wwPDB EM Validation Summary Report (i)

Mar 13, 2023 – 12:35 pm GMT

PDB ID	:	8BMW
EMDB ID	:	EMD-16126
Title	:	SsoCsm
Authors	:	Spagnolo, L.; White, M.F.
Deposited on	:	2022-11-11
Resolution	:	3.50 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 3.50 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		12
Ramachandran outliers		0.1%
Sidechain outliers		1.5%
RNA backbone		0.29

Worse ← → *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
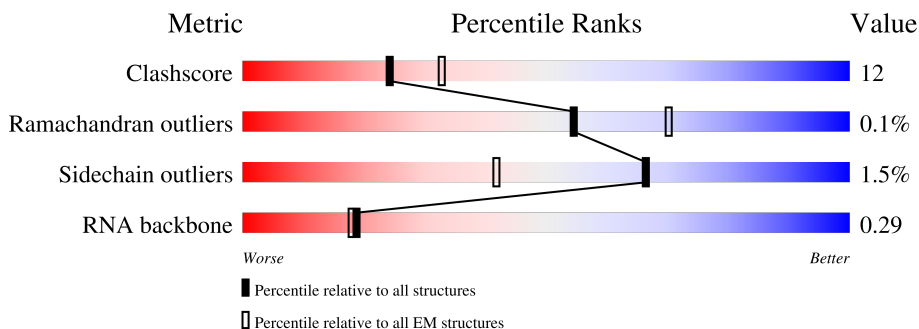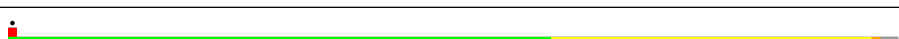
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	139	70% 17% · 13%
1	B	139	62% 24% 14%
1	C	139	61% 24% · 14%
1	D	139	63% 24% 13%
1	E	139	61% 25% · 12%
2	J	272	68% 30% ··
3	L	202	67% 32% ·

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Mol	Chain	Length	Quality of chain
4	N	252	70% · · · 28%
5	R	48	31% · 52% · 17%
6	F	248	60% · 36%
6	G	248	66% · 29%
7	H	278	71% · 28%
7	I	278	70% · 28%
8	K	829	74% · 24%
9	M	300	61% · 36%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 28658 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 CRISPR-associated small subunit protein (Type III-D).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			964	617	164	182	1		
1	B	119	Total	C	N	O	S	0	0
			948	606	161	180	1		
1	C	120	Total	C	N	O	S	0	0
			957	612	163	181	1		
1	D	121	Total	C	N	O	S	0	0
			964	617	164	182	1		
1	E	122	Total	C	N	O	S	0	0
			973	622	166	184	1		

- Molecule 2 is a protein called CRISPR-associated Cas7 paralog (Type III-D).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	270	Total	C	N	O	S	0	0
			2121	1350	371	390	10		

- Molecule 3 is a protein called CRISPR-associated Cas7 paralog (Type III-D).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	201	Total	C	N	O	S	0	0
			1585	1000	268	307	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	ASP	GLU	conflict	UNP A0A157T2I3

- Molecule 4 is a protein called CRISPR-associated Cas7 paralog (Type III-D).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	251	Total	C	N	O	S	0	0
			2029	1283	359	383	4		

- Molecule 5 is a RNA chain called RNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	48	Total 971	C 438	N 114	O 372	P 47	0	0

- Molecule 6 is a protein called CRISPR-associated Cas7 paralog (Type III-D).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	238	Total 1877	C 1209	N 309	O 348	S 11	0	0
6	F	239	Total 1876	C 1204	N 309	O 351	S 12	0	0

- Molecule 7 is a protein called CRISPR-associated Cas7 paralog (Type III-D).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	275	Total 2168	C 1381	N 374	O 401	S 12	0	0
7	I	275	Total 2164	C 1381	N 374	O 401	S 8	0	0

- Molecule 8 is a protein called CRISPR-associated protein Cas10 (Type III-D).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	829	Total 6678	C 4277	N 1101	O 1274	S 26	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	421	ASP	ASN	conflict	UNP A0A157T112

- Molecule 9 is a protein called CRISPR-associated protein Cas5 (Type III-D).

| Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	294	Total 2383	C 1541	N 389	O 444	S 9	0	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.
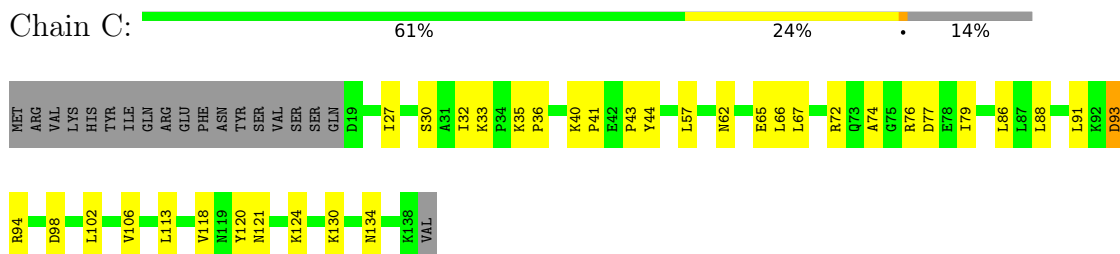
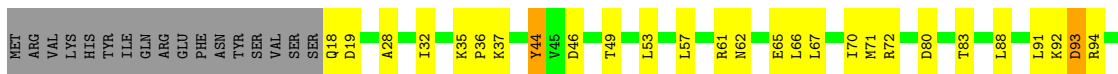• Molecule 1: CRISPR-associated small subunit protein (Type III-D)
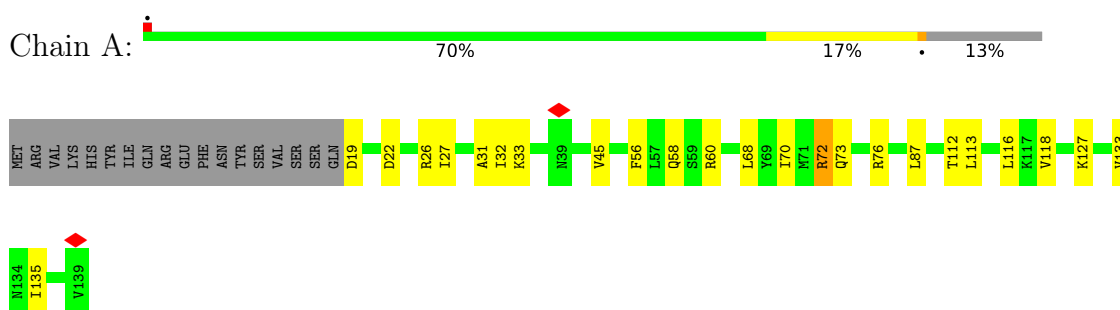
Chain A:

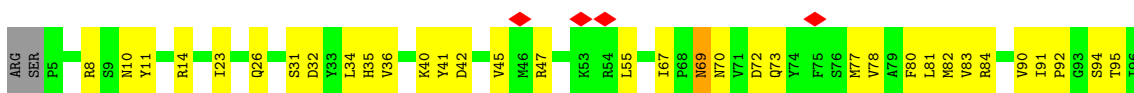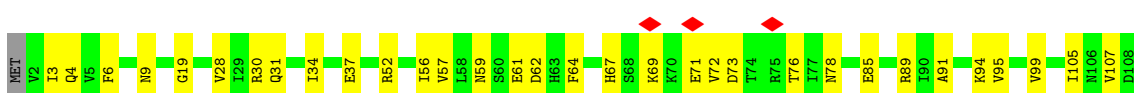• Molecule 1: CRISPR-associated small subunit protein (Type III-D)

Chain B:

• Molecule 1: CRISPR-associated small subunit protein (Type III-D)

Chain C:
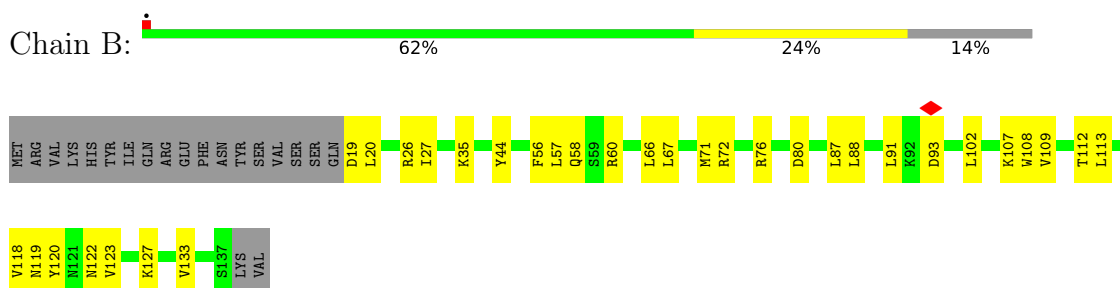
• Molecule 1: CRISPR-associated small subunit protein (Type III-D)

Chain D:

• Molecule 1: CRISPR-associated small subunit protein (Type III-D)

Chain E:

• Molecule 2: CRISPR-associated Cas7 paralog (Type III-D)
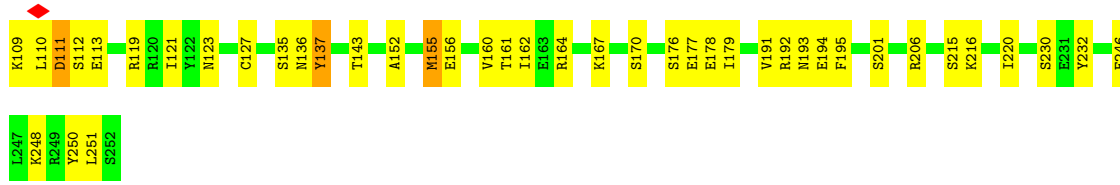
Chain J:
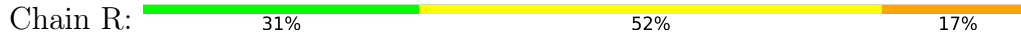

• Molecule 3: CRISPR-associated Cas7 paralog (Type III-D)

Chain L:

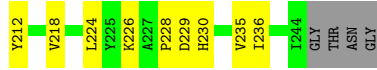• Molecule 4: CRISPR-associated Cas7 paralog (Type III-D)

Chain N:

K109 L110 D111 S112 E113 R119 R120 I121 Y122 N123 C127 S135 N136 Y137 T143 A152 M155 E156 V160 T161 I162 E163 R164 K167 S170 S176 E177 E178 I179 V191 R192 N193 E194 F195 S201 R206 S215 K216 I220 S230 E231 Y232 E246

L247 K248 R249 Y250 L251 S252

• Molecule 5: RNA (48-MER)

Chain R: 31%   52%   17%

A1 U2 U3 G4 A5 A6 A7 G8 U9 U10 U11 U12 U13 U14 U15 U16 U17 U20 U21 U22 U23 U24 U25 U26 U27 U28 U29 U30 U31 U32 U33 U34 U35 U39 U42 U43 U44 U45 U46 U47 U48
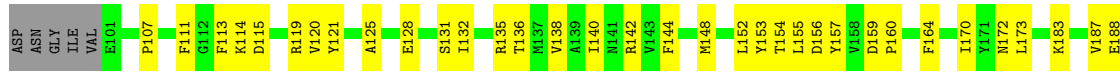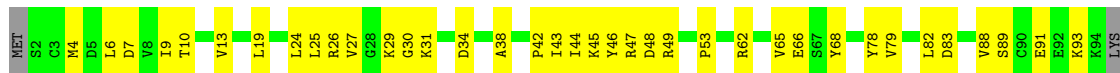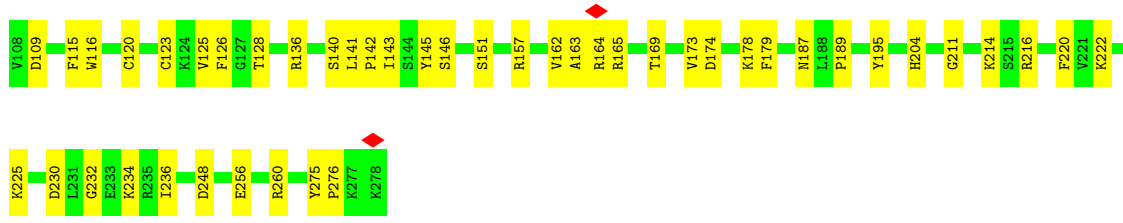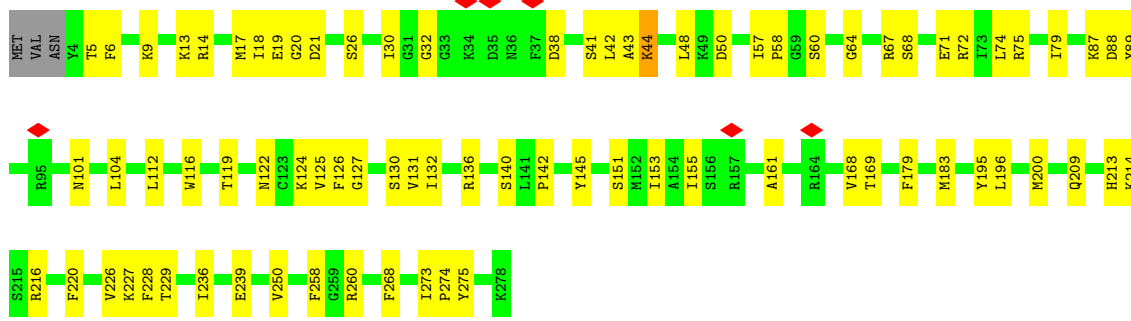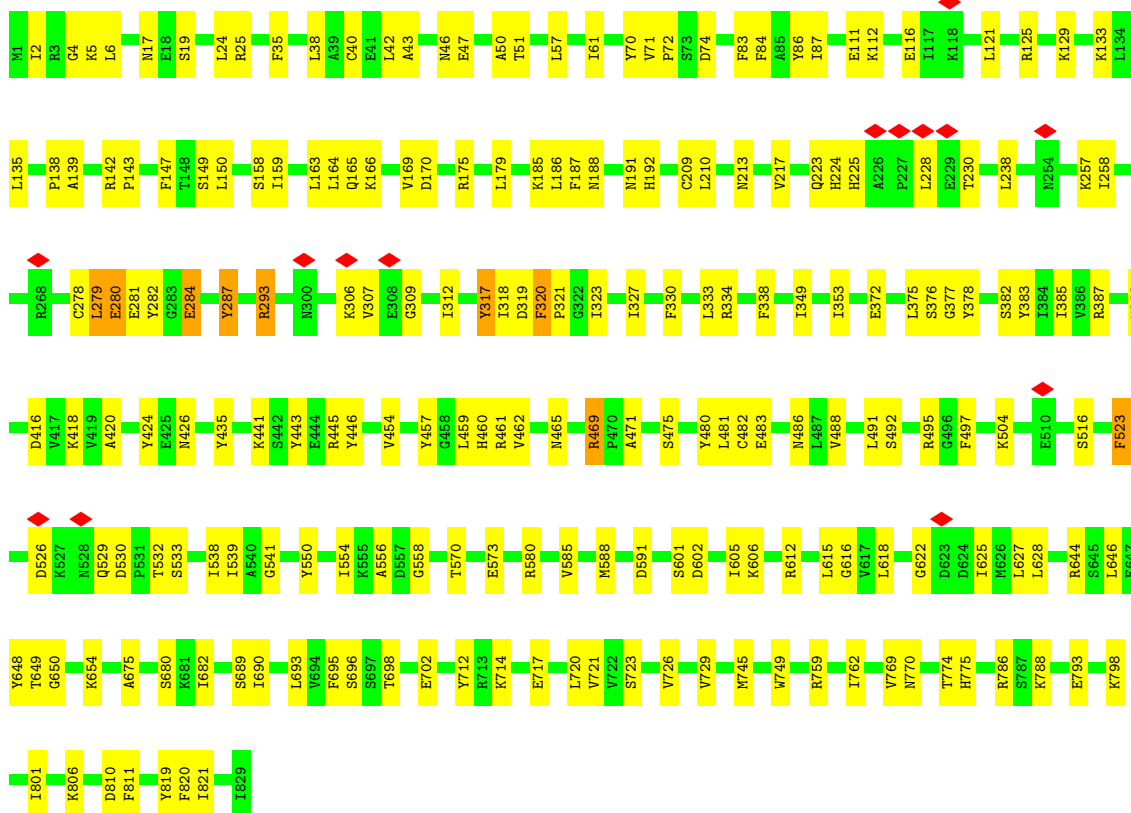
• Molecule 6: CRISPR-associated Cas7 paralog (Type III-D)

Chain G: 66%   29%

MET SER CYS M4 D5 L6 V13 L19 R20 N21 E22 T23 L24 L25 R26 V27 G28 K29 T32 Q33 E37 N41 P42 I43 I44 K45 Y46 R47 D48 R49 K58 F61 S75 Y78 V79 C80 D81 L82 N85 V88 E91 K95 ASP ASN GLY I99

R103 P107 F111 G112 F113 K114 V120 Y121 I122 L123 A127 E128 K129 V130 S131 I140 N141 R142 V143 F144 G145 G146 P149 Y157 V158 D159 E163 F164 S165 F166 M169 I170 L175 W182 K183 A184 K185 S186 L190 L193 R199 R207 K208 S209

Y212 V218 L224 Y225 K226 A227 P228 D229 H230 V235 I236 I244 GLY THR ASN GLY

• Molecule 6: CRISPR-associated Cas7 paralog (Type III-D)

Chain F: 60%   36%

MET S2 C3 M4 D5 L6 D7 V8 I9 T10 V13 L19 L24 L25 R26 V27 G28 K29 G30 K31 D34 A38 P42 I43 I44 K45 Y46 R47 D48 R49 P53 R62 V65 E66 S67 Y68 Y78 V79 L82 D83 V88 S89 C90 E91 E92 K93 K94 LYS

ASP ASN GLY ILE VAL E101 P107 F111 G112 F113 K114 D115 R119 V120 Y121 A125 E128 S131 I132 R135 T136 M137 V138 A139 I140 N141 R142 V143 F144 M148 L152 Y153 T154 L155 D156 Y157 V158 D159 P160 F164 I170 Y171 N172 L173 K183 V187 E188

L197 V198 R199 I202 A206 R207 K208 S209 V210 G211 Y212 G213 L214 I215 K216 L217 A220 K221 L224 P228 D229 H230 V235 I236 K239 T246 ASN GLY

• Molecule 7: CRISPR-associated Cas7 paralog (Type III-D)

Chain H: 71%   28%

MET VAL ASN Y4 T5 F6 I7 D8 K9 R10 R14 D21 S26 P27 L28 G31 G32 G33 K34 F37 L42 L48 K49 D50 V51 R54 P58 R67 G70 E71 R72 C82 S83 G84 I85 D88 Y89 C90 N93 F100 A103 E106 N107

V108 D109 F115 W116 C120 C123 K124 V125 F126 G127 T128 R136 S140 L141 P142 I143 S144 Y145 S146 S151 R157 V162 A163 R164 R165 T169 V173 D174 K178 F179 N187 L188 P189 Y195 H204 G211 K214 S215 R216 F220 V221 K222

K225 D230 L231 G232 E233 K234 R235 I236 D248 E256 R260 Y275 P277 K277 K278

• Molecule 7: CRISPR-associated Cas7 paralog (Type III-D)

Chain I:

MET VAL ASN Y4 T5 F6 K9 K13 R14 M17 I18 E19 G20 D21 S26 I30 G31 G32 G33 K34 D35 N36 F37 D38 S41 L42 A43 K44 L48 K49 D50 I57 P58 G59 S60 G64 R67 S68 E71 R72 I73 L74 R75 I79 K87 D88 Y89

R95 N101 L104 L112 W116 T119 N122 C123 K124 V125 F126 G127 S130 V131 I132 R136 S140 L141 P142 Y145 S151 M152 I153 A154 I155 S156 R157 A161 R164 V168 T169 F179 M183 Y195 L196 M200 Q209 H213 K214

S215 R216 F220 V226 K227 F228 T229 I236 E239 V250 F258 G259 R260 F268 I273 P274 Y275 K278

• Molecule 8: CRISPR-associated protein Cas10 (Type III-D)

Chain K:

M1 I2 R3 G4 K5 L6 N17 E18 S19 L24 R25 F35 L38 A39 C40 E41 L42 A43 N46 E47 A50 T51 L57 I61 Y70 V71 P72 S73 D74 F83 F84 A85 Y86 I87 E111 K112 E116 I117 K118 L121 R125 K129 K133 L134

L135 P138 A139 R142 P143 F147 T148 S149 L150 S158 I159 L163 L164 Q165 K166 V169 D170 R175 L179 K185 L186 F187 N188 N191 H192 C209 L210 N213 V217 Q223 H224 H225 A226 P227 L228 E229 T230 L238 N254 K257 I258 C265

R268 C278 L279 E280 E281 Y282 G283 E284 Y287 R293 N300 K306 V307 E308 G309 I312 Y317 I318 D319 P320 P321 G322 I323 I327 F330 L333 R334 F338 I349 I353 E372 L375 S376 G377 Y378 S382 Y383 I384 I385 V386 R387 K393

D416 V417 K418 V419 A420 Y424 E425 N426 Y435 K441 S442 Y443 E444 R445 Y446 V454 Y457 G458 L459 H460 R461 V462 N465 R469 P470 A471 S475 Y480 L481 C482 E483 N486 L487 V488 L491 S492 R495 G496 F497 K504 E510 S516 F523

D526 K527 N528 Q529 D530 P531 T532 S533 I538 I539 A540 G541 Y550 I554 K555 A556 D557 G558 T570 E573 R580 V585 M588 D591 S601 D602 I605 K606 R612 L615 G616 V617 L618 G622 D623 D624 I625 M626 L627 L628 R644 S645 L646 E647

Y648 T649 G650 K654 A675 S680 K681 I682 S689 I690 L693 V694 F695 S696 S697 T698 E702 Y712 R713 K714 E717 L720 V721 V722 S723 V726 V729 M745 W749 R759 I762 V769 N770 T774 H775 R786 S787 K788 E793 K798

I801 K806 D810 F811 Y819 F820 I821 I829

• Molecule 9: CRISPR-associated protein Cas5 (Type III-D)

Chain M:

61%　　　　36%

MET I2 L3 I4 K5 L6 K9 G10 Y11 Q15 M16 I19 R20 N21 F24 I30 P31 S32 R36 G37 A38 I39 E42 Y43 Q46 V56 Y60 P61 I62 K63 T64 A67 H68 Y69 E75 R76 K77 G78 D79 E80 F81 V84 K85 R86 I87 K91

E92 K93 E94 F95 E96 A97 N98 K99 P100 I101 E102 E103 I104 M105 K106 L107 E108 H113 P114 K115 I118 G119 S120 L121 I122 E127 T128 D129 K130 E131 N132 K133 Y134 R135 E136 F137 K140 S141 I142 I143 Q144 M145 H146 I149 D150 LYS THR SER ILE SER S156 Y157 K158 L161

F162 A163 E168 M172 W173 A174 I175 A176 T184 V185 K186 R187 I188 R192 D202 V203 E204 K205 V206 D212 L217 L218 Y219 C220 L221 S222 I225 I240 G241 T251 V252 D253 P260 V261 T264 L265 R266 L270 V271 Y272 F289 M290 L291 R292 I299

L300

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192787	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 $(e^-/\text{Å}^2)$	34	Depositor
Minimum defocus (nm)	0	Depositor
Maximum defocus (nm)	0	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	313.8, 313.8, 313.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.046, 1.046, 1.046	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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 RMSZ	Bond lengths $\#|Z| > 5$	Bond angles RMSZ	Bond angles $\#|Z| > 5$
1	A	0.24	0/976	0.42	0/1318
1	B	0.24	0/960	0.42	0/1297
1	C	0.25	0/969	0.42	0/1308
1	D	0.24	0/976	0.42	0/1318
1	E	0.25	0/985	0.43	0/1330
2	J	0.29	0/2161	0.51	0/2909
3	L	0.29	0/1613	0.50	0/2188
4	N	0.27	0/2060	0.50	0/2763
5	R	0.27	0/1072	0.78	0/1658
6	F	0.27	0/1907	0.46	0/2568
6	G	0.27	0/1908	0.46	0/2569
7	H	0.32	0/2209	0.51	0/2966
7	I	0.31	0/2205	0.51	0/2962
8	K	0.27	0/6803	0.45	0/9173
9	M	0.30	0/2433	0.51	0/3266
All	All	0.28	0/29237	0.49	0/39593

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	964	0	1019	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	948	0	997	21	0
1	C	957	0	1010	23	0
1	D	964	0	1019	21	0
1	E	973	0	1027	33	0
2	J	2121	0	2149	66	0
3	L	1585	0	1591	57	0
4	N	2029	0	2059	57	0
5	R	971	0	488	41	0
6	F	1876	0	1921	66	0
6	G	1877	0	1936	50	0
7	H	2168	0	2180	52	0
7	I	2164	0	2172	58	0
8	K	6678	0	6719	135	0
9	M	2383	0	2416	69	0
All	All	28658	0	28703	680	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 12.

The worst 5 of 680 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:22:ILE:HD11	8:K:720:LEU:HD22	1.54	0.88
3:L:58:CYS:N	3:L:75:CYS:SG	2.47	0.86
6:F:26:ARG:HG2	6:F:206:ALA:HB2	1.58	0.85
8:K:38:LEU:HD11	8:K:116:GLU:HG3	1.55	0.85
3:L:159:ARG:HD3	3:L:200:LEU:HB2	1.60	0.81

There are no symmetry-related clashes.

5.3　Torsion angles　ⓘ

5.3.1　Protein backbone　ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/139 (86%)	113 (95%)	6 (5%)	0	100	100
1	B	117/139 (84%)	113 (97%)	4 (3%)	0	100	100
1	C	118/139 (85%)	115 (98%)	3 (2%)	0	100	100
1	D	119/139 (86%)	116 (98%)	3 (2%)	0	100	100
1	E	120/139 (86%)	115 (96%)	5 (4%)	0	100	100
2	J	268/272 (98%)	250 (93%)	16 (6%)	2 (1%)	22	61
3	L	199/202 (98%)	185 (93%)	14 (7%)	0	100	100
4	N	249/252 (99%)	230 (92%)	19 (8%)	0	100	100
6	F	235/248 (95%)	212 (90%)	23 (10%)	0	100	100
6	G	234/248 (94%)	217 (93%)	17 (7%)	0	100	100
7	H	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
7	I	273/278 (98%)	252 (92%)	21 (8%)	0	100	100
8	K	827/829 (100%)	790 (96%)	37 (4%)	0	100	100
9	M	290/300 (97%)	258 (89%)	30 (10%)	2 (1%)	22	61
All	All	3441/3602 (96%)	3227 (94%)	210 (6%)	4 (0%)	54	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	45	VAL
9	M	20	ARG
9	M	93	LYS
2	J	69	ASN

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	110/128 (86%)	108 (98%)	2 (2%)	59	81
1	B	108/128 (84%)	107 (99%)	1 (1%)	78	90
1	C	109/128 (85%)	108 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	110/128 (86%)	109 (99%)	1 (1%)	78	90
1	E	111/128 (87%)	109 (98%)	2 (2%)	59	81
2	J	239/244 (98%)	236 (99%)	3 (1%)	69	86
3	L	185/186 (100%)	183 (99%)	2 (1%)	73	88
4	N	225/226 (100%)	222 (99%)	3 (1%)	69	86
6	F	209/216 (97%)	207 (99%)	2 (1%)	76	88
6	G	209/216 (97%)	206 (99%)	3 (1%)	67	85
7	H	236/239 (99%)	233 (99%)	3 (1%)	69	86
7	I	232/239 (97%)	227 (98%)	5 (2%)	52	78
8	K	745/745 (100%)	734 (98%)	11 (2%)	65	84
9	M	262/268 (98%)	254 (97%)	8 (3%)	40	70
All	All	3090/3219 (96%)	3043 (98%)	47 (2%)	66	84

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	K	166	LYS
8	K	320	PHE
8	K	279	LEU
8	K	287	TYR
8	K	469	ARG

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

Mol	Chain	Res	Type
1	E	18	GLN
1	E	134	ASN
3	L	125	GLN
9	M	15	GLN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	47/48 (97%)	15 (31%)	1 (2%)

5 of 15 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	R	3	U
5	R	5	A
5	R	6	A
5	R	7	A
5	R	8	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	R	4	G

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-16126. 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 |
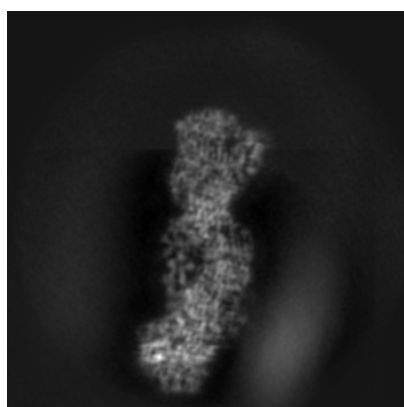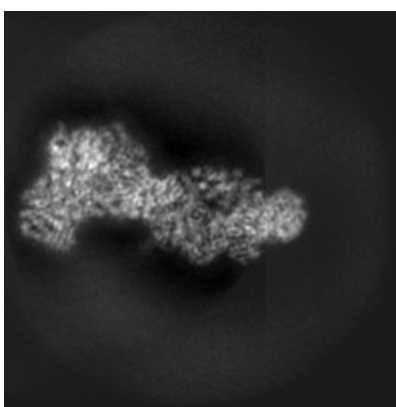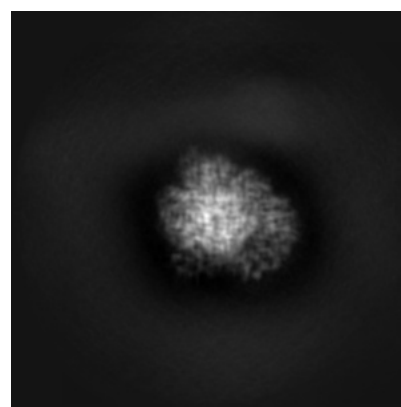
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
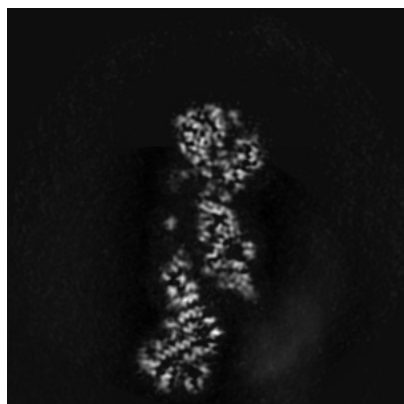
6.2.1 Primary map
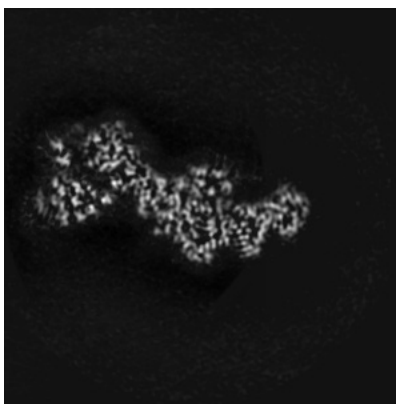
| X Index: 150 | Y Index: 150 | Z Index: 150 |
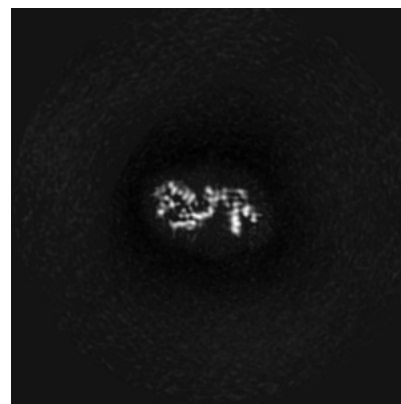
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
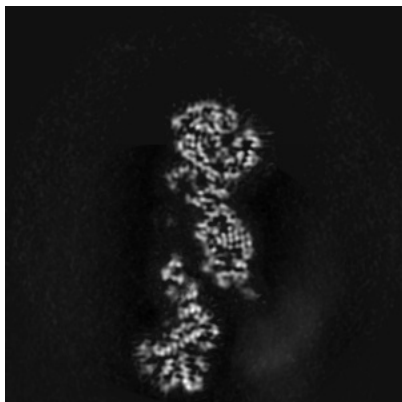
6.3.1   Primary map
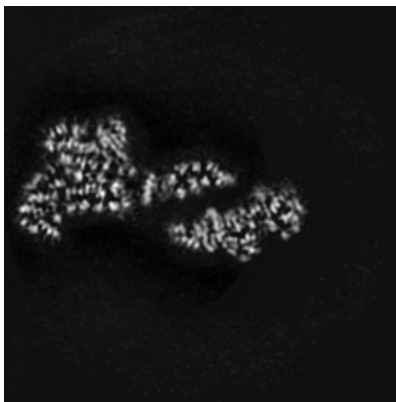
| X Index: 147 | Y Index: 137 | Z Index: 39 |
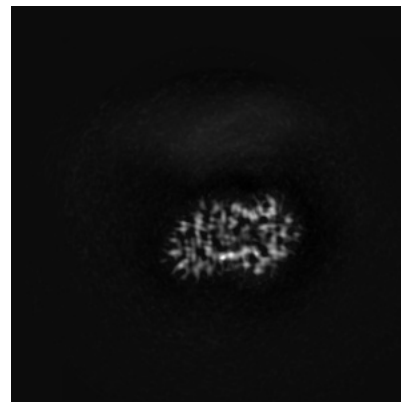
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views ⓘ

6.4.1   Primary map

| X | Y | Z |
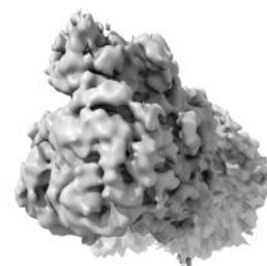
The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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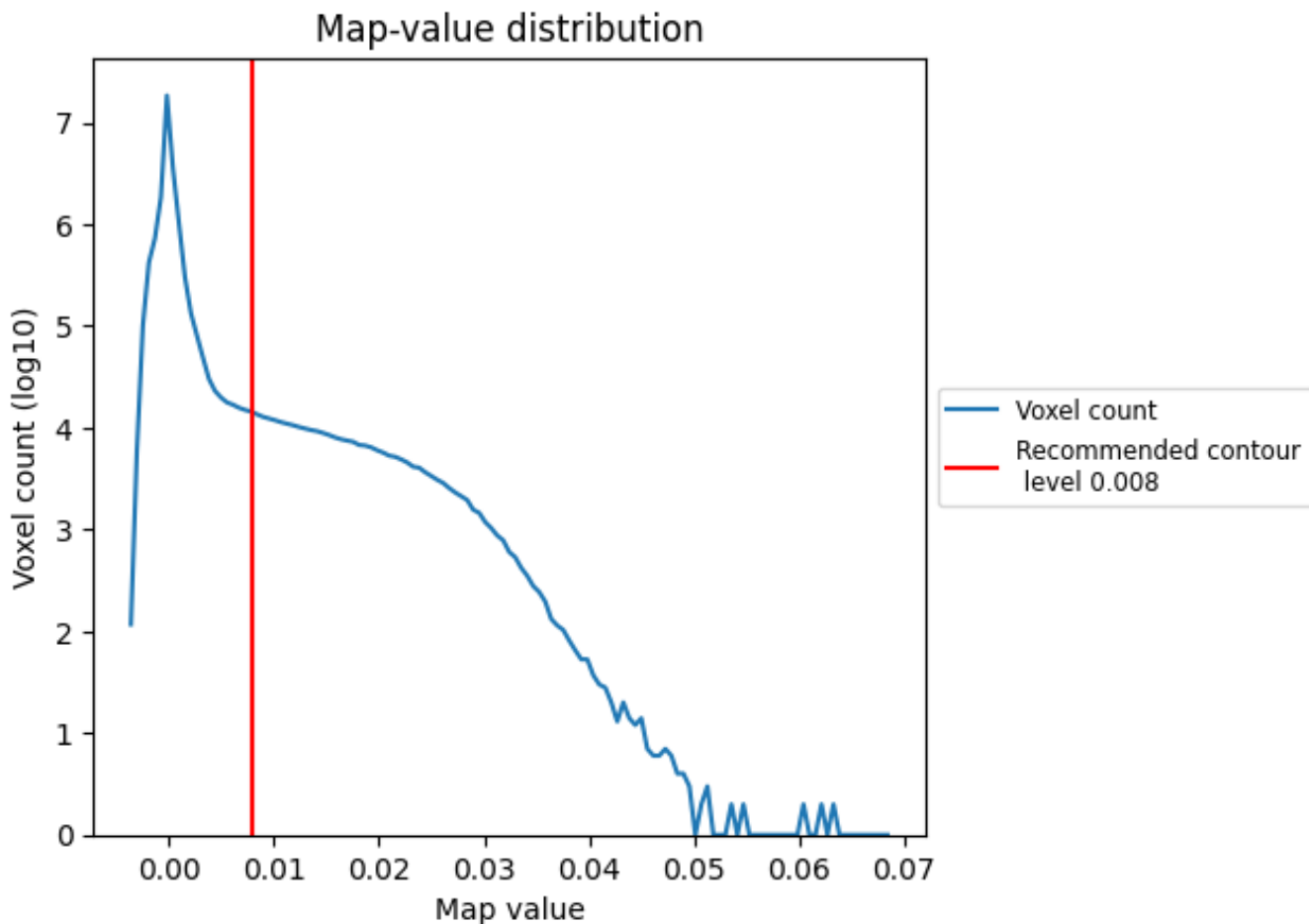
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
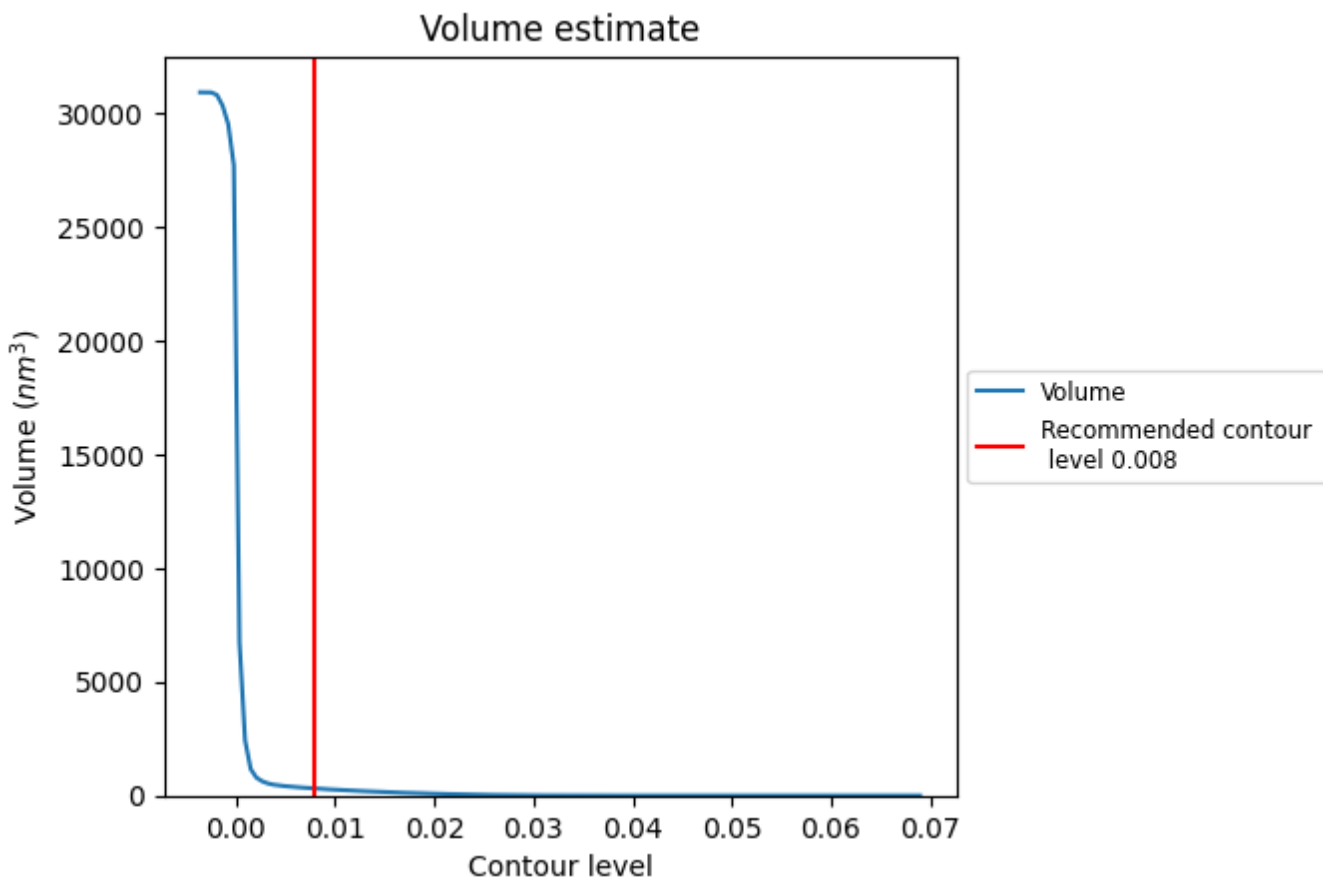
The volume at the recommended contour level is 311 nm^3; this corresponds to an approximate mass of 281 kDa.

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 ⓘ
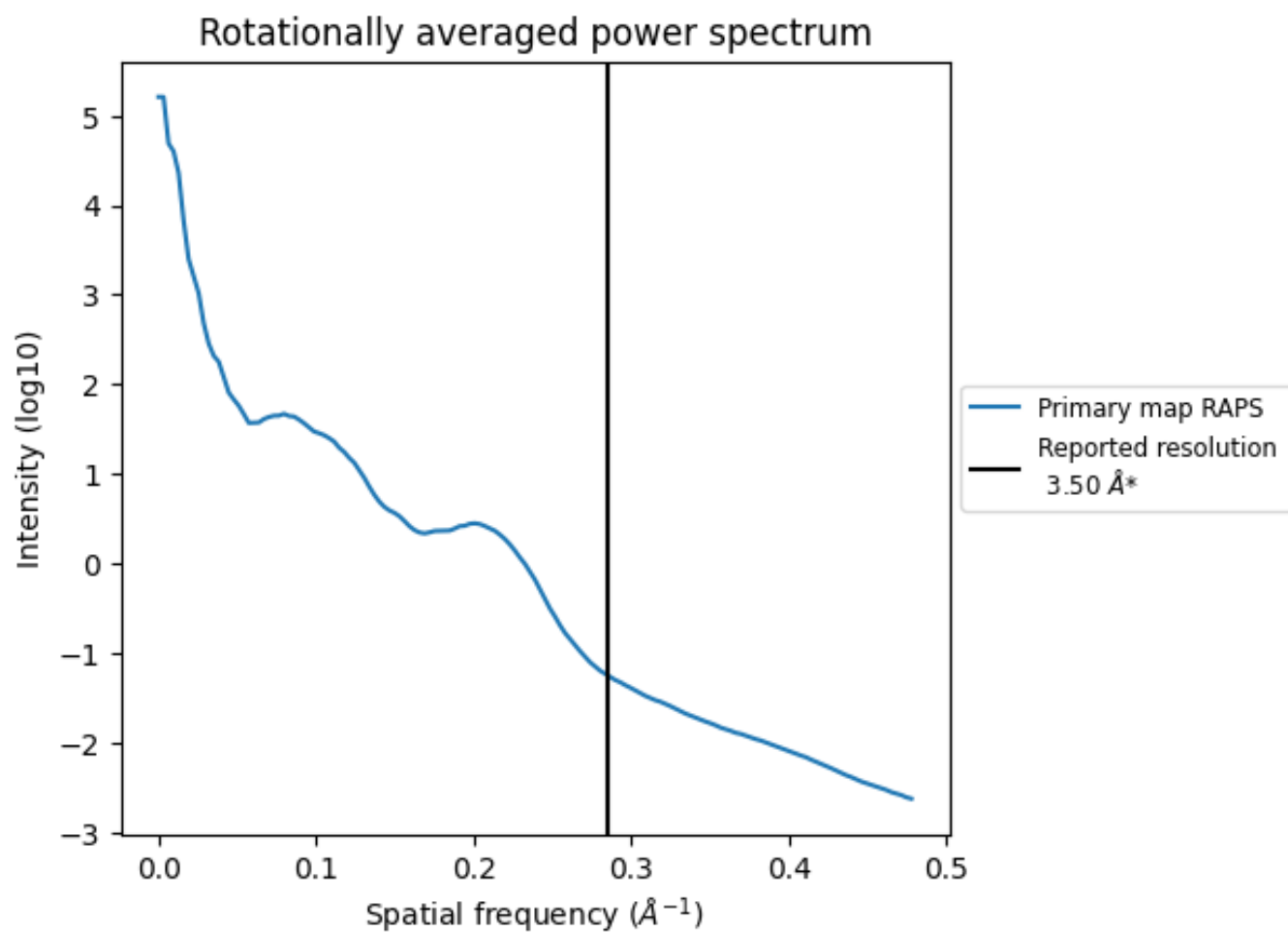
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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-16126 and PDB model 8BMW. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

| X | Y | Z |
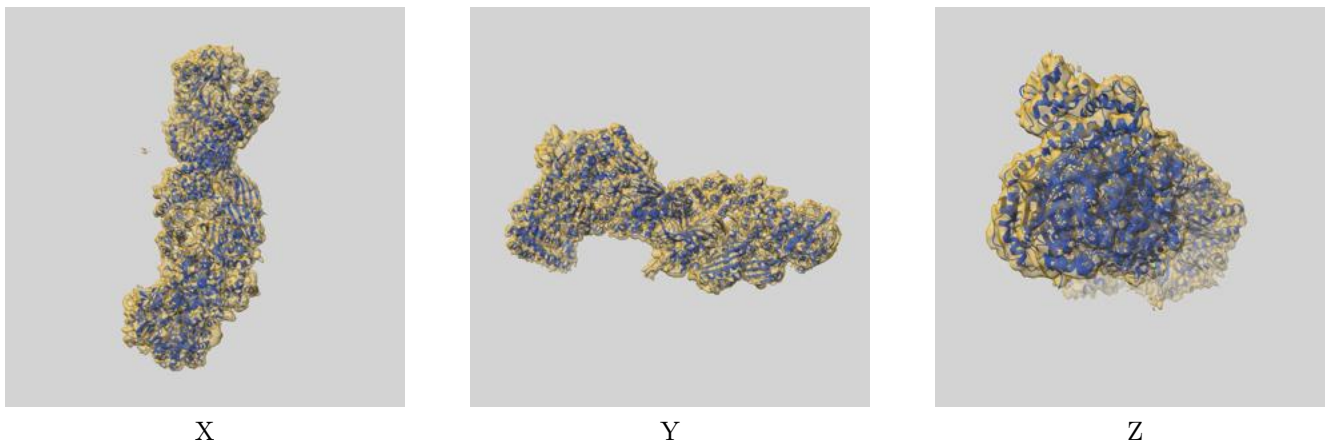
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X Y Z
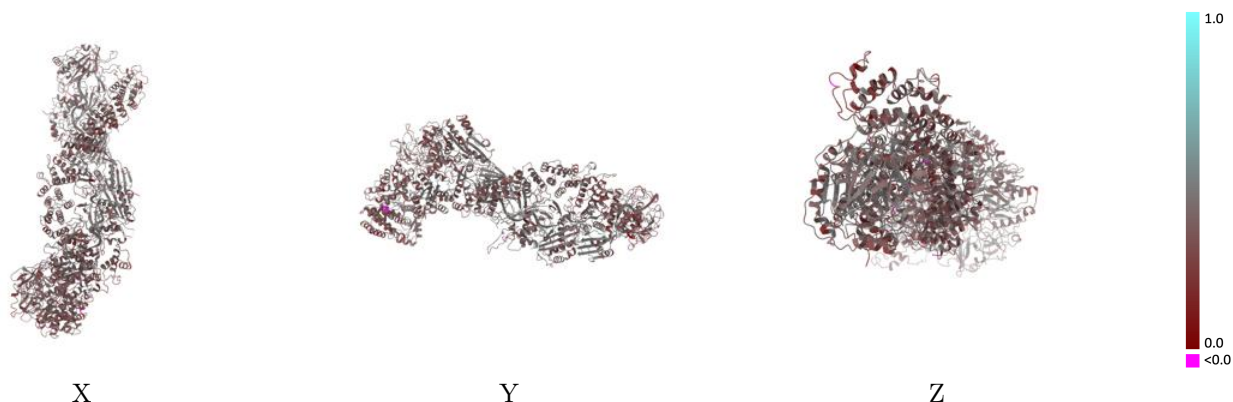
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
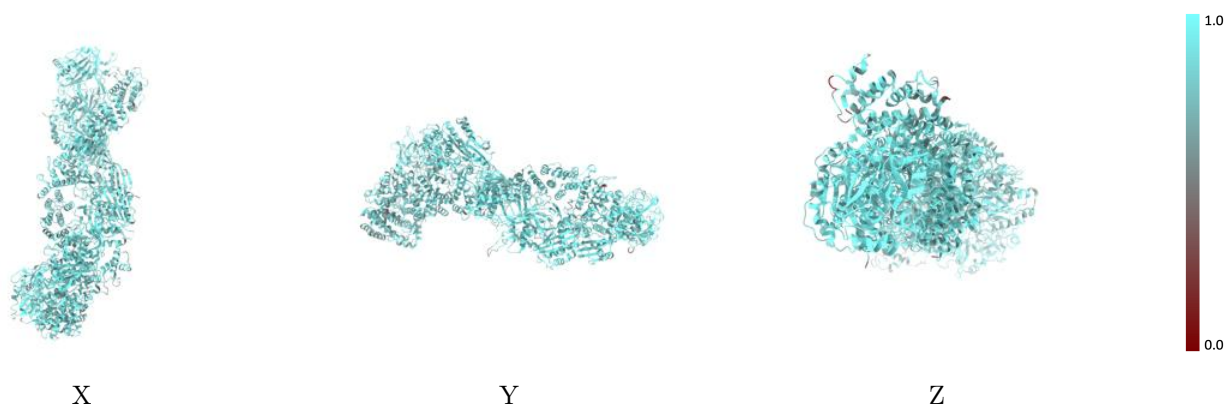
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4   Atom inclusion ⓘ
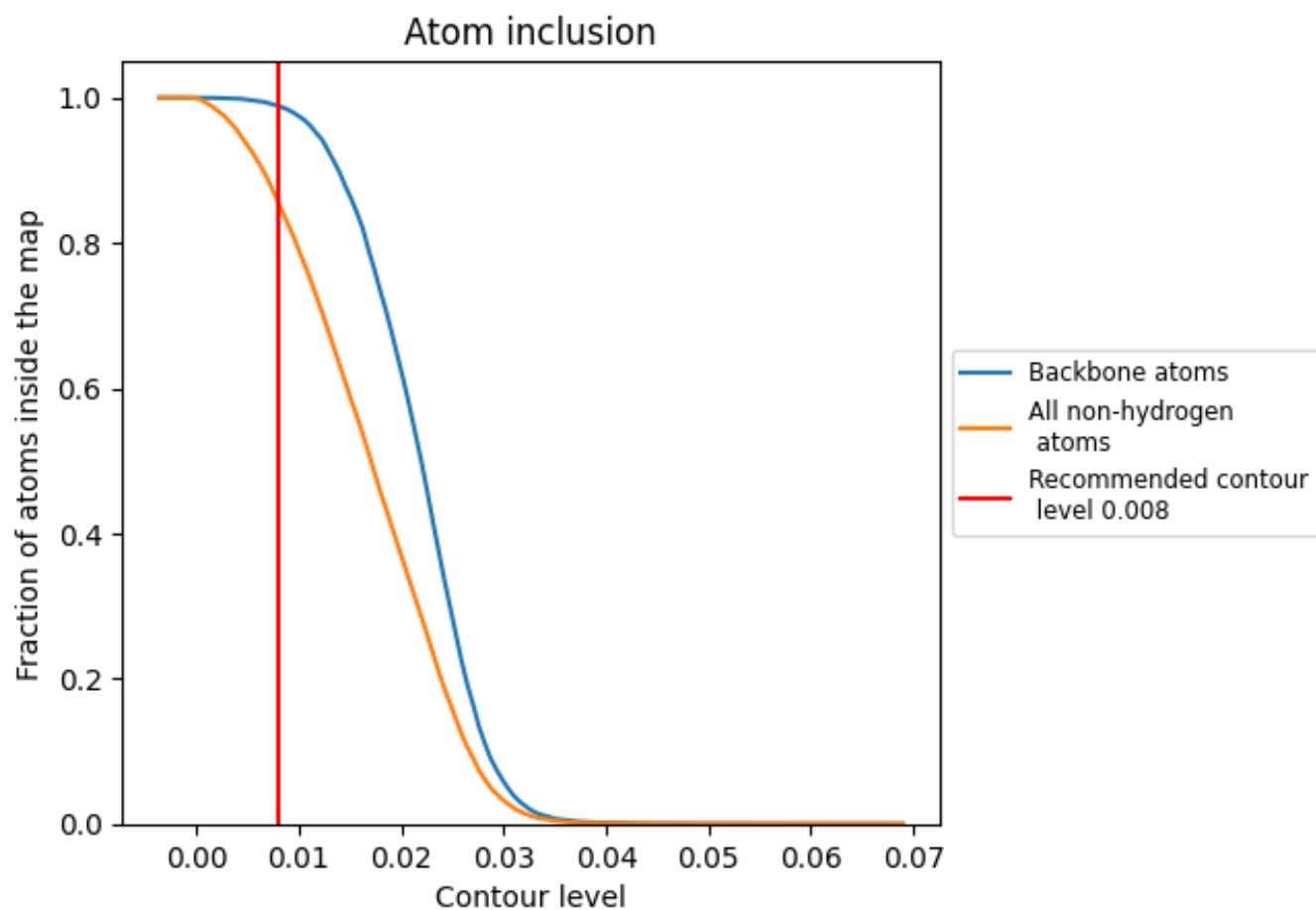
At the recommended contour level, 99% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8557	0.3700
A	0.8245	0.3500
B	0.8505	0.3690
C	0.8626	0.3660
D	0.8488	0.3670
E	0.8335	0.3290
F	0.8664	0.3900
G	0.8567	0.3980
H	0.8775	0.4020
I	0.8660	0.3840
J	0.8746	0.3650
K	0.8207	0.3430
L	0.8582	0.3660
M	0.8810	0.3650
N	0.8368	0.3780
R	0.9887	0.4290

1.0

0.0
<0.0