W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 10:35 am GMT

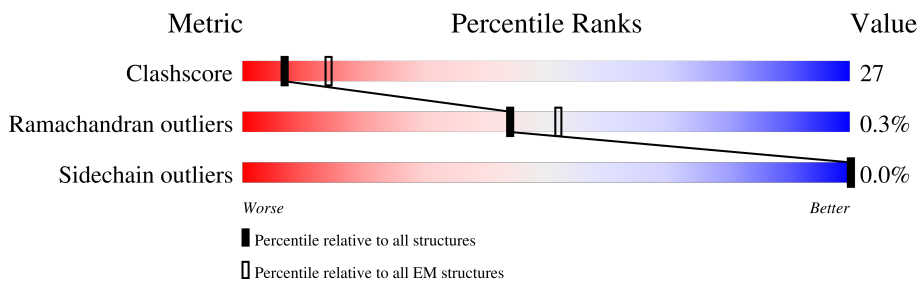|		
PDB ID	:	5M0R
EMDB ID	:	EMD-4139
Title	:	Cryo-EM reconstruction of the maedi-visna virus (MVV) strand transfer complex
Authors	:	Pye, V.E.; Ballandras-Colas, A.; Maskell, D.; Locke, J.; Kotecha, A.; Costa, A.; Cherepanov, P.
Deposited on	:	2016-10-05
Resolution	:	8.20 Å(reported)

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 8.20 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.
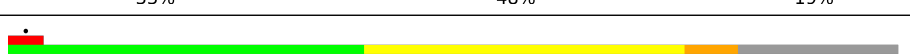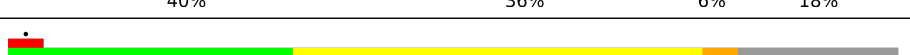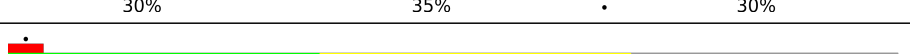
Metric	Percentile Ranks	Value
Clashscore		27
Ramachandran outliers		0.3%
Sidechain outliers		0.0%

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	281	· 51% 44% · ·
1	B	281	15% 68% 22% 9%
1	C	281	13% 70% 23% 7%
1	D	281	5% 58% 16% ·· 23%
1	E	281	10% 72% 19% 9%
1	F	281	14% 72% 23% 5%
1	G	281	8% 58% 15% 27%
1	H	281	8% 60% 17% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	281	47% 47%
1	J	281	16% 69% 21% 9%
1	K	281	12% 71% 22% 7%
1	L	281	5% 55% 21% 23%
1	M	281	10% 67% 25% 9%
1	N	281	12% 72% 22% 5%
1	O	281	6% 60% 13% 27%
1	P	281	8% 61% 16% 23%
2	Q	21	43% 57%
2	S	21	33% 48% 19%
3	R	50	40% 36% 6% 18%
3	T	50	32% 46% 18%
4	U	23	17% 30% 35% 30%
4	V	23	35% 35% 30%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 34774 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 integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	276	Total	C	N	O	S	0	0
			2216	1411	387	409	9		
1	B	256	Total	C	N	O	S	0	0
			2075	1321	363	383	8		
1	C	261	Total	C	N	O	S	0	0
			2123	1353	371	391	8		
1	D	216	Total	C	N	O	S	0	0
			1729	1110	297	316	6		
1	E	257	Total	C	N	O	S	0	0
			2090	1333	365	384	8		
1	F	266	Total	C	N	O	S	0	0
			2140	1362	377	393	8		
1	G	205	Total	C	N	O	S	0	0
			1657	1051	284	314	8		
1	H	217	Total	C	N	O	S	0	0
			1761	1129	308	318	6		
1	I	276	Total	C	N	O	S	0	0
			2216	1411	387	409	9		
1	J	256	Total	C	N	O	S	0	0
			2075	1321	363	383	8		
1	K	261	Total	C	N	O	S	0	0
			2123	1353	371	391	8		
1	L	216	Total	C	N	O	S	0	0
			1729	1110	297	316	6		
1	M	257	Total	C	N	O	S	0	0
			2090	1333	365	384	8		
1	N	266	Total	C	N	O	S	0	0
			2140	1362	377	393	8		
1	O	205	Total	C	N	O	S	0	0
			1657	1051	284	314	8		
1	P	217	Total	C	N	O	S	0	0
			1761	1129	308	318	6		

- Molecule 2 is a DNA chain called vDNA, non-transfered strand.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	21	Total	C	N	O	P	0	0
			431	203	79	128	21		
2	S	21	Total	C	N	O	P	0	0
			431	203	79	128	21		

- Molecule 3 is a DNA chain called vDNA-tDNA, transferred strand, joined to a model tDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	41	Total	C	N	O	P	0	0
			834	396	153	244	41		
3	T	41	Total	C	N	O	P	0	0
			834	396	153	244	41		

- Molecule 4 is a DNA chain called tDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	16	Total	C	N	O	P	0	0
			331	159	63	94	15		
4	V	16	Total	C	N	O	P	0	0
			331	159	63	94	15		

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: integrase

Chain A:

- Molecule 1: integrase

Chain B:

- Molecule 1: integrase

Chain C:

• Molecule 1: integrase

Chain D:

• Molecule 1: integrase

Chain E:

• Molecule 1: integrase

Chain F:

G194 T195 I202 F203 N204 K205 E206 Q207 Q208 R209 I210 Q211 Q212 Q213 S214 K215 T228 R229 K230 R231 G232 G235 V253 K254 D255 D259 L262 N266 K267 K270 F271 P274 P275 I278 GLN LYS GLU

● Molecule 1: integrase

Chain G:

8%

58%　　　　　15%　　　　　27%

TRP ILE GLU N4 E11 H12 H16 V20 S21 L22 H23 L24 E25 I28 P29 R30 K47 M48 PRO SER THR LEU ARG GLY SER ASN LYS ARG GLY I60 D61 H62 V65 T68 H69 Y70 E71 D72 I75 L76 V77 W78 V79 E80 S83 K92 Q97 K105

W106 Y107 A108 A111 S114 L115 E138 I143 L152 E165 P169 M170 A173 S176 L185 K188 R189 G192 L193 G194 I202 F203 N204 K205 E206 Q207 Q208 R209 I210 Q211 Q212 Q213 S214 K215 S216 K217 Q218 E219 LYS ILE ARG PHE CYS TYR TYR ARG THR

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

● Molecule 1: integrase

Chain H:

8%

60%　　　　　17%　　　　　23%

TRP ILE GLU ASN ILE PRO LEU ALA GLU GLU GLU HIS ASN LYS TRP HIS GLN ASP ALA VAL SER GLU LEU HIS LEU GLU PHE GLY ILE PRO ARG THR ALA ALA GLU ASP ILE VAL GLN GLN CYS ASP VAL CYS GLN GLU ASN LYS MET PRO SER THR LEU ARG GLY SER ASN LYS ARG GLY I60

Q64 T68 E71 D72 I75 V79 E80 S83 E89 G93 E98 K105 W106 Y107 A108 M109 F110 A111 L115 N119 A125 E126 S127 K133 T140 T141 G142 W145 N146 P147 Q148 S149 Q150 A151 L152 T156 L164 A173 S176 A177

L178 T181 T184 L185 R189 K190 G191 G192 I202 F203 N204 Q207 Q208 R209 I210 Q211 Q212 Q213 S214 K215 S216 K217 F223 Y226 R227 T228 G235 E236 W237 G238 G239 V252 R256 G257 T258 D259 V263 P275 K276 GLU ILE GLN LYS GLU

● Molecule 1: integrase

Chain I:

47%　　　　　47%　　● ● ●

W1 I2 I5 A8 E9 E10 E11 H12 N13 K14 W15 H16 Q17 S21 F26 G27 I28 P29 R30 A33 I36 V37 Q38 Q39 C40 D41 V42 C43 K47 M48 P49 S50 T51 L52 R53 G54 S55 N56 K57 R58 D61 H62 W63 Q64 V65 D66 Y67 T68 H69 D72 K73

I74 I75 L76 V77 W78 V79 E80 T81 N82 S83 G84 L85 I86 Y87 A88 E94 T95 F99 A108 A111 P112 K113 S114 L115 Q116 S117 D118 N119 G120 P121 A122 F123 V124 A125 E126 E138 H139 T140 T141 G142 I143 P144 W145 N146 P147 Q148 S149 Q150 V153 E154 R155 T156 H157 Q158

T159 L160 K161 N162 T163 E175 L178 L182 I183 T184 L185 N186 I187 K188 R189 K190 G191 G192 L193 S196 P197 M198 D199 F203 N204 K205 E206 Q207 Q208 R209 Q212 Q213 S214 K215 S216 K217 I221 R222 F223 C224 Y225 Y226 R227 T228 R231 G232 H233 P234 G235 E236 W237 Q238

G239 P240 T241 Q242 V243 G246 I251 V252 V253 K254 D255 R256 G257 T258 D259 L262 V263 I264 V269 K270 F271 I272 P273 K276 GLU ILE GLN LYS GLU

● Molecule 1: integrase

Chain J:

16%

69%

21%

9%

TRP ILE E3 H23 G27 I28 P29 A33 I36 C40 Q44 GLU ASN LYS MET PRO SER THR LEU ARG GLY SER ASN LYS ARG GLY I60 D61 H62 W63 Q64 T68 H69 I75 W78 V79 E80 S83 G84 L85 I86 Y87 A88 E89 R90 V91 K92 G93 M104

K105 W106 Y107 A108 M109 S114 L115 Y134 L135 E138 T159 L160 K161 N162 T163 A173 S176 A177 L178 A179 G180 T181 T184 I187 K190 L193 G194 T195 M198 D199 I200 F201 I202 Q208 R209 I210 Q211 Q212 Q213 S214 K215 S216 K217 Q218 E219 K220 I221 R222

F223 Y226 R227 T228 R229 K230 R231 G232 H233 P234 G235 E236 G239 P240 T241 Q242 V243 L244 W245 G246 G247 A250 I251 V252 V253 K254 D255 R256 G257 L262 K267 D268 V269 K270 F271 I272 P273 PRO PRO LYS GLU ILE GLN LYS GLU

• Molecule 1: integrase

Chain K:

12%

71%

22%

7%

W1 I2 E3 N4 I5 P6 L7 A8 E9 S21 L22 H23 L24 E25 F26 G27 I28 P29 R30 T31 A32 I36 C40 K47 MET PRO SER THR LEU ARG GLY SER ASN LYS ARG GLY I60 D61 H62 W63 Q64 V65 W78 V79 E80 T81 N82 S83 W106 F110 S114 L115

G136 T140 I143 Q148 S149 Q150 V153 A173 S176 L185 R189 K190 G191 G192 L193 G194 T195 I200 F203 N204 K205 E206 Q207 Q208 Q211 Q212 K215 S216 K217 Q218 E219 C224 Y225 Y226 R227 T228 R231 Q238 T241 Q242 V243 L244 W245

D248 G249 A250 V253 K254 D255 R256 G257 T258 D259 L262 V263 I264 A265 N266 V269 K270 F271 I272 P273 PRO PRO LYS GLU ILE GLN LYS GLU

• Molecule 1: integrase

Chain L:

5%

55%

21%

23%

TRP ILE GLU ASN ILE PRO LEU ALA GLU GLU GLU HIS ASN LYS TRP HIS GLN ASP ALA VAL SER LEU HIS LEU GLU PHE GLY ILE PRO ARG THR ALA ALA GLU ASP ILE VAL GLN GLN CYS ASP VAL CYS GLN GLU ASN LYS MET PRO SER THR LEU ARG GLY SER ASN LYS ARG GLY I60

D61 H62 V65 E80 T81 N82 S83 W106 Y107 A108 M109 F110 A111 P112 K113 S114 L115 L130 K133 G136 I137 E138 H139 T140 I143 P144 W145 Q148 L164 A173 S176 T181 T184 R189 K190 G191 G192 L193 G194 T195 I202 E206 R209

I210 S214 K217 K220 I221 R222 F223 C224 Y225 Y226 R227 T228 R229 K230 R231 G232 H233 P234 G235 E236 W237 Q238 G239 P240 T241 Q242 V243 L244 W245 G246 G247 I251 V252 V253 K254 D255 D259 L262 A265 N266 K267 D268 V269 K270 F271 I272 P273 P274 P275 LYS GLU ILE GLN

LYS GLU

• Molecule 1: integrase

Chain M:

10%

67%

25%

9%

• Molecule 1: integrase

• Molecule 1: integrase

• Molecule 1: integrase

• Molecule 2: vDNA, non-transfered strand

Chain Q:

• Molecule 2: vDNA, non-transfered strand

Chain S:

• Molecule 3: vDNA-tDNA, transferred strand, joined to a model tDNA

Chain R:

• Molecule 3: vDNA-tDNA, transferred strand, joined to a model tDNA

Chain T:

• Molecule 4: tDNA

Chain U:

• Molecule 4: tDNA

Chain V:
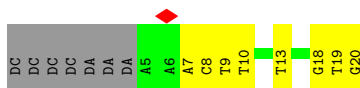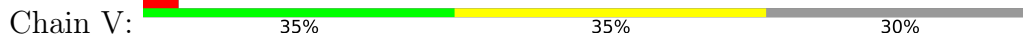
4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	37021	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 $(e^-/\text{Å}^2)$	1.47	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	0.333	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.7, 2.7, 2.7	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	0.83	4/2269 (0.2%)	0.85	7/3071 (0.2%)
1	B	0.58	1/2124 (0.0%)	0.73	2/2874 (0.1%)
1	C	0.48	1/2174 (0.0%)	0.65	0/2942
1	D	0.57	3/1772 (0.2%)	0.79	4/2401 (0.2%)
1	E	0.53	1/2140 (0.0%)	0.67	0/2896
1	F	0.62	2/2191 (0.1%)	0.72	0/2966
1	G	0.43	1/1693 (0.1%)	0.60	0/2290
1	H	0.47	1/1805 (0.1%)	0.66	0/2441
1	I	0.89	6/2271 (0.3%)	1.22	12/3077 (0.4%)
1	J	0.59	2/2124 (0.1%)	0.74	1/2874 (0.0%)
1	K	0.47	1/2174 (0.0%)	0.65	1/2942 (0.0%)
1	L	0.66	3/1772 (0.2%)	0.68	1/2401 (0.0%)
1	M	0.54	0/2140	0.67	0/2896
1	N	0.61	0/2191	0.71	1/2966 (0.0%)
1	O	0.43	1/1693 (0.1%)	0.60	0/2290
1	P	0.49	1/1805 (0.1%)	0.68	0/2441
2	Q	0.52	0/482	0.85	0/742
2	S	0.75	3/482 (0.6%)	1.07	4/742 (0.5%)
3	R	1.38	3/934 (0.3%)	0.96	3/1437 (0.2%)
3	T	0.66	2/934 (0.2%)	0.98	4/1437 (0.3%)
4	U	0.69	2/372 (0.5%)	0.92	0/574
4	V	0.48	0/372	0.88	0/574
All	All	0.63	38/35914 (0.1%)	0.77	40/49274 (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	1
1	I	0	3
All	All	0	4

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	40	DT	O3'-P	-38.12	1.15	1.61
1	I	238	GLN	C-N	17.98	1.65	1.33
1	A	239	GLY	C-N	16.57	1.65	1.34
1	L	221	ILE	C-N	14.47	1.67	1.34
1	I	146	ASN	C-N	10.20	1.53	1.34

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	238	GLN	O-C-N	30.56	175.16	123.20
1	I	238	GLN	CA-C-N	-29.87	56.45	116.20
1	I	238	GLN	C-N-CA	-16.82	86.99	122.30
1	D	274	PRO	C-N-CD	-15.44	86.63	120.60
2	S	13	DG	OP1-P-O3'	-10.65	81.76	105.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	THR	Mainchain
1	I	142	GLY	Peptide
1	I	225	TYR	Mainchain
1	I	51	THR	Mainchain

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	2216	0	2173	407	0
1	B	2075	0	2046	51	0
1	C	2123	0	2091	85	0
1	D	1729	0	1705	152	0
1	E	2090	0	2061	100	0
1	F	2140	0	2106	51	0
1	G	1657	0	1626	57	0
1	H	1761	0	1764	101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2216	0	2175	484	0
1	J	2075	0	2046	116	0
1	K	2123	0	2095	77	0
1	L	1729	0	1702	160	0
1	M	2090	0	2059	96	0
1	N	2140	0	2105	107	0
1	O	1657	0	1626	60	0
1	P	1761	0	1764	82	0
2	Q	431	0	236	58	0
2	S	431	0	236	93	0
3	R	834	0	461	127	0
3	T	834	0	460	150	0
4	U	331	0	183	12	0
4	V	331	0	182	36	0
All	All	34774	0	32902	1839	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 27.

The worst 5 of 1839 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)
1:A:212:GLN:HB2	1:D:217:LYS:CD	1.21	1.64
1:A:14:LYS:HB3	1:J:134:TYR:CE1	1.27	1.61
1:I:145:TRP:CB	1:N:229:ARG:HD2	1.28	1.61
1:C:270:LYS:HD3	1:H:145:TRP:CE2	1.31	1.59
1:I:119:ASN:HB2	4:V:19:DT:C4'	1.25	1.59

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	270/281 (96%)	253 (94%)	16 (6%)	1 (0%)	34	72
1	B	252/281 (90%)	242 (96%)	8 (3%)	2 (1%)	19	60
1	C	257/281 (92%)	249 (97%)	8 (3%)	0	100	100
1	D	214/281 (76%)	203 (95%)	8 (4%)	3 (1%)	11	46
1	E	253/281 (90%)	244 (96%)	8 (3%)	1 (0%)	34	72
1	F	262/281 (93%)	248 (95%)	12 (5%)	2 (1%)	19	60
1	G	201/281 (72%)	197 (98%)	4 (2%)	0	100	100
1	H	215/281 (76%)	211 (98%)	4 (2%)	0	100	100
1	I	274/281 (98%)	255 (93%)	18 (7%)	1 (0%)	34	72
1	J	252/281 (90%)	237 (94%)	15 (6%)	0	100	100
1	K	257/281 (92%)	253 (98%)	4 (2%)	0	100	100
1	L	214/281 (76%)	203 (95%)	9 (4%)	2 (1%)	17	57
1	M	253/281 (90%)	244 (96%)	9 (4%)	0	100	100
1	N	262/281 (93%)	252 (96%)	9 (3%)	1 (0%)	34	72
1	O	201/281 (72%)	194 (96%)	7 (4%)	0	100	100
1	P	215/281 (76%)	209 (97%)	6 (3%)	0	100	100
All	All	3852/4496 (86%)	3694 (96%)	145 (4%)	13 (0%)	44	77

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	231	ARG
1	D	233	HIS
1	I	240	PRO
1	L	233	HIS
1	D	234	PRO

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	237/246 (96%)	236 (100%)	1 (0%)	91	94
1	B	223/246 (91%)	223 (100%)	0	100	100
1	C	228/246 (93%)	228 (100%)	0	100	100
1	D	183/246 (74%)	183 (100%)	0	100	100
1	E	224/246 (91%)	224 (100%)	0	100	100
1	F	228/246 (93%)	228 (100%)	0	100	100
1	G	181/246 (74%)	181 (100%)	0	100	100
1	H	189/246 (77%)	189 (100%)	0	100	100
1	I	237/246 (96%)	237 (100%)	0	100	100
1	J	223/246 (91%)	223 (100%)	0	100	100
1	K	228/246 (93%)	228 (100%)	0	100	100
1	L	183/246 (74%)	183 (100%)	0	100	100
1	M	224/246 (91%)	224 (100%)	0	100	100
1	N	228/246 (93%)	228 (100%)	0	100	100
1	O	181/246 (74%)	181 (100%)	0	100	100
1	P	189/246 (77%)	189 (100%)	0	100	100
All	All	3386/3936 (86%)	3385 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	I	2
1	L	1
3	R	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	44:GLN	C	45:GLU	N	2.19
1	A	224:CYS	C	225:TYR	N	2.02
1	L	221:ILE	C	222:ARG	N	1.67
1	A	239:GLY	C	240:PRO	N	1.65
1	I	238:GLN	C	239:GLY	N	1.65

6　Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-4139. 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 ⓘ
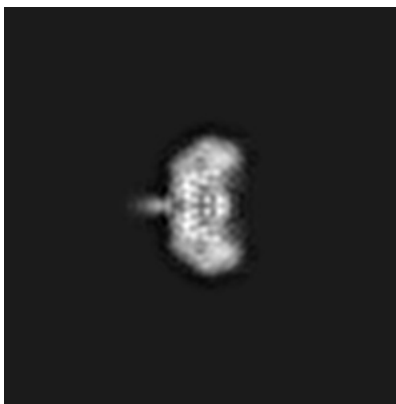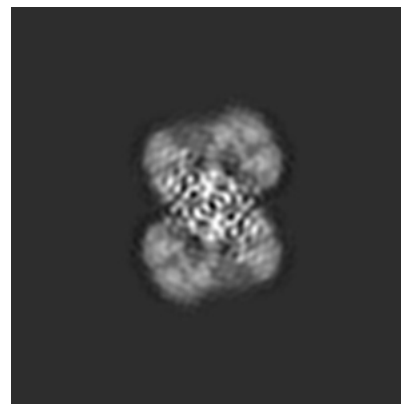
6.1.1　Primary map

X　　　　　　　　　　Y　　　　　　　　　　Z

6.1.2　Raw map

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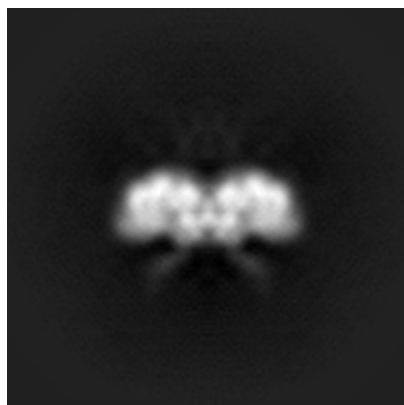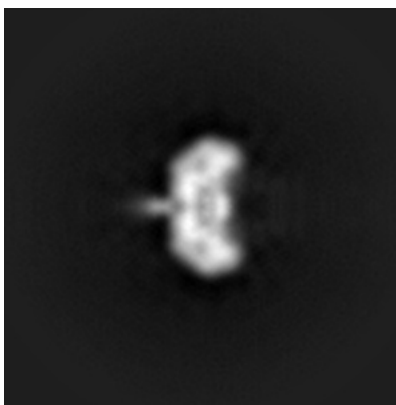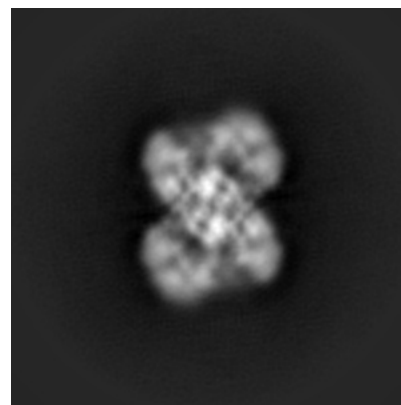
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ

6.2.1   Primary map
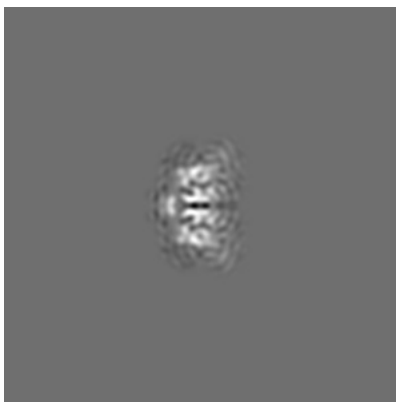
X Index: 75   Y Index: 75   Z Index: 75

6.2.2   Raw map
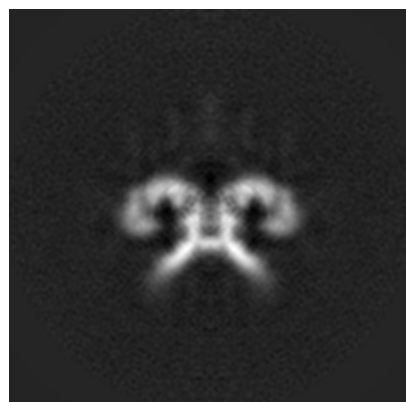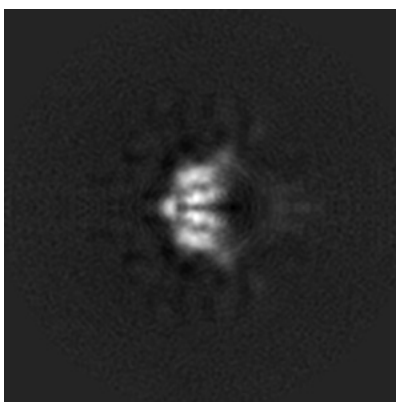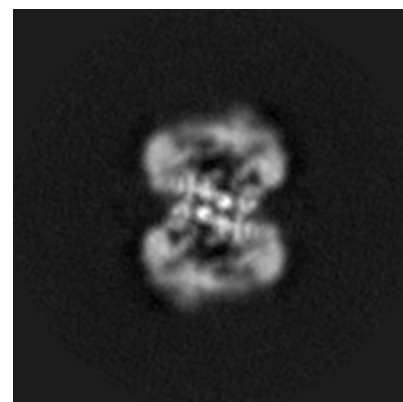
X Index: 75   Y Index: 75   Z Index: 75

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

6.3 Largest variance slices ⓘ
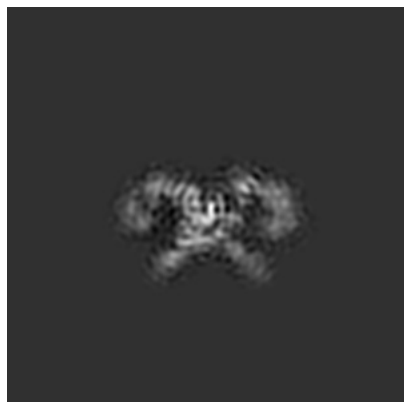
6.3.1 Primary map
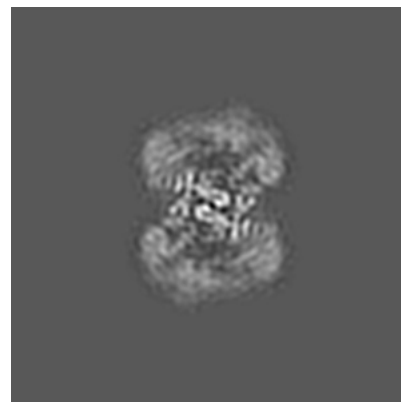
X Index: 77   Y Index: 68   Z Index: 75

6.3.2 Raw map
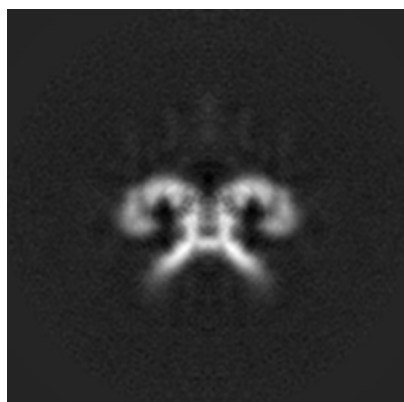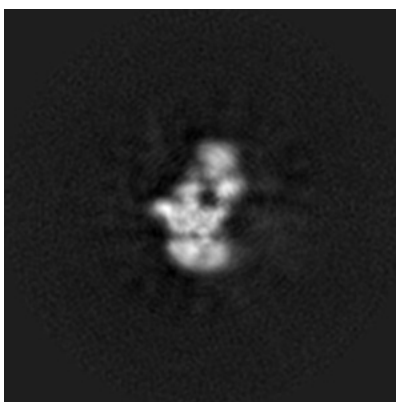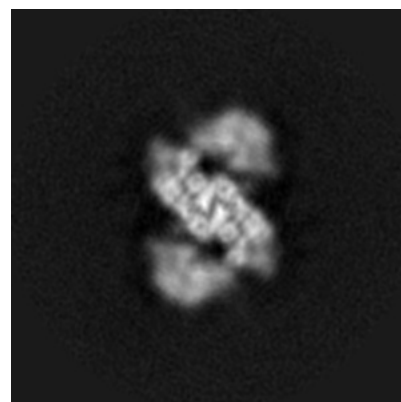
X Index: 75   Y Index: 83   Z Index: 69

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 |
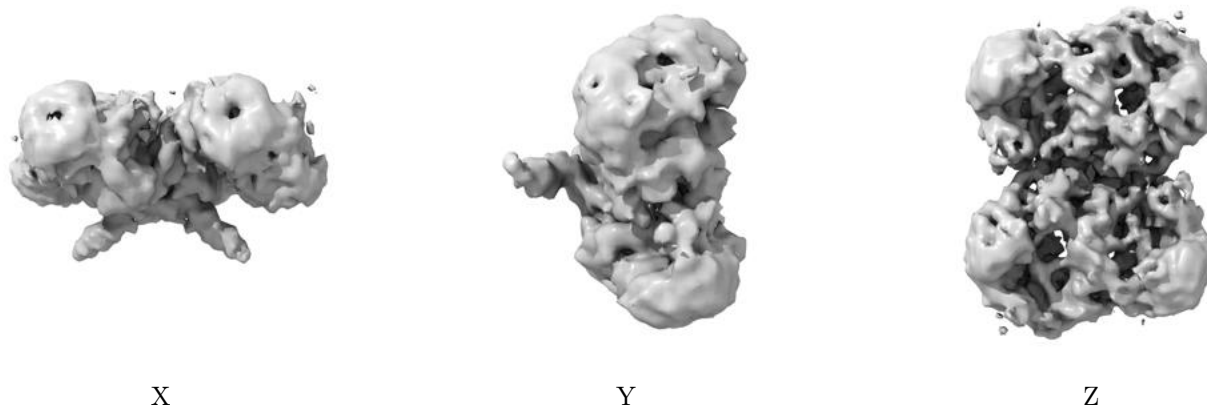
The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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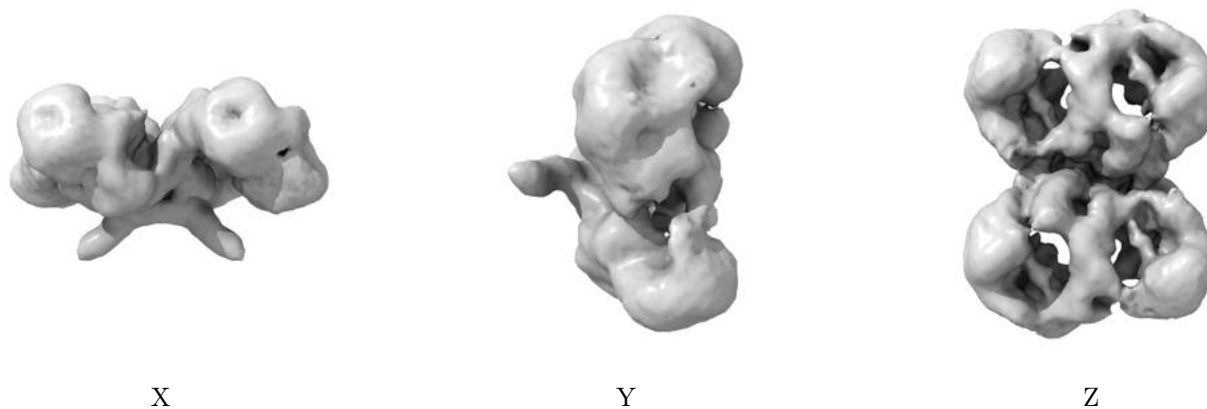
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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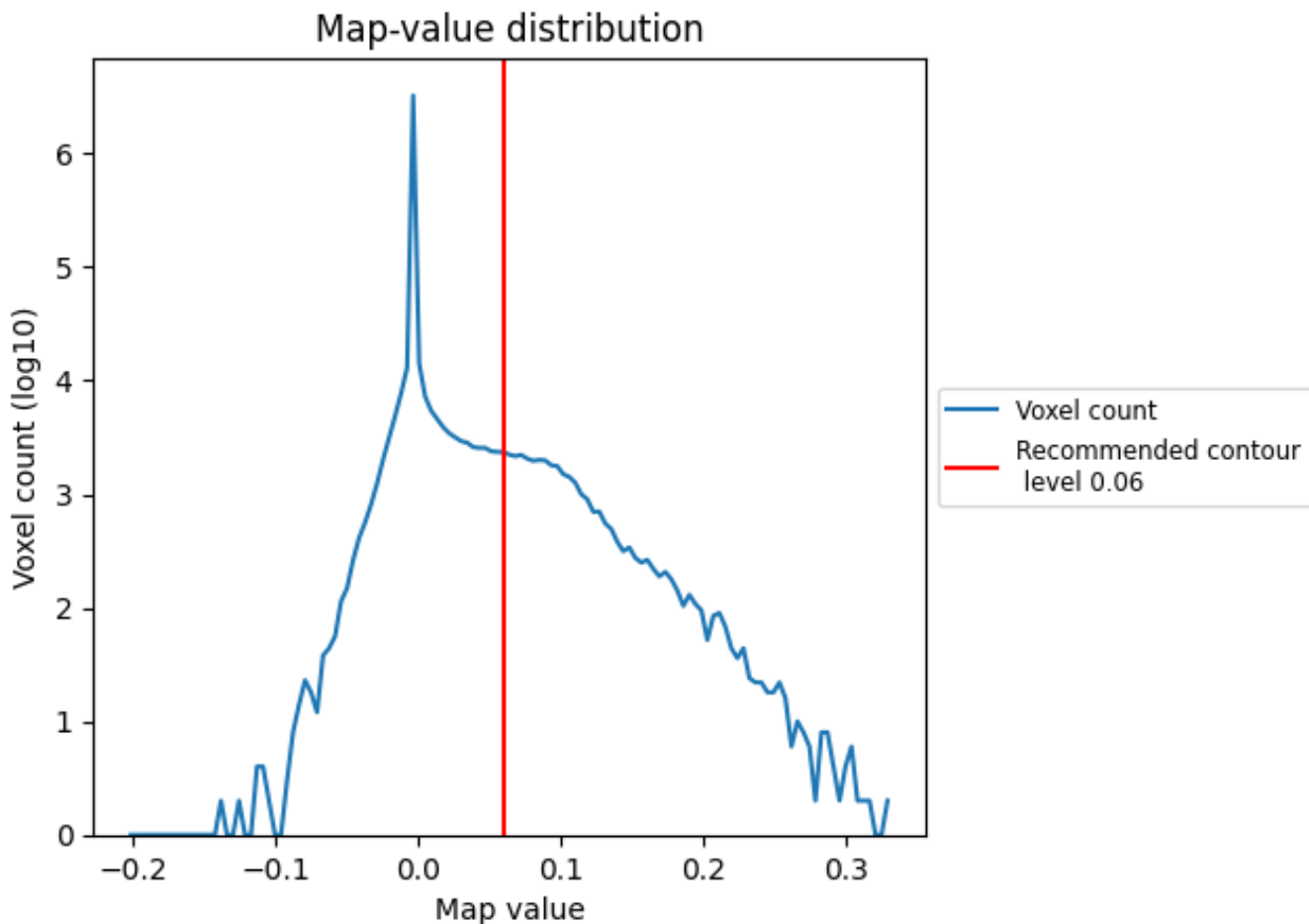
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
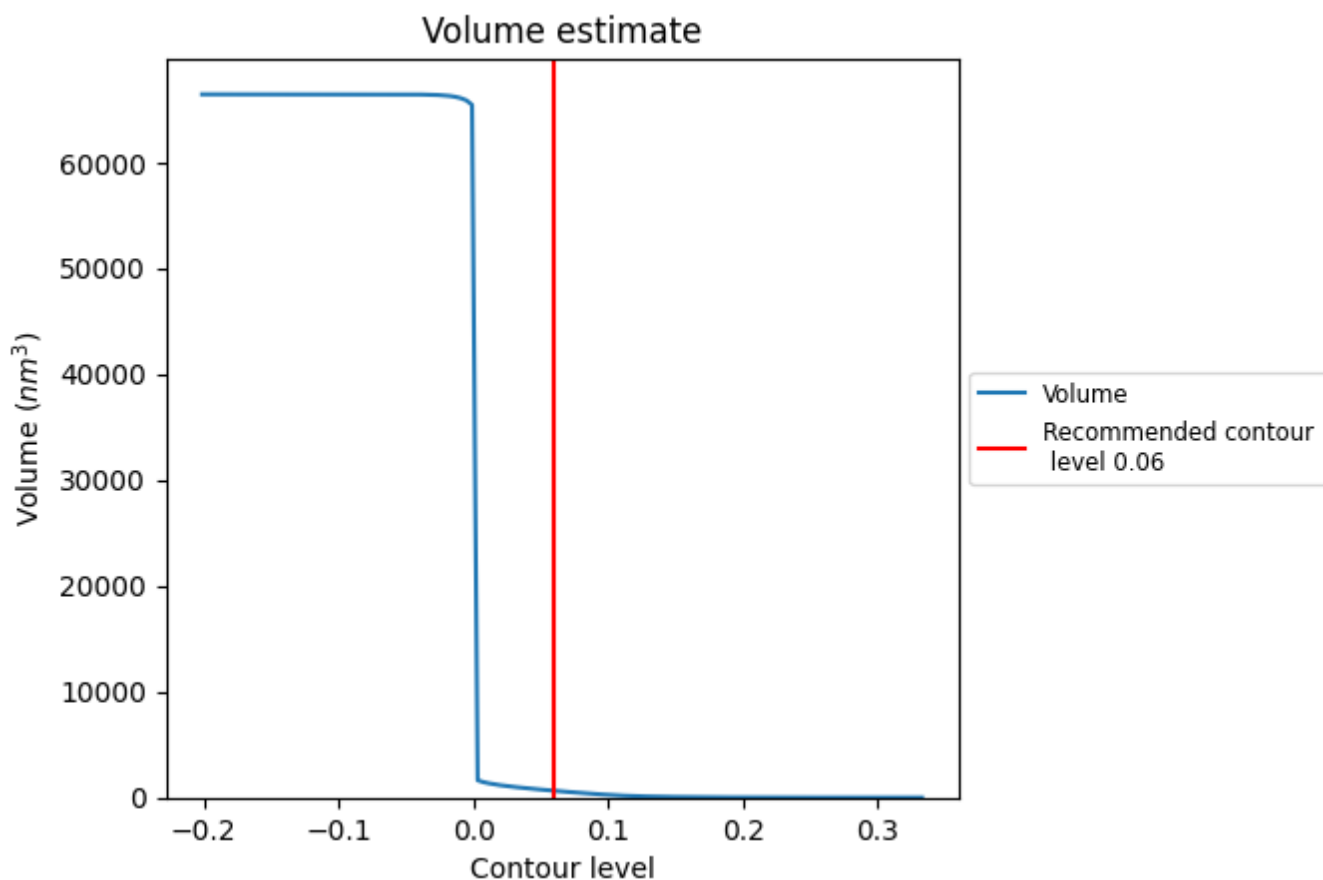
The volume at the recommended contour level is 644 nm^3; this corresponds to an approximate mass of 582 kDa.

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 ⓘ
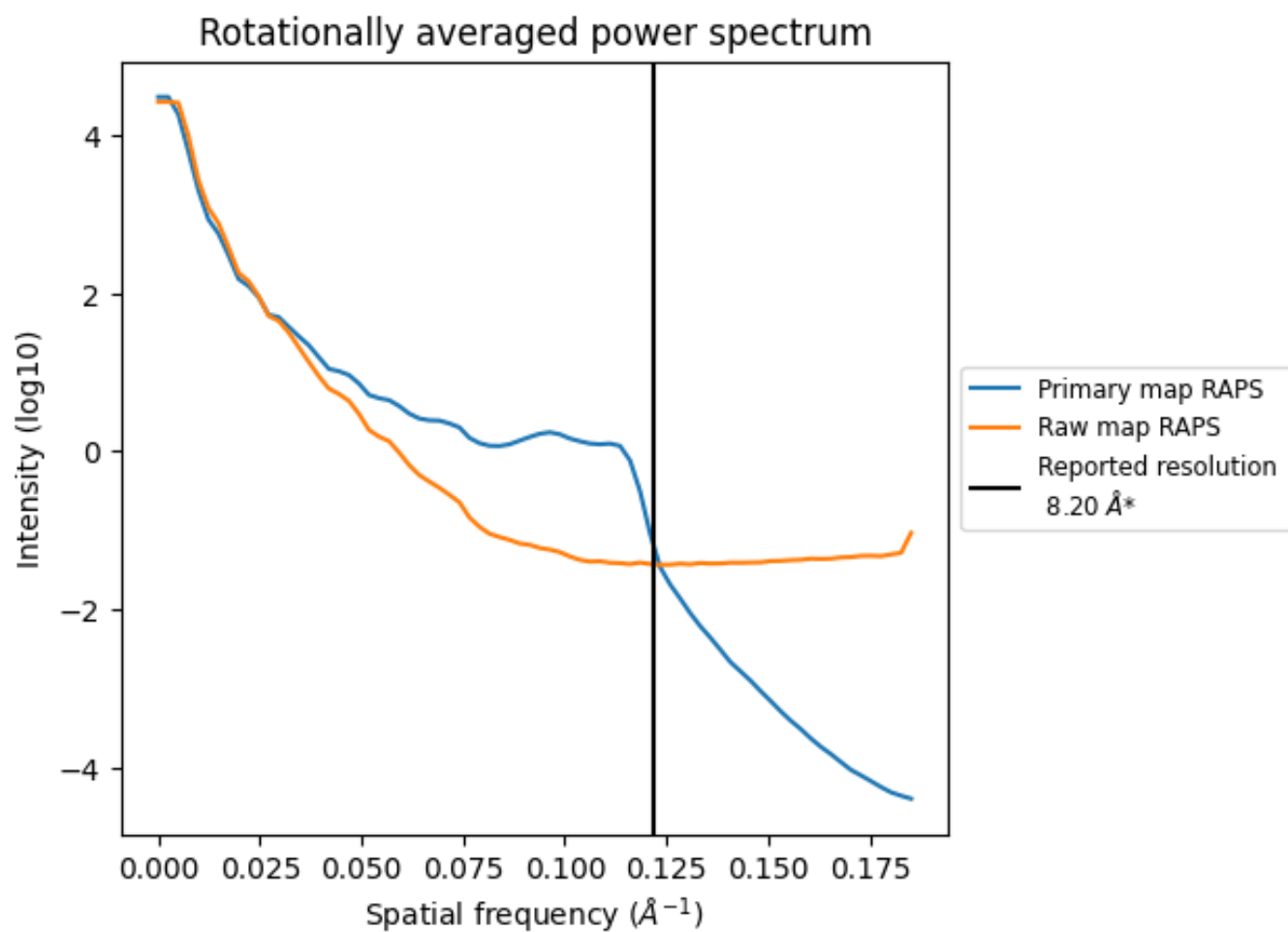
*Reported resolution corresponds to spatial frequency of 0.122 Å^{-1}

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 ⓘ
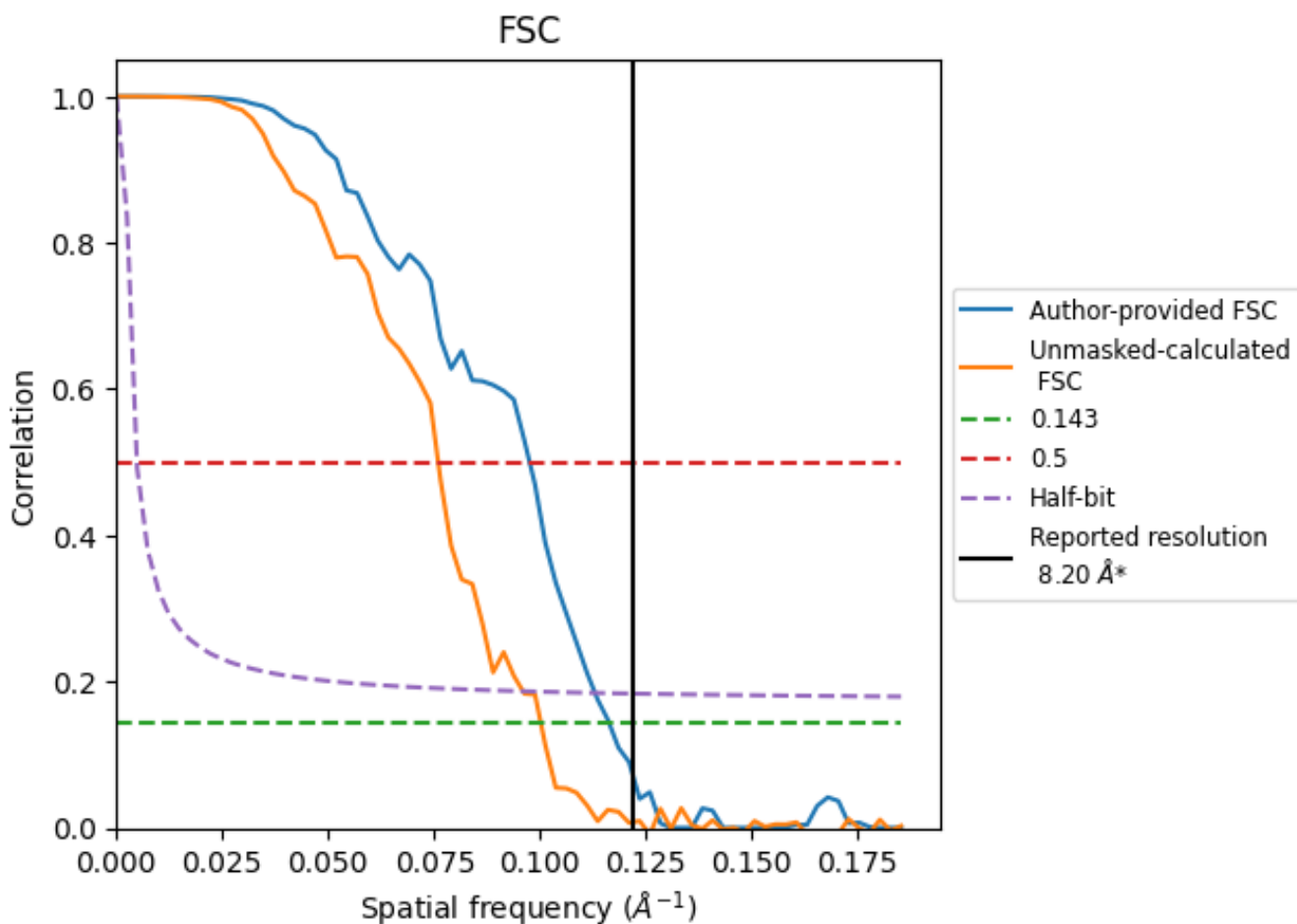
*Reported resolution corresponds to spatial frequency of 0.122 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	8.60	10.26	8.85
Unmasked-calculated*	9.98	13.16	10.42

*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 9.98 differs from the reported value 8.2 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-4139 and PDB model 5M0R. Per-residue inclusion information can be found in section 3 on page 6.

9.1   Map-model overlay ⓘ

X   Y   Z
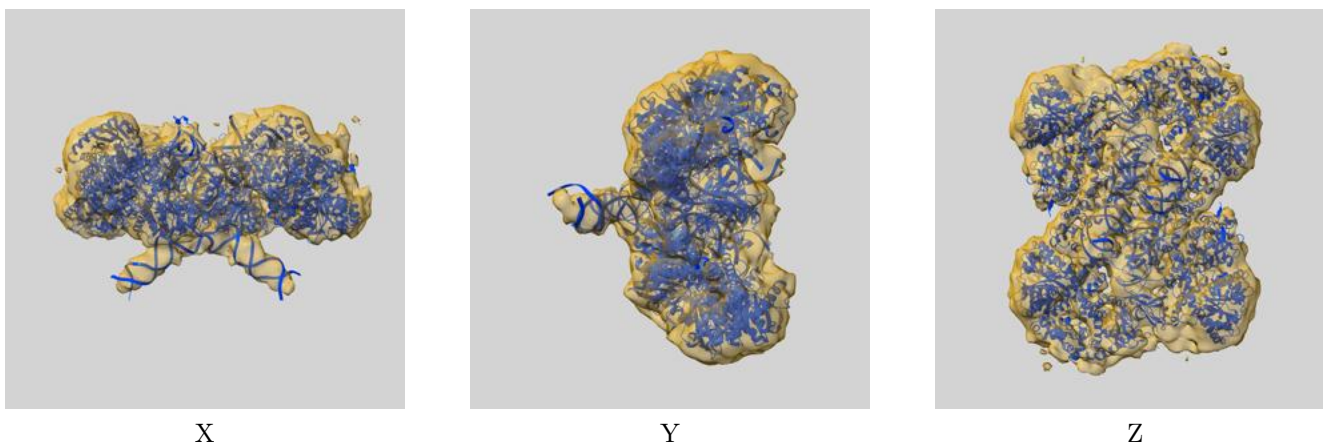
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ
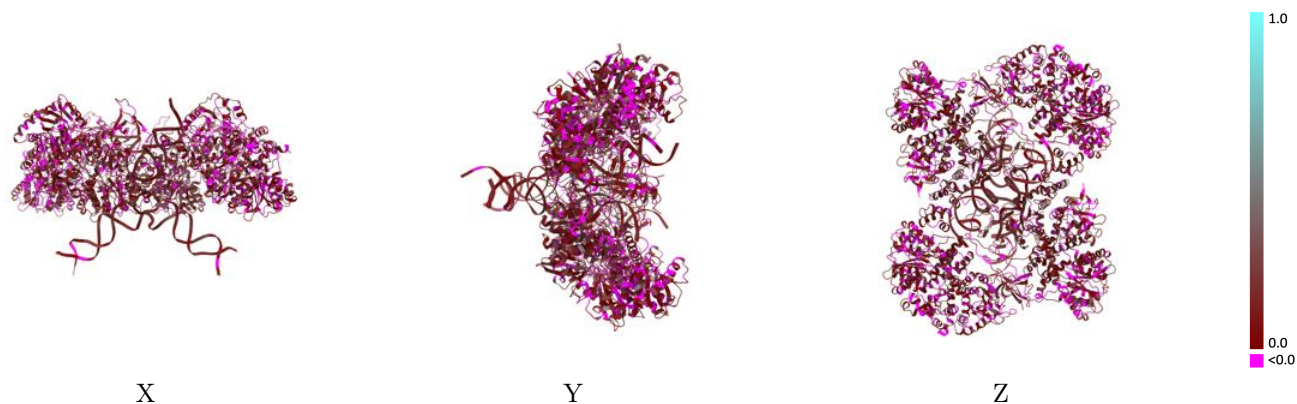
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
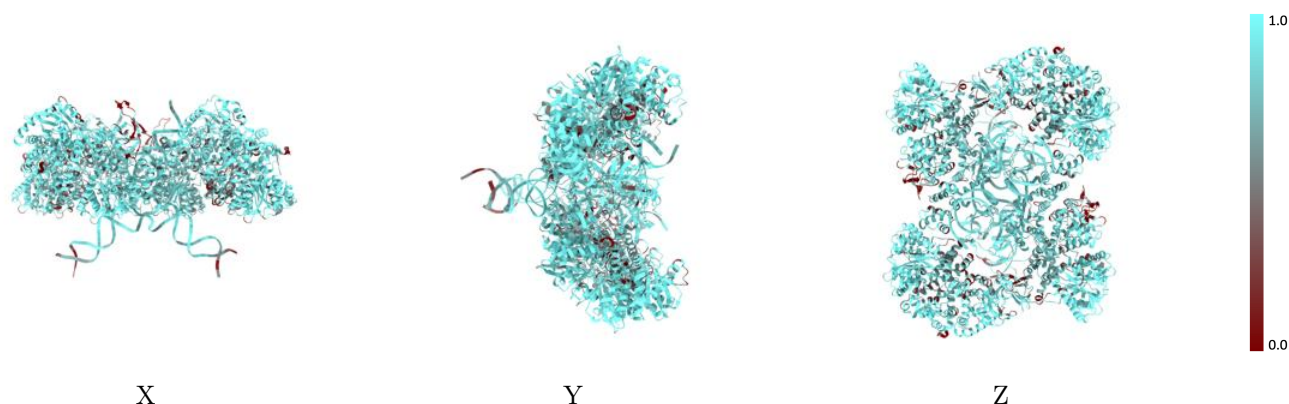
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4   Atom inclusion ⓘ
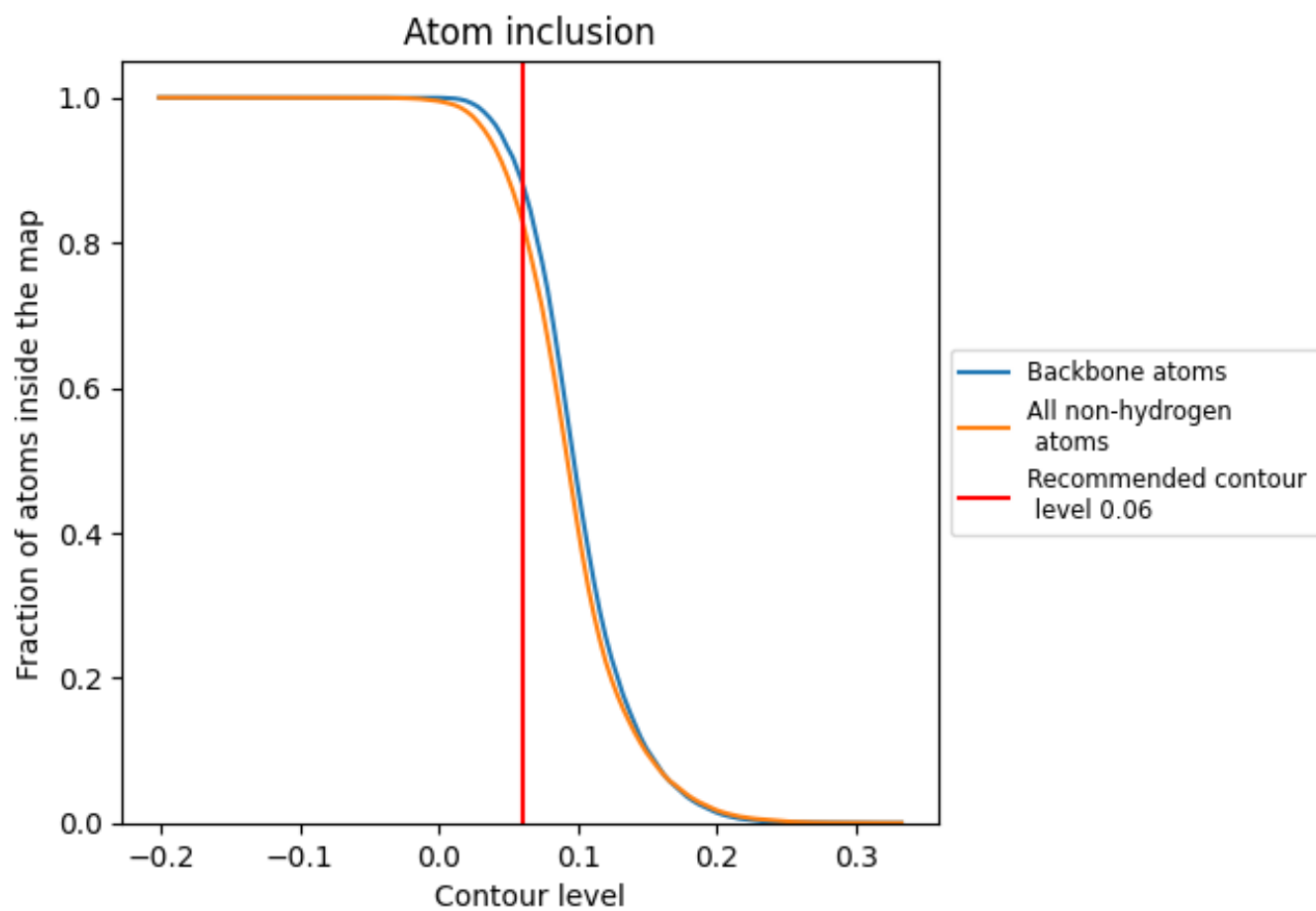
At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8315	0.0980
A	0.8676	0.1220
B	0.7760	0.1040
C	0.7979	0.0890
D	0.8633	0.0810
E	0.8249	0.0700
F	0.7880	0.0910
G	0.8440	0.0630
H	0.8649	0.0840
I	0.8676	0.1310
J	0.7706	0.1050
K	0.8022	0.0920
L	0.8686	0.0870
M	0.8312	0.0840
N	0.8085	0.1040
O	0.8563	0.0650
P	0.8690	0.0900
Q	0.9420	0.1650
R	0.8477	0.1480
S	0.9350	0.1410
T	0.8537	0.1620
U	0.7100	0.1160
V	0.7674	0.1380

1.0

0.0
<0.0