WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

May 15, 2023 – 01:47 PM EDT

PDB ID	:	8F2U
EMDB ID	:	EMD-28827
Title	:	Human CCC complex
Authors	:	Healy, M.D.; McNally, K.E.; Butkovic, R.; Chilton, M.; Kato, K.; Sacharz, J.; McConville, C.; Moody, E.R.R.; Shaw, S.; Planelles-Herrero, V.J.; Kadapalakere, S.Y.; Ross, J.; Borucu, U.; Palmer, C.S.; Chen, K.; Croll, T.I.; Hall, R.J.; Caruana, N.J.; Ghai, R.; Nguyen, T.H.D.; Heesom, K.J.; Saitoh, S.; Berger, I.; Berger-Schaffitzel, C.; Williams, T.A.; Stroud, D.A.; Derivery, E.; Collins, B.M.; Cullen, P.J.
Deposited on	:	2022-11-08
Resolution	:	3.53 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
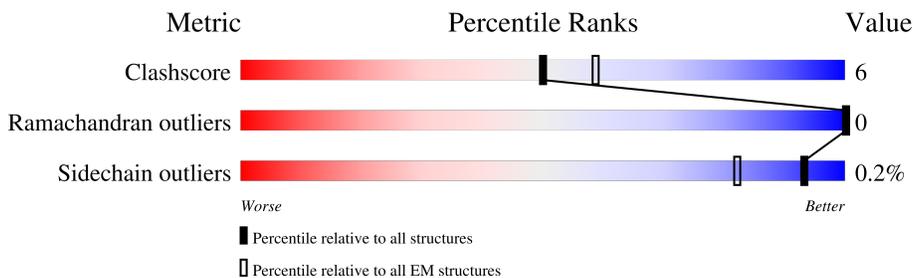http://www.wwpdb.org/validation/2017/FAQs#types.

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 3.53 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		6
Ramachandran outliers		0
Sidechain outliers		0.2%

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	190	45% / 84% 14% ••
2	B	199	10% / 86% 14%
3	C	195	• / 89% 11%
4	D	199	• / 89% 11%
5	E	260	• / 67% 12% 21%
6	F	85	75% 15% 9%
7	G	200	50% / 90% 10%
8	H	183	• / 86% 11% •

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Mol	Chain	Length	Quality of chain
9	I	198	15% 83% 17%
10	J	212	10% 75% 17% 7%
11	N	631	16% 29% 7% 64%
12	T	627	10% 24% 72%

2   Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 17684 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 COMM domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	187	Total	C	N	O	S	0	0
			1466	928	251	282	5		

- Molecule 2 is a protein called COMM domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	199	Total	C	N	O	S	0	0
			1601	1012	285	300	4		

- Molecule 3 is a protein called COMM domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	195	Total	C	N	O	S	0	0
			1555	977	268	302	8		

- Molecule 4 is a protein called COMM domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	199	Total	C	N	O	S	0	0
			1520	960	261	287	12		

- Molecule 5 is a protein called COMM domain-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	205	Total	C	N	O	S	0	0
			1598	1009	287	295	7		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	225	GLY	-	expression tag	UNP Q9GZQ3
E	226	SER	-	expression tag	UNP Q9GZQ3
E	227	LEU	-	expression tag	UNP Q9GZQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	228	PHE	-	expression tag	UNP Q9GZQ3
E	229	GLN	-	expression tag	UNP Q9GZQ3
E	230	GLY	-	expression tag	UNP Q9GZQ3
E	231	PRO	-	expression tag	UNP Q9GZQ3
E	232	TRP	-	expression tag	UNP Q9GZQ3
E	233	SER	-	expression tag	UNP Q9GZQ3
E	234	HIS	-	expression tag	UNP Q9GZQ3
E	235	PRO	-	expression tag	UNP Q9GZQ3
E	236	GLN	-	expression tag	UNP Q9GZQ3
E	237	PHE	-	expression tag	UNP Q9GZQ3
E	238	GLU	-	expression tag	UNP Q9GZQ3
E	239	LYS	-	expression tag	UNP Q9GZQ3
E	240	GLY	-	expression tag	UNP Q9GZQ3
E	241	GLY	-	expression tag	UNP Q9GZQ3
E	242	GLY	-	expression tag	UNP Q9GZQ3
E	243	SER	-	expression tag	UNP Q9GZQ3
E	244	GLY	-	expression tag	UNP Q9GZQ3
E	245	GLY	-	expression tag	UNP Q9GZQ3
E	246	GLY	-	expression tag	UNP Q9GZQ3
E	247	SER	-	expression tag	UNP Q9GZQ3
E	248	GLY	-	expression tag	UNP Q9GZQ3
E	249	GLY	-	expression tag	UNP Q9GZQ3
E	250	SER	-	expression tag	UNP Q9GZQ3
E	251	SER	-	expression tag	UNP Q9GZQ3
E	252	ALA	-	expression tag	UNP Q9GZQ3
E	253	TRP	-	expression tag	UNP Q9GZQ3
E	254	SER	-	expression tag	UNP Q9GZQ3
E	255	HIS	-	expression tag	UNP Q9GZQ3
E	256	PRO	-	expression tag	UNP Q9GZQ3
E	257	GLN	-	expression tag	UNP Q9GZQ3
E	258	PHE	-	expression tag	UNP Q9GZQ3
E	259	GLU	-	expression tag	UNP Q9GZQ3
E	260	LYS	-	expression tag	UNP Q9GZQ3

- Molecule 6 is a protein called COMM domain-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	77	617	397	101	114	5	0	0

- Molecule 7 is a protein called COMM domain-containing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	200	Total 1583	C 1014	N 262	O 298	S 9	0	0

- Molecule 8 is a protein called COMM domain-containing protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	179	Total 1449	C 927	N 246	O 270	S 6	0	0

- Molecule 9 is a protein called COMM domain-containing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	198	Total 1526	C 955	N 264	O 299	S 8	0	0

- Molecule 10 is a protein called COMM domain-containing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	198	Total 1589	C 1010	N 274	O 301	S 4	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	203	HIS	-	expression tag	UNP Q9Y6G5
J	204	HIS	-	expression tag	UNP Q9Y6G5
J	205	HIS	-	expression tag	UNP Q9Y6G5
J	206	HIS	-	expression tag	UNP Q9Y6G5
J	207	HIS	-	expression tag	UNP Q9Y6G5
J	208	HIS	-	expression tag	UNP Q9Y6G5
J	209	HIS	-	expression tag	UNP Q9Y6G5
J	210	HIS	-	expression tag	UNP Q9Y6G5
J	211	HIS	-	expression tag	UNP Q9Y6G5
J	212	HIS	-	expression tag	UNP Q9Y6G5

- Molecule 11 is a protein called Coiled-coil domain-containing protein 93.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	225	Total 1816	C 1155	N 310	O 343	S 8	0	0

- Molecule 12 is a protein called Coiled-coil domain-containing protein 22.

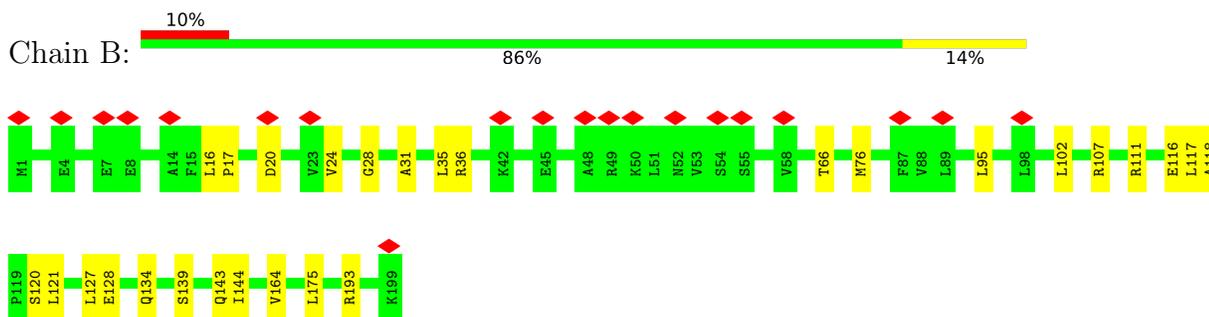| Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	174	Total	C	N	O	S	0	0
			1364	854	267	242	1		

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.
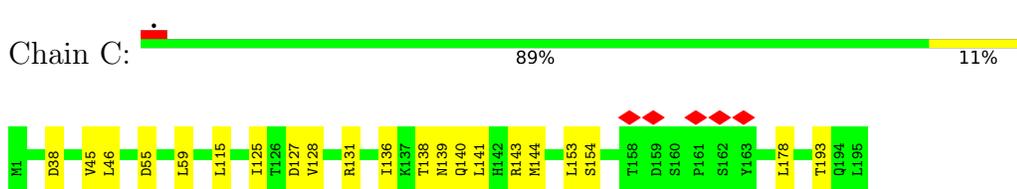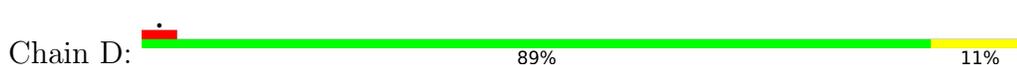
- Molecule 1: COMM domain-containing protein 1

Chain A:

- Molecule 2: COMM domain-containing protein 2

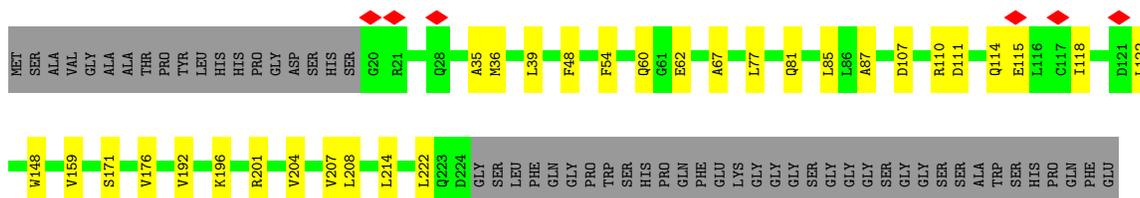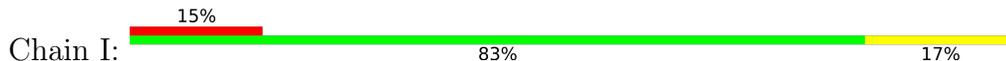Chain B:

- Molecule 3: COMM domain-containing protein 3

Chain C:

- Molecule 4: COMM domain-containing protein 4

Chain D:

M1 F5 E18 T21 L22 L33 C34 V37 A56 D57 E61 D64 V71 S78 S83 L93 L96 A103 P116 K119 L126 R127 S149 V150 E151 R158 V161 P168 A169 Q170 P171 G199

• Molecule 5: COMM domain-containing protein 5

Chain E:

67%   12%   21%

MET ALA VAL GLY ALA ALA THR PRO TYR LEU HIS HIS PRO GLY ASP SER HIS SER G20 R21 Q28 A35 M36 L39 F48 F54 Q60 G61 E62 A67 L77 Q81 L85 L86 A87 D107 R110 D111 Q114 E115 L116 C117 I118 D121 L122

W148 V159 S171 V176 V192 K196 R201 V204 V207 L208 L214 L222 Q223 D224 GLY SER LEU PHE GLN GLY PRO TRP SER HIS PRO GLN PHE GLU LYS GLY GLY SER GLY GLY SER GLY GLY SER SER ALA TRP SER HIS PRO GLN PHE GLU

LYS

• Molecule 6: COMM domain-containing protein 6

Chain F:

75%   15%   9%

MET GLU ALA SER GLU PRO PRO L9 K12 L19 V20 D21 F22 Q23 W24 D33 L38 K39 Y40 F71 I78 V81 T84 V85

• Molecule 7: COMM domain-containing protein 7

Chain G:

50%

90%   10%

M1 G2 R3 L4 H5 C6 T7 E8 D9 P10 V11 P12 E13 A14 V15 G16 G17 D18 M19 Q20 Q21 L22 N23 Q24 L25 G26 A27 Q28 Q29 F30 S31 A32 L33 T34 E35 V36 L37 F38 H39 F40 L41 T42 E43 P44 K45 E46 V47 E48 R49 F50 L51 A52 Q53 L54 S55 E56 F57 A58 T59 T60

N61 Q62 I63 S64 L65 G66 S67 L68 R69 S70 I71 V72 L76 N80 G81 A82 K85 S86 L87 T88 A89 K90 Q91 V92 Q93 A94 D95 F96 I97 T98 L99 G100 L101 S102 E103 E104 K105 A106 T107 Y108 F109 S110 E111 K112 W113 K114 A117 P118 T119 L120 A121 L129 M130 I131

D136 M137 E138 W139 R191 T194 C200

• Molecule 8: COMM domain-containing protein 8

Chain H:

86%   11%

MET GLU PRO GLU E5 L9 Q13 K14 L15 P16 A17 E18 L19 D29 E47 S48 E49 E50 W51 F61 N80 Q81 L82 N83 S84 L85 R97 E108 A111 D131 K183

• Molecule 9: COMM domain-containing protein 9

Chain I:

15%

83%   17%

M1 A2 A3 H8 F9 A10 A11 L12 Q13 S14 K17 A18 S19 D22 V23 L27 E30 S31 F32 S35 A36 L37 G38 K41 L42 L43 D44 V45 T46 C47 S48 S49 L50 S51 V52 E55 E56 A57 L60 L61 Q62 R66 R69 L76 A81 E88

N96 L97 S119 L120 P121 R122 D125 L126 K133 I139 M142 I153 Q154 E155 D156 D162 K163 P164 I188 R189 A194 V195 A196 S197 K198

• Molecule 10: COMM domain-containing protein 10

Chain J:

10%

75%   17%   •   7%

MET ALA VAL PRO A5 A6 L7 I8 L9 K17 A18 V19 N23 A24 I25 D26 L38 Q39 E46 F49 S50 E51 E52 K56 L57 Q58 A59 S62 L63 E64 K65 L68 H69 L70 V71 L72 I75 E80 L92 Q95 L96 E97 N98 I99 H100 L101 D104

K105 A106 E107 A108 F109 V110 S115 M116 G117 Q118 V121 R125 L134 W139 H147 N166 E167 D168 S169 K170 E173 L184 Y188 N189 E192 L201 T202 HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 11: Coiled-coil domain-containing protein 93

Chain N:

16%

29%   7%   64%

MET GLY LEU PRO ARG GLY PRO GLU GLY GLN GLY LEU PRO GLU VAL THR ARG GLU ASP GLU Q23 N24 V25 K26 L27 T28 E29 I30 L31 E32 L33 L34 V35 A42 R43 I44 K45 G46 L47 S48 P49 F50 D51 K52 V53 V54 M57 C60 I61 C64 D67 V68 D69

V70 D71 L72 L73 F74 Q75 E76 N77 I80 G81 Q82 K83 I84 A85 L86 S87 E88 K89 I90 V91 S92 V93 L94 P95 R96 M97 P100 H101 Q102 L103 E104 P105 H106 Q107 I108 M111 D112 F113 I114 H115 I116 F117 V120 Q121 W122 L123 V124 K125 R126 A127 I128 E129 T130 K131 E132 E133

M134 G135 D136 R139 E154 D155 D156 I159 K160 R161 K162 I166 V169 E174 K181 R184 H185 Q186 G187 A188 E189 E190 R197 T201 R207 R208 Y209 GLY PHE SER ARG GLN SER LYS MET GLU LYS ALA GLU ASP LYS LYS THR ALA LEU PRO ALA GLY LEU

SER ALA THR GLU LYS ALA ASP ALA HIS GLU GLU ASP GLU LEU ARG ALA ALA GLU GLU GLN ARG ILE GLN SER LEU MET THR LYS MET THR ALA MET ALA ASN GLU GLU SER R269 L270 T271 A272 S273 S274 V275 G276 Q277 I278 L281 E285 I286 K287 Q288 I289 V290 S291 E292 Y293 A294

E295 K296 Q297 S298 E299 L300 S301 A302 E303 E304 S305 P306 GLU LYS LEU GLY THR GLN LEU HIS ARG ARG LYS VAL ILE SER LEU ASN LYS GLN ILE ALA GLN LYS LEU HIS LYS HIS GLU GLU GLU LEU ARG ALA SER HIS THR SER LEU GLN ALA ARG TYR ASN GLU ALA LYS LYS THR LEU

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

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

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

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

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

• Molecule 12: Coiled-coil domain-containing protein 22

Chain T:

10%

24%　　　•　　　72%

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

MET SER ALA ARG PHE ARG LEU ALA MET SER LEU ALA GLN ALA CYS MET ASP LEU GLU GLY TYR PRO LEU GLU LEU GLY TYR GLN ASN PHE LEU GLU TYR PRO SER GLU PRO ASP LEU GLU ARG ASP LEU LEU PHE LEU ALA GLU GLU ARG PRO THR ASP SER ALA ASP GLU SER ASP ALA ASP GLN PRO ALA

G121 D122 S123 L127 R135 V143 R148 Q156 A159 V171 R177 R181 V192 R202 R220 D221 R222 P223 G224 D225 E226 D227 W228 V229 H230 R231 T232 S233 R234 L235 P236 P237 Q238 E239 D240 T241 R242 A243 R247 L248 Q249 T253 L256 G261

L262 L263 G264 A265 P266 I267 Q268 A269 R270 D271 L272 G273 E274 L275 L276 Q277 A278 W279 G280 A281 G282 A283 K284 T285 G286 A287 P288 K289 G290 S291 R292 F293 T294 HIS SER GLU LYS PHE THR PHE HIS LEU GLU PRO GLN ALA GLN ALA THR GLN VAL SER ASP VAL PRO ALA THR SER ARG ARG

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

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

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

GLY ASN ILE ARG LYS GLN LYS GLU GLU ILE THR LYS ILE LEU SER ASP THR LYS ILE GLU LEU GLN LYS GLU ILE ASN SER LEU SER GLY LYS LEU ASP ARG THR ALA VAL THR ASP GLU LEU VAL PHE LYS ASP ALA LYS LYS ASP ASP ALA VAL ARG LYS ALA TYR LYS LYS TYR LEU ALA

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

GLY ARG VAL ARG GLU ALA

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20034	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 $(e^-/\text{Å}^2)$	43.14	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.035	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	286.176, 286.176, 286.176	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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	0.25	0/1493	0.47	0/2011
2	B	0.23	0/1626	0.48	0/2198
3	C	0.24	0/1584	0.48	0/2142
4	D	0.24	0/1542	0.46	0/2080
5	E	0.25	0/1624	0.53	0/2198
6	F	0.25	0/629	0.46	0/849
7	G	0.24	0/1612	0.45	0/2176
8	H	0.24	0/1476	0.43	0/1994
9	I	0.24	0/1543	0.48	0/2087
10	J	0.25	0/1614	0.53	4/2176 (0.2%)
11	N	0.25	0/1848	0.48	0/2489
12	T	0.23	0/1398	0.52	0/1901
All	All	0.24	0/17989	0.48	4/24301 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	8	ILE	CG1-CB-CG2	6.95	126.70	111.40
10	J	68	LEU	CB-CG-CD1	6.00	121.20	111.00
10	J	68	LEU	CB-CG-CD2	5.05	119.58	111.00
10	J	99	ILE	CG1-CB-CG2	5.02	122.45	111.40

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	1466	0	1474	23	0
2	B	1601	0	1638	29	0
3	C	1555	0	1540	20	0
4	D	1520	0	1573	15	0
5	E	1598	0	1638	27	0
6	F	617	0	619	11	0
7	G	1583	0	1603	15	0
8	H	1449	0	1476	13	0
9	I	1526	0	1578	24	0
10	J	1589	0	1620	30	0
11	N	1816	0	1836	34	0
12	T	1364	0	1383	14	0
All	All	17684	0	17978	214	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 214 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:46:LEU:HD12	3:C:59:LEU:HD21	1.52	0.90
9:I:42:LEU:HD22	9:I:61:LEU:HD13	1.53	0.87
11:N:120:VAL:HG22	11:N:124:VAL:HG23	1.59	0.83
7:G:136:ASP:OD1	7:G:137:MET:N	2.12	0.82
7:G:23:ASN:OD1	7:G:102:SER:OG	1.98	0.81

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	185/190 (97%)	176 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
3	C	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
4	D	197/199 (99%)	197 (100%)	0	0	100	100
5	E	203/260 (78%)	198 (98%)	5 (2%)	0	100	100
6	F	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
7	G	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
8	H	177/183 (97%)	173 (98%)	4 (2%)	0	100	100
9	I	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
10	J	196/212 (92%)	191 (97%)	5 (3%)	0	100	100
11	N	221/631 (35%)	216 (98%)	5 (2%)	0	100	100
12	T	172/627 (27%)	159 (92%)	13 (8%)	0	100	100
All	All	2210/3179 (70%)	2148 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	160/163 (98%)	158 (99%)	2 (1%)	69	87
2	B	180/180 (100%)	180 (100%)	0	100	100
3	C	174/174 (100%)	174 (100%)	0	100	100
4	D	170/170 (100%)	170 (100%)	0	100	100
5	E	174/213 (82%)	174 (100%)	0	100	100
6	F	69/76 (91%)	68 (99%)	1 (1%)	67	85
7	G	176/176 (100%)	176 (100%)	0	100	100
8	H	161/165 (98%)	161 (100%)	0	100	100
9	I	175/175 (100%)	175 (100%)	0	100	100
10	J	176/189 (93%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	N	202/563 (36%)	201 (100%)	1 (0%)	88	95
12	T	145/538 (27%)	145 (100%)	0	100	100
All	All	1962/2782 (70%)	1958 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	106	ARG
6	F	12	LYS
11	N	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	102	HIS
6	F	52	HIS
10	J	69	HIS
11	N	115	HIS

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 (i)

This section contains visualisations of the EMDB entry EMD-28827. 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 (i)

6.1.1   Primary map
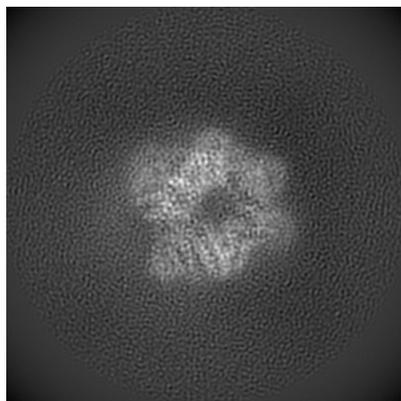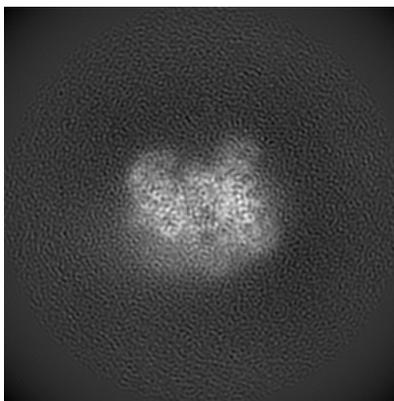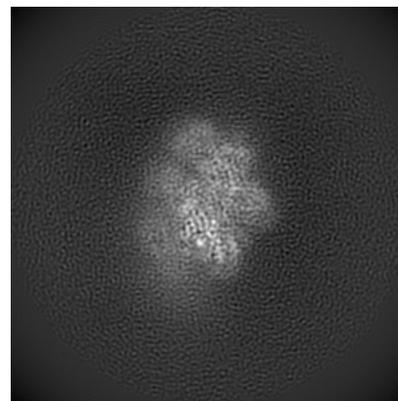
X   Y   Z

6.1.2   Raw map

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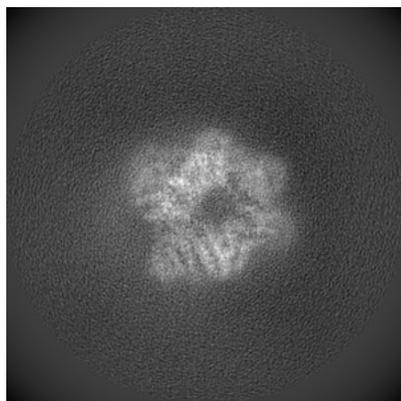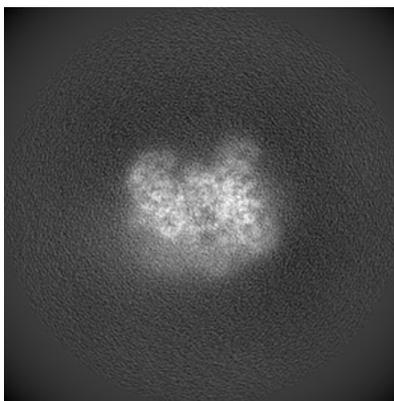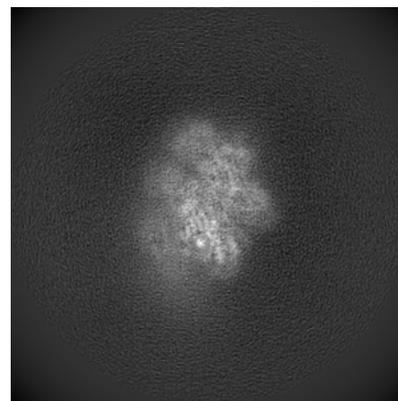
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
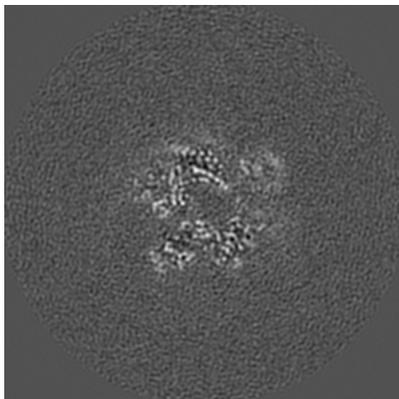
6.2.1   Primary map
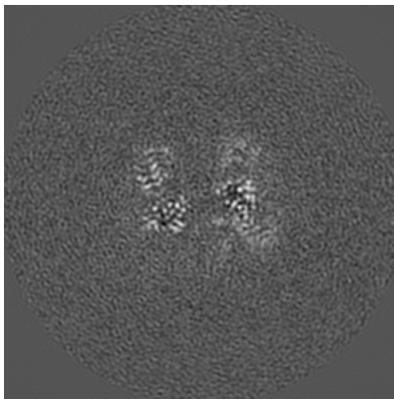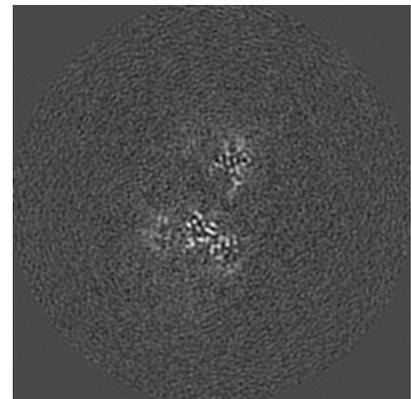
X Index: 132   Y Index: 132   Z Index: 132

6.2.2   Raw map
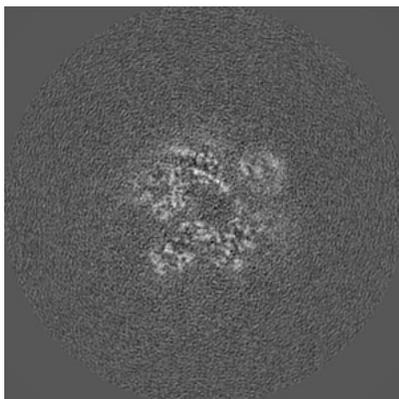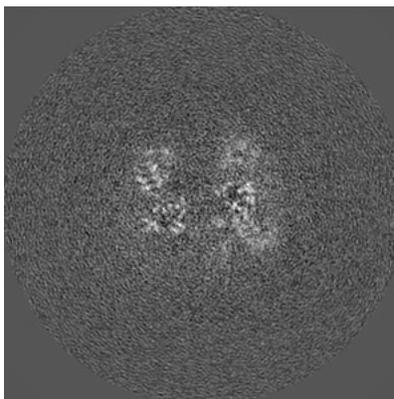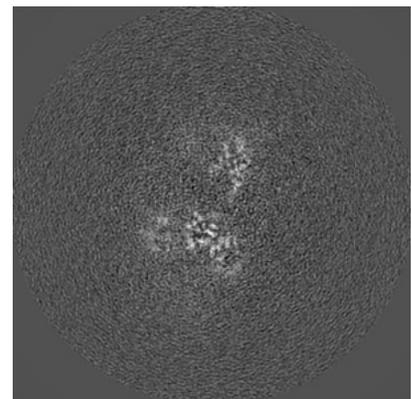
X Index: 132   Y Index: 132   Z Index: 132

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

6.3 Largest variance slices (i)

6.3.1 Primary map
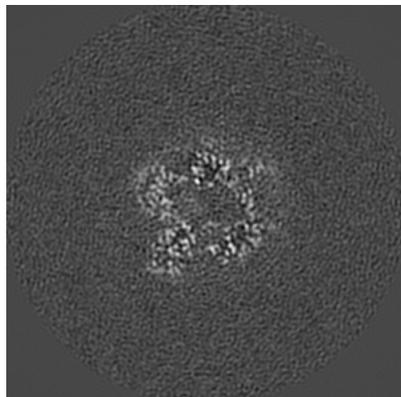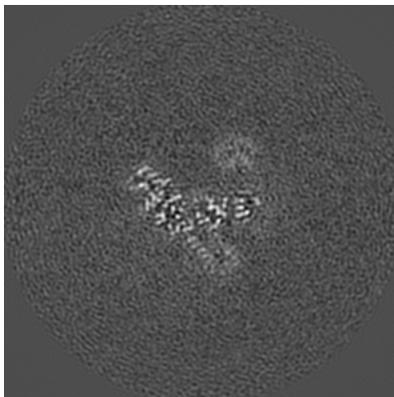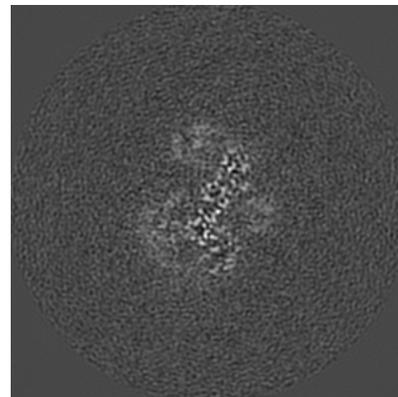
| X Index: 137 | Y Index: 121 | Z Index: 146 |

6.3.2 Raw map
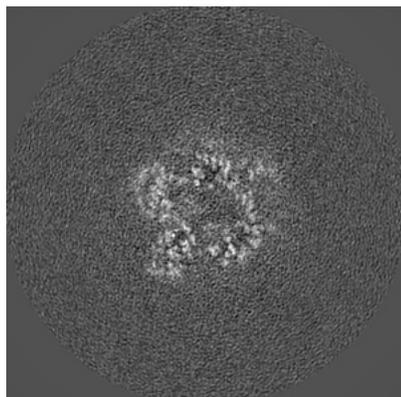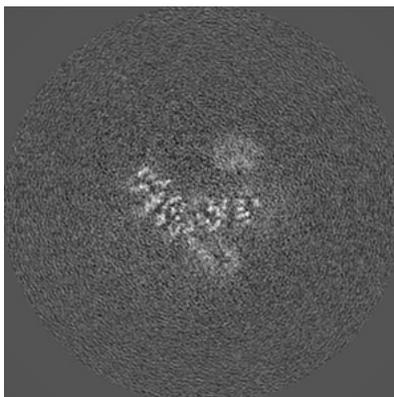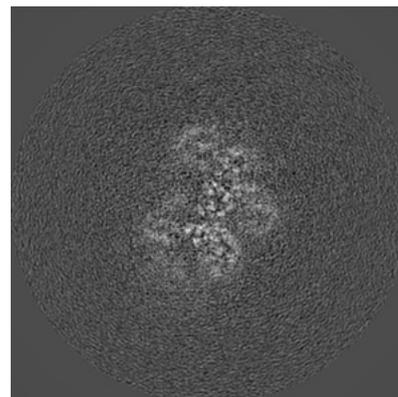
| X Index: 137 | Y Index: 121 | Z Index: 148 |

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
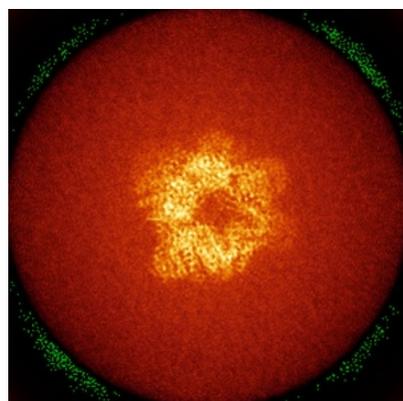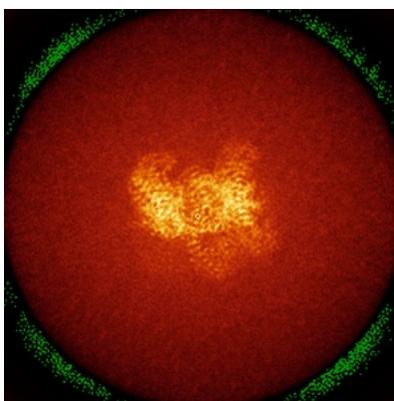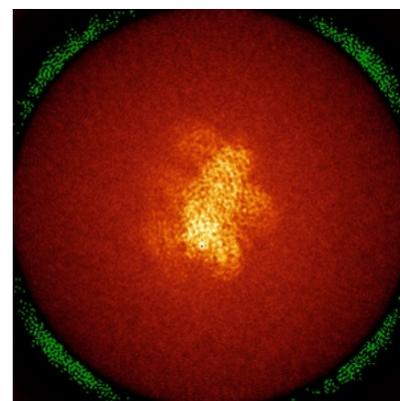
X   Y   Z

6.4.2   Raw map

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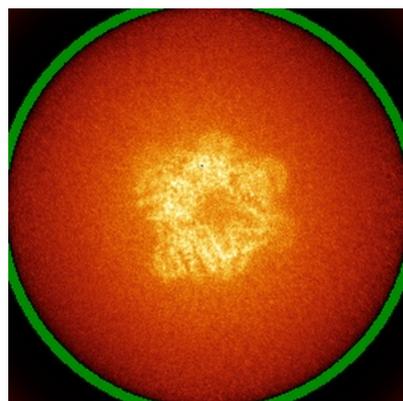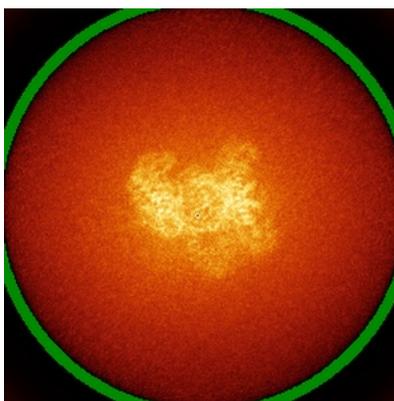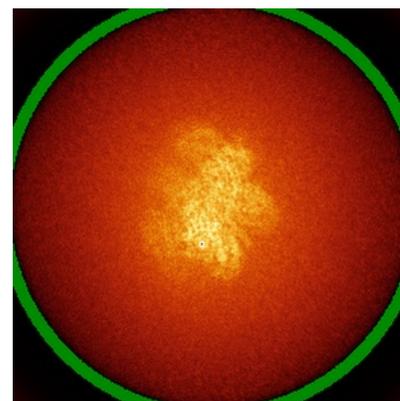
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
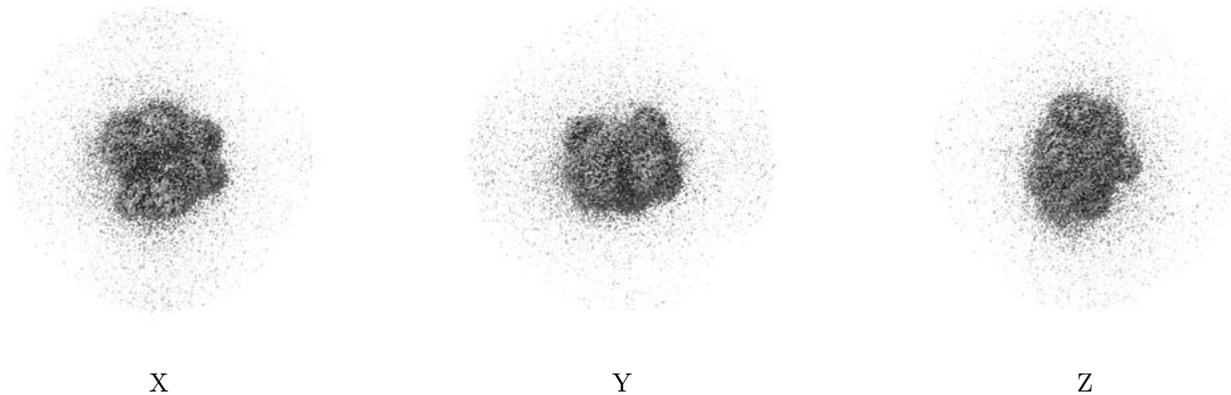
The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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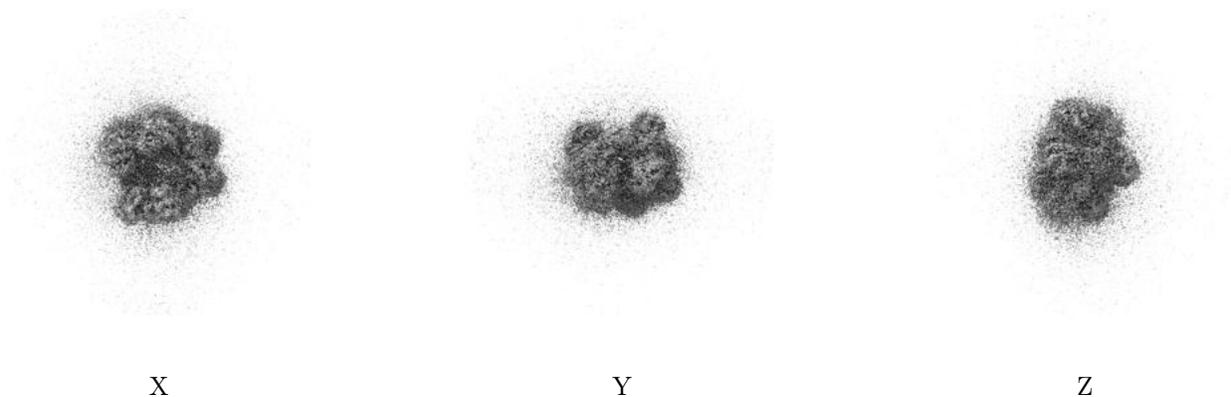
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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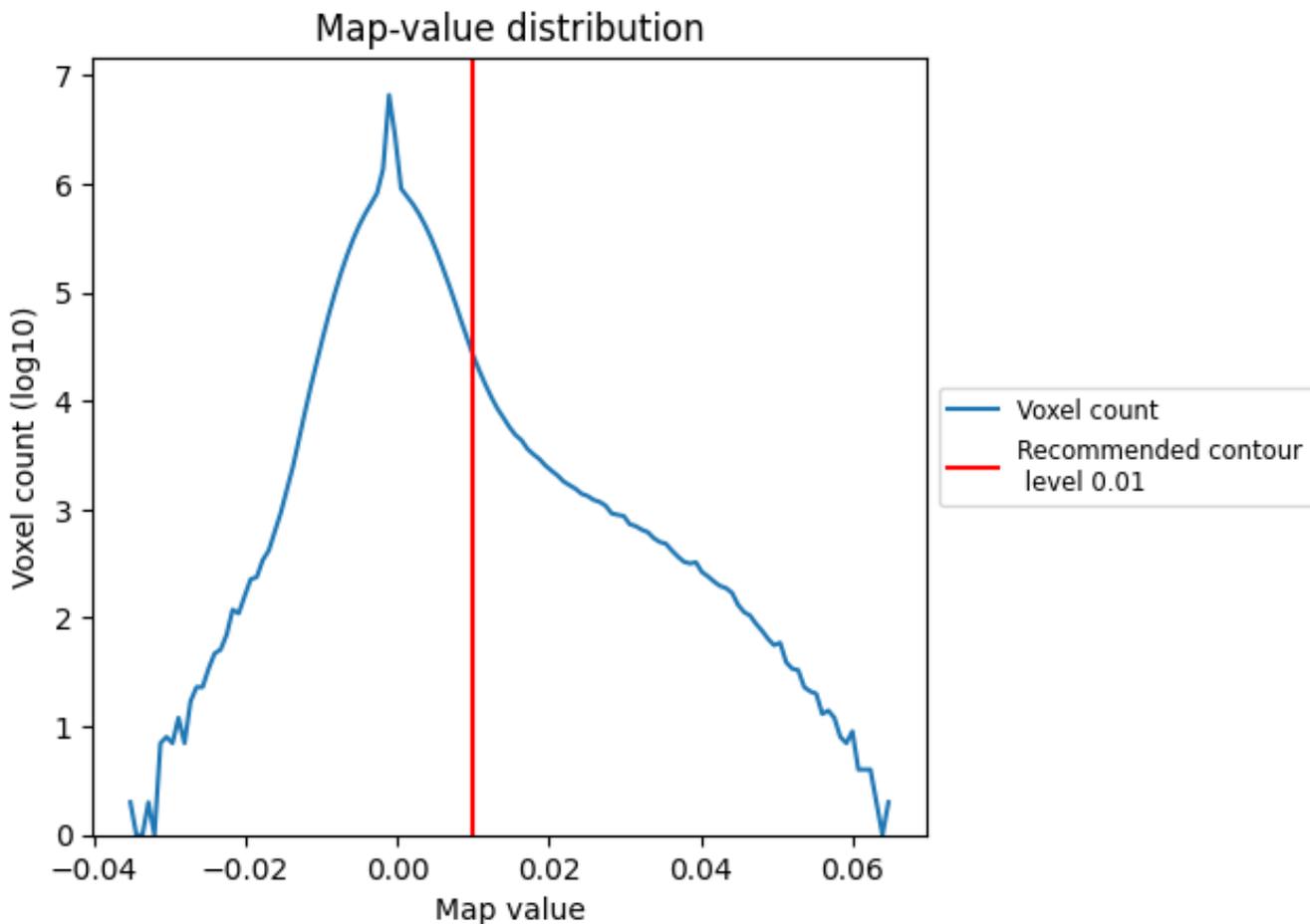
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
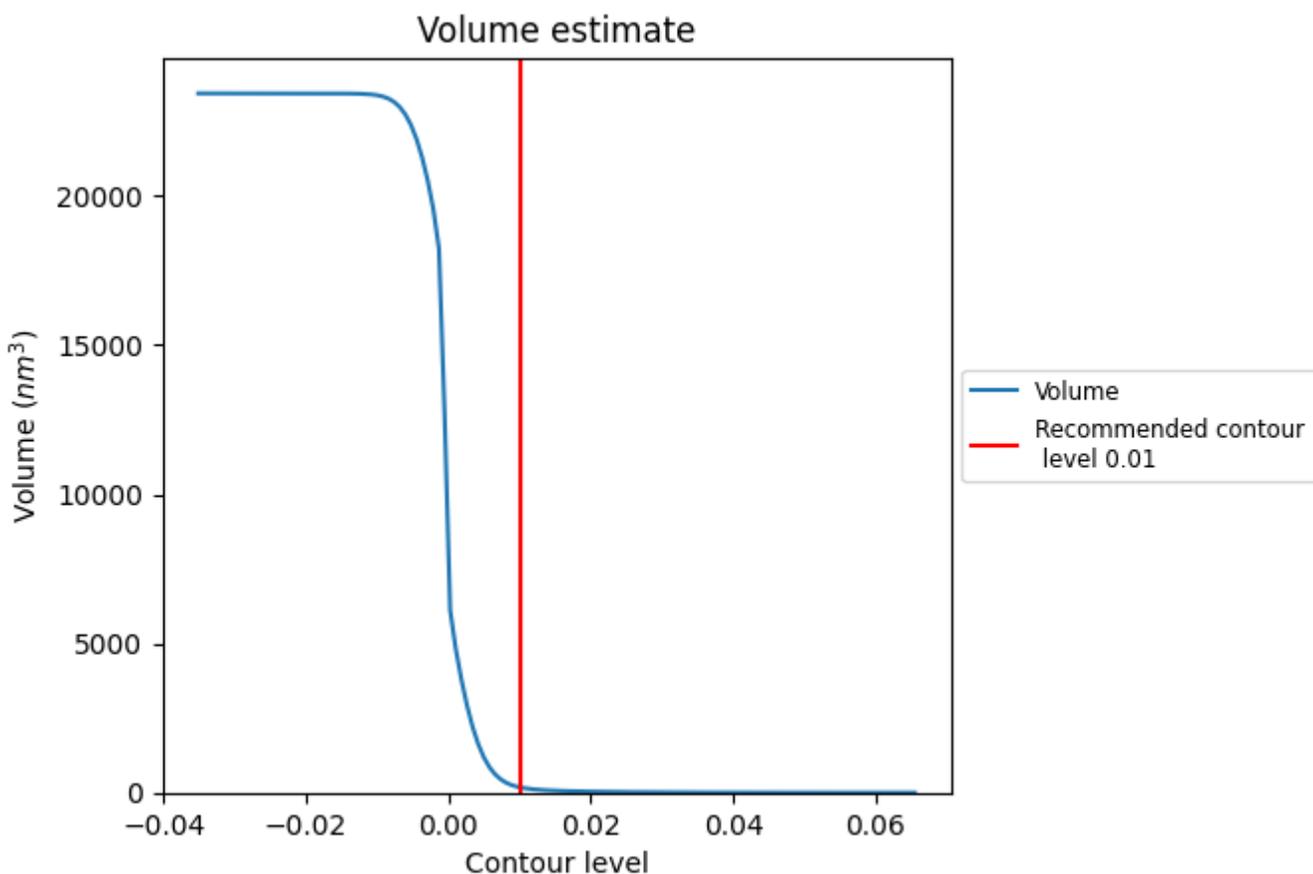
The volume at the recommended contour level is 181 nm^3; this corresponds to an approximate mass of 163 kDa.

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 ⓘ
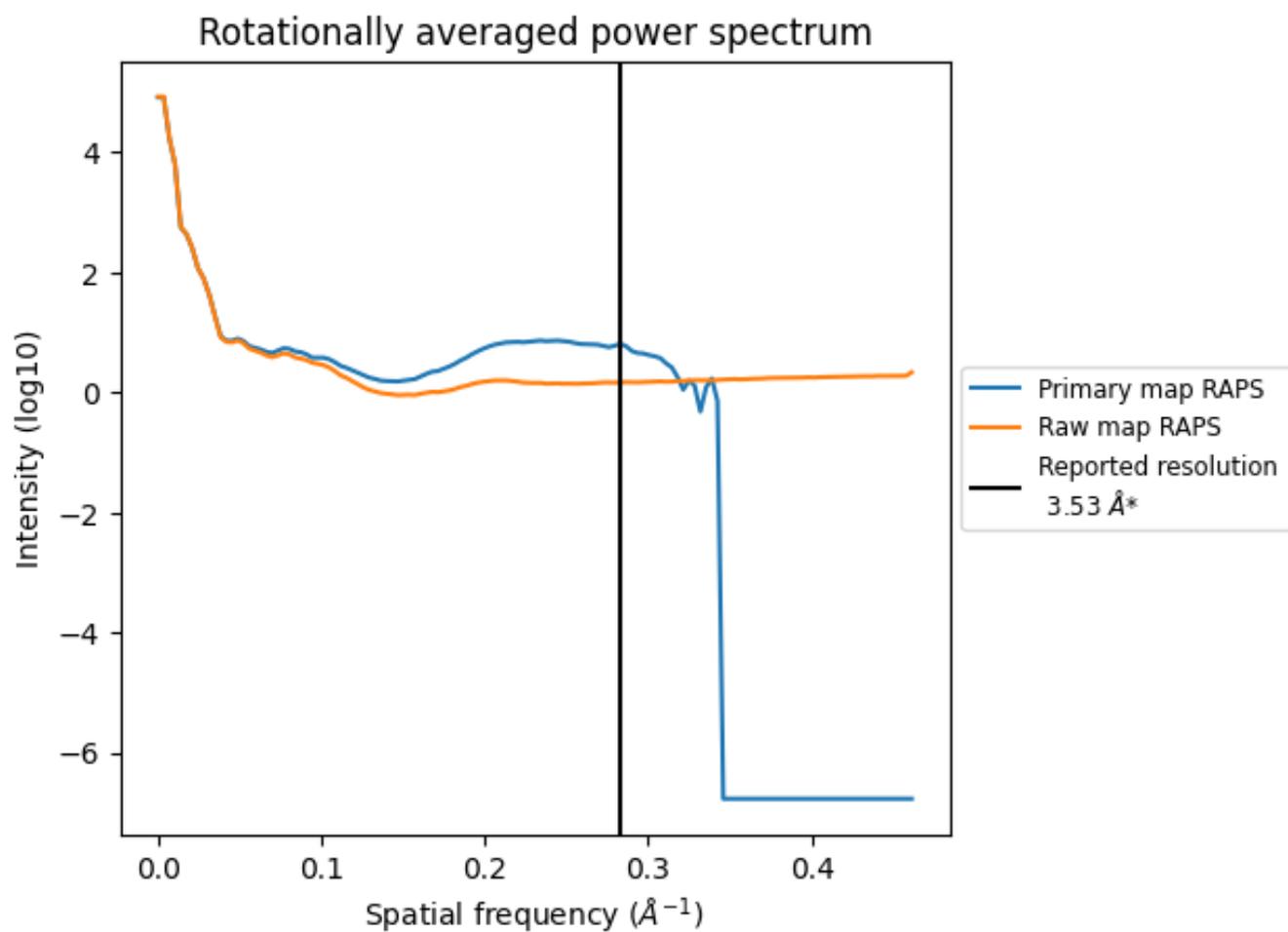
*Reported resolution corresponds to spatial frequency of 0.283 Å^{-1}

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 ⓘ
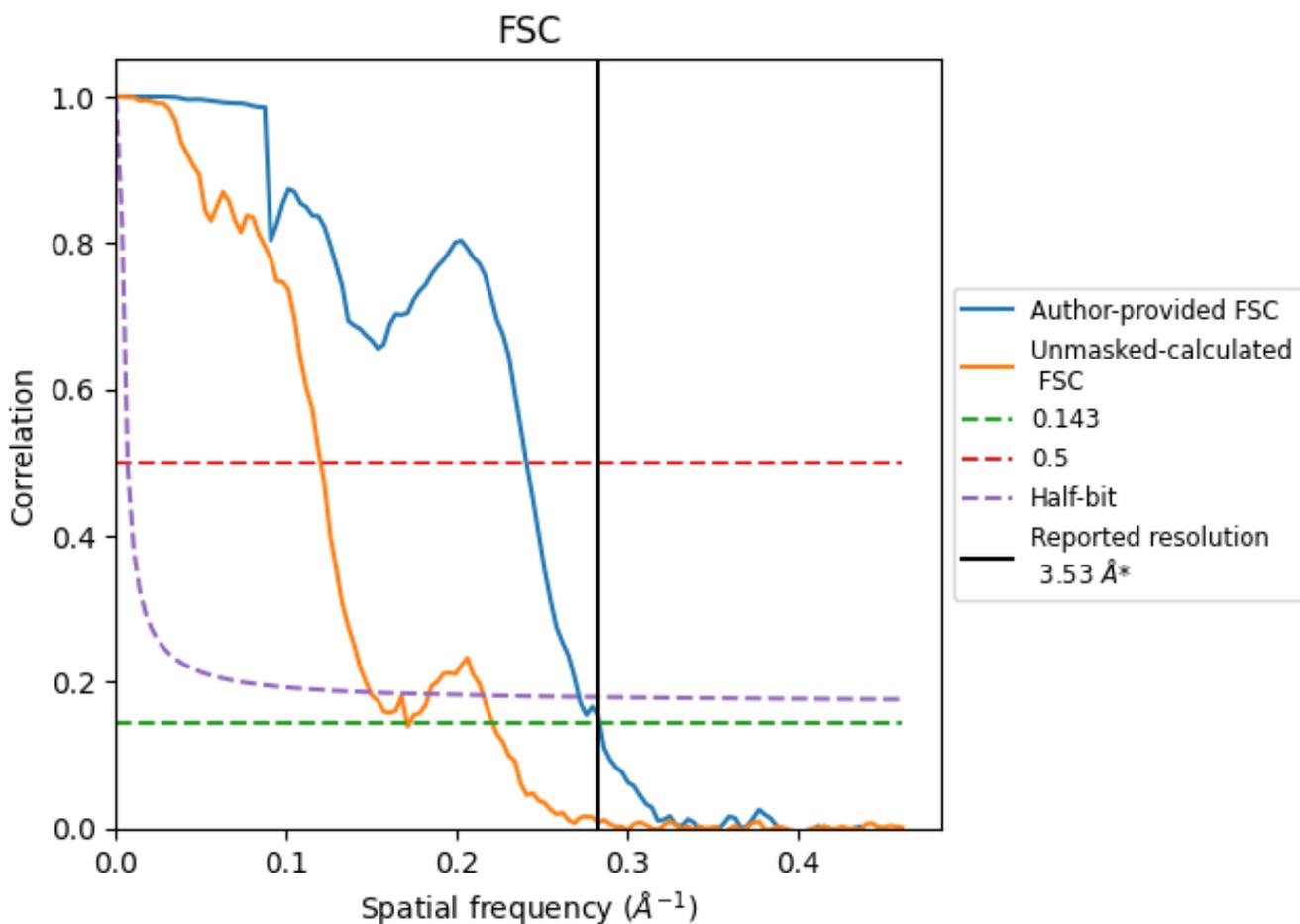
*Reported resolution corresponds to spatial frequency of 0.283 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.52	4.15	3.68
Unmasked-calculated*	5.85	8.33	6.69

*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 5.85 differs from the reported value 3.53 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-28827 and PDB model 8F2U. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay ⓘ


X   Y   Z
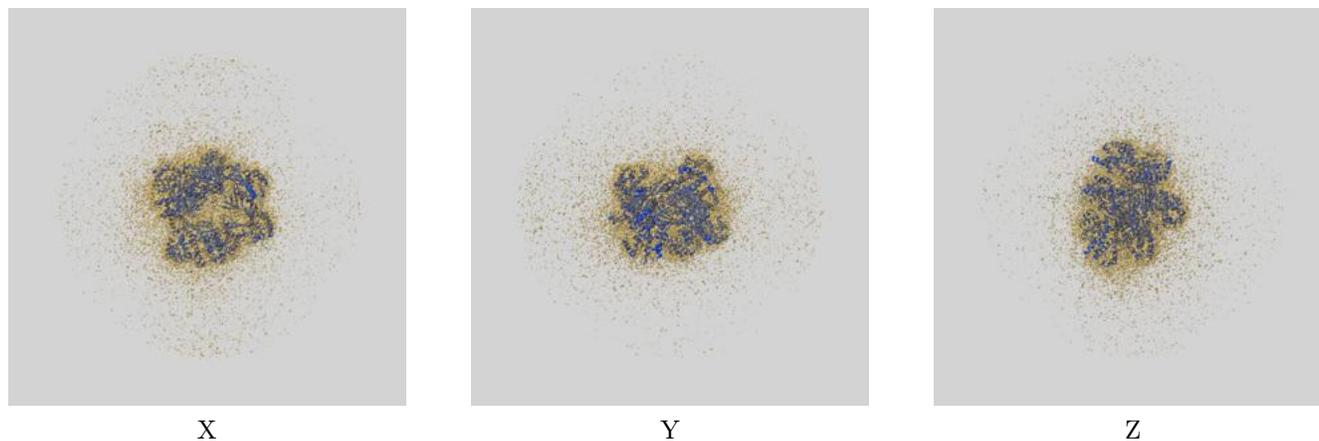
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ


X   Y   Z
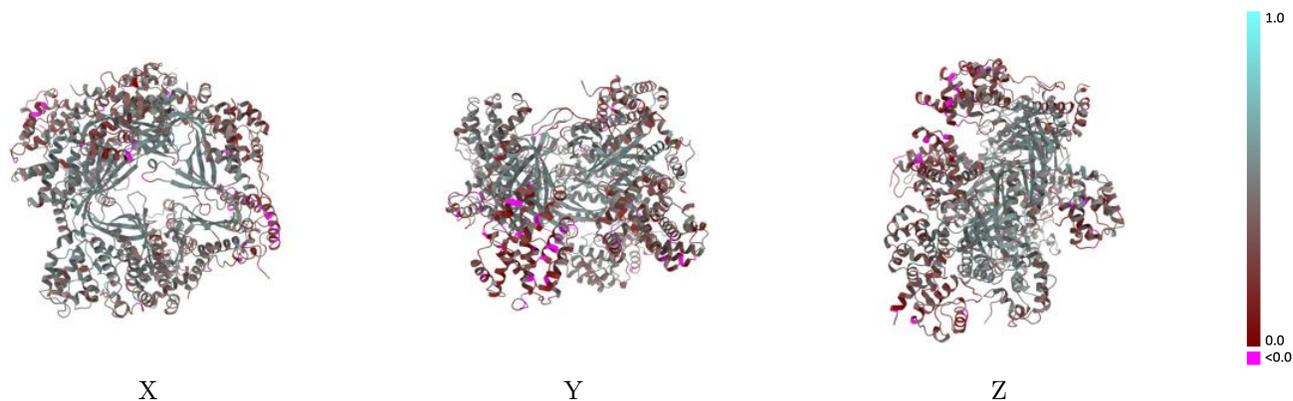
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
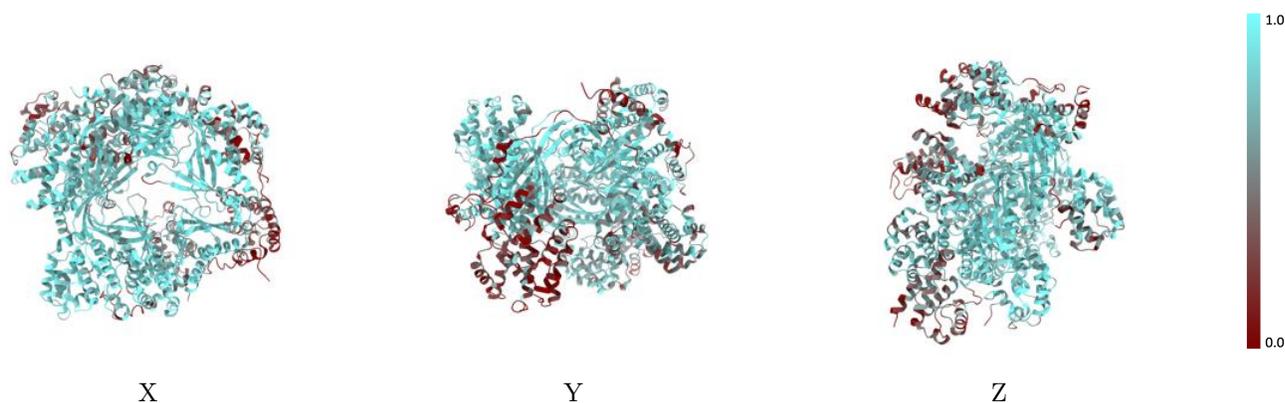
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4   Atom inclusion   ⓘ
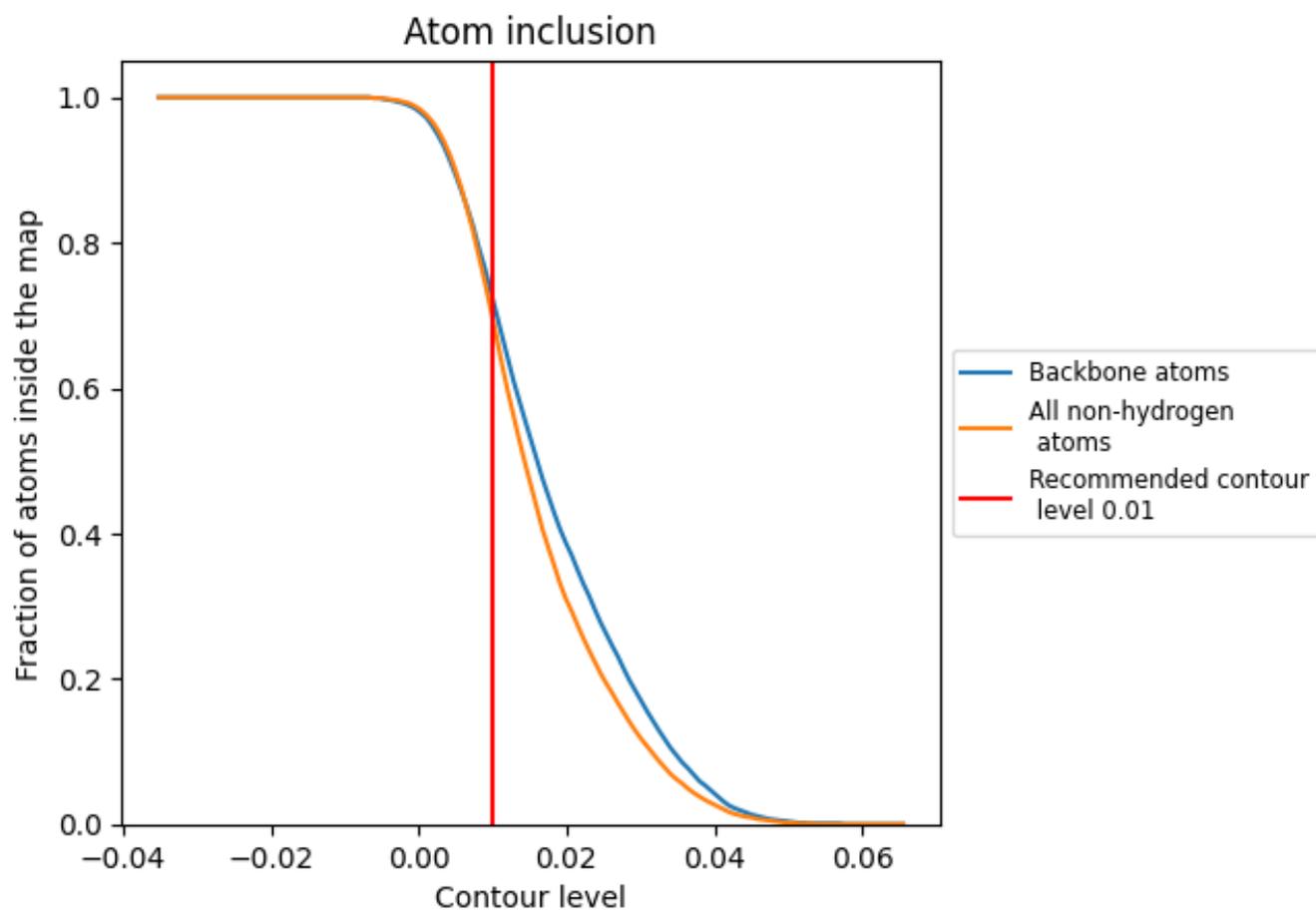
At the recommended contour level, 72% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.4080
A	0.5060	0.3460
B	0.7580	0.4270
C	0.8510	0.4840
D	0.7900	0.4500
E	0.8470	0.4710
F	0.8720	0.4880
G	0.4860	0.3050
H	0.8540	0.4830
I	0.7130	0.3880
J	0.7550	0.4040
N	0.4540	0.3270
T	0.6000	0.3800

1.0

0.0
<0.0