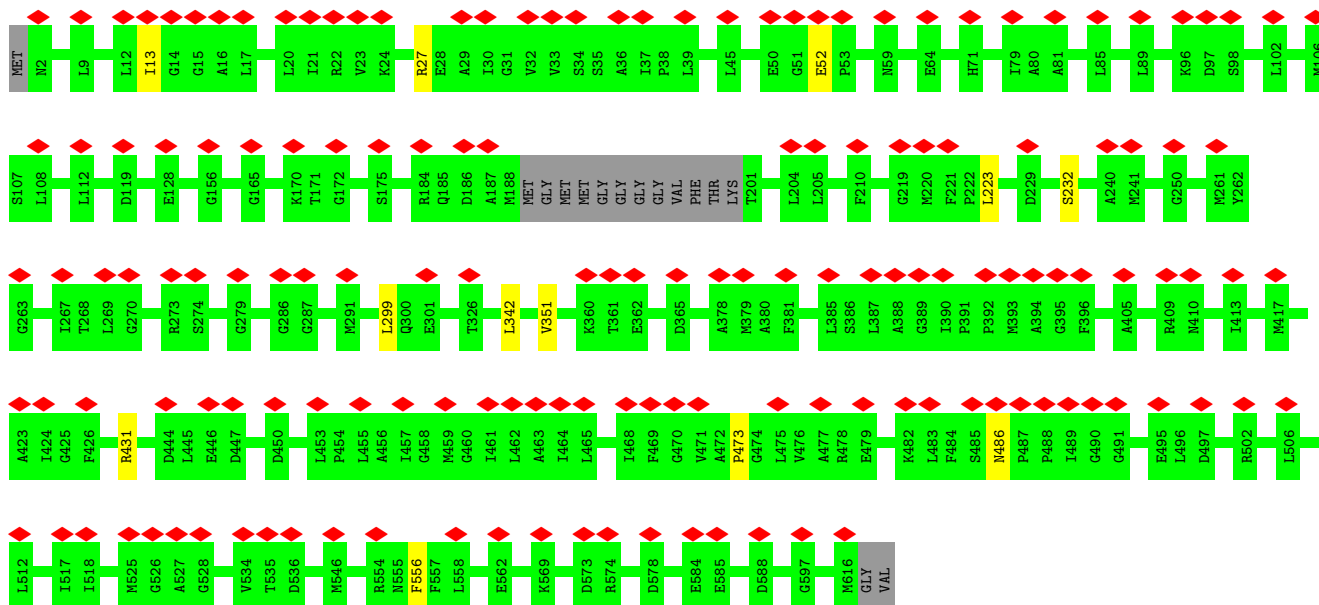


• Molecule 8: NADH dehydrogenase subunit M

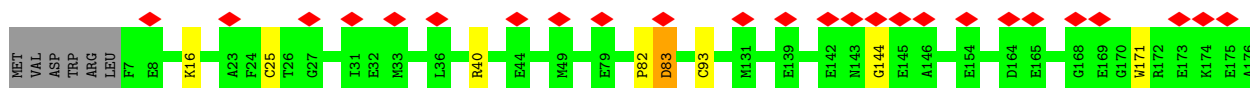
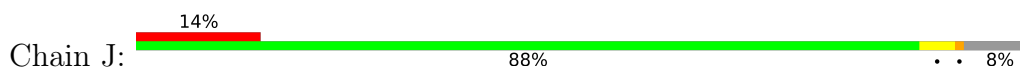
Chain X: 25% 96%

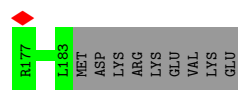


• Molecule 8: NADH dehydrogenase subunit M

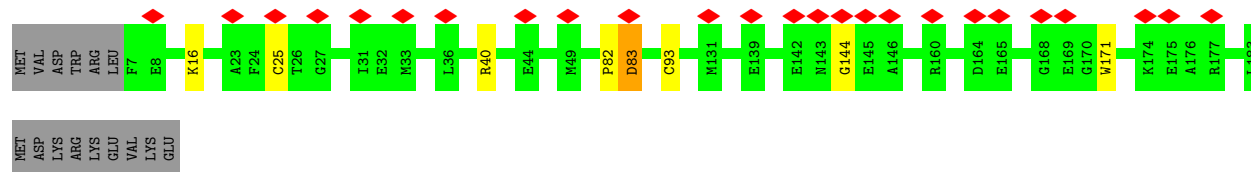
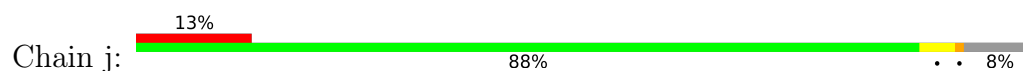


• Molecule 9: NADH dehydrogenase subunit B

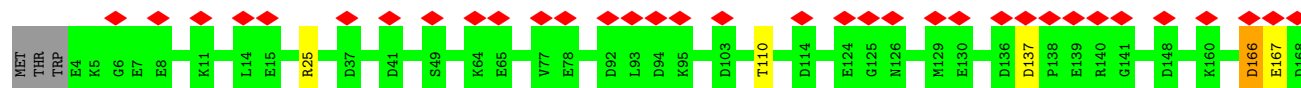




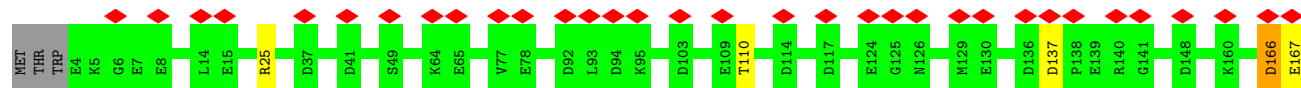
• Molecule 9: NADH dehydrogenase subunit B



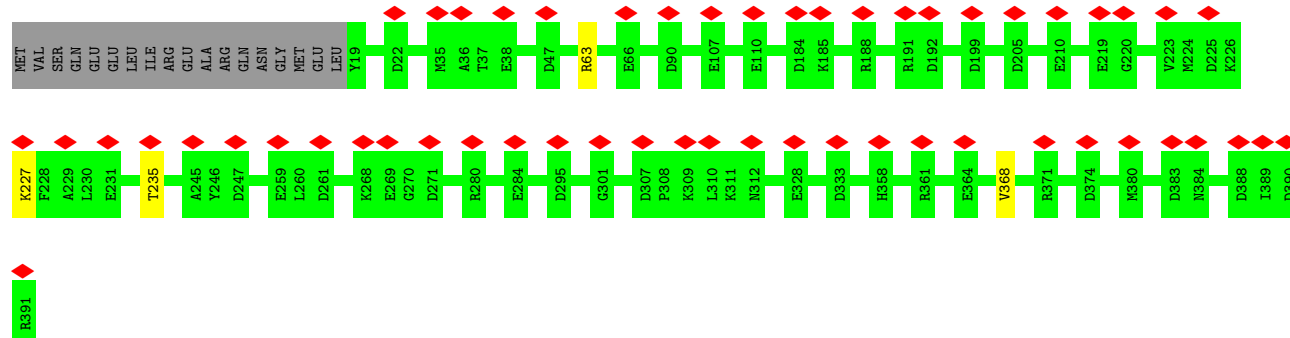
• Molecule 10: NADH dehydrogenase subunit C



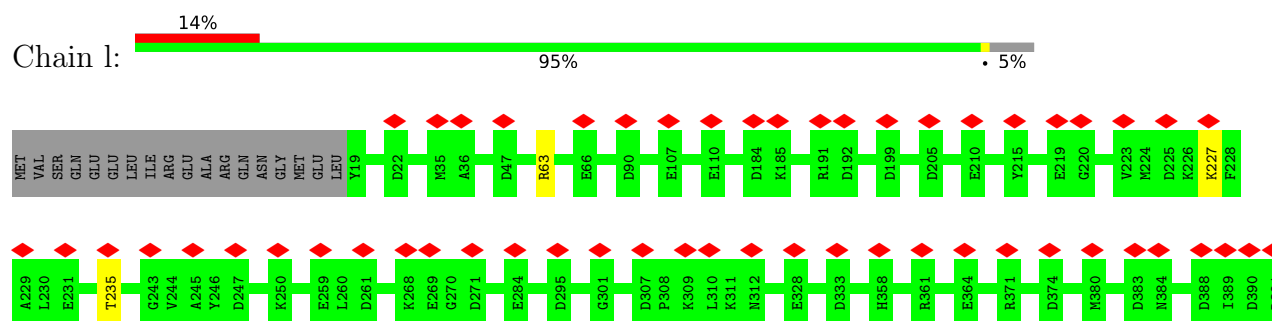
• Molecule 10: NADH dehydrogenase subunit C



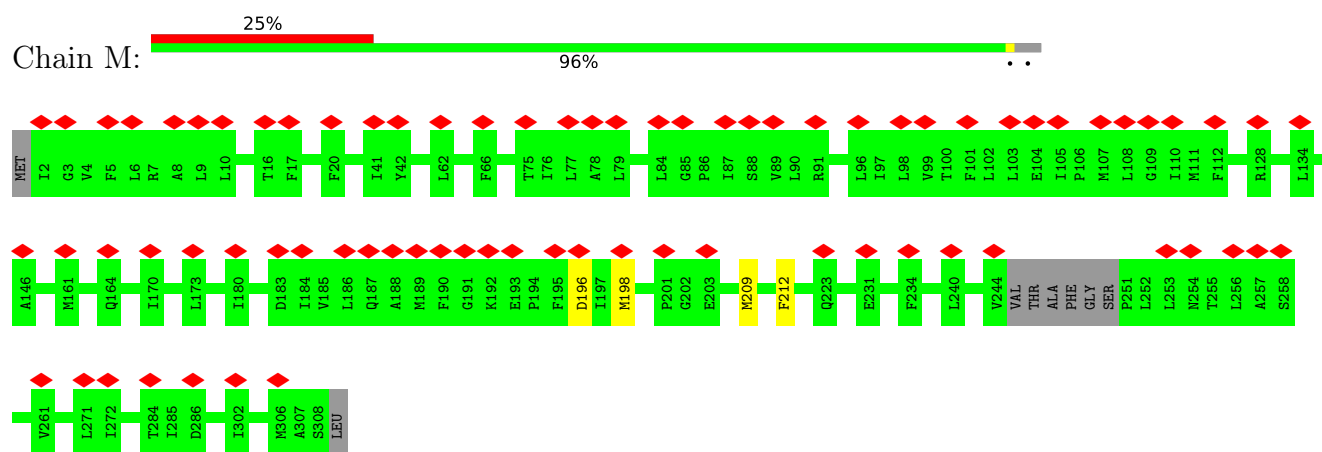
• Molecule 11: NADH dehydrogenase subunit D



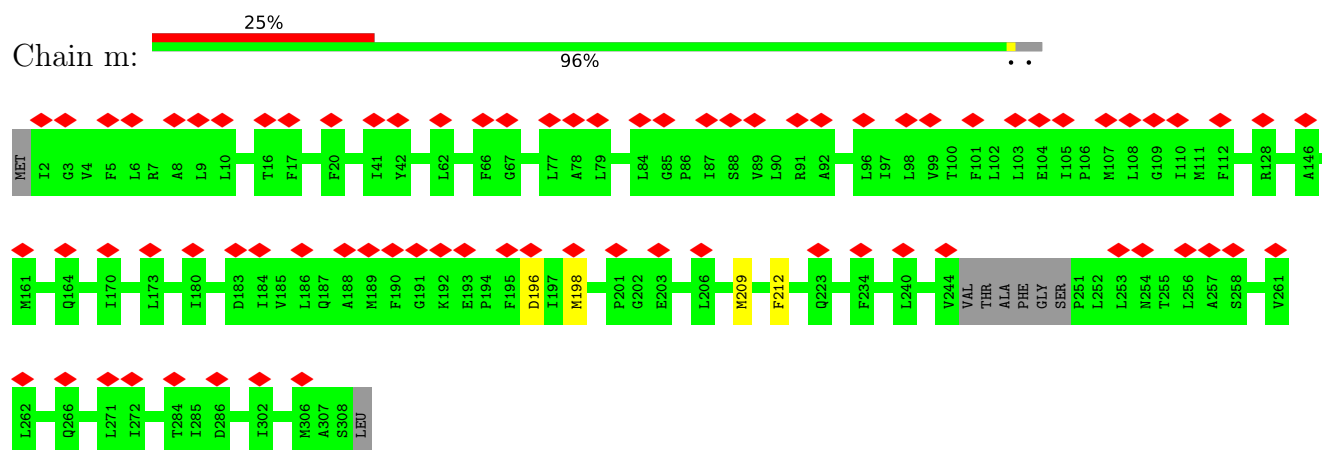
- Molecule 11: NADH dehydrogenase subunit D



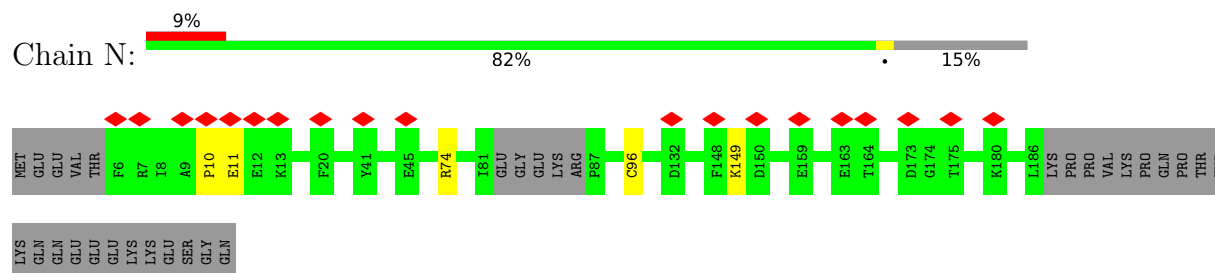
- Molecule 12: NADH dehydrogenase subunit



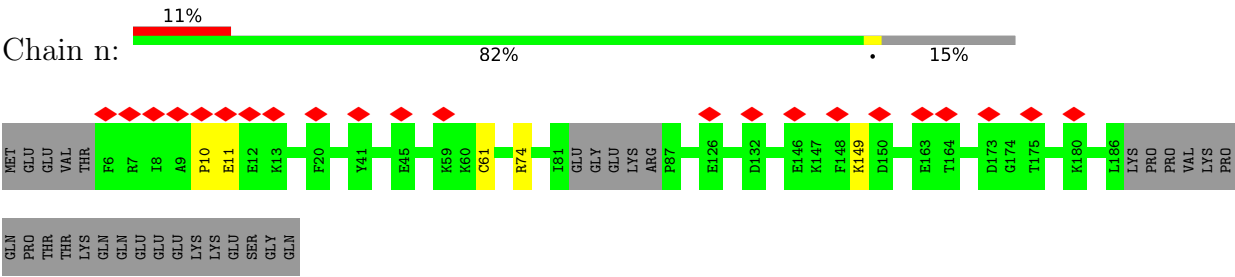
- Molecule 12: NADH dehydrogenase subunit



- Molecule 13: NADH dehydrogenase subunit I



● Molecule 13: NADH dehydrogenase subunit I



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	203673	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.263	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	329.28003, 329.28003, 329.28003	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.029, 1.029, 1.029	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	0.35	0/1337	0.62	0/1824
1	a	0.36	0/1337	0.62	0/1824
2	B	0.36	0/635	0.61	0/865
2	b	0.36	0/635	0.61	0/865
3	C	0.35	0/876	0.62	1/1190 (0.1%)
3	c	0.35	0/876	0.62	1/1190 (0.1%)
4	D	0.42	0/701	0.61	1/956 (0.1%)
4	d	0.42	0/701	0.61	1/956 (0.1%)
5	E	0.38	0/1838	0.64	1/2497 (0.0%)
5	e	0.38	0/1838	0.66	1/2497 (0.0%)
6	G	0.34	0/825	0.59	0/1123
6	g	0.34	0/825	0.60	0/1123
7	H	0.38	0/3783	0.66	4/5156 (0.1%)
7	h	0.39	0/3783	0.66	4/5156 (0.1%)
8	X	0.39	0/4802	0.64	2/6530 (0.0%)
8	x	0.39	0/4802	0.64	2/6530 (0.0%)
9	J	0.51	0/1508	0.69	1/2045 (0.0%)
9	j	0.51	0/1508	0.69	1/2045 (0.0%)
10	K	0.40	0/1471	0.61	0/1978
10	k	0.40	0/1471	0.61	0/1978
11	L	0.44	0/3091	0.61	0/4199
11	l	0.44	0/3091	0.61	0/4199
12	M	0.37	0/2377	0.60	0/3227
12	m	0.37	0/2377	0.60	0/3227
13	N	0.55	0/1532	0.66	0/2067
13	n	0.53	0/1532	0.65	0/2067
All	All	0.41	0/49552	0.63	20/67314 (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	1
1	a	0	1
3	C	0	1
3	c	0	1
4	D	0	1
4	d	0	1
5	E	0	1
5	e	0	1
6	G	0	1
6	g	0	1
7	H	0	1
7	h	0	1
8	X	0	3
8	x	0	3
9	J	0	2
9	j	0	2
10	K	0	2
10	k	0	2
12	M	0	1
12	m	0	1
13	N	0	1
13	n	0	1
All	All	0	30

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	203	LEU	CB-CA-C	-9.84	91.50	110.20
8	x	223	LEU	CA-CB-CG	6.18	129.52	115.30
8	X	223	LEU	CA-CB-CG	6.18	129.50	115.30
7	h	413	LEU	CA-CB-CG	6.03	129.16	115.30
7	H	413	LEU	CA-CB-CG	6.02	129.15	115.30
7	h	119	LEU	CB-CG-CD1	-5.79	101.17	111.00
7	H	119	LEU	CB-CG-CD1	-5.76	101.20	111.00
3	C	41	LYS	CD-CE-NZ	-5.56	98.92	111.70
3	c	41	LYS	CD-CE-NZ	-5.56	98.91	111.70
7	H	289	LEU	CA-CB-CG	5.49	127.93	115.30
7	h	289	LEU	CA-CB-CG	5.47	127.87	115.30
7	H	406	LEU	CA-CB-CG	5.46	127.87	115.30
5	E	201	GLY	N-CA-C	-5.45	99.48	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	h	406	LEU	CA-CB-CG	5.43	127.79	115.30
4	d	40	LEU	CA-CB-CG	5.15	127.15	115.30
8	X	342	LEU	CA-CB-CG	5.14	127.13	115.30
4	D	40	LEU	CA-CB-CG	5.14	127.12	115.30
8	x	342	LEU	CA-CB-CG	5.13	127.10	115.30
9	j	83	ASP	CB-CG-OD2	5.10	122.89	118.30
9	J	83	ASP	CB-CG-OD2	5.09	122.89	118.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	THR	Peptide
3	C	112	HIS	Mainchain
4	D	80	TYR	Mainchain
5	E	95	LYS	Peptide
6	G	57	ILE	Peptide
7	H	221	GLU	Peptide
9	J	144	GLY	Mainchain,Peptide
10	K	166	ASP	Peptide
10	K	25	ARG	Peptide
12	M	196	ASP	Peptide
13	N	10	PRO	Peptide
8	X	232	SER	Peptide
8	X	486	ASN	Peptide
8	X	52	GLU	Peptide
1	a	123	THR	Peptide
3	c	112	HIS	Mainchain
4	d	80	TYR	Mainchain
5	e	95	LYS	Peptide
6	g	57	ILE	Peptide
7	h	221	GLU	Peptide
9	j	144	GLY	Mainchain,Peptide
10	k	166	ASP	Peptide
10	k	25	ARG	Peptide
12	m	196	ASP	Peptide
13	n	10	PRO	Peptide
8	x	232	SER	Peptide
8	x	486	ASN	Peptide
8	x	52	GLU	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	159/168 (95%)	133 (84%)	26 (16%)	0	100	100
1	a	159/168 (95%)	133 (84%)	26 (16%)	0	100	100
2	B	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
2	b	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
3	C	110/124 (89%)	99 (90%)	11 (10%)	0	100	100
3	c	110/124 (89%)	99 (90%)	11 (10%)	0	100	100
4	D	85/94 (90%)	81 (95%)	4 (5%)	0	100	100
4	d	85/94 (90%)	81 (95%)	4 (5%)	0	100	100
5	E	230/235 (98%)	194 (84%)	35 (15%)	1 (0%)	34	71
5	e	230/235 (98%)	194 (84%)	35 (15%)	1 (0%)	34	71
6	G	108/114 (95%)	95 (88%)	13 (12%)	0	100	100
6	g	108/114 (95%)	95 (88%)	13 (12%)	0	100	100
7	H	485/493 (98%)	436 (90%)	48 (10%)	1 (0%)	47	79
7	h	485/493 (98%)	436 (90%)	48 (10%)	1 (0%)	47	79
8	X	599/618 (97%)	538 (90%)	59 (10%)	2 (0%)	41	75
8	x	599/618 (97%)	538 (90%)	59 (10%)	2 (0%)	41	75
9	J	175/192 (91%)	141 (81%)	31 (18%)	3 (2%)	9	43
9	j	175/192 (91%)	141 (81%)	31 (18%)	3 (2%)	9	43
10	K	168/174 (97%)	138 (82%)	28 (17%)	2 (1%)	13	49
10	k	168/174 (97%)	138 (82%)	28 (17%)	2 (1%)	13	49
11	L	371/391 (95%)	322 (87%)	49 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	371/391 (95%)	322 (87%)	49 (13%)	0	100	100
12	M	297/309 (96%)	268 (90%)	29 (10%)	0	100	100
12	m	297/309 (96%)	268 (90%)	29 (10%)	0	100	100
13	N	172/208 (83%)	137 (80%)	34 (20%)	1 (1%)	25	63
13	n	172/208 (83%)	136 (79%)	35 (20%)	1 (1%)	25	63
All	All	6072/6408 (95%)	5315 (88%)	737 (12%)	20 (0%)	44	75

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	200	ILE
5	e	200	ILE
8	X	556	PHE
9	J	82	PRO
8	x	556	PHE
9	j	82	PRO
10	K	167	GLU
10	k	167	GLU
9	J	40	ARG
13	N	149	LYS
9	j	40	ARG
13	n	149	LYS
10	K	166	ASP
10	k	166	ASP
8	X	473	PRO
8	x	473	PRO
7	h	61	ILE
7	H	61	ILE
9	J	83	ASP
9	j	83	ASP

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	141/147 (96%)	135 (96%)	6 (4%)	29	56
1	a	141/147 (96%)	135 (96%)	6 (4%)	29	56
2	B	66/69 (96%)	63 (96%)	3 (4%)	27	55
2	b	66/69 (96%)	63 (96%)	3 (4%)	27	55
3	C	90/101 (89%)	85 (94%)	5 (6%)	21	49
3	c	90/101 (89%)	85 (94%)	5 (6%)	21	49
4	D	66/75 (88%)	63 (96%)	3 (4%)	27	55
4	d	66/75 (88%)	63 (96%)	3 (4%)	27	55
5	E	181/184 (98%)	176 (97%)	5 (3%)	43	65
5	e	181/184 (98%)	176 (97%)	5 (3%)	43	65
6	G	90/93 (97%)	88 (98%)	2 (2%)	52	71
6	g	90/93 (97%)	88 (98%)	2 (2%)	52	71
7	H	386/391 (99%)	377 (98%)	9 (2%)	50	70
7	h	386/391 (99%)	377 (98%)	9 (2%)	50	70
8	X	478/487 (98%)	473 (99%)	5 (1%)	76	86
8	x	478/487 (98%)	473 (99%)	5 (1%)	76	86
9	J	152/167 (91%)	148 (97%)	4 (3%)	46	67
9	j	152/167 (91%)	148 (97%)	4 (3%)	46	67
10	K	154/158 (98%)	152 (99%)	2 (1%)	69	82
10	k	154/158 (98%)	152 (99%)	2 (1%)	69	82
11	L	316/332 (95%)	312 (99%)	4 (1%)	69	82
11	l	316/332 (95%)	313 (99%)	3 (1%)	78	88
12	M	237/243 (98%)	234 (99%)	3 (1%)	69	82
12	m	237/243 (98%)	234 (99%)	3 (1%)	69	82
13	N	161/191 (84%)	158 (98%)	3 (2%)	57	75
13	n	161/191 (84%)	158 (98%)	3 (2%)	57	75
All	All	5036/5276 (96%)	4929 (98%)	107 (2%)	56	72

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	27	SER
1	A	28	LEU

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Mol	Chain	Res	Type
1	A	35	ILE
1	A	42	ILE
1	A	114	MET
2	B	16	LEU
2	B	35	VAL
2	B	73	VAL
3	C	10	LEU
3	C	26	LEU
3	C	65	VAL
3	C	68	LEU
3	C	115	ARG
4	D	20	ILE
4	D	31	SER
4	D	39	SER
5	E	103	THR
5	E	122	ILE
5	E	200	ILE
5	E	202	ARG
5	E	225	SER
6	G	2	ILE
6	G	95	ILE
7	H	13	LEU
7	H	61	ILE
7	H	104	VAL
7	H	143	SER
7	H	207	VAL
7	H	225	LEU
7	H	332	LEU
7	H	384	VAL
7	H	447	ILE
8	X	13	ILE
8	X	27	ARG
8	X	299	LEU
8	X	351	VAL
8	X	431	ARG
9	J	16	LYS
9	J	25	CYS
9	J	93	CYS
9	J	171	TRP
10	K	110	THR
10	K	137	ASP
11	L	63	ARG

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Mol	Chain	Res	Type
11	L	227	LYS
11	L	235	THR
11	L	368	VAL
12	M	198	MET
12	M	209	MET
12	M	212	PHE
13	N	11	GLU
13	N	74	ARG
13	N	96	CYS
1	a	25	THR
1	a	27	SER
1	a	28	LEU
1	a	35	ILE
1	a	42	ILE
1	a	114	MET
2	b	16	LEU
2	b	35	VAL
2	b	73	VAL
3	c	10	LEU
3	c	26	LEU
3	c	65	VAL
3	c	68	LEU
3	c	115	ARG
4	d	20	ILE
4	d	31	SER
4	d	39	SER
5	e	103	THR
5	e	122	ILE
5	e	200	ILE
5	e	202	ARG
5	e	225	SER
6	g	2	ILE
6	g	95	ILE
7	h	13	LEU
7	h	61	ILE
7	h	104	VAL
7	h	143	SER
7	h	207	VAL
7	h	225	LEU
7	h	332	LEU
7	h	384	VAL
7	h	447	ILE

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Mol	Chain	Res	Type
8	x	13	ILE
8	x	27	ARG
8	x	299	LEU
8	x	351	VAL
8	x	431	ARG
9	j	16	LYS
9	j	25	CYS
9	j	93	CYS
9	j	171	TRP
10	k	110	THR
10	k	137	ASP
11	l	63	ARG
11	l	227	LYS
11	l	235	THR
12	m	198	MET
12	m	209	MET
12	m	212	PHE
13	n	11	GLU
13	n	61	CYS
13	n	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	118	ASN
6	G	66	ASN
7	H	41	GLN
7	H	189	ASN
7	H	308	GLN
7	H	334	HIS
8	X	236	GLN
8	X	340	HIS
10	K	12	GLN
10	K	126	ASN
11	L	77	ASN
11	L	326	HIS
12	M	34	HIS
12	M	43	GLN
12	M	164	GLN
12	M	187	GLN
13	N	100	GLN

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Mol	Chain	Res	Type
1	a	58	ASN
1	a	118	ASN
6	g	66	ASN
7	h	41	GLN
7	h	132	ASN
7	h	189	ASN
7	h	226	ASN
7	h	308	GLN
7	h	334	HIS
8	x	236	GLN
8	x	340	HIS
10	k	12	GLN
10	k	126	ASN
11	l	77	ASN
11	l	326	HIS
12	m	43	GLN
12	m	164	GLN
12	m	187	GLN
13	n	100	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
14	SF4	n	301	13	0,12,12	-	-	-		
14	SF4	j	201	9	0,12,12	-	-	-		
14	SF4	n	302	13	0,12,12	-	-	-		
14	SF4	N	301	-	0,12,12	-	-	-		
14	SF4	N	302	-	0,12,12	-	-	-		
14	SF4	J	201	9	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
14	SF4	n	301	13	-	-	0/6/5/5
14	SF4	j	201	9	-	-	0/6/5/5
14	SF4	n	302	13	-	-	0/6/5/5
14	SF4	N	301	-	-	-	0/6/5/5
14	SF4	N	302	-	-	-	0/6/5/5
14	SF4	J	201	9	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

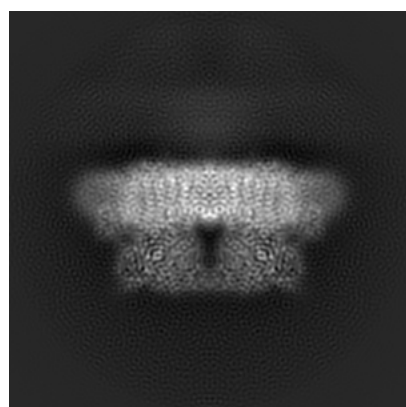
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20692. These allow visual inspection of the internal detail of the map and identification of artifacts.

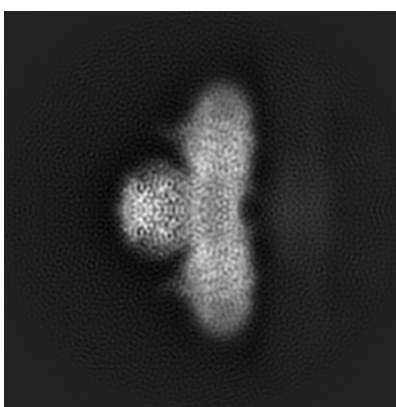
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

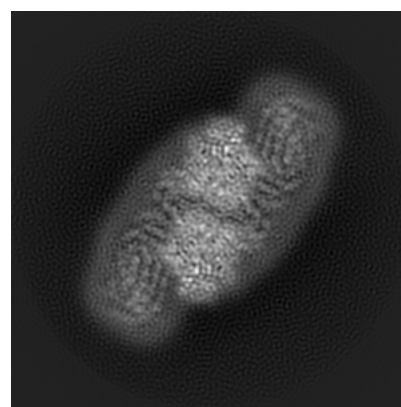
6.1.1 Primary map



X



Y

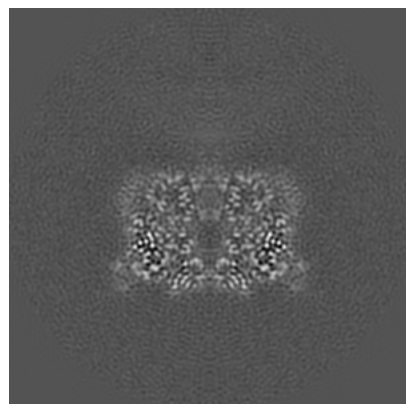


Z

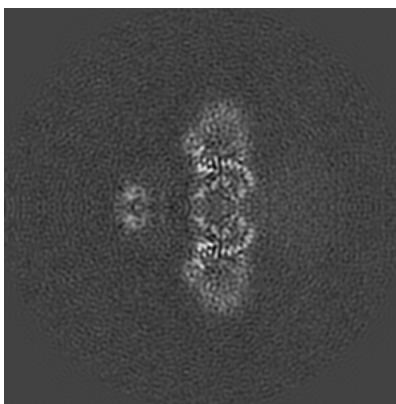
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

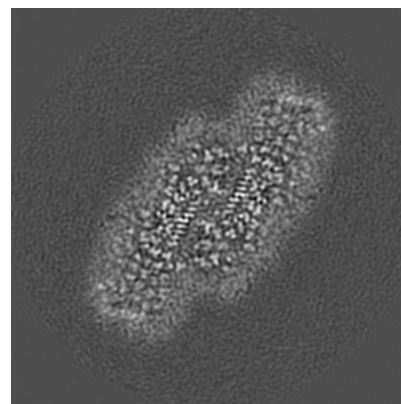
6.2.1 Primary map



X Index: 160



Y Index: 160

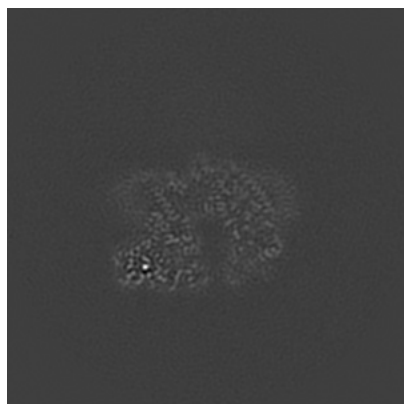


Z Index: 160

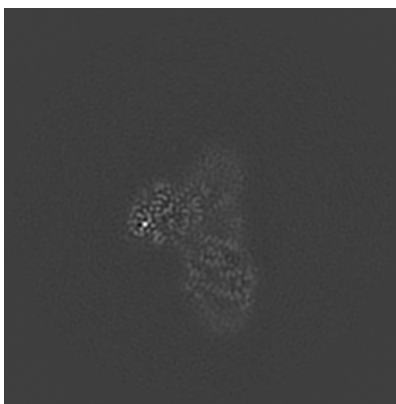
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

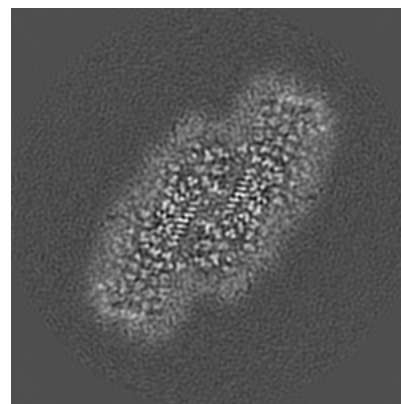
6.3.1 Primary map



X Index: 146



Y Index: 110



Z Index: 160

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

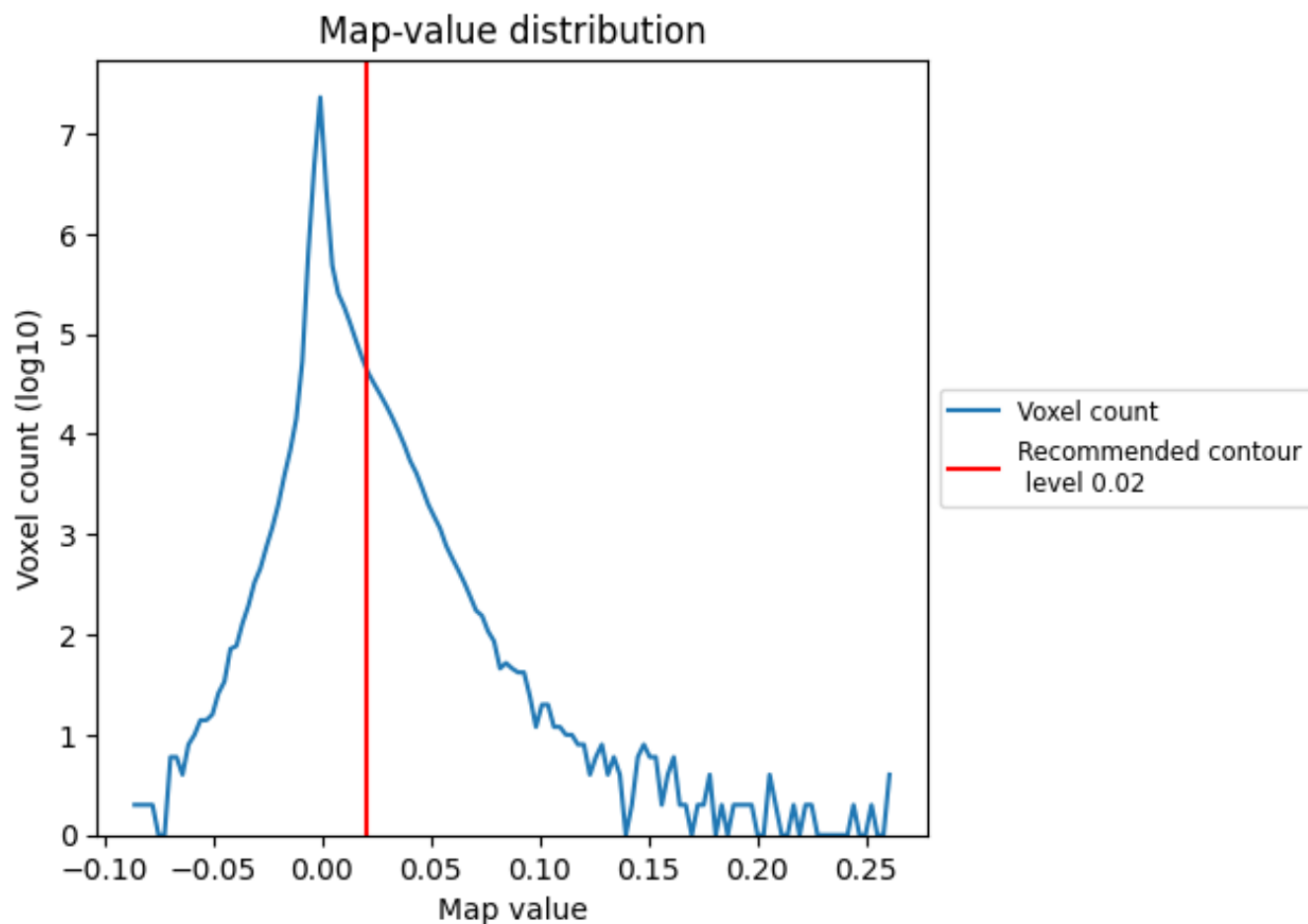
6.5 Mask visualisation

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

7 Map analysis [i](#)

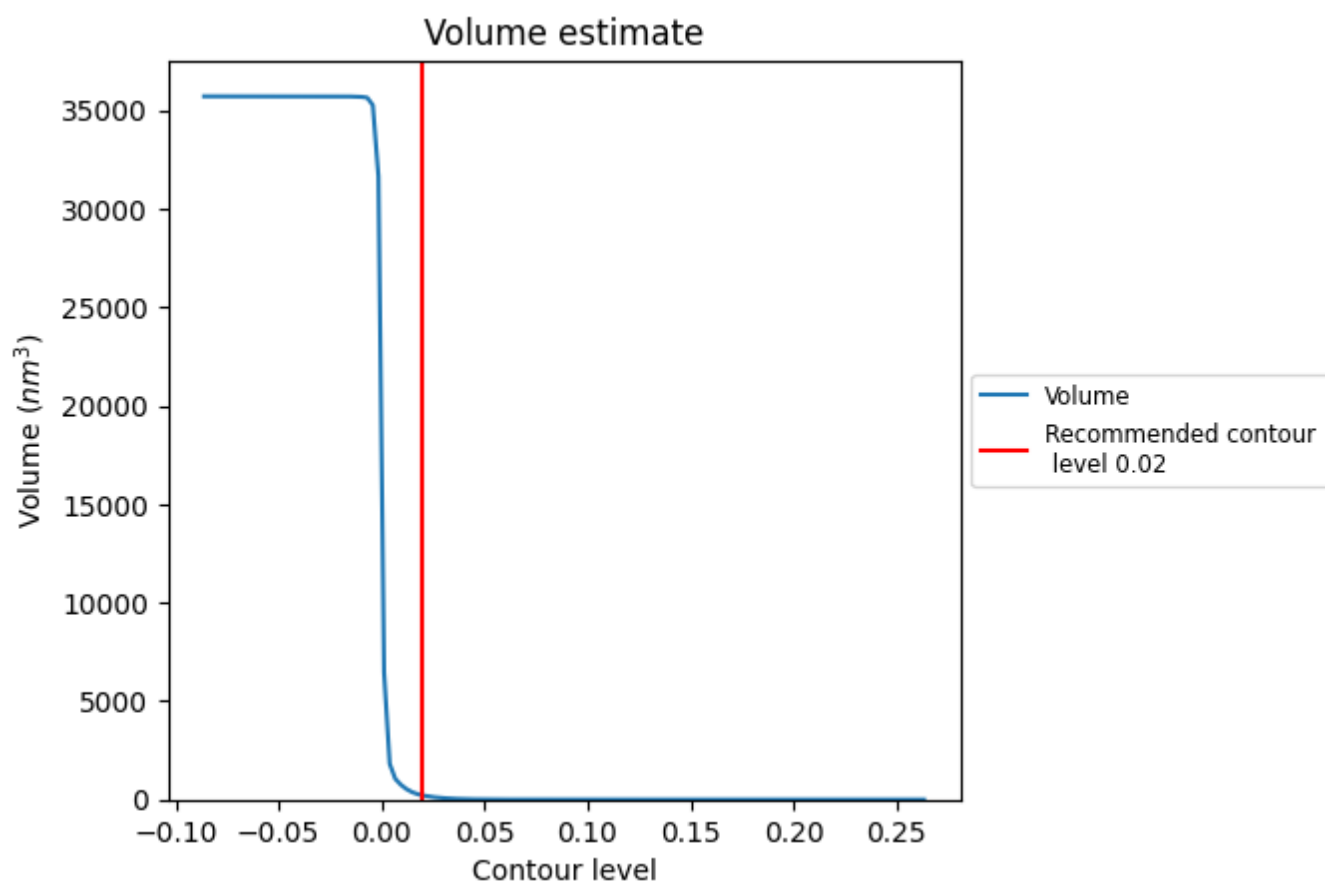
This section contains the results of statistical analysis of the map.

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.

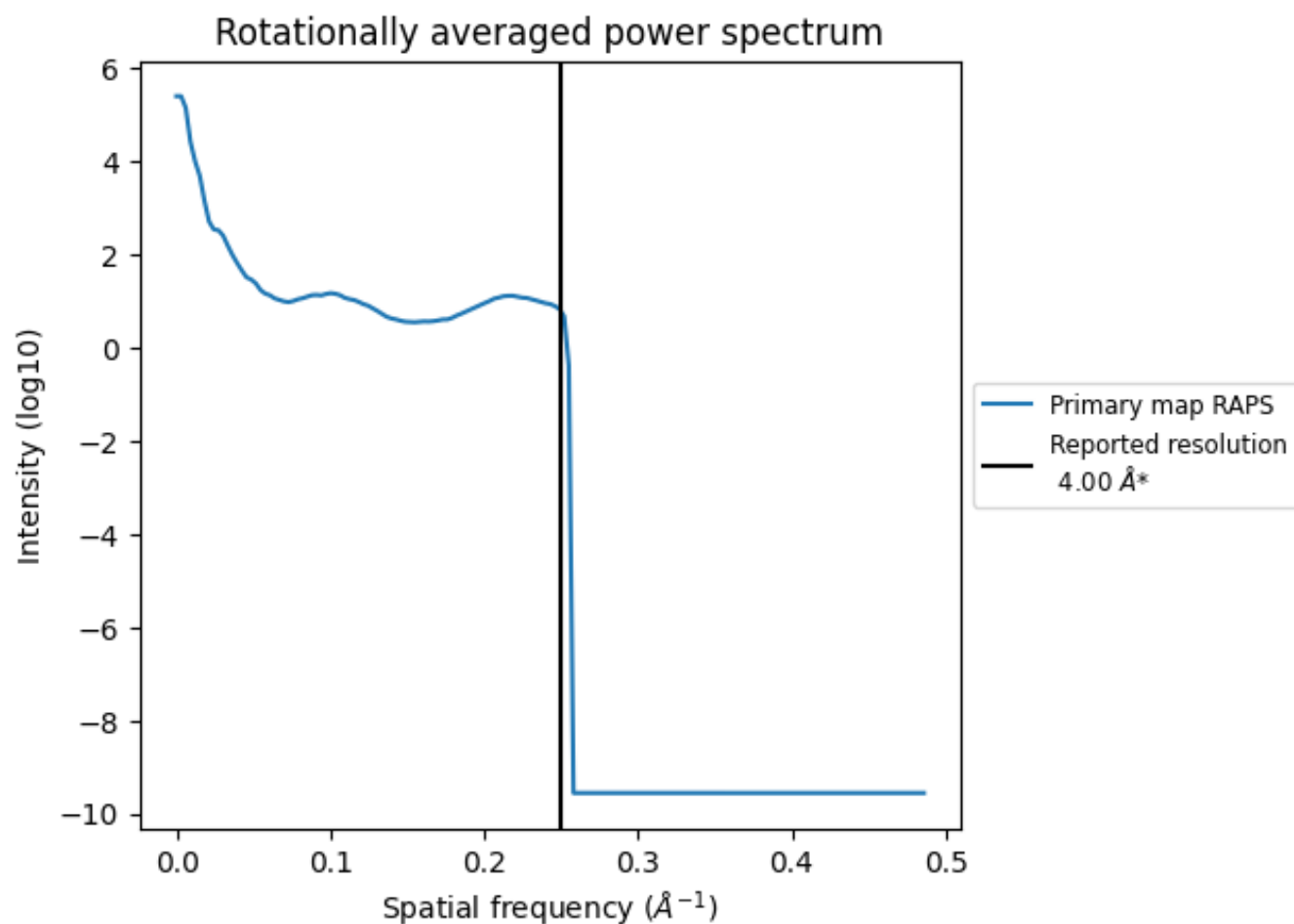
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 ⓘ

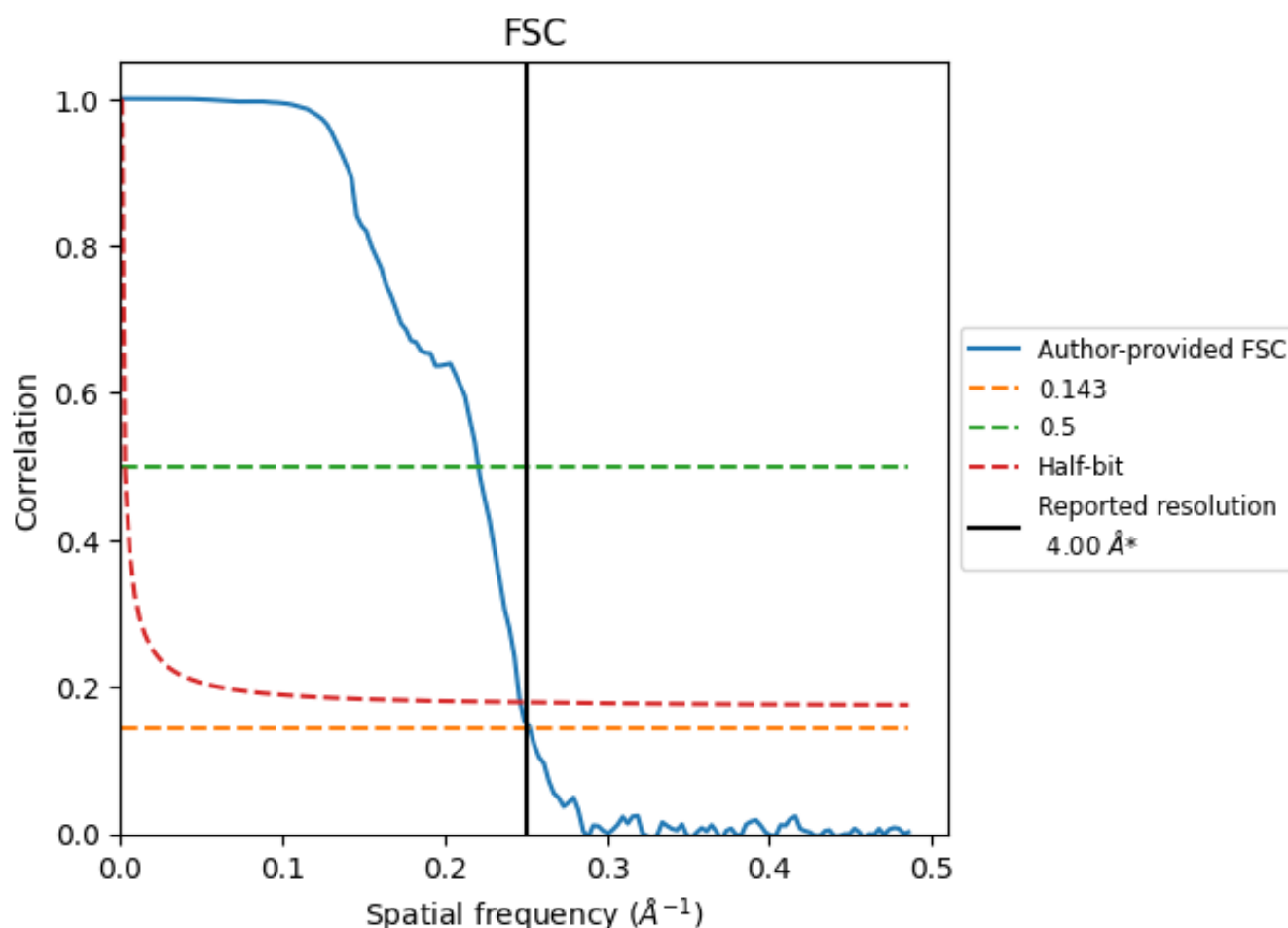


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

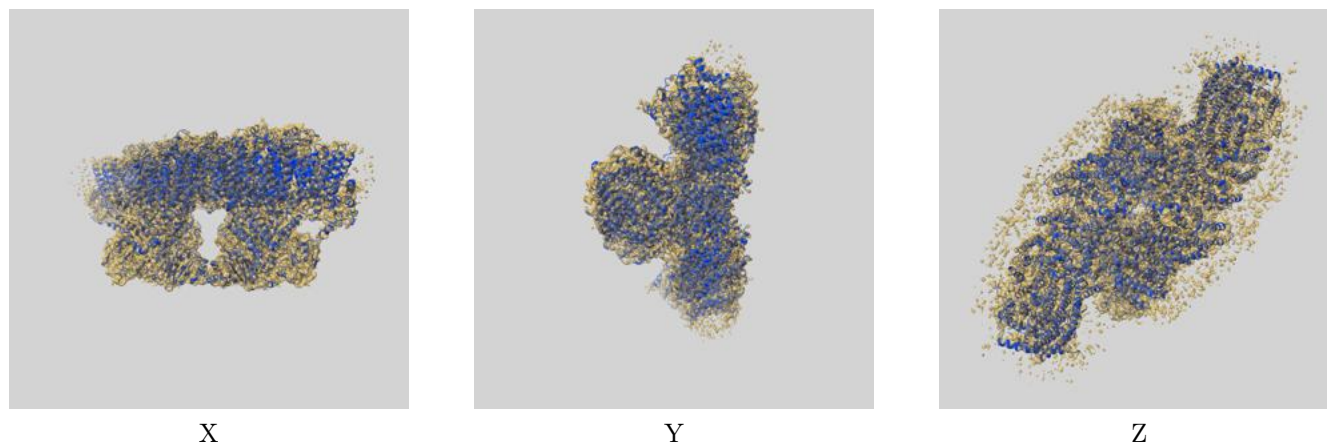
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.96	4.53	4.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

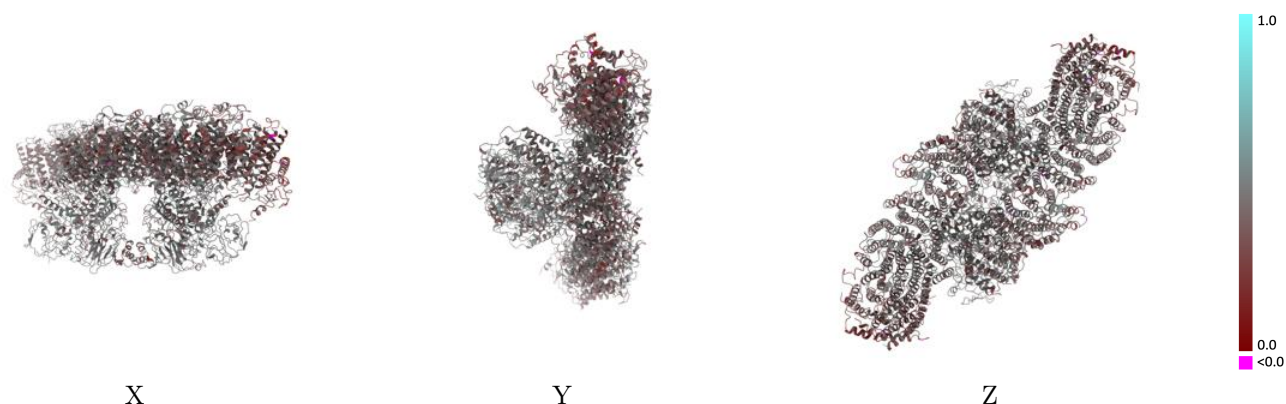
This section contains information regarding the fit between EMDB map EMD-20692 and PDB model 6U8Y. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



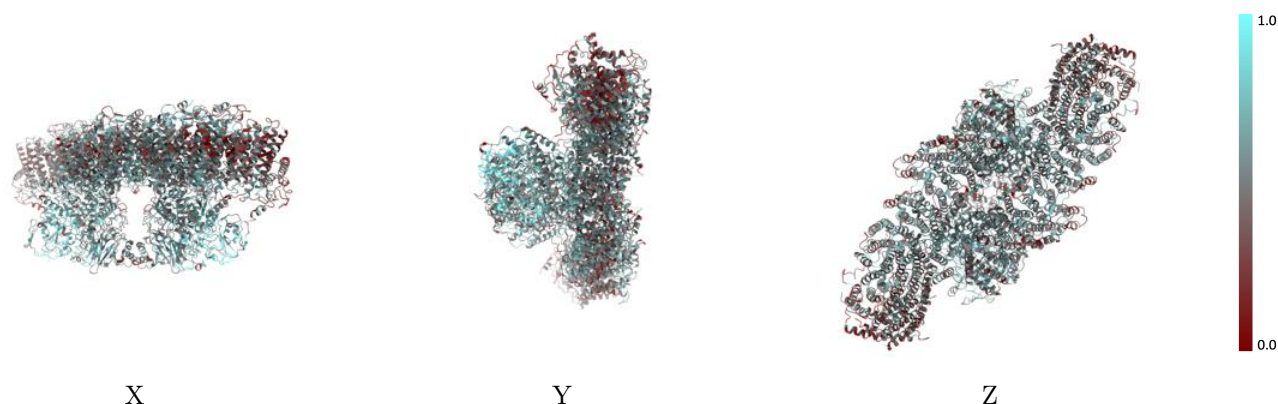
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



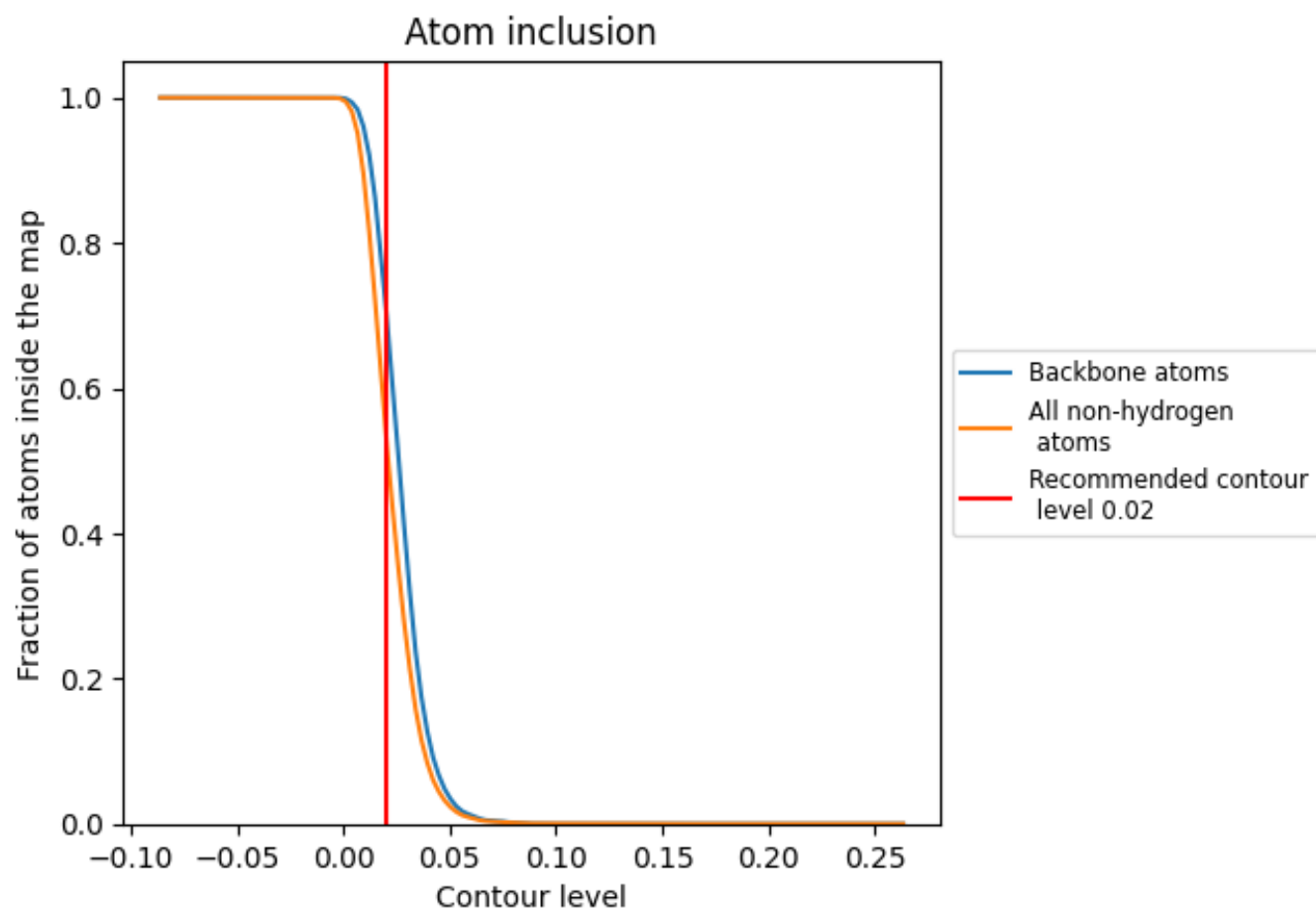
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).























































9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 54% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5353	 0.4140
A	 0.3774	 0.3200
B	 0.4290	 0.3820
C	 0.3796	 0.3450
D	 0.4567	 0.3970
E	 0.4580	 0.3940
G	 0.4801	 0.4150
H	 0.5141	 0.4130
J	 0.6725	 0.4500
K	 0.5873	 0.4340
L	 0.6312	 0.4540
M	 0.5269	 0.4250
N	 0.6776	 0.4520
X	 0.5273	 0.4100
a	 0.3696	 0.3080
b	 0.4373	 0.3840
c	 0.3962	 0.3480
d	 0.4597	 0.4020
e	 0.4529	 0.3910
g	 0.4826	 0.4190
h	 0.5144	 0.4140
j	 0.6697	 0.4530
k	 0.5873	 0.4320
l	 0.6346	 0.4530
m	 0.5286	 0.4230
n	 0.6755	 0.4530
x	 0.5271	 0.4090

