



wwPDB EM Validation Summary Report ⓘ

May 19, 2024 – 09:50 PM JST

PDB ID : 6LTJ
EMDB ID : EMD-0974
Title : Structure of nucleosome-bound human BAF complex
Authors : He, S.; Wu, Z.; Tian, Y.; Yu, Z.; Yu, J.; Wang, X.; Li, J.; Liu, B.; Xu, Y.
Deposited on : 2020-01-22
Resolution : 3.70 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:

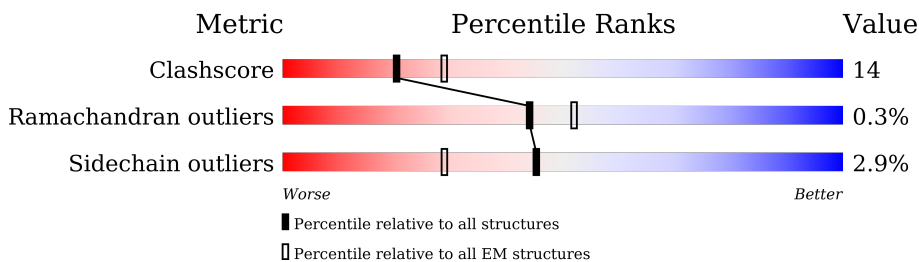
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
3	G	130	
4	D	126	
4	H	126	

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Mol	Chain	Length	Quality of chain
5	I	1647	
6	J	407	
7	K	375	
8	L	1295	
9	M	336	
10	N	1214	
10	O	1214	
11	P	515	
12	Q	411	
13	R	292	
14	X	119	
15	Y	119	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 34283 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 Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	91	739	466	141	130	2	0	0
1	E	91	739	466	141	130	2	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	78	622	393	120	108	1	0	0
2	F	77	614	389	119	105	1	0	0

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	95	726	455	142	129	0	0
3	G	95	727	457	142	128	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	88	682	430	121	129	2	0	0
4	H	90	700	441	124	133	2	0	0

- Molecule 5 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	551	4606	2932	841	809	24	0	0

- Molecule 6 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	334	2612	1656	441	495	20	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	418	PRO	-	expression tag	UNP O96019

- Molecule 7 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	317	2482	1575	409	480	18	0	0

- Molecule 8 is a protein called AT-rich interactive domain-containing protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	466	3670	2341	620	688	21	0	0

- Molecule 9 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	283	2277	1437	388	440	12	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	163	GLY	-	linker	UNP Q12824
M	164	GLY	-	linker	UNP Q12824
M	165	SER	-	linker	UNP Q12824
M	166	GLY	-	linker	UNP Q12824
M	167	GLY	-	linker	UNP Q12824
M	168	SER	-	linker	UNP Q12824

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Chain	Residue	Modelled	Actual	Comment	Reference
M	169	GLY	-	linker	UNP Q12824
M	170	GLY	-	linker	UNP Q12824
M	171	SER	-	linker	UNP Q12824

- Molecule 10 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	261	2120	1346	374	388	12	0	0
10	O	325	2632	1676	458	485	13	0	0

- Molecule 11 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	239	2015	1281	362	361	11	0	0

- Molecule 12 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Q	105	860	530	161	165	4	0	0

- Molecule 13 is a protein called Zinc finger protein ubi-d4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	R	70	580	361	112	102	5	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	101	GLY	-	linker	UNP Q92785
R	102	GLY	-	linker	UNP Q92785
R	103	SER	-	linker	UNP Q92785
R	104	GLY	-	linker	UNP Q92785
R	105	GLY	-	linker	UNP Q92785
R	106	SER	-	linker	UNP Q92785

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Chain	Residue	Modelled	Actual	Comment	Reference
R	107	GLY	-	linker	UNP Q92785
R	108	GLY	-	linker	UNP Q92785
R	109	SER	-	linker	UNP Q92785

- Molecule 14 is a DNA chain called DNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	X	119	2424	1150	440	715	119	0	0

- Molecule 15 is a DNA chain called DNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	Y	119	2455	1160	463	713	119	0	0

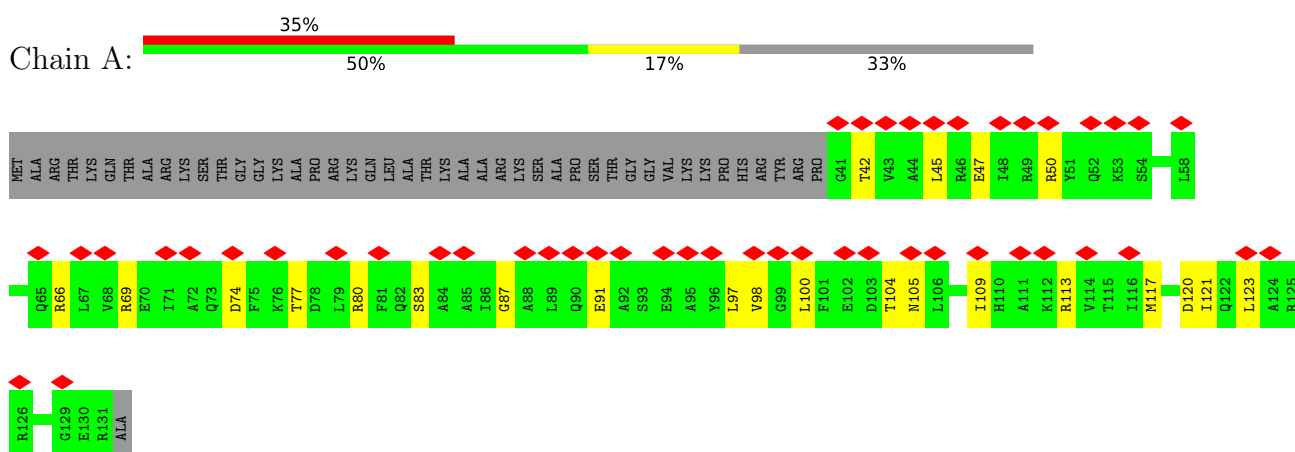
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	L	1	Total	Zn	0
			1	1	

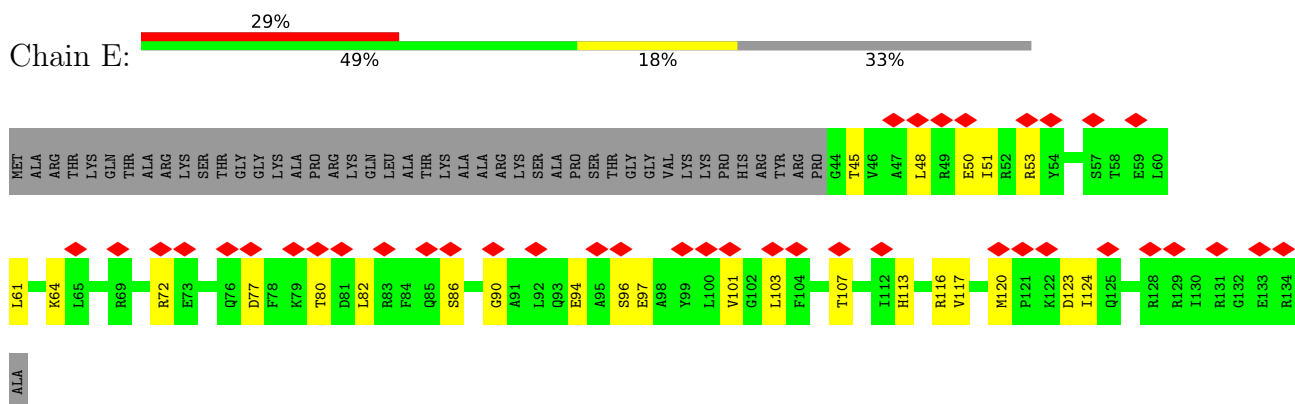
3 Residue-property plots [i](#)

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

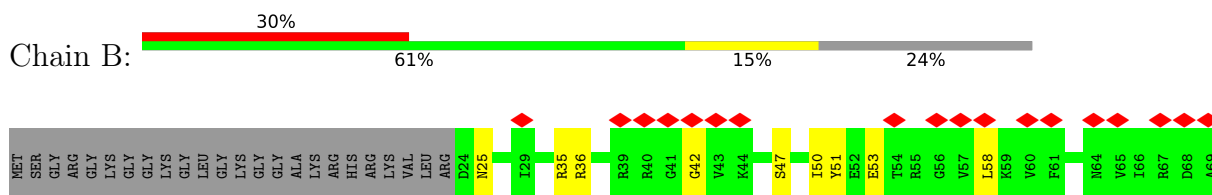
- Molecule 1: Histone H3.3

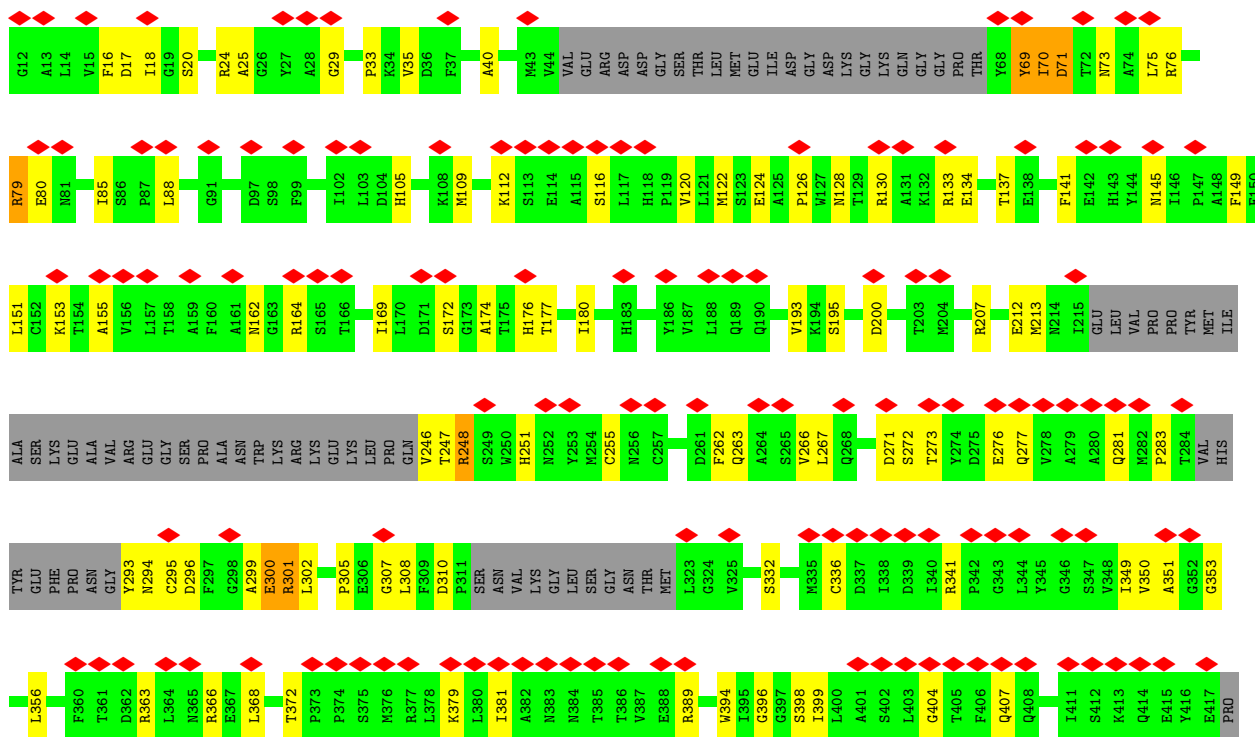


- Molecule 1: Histone H3.3

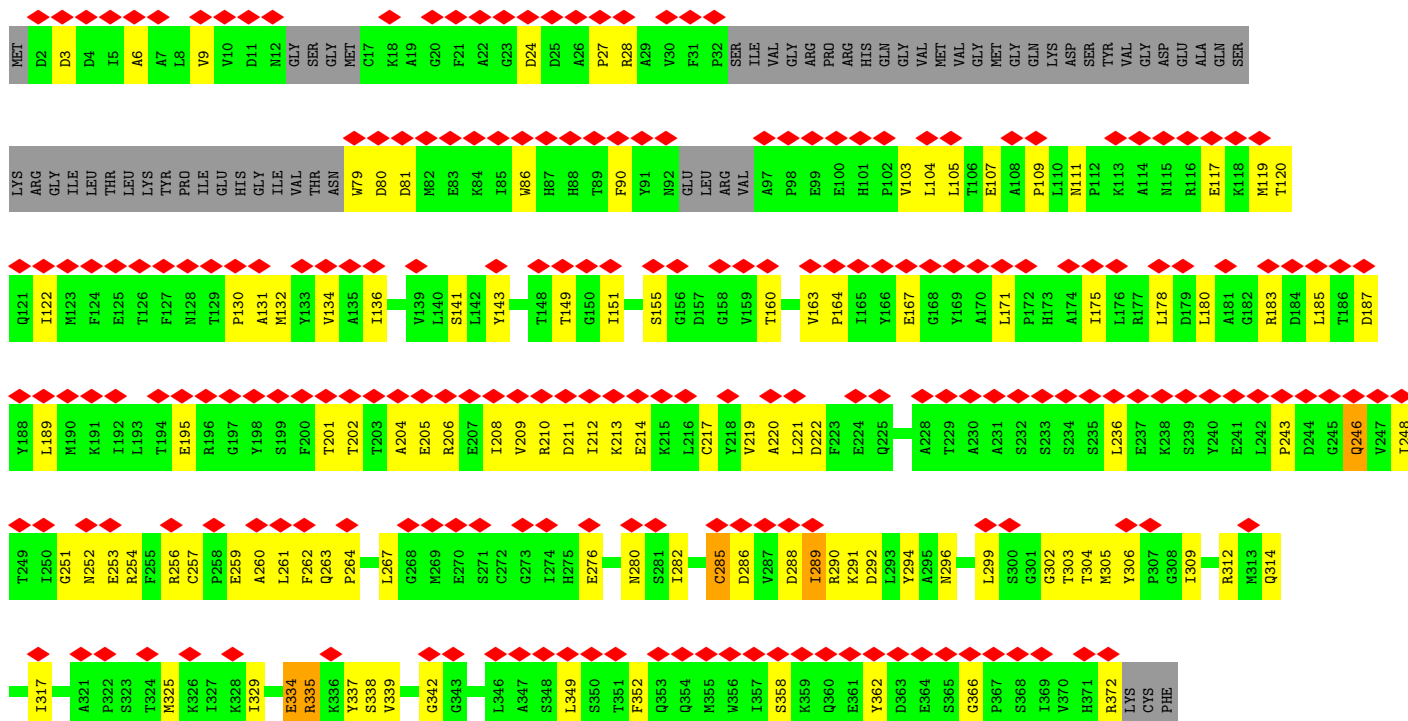


- Molecule 2: Histone H4



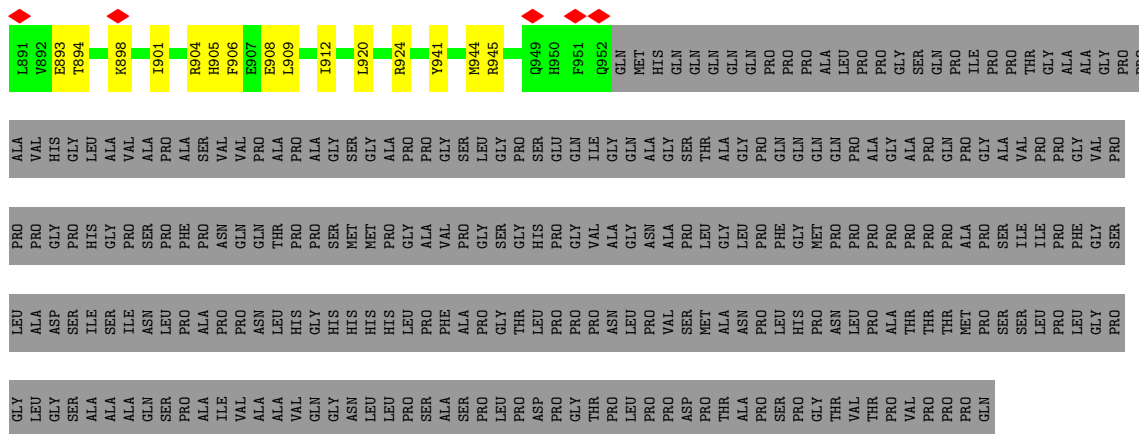


• Molecule 7: Actin, cytoplasmic 1

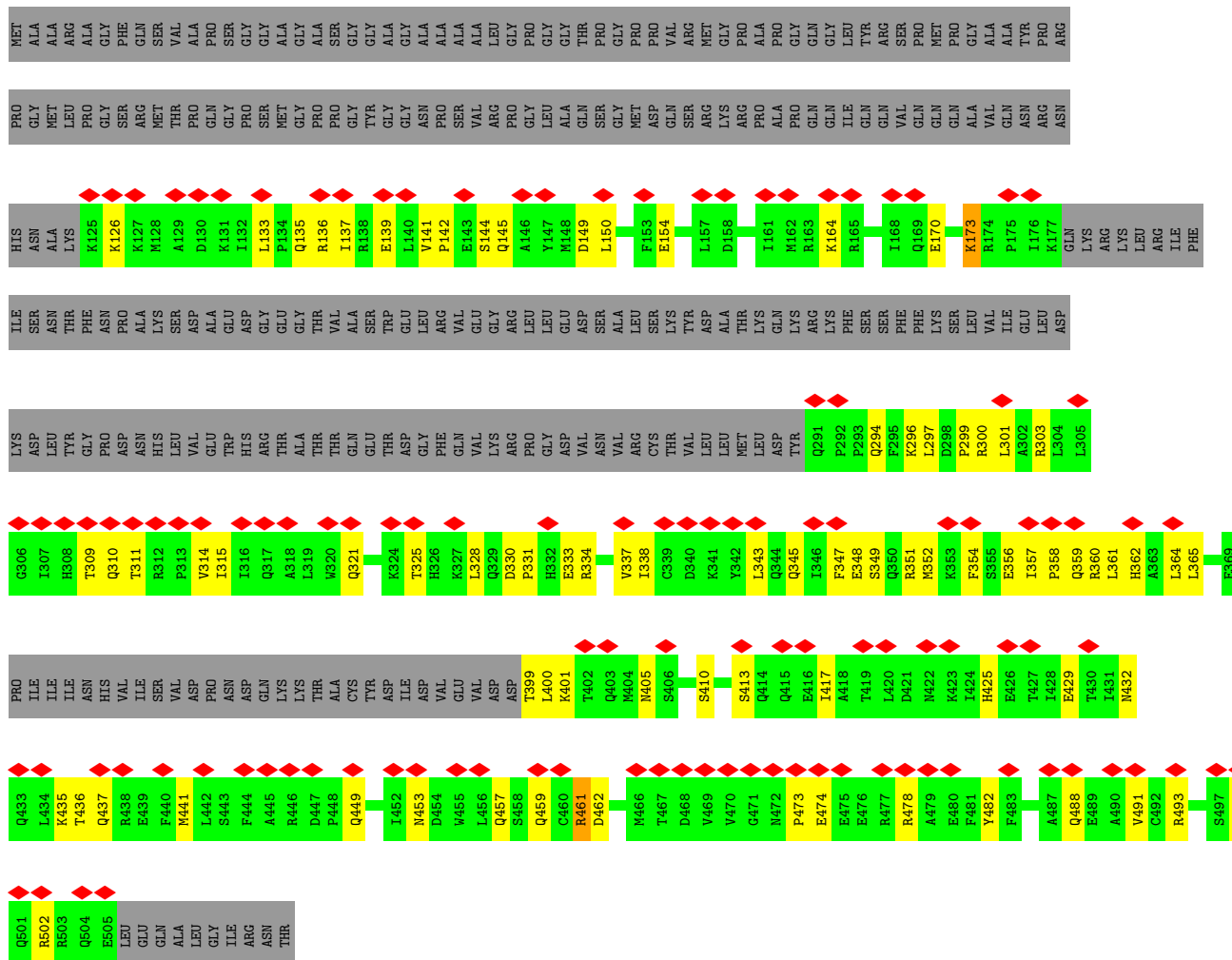
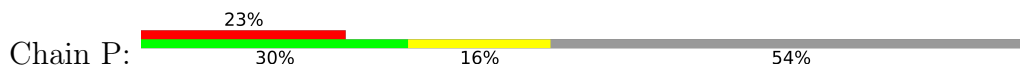


• Molecule 8: AT-rich interactive domain-containing protein 1A

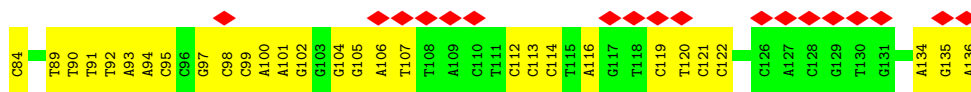




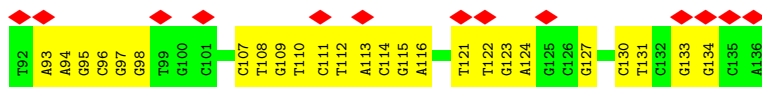
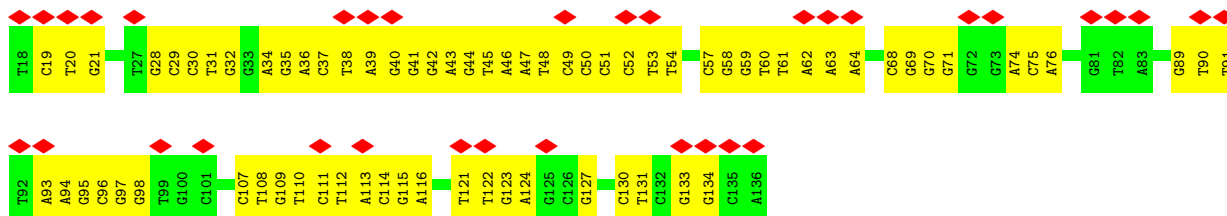
• Molecule 11: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family D member 1



• Molecule 12: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family E member 1



- Molecule 15: DNA (119-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	320658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	3.306	Depositor
Minimum map value	-1.288	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.48	Depositor
Map size (\AA)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.74	0/747	0.67	0/1001
1	E	0.74	0/747	0.67	0/1001
2	B	0.78	0/629	0.70	0/843
2	F	0.81	0/621	0.77	0/832
3	C	0.73	0/735	0.68	0/993
3	G	0.72	0/736	0.66	0/993
4	D	0.74	0/693	0.64	0/934
4	H	0.75	0/711	0.62	0/957
5	I	0.51	0/4682	0.75	0/6281
6	J	0.46	0/2667	0.67	0/3615
7	K	0.42	0/2535	0.62	0/3436
8	L	0.32	0/3739	0.46	0/5070
9	M	0.37	0/2317	0.52	0/3129
10	N	0.34	0/2158	0.46	0/2908
10	O	0.33	0/2692	0.46	0/3646
11	P	0.31	0/2055	0.45	0/2764
12	Q	0.29	0/871	0.45	0/1168
13	R	0.36	0/595	0.47	0/799
14	X	0.98	0/2715	1.05	0/4184
15	Y	0.97	0/2757	0.99	0/4257
All	All	0.59	0/35402	0.69	0/48811

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	739	0	778	17	0
1	E	739	0	778	17	0
2	B	622	0	660	11	0
2	F	614	0	656	14	0
3	C	726	0	761	12	0
3	G	727	0	768	31	0
4	D	682	0	697	10	0
4	H	700	0	716	11	0
5	I	4606	0	4726	197	0
6	J	2612	0	2557	71	0
7	K	2482	0	2432	71	0
8	L	3670	0	3724	85	0
9	M	2277	0	2248	84	0
10	N	2120	0	2116	80	0
10	O	2632	0	2606	87	0
11	P	2015	0	2046	68	0
12	Q	860	0	864	30	0
13	R	580	0	557	19	0
14	X	2424	0	1335	69	0
15	Y	2455	0	1334	85	0
16	L	1	0	0	0	0
All	All	34283	0	32359	904	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 14.

The worst 5 of 904 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)
3:G:74:LYS:HZ1	9:M:195:ILE:HG21	1.08	1.16
3:G:74:LYS:NZ	9:M:195:ILE:HG21	1.68	1.05
3:G:74:LYS:NZ	9:M:232:THR:HG23	1.74	1.02
6:J:305:PRO:O	6:J:308:LEU:HB2	1.61	1.00
6:J:248:ARG:HA	6:J:248:ARG:CZ	1.92	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/136 (65%)	87 (98%)	2 (2%)	0	100	100
1	E	89/136 (65%)	87 (98%)	2 (2%)	0	100	100
2	B	76/103 (74%)	73 (96%)	3 (4%)	0	100	100
2	F	75/103 (73%)	74 (99%)	1 (1%)	0	100	100
3	C	93/130 (72%)	88 (95%)	5 (5%)	0	100	100
3	G	93/130 (72%)	90 (97%)	3 (3%)	0	100	100
4	D	86/126 (68%)	82 (95%)	4 (5%)	0	100	100
4	H	88/126 (70%)	84 (96%)	4 (4%)	0	100	100
5	I	527/1647 (32%)	445 (84%)	75 (14%)	7 (1%)	12	47
6	J	324/407 (80%)	288 (89%)	34 (10%)	2 (1%)	25	62
7	K	309/375 (82%)	290 (94%)	18 (6%)	1 (0%)	41	74
8	L	456/1295 (35%)	434 (95%)	22 (5%)	0	100	100
9	M	273/336 (81%)	263 (96%)	10 (4%)	0	100	100
10	N	253/1214 (21%)	247 (98%)	6 (2%)	0	100	100
10	O	317/1214 (26%)	304 (96%)	13 (4%)	0	100	100
11	P	233/515 (45%)	220 (94%)	13 (6%)	0	100	100
12	Q	103/411 (25%)	96 (93%)	7 (7%)	0	100	100
13	R	68/292 (23%)	61 (90%)	7 (10%)	0	100	100
All	All	3552/8696 (41%)	3313 (93%)	229 (6%)	10 (0%)	44	74

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	811	PRO

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Mol	Chain	Res	Type
5	I	874	ARG
5	I	1050	TYR
5	I	1162	GLY
7	K	288	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	77/110 (70%)	71 (92%)	6 (8%)	12	42
1	E	77/110 (70%)	71 (92%)	6 (8%)	12	42
2	B	64/79 (81%)	63 (98%)	1 (2%)	62	80
2	F	63/79 (80%)	63 (100%)	0	100	100
3	C	73/100 (73%)	73 (100%)	0	100	100
3	G	73/100 (73%)	73 (100%)	0	100	100
4	D	74/104 (71%)	74 (100%)	0	100	100
4	H	76/104 (73%)	76 (100%)	0	100	100
5	I	501/1422 (35%)	459 (92%)	42 (8%)	11	40
6	J	287/348 (82%)	272 (95%)	15 (5%)	23	55
7	K	270/318 (85%)	260 (96%)	10 (4%)	34	61
8	L	418/1117 (37%)	415 (99%)	3 (1%)	84	91
9	M	252/294 (86%)	248 (98%)	4 (2%)	62	80
10	N	222/1030 (22%)	222 (100%)	0	100	100
10	O	282/1030 (27%)	279 (99%)	3 (1%)	73	85
11	P	223/442 (50%)	220 (99%)	3 (1%)	69	83
12	Q	98/361 (27%)	98 (100%)	0	100	100
13	R	59/253 (23%)	59 (100%)	0	100	100
All	All	3189/7401 (43%)	3096 (97%)	93 (3%)	45	66

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	J	71	ASP
7	K	206	ARG
6	J	80	GLU
6	J	293	TYR
7	K	285	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
8	L	1858	HIS
13	R	61	HIS
10	N	604	GLN
12	Q	268	ASN
11	P	432	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

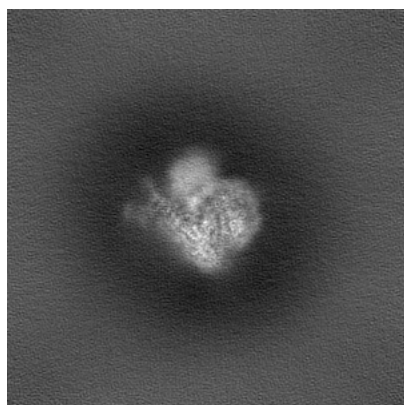
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0974. These allow visual inspection of the internal detail of the map and identification of artifacts.

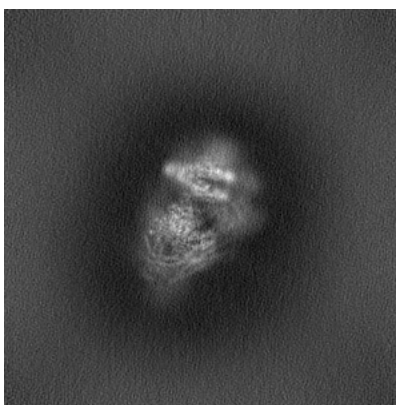
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

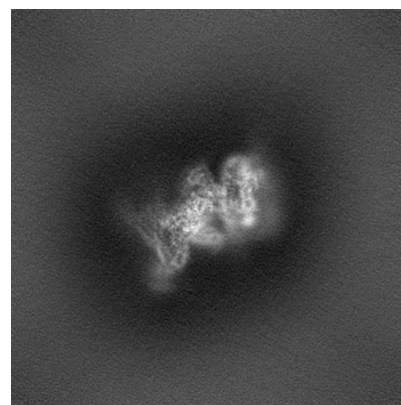
6.1.1 Primary map



X



Y

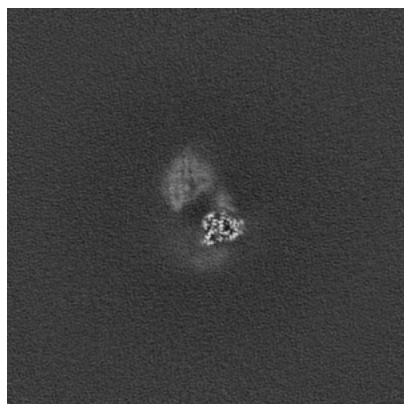


Z

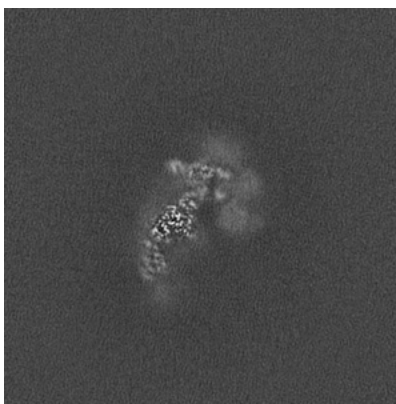
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

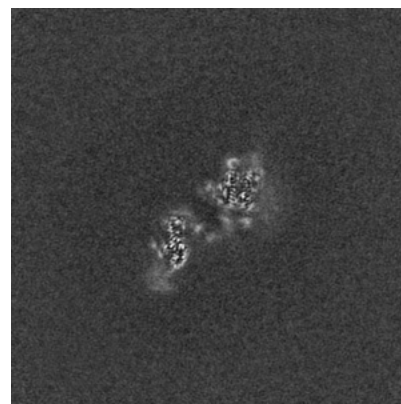
6.2.1 Primary map



X Index: 256



Y Index: 256

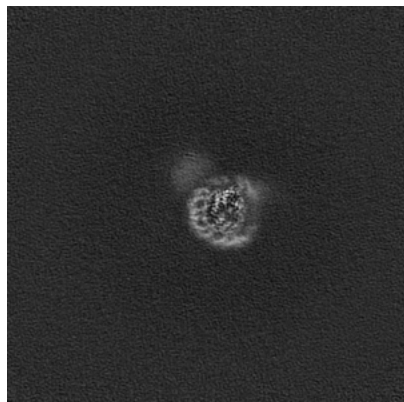


Z Index: 256

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

6.3 Largest variance slices [i](#)

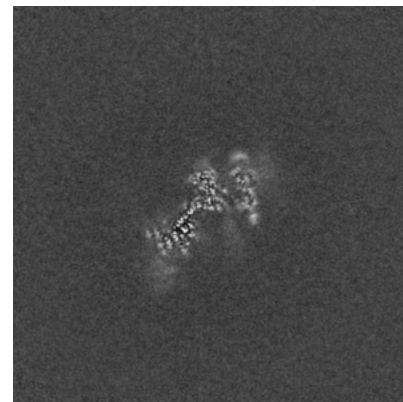
6.3.1 Primary map



X Index: 304



Y Index: 253

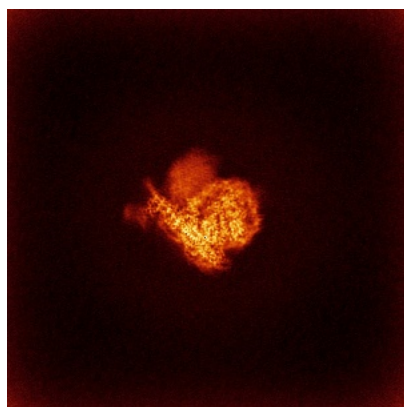


Z Index: 238

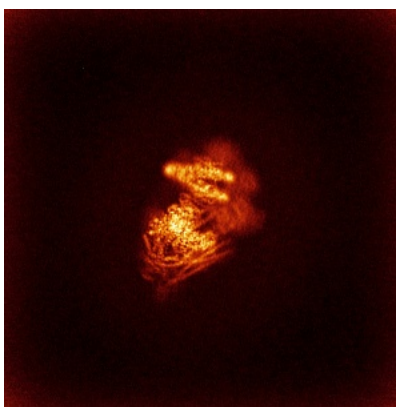
The images above show the largest variance slices of the map in three orthogonal directions.

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

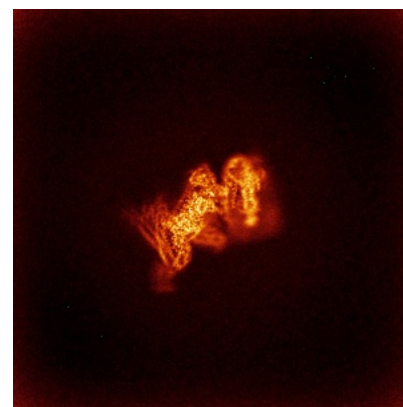
6.4.1 Primary map



X



Y

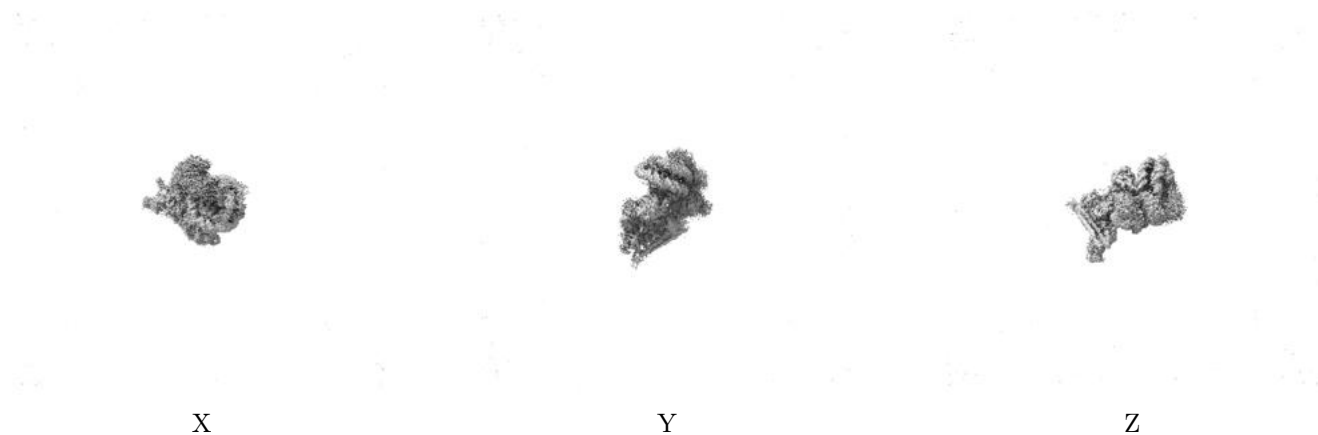


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.48. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

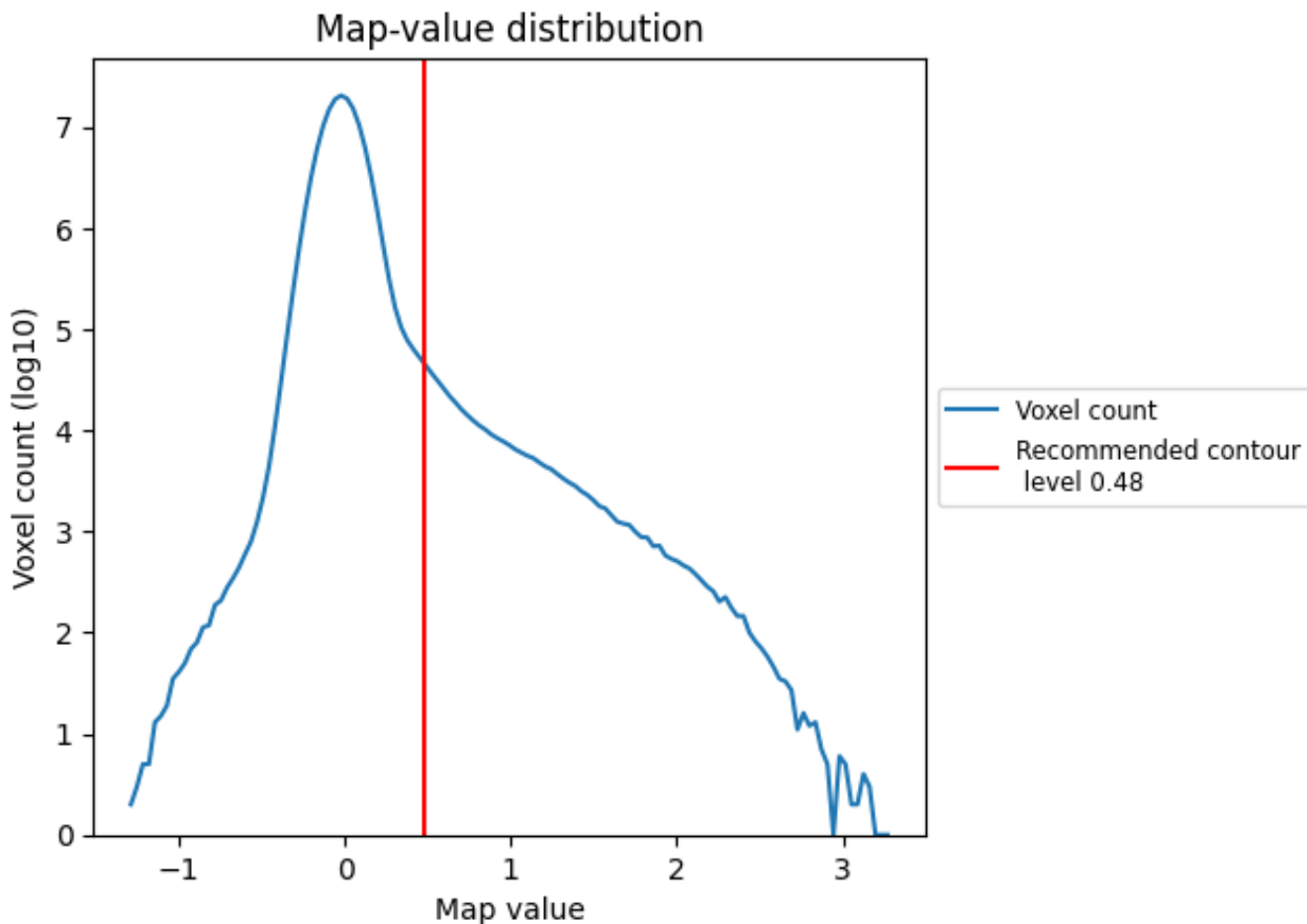
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

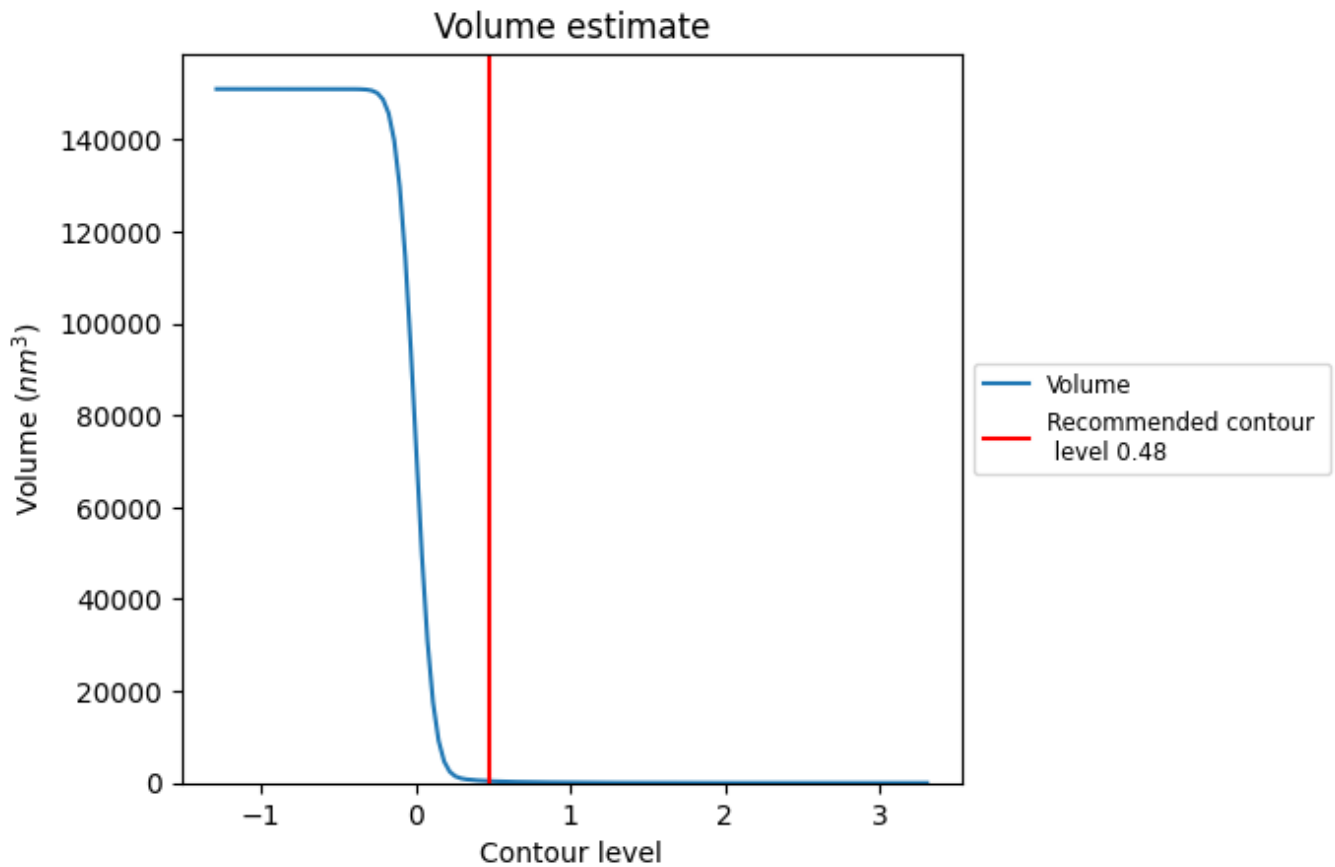
This section contains the results of statistical analysis of the map.

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.

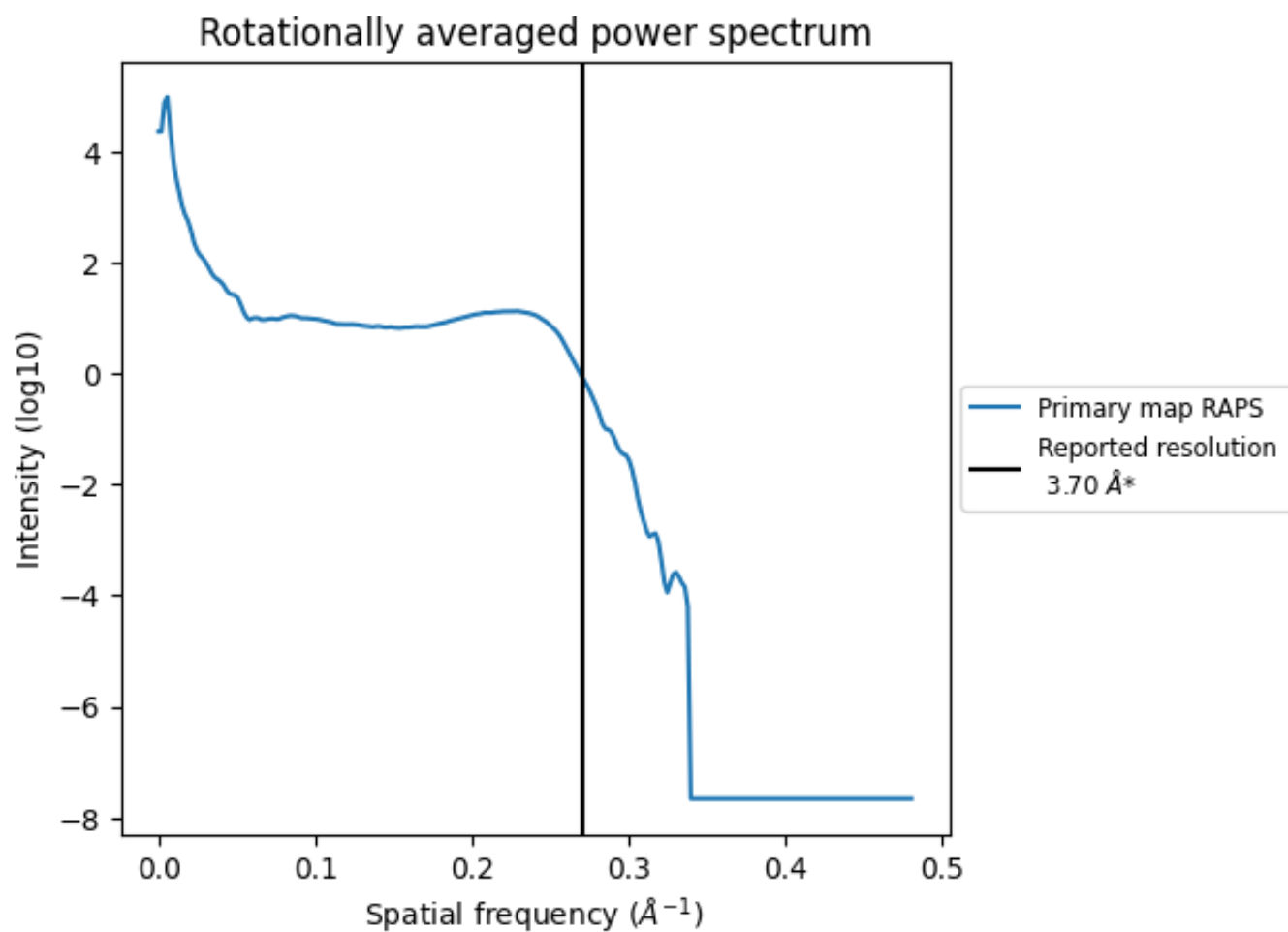
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm^3 ; this corresponds to an approximate mass of 365 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

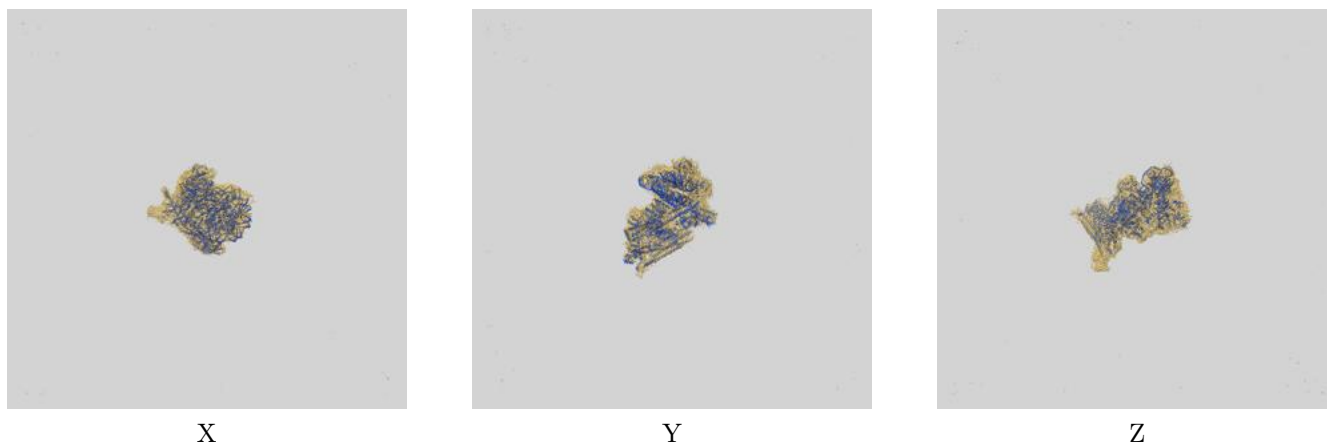
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

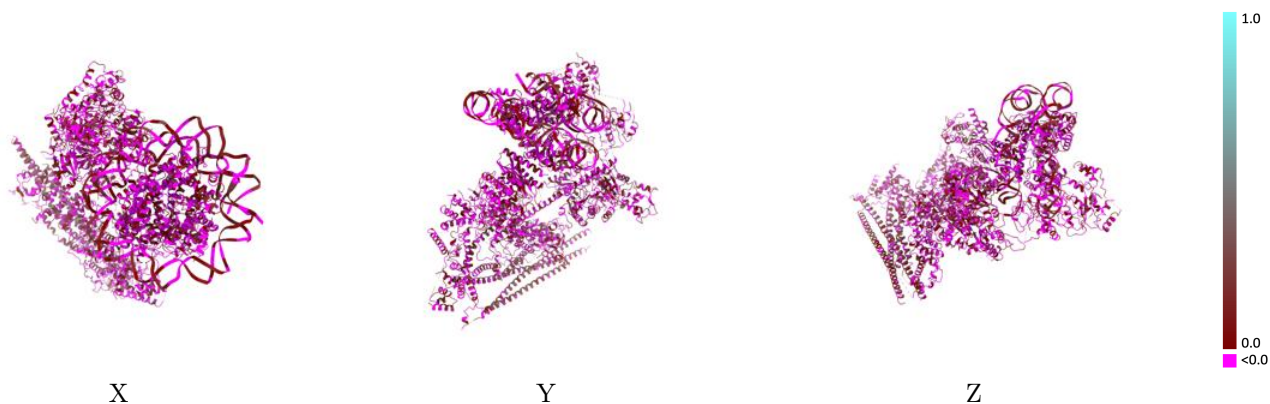
This section contains information regarding the fit between EMDB map EMD-0974 and PDB model 6LTJ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



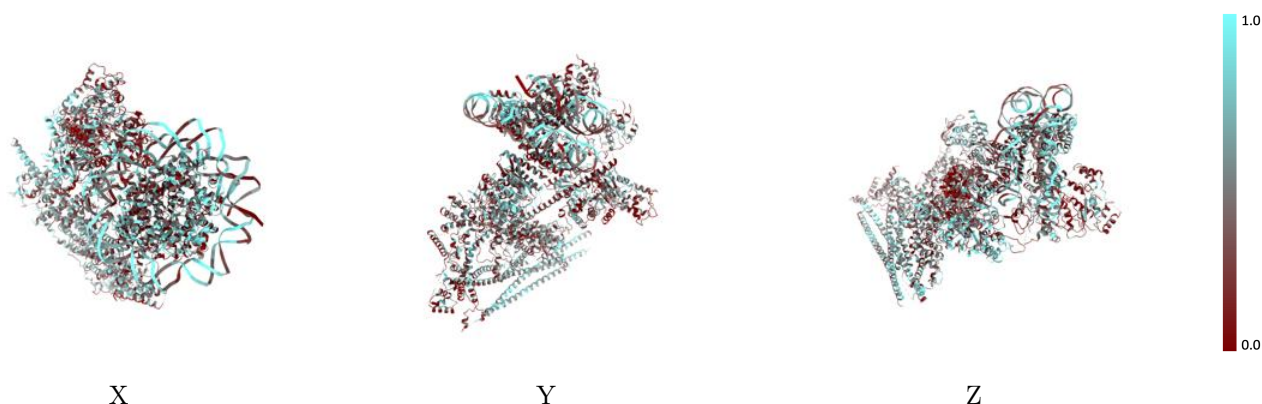
The images above show the 3D surface view of the map at the recommended contour level 0.48 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



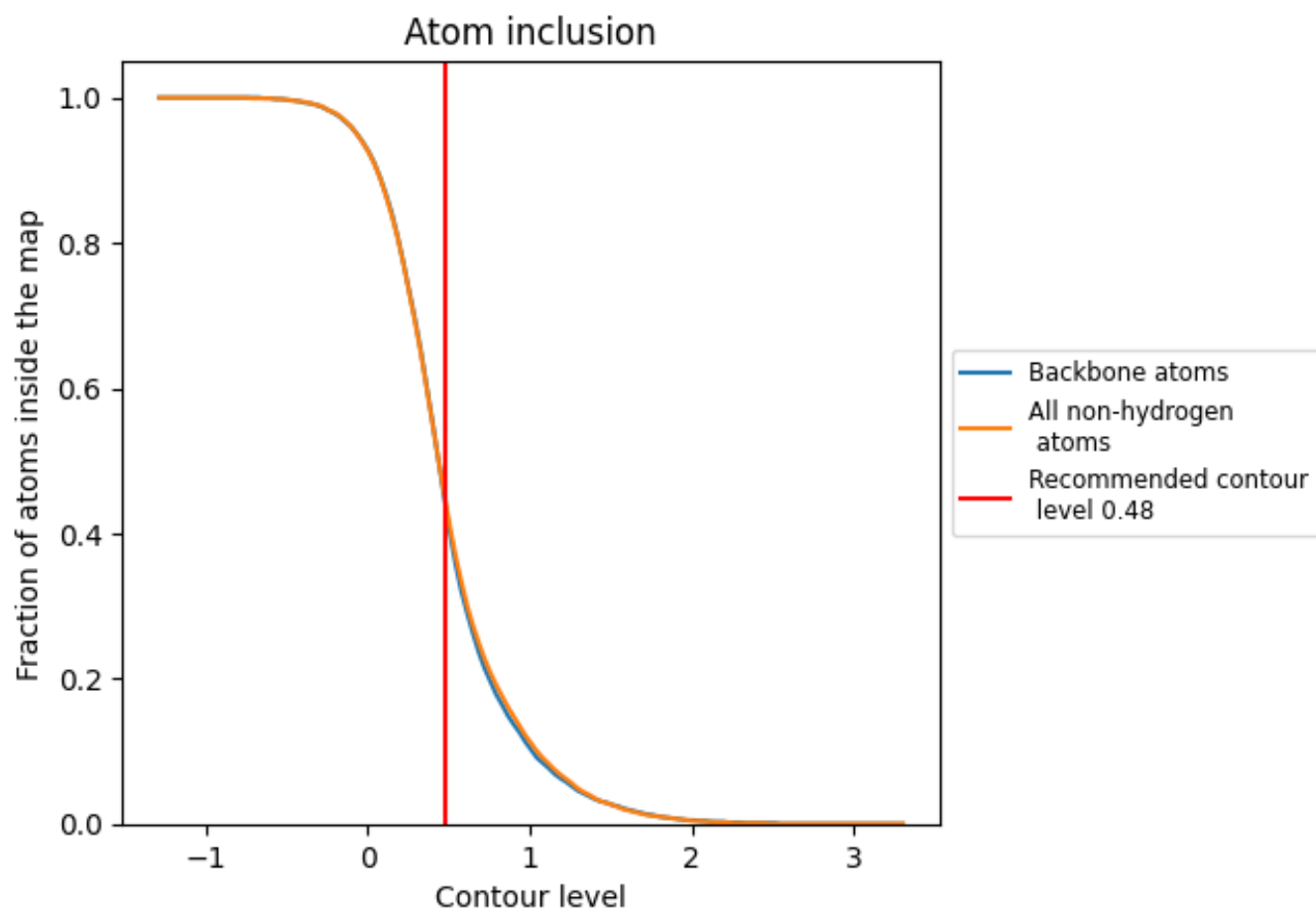
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.48).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 44% 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 (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4430	 0.0070
A	 0.4520	 -0.0070
B	 0.4970	 -0.0090
C	 0.5020	 -0.0140
D	 0.4630	 -0.0280
E	 0.4610	 -0.0760
F	 0.4680	 0.0050
G	 0.4390	 -0.0310
H	 0.3810	 -0.0530
I	 0.2940	 -0.0020
J	 0.5410	 0.0100
K	 0.2800	 0.0300
L	 0.3890	 -0.0050
M	 0.4570	 -0.0130
N	 0.4210	 0.0210
O	 0.5190	 0.0290
P	 0.4480	 0.0110
Q	 0.5510	 0.0880
R	 0.4300	 -0.0440
X	 0.5640	 0.0270
Y	 0.5850	 0.0320

