WORLD WIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Oct 6, 2024 – 01:07 PM JST

PDB ID	:	7YC5
EMDB ID	:	EMD-33734
Title	:	Cryo-EM structure of SARS-CoV-2 spike in complex with K202.B bispecific antibody
Authors	:	Yoo, Y.; Cho, H.S.
Deposited on	:	2022-06-30
Resolution	:	3.10 Å(reported)
Based on initial models	:	7D85, 2A9N, 7VXM

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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 3.10 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		17
Ramachandran outliers		0
Sidechain outliers		1.7%

Worse .... *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures
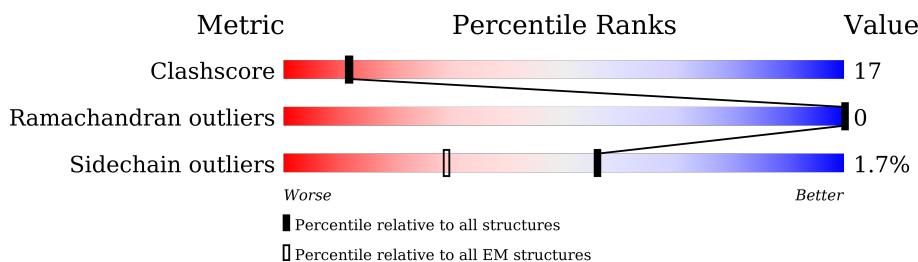
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1208	9% / 55% / 30% · 14%
1	B	1208	5% / 53% / 32% · 14%
1	C	1208	· / 55% / 30% / 14%
2	D	478	71% / 63% / 30% / 8%
2	E	478	68% / 64% / 28% / 8%
2	F	478	64% / 64% / 29% / 8%
3	G	454	37% / 25% / 19% / 56%
3	H	454	39% / 27% / 16% / 56%
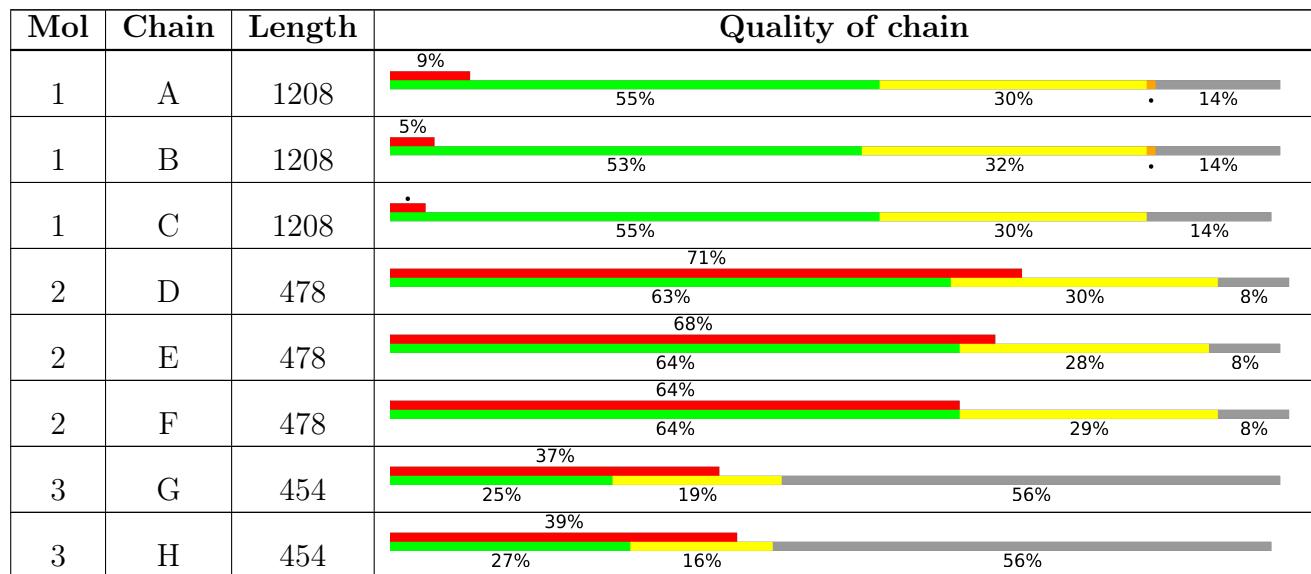
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Mol	Chain	Length	Quality of chain
3	I	454	36% 26% 18% 56%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 39157 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 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1037	Total	C	N	O	S	0	0
			8094	5170	1343	1545	36		
1	B	1037	Total	C	N	O	S	0	0
			8094	5170	1343	1545	36		
1	C	1037	Total	C	N	O	S	0	0
			8094	5170	1343	1545	36		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Light chain from K202.B, bispecific antibody.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	441	Total	C	N	O	S	0	0
			3313	2069	559	675	10		
2	E	441	Total	C	N	O	S	0	0
			3313	2069	559	675	10		
2	F	441	Total	C	N	O	S	0	0
			3313	2069	559	675	10		

- Molecule 3 is a protein called Heavy chain from K202.B, bispecific antibody.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	198	Total	C	N	O	S	0	0
			1496	945	252	292	7		
3	H	198	Total	C	N	O	S	0	0
			1496	945	252	292	7		
3	I	198	Total	C	N	O	S	0	0
			1496	945	252	292	7		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0

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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	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 glycoprotein

• Molecule 1: Spike glycoprotein

Chain B:

5%

53% 32% • 14%

• Molecule 1: Spike glycoprotein

Chain C:

55%   30%   14%

• Molecule 2: Light chain from K202.B, bispecific antibody

Chain D:

71%

63% 30% 8%

• Molecule 2: Light chain from K202.B, bispecific antibody

Chain E:

• Molecule 2: Light chain from K202.B, bispecific antibody

Chain F:

• Molecule 3: Heavy chain from K202.B, bispecific antibody

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

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

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

• Molecule 3: Heavy chain from K202.B, bispecific antibody

39%

Chain H: 27%   16%   56%

GLU V2 Q3 L4 L5 E6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 A23 A24 S25 G26 F27 T28 F29 S30 D31 Y32 A33 M34 S35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 V48 S49 W50 I51 Y52 S53 G54 S55 G56 N57 K58 Y59 Y60 A61

D62 S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 N74 S75 K76 N77 T78 L79 Y80 L81 Q82 M83 N84 S85 L86 R87 A88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 F99 P100 I101 A102 R103 T104 S105 N106 S107 Q108 S109 S110 Y111 D112 G113 M114 D115 V116 W117 G118 Q119 G120 T121

L122 V123 T124 V125 S126 S127 A128 S129 T130 K131 G132 P133 S134 V135 F136 P137 L138 ALA PRO CYS SER ARG SER THR SER GLU SER THR ALA A151 L152 G153 C154 L155 V156 K157 D158 Y159 F160 P161 E162 P163 V164 T165 V166 S167 W168 N169 S170 G171 A172 L173 T174 S175 G176 V177 H178 T179 F180 P181

A182 V183 L184 Q185 S186 S187 G188 L189 Y190 S191 L192 S193 S194 V195 V196 THR VAL PRO SER SER LEU GLY THR LYS THR TYR T209 C210 N211 V212 D213 H214 K215 P216 S217 N218 T219 K220 V221 D222 K223 ARG VAL GLU SER LYS TYR GLY PRO PRO CYS PRO CYS PRO ALA PRO GLU PHE

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

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

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

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

• Molecule 3: Heavy chain from K202.B, bispecific antibody

36%

Chain I: 26%   18%   56%

GLU V2 Q3 L4 L5 E6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 A23 A24 S25 G26 F27 T28 Y32 A33 M34 S35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 V48 S49 W50 I51 Y52 S53 G54 S55 G56 N57 K58 Y59 Y60 A61 D62

S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 S75 K76 N77 T78 L79 Y80 L81 Q82 M83 N84 S85 L86 R87 A88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 F99 P100 I101 A102 R103 T104 S105 N106 S107 Q108 S109 S110 Y111 D112 G113 M114 D115 V116 W117 G118 Q119 G120 T121 L122 V123

T124 V125 S126 S127 A128 S129 T130 K131 G132 P133 S134 V135 F136 P137 L138 ALA PRO CYS SER ARG SER THR SER GLU SER THR ALA A151 L152 G153 C154 L155 V156 K157 D158 Y159 F160 P161 E162 P163 V164 T165 V166 S167 W168 N169 S170 G171 A172 L173 T174 S175 G176 V177 H178 T179 F180 P181 A182 V183

Row 1: L184 Q185 S186 S187 G188 L189 Y190 S191 L192 S193 S194 V195 V196 THR VAL PRO SER SER SER LEU GLY THR LYS THR TYR T209 C210 N211 V212 D213 H214 K215 P216 S217 N218 T219 K220 V221 D222 K223 ARG VAL GLU SER LYS TYR GLY PRO PRO CYS PRO PRO CYS PRO ALA PRO GLU PHE LEU GLY

Row 2: GLY PRO SER VAL PHE LEU PHE PRO PRO LYS PRO LYS ASP THR LEU MET ILE SER ARG THR PRO GLU VAL THR CYS VAL VAL VAL ASP VAL SER GLN GLU ASP PRO GLU VAL GLN PHE ASN TRP TYR VAL ASP GLY VAL GLU VAL HIS ASN ALA LYS THR LYS PRO ARG GLU GLU GLN PHE

Row 3: ASN SER THR TYR ARG VAL VAL SER VAL LEU THR VAL LEU HIS GLN ASP TRP LEU ASN GLY LYS GLU TYR LYS CYS LYS VAL SER ASN LYS GLY LEU PRO SER SER ILE GLU LYS THR ILE SER LYS ALA LYS GLY GLN PRO ARG GLU PRO GLN VAL TYR THR LEU PRO PRO SER GLN GLU

Row 4: GLU MET THR LYS ASN GLN VAL SER LEU THR CYS LEU VAL LYS GLY PHE TYR PRO SER ASP ILE ALA VAL GLU TRP GLU SER ASN GLY GLN PRO GLU ASN ASN TYR LYS THR THR PRO PRO VAL LEU ASP SER ASP GLY SER PHE PHE LEU TYR SER ARG LEU THR VAL ASP LYS SER ARG

Row 5: TRP GLN GLU GLY ASN VAL PHE SER CYS SER VAL MET HIS GLU ALA LEU HIS ASN HIS TYR THR GLN LYS SER LEU SER LEU SER LEU GLY LYS

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182595	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	11.289	Depositor
Minimum map value	-7.992	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.202	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	360.52002, 360.52002, 360.52002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9013001, 0.9013001, 0.9013001	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	0.38	0/8280	0.54	3/11274 (0.0%)
1	B	0.38	0/8280	0.53	2/11274 (0.0%)
1	C	0.38	0/8280	0.52	1/11274 (0.0%)
2	D	0.32	0/3386	0.54	0/4606
2	E	0.29	0/3386	0.54	0/4606
2	F	0.30	0/3386	0.54	0/4606
3	G	0.37	0/1531	0.56	0/2080
3	H	0.34	0/1531	0.56	0/2080
3	I	0.38	0/1531	0.57	0/2080
All	All	0.36	0/39591	0.54	6/53880 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	796	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	273	ARG	N-CA-CB	5.57	120.62	110.60
1	A	574	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	80	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	80	ASP	CB-CG-OD2	5.18	122.97	118.30

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	8094	0	7885	300	0
1	B	8094	0	7883	350	0
1	C	8094	0	7884	322	0
2	D	3313	0	3186	107	0
2	E	3313	0	3186	87	0
2	F	3313	0	3186	99	0
3	G	1496	0	1446	57	0
3	H	1496	0	1446	46	0
3	I	1496	0	1446	53	0
4	A	154	0	143	6	0
4	B	154	0	143	4	0
4	C	140	0	130	2	0
All	All	39157	0	37964	1345	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 17.

The worst 5 of 1345 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:855:PHE:HB3	1:C:589:PRO:HG2	1.31	1.12
1:A:369:TYR:CE2	2:D:53:TYR:CE2	2.56	0.94
1:B:18:LEU:HG	1:B:20:THR:H	1.37	0.88
1:A:105:ILE:HG12	1:A:118:LEU:HD13	1.56	0.87
1:C:17:ASN:HA	1:C:138:ASP:HB2	1.57	0.87

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	1019/1208 (84%)	954 (94%)	65 (6%)	0	100	100
1	B	1019/1208 (84%)	960 (94%)	59 (6%)	0	100	100
1	C	1019/1208 (84%)	954 (94%)	65 (6%)	0	100	100
2	D	435/478 (91%)	411 (94%)	24 (6%)	0	100	100
2	E	435/478 (91%)	412 (95%)	23 (5%)	0	100	100
2	F	435/478 (91%)	409 (94%)	26 (6%)	0	100	100
3	G	192/454 (42%)	184 (96%)	8 (4%)	0	100	100
3	H	192/454 (42%)	185 (96%)	7 (4%)	0	100	100
3	I	192/454 (42%)	182 (95%)	10 (5%)	0	100	100
All	All	4938/6420 (77%)	4651 (94%)	287 (6%)	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	909/1056 (86%)	887 (98%)	22 (2%)	44	70
1	B	909/1056 (86%)	894 (98%)	15 (2%)	56	78
1	C	909/1056 (86%)	900 (99%)	9 (1%)	73	86
2	D	369/381 (97%)	363 (98%)	6 (2%)	58	79
2	E	369/381 (97%)	364 (99%)	5 (1%)	62	81
2	F	369/381 (97%)	364 (99%)	5 (1%)	62	81
3	G	166/402 (41%)	162 (98%)	4 (2%)	44	70
3	H	166/402 (41%)	162 (98%)	4 (2%)	44	70
3	I	166/402 (41%)	162 (98%)	4 (2%)	44	70
All	All	4332/5517 (78%)	4258 (98%)	74 (2%)	56	78

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	73	ASP
3	I	53	SER
2	F	325	SER
3	G	108	GLN
1	B	125	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	168	ASN
2	F	289	ASN
2	D	289	ASN
2	E	289	ASN
2	F	388	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

32 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	$\#\|Z\| > 2$
4	NAG	C	1401	1	14,14,15	0.38	0	17,19,21	0.60	0
4	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	B	1307	1	14,14,15	0.30	0	17,19,21	0.66	0
4	NAG	A	1309	1	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	B	1310	1	14,14,15	0.24	0	17,19,21	0.59	0
4	NAG	A	1308	1	14,14,15	0.46	0	17,19,21	0.95	1 (5%)
4	NAG	A	1310	1	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	B	1302	1	14,14,15	0.27	0	17,19,21	0.64	0
4	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.71	0
4	NAG	C	1406	1	14,14,15	0.33	0	17,19,21	0.61	0
4	NAG	B	1308	1	14,14,15	0.83	1 (7%)	17,19,21	1.13	1 (5%)
4	NAG	B	1309	1	14,14,15	0.29	0	17,19,21	0.82	0
4	NAG	A	1307	1	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	B	1301	1	14,14,15	0.36	0	17,19,21	0.64	0
4	NAG	B	1306	1	14,14,15	0.28	0	17,19,21	0.74	0
4	NAG	C	1405	1	14,14,15	0.69	0	17,19,21	0.88	1 (5%)
4	NAG	A	1301	1	14,14,15	0.34	0	17,19,21	0.63	0
4	NAG	A	1306	1	14,14,15	0.28	0	17,19,21	0.66	0
4	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.69	0
4	NAG	C	1409	1	14,14,15	0.24	0	17,19,21	0.59	0
4	NAG	C	1407	1	14,14,15	0.93	1 (7%)	17,19,21	1.12	1 (5%)
4	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	C	1404	1	14,14,15	0.34	0	17,19,21	0.73	0
4	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.77	0
4	NAG	C	1402	1	14,14,15	0.89	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	C	1410	-	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	B	1311	-	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	A	1311	-	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	C	1408	1	14,14,15	0.67	1 (7%)	17,19,21	1.03	2 (11%)
4	NAG	C	1403	1	14,14,15	0.28	0	17,19,21	0.67	0
4	NAG	B	1303	1	14,14,15	0.28	0	17,19,21	0.56	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
4	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1410	-	-	5/6/23/26	0/1/1/1
4	NAG	B	1311	-	-	5/6/23/26	0/1/1/1
4	NAG	A	1311	-	-	5/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1407	NAG	C1-C2	3.29	1.57	1.52
4	C	1402	NAG	C1-C2	3.02	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1308	NAG	C1-C2	2.91	1.56	1.52
4	C	1408	NAG	C1-C2	2.29	1.55	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1308	NAG	C4-C3-C2	-3.49	105.91	111.02
4	C	1407	NAG	C4-C3-C2	-3.31	106.17	111.02
4	A	1308	NAG	O5-C1-C2	-2.28	107.68	111.29
4	C	1405	NAG	C4-C3-C2	-2.25	107.72	111.02
4	C	1402	NAG	C2-N2-C7	-2.08	119.94	122.90

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1304	NAG	C3-C2-N2-C7
4	A	1304	NAG	C8-C7-N2-C2
4	A	1304	NAG	O7-C7-N2-C2
4	A	1305	NAG	C8-C7-N2-C2
4	A	1305	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1308	NAG	2	0
4	B	1309	NAG	2	0
4	B	1301	NAG	1	0
4	A	1301	NAG	1	0
4	A	1306	NAG	1	0
4	B	1304	NAG	1	0
4	A	1305	NAG	1	0
4	C	1402	NAG	1	0
4	A	1311	NAG	1	0
4	C	1408	NAG	1	0

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-33734. 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
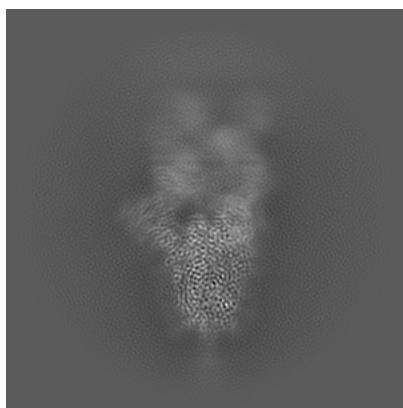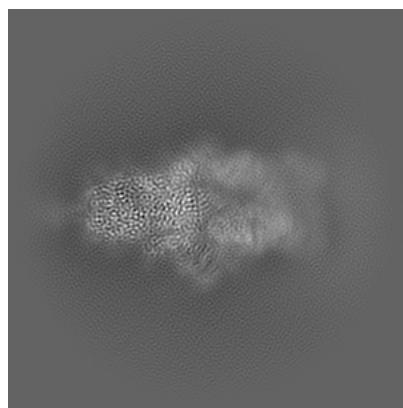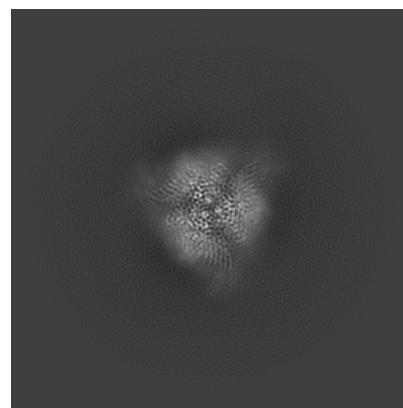
X   Y   Z

6.1.2 Raw map

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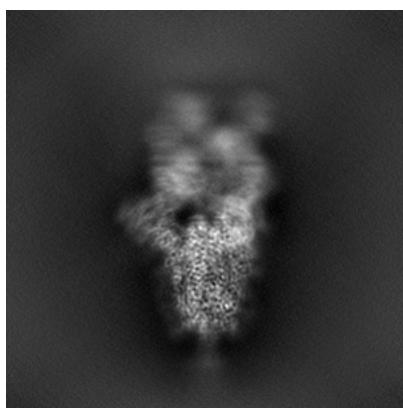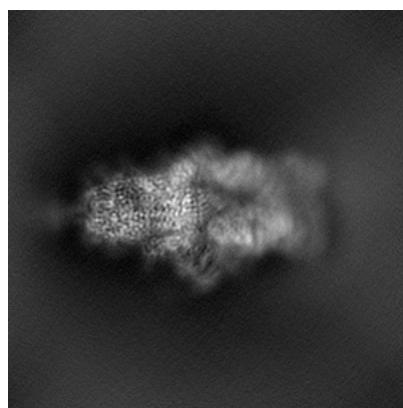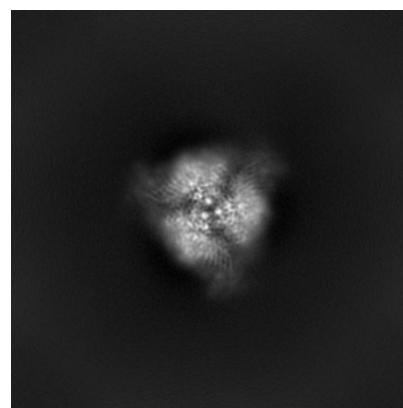
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
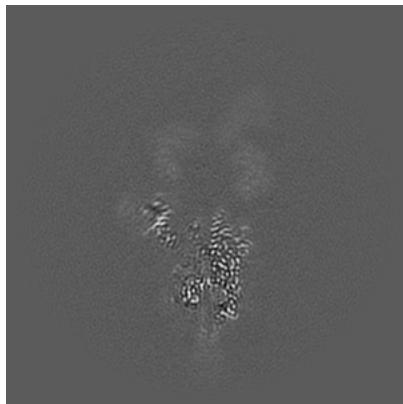
6.2.1   Primary map
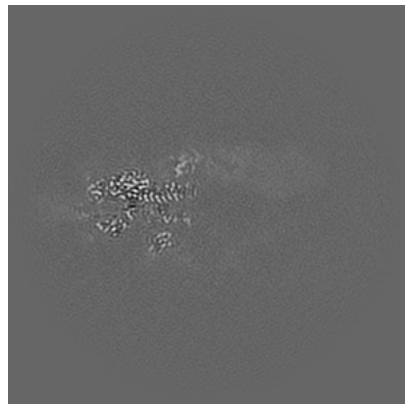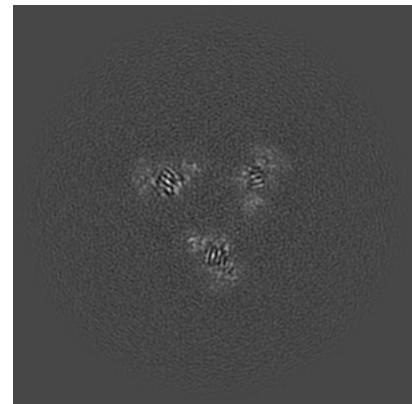
| X Index: 200 | Y Index: 200 | Z Index: 200 |

6.2.2   Raw map
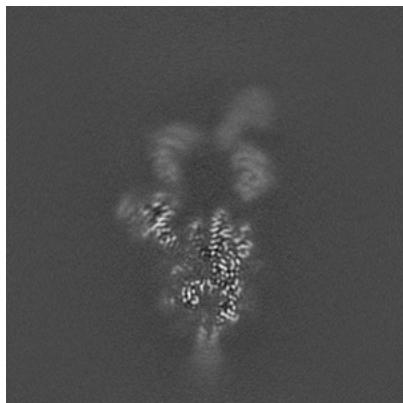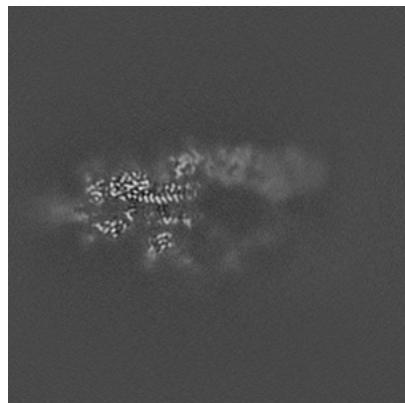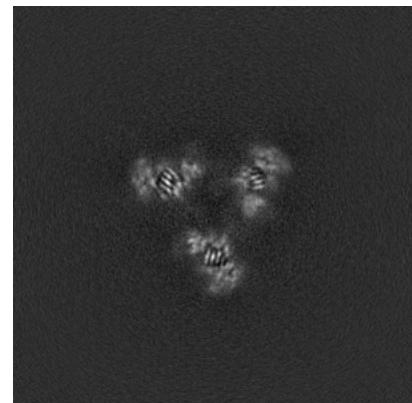
| X Index: 200 | Y Index: 200 | Z Index: 200 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
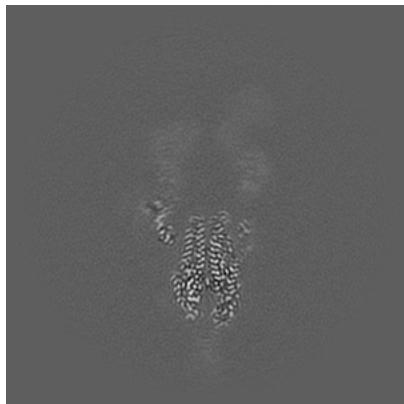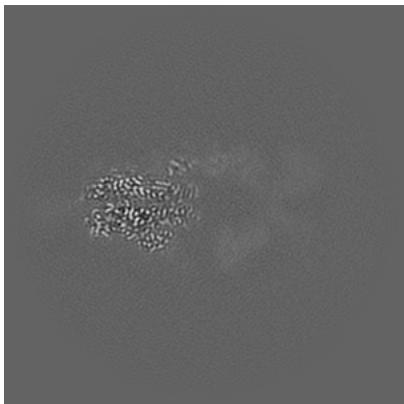
| X Index: 195 | Y Index: 191 | Z Index: 122 |
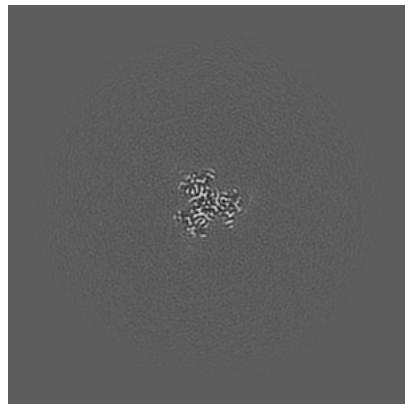
6.3.2 Raw map
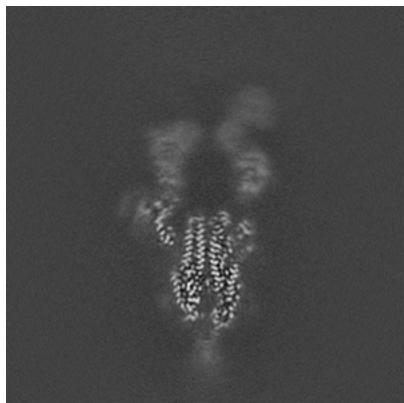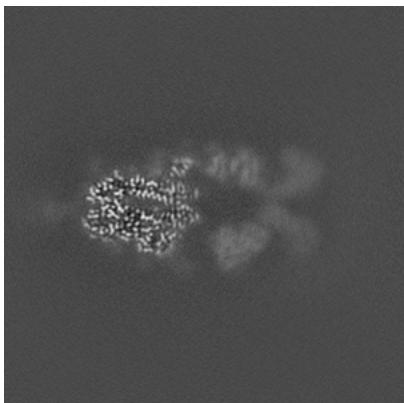
| X Index: 195 | Y Index: 188 | Z Index: 169 |
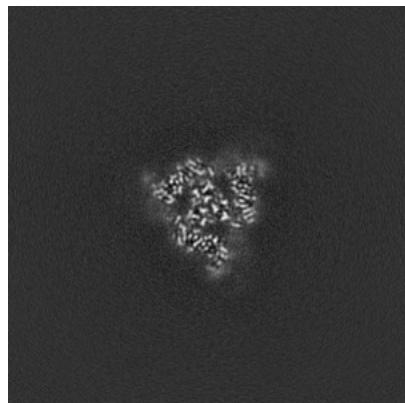
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1　Primary map
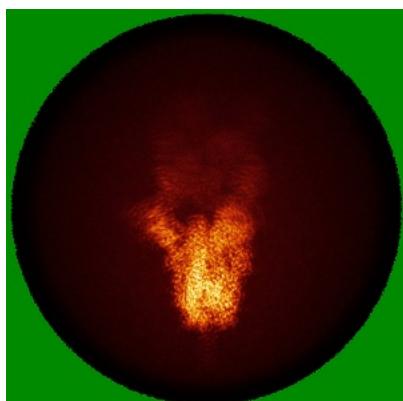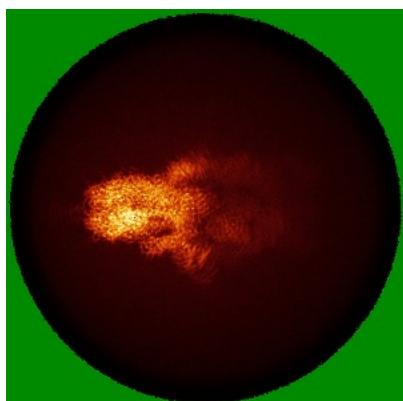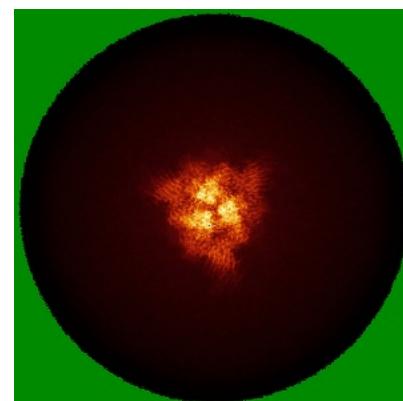
X	Y	Z

6.4.2　Raw map

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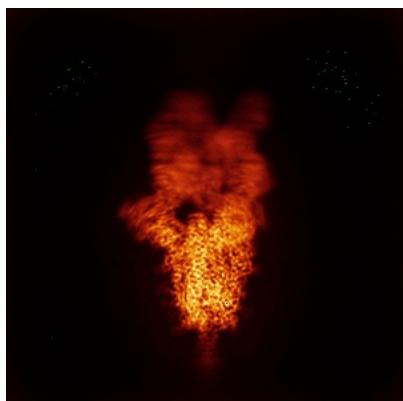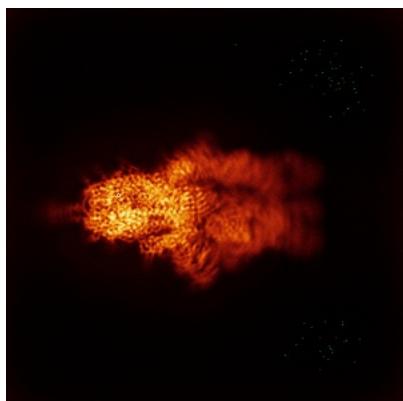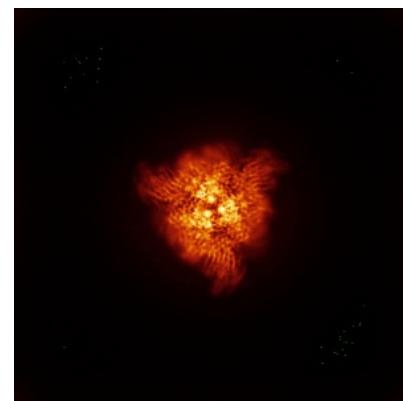
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X	Y	Z
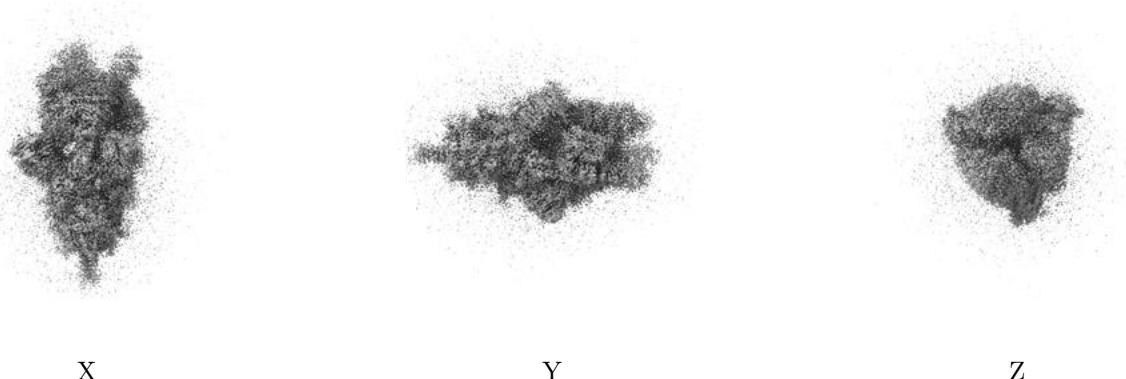
The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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 ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

### 6.6.1 emd_33734_msk_1.map ⓘ
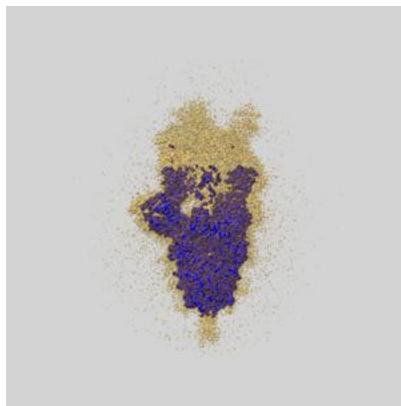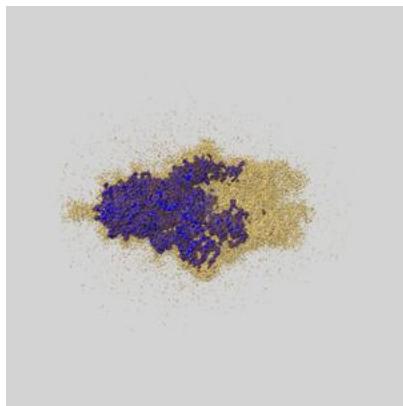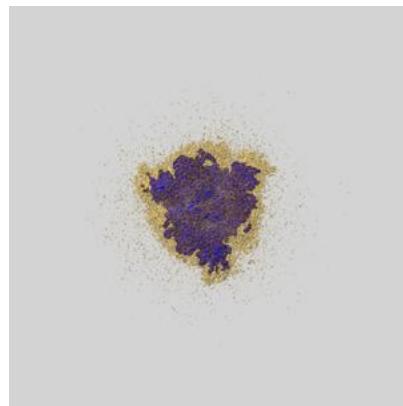
X Y Z

7 Map analysis (i)

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

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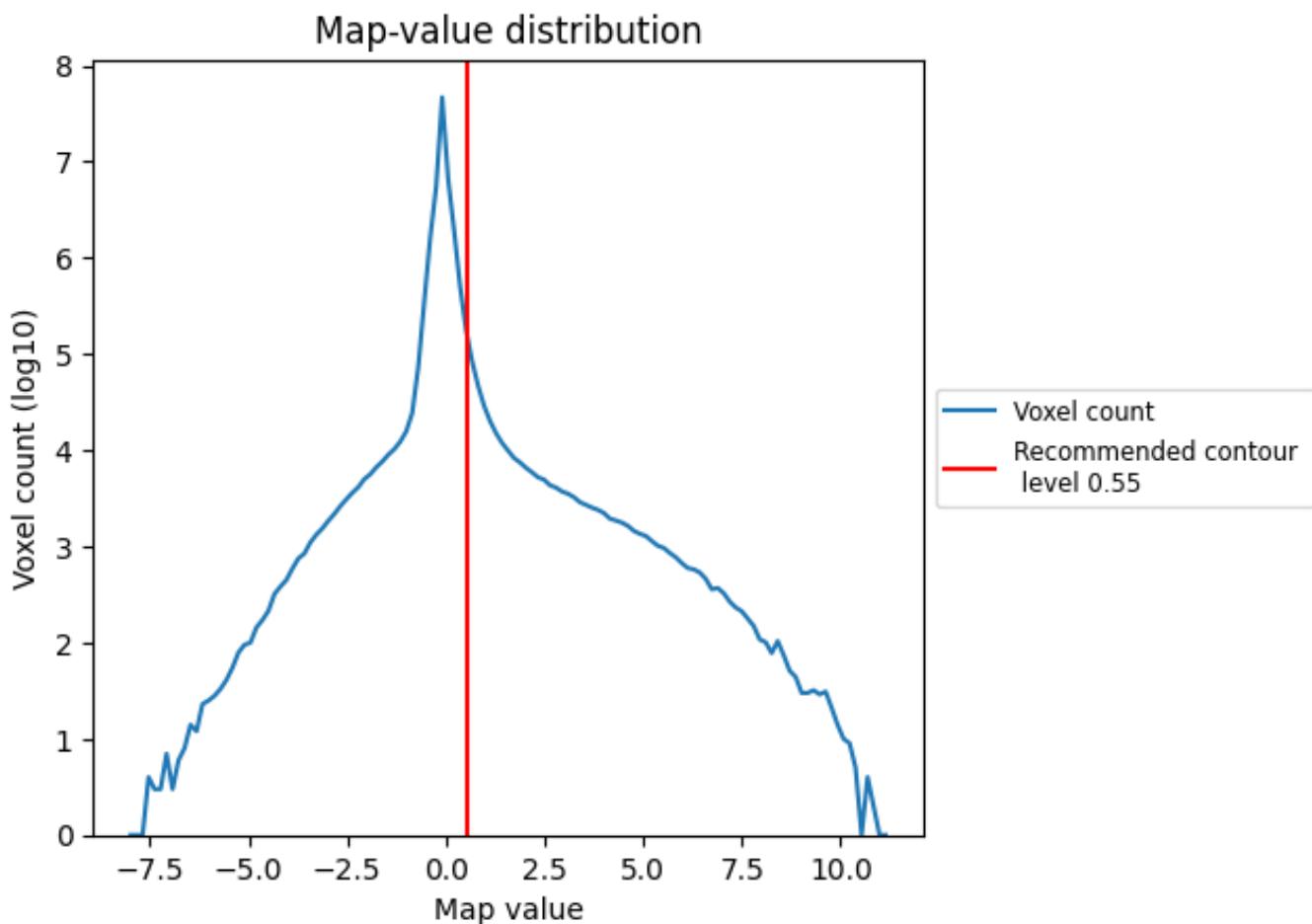
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
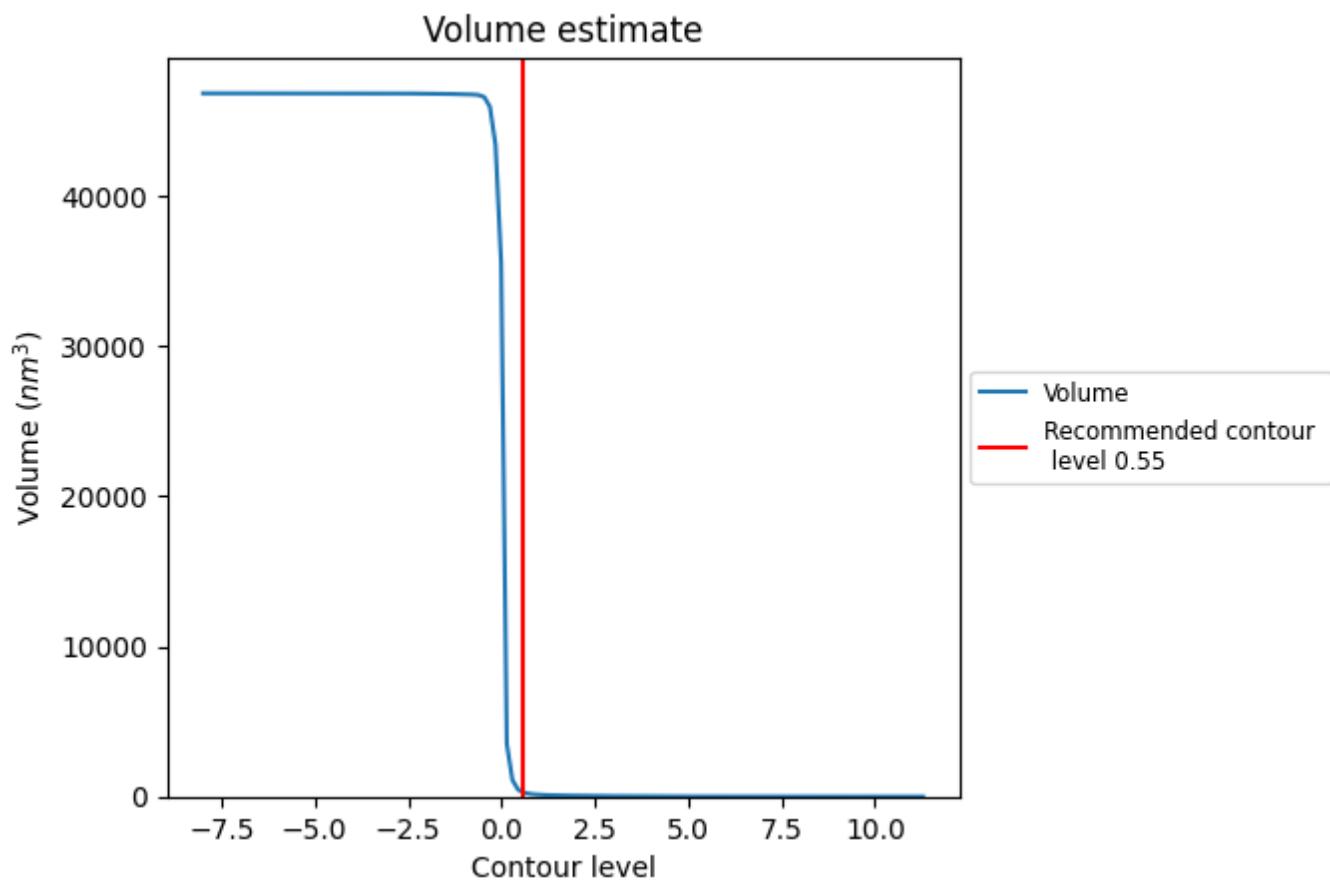
The volume at the recommended contour level is 327 nm^3; this corresponds to an approximate mass of 295 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)
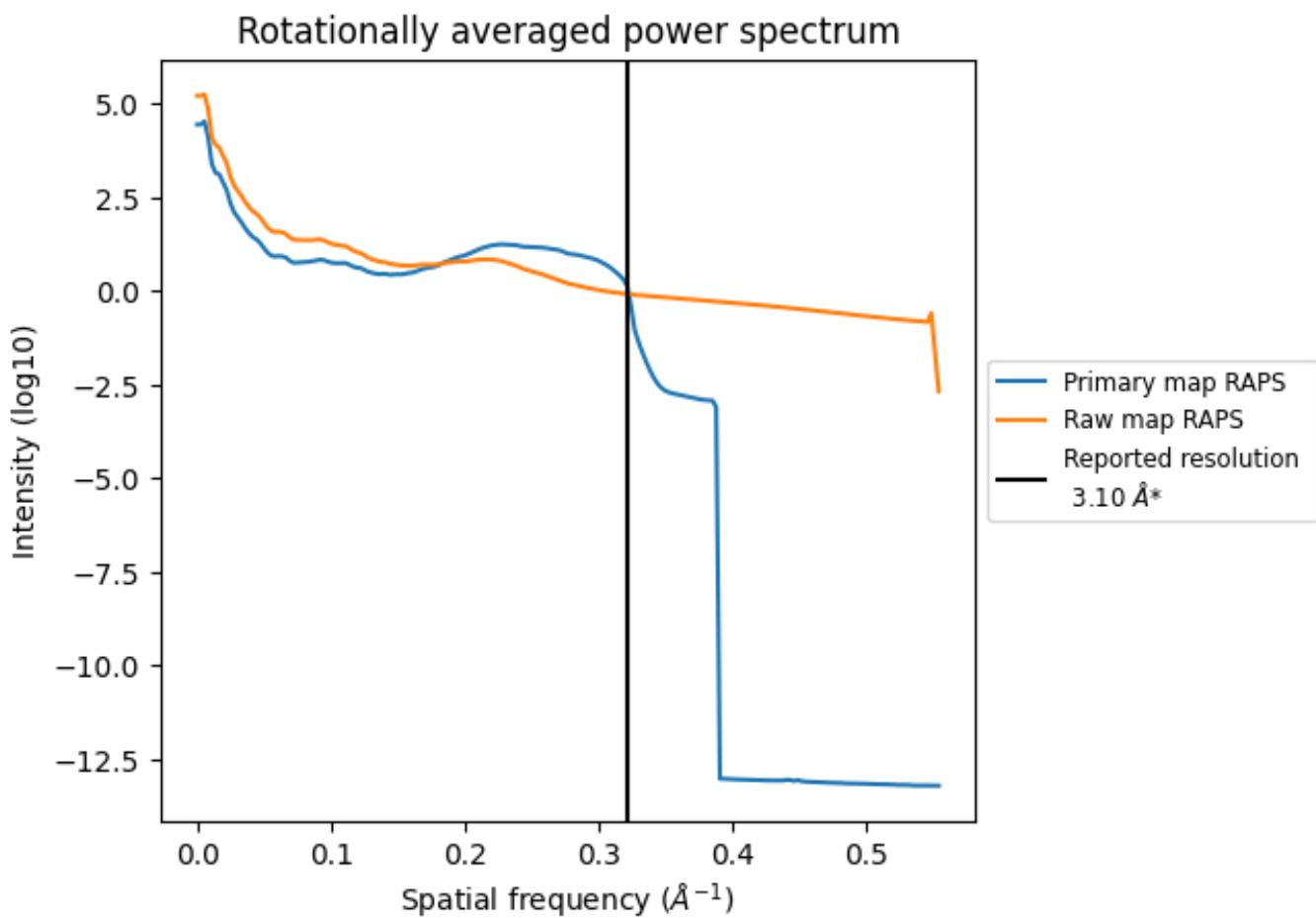
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 ⓘ
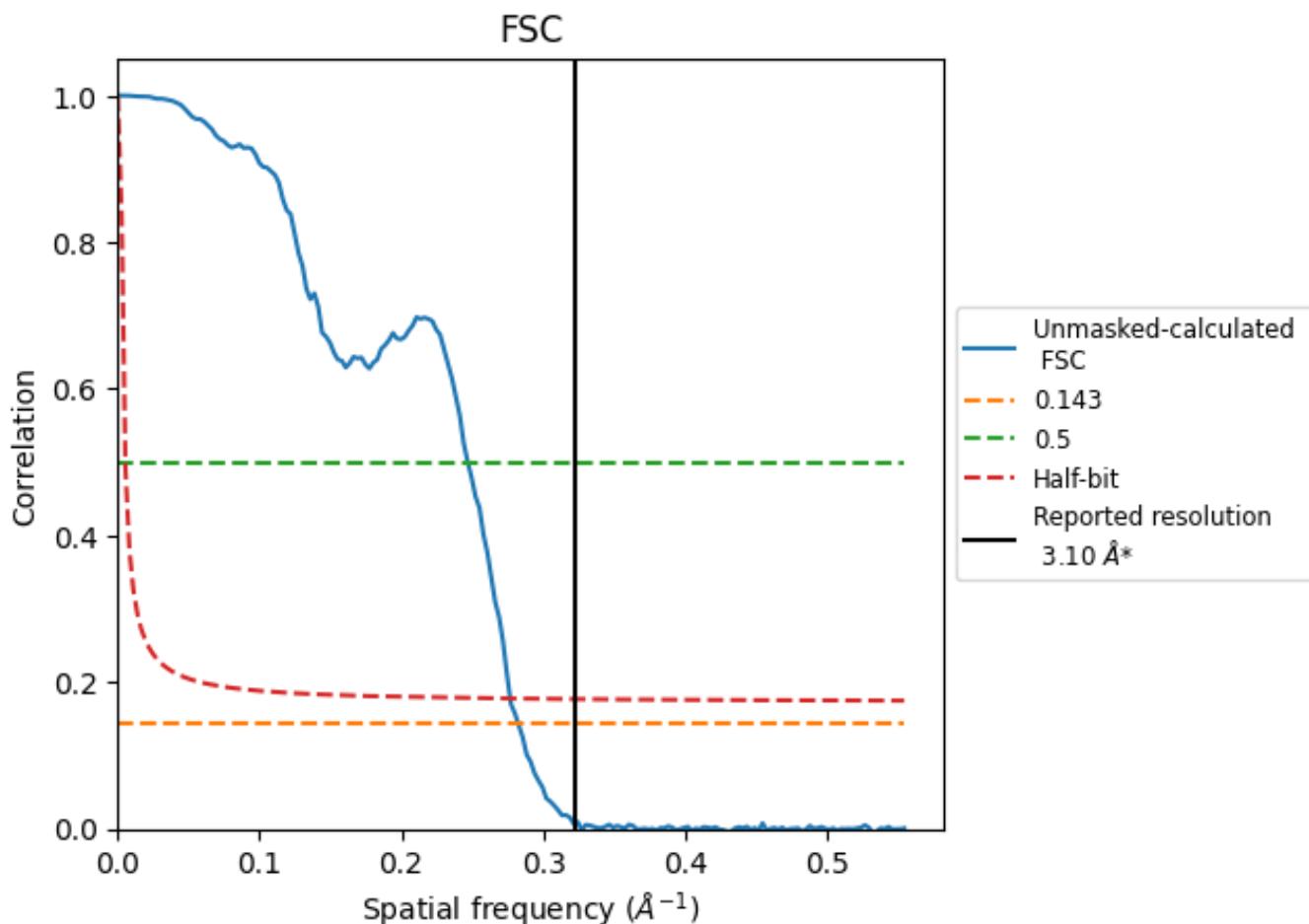
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.05	3.61

*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 3.54 differs from the reported value 3.1 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-33734 and PDB model 7YC5. Per-residue inclusion information can be found in section 3 on page 8.

## 9.1 Map-model overlay ⓘ

| X | Y | Z |
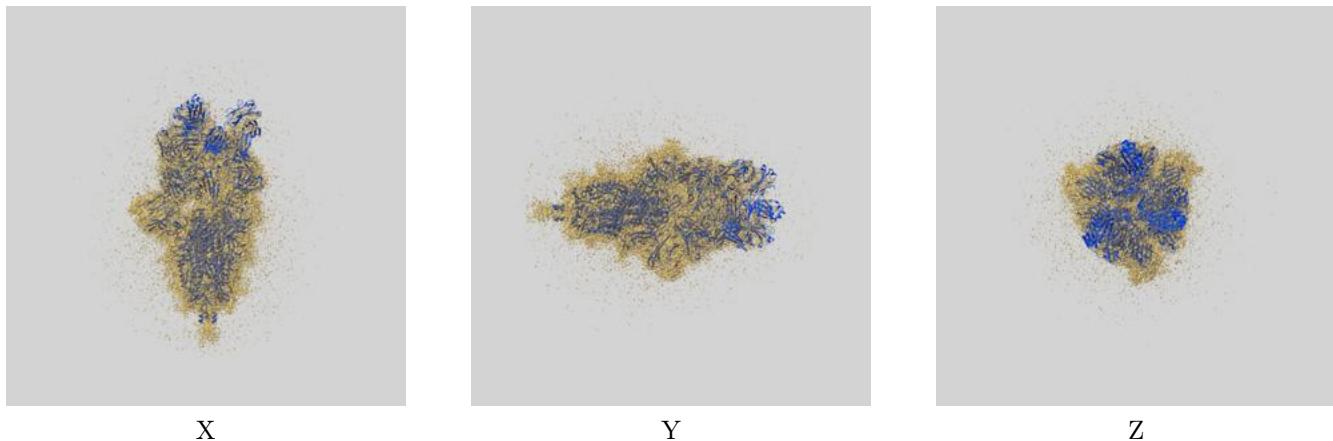
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
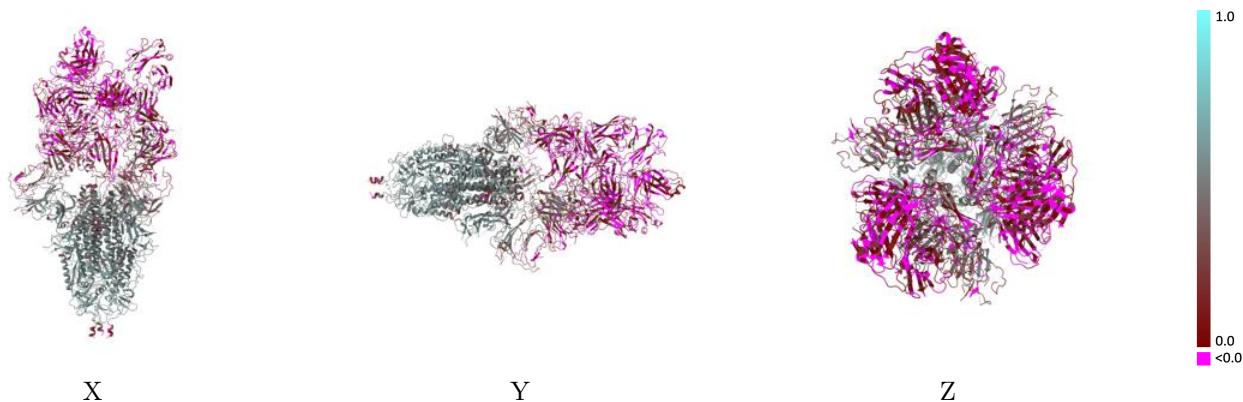
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
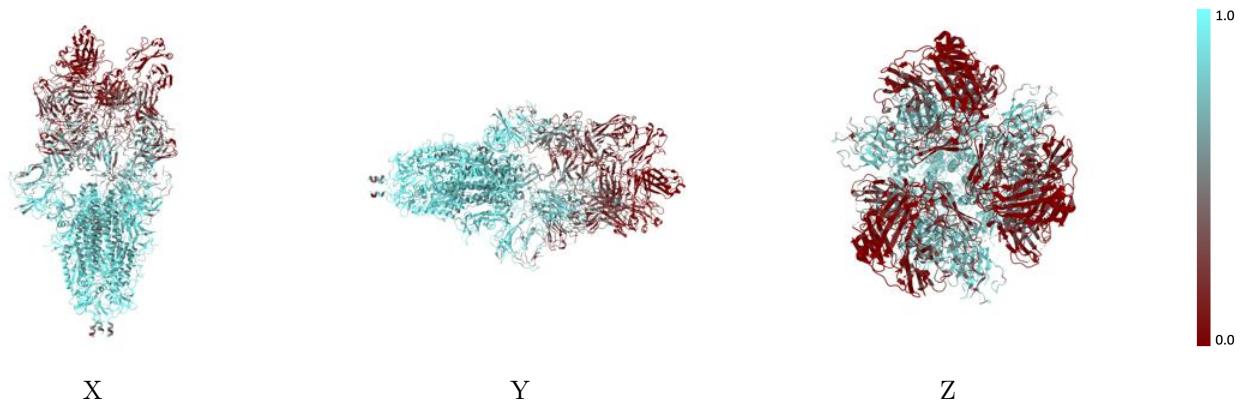
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion ⓘ
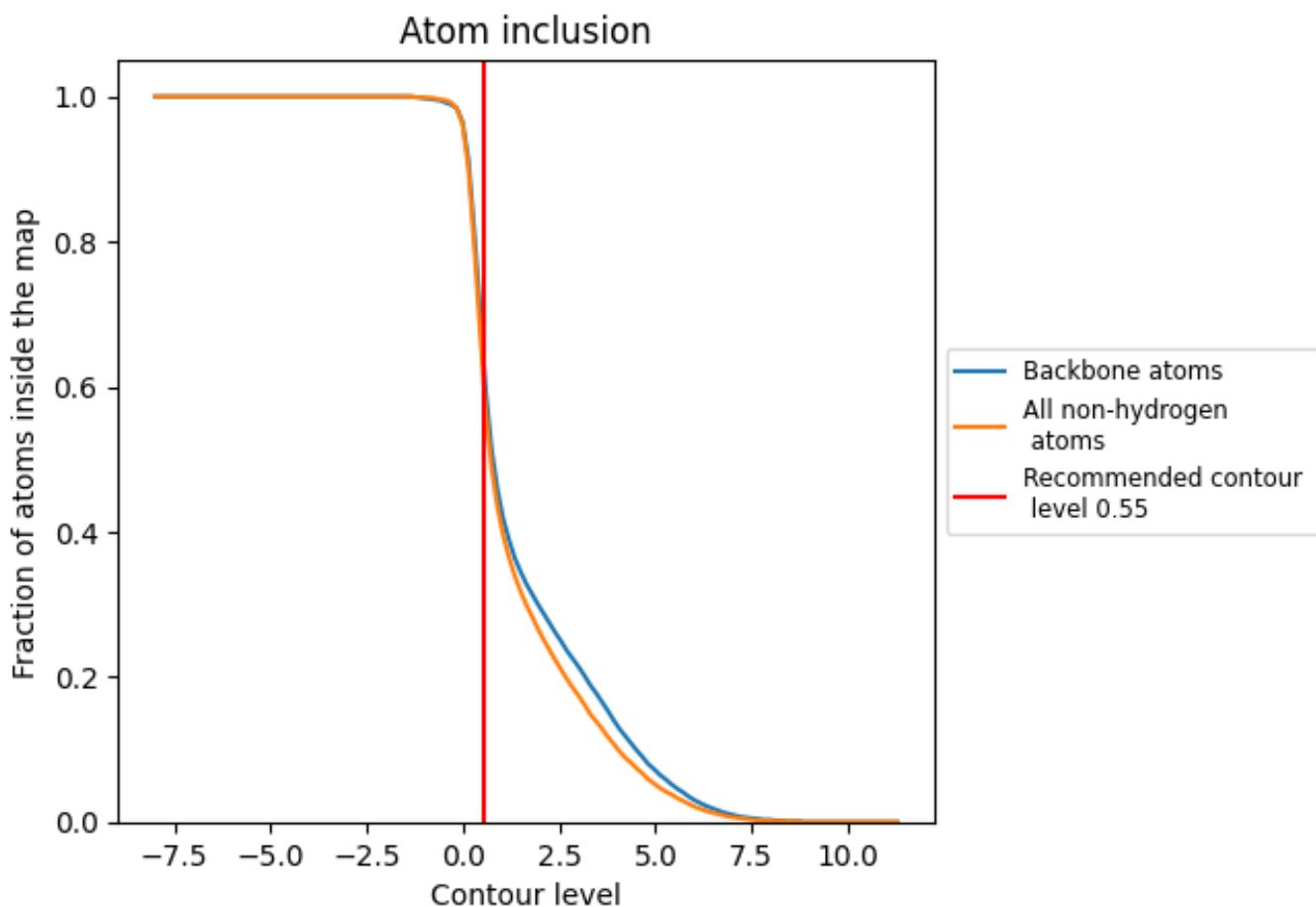
At the recommended contour level, 62% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5950	0.2840
A	0.7820	0.3930
B	0.8100	0.4220
C	0.8270	0.4380
D	0.2330	0.0450
E	0.2560	0.0680
F	0.2830	0.0680
G	0.1730	0.0320
H	0.1460	0.0350
I	0.2060	0.0580

1.0

0.0
<0.0