wwPDB EM Validation Summary Report ⓘ

Mar 19, 2024 – 06:08 PM JST

PDB ID	:	6IGM
EMDB ID	:	EMD-9668
Title	:	Cryo-EM Structure of Human SRCAP Complex
Authors	:	Feng, Y.; Tian, Y.; Wu, Z.; Xu, Y.
Deposited on	:	2018-09-25
Resolution	:	4.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

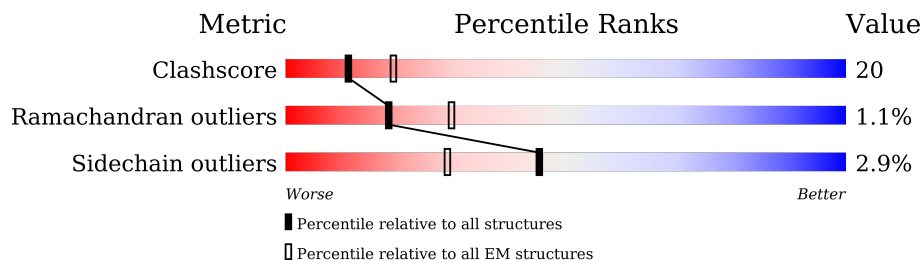|		
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Clashscore		20
Ramachandran outliers		1.1%
Sidechain outliers		2.9%

Worse   *Better*

▊ Percentile relative to all structures
▯ Percentile relative to all EM structures

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 <=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	456	12% / 65% 21% • 11%
1	C	456	16% / 66% 14% • 19%
1	E	456	14% / 68% 16% 17%
2	B	463	16% / 69% 16% • 14%
2	D	463	17% / 72% 12% • 14%
2	F	463	15% / 65% 13% • 21%
3	G	396	32% / 67% 19% •• 8%
4	H	3230	8% / 8% •• 88%

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Mol	Chain	Length	Quality of chain
5	X	62	23% / 65% / 35%

2　Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 24257 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	405	Total	C	N	O	S	0	0
			3123	1970	536	604	13		
1	C	370	Total	C	N	O	S	0	0
			2852	1801	495	544	12		
1	E	380	Total	C	N	O	S	0	0
			2935	1857	503	564	11		

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	398	Total	C	N	O	S	0	0
			3090	1931	540	604	15		
2	D	396	Total	C	N	O	S	0	0
			3078	1927	540	597	14		
2	F	366	Total	C	N	O	S	0	0
			2852	1785	501	553	13		

- Molecule 3 is a protein called Actin-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	366	Total	C	N	O	S	0	0
			2987	1913	489	569	16		

- Molecule 4 is a protein called Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	373	Total	C	N	O	S	0	0
			3030	1925	559	525	21		

- Molecule 5 is a protein called unknown subunit.

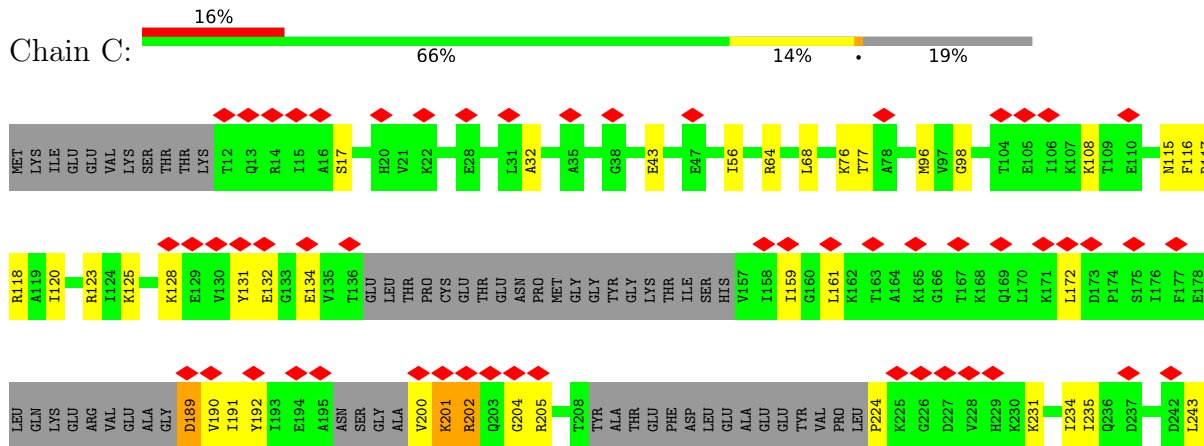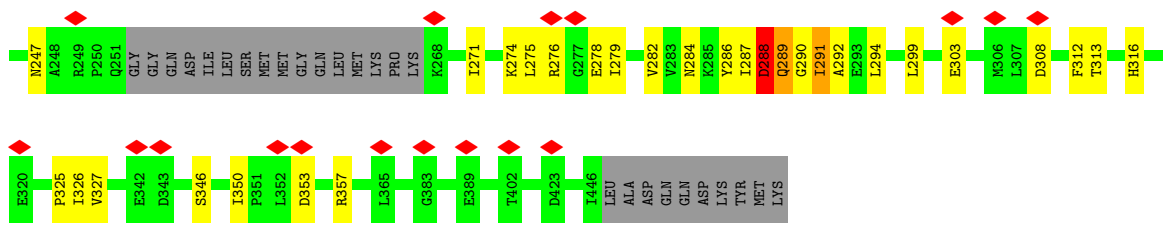| Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	X	62	310	186	62	62	0	0

3   Residue-property plots ⓘ

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.
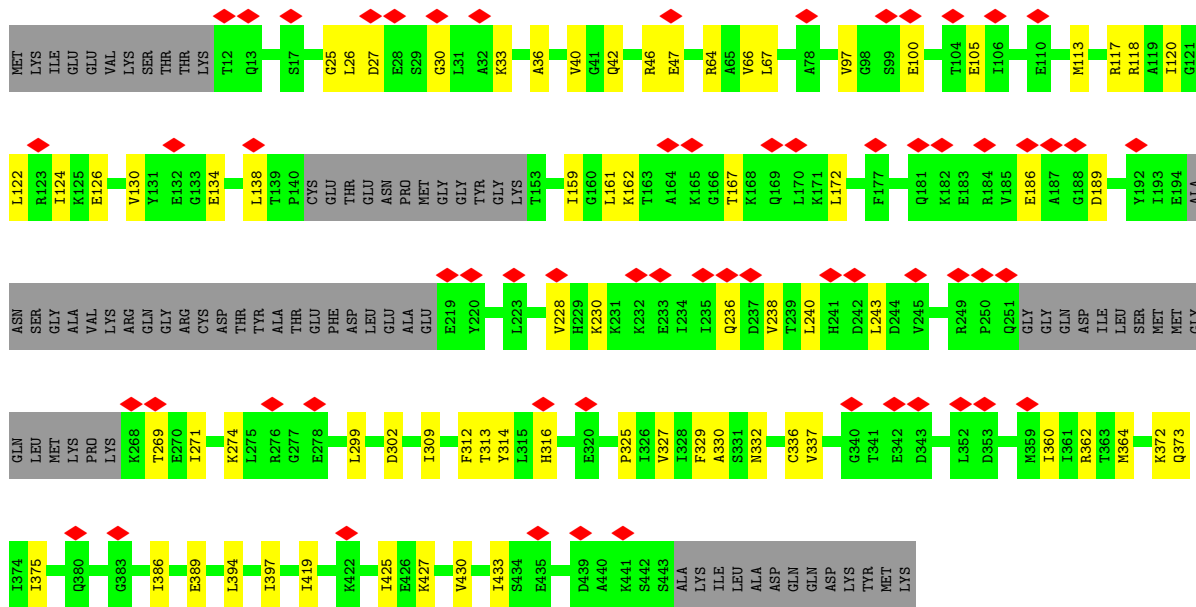
- Molecule 1: RuvB-like 1

- Molecule 1: RuvB-like 1
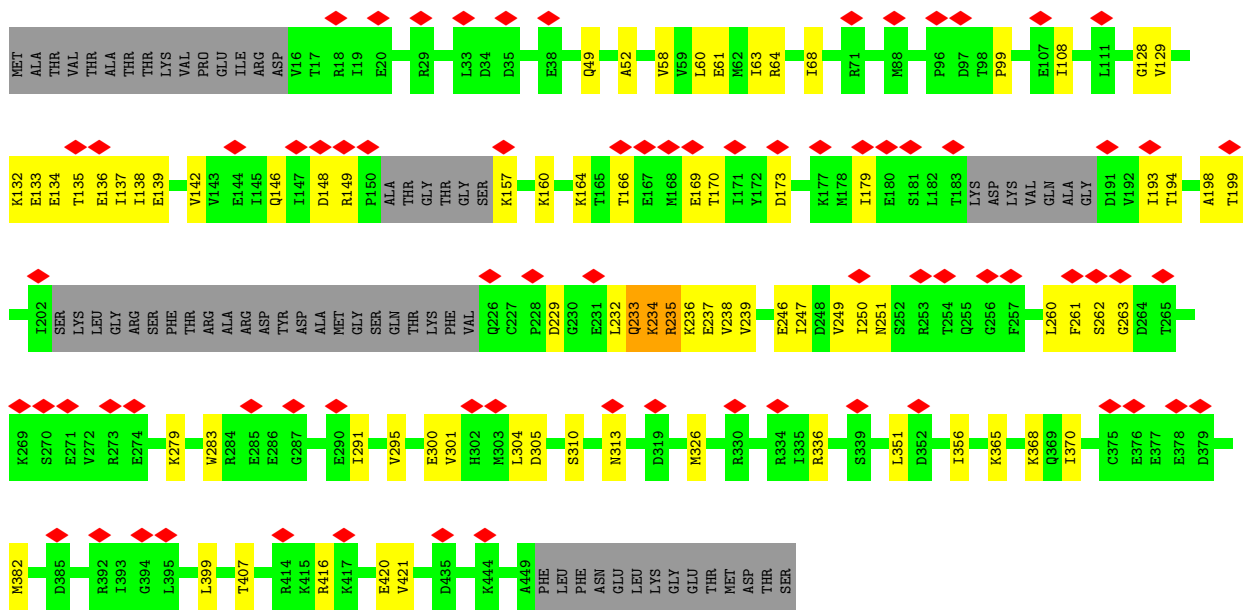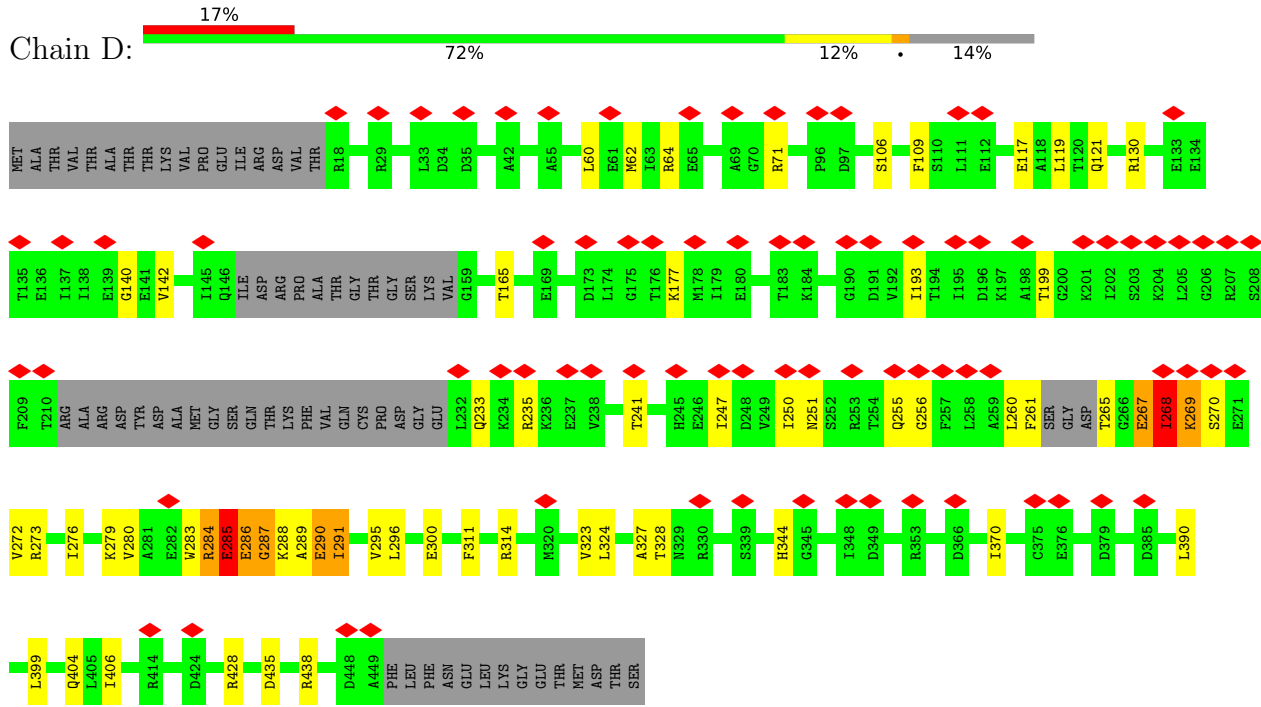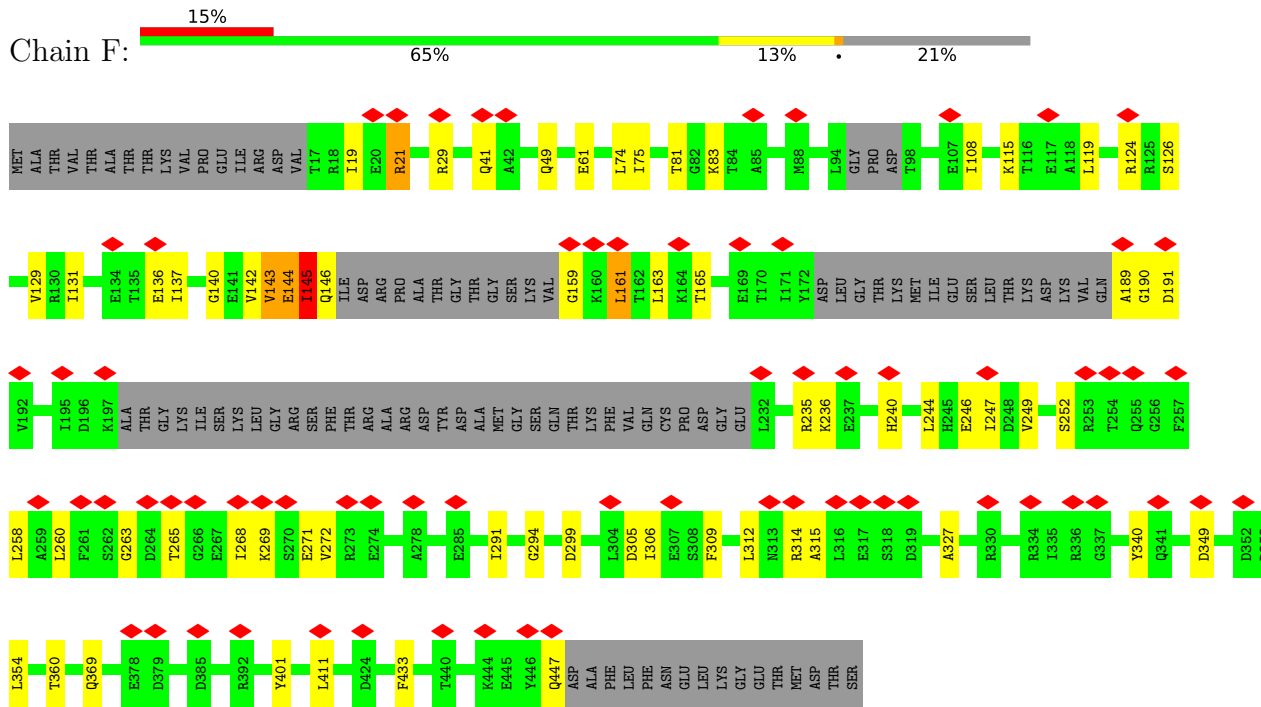
• Molecule 1: RuvB-like 1

Chain E:

• Molecule 2: RuvB-like 2

Chain B:

● Molecule 2: RuvB-like 2

Chain D:

● Molecule 2: RuvB-like 2

Chain F:

● Molecule 3: Actin-related protein 6

Chain G:

• Molecule 4: Helicase SRCAP

Chain H:

CYS ILE THR SER TYR LYS LEU VAL LEU LEU GLN ASP HIS GLN ALA PHE ARG ARG LYS ASN TRP ARG TYR LEU ILE LEU LEU ASP GLU ALA GLN ASN ILE LYS ASN PHE LYS SER GLN ARG TRP GLN SER LEU LEU ASN PHE ASN SER GLN ARG ARG LEU LEU LEU THR GLY THR PRO LEU GLN ASN

SER LEU MET GLU LEU TRP SER LEU MET HIS PHE LEU MET PRO HIS VAL PHE GLN SER HIS ARG GLU GLU PHE LYS GLU TRP PHE SER ASN PRO LEU GLU THR GLY MET ILE GLU GLU GLY LEU SER GLU GLU TYR ASN GLU GLN GLY LEU VAL LYS ARG LEU GLU HIS LYS VAL LEU GLU ARG PRO PHE LEU LEU GLU ARG ARG

VAL LYS VAL ASP VAL GLU LYS GLN MET PRO **K851** **K852** **Y853** **E854** **H855** **V856** **I857** **R858** **C859** **R860** **L861** **S862** **K863** **R864** **Q865** **R866** **C867** **L868** **Y869** **D870** **D871** **F872** **M873** **A874** GLN THR THR THR LYS GLU THR LEU ALA THR GLY HIS PHE MET SER VAL ILE ASN **I893** **L894** **M895** **Q896** **L897** **R898** **K899** **V900**

C901 **N902** **N905** **L906** **F907** **D908** **P909** **R910** **P911** **V912** **T913** **S914** **P915** **F916** **I917** **T918** **P919** **G920** **I921** **C922** **F923** **L928** **T933** **D934** **V935** **H936** **P937** **L938** **Q939** **R940** **I941** **D942** **M943** **G944** **R945** **F946** **D947** **L948** **I949** **G950** **L951** **E952** **G953** **R954** **R957** **Y958** **E959** **A960** **F963** **L964** **P965** **R966** **H967** **R968** **L969**

S970 **R971** **R972** **V973** **L974** LEU GLU VAL ALA THR PRO ASP PRO PRO ARG PRO LYS PRO VAL LYS MET LYS VAL ASN ARG MET LEU GLN PRO VAL PRO LYS PRO VAL PRO LYS PRO GLY SER ARG PRO ALA GLY PRO ARG ALA THR VAL VAL ASN VAL ASN PRO ARG ALA PRO ALA PRO LEU ILE ALA SER ARG ALA PRO LEU GLN PRO ASN ALA SER SER GLY SER LEU ASN SER SER GLY SER LEU PRO GLN VAL LEU LEU PRO GLN VAL LEU

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LEU GLY VAL LEU SER GLY THR THR SER ARG PRO PRO THR PRO THR LEU SER LEU LYS PRO THR PRO PRO ALA PRO VAL ARG LEU SER PRO ALA PRO PRO LEU PRO PRO GLY SER GLU SER ARG SER LEU GLN LEU LEU LYS PRO LEU THR VAL PRO PRO GLY TYR THR PHE PRO PRO ALA ALA THR THR SER THR

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GLN ILE GLN GLY ASN LYS SER LEU LEU THR LEU GLY ALA GLN GLY VAL ARG GLN LEU ALA VAL GLY PRO ARG PRO GLN LEU SER PRO ASP MET GLN ALA ARG LEU PRO SER GLY GLU GLU VAL HIS LEU VAL SER ALA GLY VAL VAL SER ILE GLY GLN LEU ALA SER GLN ALA HIS VAL ALA LEU ILE GLN ALA VAL ALA PRO THR PRO GLY PRO

THR PRO VAL SER VAL LEU PRO SER SER THR PRO SER THR THR PRO ALA PRO THR GLY LEU LEU PRO LEU LEU ALA ALA ASN GLN VAL PRO PRO THR MET VAL ASN ASN THR GLY VAL VAL LYS ILE VAL LEU VAL ARG GLN GLN ALA HIS VAL ALA LEU ILE GLN ALA VAL ALA ARG GLY ASP GLY LEU THR PRO VAL PRO LEU ALA PRO

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VAL LEU GLU SER CYS GLY LEU GLY ARG ARG GLN PRO GLN GLY GLN GLY GLU SER GLU GLY SER SER ASP GLU ASP GLY SER SER ARG PRO LEU THR ARG LEU ALA LEU ARG LEU ARG GLU GLU ALA GLU GLU ALA GLY MET ARG GLY ARG LYS SER GLY GLY SER SER MET VAL VAL ALA VAL ILE GLN

ASP ASP LEU ASP LEU ALA ASP SER GLY PRO GLY GLY LEU GLU LEU THR PRO PRO VAL VAL SER LEU THR PRO LYS LEU ARG SER THR ARG LEU ARG PRO GLY SER LEU VAL PRO LEU GLU THR GLU LYS LEU PRO ARG LYS ARG ALA ALA PRO VAL GLY GLY PRO GLY LEU

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ALA PRO PRO SER LEU ALA GLY PRO ALA VAL SER HIS ARG GLY ARG LYS ALA LYS THR

• Molecule 5: unknown subunit

Chain X:

23% 65% 35%

X1 X4 X5 X6 X9 X10 X11 X12 X13 X14 X15 X16 X17 X18 X19 X20 X21 X22 X25 X26 X27 X28 X29 X30 X31 X32 X33 X39 X47 X48 X49 X50 X51 X52 X55 X56 X57 X58 X59 X60 X61 X62

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130318	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 $(e^-/\text{Å}^2)$	1.5625	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	0.269	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.058	Depositor
Map size (Å)	432.0, 432.0, 432.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	0.28	1/3163 (0.0%)	0.54	2/4266 (0.0%)
1	C	0.25	0/2883	0.48	0/3878
1	E	0.25	0/2972	0.51	1/4008 (0.0%)
2	B	0.25	0/3122	0.51	1/4203 (0.0%)
2	D	0.25	0/3109	0.49	0/4180
2	F	0.25	0/2880	0.51	1/3873 (0.0%)
3	G	0.32	1/3055 (0.0%)	0.57	4/4141 (0.1%)
4	H	0.26	0/3098	0.50	2/4191 (0.0%)
All	All	0.26	2/24282 (0.0%)	0.51	11/32740 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	PRO	N-CD	5.03	1.54	1.47
3	G	306	PRO	N-CD	5.03	1.54	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	50	ASP	C-N-CD	6.29	141.61	128.40
1	A	173	ASP	C-N-CD	5.81	140.59	128.40
3	G	305	LEU	C-N-CD	5.78	140.54	128.40
2	F	161	LEU	CA-CB-CG	5.60	128.17	115.30
2	B	146	GLN	CA-CB-CG	5.29	125.04	113.40

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	A	3123	0	3214	205	0
1	C	2852	0	2968	95	0
1	E	2935	0	3043	70	0
2	B	3090	0	3163	104	0
2	D	3078	0	3159	65	0
2	F	2852	0	2922	60	0
3	G	2987	0	2905	250	0
4	H	3030	0	3058	247	0
5	X	310	0	74	51	0
All	All	24257	0	24506	989	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 20.

The worst 5 of 989 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:198:ALA:HB1	4:H:1998:TRP:CE2	1.35	1.57
3:G:306:PRO:CA	3:G:309:MET:HB2	1.25	1.55
1:A:124:ILE:CG2	1:A:292:ALA:CA	1.87	1.49
3:G:30:PHE:HB2	3:G:47:GLU:CG	1.02	1.48
3:G:30:PHE:HB2	3:G:47:GLU:CD	1.20	1.48

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	399/456 (88%)	365 (92%)	29 (7%)	5 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	358/456 (78%)	330 (92%)	25 (7%)	3 (1%)	19	58
1	E	372/456 (82%)	346 (93%)	26 (7%)	0	100	100
2	B	390/463 (84%)	370 (95%)	20 (5%)	0	100	100
2	D	388/463 (84%)	370 (95%)	13 (3%)	5 (1%)	12	48
2	F	356/463 (77%)	330 (93%)	24 (7%)	2 (1%)	25	63
3	G	362/396 (91%)	311 (86%)	42 (12%)	9 (2%)	5	35
4	H	363/3230 (11%)	316 (87%)	38 (10%)	9 (2%)	5	35
All	All	2988/6383 (47%)	2738 (92%)	217 (7%)	33 (1%)	18	51

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	SER
1	A	176	ILE
1	C	288	ASP
1	C	291	ILE
2	D	286	GLU

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	343/387 (89%)	334 (97%)	9 (3%)	46	67
1	C	314/387 (81%)	308 (98%)	6 (2%)	57	75
1	E	325/387 (84%)	325 (100%)	0	100	100
2	B	337/390 (86%)	334 (99%)	3 (1%)	78	88
2	D	334/390 (86%)	326 (98%)	8 (2%)	49	69
2	F	309/390 (79%)	305 (99%)	4 (1%)	69	82
3	G	334/361 (92%)	316 (95%)	18 (5%)	22	50
4	H	333/2721 (12%)	304 (91%)	29 (9%)	10	35
All	All	2629/5413 (49%)	2552 (97%)	77 (3%)	45	65

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	946	PHE
4	H	2025	VAL
4	H	949	ILE
4	H	1978	PHE
4	H	2032	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	903	HIS
4	H	1991	HIS
4	H	2153	HIS
4	H	2022	HIS
1	E	42	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 monosaccharides 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-9668. 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 ⓘ

6.1.1 Primary map

| X | Y | Z |
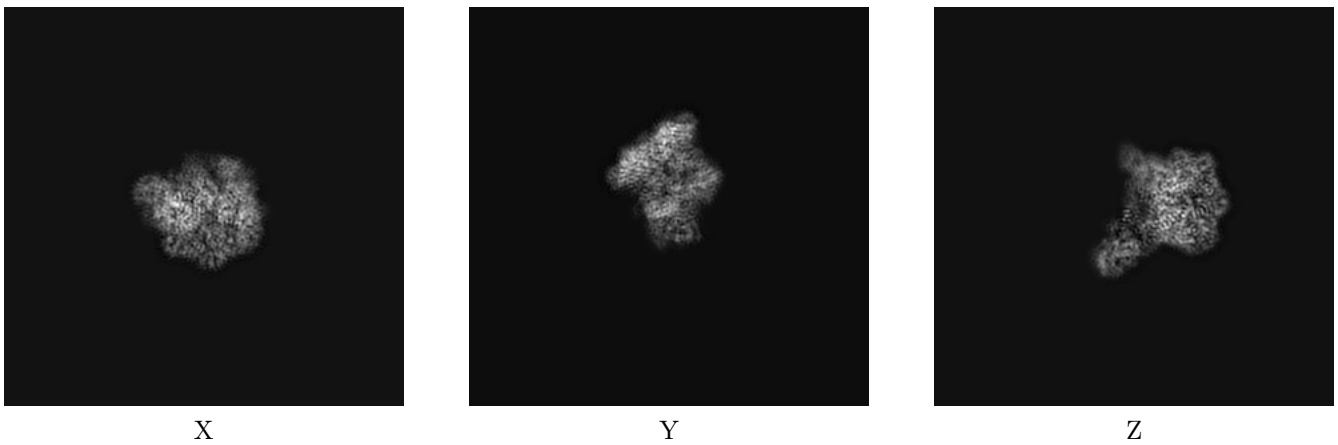
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 160 | Y Index: 160 | Z Index: 160 |
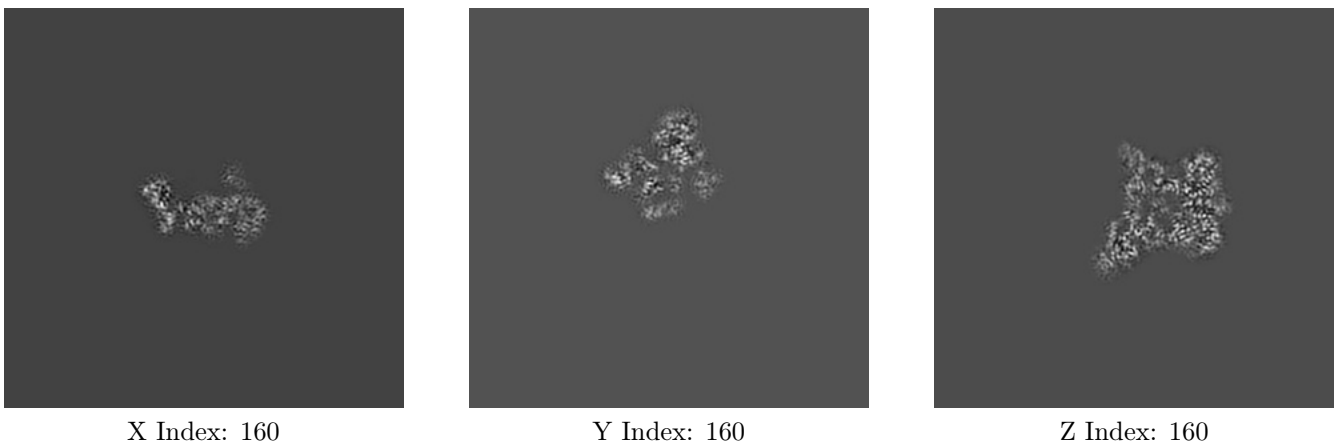
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
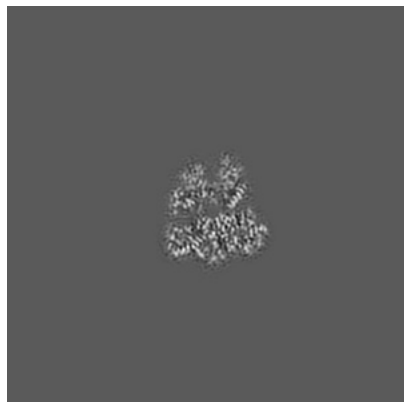
6.3.1 Primary map
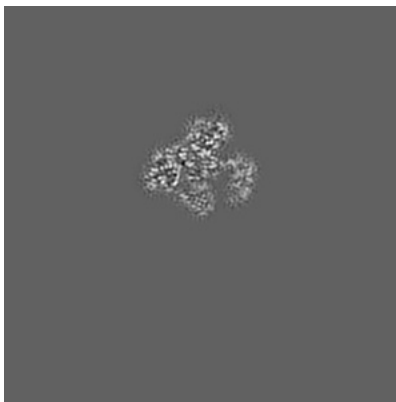
| X Index: 193 | Y Index: 175 | Z Index: 166 |
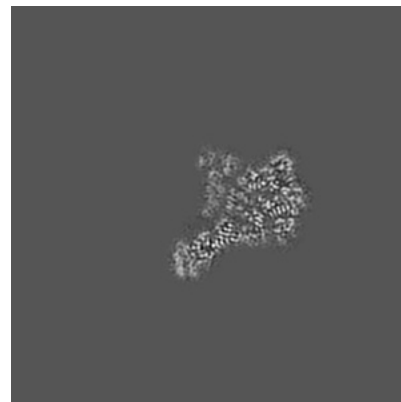
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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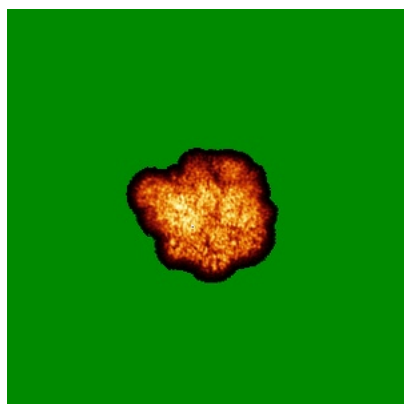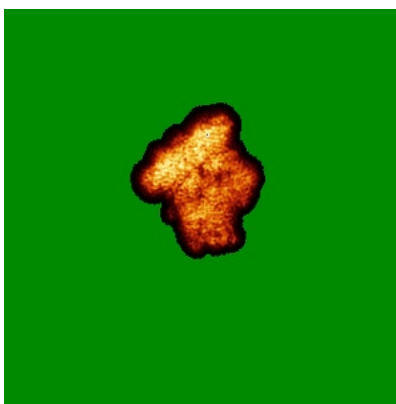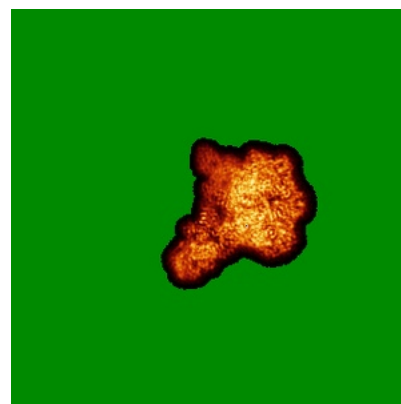
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views ⓘ

6.5.1   Primary map

X   Y   Z
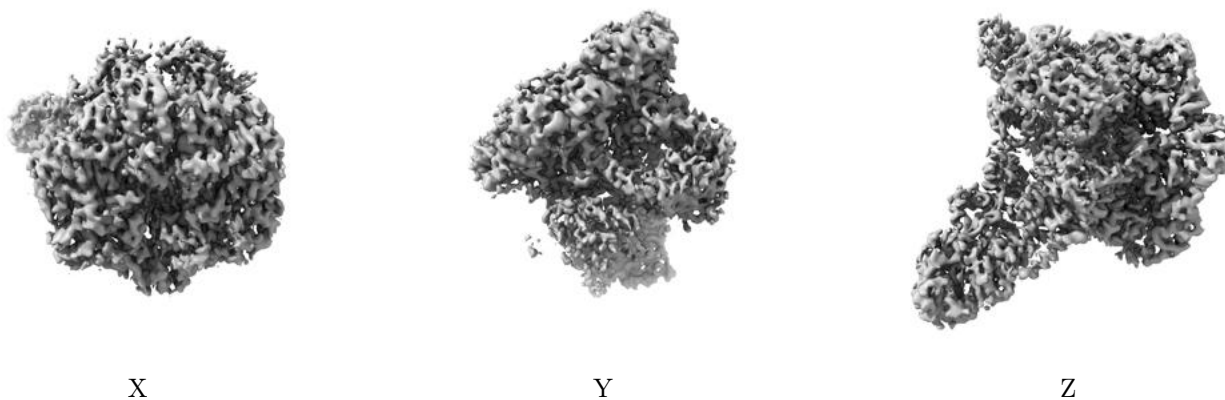
The images above show the 3D surface view of the map at the recommended contour level 0.058. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6   Mask visualisation ⓘ

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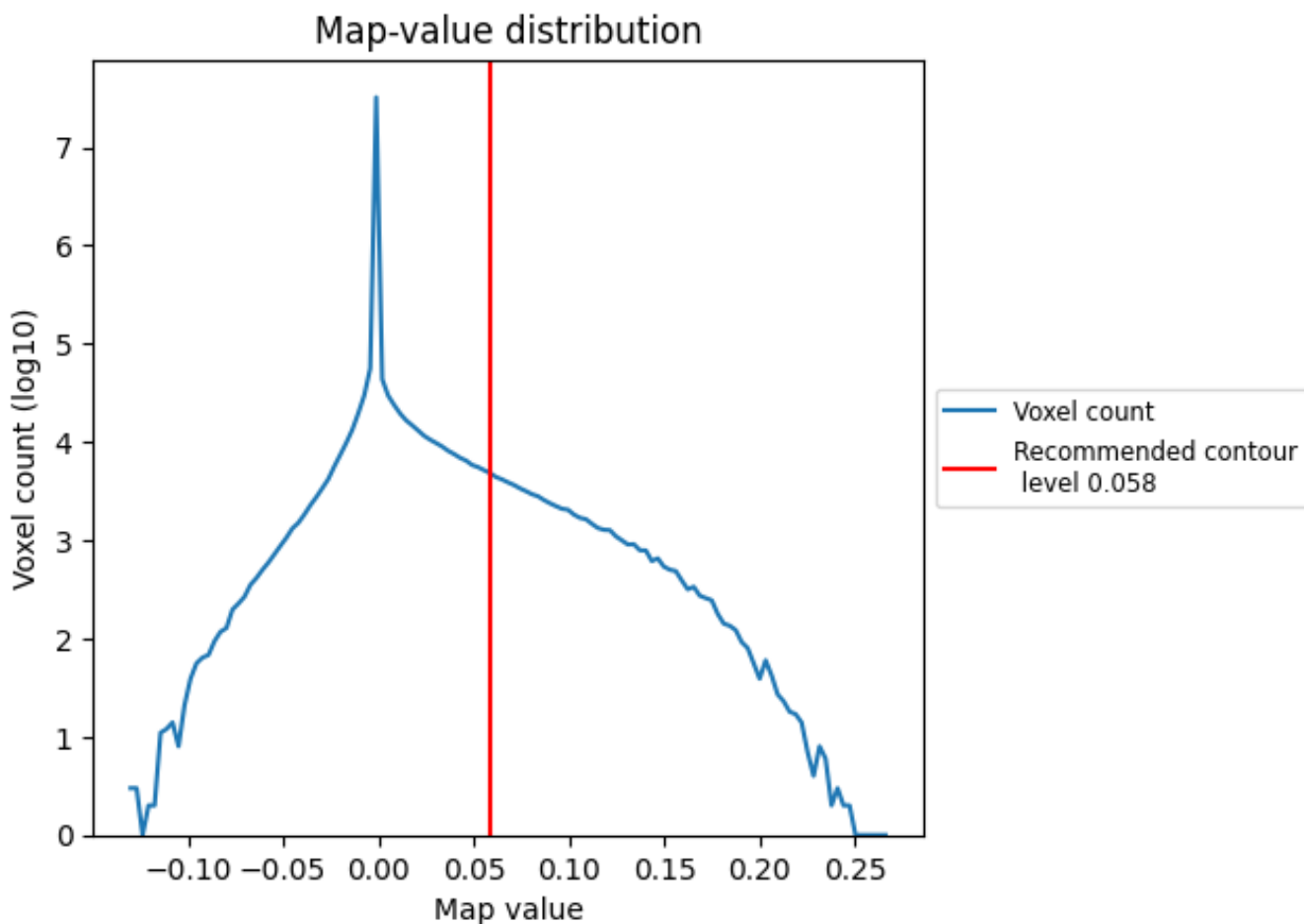
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
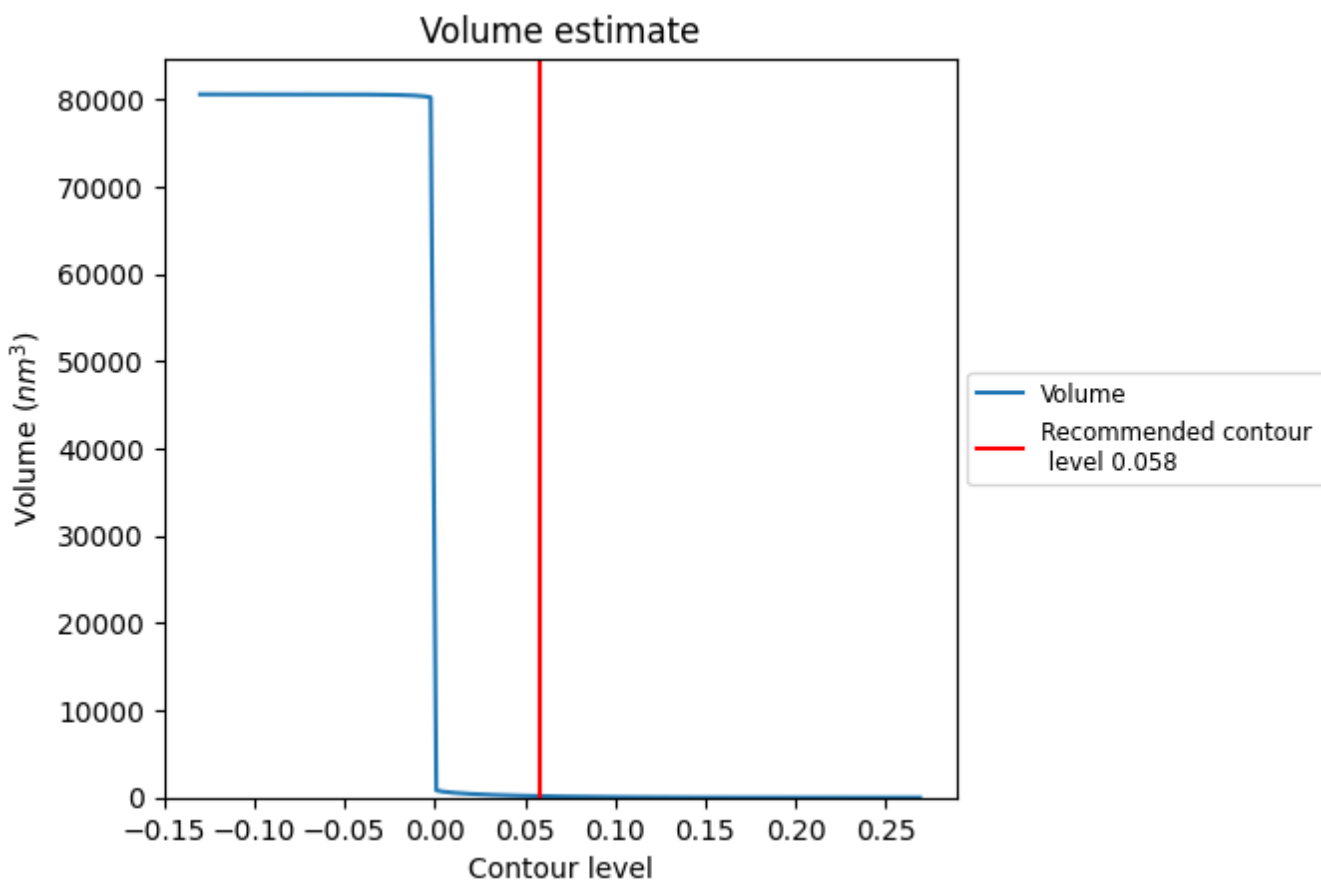
The volume at the recommended contour level is 165 nm^3; this corresponds to an approximate mass of 149 kDa.

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 ⓘ
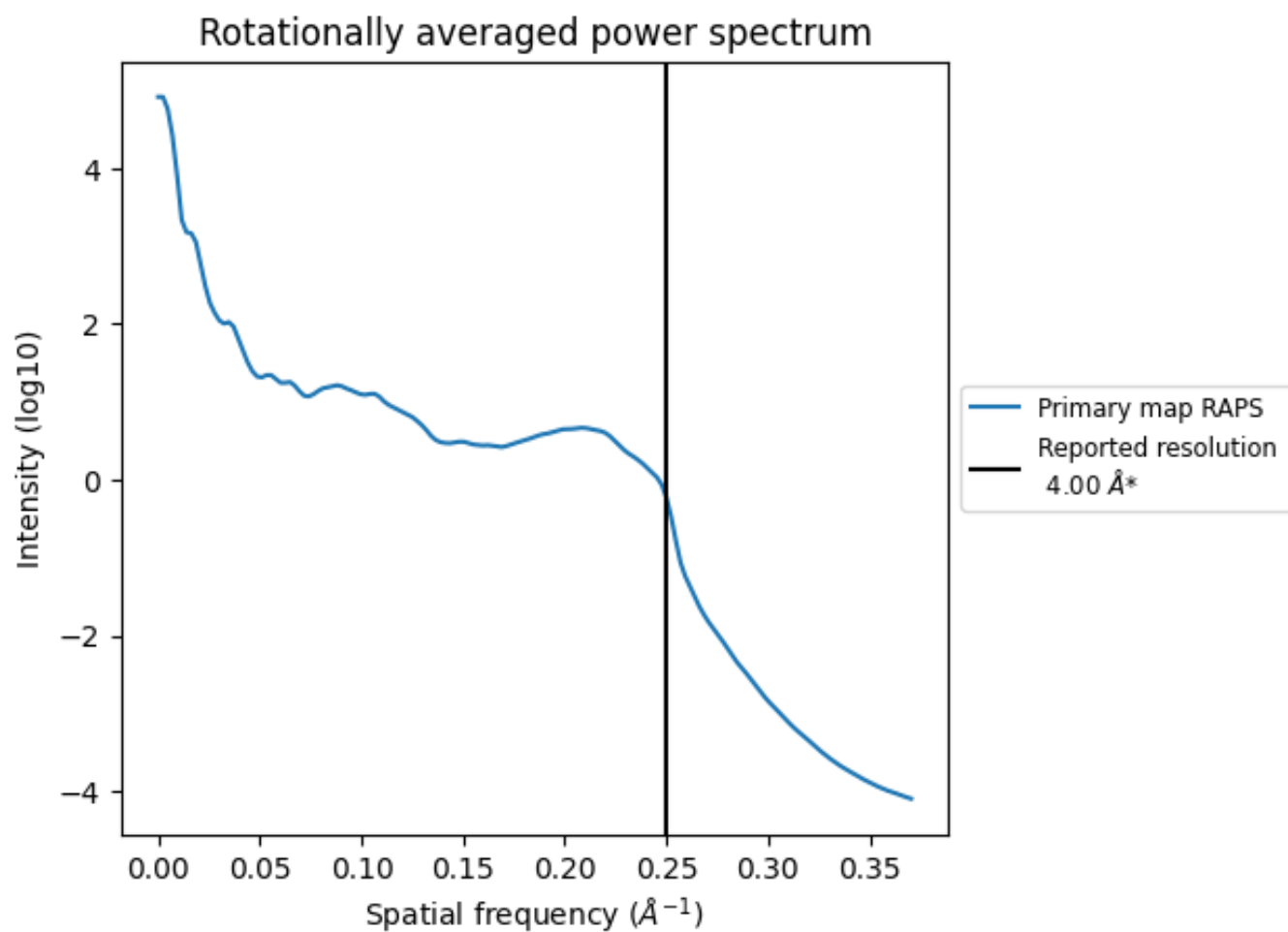
*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9668 and PDB model 6IGM. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

| X | Y | Z |
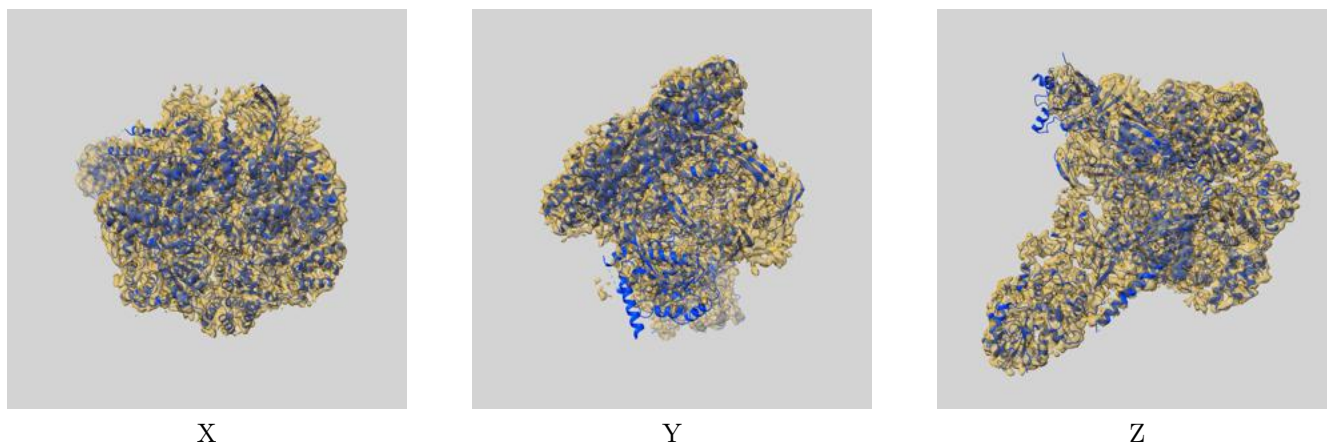
The images above show the 3D surface view of the map at the recommended contour level 0.058 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ
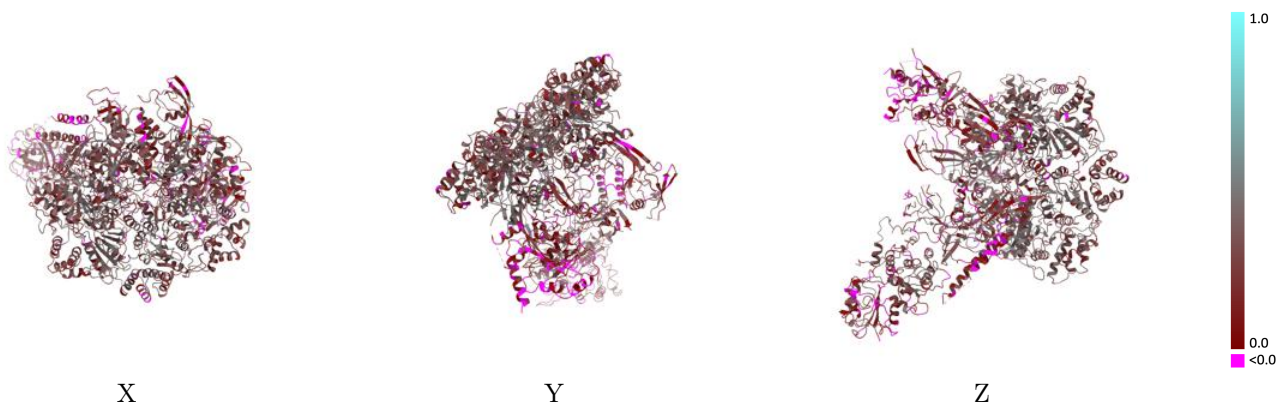
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
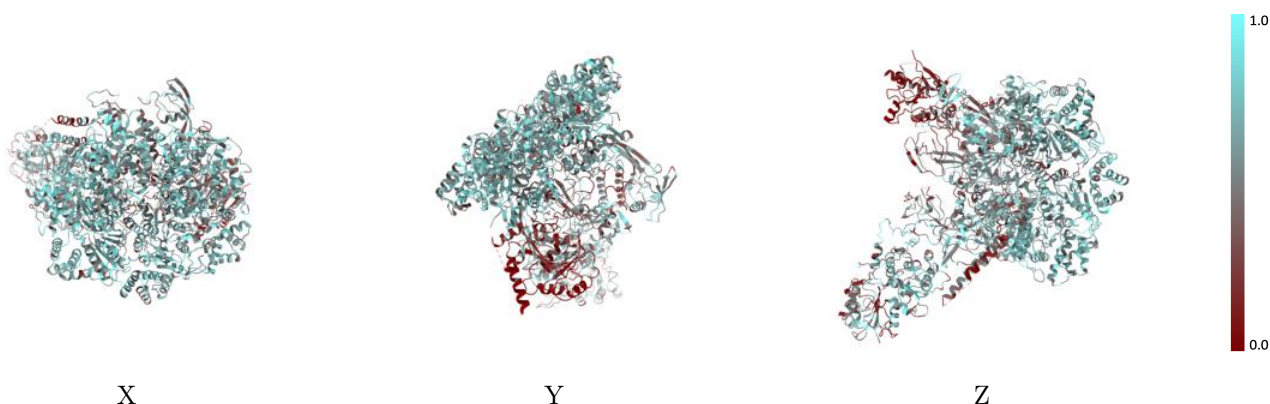
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.058).

9.4   Atom inclusion ⓘ
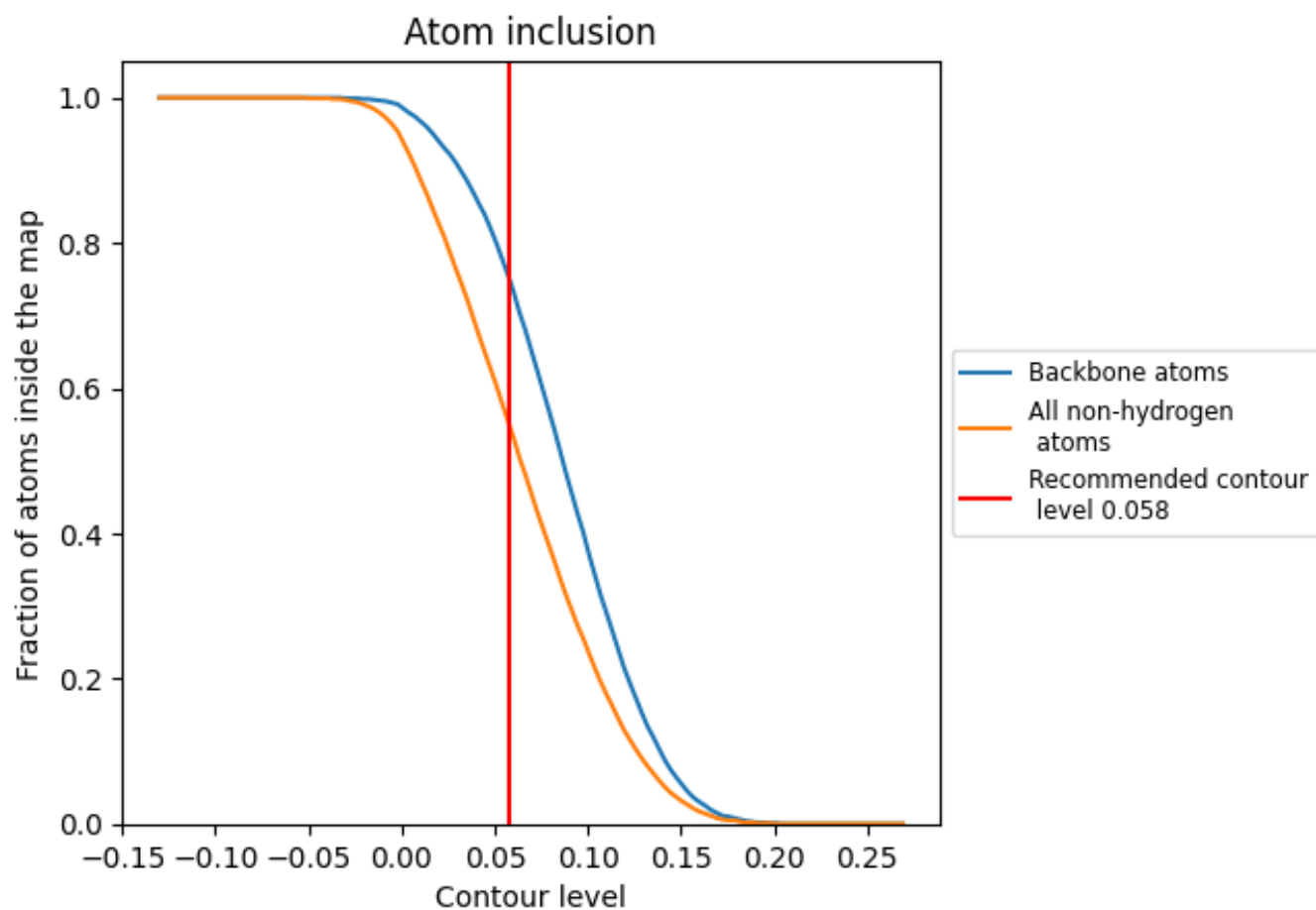
At the recommended contour level, 75% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.058) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.2530
A	0.6250	0.2990
B	0.5960	0.2870
C	0.5840	0.2840
D	0.5850	0.2860
E	0.6040	0.2760
F	0.6130	0.2770
G	0.4930	0.1930
H	0.2670	0.1140
X	0.6900	0.3310

1.0

0.0
<0.0