wwPDB EM Validation Summary Report (i)

Jan 22, 2024 – 03:44 PM JST

PDB ID	:	8HPQ
EMDB ID	:	EMD-34940
Title	:	Cryo-EM structure of SARS-CoV-2 Omicron BA.4 S-trimer in complex with fab L4.65 and L5.34
Authors	:	Gao, G.F.; Liu, S.
Deposited on	:	2022-12-12
Resolution	:	2.85 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 2.85 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		10
Ramachandran outliers		0.1%
Sidechain outliers		0.5%

Worse *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
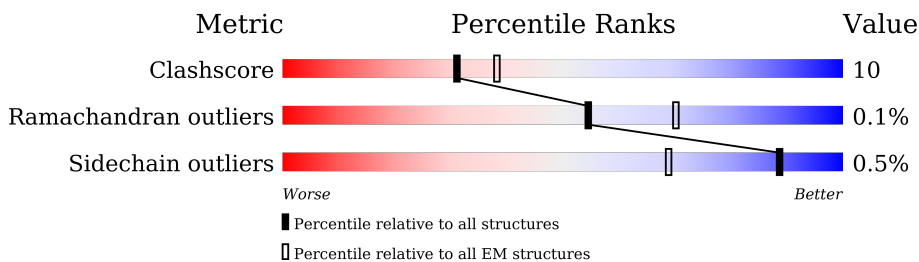
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1129	75% 15% · 9%
1	B	1129	75% 15% · 9%
1	C	1129	76% 15% 9%
2	H	231	39% 77% 22% ·
2	I	231	55% 78% 21% ·
2	P	231	63% 78% 21% ·
3	J	215	71% 73% 27%
3	L	215	52% 72% 28%

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Mol	Chain	Length	Quality of chain
3	Q	215	73% / 73% 27%
4	E	224	58% / 80% 20%
4	M	224	28% / 81% 19%
4	R	224	54% / 80% 20%
5	F	216	60% / 71% 29%
5	N	216	40% / 71% 29%
5	S	216	59% / 72% 28%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 44355 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 Spike protein S2'.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1029	Total 8059	C 5158	N 1342	O 1522	S 37	1	0
1	B	1029	Total 8059	C 5158	N 1342	O 1522	S 37	1	0
1	C	1029	Total 8059	C 5158	N 1342	O 1522	S 37	1	0

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ILE	THR	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	43	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	156	ASP	GLY	variant	UNP P0DTC2
A	353	ASP	GLY	variant	UNP P0DTC2
A	385	PHE	SER	variant	UNP P0DTC2
A	387	PRO	SER	variant	UNP P0DTC2
A	389	PHE	SER	variant	UNP P0DTC2
A	390	ALA	THR	variant	UNP P0DTC2
A	419	ASN	ASP	variant	UNP P0DTC2
A	422	SER	ARG	variant	UNP P0DTC2
A	431	ASN	LYS	variant	UNP P0DTC2
A	454	LYS	ASN	variant	UNP P0DTC2
A	466	ARG	LEU	variant	UNP P0DTC2
A	491	ASN	SER	variant	UNP P0DTC2
A	492	LYS	THR	variant	UNP P0DTC2
A	498	ALA	GLU	variant	UNP P0DTC2
A	500	VAL	PHE	variant	UNP P0DTC2
A	512	ARG	GLN	variant	UNP P0DTC2
A	515	TYR	ASN	variant	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	519	HIS	TYR	variant	UNP P0DTC2
A	628	GLY	ASP	variant	UNP P0DTC2
A	669	TYR	HIS	variant	UNP P0DTC2
A	778	LYS	ASN	variant	UNP P0DTC2
A	810	TYR	ASP	variant	UNP P0DTC2
A	831	PRO	PHE	conflict	UNP P0DTC2
A	906	PRO	ALA	conflict	UNP P0DTC2
A	913	PRO	ALA	conflict	UNP P0DTC2
A	956	PRO	ALA	conflict	UNP P0DTC2
A	968	HIS	GLN	variant	UNP P0DTC2
A	983	LYS	ASN	variant	UNP P0DTC2
A	1000	PRO	LYS	conflict	UNP P0DTC2
A	1001	PRO	VAL	conflict	UNP P0DTC2
B	38	ILE	THR	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	43	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	156	ASP	GLY	variant	UNP P0DTC2
B	353	ASP	GLY	variant	UNP P0DTC2
B	385	PHE	SER	variant	UNP P0DTC2
B	387	PRO	SER	variant	UNP P0DTC2
B	389	PHE	SER	variant	UNP P0DTC2
B	390	ALA	THR	variant	UNP P0DTC2
B	419	ASN	ASP	variant	UNP P0DTC2
B	422	SER	ARG	variant	UNP P0DTC2
B	431	ASN	LYS	variant	UNP P0DTC2
B	454	LYS	ASN	variant	UNP P0DTC2
B	466	ARG	LEU	variant	UNP P0DTC2
B	491	ASN	SER	variant	UNP P0DTC2
B	492	LYS	THR	variant	UNP P0DTC2
B	498	ALA	GLU	variant	UNP P0DTC2
B	500	VAL	PHE	variant	UNP P0DTC2
B	512	ARG	GLN	variant	UNP P0DTC2
B	515	TYR	ASN	variant	UNP P0DTC2
B	519	HIS	TYR	variant	UNP P0DTC2
B	628	GLY	ASP	variant	UNP P0DTC2
B	669	TYR	HIS	variant	UNP P0DTC2
B	778	LYS	ASN	variant	UNP P0DTC2
B	810	TYR	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	831	PRO	PHE	conflict	UNP P0DTC2
B	906	PRO	ALA	conflict	UNP P0DTC2
B	913	PRO	ALA	conflict	UNP P0DTC2
B	956	PRO	ALA	conflict	UNP P0DTC2
B	968	HIS	GLN	variant	UNP P0DTC2
B	983	LYS	ASN	variant	UNP P0DTC2
B	1000	PRO	LYS	conflict	UNP P0DTC2
B	1001	PRO	VAL	conflict	UNP P0DTC2
C	38	ILE	THR	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	43	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	156	ASP	GLY	variant	UNP P0DTC2
C	353	ASP	GLY	variant	UNP P0DTC2
C	385	PHE	SER	variant	UNP P0DTC2
C	387	PRO	SER	variant	UNP P0DTC2
C	389	PHE	SER	variant	UNP P0DTC2
C	390	ALA	THR	variant	UNP P0DTC2
C	419	ASN	ASP	variant	UNP P0DTC2
C	422	SER	ARG	variant	UNP P0DTC2
C	431	ASN	LYS	variant	UNP P0DTC2
C	454	LYS	ASN	variant	UNP P0DTC2
C	466	ARG	LEU	variant	UNP P0DTC2
C	491	ASN	SER	variant	UNP P0DTC2
C	492	LYS	THR	variant	UNP P0DTC2
C	498	ALA	GLU	variant	UNP P0DTC2
C	500	VAL	PHE	variant	UNP P0DTC2
C	512	ARG	GLN	variant	UNP P0DTC2
C	515	TYR	ASN	variant	UNP P0DTC2
C	519	HIS	TYR	variant	UNP P0DTC2
C	628	GLY	ASP	variant	UNP P0DTC2
C	669	TYR	HIS	variant	UNP P0DTC2
C	778	LYS	ASN	variant	UNP P0DTC2
C	810	TYR	ASP	variant	UNP P0DTC2
C	831	PRO	PHE	conflict	UNP P0DTC2
C	906	PRO	ALA	conflict	UNP P0DTC2
C	913	PRO	ALA	conflict	UNP P0DTC2
C	956	PRO	ALA	conflict	UNP P0DTC2
C	968	HIS	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	983	LYS	ASN	variant	UNP P0DTC2
C	1000	PRO	LYS	conflict	UNP P0DTC2
C	1001	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called fab L4.65.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		
2	P	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		
2	I	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		

- Molecule 3 is a protein called fab L4.65.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		
3	Q	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		
3	J	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		

- Molecule 4 is a protein called fab L5.34.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	224	Total	C	N	O	S	0	0
			1656	1040	279	329	8		
4	E	224	Total	C	N	O	S	0	0
			1656	1040	279	329	8		
4	R	224	Total	C	N	O	S	0	0
			1656	1040	279	329	8		

- Molecule 5 is a protein called fab L5.34.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	216	Total	C	N	O	S	0	0
			1642	1020	280	336	6		
5	F	216	Total	C	N	O	S	0	0
			1642	1020	280	336	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	216	1642	1020	280	336	6	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
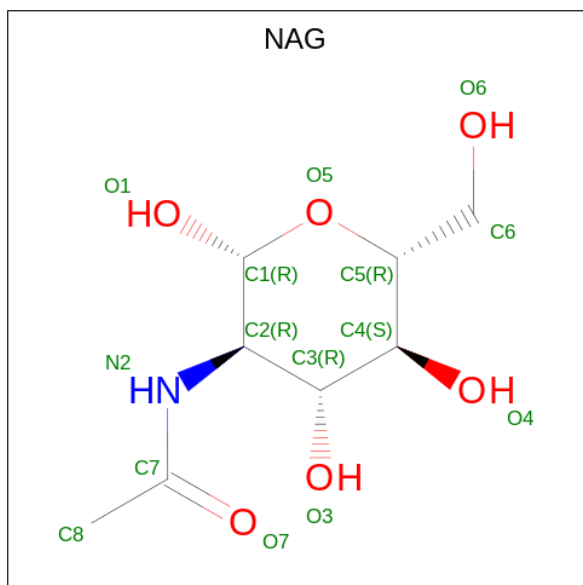
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

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: Spike protein S2'

Chain A:

- Molecule 1: Spike protein S2'

Chain B:

• Molecule 1: Spike protein S2'

Chain C:

76%   15%   9%

G662 V670 N671 N672 S673 I678 Q689 THR GLN ASN SER PRO ARG ARG ALA ARG SER VAL ALA SER GLN S705 S712 L713 N717 S718 V719 A720 Y721 S722 N723 I726 A727 I728 P729 I734 S735 V736 T737 T738 V750 M754 D759 Y770 K790

E794 L835 T841 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN LYS PHE N870 G871 L872 M883 Q886 T897 L908 Q909 L930 Y931 E932 I937 Q940 I948 S953 L973

L976 V977 K978 D999 P1000 A1003 D1008 R1009 L1010 L1018 K1042 F1056 H1062 V1079 T1080 K1100 Y1124 V1136 V1142 L1155 L1159 D1160 S1161

• Molecule 2: fab L4.65

Chain H:

39%

77%   22%

Q1 I2 P9 T10 L11 V12 K13 P14 T15 Q16 T17 L18 G26 L29 V36 Q41 P42 P43 L47 N67 R68 I71 T85 N86 M87 D88 P89 E90 D91 T92 N108 Y109 Y110 W114 F115 D116 V124 T125 V126 S127 S128 A129 S130 T131 K132 S135 V136

F137 P138 L139 A140 P141 S142 S143 K144 S145 T146 S147 G148 G149 T150 A151 A152 L153 G154 C155 L156 V157 K158 D159 Y160 F161 P162 E163 P164 V165 T166 V167 S168 W169 N170 S171 G172 A173 L174 T175 S176 G177 V178 H179 T180 L185 Q186 S187 S188 G189 L190 Y191 S192 L193 V197 T198 V199 P200 S201

S202 S203 L204 G205 T206 Q207 T208 Y209 I210 C211 N212 V213 N214 H215 K216 P217 S218 N219 T220 K221 V222 D223 K224 R225 V226 E227 P228 K229 S230 C231

• Molecule 2: fab L4.65

Chain P:

63%

78%   21%

Q1 I2 S7 G8 P9 T10 L11 V12 K13 P14 T15 Q16 T17 L18 T19 G26 L29 S30 V36 R40 Q41 P42 P43 G44 K45 A46 L47 A51 N57 D58 K59 R60 S61 S64 L65 N66 N67 R68 L69 T70 I71 T72 K73 D74 T75 S76 T83 M84 T85 N86 M87

D88 P89 E90 D91 T92 S106 S107 N108 Y109 Y110 W114 F115 D116 Q120 G121 T122 L123 V124 T125 V126 S127 S128 A129 S130 T131 K132 G133 P134 S135 V136 F137 P138 L139 A140 P141 S142 S143 K144 S145 T146 S147 G148 G149 T150 A151 A152 L153 G154 C155 L156 V157 K158 D159 Y160 F161 P162 E163

P164 V165 T166 V167 S168 W169 N170 S171 G172 A173 L174 T175 S176 G177 V178 H179 T180 F181 P182 A183 V184 L185 Q186 S187 S188 G189 L190 Y191 S192 L193 V197 T198 V199 P200 S201 S202 S203 L204 G205 T206 Q207 T208 Y209 I210 C211 N212 V213 N214 H215 K216 P217 S218 N219 T220 K221 V222 D223 K224 R225

V226 E227 P228 K229 S230 C231

• Molecule 2: fab L4.65

Chain I:

55%

78%   21%

Q1 I2 S7 T10 L11 V12 K13 P14 T15 Q16 T17 L18 T19 G26 L29 V36 Q41 P42 P43 G44 K45 A46 L47 N57 S61 S62 P63 S64 L65 N66 N67 R68 L69 T70 D74 T75 S76 K77 M84 T85 N86 M87 D88 P89 E90 D91 T92 N108 Y109

Y110 W114 F115 D116 Q120 L123 V124 T125 V126 S127 S128 A129 S130 T131 K132 G133 P134 S135 V136 F137 P138 L139 A140 P141 S142 S143 K144 S145 T146 S147 G148 G149 T150 A151 A152 L153 G154 C155 L156 V157 K158 D159 Y160 F161 P162 E163 P164 V165 T166 V167 S168 W169 N170 S171 G172 A173 L174

T175 S176 G177 V178 H179 T180 F181 P182 A183 V184 L185 Q186 S187 S188 G189 L190 Y191 S192 L193 S194 S195 V196 V197 T198 V199 P200 S201 S202 S203 L204 G205 T206 Q207 T208 Y209 I210 C211 N212 V213 N214 H215 K216 P217 S218 N219 T220 K221 V222 D223 K224 R225 V226 E227 P228 K229 S230 C231

• Molecule 3: fab L4.65

Chain L:

E1 I2 V3 L4 S7 P8 G9 T10 L11 S12 L13 S14 P15 G16 E17 R18 A19 R32 Y33 L34 Y37 Q38 Q39 K40 S41 G42 T57 G58 D61 R62 G65 S66 G67 S68 G69 F72 I76 S77 R78 L79 E80 P81 E82 A85 C89 G93 G100

T103 K104 L105 E106 I107 K108 R109 T110 V111 A112 A113 P114 S115 V116 F117 I118 F119 P120 P121 S122 D123 E124 Q125 L126 K127 S128 G129 T130 A131 L136 L137 N138 N139 F140 Y141 P142 R143 E144 A145 K146 V147 Q148 W149 K150 V151 D152 N153 A154 L155 Q156 S157 G158 N159 S160 E166 Q167 D168 S169

K170 D171 S172 T173 S177 S178 T179 L182 S183 K184 A185 D186 Y187 E188 K189 H190 K191 V192 Y193 A194 C195 E196 V197 T198 H199 Q200 G201 L202 S203 S204 P205 V206 T207 K208 S209 F210 N211 R212 G213 E214 C215

• Molecule 3: fab L4.65

Chain Q:

E1 I2 V3 L4 T5 Q6 S7 P8 G9 T10 L11 S12 L13 S14 P15 G16 E17 R18 A19 T20 L21 R24 S28 S31 R32 Y33 L34 Y37 Q38 Q39 K40 S41 G42 S54 R55 A56 T57 G58 I59 P60 D61 R62 F63 S64 G65 S66 G67 S68 G69 F72 T75 I76 S77

R78 L79 E80 P81 E82 A85 C89 G93 D94 S95 G100 Q101 K104 L105 E106 I107 K108 R109 T110 V111 A112 A113 P114 S115 V116 F117 I118 F119 P120 P121 S122 D123 E124 Q125 L126 K127 S128 G129 T130 A131 S132 V133 V134 C135 L136 L137 N138 N139 F140 Y141 P142 R143 E144 A145 K146

V147 Q148 W149 K150 V151 D152 N153 A154 L155 Q156 S157 G158 N159 S160 Q161 E162 S163 V164 T165 E166 Q167 D168 S169 K170 D171 S172 T173 Y174 S175 L176 S177 S178 T179 L180 T181 L182 S183 K184 A185 D186 Y187 E188 K189 H190 K191 V192 Y193 A194 C195 E196 V197 T198 H199 Q200 G201 L202 S203 S204 P205 V206

T207 K208 S209 F210 N211 R212 G213 E214 C215

• Molecule 3: fab L4.65

Chain J:

E1 S7 P8 G9 T10 L11 S12 L13 S14 P15 G16 E17 R18 A19 T20 L21 S22 Q27 D30 S31 R32 Y33 L34 Y37 Q38 Q39 K40 S41 G42 Q43 R55 A56 T57 G58 I59 P60 D61 R62 F63 S64 G65 S66 G67 S68 G69 F72 T73 L74 T75 I76 S77 R78 L79 E80

- Molecule 4: fab L5.34

Chain M:

- Molecule 4: fab L5.34

Chain E:

- Molecule 4: fab L5.34

Chain R:

G101 F102 P103 L104 D110 Q114 G115 T116 M117 V118 T119 V120 S121 S122 A123 S124 T125 K126 G127 P128 S129 V130 F131 P132 L133 A134 P135 S136 S137 K138 S139 T140 S141 G142 G143 T144 A145 A146 L147 G148 C149 L150 V151 K152 D153 Y154 F155 P156 E157 P158 V159 T160 V161 S162 W163 N164 S165 G166

A167 L168 T169 S170 G171 V172 H173 T174 F175 P176 A177 V178 L179 Q180 S181 S182 G183 L184 Y185 S186 L187 S188 S189 V190 P194 S195 S196 S197 L198 G199 T200 Q201 T202 Y203 I204 C205 N206 V207 N208 H209 K210 P211 S212 N213 T214 K215 V216 D217 K218 R219 V220 E221 P222 K223 S224 C225

- Molecule 5: fab L5.34

Chain N:
40%
71% 29%

D1 I2 V15 G16 D17 R18 I21 T22 L33 H34 W35 G41 K42 I48 S56 S60 R61 F71 T72 L73 T74 I75 T76 S77 L78 Q79 P80 E81 D82 F83 Q90 S93 T94 P95 R96 G97 E107 I108 K109 R110 T111 V112 A113 A114 P115 S116 V117 F118 I119

F120 P121 P122 S123 D124 E125 Q126 L127 K128 S129 G130 T131 A132 S133 V134 V135 L138 N139 N140 F141 Y142 P143 R144 E145 A146 K147 V148 Q149 W150 K151 V152 D153 N154 A155 L156 Q157 S158 G159 N160 S161 Q162 E163 S164 E167 Q168 D169 S170 K171 S178 S179 T180 L181 T182 L183 S184 K185 A186

D187 Y188 E189 K190 H191 K192 V193 Y194 A195 C196 E197 V198 T199 H200 Q201 G202 L203 S204 S205 P206 V207 T208 K209 S210 F211 N212 R213 G214 E215 C216

- Molecule 5: fab L5.34

Chain F:
60%
71% 29%

D1 I2 Q3 P8 S9 S10 L11 S12 A13 S14 V15 G16 D17 R18 V19 S20 I21 T22 S28 T31 H32 L33 H34 W35 K39 P40 G41 K42 K45 I48 A51 S56 G57 V58 P59 S60 R61 F62 F71 T72 L73 T74 I75 T76 S77 L78 Q79 P80 E81 D82 F83

Q90 S93 T94 P95 R96 G97 E107 I108 K109 R110 T111 V112 A113 A114 P115 S116 V117 F118 I119 F120 P121 P122 S123 D124 E125 Q126 L127 K128 S129 G130 T131 A132 S133 V134 V135 L138 N139 N140 F141 Y142 P143 R144 E145 A146 K147 V148 Q149 W150 K151 V152 D153 N154 A155 L156 Q157 S158

G159 N160 S161 Q162 E163 S164 V165 T166 E167 Q168 D169 S170 K171 D172 S173 S176 L177 S178 S179 T180 L181 T182 L183 S184 K185 A186 D187 Y188 E189 K190 H191 K192 V193 Y194 A195 C196 E197 V198 T199 H200 Q201 G202 L203 S204 S205 P206 V207 T208 K209 S210 F211 N212 R213 G214 E215 C216

- Molecule 5: fab L5.34

Chain S:
59%
72% 28%

D1 I2 P8 S9 S10 L11 S12 A13 S14 V15 G16 D17 R18 I21 T22 S26 L33 H34 W35 K39 P40 G41 K42 I48 S56 G57 V58 P59 S60 R61 F62 S63 D70 F71 T72 L73 T74 I75 T76 S77 L78 Q79 P80 E81 D82 F83 Q90 S93 T94 P95

R96 G97 E107 I108 K109 R110 T111 V112 A113 A114 P115 S116 V117 F118 I119 F120 P121 P122 S123 D124 E125 Q126 L127 K128 S129 G130 T131 A132 S133 V134 V135 C136 L137 L138 N139 N140 F141 Y142 P143 R144 E145 A146 K147 V148 Q149 W150 K151 V152 D153 N154 A155 L156 Q157 S158 G159 N160 S161 Q162 E163

S164 V165 T166 E167 Q168 D169 S170 K171 D172 Y175 S176 L177 S178 S179 T180 L181 T182 L183 S184 K185 A186 D187 Y188 E189 K190 H191 K192 V193 Y194 A195 C196 E197 V198 T199 H200 Q201 G202 L203 S204 S205 P206 V207 T208 K209 S210 F211 N212 R213 G214 E215 C216

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	593563	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 $(e^-/Å^2)$	1.39	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.550	Depositor
Minimum map value	-5.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	430.08, 430.08, 430.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.48	2/8248 (0.0%)	0.64	9/11214 (0.1%)
1	B	0.48	4/8249 (0.0%)	0.61	6/11217 (0.1%)
1	C	0.36	2/8249 (0.0%)	0.63	7/11217 (0.1%)
2	H	0.27	0/1805	0.54	1/2471 (0.0%)
2	I	0.27	0/1805	0.54	1/2471 (0.0%)
2	P	0.27	0/1805	0.54	1/2471 (0.0%)
3	J	0.28	0/1694	0.53	0/2294
3	L	0.28	0/1694	0.53	0/2294
3	Q	0.28	0/1694	0.53	0/2294
4	E	0.28	0/1694	0.53	0/2308
4	M	0.28	0/1694	0.53	0/2308
4	R	0.28	0/1694	0.53	0/2308
5	F	0.27	0/1676	0.51	0/2272
5	N	0.27	0/1676	0.51	0/2272
5	S	0.27	0/1676	0.51	0/2272
All	All	0.38	8/45353 (0.0%)	0.58	25/61683 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	3
2	H	0	1
2	I	0	1
2	P	0	1
All	All	0	11

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	PHE	C-N	28.21	1.87	1.34
1	A	343	PHE	C-N	27.58	1.86	1.34
1	C	43	SER	CB-OG	8.66	1.53	1.42
1	A	43	SER	CB-OG	8.60	1.53	1.42
1	B	43	SER	CB-OG	8.59	1.53	1.42

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	THR	O-C-N	-15.98	97.13	122.70
1	A	321	THR	O-C-N	-14.09	100.16	122.70
1	C	321	THR	CA-C-N	10.39	140.06	117.20
1	C	321	THR	C-N-CA	9.82	146.24	121.70
1	B	321	THR	O-C-N	-9.27	107.87	122.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	THR	Mainchain
1	A	393	CYS	Peptide
1	B	321	THR	Mainchain
1	B	393	CYS	Peptide
2	H	116	ASP	Peptide

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8059	0	7855	182	0
1	B	8059	0	7856	207	0
1	C	8059	0	7857	207	0
2	H	1756	0	1713	36	0
2	I	1756	0	1713	36	0
2	P	1756	0	1713	35	0
3	J	1658	0	1599	41	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1658	0	1599	42	0
3	Q	1658	0	1599	39	0
4	E	1656	0	1620	33	0
4	M	1656	0	1620	31	0
4	R	1656	0	1620	31	0
5	F	1642	0	1599	40	0
5	N	1642	0	1599	42	0
5	S	1642	0	1599	39	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
All	All	44355	0	43200	849	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 10.

The worst 5 of 849 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:B:182:PHE:CE1	1:C:374:ASN:ND2	1.73	1.54
1:B:181:THR:CA	1:C:371:ARG:NH1	1.67	1.50
1:B:181:THR:CB	1:C:371:ARG:HH22	1.22	1.48
1:B:182:PHE:HE1	1:C:374:ASN:ND2	0.95	1.43
1:B:181:THR:HB	1:C:371:ARG:NH2	1.27	1.40

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	1006/1129 (89%)	974 (97%)	31 (3%)	1 (0%)	51	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1008/1129 (89%)	977 (97%)	29 (3%)	2 (0%)	47	75
1	C	1008/1129 (89%)	982 (97%)	26 (3%)	0	100	100
2	H	229/231 (99%)	213 (93%)	16 (7%)	0	100	100
2	I	229/231 (99%)	213 (93%)	16 (7%)	0	100	100
2	P	229/231 (99%)	213 (93%)	16 (7%)	0	100	100
3	J	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
3	L	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
3	Q	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
4	E	222/224 (99%)	210 (95%)	12 (5%)	0	100	100
4	M	222/224 (99%)	210 (95%)	12 (5%)	0	100	100
4	R	222/224 (99%)	210 (95%)	12 (5%)	0	100	100
5	F	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
5	N	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
5	S	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
All	All	5656/6045 (94%)	5441 (96%)	212 (4%)	3 (0%)	54	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	THR
1	B	344	PRO
1	B	716	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	898/983 (91%)	891 (99%)	7 (1%)	81	93
1	B	898/983 (91%)	889 (99%)	9 (1%)	76	91
1	C	898/983 (91%)	891 (99%)	7 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	204/204 (100%)	204 (100%)	0	100	100
2	I	204/204 (100%)	204 (100%)	0	100	100
2	P	204/204 (100%)	204 (100%)	0	100	100
3	J	186/186 (100%)	186 (100%)	0	100	100
3	L	186/186 (100%)	186 (100%)	0	100	100
3	Q	186/186 (100%)	186 (100%)	0	100	100
4	E	187/187 (100%)	187 (100%)	0	100	100
4	M	187/187 (100%)	187 (100%)	0	100	100
4	R	187/187 (100%)	187 (100%)	0	100	100
5	F	189/189 (100%)	188 (100%)	1 (0%)	88	96
5	N	189/189 (100%)	188 (100%)	1 (0%)	88	96
5	S	189/189 (100%)	188 (100%)	1 (0%)	88	96
All	All	4992/5247 (95%)	4966 (100%)	26 (0%)	89	96

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	545	THR
5	F	144	ARG
1	C	713	LEU
1	B	547	LEU
1	C	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1025	GLN
5	F	126	GLN
5	S	126	GLN
1	C	940	GLN
1	C	1025	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no monosaccharides in this entry.

5.6   Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
6	NAG	A	1201	1	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	C	1201	1	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	B	1201	1	14,14,15	0.22	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1201	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1201	NAG	O5-C5-C6-O6
6	B	1201	NAG	O5-C5-C6-O6
6	C	1201	NAG	O5-C5-C6-O6
6	A	1201	NAG	C4-C5-C6-O6
6	C	1201	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	4
1	B	3
1	C	2

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	43:SER	C	44:TYR	N	10.12
1	B	43:SER	C	44:TYR	N	10.12
1	C	43:SER	C	44:TYR	N	10.12
1	A	330:SER	C	331:ASN	N	2.69
1	A	605:SER	C	606:PHE	N	2.52

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-34940. 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 ⓘ
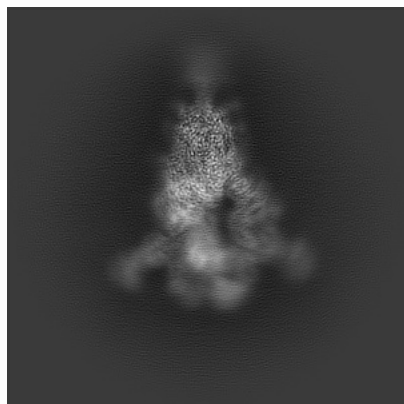
6.1.1 Primary map

X
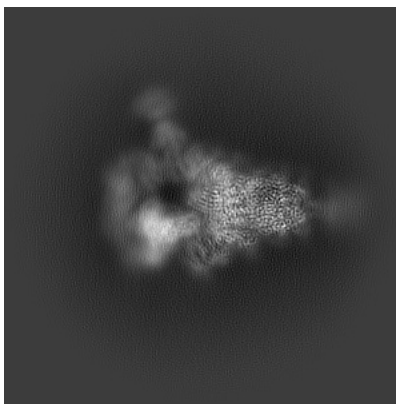
Y
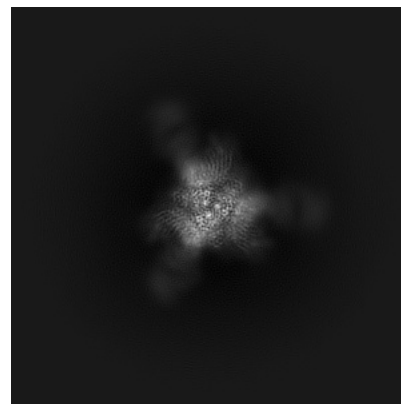
Z

6.1.2 Raw map

X

Y

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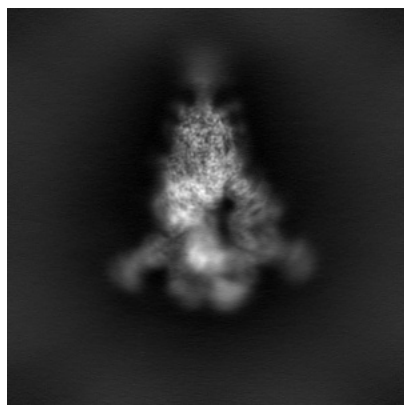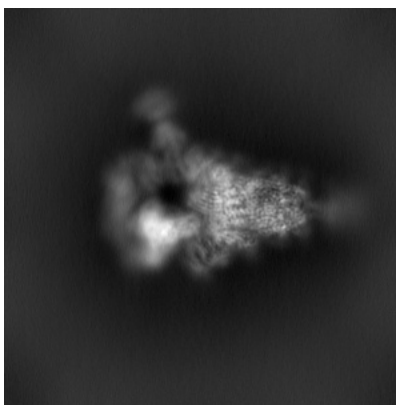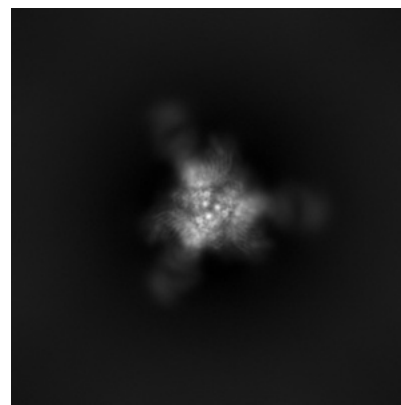
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
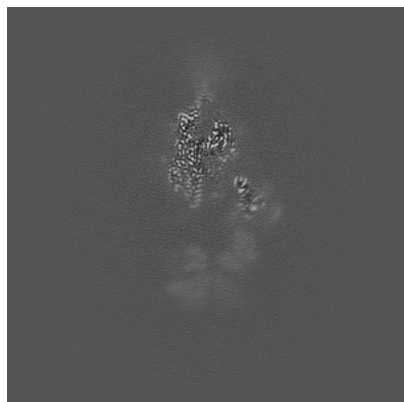
6.2.1   Primary map
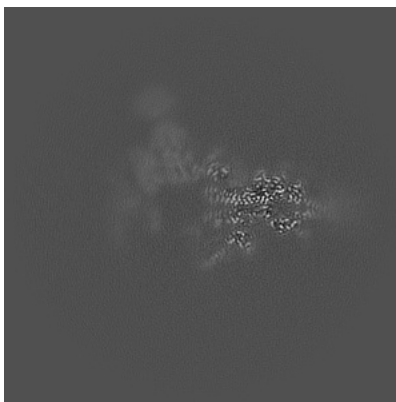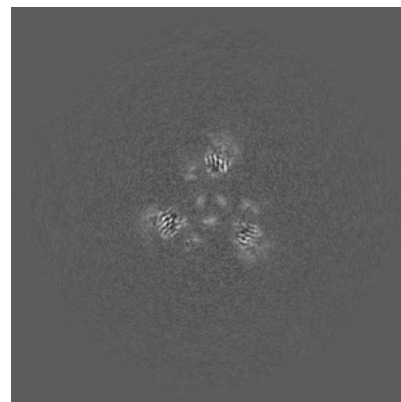
X Index: 256   Y Index: 256   Z Index: 256

6.2.2   Raw map
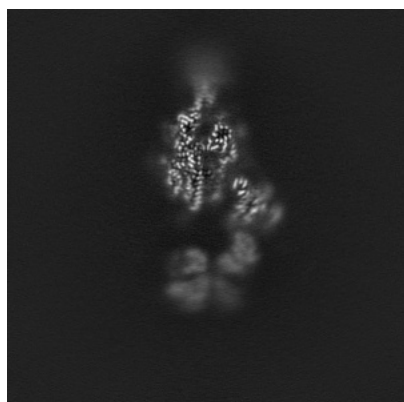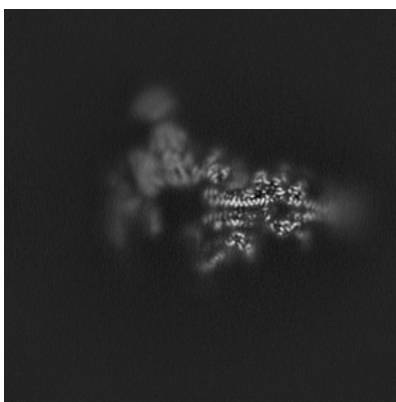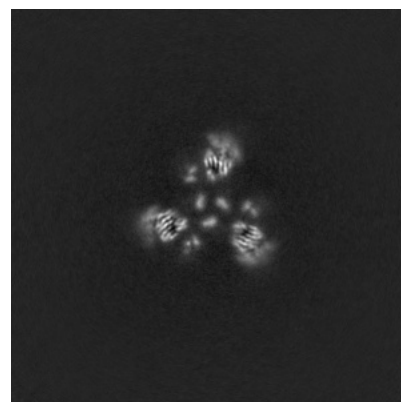
X Index: 256   Y Index: 256   Z Index: 256

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
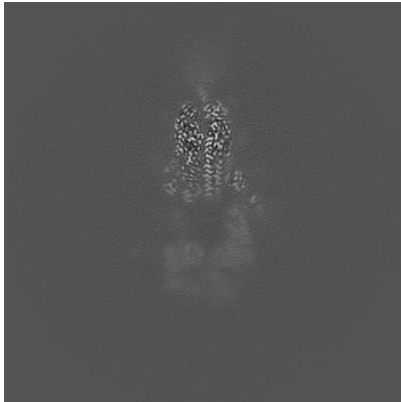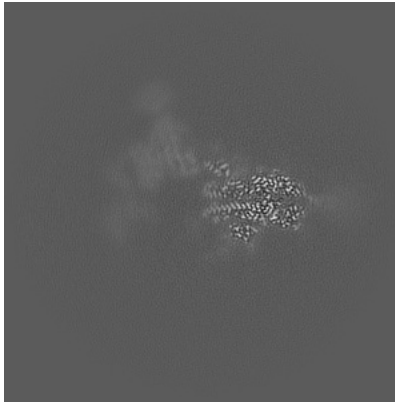
X Index: 248	Y Index: 262	Z Index: 335
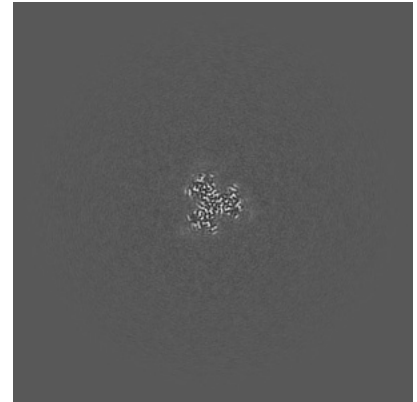
6.3.2 Raw map
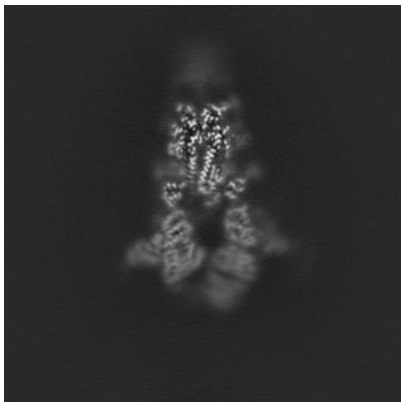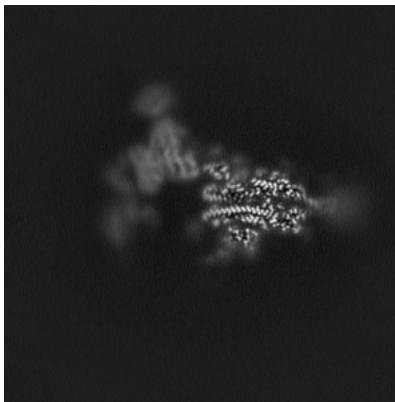
X Index: 237	Y Index: 262	Z Index: 284
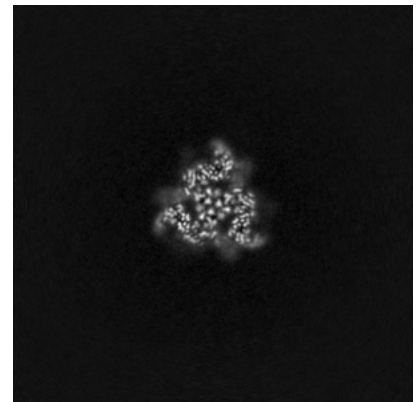
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
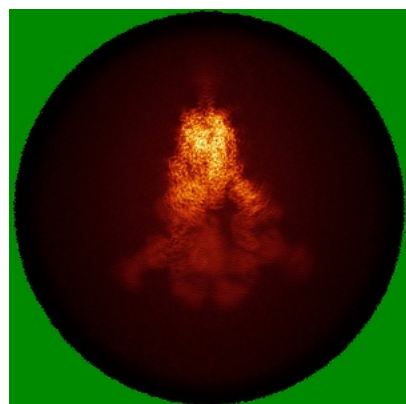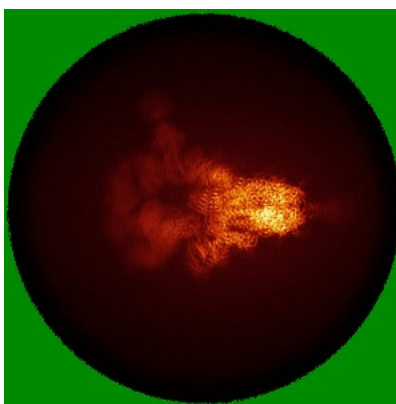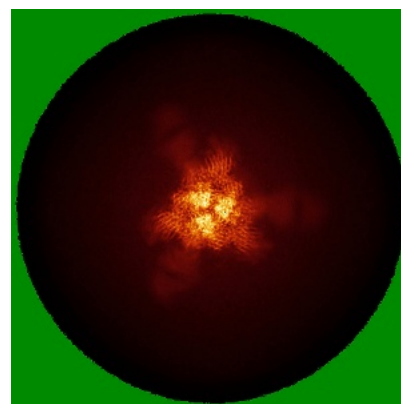
X   Y   Z

6.4.2 Raw map

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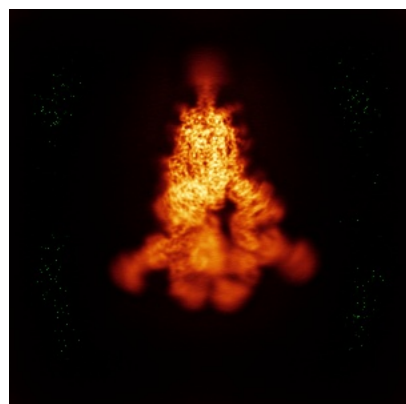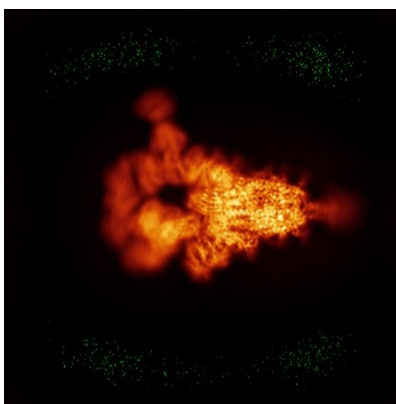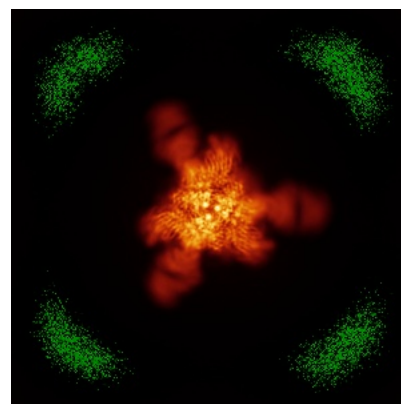
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.4. 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
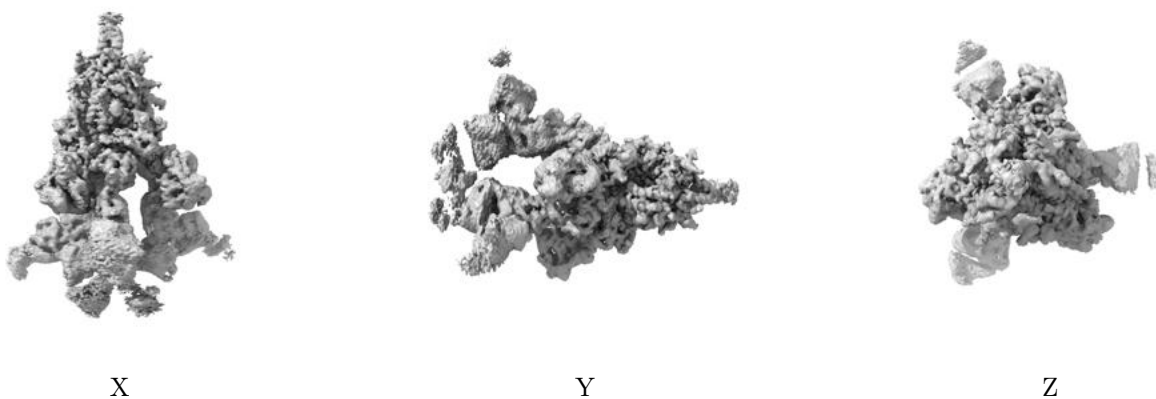
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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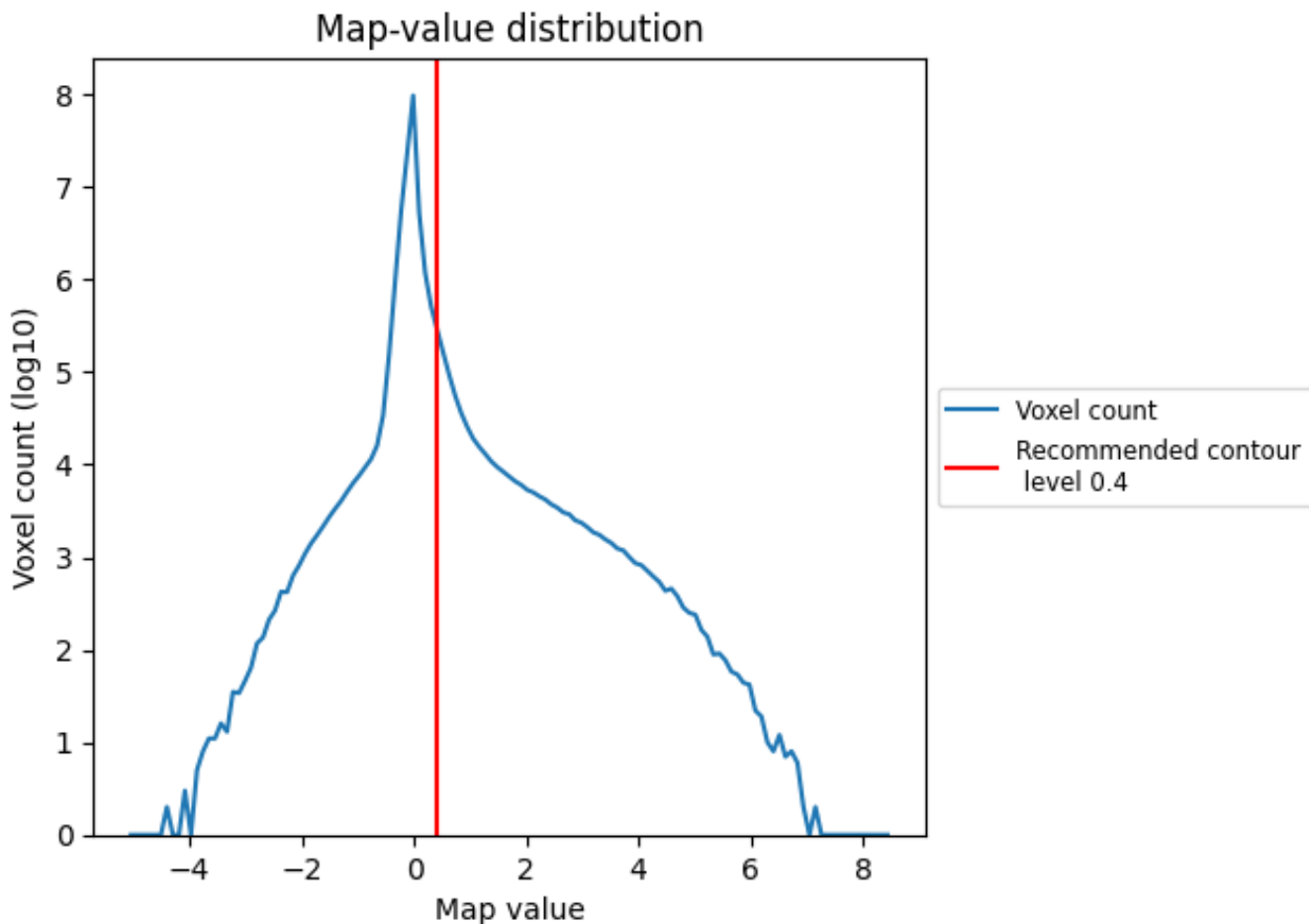
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
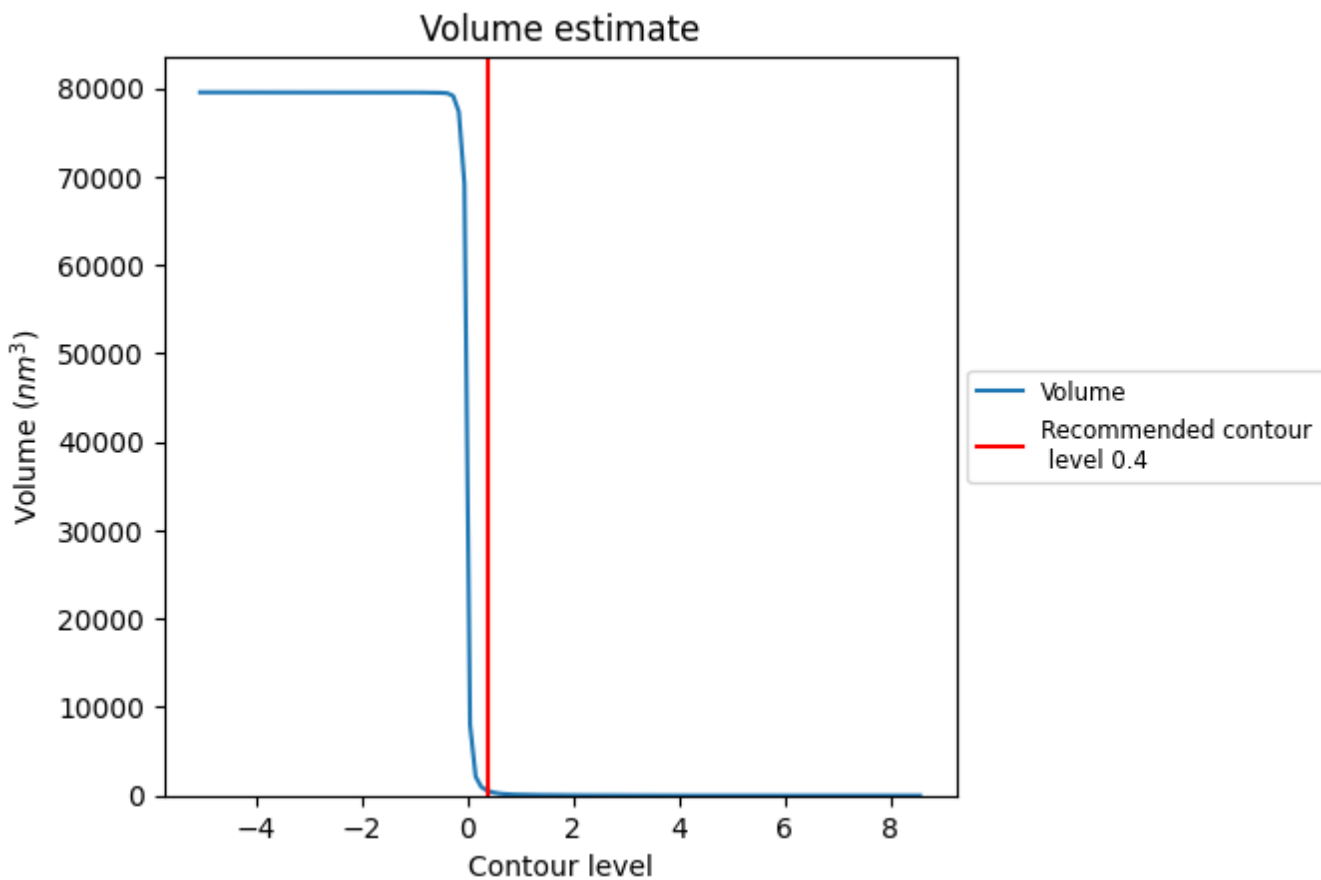
The volume at the recommended contour level is 523 nm^3; this corresponds to an approximate mass of 473 kDa.

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   ⓘ
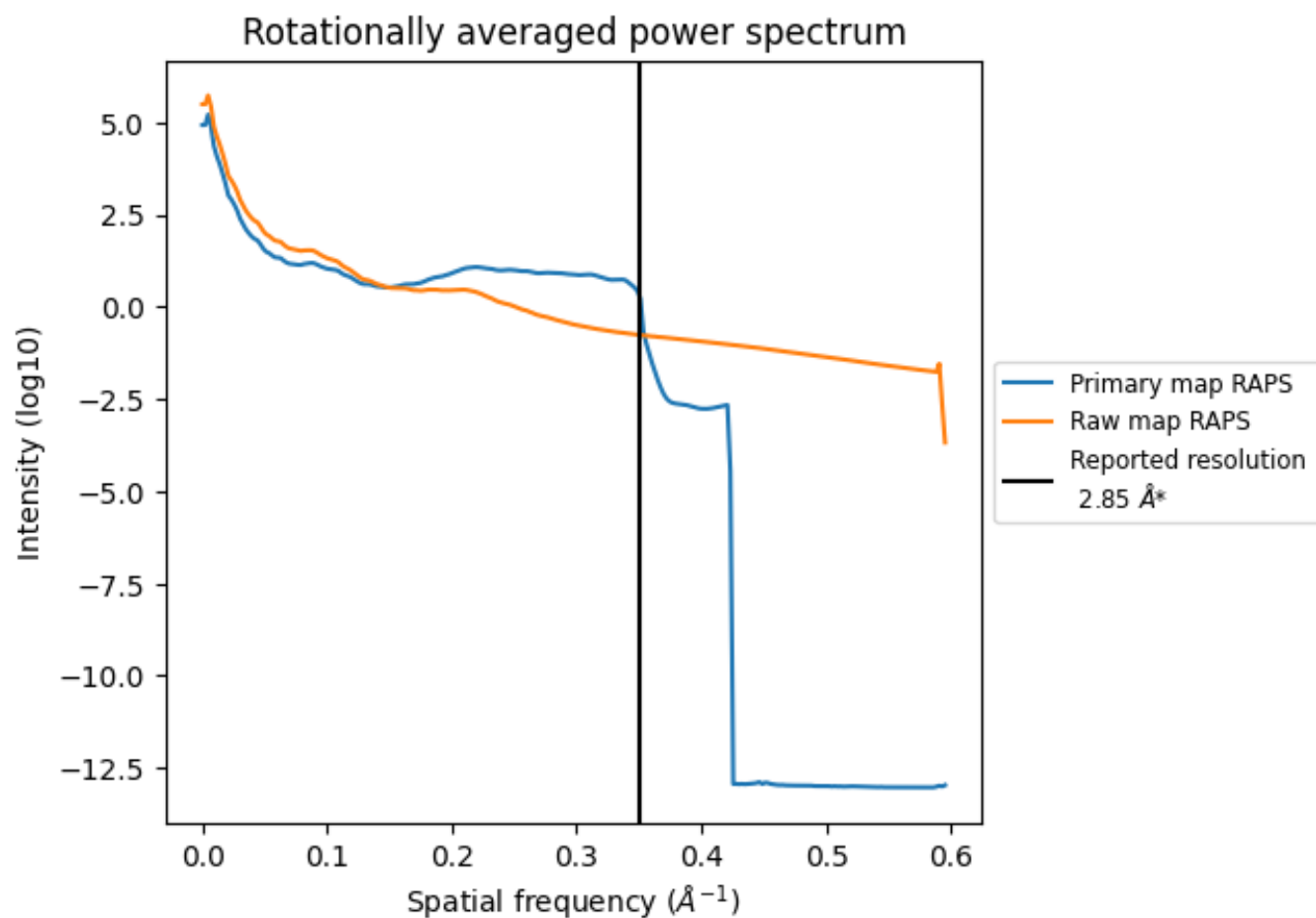
*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)
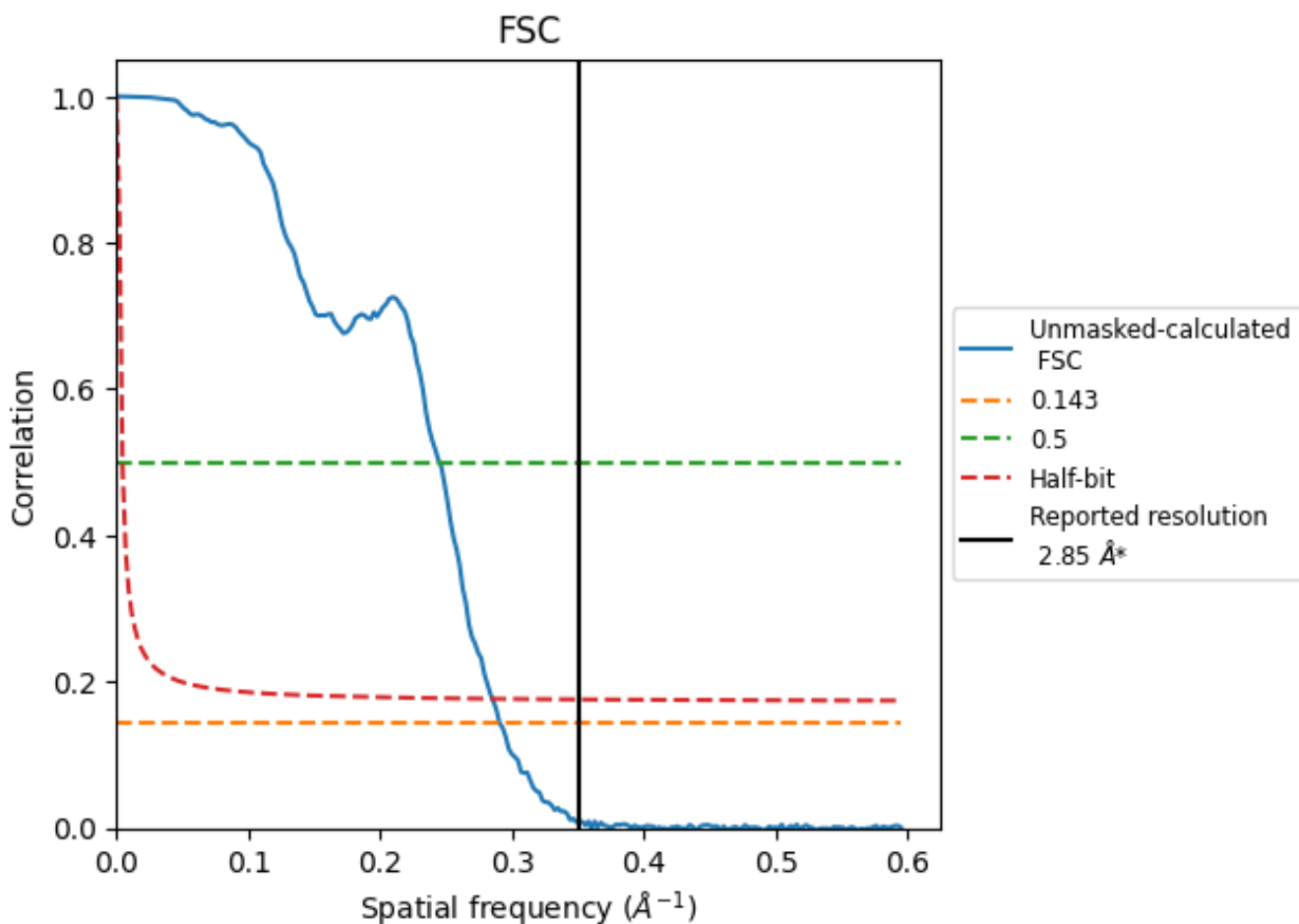
*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.08	3.51

*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 3.44 differs from the reported value 2.85 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-34940 and PDB model 8HPQ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay ⓘ

X   Y   Z
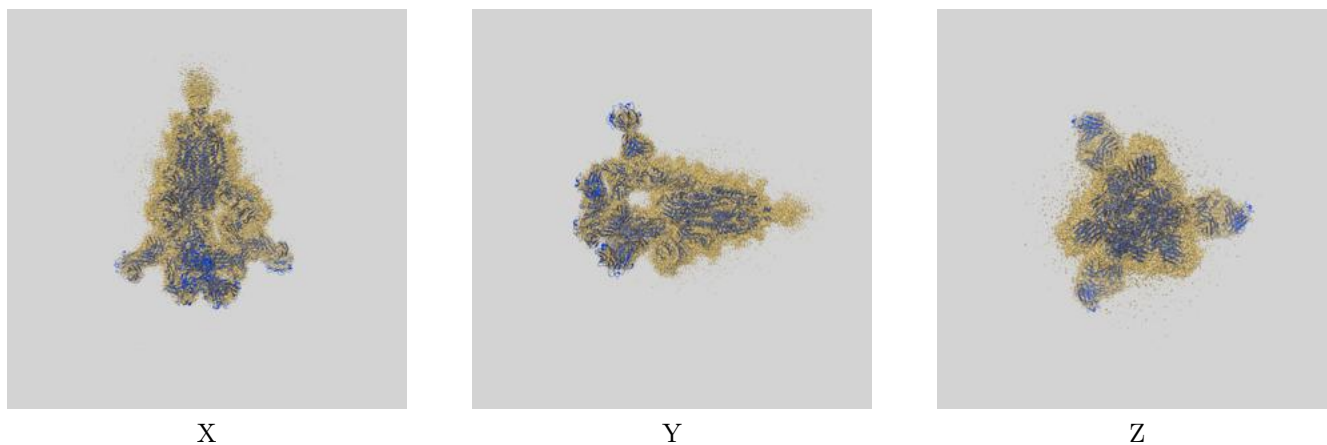
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ
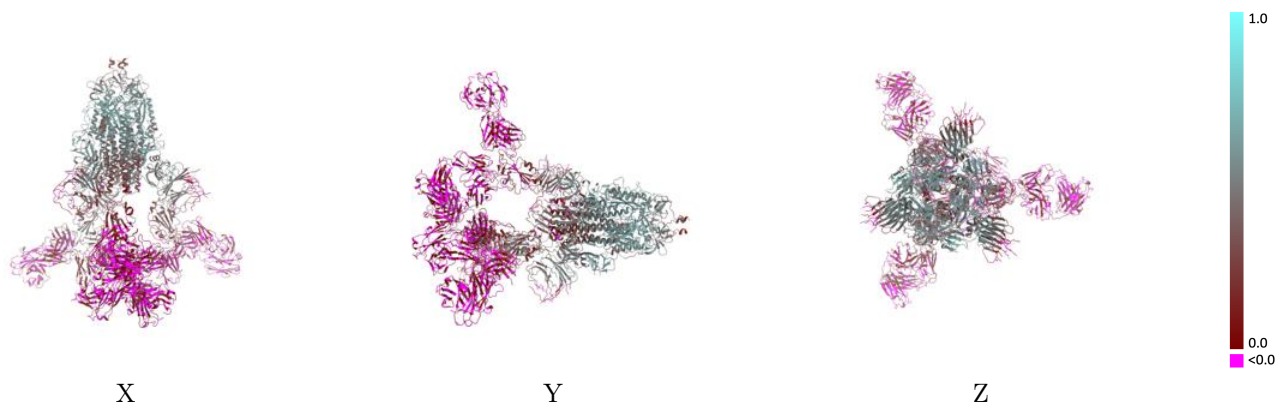
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
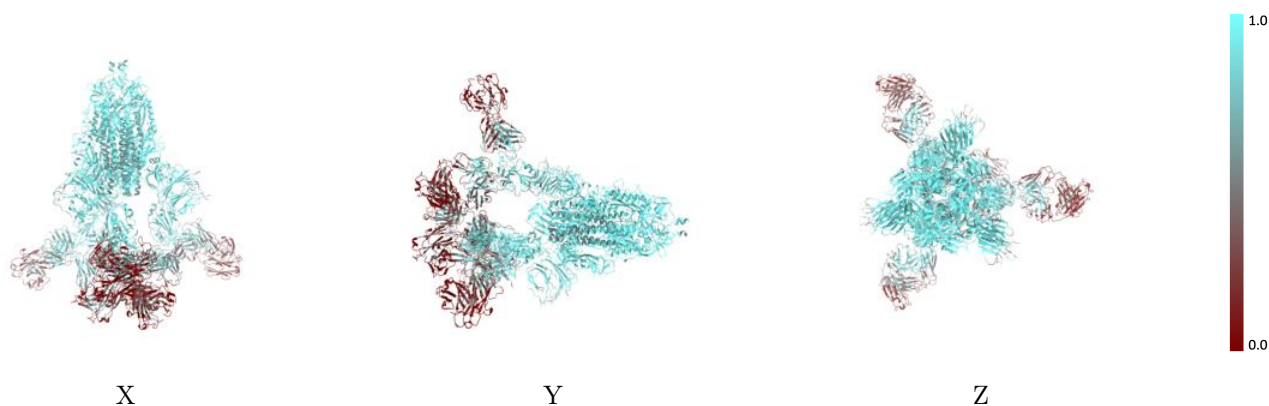
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4   Atom inclusion ⓘ
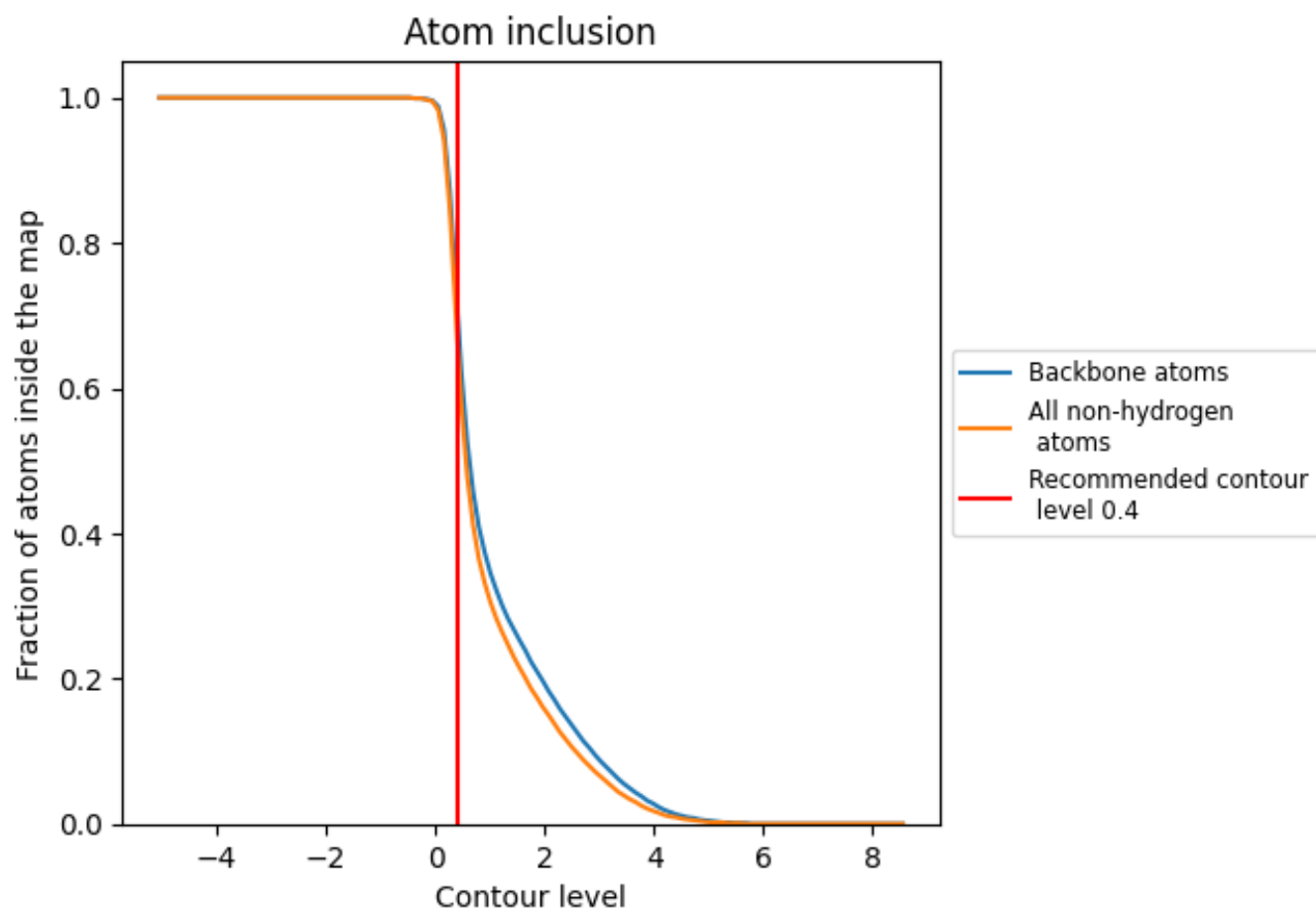
At the recommended contour level, 71% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6690	0.2430
A	0.8980	0.4180
B	0.8760	0.3850
C	0.8930	0.4050
E	0.3620	0.0280
F	0.3610	0.0290
H	0.5200	0.0790
I	0.4060	0.0520
J	0.2960	0.0350
L	0.4460	0.0710
M	0.5920	0.0990
N	0.5160	0.0910
P	0.3370	0.0300
Q	0.2590	0.0240
R	0.4060	0.0400
S	0.3580	0.0360

1.0

0.0
<0.0