



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 10:54 AM JST

PDB ID : 6LT0
EMDB ID : EMD-0966
Title : cryo-EM structure of C9ORF72-SMCR8-WDR41
Authors : Tang, D.; Sheng, J.; Xu, L.; Zhan, X.; Yan, C.; Qi, S.
Deposited on : 2020-01-21
Resolution : 3.20 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.dev43
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

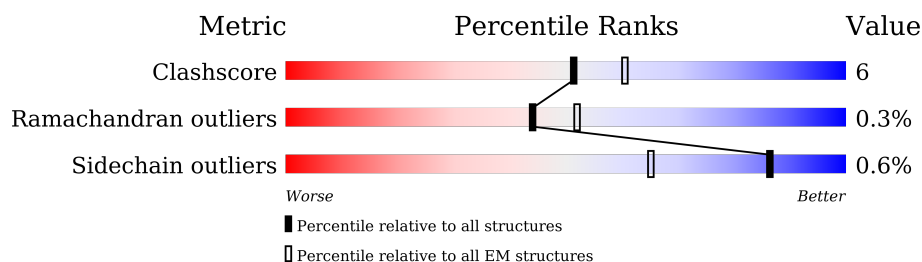
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	459	
1	D	459	
2	B	937	
2	E	937	
3	C	481	
3	F	481	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17774 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 WD repeat-containing protein 41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	343	Total	C	N	O	S	0	0
			2693	1713	471	497	12		
1	D	343	Total	C	N	O	S	0	0
			2693	1713	471	497	12		

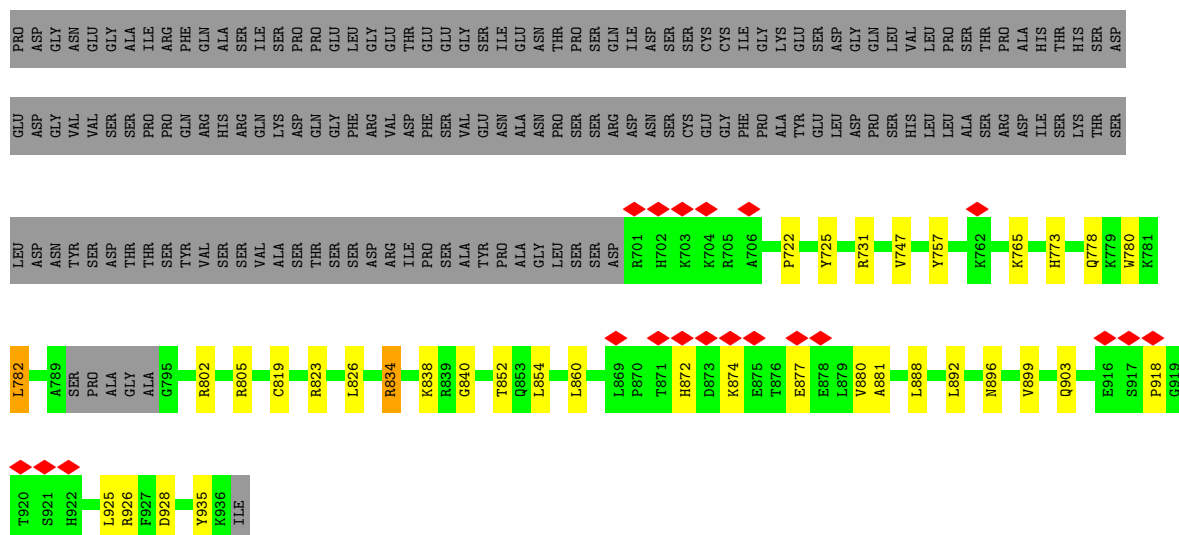
- Molecule 2 is a protein called Guanine nucleotide exchange protein SMCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	386	Total	C	N	O	S	0	0
			3134	2026	541	551	16		
2	E	386	Total	C	N	O	S	0	0
			3134	2026	541	551	16		

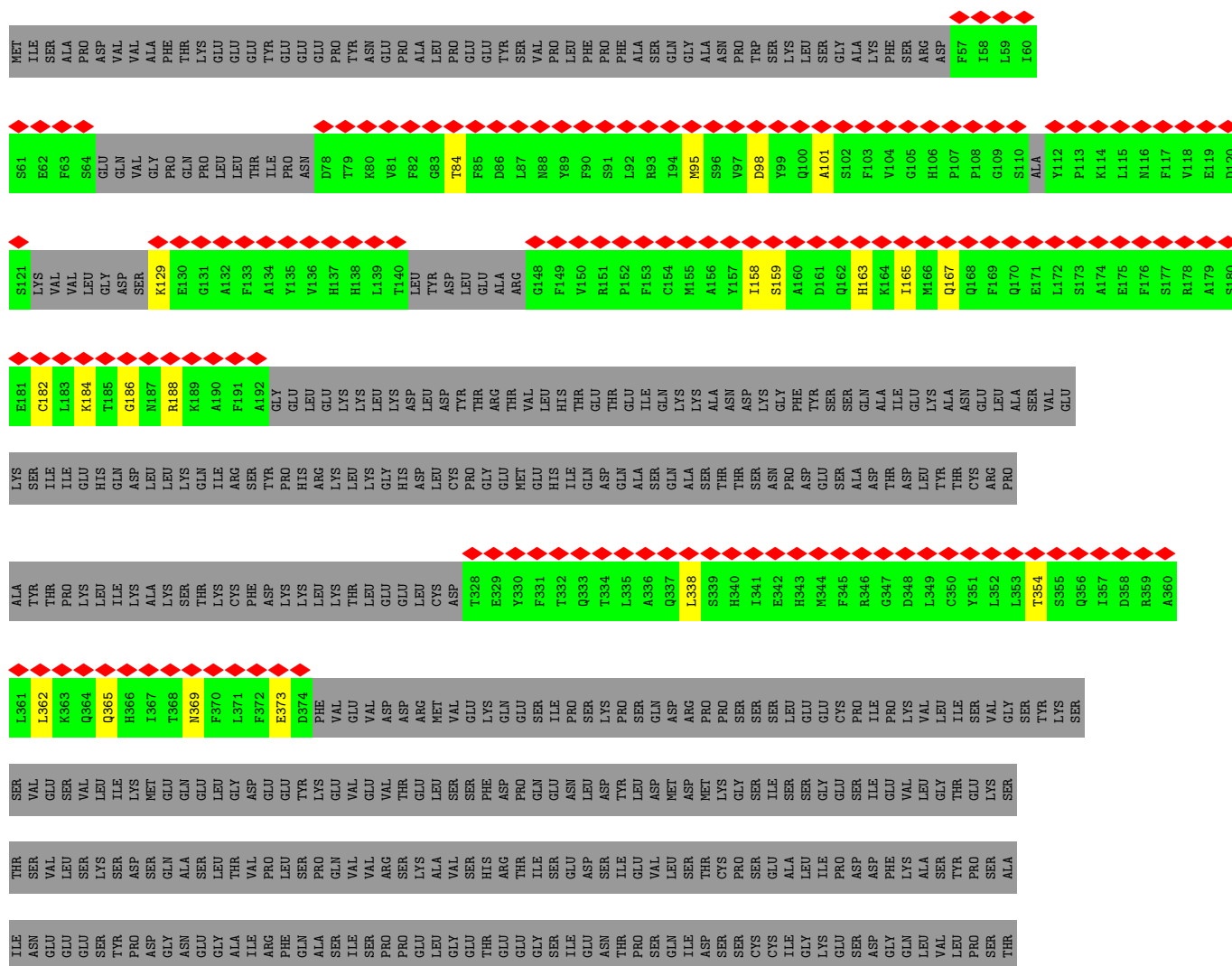
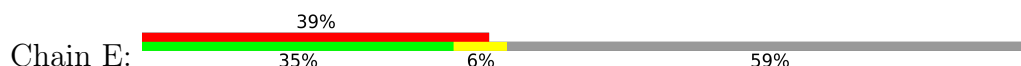
- Molecule 3 is a protein called Guanine nucleotide exchange C9orf72.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3060	1980	514	550	16		
3	F	385	Total	C	N	O	S	0	0
			3060	1980	514	550	16		





• Molecule 2: Guanine nucleotide exchange protein SMCR8



G423	R431	R436	R439	T440	A441	E442	G443	D444	L445	I447	L448	N449	A450	L451	A452	E453	K454	I455	K456	P457	G458	L459	H460	S461	F462	I463	F464	G465	ARG	PRO	PHE	TYR	THR	SER	VAL	GLN	GLU	ARG	ASP	VAL	LEU	MET	THR	PHE																	
ASP	H372	D369	A379	F380	L381	D382	Q383	V384	F385	L387	K388	P389	G390	L391	S392	L393	R394	S395	T396	F397	L398	A399	Q400	F401	L402	L403	V404	L405	H406	R407	K408	A409	L410	T411	L412	I413	K414	Y415	I416	E417	D418	D419	T420	Q421	K422																
PRO	THR	LEU	ASN	I366	F367	Q368	D369	D309	V310	D311	V312	N313	T314	V315	K316	Q317	M318	P319	P320	C321	H322	E323	H324	I325	Y326	N327	Q328	R329	G330	L331	S332	L333	R334	S335	T336	F337	L338	A339	F339	W340	ARG	ALA	THR	SER	GLU	GLU	ASP	NET	ALA	GLN	ASP	THR	ILE	ILE	TYR	THR	ASP	GLU	SER	PHE	THR
A301	V310	D311	V312	N313	T314	V315	K316	Q317	M318	P319	P320	C321	H322	E323	H324	I325	Y326	N327	Q328	R329	G330	L331	S332	L333	R334	S335	T336	F337	L338	A339	F339	W340	ARG	ALA	THR	SER	GLU	GLU	ASP	NET	ALA	GLN	ASP	THR	ILE	ILE	TYR	THR	ASP	GLU	SER	PHE	THR								
A241	R249	T250	L251	C252	L253	F254	L255	T256	P257	A258	E259	R260	K261	C262	S263	R264	L265	C266	E267	A268	E269	S270	S271	F272	K273	Y274	E275	S276	G277	L278	F279	V280	Q281	G282	L283	L284	K285	D286	S287	T288	G289	S290	F291	V292	L293	P294	F295	R296	Q297	V298	M299	Y300									
I181	P182	V183	M184	E185	L186	L187	S188	S189	M190	K191	S192	H193	S194	V195	P196	E197	E198	I199	D200	I201	A202	D203	T204	V205	L206	N207	D208	D209	D210	I211	G212	D213	S214	C215	H216	E217	G218	F219	L220	L221	N222	A223	I224	S225	S226	H227	L228	Q229	T230	C231	C232	C233	S234	V235	V236	V237	G238	S239	S240		
F61	L62	A63	H64	H65	T66	L67	H68	G69	E70	I71	LEU	ARG	ASN	ALA	GLU	SER	G78	A79	I80	D81	V82	K83	F84	F85	V86	L87	S88	E89	K90	G91	V92	I93	I94	W95	S96	L97	I98	F99	ASP	GLY	ASN	TRP	ASN	GLY	ASP	ARG	SER	T109	Y110	G111	L112	S113	I114	I115	L116	P117	Q118	T119	E120		
L121	S122	F123	Y124	L125	P126	L127	H128	R129	V130	G131	V132	D133	R134	L135	T136	H137	I138	I139	R140	K141	G142	R143	I144	W145	M146	H147	K148	E149	ARG	GLN	GLU	ASN	VAL	GLN	LYS	ILE	ILE	LEU	GLU	GLY	THR	GLU	ARG	MET	ASP	GLN	GLY	SER	I172	I173	P174	M175	L176	T177	G178	E179	V180				
MET	SER	THR	LEU	CYS	PRO	PRO	PRO	SER	PRO	ALA	ALA	VAL	A13	K14	T15	E16	I17	A18	L19	S20	G21	K22	S23	P24	L25	L26	A27	A28	T29	F30	A31	Y32	W33	ASP	ASN	ASN	ILE	LEU	GLY	PRO	R40	V41	R42	H43	I44	W45	A46	P47	K48	T49	E50	Q51	V52	L53	L54	S55	D56	G57	E58	I59	T60

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	347925	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 ($e^-/\text{\AA}^2$)	5.3	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	0.145	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	297.08, 297.08, 297.08	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

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	0.31	0/2735	0.67	5/3705 (0.1%)
1	D	0.31	0/2735	0.67	5/3705 (0.1%)
2	B	0.31	0/3211	0.60	1/4334 (0.0%)
2	E	0.31	0/3211	0.60	1/4334 (0.0%)
3	C	0.30	0/3122	0.59	0/4220
3	F	0.30	0/3122	0.59	1/4220 (0.0%)
All	All	0.31	0/18136	0.62	13/24518 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
3	C	0	2
3	F	0	2
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	LEU	CA-CB-CG	6.36	129.93	115.30
1	A	37	LEU	CA-CB-CG	6.35	129.91	115.30
1	A	146	ASP	CB-CG-OD1	5.60	123.34	118.30
1	D	218	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	218	LEU	CA-CB-CG	5.58	128.13	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	LEU	Peptide
1	A	292	ASP	Peptide
3	C	193	HIS	Peptide
3	C	195	VAL	Peptide
1	D	218	LEU	Peptide

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	2693	0	2697	28	0
1	D	2693	0	2697	27	0
2	B	3134	0	3105	47	0
2	E	3134	0	3105	34	0
3	C	3060	0	3134	46	0
3	F	3060	0	3134	59	0
All	All	17774	0	17872	205	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 6.

The worst 5 of 205 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)
2:B:834:ARG:HG2	3:F:431:ARG:NH2	1.43	1.31
3:C:431:ARG:HD3	3:F:435:ILE:CD1	1.61	1.30
2:B:896:ASN:CG	3:F:368:GLN:OE1	1.91	1.08
3:C:431:ARG:CD	3:F:435:ILE:HD12	1.85	1.05
2:B:834:ARG:O	3:F:431:ARG:NH2	1.90	1.05

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	329/459 (72%)	277 (84%)	50 (15%)	2 (1%)	25	64
1	D	329/459 (72%)	277 (84%)	50 (15%)	2 (1%)	25	64
2	B	370/937 (40%)	315 (85%)	54 (15%)	1 (0%)	41	74
2	E	370/937 (40%)	315 (85%)	54 (15%)	1 (0%)	41	74
3	C	373/481 (78%)	334 (90%)	39 (10%)	0	100	100
3	F	373/481 (78%)	334 (90%)	39 (10%)	0	100	100
All	All	2144/3754 (57%)	1852 (86%)	286 (13%)	6 (0%)	44	74

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	GLU
1	D	293	GLU
2	B	840	GLY
2	E	840	GLY
1	A	219	LEU

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	298/405 (74%)	296 (99%)	2 (1%)	84	94
1	D	298/405 (74%)	296 (99%)	2 (1%)	84	94
2	B	339/837 (40%)	335 (99%)	4 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	339/837 (40%)	335 (99%)	4 (1%)	71	88
3	C	344/431 (80%)	344 (100%)	0	100	100
3	F	344/431 (80%)	344 (100%)	0	100	100
All	All	1962/3346 (59%)	1950 (99%)	12 (1%)	86	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	441	ARG
2	E	95	MET
2	E	926	ARG
2	E	802	ARG
2	B	802	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	106	HIS
2	E	137	HIS
3	F	281	GLN
2	E	814	ASN
2	B	896	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

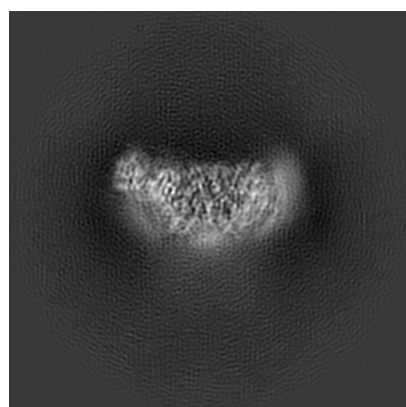
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0966. These allow visual inspection of the internal detail of the map and identification of artifacts.

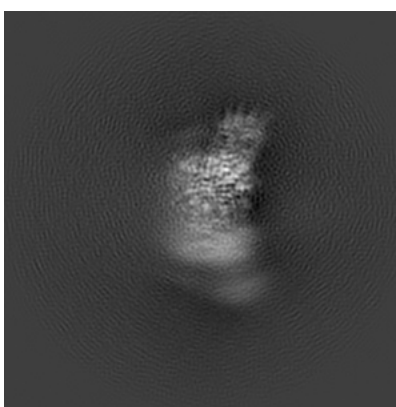
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

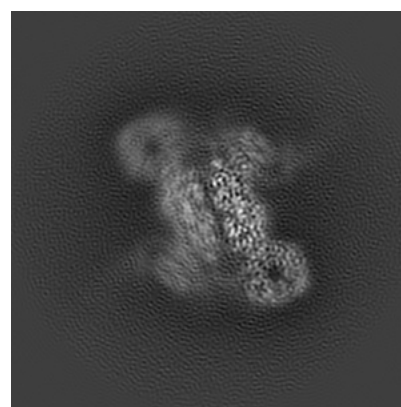
6.1.1 Primary map



X



Y

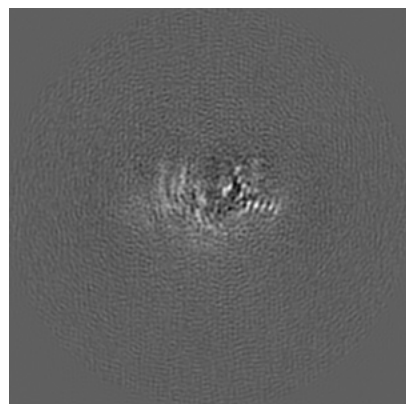


Z

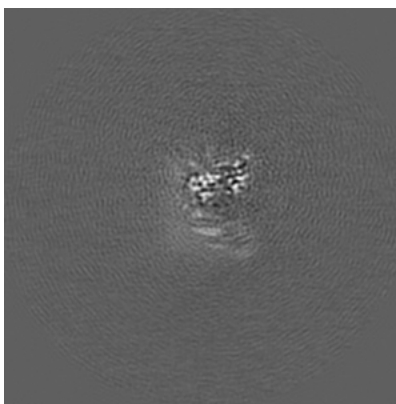
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

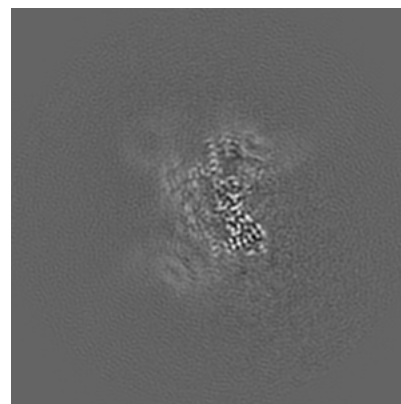
6.2.1 Primary map



X Index: 140



Y Index: 140

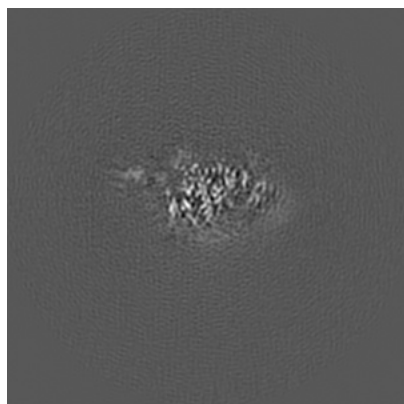


Z Index: 140

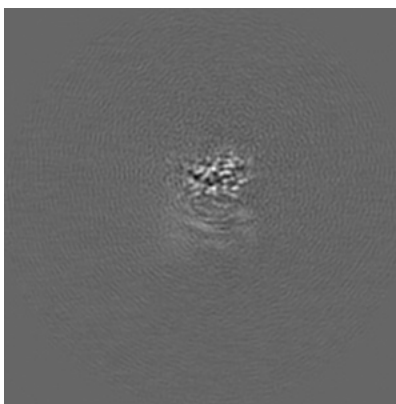
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

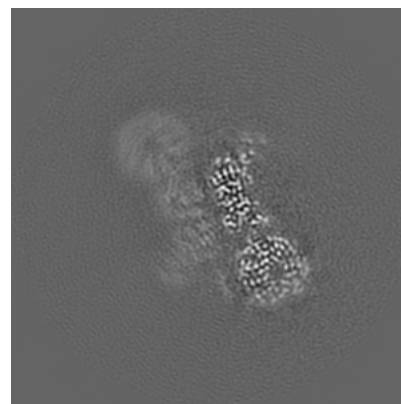
6.3.1 Primary map



X Index: 159



Y Index: 130



Z Index: 159

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 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

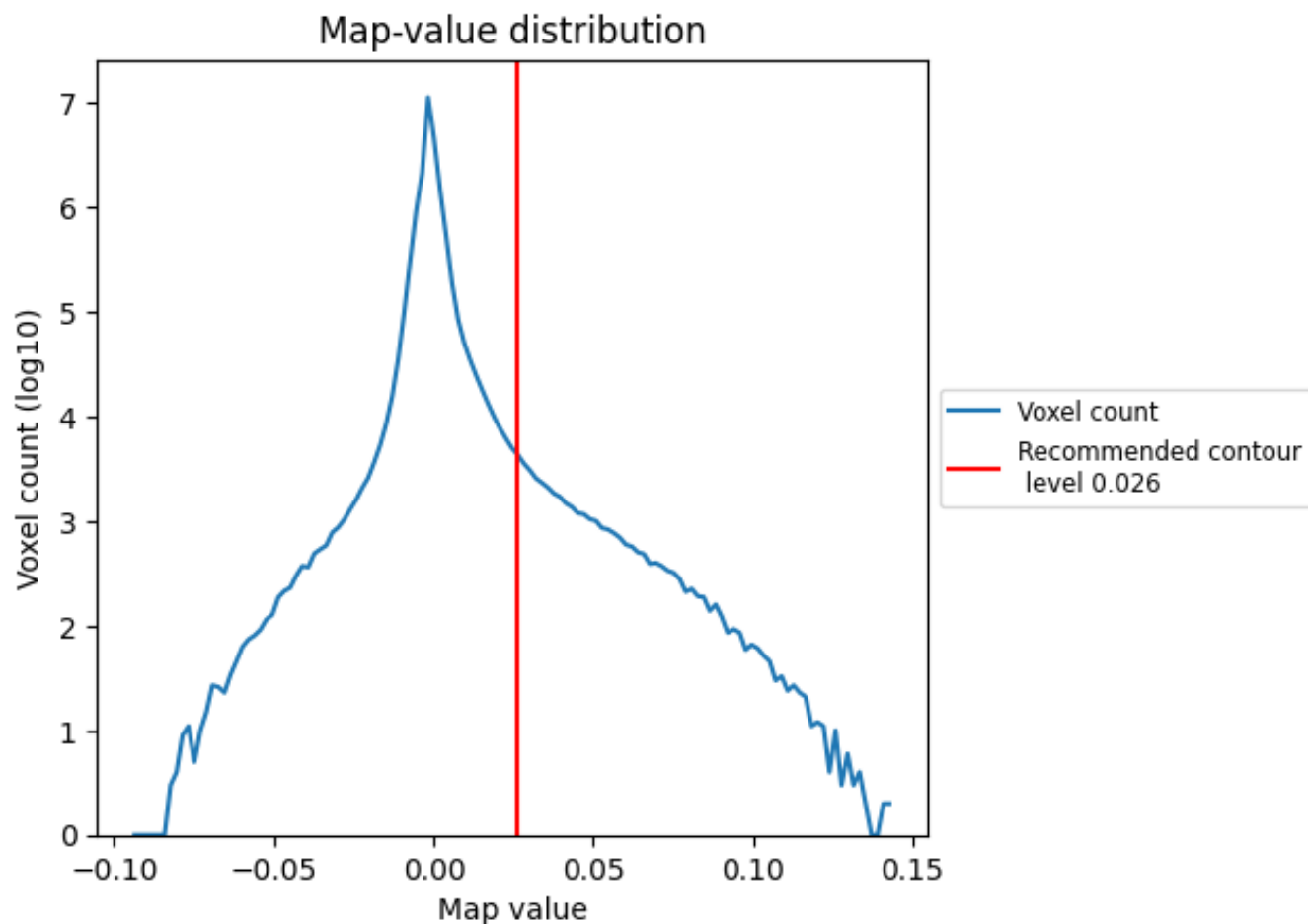
6.5 Mask visualisation

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

7 Map analysis [i](#)

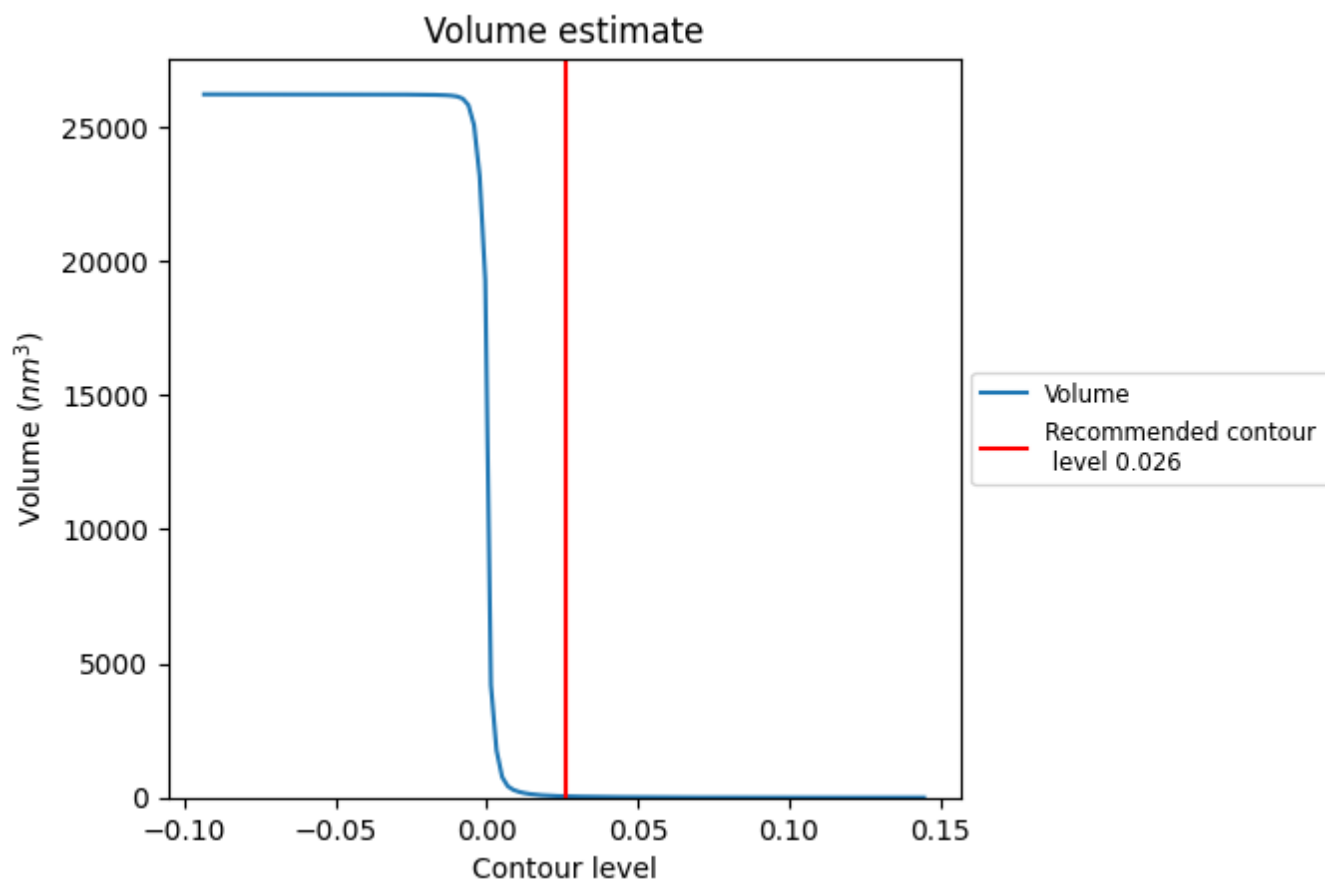
This section contains the results of statistical analysis of the map.

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.

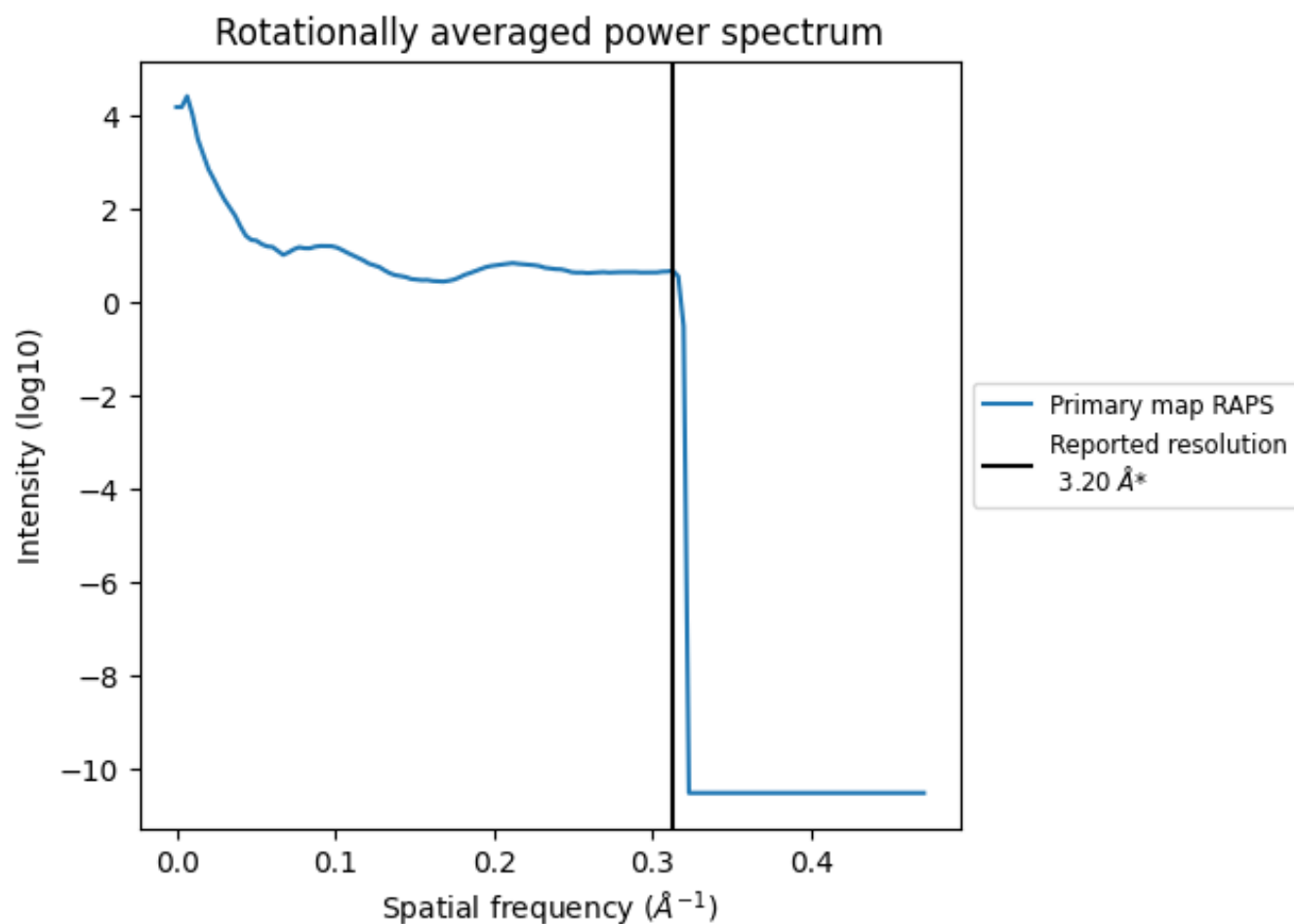
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm³; this corresponds to an approximate mass of 43 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 0.312 Å⁻¹

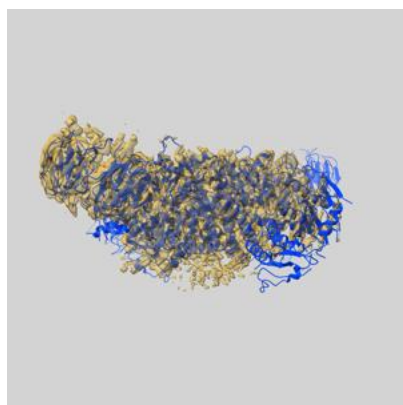
8 Fourier-Shell correlation ⓘ

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

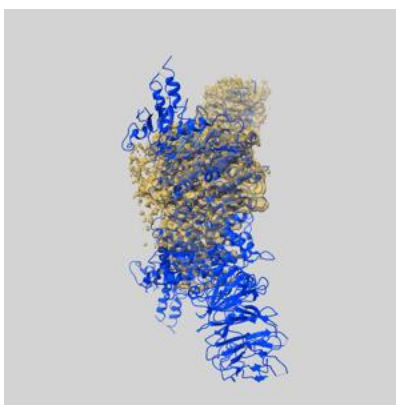
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0966 and PDB model 6LT0. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

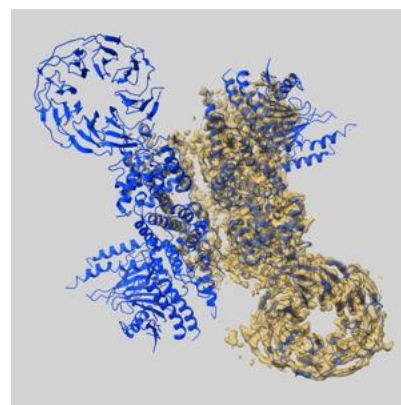
9.1 Map-model overlay [i](#)



X



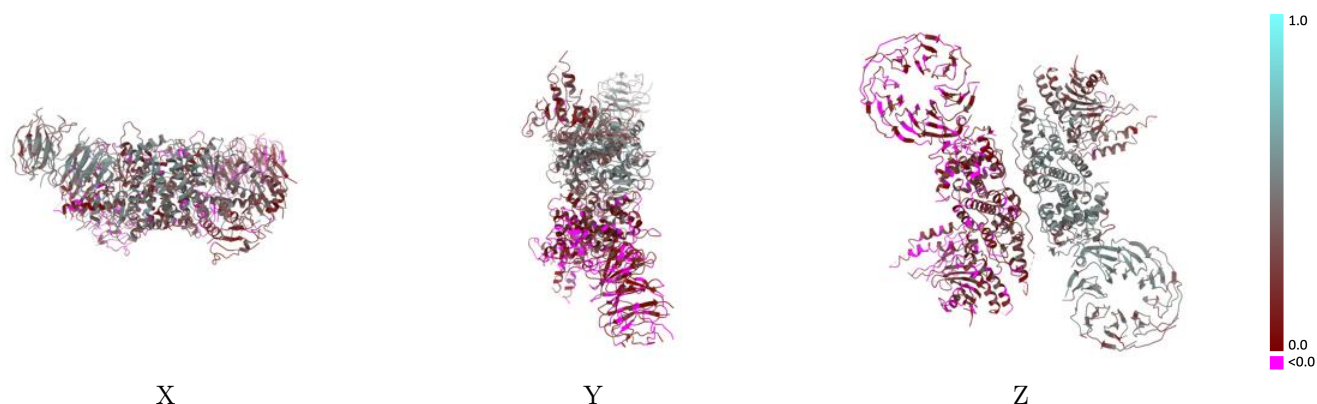
Y



Z

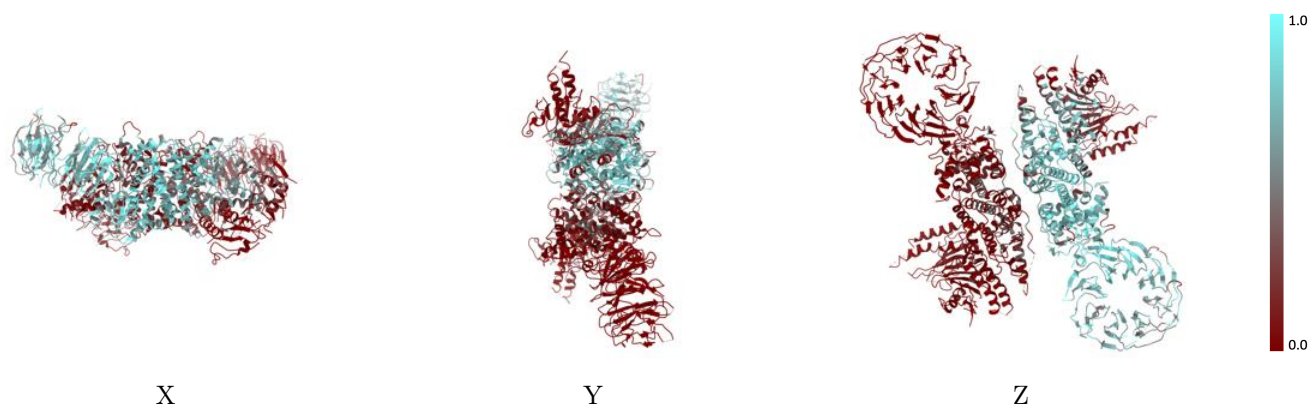
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



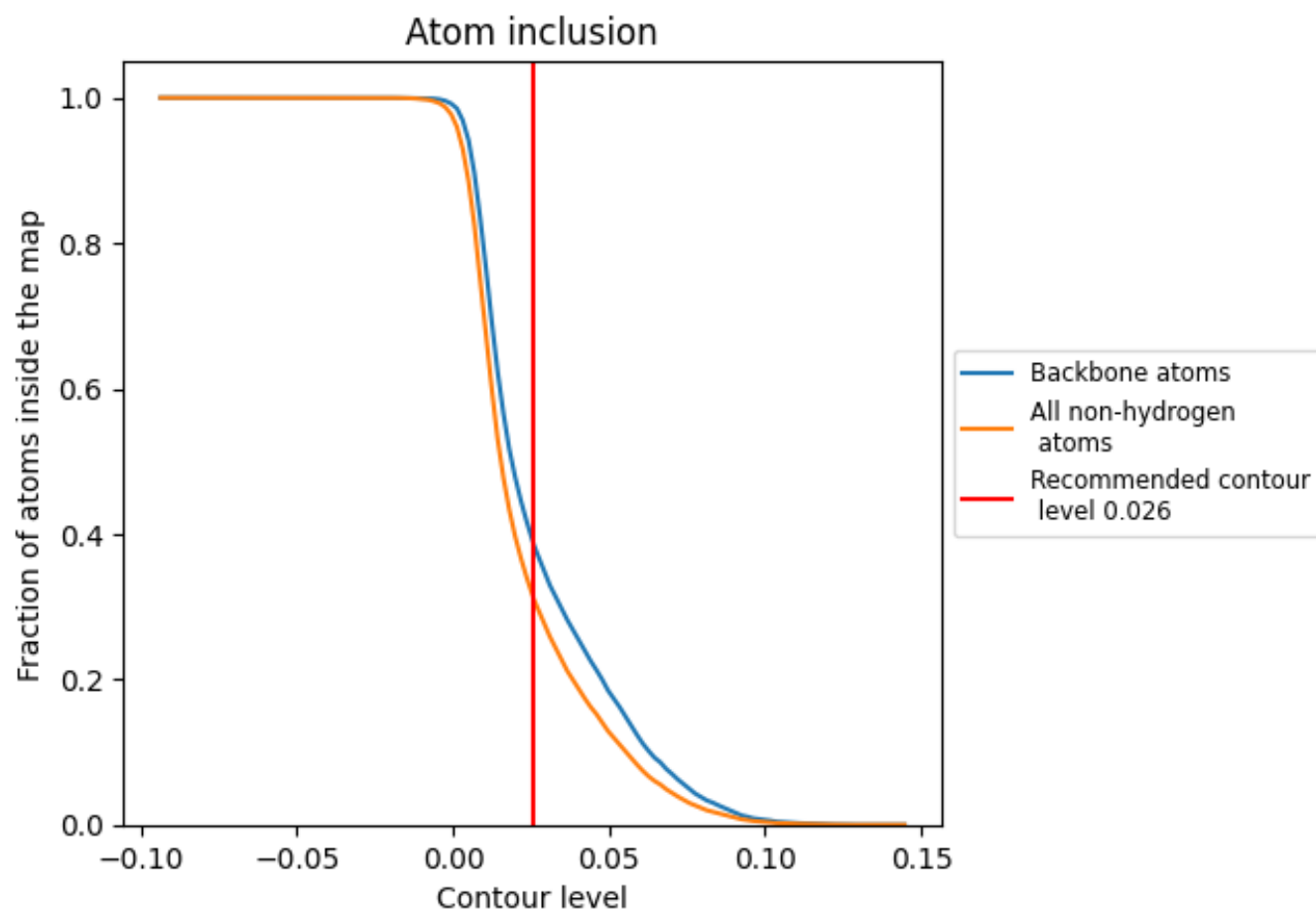
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.026).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 31% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3096	<div></div> 0.2600
A	<div></div> 0.6849	<div></div> 0.4600
B	<div></div> 0.5129	<div></div> 0.4030
C	<div></div> 0.5476	<div></div> 0.4170
D	<div></div> 0.0004	<div></div> 0.0590
E	<div></div> 0.0525	<div></div> 0.0690
F	<div></div> 0.0684	<div></div> 0.1540

1.0

0.0

<0.0