wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 06:46 PM EST

|		
PDB ID	:	7MPG
EMDB ID	:	EMD-23933
Title	:	Cryo-EM structure of Prefusion-stabilized RSV F (DS-Cav1) in complex with Fab AM14
Authors	:	Abeyrathne, P.D.; Malito, E.; Harshbarger, W.D.
Deposited on	:	2021-05-04
Resolution	:	3.40 Å(reported)

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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 3.40 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		15
Ramachandran outliers		0.2%
Sidechain outliers		0.2%

Worse   *Better*

■ Percentile relative to all structures

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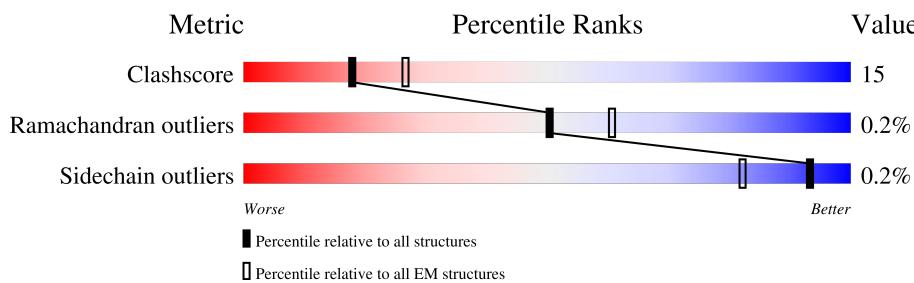
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	496	12% / 57% / 33% / 9%
1	B	496	11% / 58% / 33% / 9%
1	C	496	11% / 58% / 33% / 9%
2	D	244	37% / 64% / 25% / 11%
2	F	244	38% / 66% / 22% / 11%
2	H	244	36% / 66% / 22% / 11%
3	E	235	49% / 71% / 20% / 9%
3	G	235	51% / 69% / 21% / · / 9%
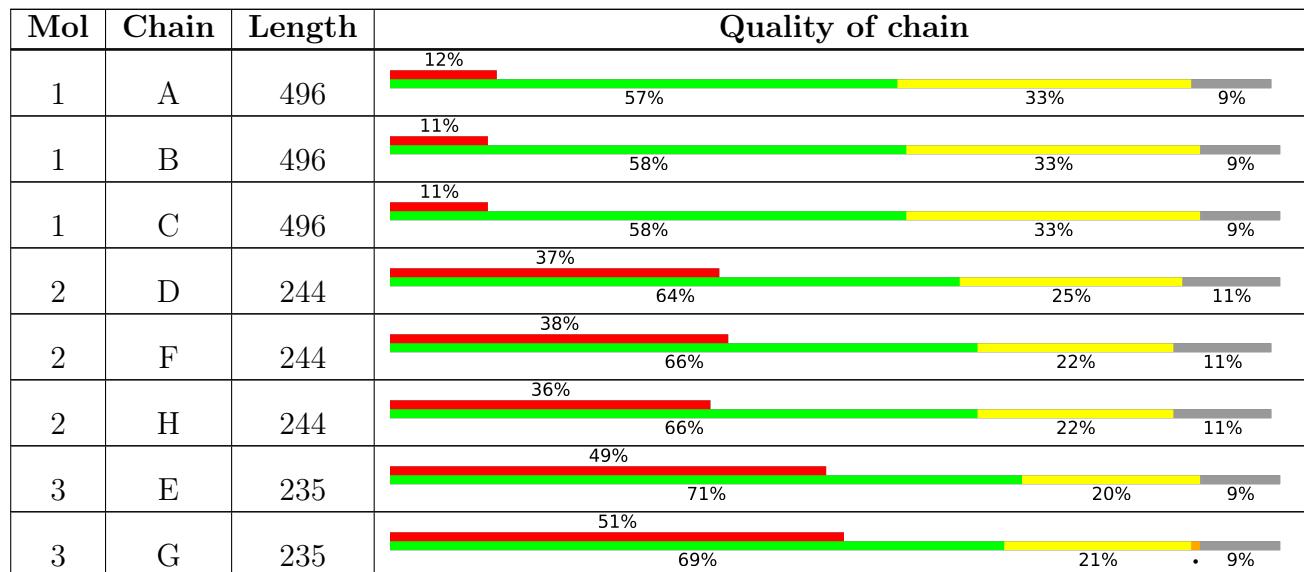
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Mol	Chain	Length	Quality of chain
3	I	235	50% · 70% · 20% · 9%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 20366 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 Fusion glycoprotein F0,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	451	Total 3497	C 2210	N 576	O 688	S 23	0	0
1	B	451	Total 3497	C 2210	N 576	O 688	S 23	0	0
1	C	451	Total 3497	C 2210	N 576	O 688	S 23	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	THR	ALA	conflict	UNP A0A0X8XQD7
A	?	-	ARG	deletion	UNP A0A0X8XQD7
A	?	-	ARG	deletion	UNP A0A0X8XQD7
A	?	-	GLU	deletion	UNP A0A0X8XQD7
A	?	-	LEU	deletion	UNP A0A0X8XQD7
A	?	-	PRO	deletion	UNP A0A0X8XQD7
A	?	-	ARG	deletion	UNP A0A0X8XQD7
A	?	-	PHE	deletion	UNP A0A0X8XQD7
A	?	-	MET	deletion	UNP A0A0X8XQD7
A	?	-	ASN	deletion	UNP A0A0X8XQD7
A	?	-	TYR	deletion	UNP A0A0X8XQD7
A	?	-	THR	deletion	UNP A0A0X8XQD7
A	?	-	LEU	deletion	UNP A0A0X8XQD7
A	?	-	ASN	deletion	UNP A0A0X8XQD7
A	?	-	ASN	deletion	UNP A0A0X8XQD7
A	?	-	THR	deletion	UNP A0A0X8XQD7
A	?	-	LYS	deletion	UNP A0A0X8XQD7
A	?	-	ASN	deletion	UNP A0A0X8XQD7
A	?	-	ASN	deletion	UNP A0A0X8XQD7
A	?	-	ASN	deletion	UNP A0A0X8XQD7
A	?	-	VAL	deletion	UNP A0A0X8XQD7
A	?	-	THR	deletion	UNP A0A0X8XQD7
A	?	-	LEU	deletion	UNP A0A0X8XQD7
A	?	-	SER	deletion	UNP A0A0X8XQD7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP A0A0X8XQD7
A	?	-	LYS	deletion	UNP A0A0X8XQD7
A	?	-	ARG	deletion	UNP A0A0X8XQD7
A	?	-	LYS	deletion	UNP A0A0X8XQD7
A	?	-	ARG	deletion	UNP A0A0X8XQD7
A	?	-	ARG	deletion	UNP A0A0X8XQD7
A	152	VAL	ILE	conflict	UNP A0A0X8XQD7
A	155	CYS	SER	engineered mutation	UNP A0A0X8XQD7
A	190	PHE	SER	engineered mutation	UNP A0A0X8XQD7
A	207	LEU	VAL	engineered mutation	UNP A0A0X8XQD7
A	290	CYS	SER	engineered mutation	UNP A0A0X8XQD7
A	514	SER	-	linker	UNP A0A0X8XQD7
A	515	ALA	-	linker	UNP A0A0X8XQD7
A	516	ILE	-	linker	UNP A0A0X8XQD7
A	517	GLY	-	linker	UNP A0A0X8XQD7
A	546	GLY	SER	conflict	UNP M1E1E4
A	547	LEU	-	expression tag	UNP M1E1E4
A	548	VAL	-	expression tag	UNP M1E1E4
A	549	PRO	-	expression tag	UNP M1E1E4
A	550	ARG	-	expression tag	UNP M1E1E4
B	132	THR	ALA	conflict	UNP A0A0X8XQD7
B	?	-	ARG	deletion	UNP A0A0X8XQD7
B	?	-	ARG	deletion	UNP A0A0X8XQD7
B	?	-	GLU	deletion	UNP A0A0X8XQD7
B	?	-	LEU	deletion	UNP A0A0X8XQD7
B	?	-	PRO	deletion	UNP A0A0X8XQD7
B	?	-	ARG	deletion	UNP A0A0X8XQD7
B	?	-	PHE	deletion	UNP A0A0X8XQD7
B	?	-	MET	deletion	UNP A0A0X8XQD7
B	?	-	ASN	deletion	UNP A0A0X8XQD7
B	?	-	TYR	deletion	UNP A0A0X8XQD7
B	?	-	THR	deletion	UNP A0A0X8XQD7
B	?	-	LEU	deletion	UNP A0A0X8XQD7
B	?	-	ASN	deletion	UNP A0A0X8XQD7
B	?	-	ASN	deletion	UNP A0A0X8XQD7
B	?	-	THR	deletion	UNP A0A0X8XQD7
B	?	-	LYS	deletion	UNP A0A0X8XQD7
B	?	-	ASN	deletion	UNP A0A0X8XQD7
B	?	-	ASN	deletion	UNP A0A0X8XQD7
B	?	-	ASN	deletion	UNP A0A0X8XQD7
B	?	-	VAL	deletion	UNP A0A0X8XQD7
B	?	-	THR	deletion	UNP A0A0X8XQD7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP A0A0X8XQD7
B	?	-	SER	deletion	UNP A0A0X8XQD7
B	?	-	LYS	deletion	UNP A0A0X8XQD7
B	?	-	LYS	deletion	UNP A0A0X8XQD7
B	?	-	ARG	deletion	UNP A0A0X8XQD7
B	?	-	LYS	deletion	UNP A0A0X8XQD7
B	?	-	ARG	deletion	UNP A0A0X8XQD7
B	?	-	ARG	deletion	UNP A0A0X8XQD7
B	152	VAL	ILE	conflict	UNP A0A0X8XQD7
B	155	CYS	SER	engineered mutation	UNP A0A0X8XQD7
B	190	PHE	SER	engineered mutation	UNP A0A0X8XQD7
B	207	LEU	VAL	engineered mutation	UNP A0A0X8XQD7
B	290	CYS	SER	engineered mutation	UNP A0A0X8XQD7
B	514	SER	-	linker	UNP A0A0X8XQD7
B	515	ALA	-	linker	UNP A0A0X8XQD7
B	516	ILE	-	linker	UNP A0A0X8XQD7
B	517	GLY	-	linker	UNP A0A0X8XQD7
B	546	GLY	SER	conflict	UNP M1E1E4
B	547	LEU	-	expression tag	UNP M1E1E4
B	548	VAL	-	expression tag	UNP M1E1E4
B	549	PRO	-	expression tag	UNP M1E1E4
B	550	ARG	-	expression tag	UNP M1E1E4
C	132	THR	ALA	conflict	UNP A0A0X8XQD7
C	?	-	ARG	deletion	UNP A0A0X8XQD7
C	?	-	ARG	deletion	UNP A0A0X8XQD7
C	?	-	GLU	deletion	UNP A0A0X8XQD7
C	?	-	LEU	deletion	UNP A0A0X8XQD7
C	?	-	PRO	deletion	UNP A0A0X8XQD7
C	?	-	ARG	deletion	UNP A0A0X8XQD7
C	?	-	PHE	deletion	UNP A0A0X8XQD7
C	?	-	MET	deletion	UNP A0A0X8XQD7
C	?	-	ASN	deletion	UNP A0A0X8XQD7
C	?	-	TYR	deletion	UNP A0A0X8XQD7
C	?	-	THR	deletion	UNP A0A0X8XQD7
C	?	-	LEU	deletion	UNP A0A0X8XQD7
C	?	-	ASN	deletion	UNP A0A0X8XQD7
C	?	-	ASN	deletion	UNP A0A0X8XQD7
C	?	-	THR	deletion	UNP A0A0X8XQD7
C	?	-	LYS	deletion	UNP A0A0X8XQD7
C	?	-	ASN	deletion	UNP A0A0X8XQD7
C	?	-	ASN	deletion	UNP A0A0X8XQD7
C	?	-	ASN	deletion	UNP A0A0X8XQD7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP A0A0X8XQD7
C	?	-	THR	deletion	UNP A0A0X8XQD7
C	?	-	LEU	deletion	UNP A0A0X8XQD7
C	?	-	SER	deletion	UNP A0A0X8XQD7
C	?	-	LYS	deletion	UNP A0A0X8XQD7
C	?	-	LYS	deletion	UNP A0A0X8XQD7
C	?	-	ARG	deletion	UNP A0A0X8XQD7
C	?	-	LYS	deletion	UNP A0A0X8XQD7
C	?	-	ARG	deletion	UNP A0A0X8XQD7
C	?	-	ARG	deletion	UNP A0A0X8XQD7
C	152	VAL	ILE	conflict	UNP A0A0X8XQD7
C	155	CYS	SER	engineered mutation	UNP A0A0X8XQD7
C	190	PHE	SER	engineered mutation	UNP A0A0X8XQD7
C	207	LEU	VAL	engineered mutation	UNP A0A0X8XQD7
C	290	CYS	SER	engineered mutation	UNP A0A0X8XQD7
C	514	SER	-	linker	UNP A0A0X8XQD7
C	515	ALA	-	linker	UNP A0A0X8XQD7
C	516	ILE	-	linker	UNP A0A0X8XQD7
C	517	GLY	-	linker	UNP A0A0X8XQD7
C	546	GLY	SER	conflict	UNP M1E1E4
C	547	LEU	-	expression tag	UNP M1E1E4
C	548	VAL	-	expression tag	UNP M1E1E4
C	549	PRO	-	expression tag	UNP M1E1E4
C	550	ARG	-	expression tag	UNP M1E1E4

- Molecule 2 is a protein called AM14 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	216	Total	C	N	O	S	0	0
			1636	1033	276	320	7		
2	H	216	Total	C	N	O	S	0	0
			1635	1033	276	319	7		
2	D	216	Total	C	N	O	S	0	0
			1636	1033	276	320	7		

- Molecule 3 is a protein called AM14 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	213	Total	C	N	O	S	0	0
			1642	1025	277	334	6		
3	I	213	Total	C	N	O	S	0	0
			1642	1025	277	334	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	213	Total 1642	C 1025	N 277	O 334	S 6	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
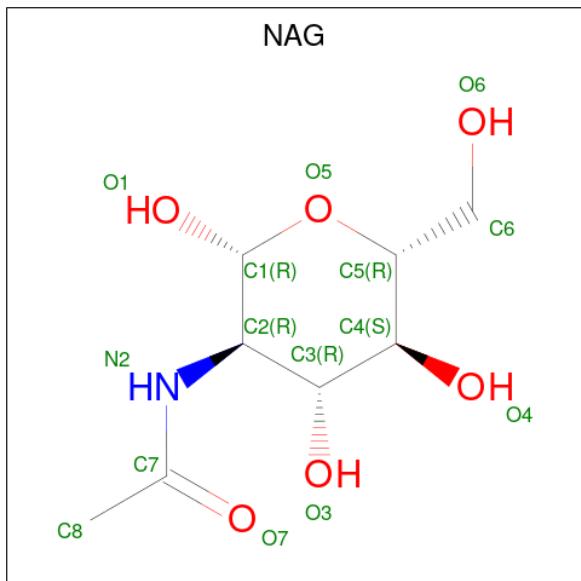
| Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fusion glycoprotein F0,Envelope glycoprotein

• Molecule 1: Fusion glycoprotein F0,Envelope glycoprotein

• Molecule 1: Fusion glycoprotein F0,Envelope glycoprotein

Chain C:

• Molecule 2: AM14 Fab Heavy Chain

Chain F:

• Molecule 2: AM14 Fab Heavy Chain

• Molecule 2: AM14 Fab Heavy Chain

• Molecule 2: AM14 Fab Heavy Chain

• Molecule 3: AM14 Fab Light Chain

Chain G:

51%

69% 21% • 9%

MET GLU THR PRO ALA GLU LEU LEU PHE LEU LEU LEU TRP LEU PRO ASP THR THR GLY D1 I2 Q3 M4 P8 L11 S14 D17 R18 V19 C23 Q24 Q27 D28 I29 Y32 L33 N34 H37 Q38 E45 L46 L47 M48 N53 V58 P59 S63

L73 S76 S77 L78 Q79 P80 E81 D82 I83 G84 T85 D92 T102 K103 V104 E105 I106 K107 R108 T109 V110 A111 A112 P113 S114 V115 F116 I117 F118 P119 P120 S121 D122 E123 Q124 L125 K126 S127 G128 T129 A130 S131 V132 V133 C134 L135 L136 N137 N138 F139 Y140 P141 R142 E143 A144 K145

V146 Q147 W148 K149 V150 D151 N152 A153 L154 Q155 S156 G157 N158 S159 Q160 E161 S162 V163 T164 E165 Q166 D167 S168 K169 D170 S171 T172 Y173 S174 L175 S176 S177 T178 L179 T180 L181 S182 K183 A184 D185 Y186 E187 K188 H189 K190 V191 Y192 A193 C194 E195 V196 T197 H198 Q199 G200 L201 S202 S203 P204 V205

T206 K207 S208 F209 N210 R211 G212 GLU CYS

• Molecule 3: AM14 Fab Light Chain

Chain I:

50%

70% 20% • 9%

MET GLU THR PRO ALA GLU LEU LEU PHE LEU LEU LEU TRP LEU PRO ASP THR THR GLY D1 P8 S14 D17 I21 Q24 Q27 L33 N34 W35 Y36 H37 Q38 E45 L46 L47 N53 L54 E55 V58 P59 S63 L73 S76 S77 L78 Q79

P80 E81 D82 I83 G84 T85 Y86 Y87 D92 N93 L94 G101 T102 E105 I106 K107 R108 T109 V110 A111 A112 P113 S114 V115 F116 I117 F118 P119 P120 S121 D122 E123 Q124 L125 K126 S127 G128 T129 A130 S131 V132 V133 C134 L135 L136 N137 N138 F139 Y140 P141 R142 E143 A144 K145 V146 Q147 W148

K149 V150 D151 N152 A153 L154 Q155 S156 G157 N158 S159 Q160 E161 S162 V163 T164 E165 Q166 D167 S168 K169 D170 S171 T172 Y173 S174 L175 S176 S177 T178 L179 T180 L181 S182 K183 A184 D185 Y186 E187 K188 H189 K190 V191 Y192 A193 C194 E195 V196 T197 H198 Q199 G200 L201 S202 S203 P204 V205 T206 K207 S208

F209 N210 R211 G212 GLU CYS

• Molecule 3: AM14 Fab Light Chain

Chain E:

49%

71% 20% 9%

MET GLU THR PRO ALA GLU LEU LEU PHE LEU LEU LEU TRP LEU PRO ASP THR THR GLY D1 P8 S14 D17 Q24 D28 L33 N34 W35 Y36 H37 Q38 E45 L46 L47 V58 P59 S63 L73 S76 S77 L78 Q79 P80 E81 D82 I83 G84 T85

Y91 D92 N93 F98 T102 E105 R108 T109 V110 A111 A112 P113 S114 V115 F116 I117 F118 P119 P120 S121 D122 E123 Q124 L125 K126 S127 G128 T129 A130 S131 V132 V133 C134 L135 L136 N137 N138 F139 Y140 P141 R142 E143 A144 K145 V146 Q147 W148 K149 V150 D151 N152 A153 L154 Q155 S156

G157 N158 S159 Q160 E161 S162 V163 T164 E165 Q166 D167 S168 K169 D170 S171 T172 Y173 S174 L175 S176 S177 T178 L179 T180 L181 S182 K183 A184 D185 Y186 E187 K188 H189 K190 V191 Y192 A193 C194 E195 V196 T197 H198 Q199 G200 L201 S202 S203 P204 V205 T206 K207 S208 F209 N210 R211 G212 GLU CYS

4   Experimental information   ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	23737	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 $(e^-/\text{Å}^2)$	26.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	30.023	Depositor
Minimum map value	-19.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.94	Depositor
Map size (Å)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.26	0/3547	0.49	1/4804 (0.0%)
1	B	0.26	0/3547	0.50	1/4804 (0.0%)
1	C	0.27	0/3547	0.50	1/4804 (0.0%)
2	D	0.27	0/1677	0.53	0/2286
2	F	0.27	0/1677	0.52	0/2286
2	H	0.26	0/1676	0.52	0/2285
3	E	0.25	0/1677	0.50	0/2277
3	G	0.25	0/1677	0.53	1/2277 (0.0%)
3	I	0.25	0/1677	0.52	2/2277 (0.1%)
All	All	0.26	0/20702	0.51	6/28100 (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})
3	G	115	VAL	CG1-CB-CG2	6.92	121.97	110.90
3	I	94	LEU	CB-CG-CD2	5.82	120.90	111.00
3	I	94	LEU	CB-CG-CD1	5.32	120.05	111.00
1	B	313	CYS	CA-CB-SG	5.25	123.45	114.00
1	C	313	CYS	CA-CB-SG	5.13	123.23	114.00

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	3497	0	3539	142	0
1	B	3497	0	3539	136	0
1	C	3497	0	3538	131	0
2	D	1636	0	1579	50	0
2	F	1636	0	1579	44	0
2	H	1635	0	1576	35	0
3	E	1642	0	1597	32	0
3	G	1642	0	1597	34	0
3	I	1642	0	1597	31	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	5	0
All	All	20366	0	20180	602	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 15.

The worst 5 of 602 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:95:LEU:HD22	1:B:278:VAL:HG12	1.42	0.99
2:H:52(A):TYR:O	2:H:71:ARG:NH1	1.97	0.96
4:C:601:NAG:H83	4:C:601:NAG:H3	1.49	0.94
1:B:95:LEU:HD22	1:C:278:VAL:HG12	1.50	0.93
1:A:278:VAL:HG12	1:C:95:LEU:HD22	1.55	0.86

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	447/496 (90%)	418 (94%)	28 (6%)	1 (0%)	47	78
1	B	447/496 (90%)	413 (92%)	34 (8%)	0	100	100
1	C	447/496 (90%)	413 (92%)	34 (8%)	0	100	100
2	D	212/244 (87%)	201 (95%)	11 (5%)	0	100	100
2	F	212/244 (87%)	203 (96%)	9 (4%)	0	100	100
2	H	212/244 (87%)	209 (99%)	3 (1%)	0	100	100
3	E	211/235 (90%)	198 (94%)	12 (6%)	1 (0%)	29	61
3	G	211/235 (90%)	197 (93%)	13 (6%)	1 (0%)	29	61
3	I	211/235 (90%)	194 (92%)	16 (8%)	1 (0%)	29	61
All	All	2610/2925 (89%)	2446 (94%)	160 (6%)	4 (0%)	50	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	110	VAL
3	I	110	VAL
3	E	110	VAL
1	A	362	SER

5.3.2 Protein sidechains (i)

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	412/446 (92%)	411 (100%)	1 (0%)	93	98
1	B	412/446 (92%)	411 (100%)	1 (0%)	93	98
1	C	412/446 (92%)	412 (100%)	0	100	100
2	D	182/207 (88%)	181 (100%)	1 (0%)	88	94
2	F	182/207 (88%)	181 (100%)	1 (0%)	88	94
2	H	181/207 (87%)	181 (100%)	0	100	100
3	E	189/209 (90%)	189 (100%)	0	100	100
3	G	189/209 (90%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	189/209 (90%)	189 (100%)	0	100	100
All	All	2348/2586 (91%)	2344 (100%)	4 (0%)	93	98

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

Mol	Chain	Res	Type
1	A	508	LYS
1	B	508	LYS
2	F	83	ARG
2	D	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	361	GLN
2	F	35	HIS
3	I	37	HIS
3	G	37	HIS
1	C	277	ASN

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 ⓘ

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	#$|Z| > 2$
4	NAG	C	601	1	14,14,15	0.68	0	17,19,21	0.96	1 (5%)
4	NAG	B	601	-	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	A	601	-	14,14,15	0.19	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
4	NAG	C	601	1	-	5/6/23/26	0/1/1/1
4	NAG	B	601	-	-	2/6/23/26	0/1/1/1
4	NAG	A	601	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	601	NAG	C1-O5-C5	3.24	116.58	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	C3-C2-N2-C7
4	C	601	NAG	O5-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
4	C	601	NAG	C8-C7-N2-C2
4	C	601	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	5	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 ⓘ

This section contains visualisations of the EMDB entry EMD-23933. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1   Orthogonal projections ⓘ

6.1.1   Primary map

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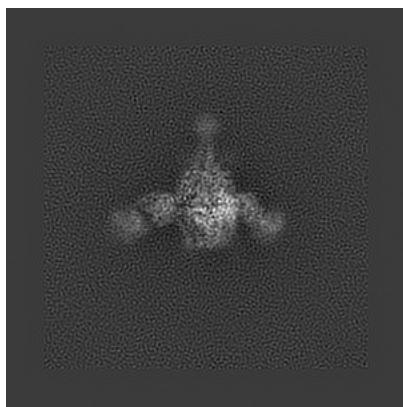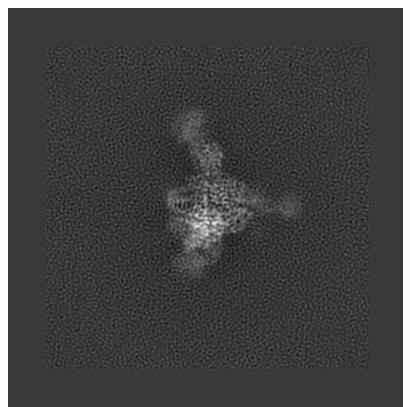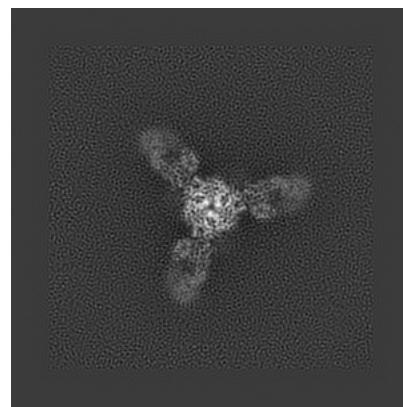
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
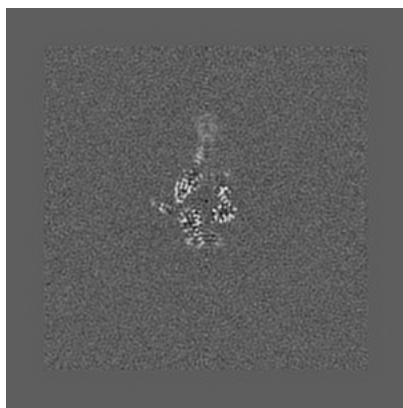
6.2.1   Primary map
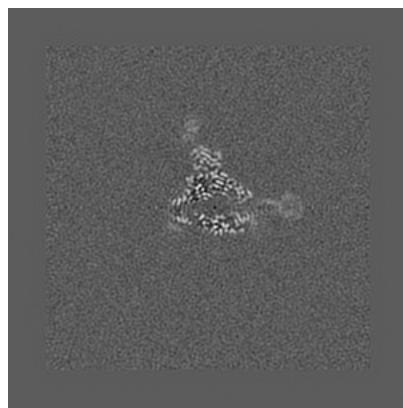
| X Index: 200 | Y Index: 200 | Z Index: 200 |
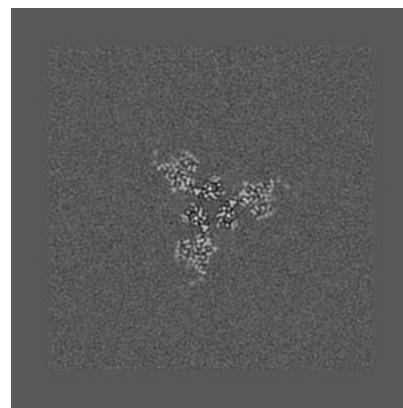
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
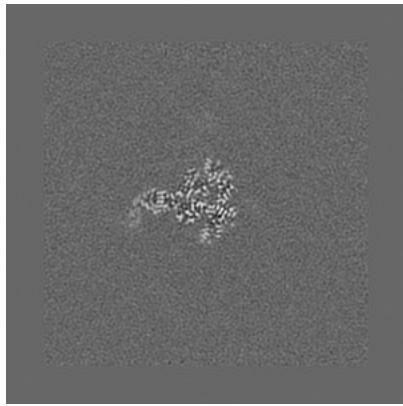
6.3.1 Primary map
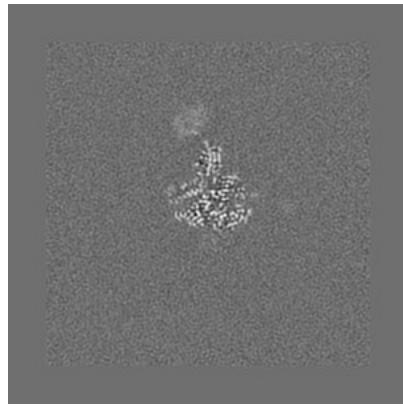
| X Index: 189 | Y Index: 213 | Z Index: 198 |
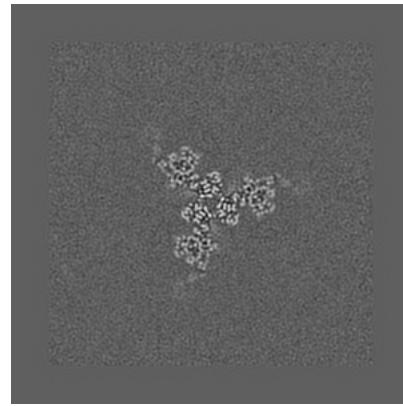
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 5.94. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7   Map analysis ⓘ

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

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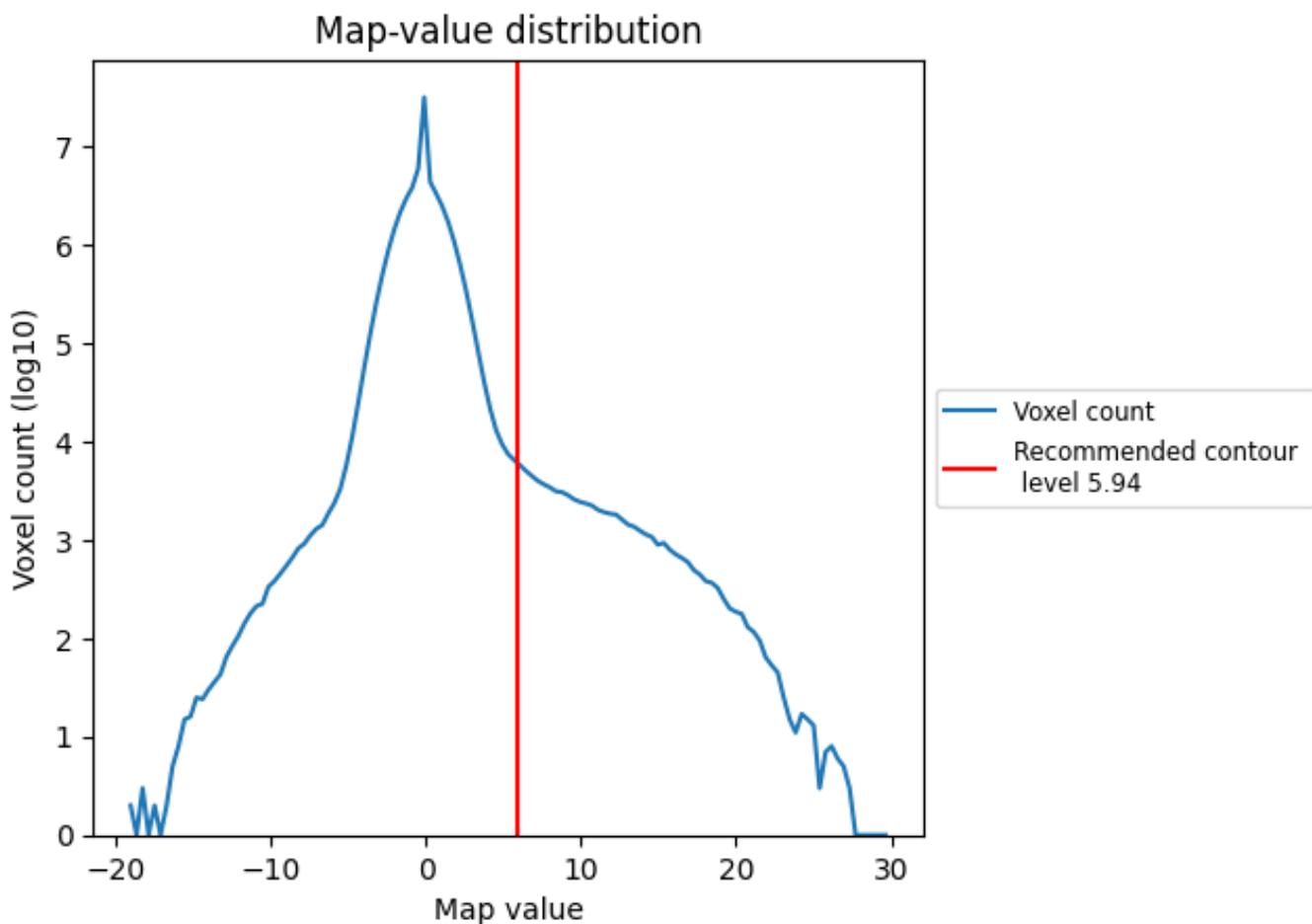
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
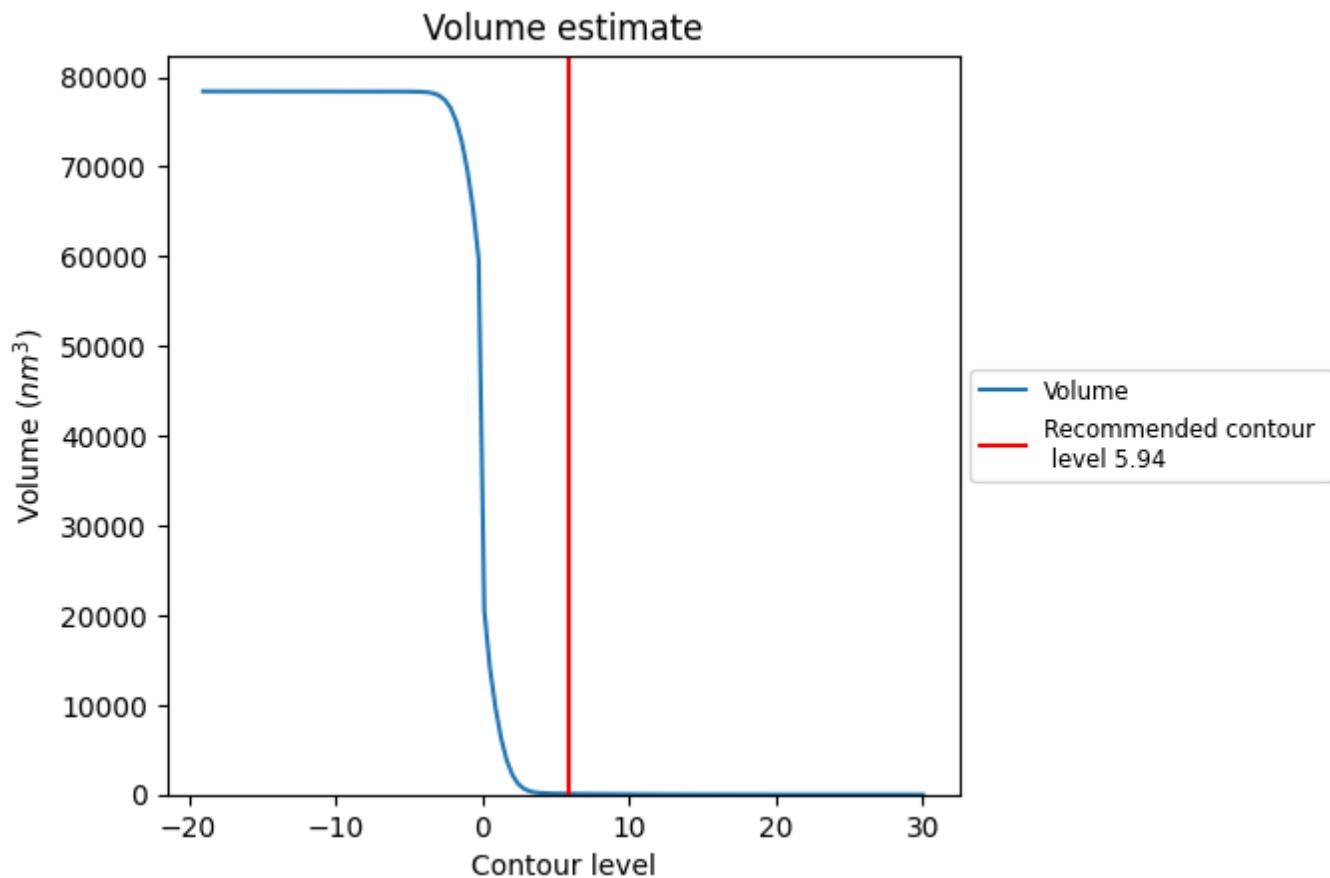
The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 78 kDa.

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 ⓘ
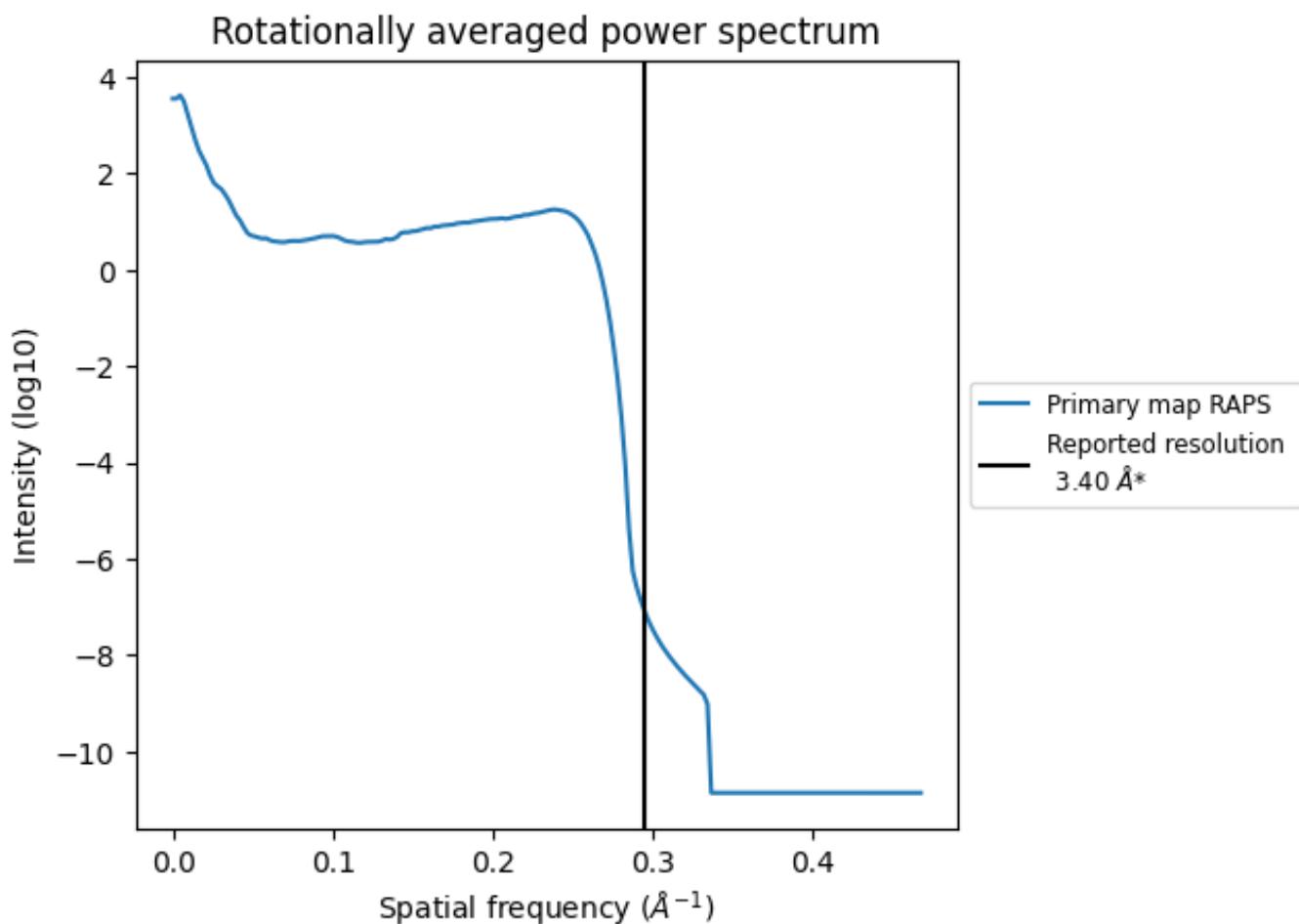
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-23933 and PDB model 7MPG. Per-residue inclusion information can be found in section 3 on page 9.

9.1   Map-model overlay ⓘ

| X | Y | Z |
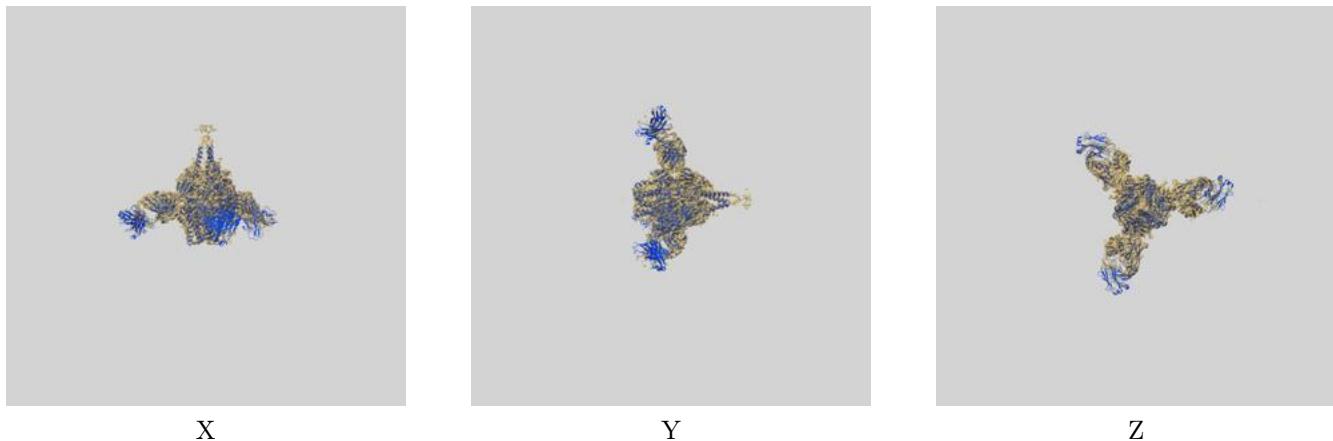
The images above show the 3D surface view of the map at the recommended contour level 5.94 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
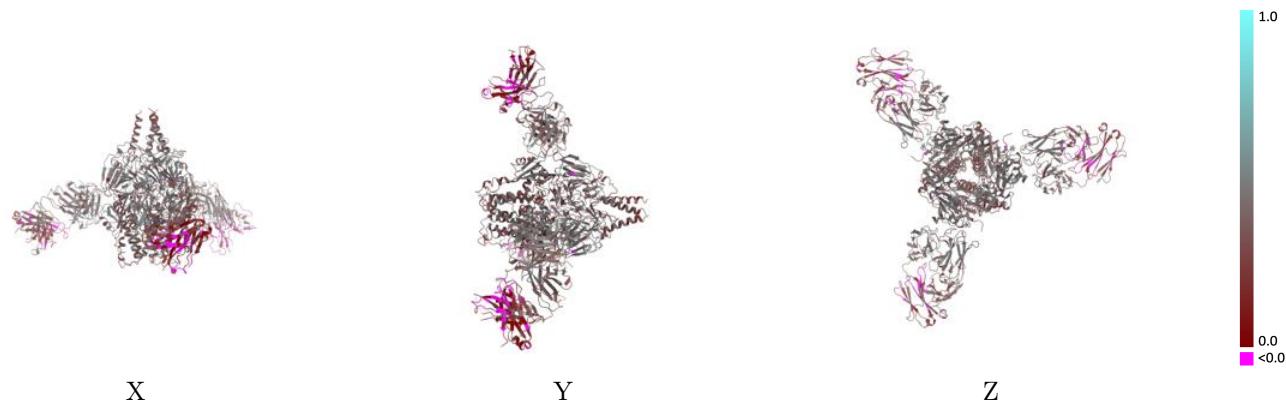
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
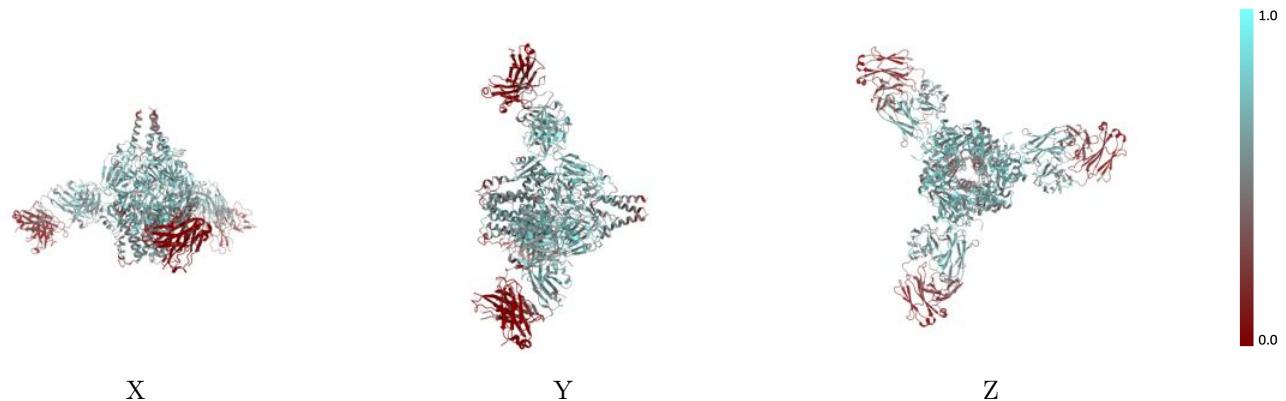
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.94).

9.4 Atom inclusion ⓘ
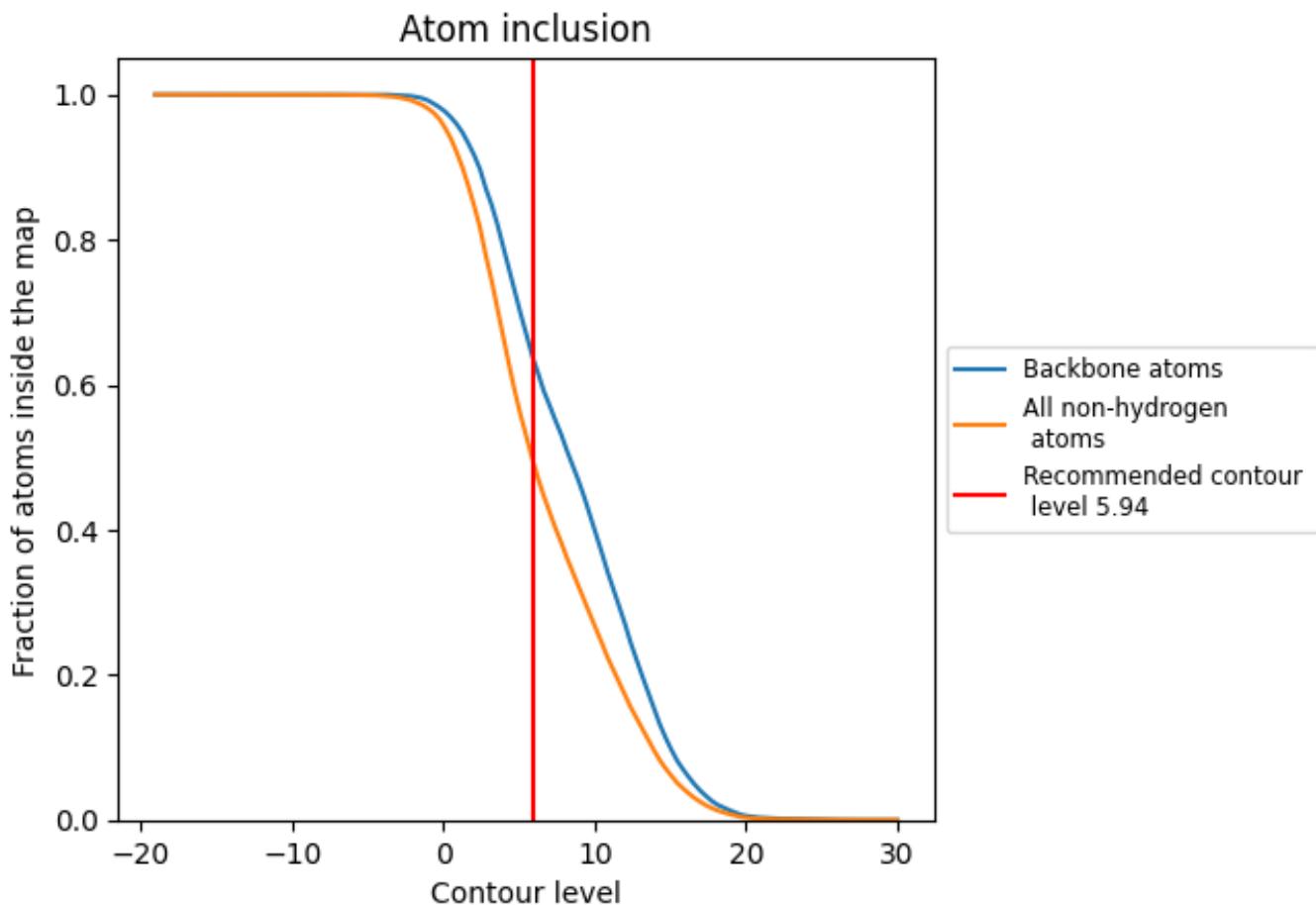
At the recommended contour level, 64% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5.94) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4945	0.3480
A	0.5998	0.3900
B	0.6050	0.3920
C	0.6078	0.3950
D	0.4267	0.2940
E	0.3261	0.2880
F	0.4261	0.2970
G	0.3292	0.2870
H	0.4263	0.3500
I	0.3243	0.2880

1.0

0.0
<0.0