wwPDB EM Validation Summary Report (i)

Apr 15, 2026 – 02:28 AM UTC

PDB ID	:	9UER / pdb_00009uer
EMDB ID	:	EMD-64090
Title	:	AcrIE10-Cas7-IR complex
Authors	:	Tsui, W.T.; Ma, J.B.
Deposited on	:	2025-04-09
Resolution	:	3.64 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 (i) 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 (i)) were used in the production of this report:

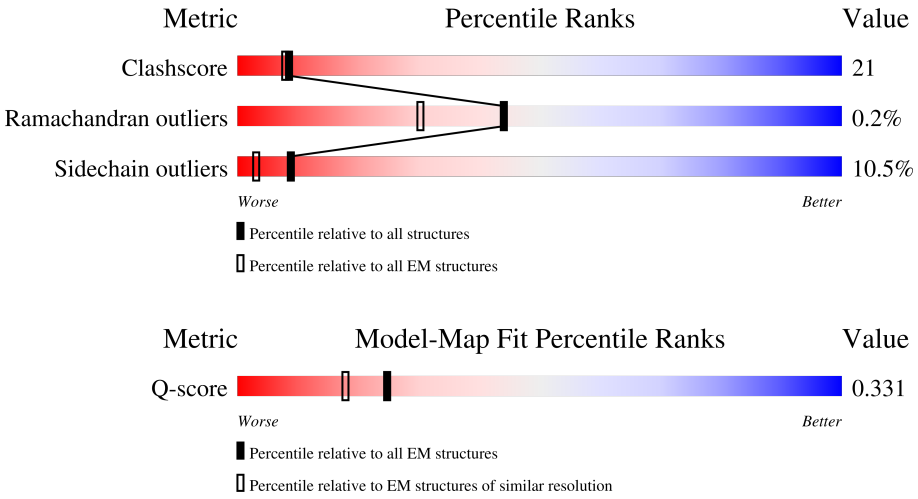
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.64 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	11633 (3.14 - 4.14)

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 <=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	G	19	32% 68%
2	H	20	20% 80%
3	A	116	66% 27% 7%
3	B	116	68% 27% 5%

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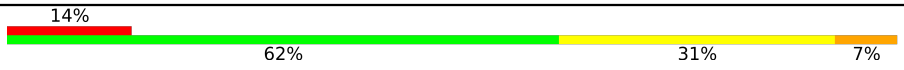
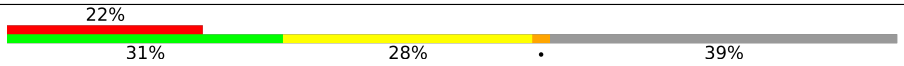
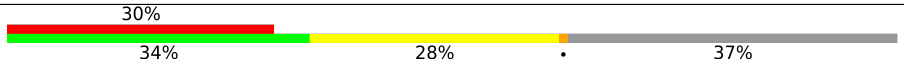
Mol	Chain	Length	Quality of chain
3	C	116	
3	D	116	
4	E	351	
4	F	351	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7873 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 DNA chain called DNA (5'-D(P*TP*GP*TP*AP*TP*GP*AP*CP*AP*TP*CP*TP*GP*TP*CP*AP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	19	Total	C	N	O	P	0	0
			387	186	66	116	19		

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*TP*AP*TP*GP*AP*CP*AP*GP*AP*TP*GP*TP*CP*AP*TP*AP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	20	Total	C	N	O	P	0	0
			413	197	79	117	20		

- Molecule 3 is a protein called AcrIE10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	116	Total	C	N	O	S	0	0
			928	581	164	181	2		
3	B	116	Total	C	N	O	S	0	0
			928	581	164	181	2		
3	C	116	Total	C	N	O	S	0	0
			928	581	164	181	2		
3	D	116	Total	C	N	O	S	0	0
			928	581	164	181	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	conflict	UNP A0A218NFC2
B	1	VAL	MET	conflict	UNP A0A218NFC2
C	1	VAL	MET	conflict	UNP A0A218NFC2
D	1	VAL	MET	conflict	UNP A0A218NFC2

- Molecule 4 is a protein called CRISPR-associated protein Cse4.

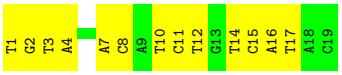
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	215	Total	C	N	O	S	0	0
			1659	1039	291	319	10		
4	F	220	Total	C	N	O	S	0	0
			1702	1068	298	326	10		

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: DNA (5'-D(P*TP*GP*TP*AP*TP*GP*AP*CP*AP*TP*CP*TP*GP*TP*CP*AP*TP*AP*C)-3')

Chain G:

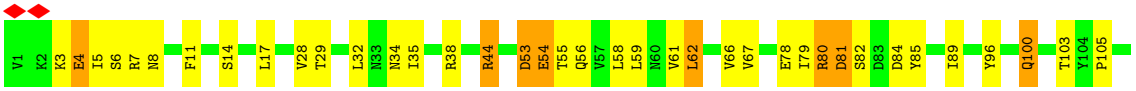


• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*GP*AP*CP*AP*GP*AP*TP*GP*TP*CP*AP*TP*AP*CP*AP*A)-3')

Chain H:

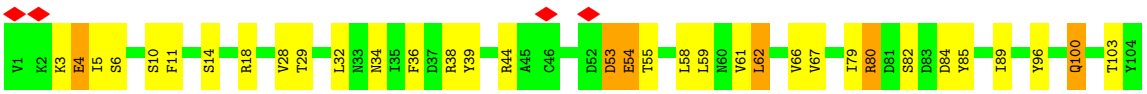
• Molecule 3: AcrIE10

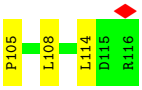
Chain A:



• Molecule 3: AcrIE10

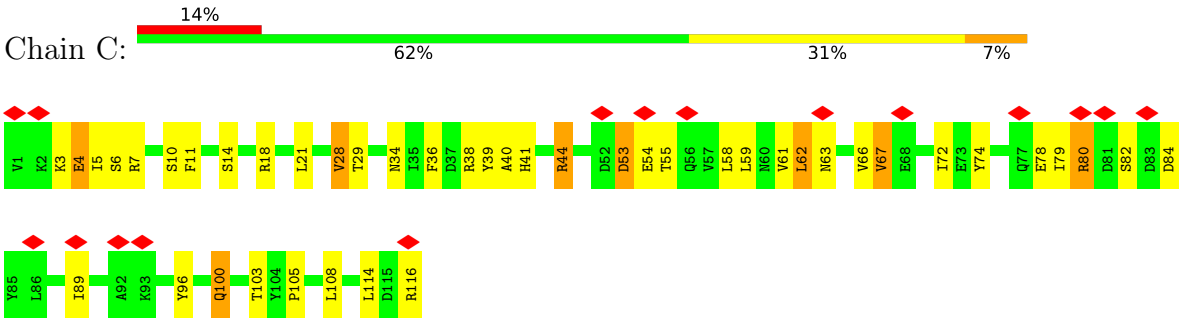
Chain B:





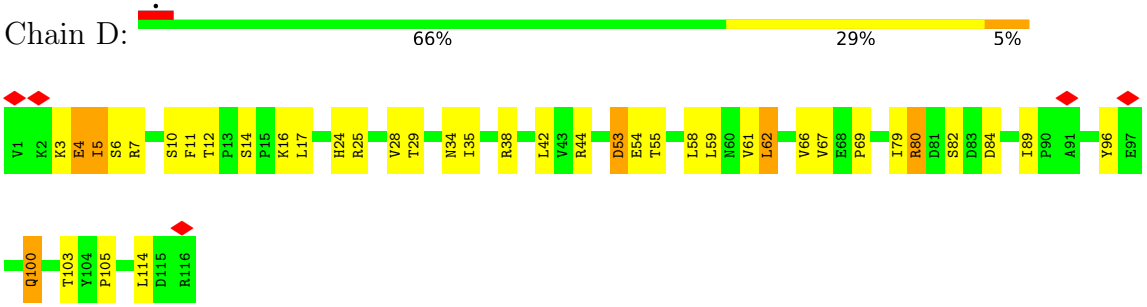
• Molecule 3: AcrIE10

Chain C:



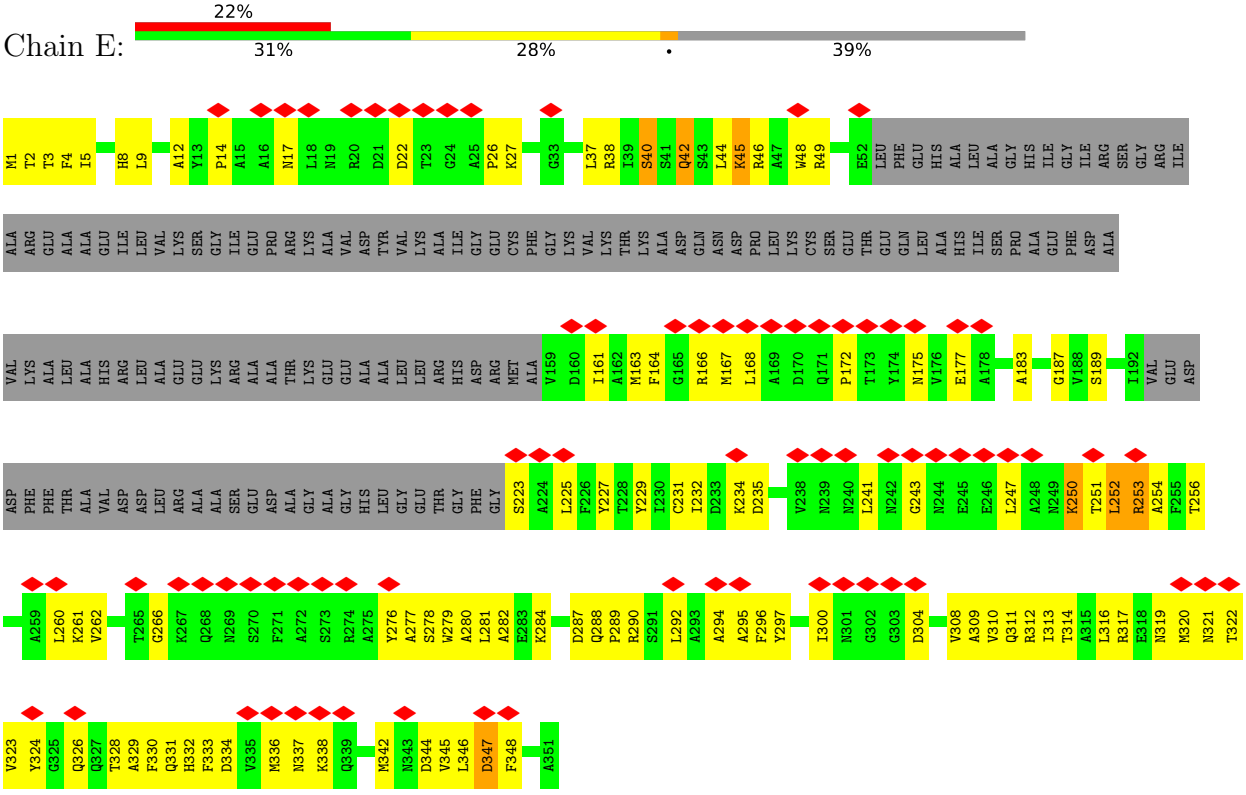
• Molecule 3: AcrIE10

Chain D:



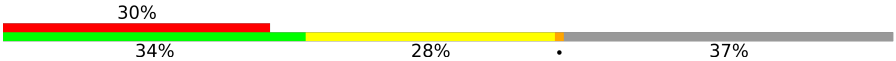
• Molecule 4: CRISPR-associated protein Cse4

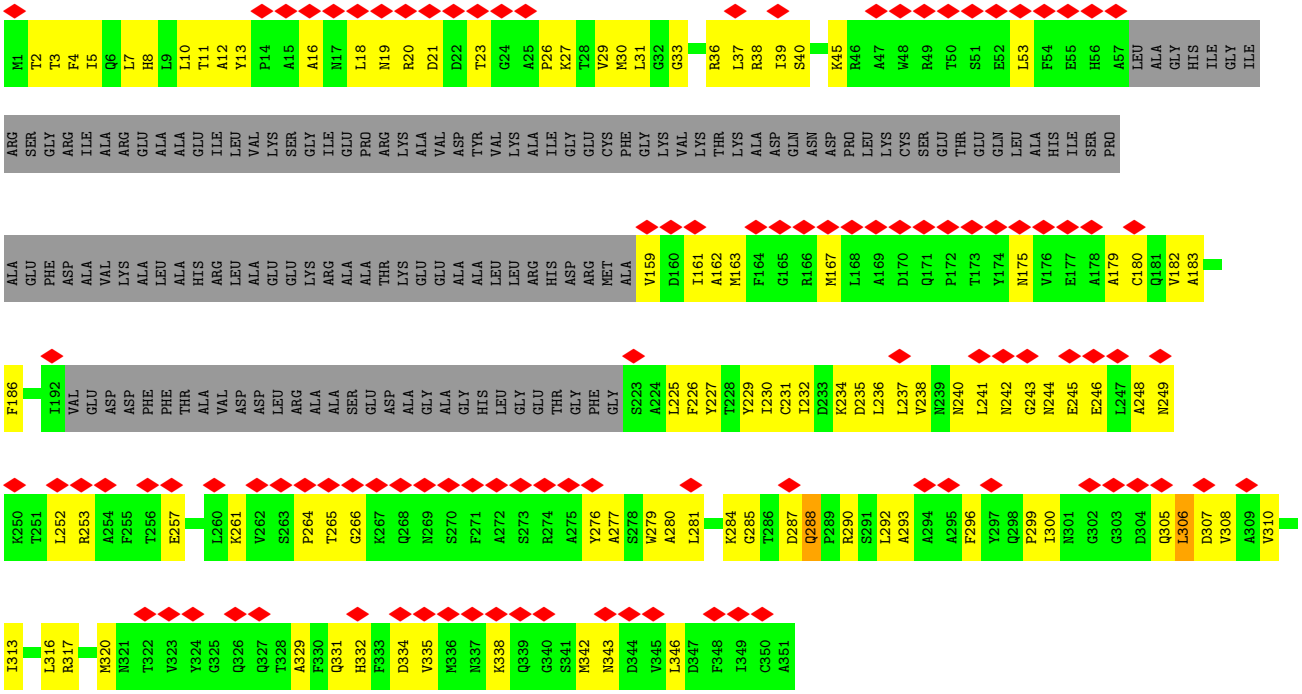
Chain E:



• Molecule 4: CRISPR-associated protein Cse4

Chain F:




M1 T2 T3 F4 I5 Q6 L7 H8 L9 L10 T11 A12 Y13 P14 A15 A16 N17 L18 N19 R20 D21 D22 T23 G24 A25 P26 K27 T28 V29 M30 L31 G32 G33 R36 L37 R38 I39 S40 K45 R46 A47 W48 R49 T50 S51 E52 L53 F54 E55 H56 A57 LEU ALA GLY HIS ILE GLY ILE
ARG SER GLY ARG ILE ALA ARG GLU ALA ALA GLU ILE LEU VAL LYS SER GLY ILE GLU PRO ARG LYS ALA VAL ASP TYR VAL LYS ALA ILE GLY GLU CYS PHE GLY LYS VAL LYS THR LYS ALA ASP GLN ASN ASP PRO LEU LYS CYS SER GLU THR GLU GLN LEU ALA HIS ILE SER PRO
ALA GLU PHE ASP ALA VAL LYS ALA LEU ALA HIS ARG LEU ALA GLU GLU LYS ARG ALA ALA THR LYS GLU GLU ALA ALA LEU LEU ARG HIS ASP ARG MET ALA V159 D160 I161 A162 M163 F164 G165 R166 M167 L168 A169 D170 Q171 P172 T173 Y174 N175 V176 E177 A178 A179 C180 Q181 V182 A183
F186 I192 VAL GLU ASP ASP PHE PHE THR ALA VAL ASP ASP LEU ARG ALA ALA SER GLU ASP ALA GLY ALA GLY HIS LEU GLY GLU THR GLY PHE GLY S223 A224 L225 F226 Y227 T228 Y229 I230 C231 I232 D233 K234 D235 L236 L237 V238 N239 N240 L241 N242 G243 N244 E245 E246 L247 A248 N249
K250 T251 L252 R253 A254 F255 T256 E257 L260 K261 V262 S263 P264 T265 G266 K267 Q268 N269 S270 F271 A272 S273 R274 A275 Y276 A277 S278 W279 A280 L281 K284 G285 T286 D287 Q288 P289 R290 S291 L292 A293 A294 A295 F296 Y297 Q298 P299 I300 N301 G302 G303 D304 Q305 L306 D307 V308 A309 V310
I313 L316 R317 M320 N321 T322 V323 Y324 G325 Q326 Q327 T328 A329 F330 Q331 H332 F333 D334 V335 M336 N337 K338 Q339 G340 S341 M342 N343 D344 V345 L346 D347 F348 I349 C350 A351

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.853	Depositor
Minimum map value	-0.546	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.119	Depositor
Map size (Å)	172.8, 172.8, 172.8	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96000004, 0.96000004, 0.96000004	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	G	0.46	0/432	0.64	0/664
2	H	0.42	0/464	0.55	0/714
3	A	0.30	0/945	0.50	0/1282
3	B	0.29	0/945	0.48	0/1282
3	C	0.29	0/945	0.49	0/1282
3	D	0.29	0/945	0.48	0/1282
4	E	0.32	0/1686	0.60	0/2282
4	F	0.23	0/1731	0.51	0/2343
All	All	0.31	0/8093	0.53	0/11131

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

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	G	387	0	217	15	0
2	H	413	0	226	27	0
3	A	928	0	922	40	0
3	B	928	0	922	24	0
3	C	928	0	922	44	0
3	D	928	0	922	37	0
4	E	1659	0	1632	101	0
4	F	1702	0	1670	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7873	0	7433	325	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 21.

The worst 5 of 325 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:C:18:ARG:HH12	3:D:7:ARG:HA	1.28	0.94
3:D:103:THR:HG22	3:D:105:PRO:HD2	1.60	0.84
2:H:5:DT:H2"	2:H:6:DG:H5"	1.58	0.84
3:B:103:THR:HG22	3:B:105:PRO:HD2	1.60	0.84
4:F:12:ALA:HB2	4:F:306:LEU:HD11	1.60	0.84

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
3	A	114/116 (98%)	107 (94%)	7 (6%)	0	100 100
3	B	114/116 (98%)	106 (93%)	8 (7%)	0	100 100
3	C	114/116 (98%)	106 (93%)	8 (7%)	0	100 100
3	D	114/116 (98%)	106 (93%)	8 (7%)	0	100 100
4	E	209/351 (60%)	188 (90%)	21 (10%)	0	100 100
4	F	214/351 (61%)	192 (90%)	20 (9%)	2 (1%)	14 43
All	All	879/1166 (75%)	805 (92%)	72 (8%)	2 (0%)	44 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	306	LEU
4	F	305	GLN

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
3	A	103/103 (100%)	85 (82%)	18 (18%)	2 11
3	B	103/103 (100%)	85 (82%)	18 (18%)	2 11
3	C	103/103 (100%)	86 (84%)	17 (16%)	2 13
3	D	103/103 (100%)	85 (82%)	18 (18%)	2 11
4	E	174/275 (63%)	166 (95%)	8 (5%)	24 47
4	F	178/275 (65%)	177 (99%)	1 (1%)	78 77
All	All	764/962 (79%)	684 (90%)	80 (10%)	9 26

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	14	SER
4	E	40	SER
3	D	44	ARG
3	D	67	VAL
4	E	252	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	331	GLN
4	F	17	ASN
4	F	288	GLN
4	E	42	GLN
4	E	6	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

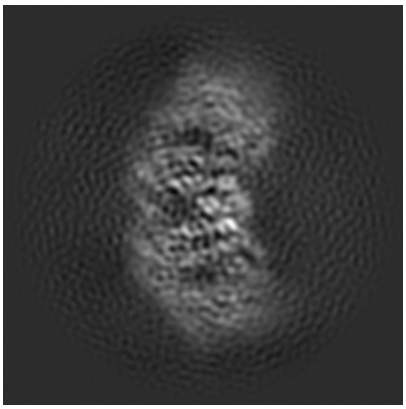
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64090. These allow visual inspection of the internal detail of the map and identification of artifacts.

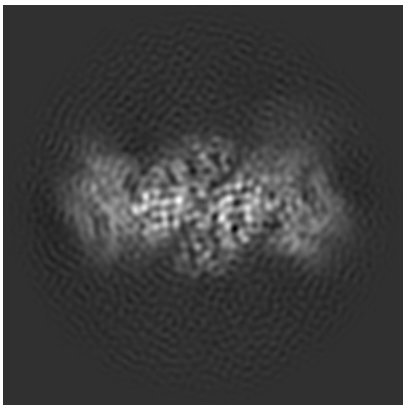
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

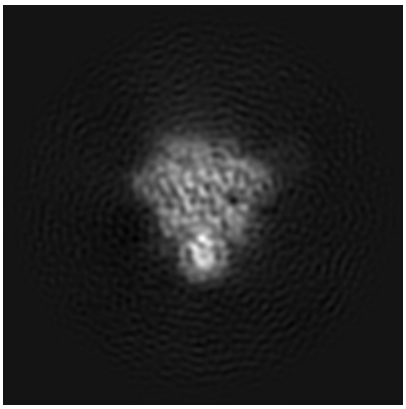
6.1.1 Primary map



X

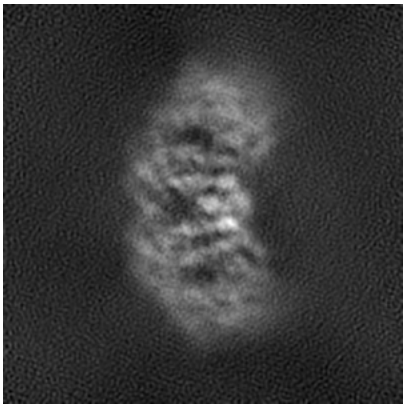


Y



Z

6.1.2 Raw map



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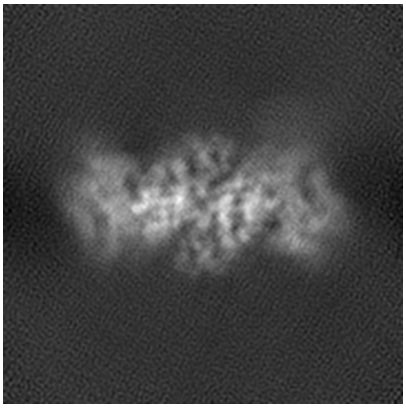
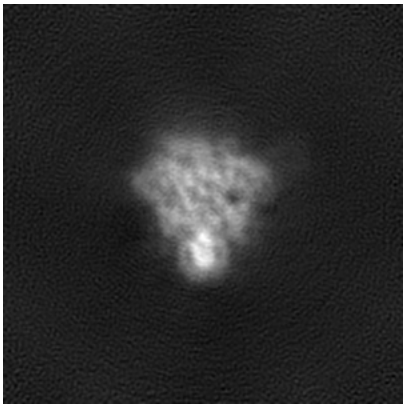


Y

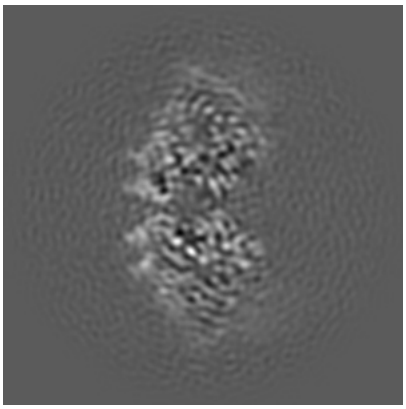


Z

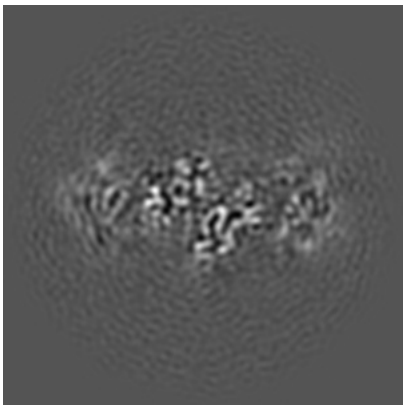
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

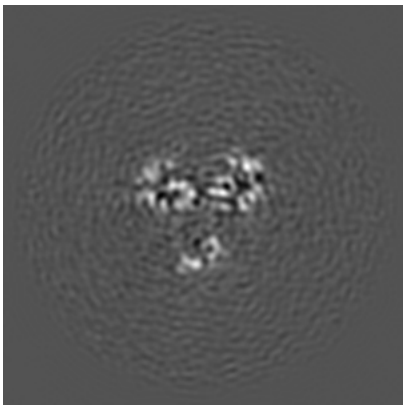
6.2.1 Primary map



X Index: 90

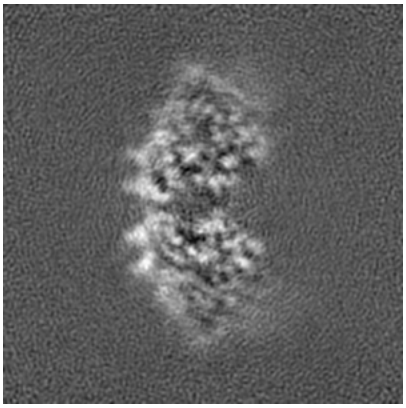


Y Index: 90

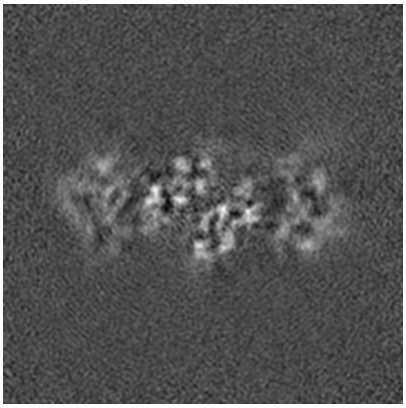


Z Index: 90

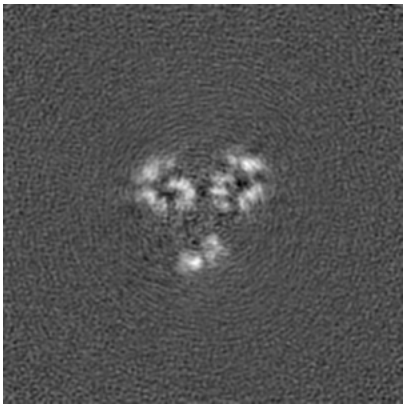
6.2.2 Raw map



X Index: 90



Y Index: 90

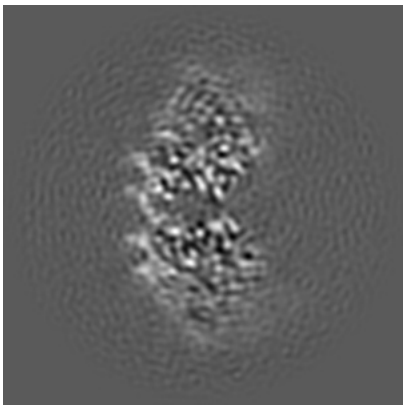


Z Index: 90

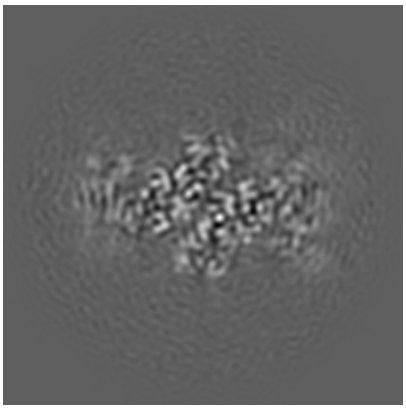
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

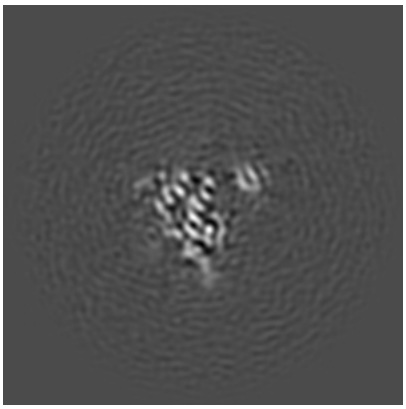
6.3.1 Primary map



X Index: 88

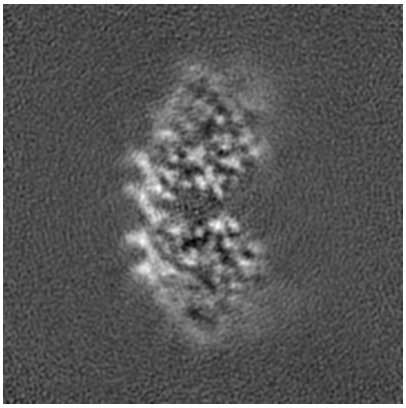


Y Index: 98

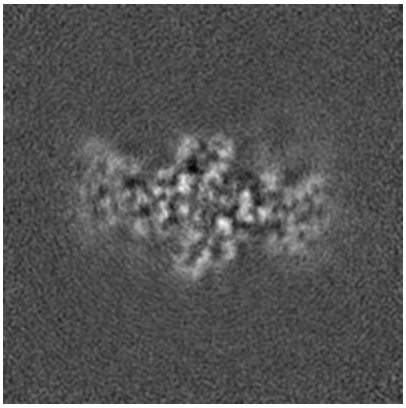


Z Index: 99

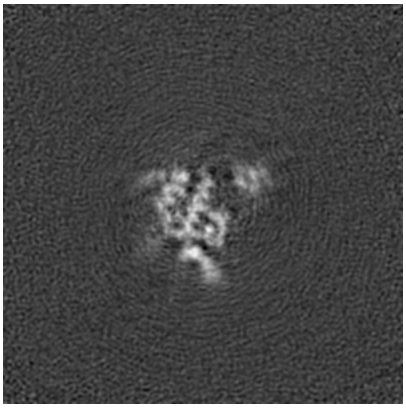
6.3.2 Raw map



X Index: 88



Y Index: 102

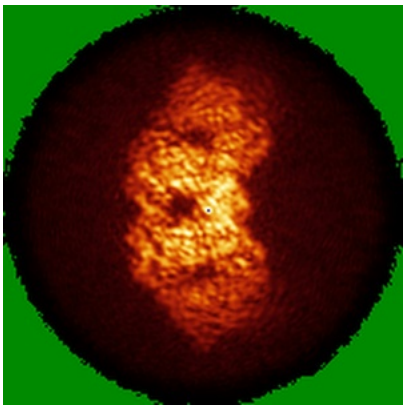


Z Index: 100

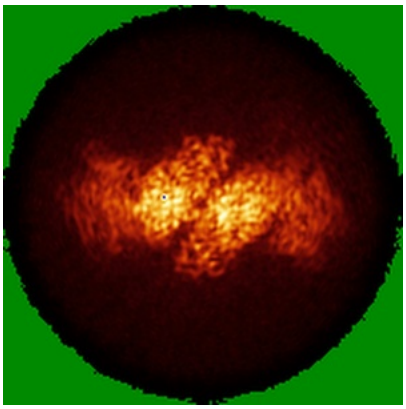
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

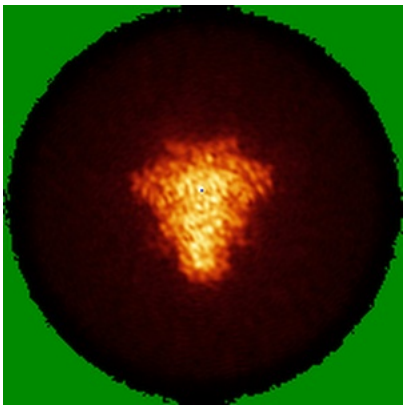
6.4.1 Primary map



X

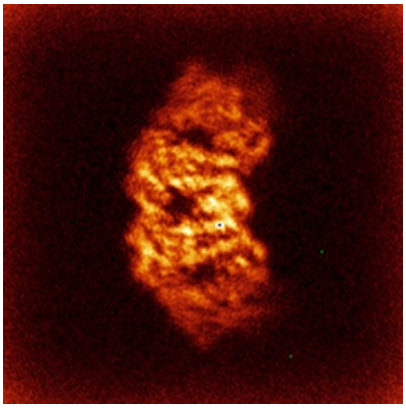


Y

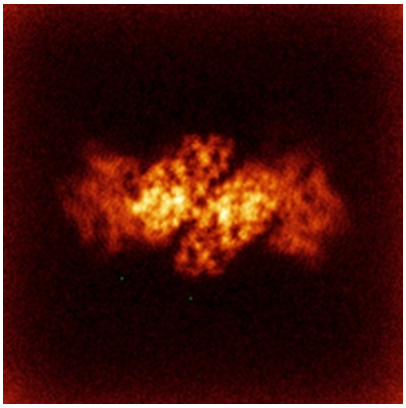


Z

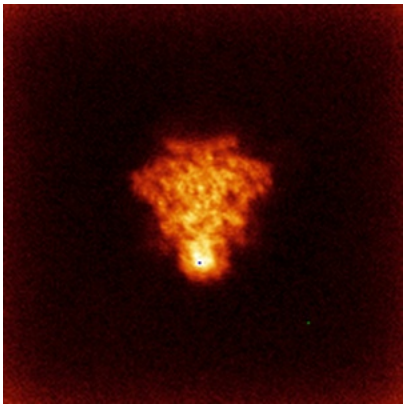
6.4.2 Raw map



X



Y

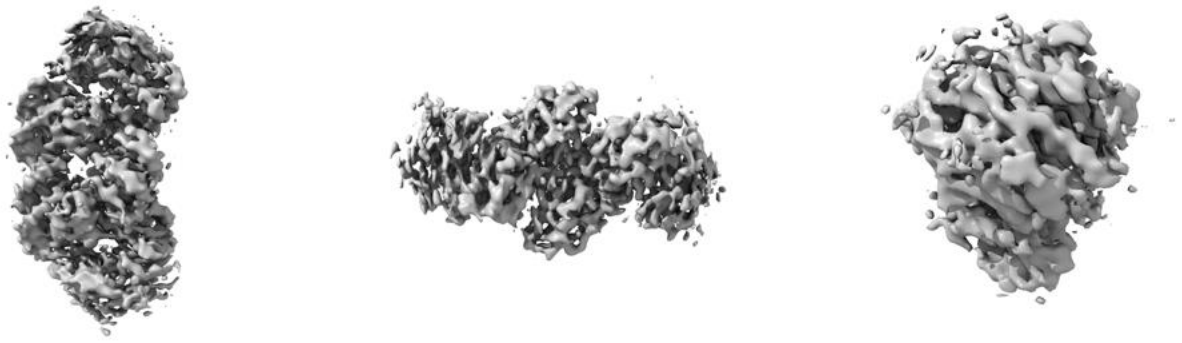


Z

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

6.5 Orthogonal surface views (i)

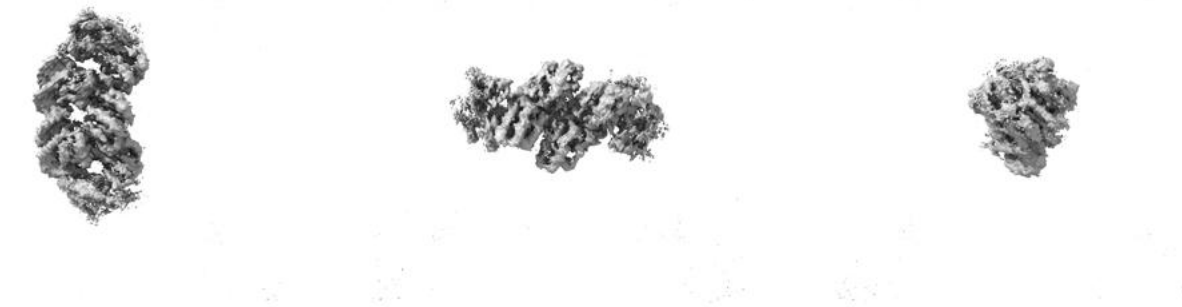
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

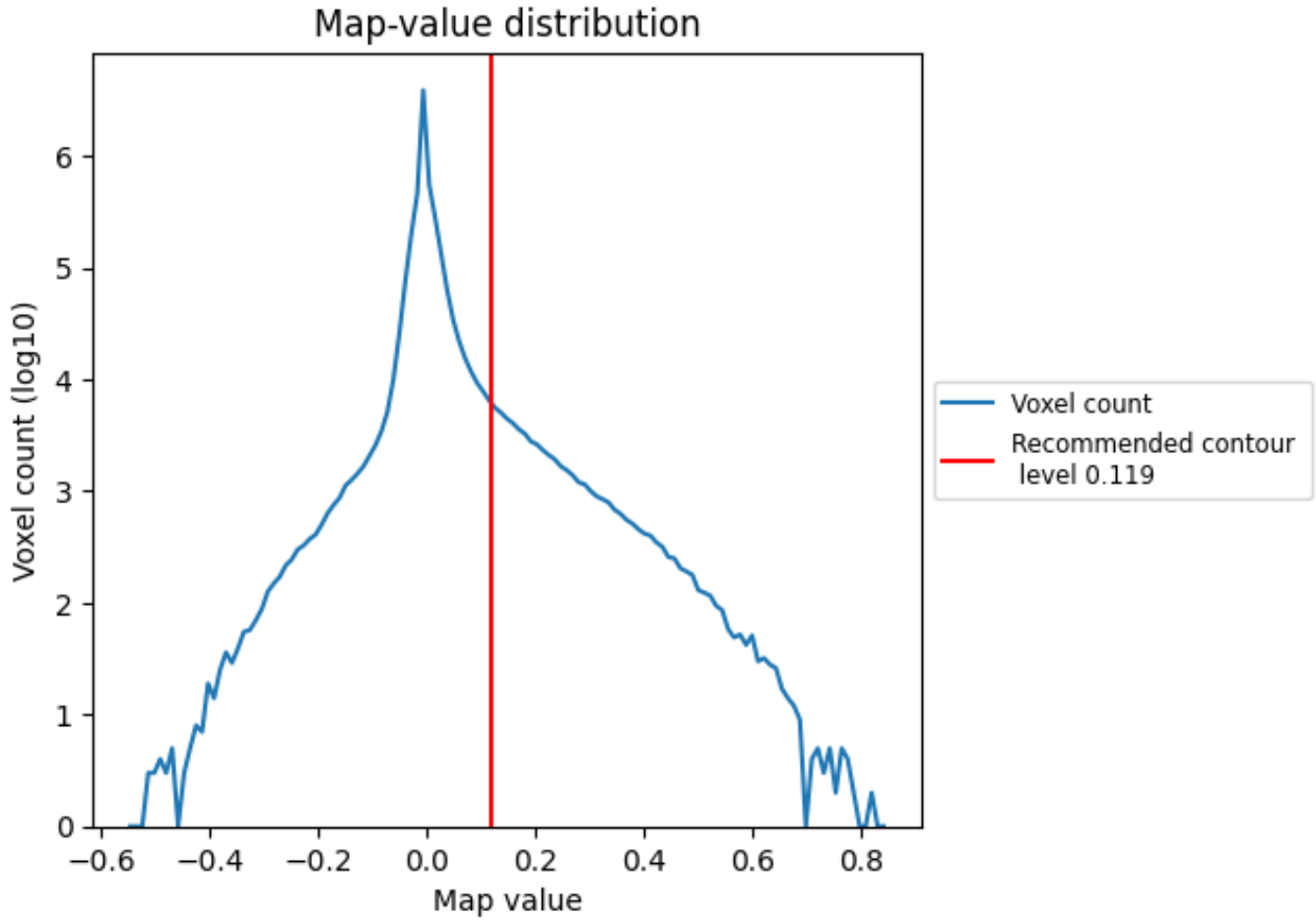
6.6 Mask visualisation (i)

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

7 Map analysis

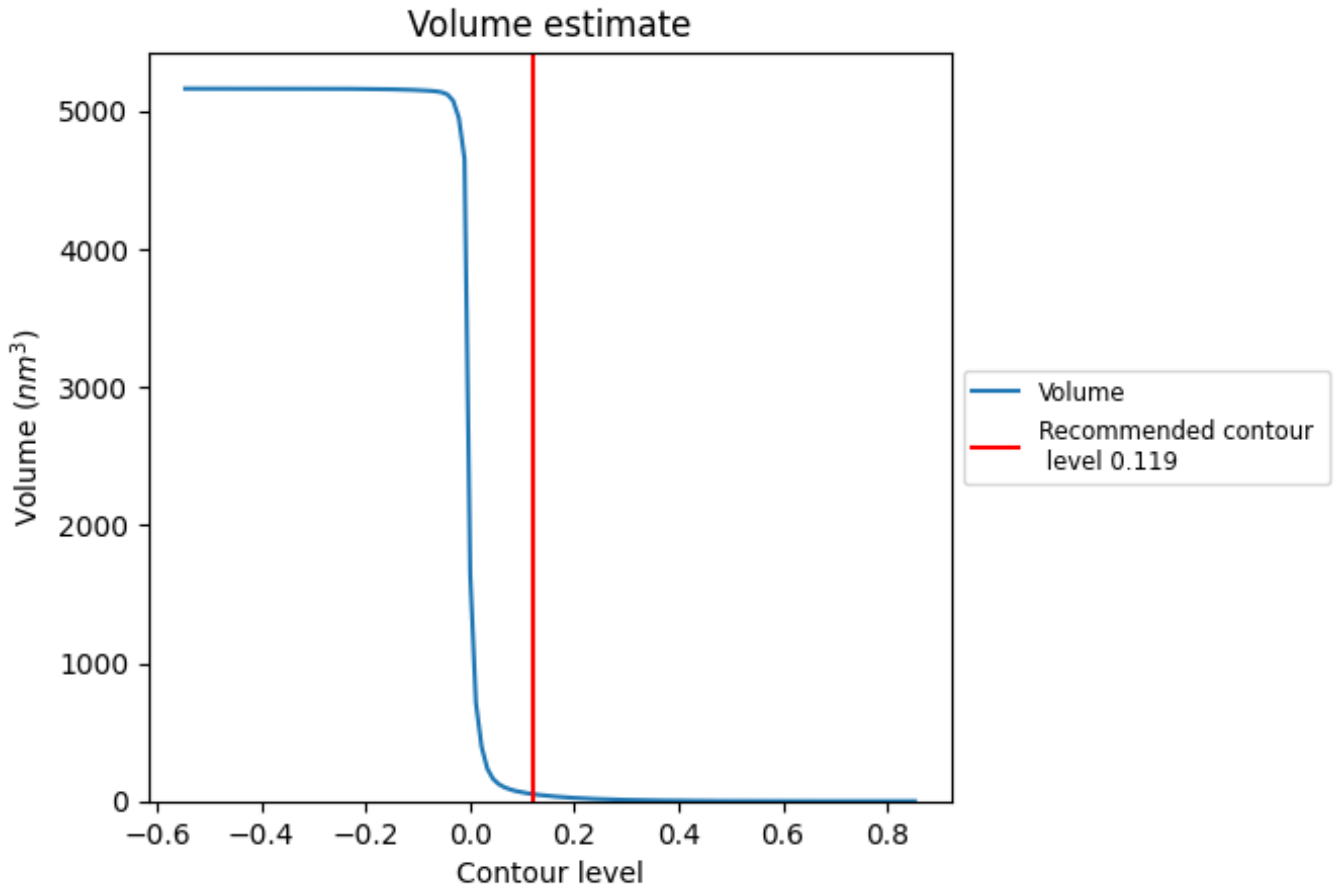
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

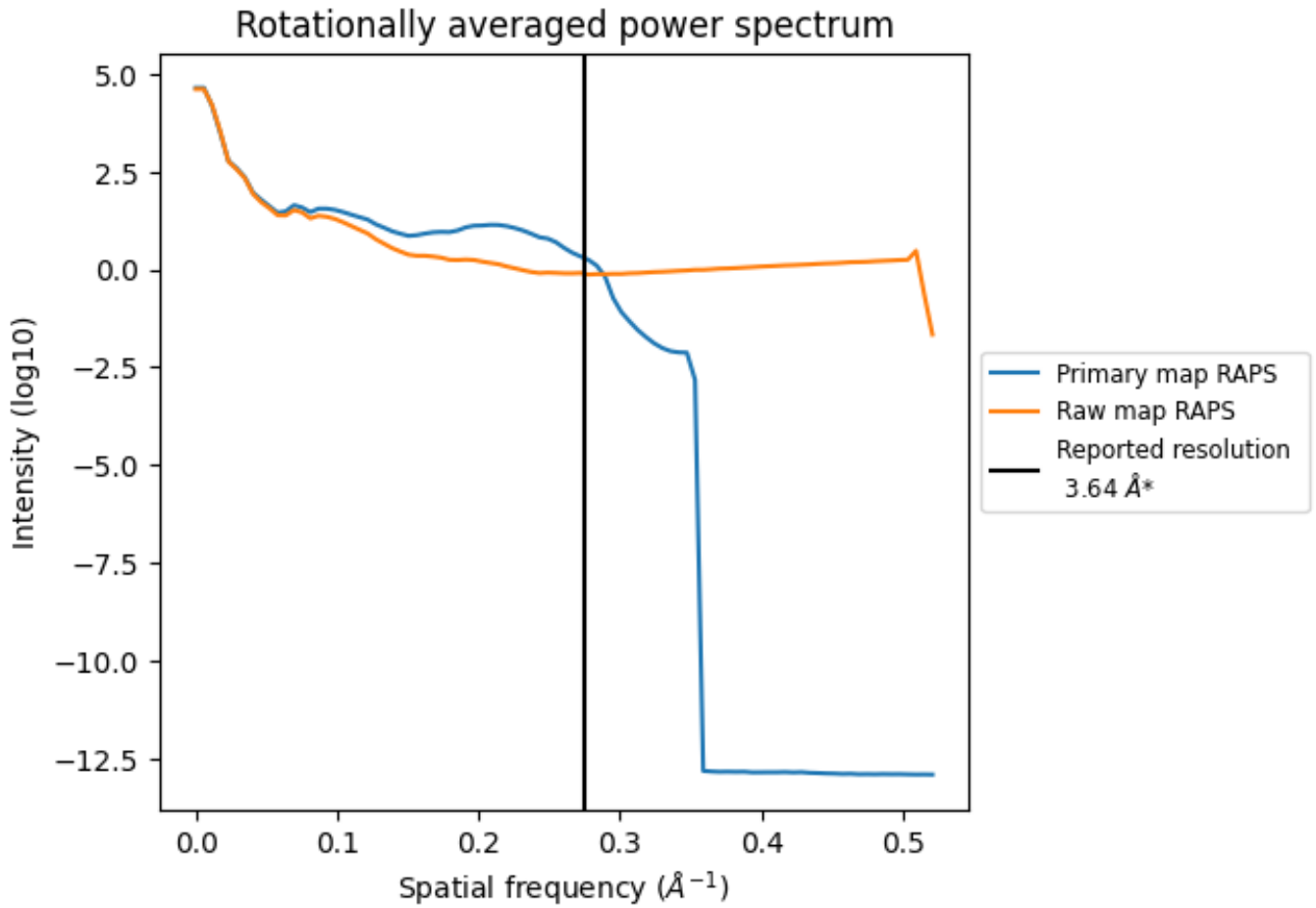
7.2 Volume estimate (i)



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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)

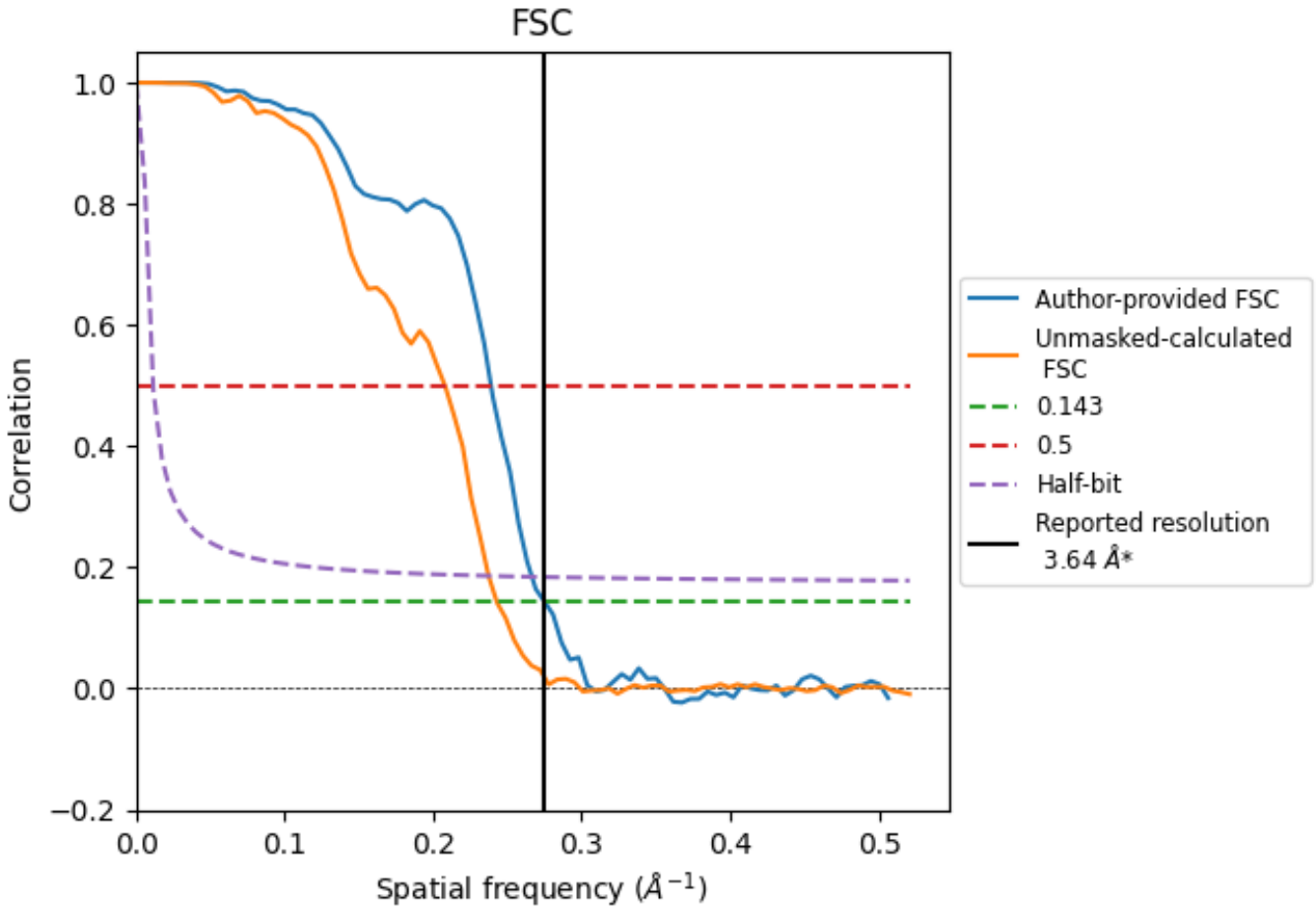


*Reported resolution corresponds to spatial frequency of 0.275 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

8.2 Resolution estimates (i)

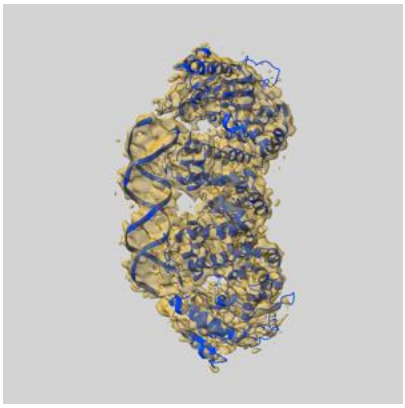
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	3.64	4.19	3.75
Unmasked-calculated*	4.12	4.81	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.64 by more than 10 %

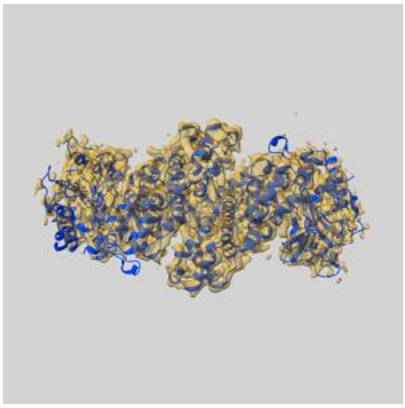
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64090 and PDB model 9UER. Per-residue inclusion information can be found in section 3 on page 6.

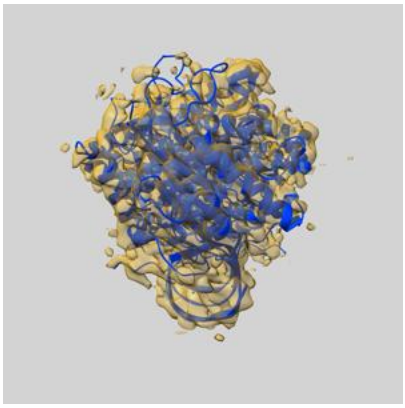
9.1 Map-model overlay



X



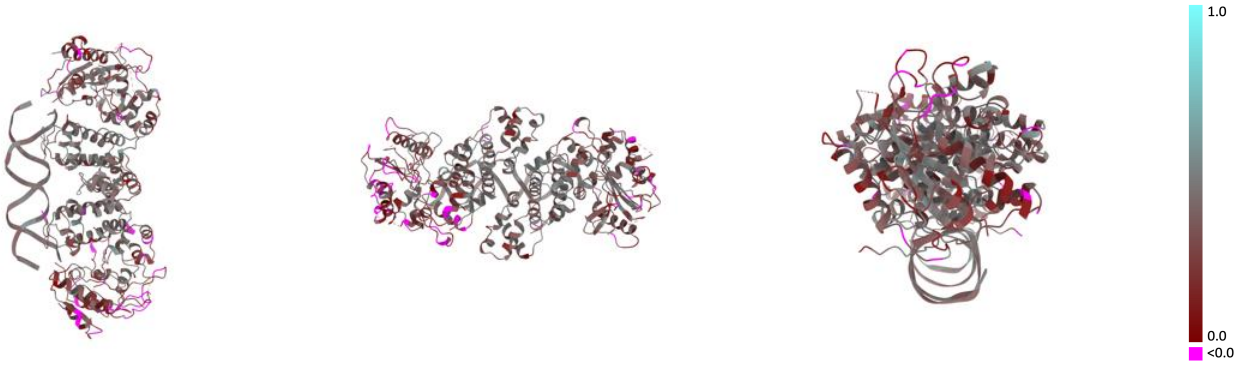
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.119 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.

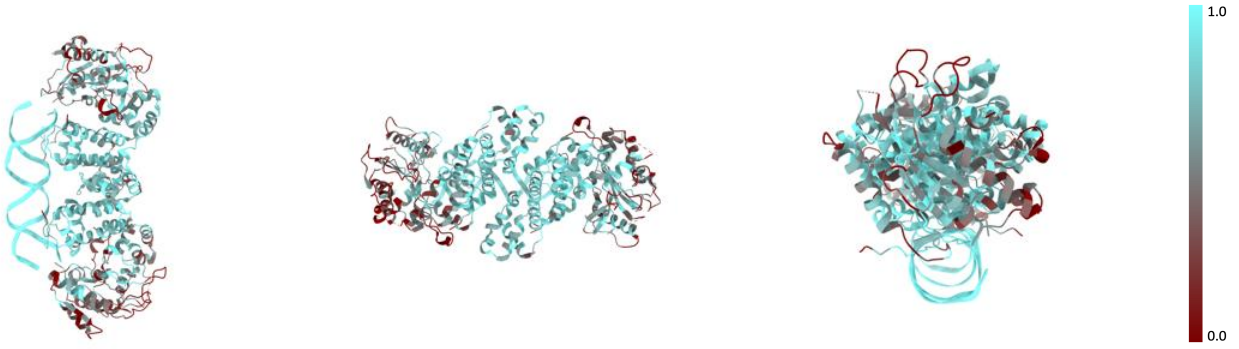
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

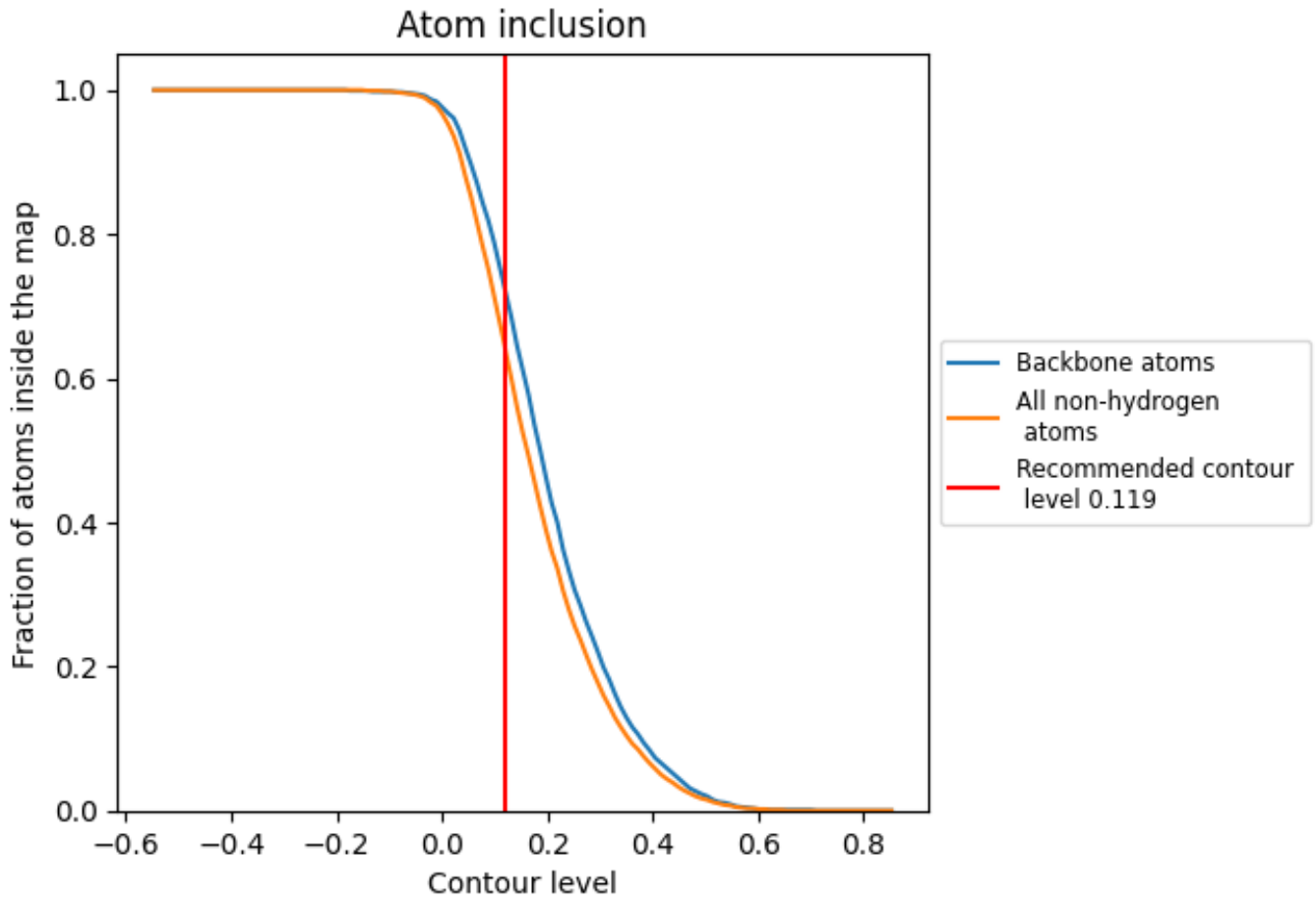
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.119).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.3310
A	0.7930	0.4050
B	0.7960	0.3930
C	0.7090	0.3400
D	0.8020	0.3950
E	0.4850	0.2860
F	0.3880	0.2220
G	0.9300	0.4020
H	0.9080	0.4170