wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 11:01 am GMT

PDB ID	:	7AEF
EMDB ID	:	EMD-11745
Title	:	Cryo-EM structure of an extracellular contractile injection system in marine bacterium Algoriphagus machipongonensis, the baseplate complex in extended state applied 3-fold symmetry.
Authors	:	Xu, J.; Ericson, C.; Feldmueller, M.; Lien, Y.W.; Pilhofer, M.
Deposited on	:	2020-09-17
Resolution	:	2.80 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

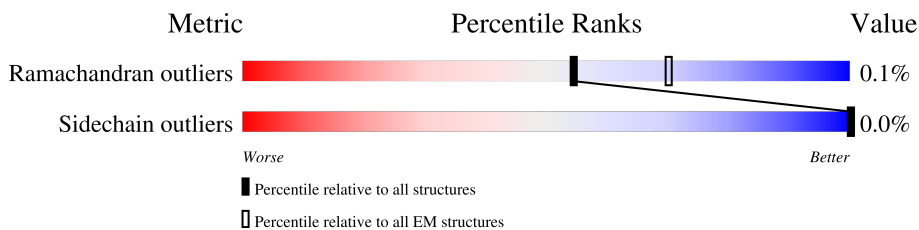|		
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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
Ramachandran outliers		0.1%
Sidechain outliers		0.0%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
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	933	10% / 58% / 41%
1	B	933	11% / 58% / 41%
1	C	933	10% / 58% / 41%
1	D	933	12% / 58% / 41%
1	E	933	9% / 58% / 41%
1	F	933	12% / 58% / 41%
2	G	1050	12% / 93% / · ·
2	H	1050	12% / 94% / · ·
2	I	1050	15% / 93% / · ·

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Mol	Chain	Length	Quality of chain
2	J	1050	15% / 93%
2	K	1050	14% / 93%
2	L	1050	14% / 94%
3	M	228	99%
3	N	228	98%
3	O	228	99%
3	P	228	98%
3	Q	228	99%
3	R	228	99%
4	S	137	96%
4	T	137	96%
4	U	137	96%
4	V	137	96%
4	W	137	96%
4	X	137	96%
5	Y	147	96%
5	Z	147	96%
5	a	147	95%
5	b	147	96%
5	c	147	96%
5	d	147	96%
6	e	692	27% / 93% / 5%
6	f	692	27% / 93% / 5%
6	g	692	26% / 93% / 5%
6	h	692	27% / 93% / 5%

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Mol	Chain	Length	Quality of chain
6	i	692	27% 93% 5%
6	j	692	27% 93% 5%
7	k	142	26% 98%
7	l	142	27% 98%
7	m	142	27% 98%
7	n	142	27% 98%
7	o	142	27% 98%
7	p	142	27% 98%
8	t	52	77% 23%
8	u	52	77% 23%
8	v	52	77% 23%
9	q	581	98%
9	r	581	98%
9	s	581	98%

2   Entry composition   ⓘ

There are 9 unique types of molecules in this entry. The entry contains 149535 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 baseplate protein (Algo12).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	549	Total 4447	C 2845	N 730	O 858	S 14	0	0
1	B	549	Total 4447	C 2845	N 730	O 858	S 14	0	0
1	C	549	Total 4447	C 2845	N 730	O 858	S 14	0	0
1	D	549	Total 4447	C 2845	N 730	O 858	S 14	0	0
1	E	549	Total 4447	C 2845	N 730	O 858	S 14	0	0
1	F	549	Total 4447	C 2845	N 730	O 858	S 14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	1011	Total 7762	C 4951	N 1284	O 1512	S 15	0	0
2	H	1011	Total 7762	C 4951	N 1284	O 1512	S 15	0	0
2	I	1011	Total 7762	C 4951	N 1284	O 1512	S 15	0	0
2	J	1011	Total 7762	C 4951	N 1284	O 1512	S 15	0	0
2	K	1011	Total 7762	C 4951	N 1284	O 1512	S 15	0	0
2	L	1011	Total 7762	C 4951	N 1284	O 1512	S 15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	225	Total 1849	C 1185	N 304	O 355	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	225	Total 1849	C 1185	N 304	O 355	S 5	0	0
3	O	225	Total 1849	C 1185	N 304	O 355	S 5	0	0
3	P	225	Total 1849	C 1185	N 304	O 355	S 5	0	0
3	Q	225	Total 1849	C 1185	N 304	O 355	S 5	0	0
3	R	225	Total 1849	C 1185	N 304	O 355	S 5	0	0

- Molecule 4 is a protein called Putative tail lysozyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	133	Total 1074	C 690	N 174	O 207	S 3	0	0
4	T	133	Total 1074	C 690	N 174	O 207	S 3	0	0
4	U	133	Total 1074	C 690	N 174	O 207	S 3	0	0
4	V	133	Total 1074	C 690	N 174	O 207	S 3	0	0
4	W	133	Total 1074	C 690	N 174	O 207	S 3	0	0
4	X	133	Total 1074	C 690	N 174	O 207	S 3	0	0

- Molecule 5 is a protein called Phospholipid/glycerol acyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	145	Total 1192	C 773	N 190	O 226	S 3	0	0
5	Z	145	Total 1192	C 773	N 190	O 226	S 3	0	0
5	a	145	Total 1192	C 773	N 190	O 226	S 3	0	0
5	b	145	Total 1192	C 773	N 190	O 226	S 3	0	0
5	c	145	Total 1192	C 773	N 190	O 226	S 3	0	0
5	d	145	Total 1192	C 773	N 190	O 226	S 3	0	0

- Molecule 6 is a protein called Putative phage tail sheath protein FI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	f	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	g	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	h	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	i	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	j	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		

- Molecule 7 is a protein called Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	l	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	m	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	n	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	o	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	p	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		

- Molecule 8 is a protein called inner protein (Algo6).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	t	40	Total	C	N	O	S	0	0
			324	202	55	66	1		
8	u	40	Total	C	N	O	S	0	0
			324	202	55	66	1		
8	v	40	Total	C	N	O	S	0	0
			324	202	55	66	1		

- Molecule 9 is a protein called Phosphoserine phosphatase SerB.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	q	580	Total 4469	C 2771	N 765	O 920	S 13	0	0
9	r	580	Total 4469	C 2771	N 765	O 920	S 13	0	0
9	s	580	Total 4469	C 2771	N 765	O 920	S 13	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: baseplate protein (Algo12)

- Molecule 1: baseplate protein (Algo12)

• Molecule 1: baseplate protein (Algo12)

Chain C:

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

THR GLY LEU HIS THR ILE TYR PRO THR GLY ARG LEU TYR ASP CYS ASP GLU GLU GLU GLU LEU ASP GLY LYS LEU ILE LEU GLY LYS THR ASN GLY THR LEU

● Molecule 1: baseplate protein (Algo12)

Chain D:

12%

58%   41%

MET SER T3 R26 D110 C117 W118 I119 E122 R123 V124 T125 V126 F127 A128 D129 L130 K131 N132 Q133 K134 L135 S136 Y137 E138 K139 T140 I141 W142 E143 D144 L145 K146 E147 N148 Q149 K150 A151 Q152 F153 D154 L155 L158 Y159 R160 E166 D167 A168 D169 K170 V171 L172 S173 E174

S175 L176 E177 L190 C191 E192 D193 L194 I195 K196 V197 E198 A201 C208 E216 A217 D218 D248 L262 A274 E280 D285 D294 G295 V296 K297 E301 I302 T303 L304 G305 N306 C307 D308 E309 N310 D311 G312 I313 E314 N315 N316 Q317 W318 V319 I322 P323 E324

K332 K333 T334 T335 I336 G341 I342 I345 N346 L347 N348 R351 A361 D372 D450 D467 R509 S516 Y517 A518 L524 E527 D530 E531 R551 GLY GLU GLY PHE ASN PHE TYR GLU GLN SER ASN ASP ASN LEU TRP ASP THR LEU ASN VAL SER

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

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

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

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

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

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

LEU

● Molecule 1: baseplate protein (Algo12)

Chain E:

9%

58%   41%

MET SER T3 L4 R26 E112 C117 R123 F127 A128 D129 L130 K131 N132 Q133 K134 L135 S136 Y137 E138 K139 T140 I141 W142 E143 D144 L145 K146 E147 N148 Q149 K150 A151 Q152 F153 D154 R160 E166 D167 A168 D169 K170 V171 L172 S173 E174 S175 L176 E177 E192 D193

K196 V197 E198 E203 E216 A217 D218 E219 D248 D285 D294 I298 E301 I302 T303 L304 G305 N306 C307 D308 E309 N310 D311 G312 I313 E314 N315 N316 Q317 E324 K332 K333 T334 G341 I342 I345 N346 R351 D372 D450 D464 R509 S516

• Molecule 1: baseplate protein (Algo12)

Chain F:

12%

58%   41%

• Molecule 2: Baseplate_J domain-containing protein

Chain G:

• Molecule 2: Baseplate_J domain-containing protein

Chain H:

• Molecule 2: Baseplate_J domain-containing protein

Chain I:

• Molecule 2: Baseplate_J domain-containing protein

Chain J:

• Molecule 2: Baseplate_J domain-containing protein

Chain K:

A727 D730 D750 V766 E778 K779 G780 L793 K847 N855 S859 S860 S861 F862 N867 L870 D875 T876 V877 Q878 Q879 S880 V881 F882 D883 I884 Y885 Q886 S890 D896 F900 V901 E903 F907 A911 N917 E920 V921 K922 V923

D924 V925 K926 V927 K928 F929 R930 E931 G932 L933 D934 V935 S936 L939 T940 K941 V942 K943 E944 D945 I946 K947 P952 W953 D956 Q957 E958 S959 S960 V961 E962 F963 G964 V965 T966 L967 Q978 L979 T980 Y981 Y984 I985 T986 D987 L988 R989 L990 L991 K992 R993 Q994 A995 G996 S997 S998

P999 C1000 N1001 P1002 I1003 F1004 I1005 E1006 T1007 T1008 E1009 K1010 E1011 Q1014 P1015 K1019 S1020 I1021 L1022 V1023 S1024 ALA LYS GLU HIS LEU VAL THR PRO ILE THR GLN ASN CYS SER SER ILE SER LEU ASN ASN GLU GLU GLU CYS GLN HIS

• Molecule 2: Baseplate_J domain-containing protein

Chain L:

14%

94%

MET SER GLU ASN CYS ASN HIS ILE VAL THR THR LEU LYS R14 D15 G16 R20 D21 L22 L23 D24 D59 L60 A61 N62 S77 D78 D84 I85 E86 N87 L88 D89 E92 E99 D106 K110 G183 D187 K190 Y214 E220 K221 E222 E223 I231

E250 K254 C268 N269 A270 S271 F304 D345 N349 S350 G351 L357 E407 V433 L434 R446 P447 K506 P509 S523 G524 E536 E547 A587 G596 S609 S610 E611 D634 T678 D679 T682 S702 R712 I718

N731 D750 A765 D769 K797 A831 K847 K852 N855 C858 S859 S860 S861 F862 N867 A868 T869 L870 I871 L872 D875 T876 V877 Q878 Q879 S880 V881 F882 D883 I884 Y885 Q886 P887 R888 V889 S890 Q891 E903 S906 F907 N917 Y918 E919 E920 V921 K922

V923 D924 V925 K926 V927 K928 F929 R930 E931 G932 L933 D934 V935 S936 F937 Y938 L939 T940 K941 V942 K943 E944 D945 I946 K947 P952 W953 A954 Y955 D956 Q957 E958 S959 S960 V961 E962 F963 G964 V965 T966 E977 Q978 L979 T980 Y981 T986 D987 L988 R989 L990 L991 K992 R993 Q994 A995 G996 S997

S998 P999 C1000 N1001 P1002 I1003 F1004 I1005 E1006 T1007 T1008 E1009 K1010 E1011 Q1014 P1015 S1016 N1017 P1018 K1019 S1020 V1023 S1024 ALA LYS GLU HIS LEU VAL THR PRO ILE THR GLN ASN CYS SER SER ILE SER LEU ASN ASN GLU GLU GLU CYS GLN HIS

• Molecule 3: LysM domain-containing protein

Chain M:

99%

MET S2 Q168 SER P170 Q227 LYS

• Molecule 3: LysM domain-containing protein

Chain N:

98%

MET S2 L136 Q168 SER P170 Q227 LYS

• Molecule 3: LysM domain-containing protein

Chain O:

• Molecule 3: LysM domain-containing protein

Chain P:

• Molecule 3: LysM domain-containing protein

Chain Q:

• Molecule 3: LysM domain-containing protein

Chain R:

• Molecule 4: Putative tail lysozyme

Chain S:

• Molecule 4: Putative tail lysozyme

Chain T:

• Molecule 4: Putative tail lysozyme

Chain U:

• Molecule 4: Putative tail lysozyme

Chain V:

• Molecule 4: Putative tail lysozyme

Chain W:

• Molecule 4: Putative tail lysozyme

Chain X:

• Molecule 5: Phospholipid/glycerol acyltransferase

Chain Y:

• Molecule 5: Phospholipid/glycerol acyltransferase

Chain Z:

• Molecule 5: Phospholipid/glycerol acyltransferase

Chain a:

• Molecule 5: Phospholipid/glycerol acyltransferase

Chain b:

• Molecule 5: Phospholipid/glycerol acyltransferase

Chain c:

• Molecule 5: Phospholipid/glycerol acyltransferase

Chain d:

• Molecule 6: Putative phage tail sheath protein FI

Chain e:

• Molecule 6: Putative phage tail sheath protein FI

Chain f:

• Molecule 6: Putative phage tail sheath protein FI

Chain g:

• Molecule 6: Putative phage tail sheath protein FI

Chain h:

• Molecule 6: Putative phage tail sheath protein FI

• Molecule 6: Putative phage tail sheath protein FI

A404 D405 T406 N407 T408 K409 V410 E411 N412 V413 L414 S415 I416 N417 A418 L419 N420 F421 S422 A423 E424 F425 E426 K427 L428 L429 T430 Y431 D432 V433 N434 T435 G436 L437 T438 A439 S440 V441 T442 L443 D444 L445 F446 A447 N448 I449 G450 T451 R452 L463 D454 D455 I456 I457 A458 A459 V460 S461 A462 A463

E464 P465 I466 D467 E482 P483 L484 D485 N486 V533 R562 Q659 Q690 GLU SER

• Molecule 7: Phage tail protein

Chain k:

26%

98%

MET S2 Y3 P4 L5 S6 K7 F8 H9 F10 S11 T17 K18 I19 G20 F21 T22 G63 T64 F65 K66 S67 D68 Y71 L92 L93 N94 E95 E96 H97 E98 P99 V100 K119 G120 D121 G122 N123 E124 V125 A126 E142

• Molecule 7: Phage tail protein

Chain l:

27%

98%

MET S2 Y3 P4 L5 S6 K7 F8 H9 F10 S11 K18 I19 G20 F21 T22 G63 T64 F65 K66 S67 D68 Y71 L92 L93 N94 E95 E96 H97 E98 P99 V100 K119 G120 D121 G122 N123 E124 V125 A126 I127 E142

• Molecule 7: Phage tail protein

Chain m:

27%

98%

MET S2 Y3 P4 L5 S6 K7 F8 H9 F10 S11 T17 K18 I19 G20 F21 T22 G63 T64 F65 K66 S67 D68 Y71 L92 L93 N94 E95 E96 H97 E98 P99 V100 K119 G120 D121 G122 N123 E124 V125 A126 E142

• Molecule 7: Phage tail protein

Chain n:

27%

98%

MET S2 Y3 P4 L5 S6 K7 F8 H9 F10 S11 K18 I19 G20 F21 T22 G63 T64 F65 K66 S67 D68 Y71 L92 L93 N94 E95 E96 H97 E98 P99 V100 K119 G120 D121 G122 N123 E124 V125 A126 E142

• Molecule 7: Phage tail protein

Chain o:

27%

98%

MET S2 Y3 P4 L5 S6 K7 F8 H9 F10 S11 K18 I19 G20 F21 T22 G63 T64 F65 K66 S67 D68 Y71 D87 L92 L93 N94 E95 E96 H97 E98 P99 V100 K119 G120 D121 G122 N123 E124 V125 A126 E142

• Molecule 7: Phage tail protein

Chain p:

27%

98%

- Molecule 8: inner protein (Algo6)

Chain t:

- Molecule 8: inner protein (Algo6)

Chain u:

- Molecule 8: inner protein (Algo6)

Chain v:

- Molecule 9: Phosphoserine phosphatase SerB

Chain q:

- Molecule 9: Phosphoserine phosphatase SerB

Chain r:

- Molecule 9: Phosphoserine phosphatase SerB

Chain s:

4　Experimental information　ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	82969	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 $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.219	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.76	2/4531 (0.0%)	0.77	2/6117 (0.0%)
1	B	0.75	1/4531 (0.0%)	0.78	3/6117 (0.0%)
1	C	0.76	2/4531 (0.0%)	0.77	2/6117 (0.0%)
1	D	0.75	1/4531 (0.0%)	0.78	3/6117 (0.0%)
1	E	0.76	2/4531 (0.0%)	0.77	2/6117 (0.0%)
1	F	0.75	1/4531 (0.0%)	0.78	3/6117 (0.0%)
2	G	0.69	11/7935 (0.1%)	0.90	29/10781 (0.3%)
2	H	0.80	12/7935 (0.2%)	0.87	26/10781 (0.2%)
2	I	0.69	11/7935 (0.1%)	0.90	29/10781 (0.3%)
2	J	0.80	12/7935 (0.2%)	0.87	27/10781 (0.3%)
2	K	0.69	11/7935 (0.1%)	0.90	29/10781 (0.3%)
2	L	0.80	12/7935 (0.2%)	0.87	26/10781 (0.2%)
3	M	0.41	0/1889	0.58	0/2544
3	N	0.43	0/1889	0.57	1/2544 (0.0%)
3	O	0.41	0/1889	0.58	0/2544
3	P	0.43	0/1889	0.57	1/2544 (0.0%)
3	Q	0.41	0/1889	0.58	0/2544
3	R	0.43	0/1889	0.57	0/2544
4	S	0.68	1/1096 (0.1%)	0.80	0/1483
4	T	0.70	1/1096 (0.1%)	0.80	0/1483
4	U	0.69	1/1096 (0.1%)	0.80	0/1483
4	V	0.70	1/1096 (0.1%)	0.80	0/1483
4	W	0.69	1/1096 (0.1%)	0.80	0/1483
4	X	0.70	1/1096 (0.1%)	0.79	0/1483
5	Y	0.73	0/1226	0.89	5/1664 (0.3%)
5	Z	0.73	0/1226	0.89	5/1664 (0.3%)
5	a	0.73	0/1226	0.89	6/1664 (0.4%)
5	b	0.73	0/1226	0.89	5/1664 (0.3%)
5	c	0.73	0/1226	0.89	5/1664 (0.3%)
5	d	0.73	0/1226	0.89	5/1664 (0.3%)
6	e	0.78	0/5155	0.83	10/7021 (0.1%)
6	f	0.78	0/5155	0.83	10/7021 (0.1%)
6	g	0.78	0/5155	0.83	10/7021 (0.1%)
6	h	0.78	0/5155	0.83	10/7021 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	i	0.78	0/5155	0.83	10/7021 (0.1%)
6	j	0.79	0/5155	0.83	10/7021 (0.1%)
7	k	0.97	0/1172	0.85	2/1584 (0.1%)
7	l	0.97	0/1172	0.85	2/1584 (0.1%)
7	m	0.97	0/1172	0.85	2/1584 (0.1%)
7	n	0.97	0/1172	0.85	2/1584 (0.1%)
7	o	0.97	0/1172	0.85	2/1584 (0.1%)
7	p	0.97	0/1172	0.85	2/1584 (0.1%)
8	t	0.32	0/324	0.47	0/432
8	u	0.32	0/324	0.47	0/432
8	v	0.32	0/324	0.47	0/432
9	q	0.96	3/4536 (0.1%)	0.86	6/6145 (0.1%)
9	r	0.96	4/4536 (0.1%)	0.86	6/6145 (0.1%)
9	s	0.96	4/4536 (0.1%)	0.86	6/6145 (0.1%)
All	All	0.76	95/152604 (0.1%)	0.83	304/206895 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	5
2	H	0	2
2	I	0	4
2	J	0	2
2	K	0	4
2	L	0	2
All	All	0	19

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	509	PRO	C-N	15.90	1.70	1.34
2	I	509	PRO	C-N	15.90	1.70	1.34
2	G	509	PRO	C-N	15.89	1.70	1.34
2	L	506	LYS	C-N	14.66	1.67	1.34
2	H	506	LYS	C-N	14.61	1.67	1.34

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	175	LEU	CA-CB-CG	10.64	139.77	115.30
9	s	175	LEU	CA-CB-CG	10.63	139.76	115.30
9	q	175	LEU	CA-CB-CG	10.62	139.73	115.30
2	K	506	LYS	O-C-N	-10.34	106.15	122.70
2	G	506	LYS	O-C-N	-10.34	106.16	122.70

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	364	GLU	Sidechain
2	G	48	ASN	Sidechain
2	G	492	ASP	Sidechain
2	G	635	ASN	Sidechain
2	G	642	ASP	Sidechain

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	B	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	C	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	D	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	E	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	F	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
2	G	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	I	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	J	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	K	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	L	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
3	M	221/228 (97%)	218 (99%)	3 (1%)	0	100	100
3	N	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
3	O	221/228 (97%)	218 (99%)	3 (1%)	0	100	100
3	P	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
3	Q	221/228 (97%)	219 (99%)	2 (1%)	0	100	100
3	R	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
4	S	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	T	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	U	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	V	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	W	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	X	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
5	Y	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	Z	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	a	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	b	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	c	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	d	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
6	e	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	f	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	g	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	h	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	i	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	j	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
7	k	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	l	139/142 (98%)	137 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	m	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	n	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	o	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	p	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
8	t	36/52 (69%)	36 (100%)	0	0	100	100
8	u	36/52 (69%)	36 (100%)	0	0	100	100
8	v	36/52 (69%)	36 (100%)	0	0	100	100
9	q	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
9	r	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
9	s	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
All	All	18888/21873 (86%)	18397 (97%)	473 (2%)	18 (0%)	54	81

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	1001	ASN
2	G	1015	PRO
2	G	1018	PRO
2	H	1001	ASN
2	H	1015	PRO

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	497/842 (59%)	497 (100%)	0	100	100
1	B	497/842 (59%)	497 (100%)	0	100	100
1	C	497/842 (59%)	497 (100%)	0	100	100
1	D	497/842 (59%)	497 (100%)	0	100	100
1	E	497/842 (59%)	497 (100%)	0	100	100
1	F	497/842 (59%)	497 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	814/955 (85%)	813 (100%)	1 (0%)	93	98
2	H	814/955 (85%)	814 (100%)	0	100	100
2	I	814/955 (85%)	813 (100%)	1 (0%)	93	98
2	J	814/955 (85%)	814 (100%)	0	100	100
2	K	814/955 (85%)	813 (100%)	1 (0%)	93	98
2	L	814/955 (85%)	814 (100%)	0	100	100
3	M	201/204 (98%)	201 (100%)	0	100	100
3	N	201/204 (98%)	201 (100%)	0	100	100
3	O	201/204 (98%)	201 (100%)	0	100	100
3	P	201/204 (98%)	201 (100%)	0	100	100
3	Q	201/204 (98%)	201 (100%)	0	100	100
3	R	201/204 (98%)	201 (100%)	0	100	100
4	S	121/125 (97%)	121 (100%)	0	100	100
4	T	121/125 (97%)	121 (100%)	0	100	100
4	U	121/125 (97%)	121 (100%)	0	100	100
4	V	121/125 (97%)	121 (100%)	0	100	100
4	W	121/125 (97%)	121 (100%)	0	100	100
4	X	121/125 (97%)	121 (100%)	0	100	100
5	Y	134/135 (99%)	134 (100%)	0	100	100
5	Z	134/135 (99%)	134 (100%)	0	100	100
5	a	134/135 (99%)	134 (100%)	0	100	100
5	b	134/135 (99%)	134 (100%)	0	100	100
5	c	134/135 (99%)	134 (100%)	0	100	100
5	d	134/135 (99%)	134 (100%)	0	100	100
6	e	547/593 (92%)	547 (100%)	0	100	100
6	f	547/593 (92%)	547 (100%)	0	100	100
6	g	547/593 (92%)	547 (100%)	0	100	100
6	h	547/593 (92%)	547 (100%)	0	100	100
6	i	547/593 (92%)	547 (100%)	0	100	100
6	j	547/593 (92%)	547 (100%)	0	100	100
7	k	127/128 (99%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	l	127/128 (99%)	127 (100%)	0	100	100
7	m	127/128 (99%)	127 (100%)	0	100	100
7	n	127/128 (99%)	127 (100%)	0	100	100
7	o	127/128 (99%)	127 (100%)	0	100	100
7	p	127/128 (99%)	127 (100%)	0	100	100
8	t	39/45 (87%)	39 (100%)	0	100	100
8	u	39/45 (87%)	39 (100%)	0	100	100
8	v	39/45 (87%)	39 (100%)	0	100	100
9	q	499/500 (100%)	499 (100%)	0	100	100
9	r	499/500 (100%)	499 (100%)	0	100	100
9	s	499/500 (100%)	499 (100%)	0	100	100
All	All	16260/19527 (83%)	16257 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	359	LEU
2	I	359	LEU
2	K	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
4	U	36	GLN
9	r	467	HIS
4	V	36	GLN
8	t	9	HIS
2	J	54	HIS

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	3
2	J	3
2	L	3
2	G	1
2	I	1
2	K	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	509:PRO	C	510:LYS	N	1.70
1	I	509:PRO	C	510:LYS	N	1.70
1	K	509:PRO	C	510:LYS	N	1.70
1	H	506:LYS	C	507:SER	N	1.67
1	J	506:LYS	C	507:SER	N	1.67

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-11745. 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
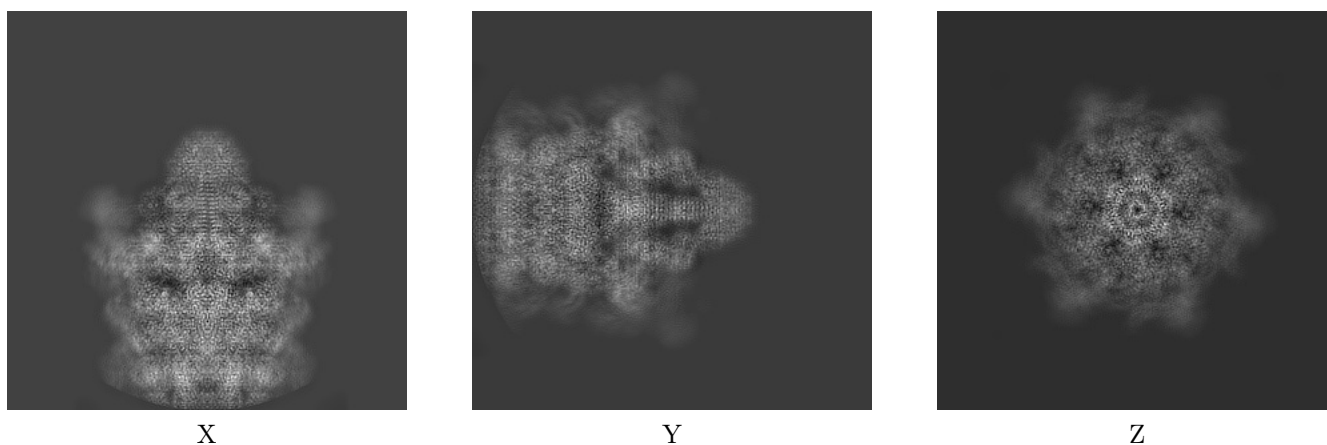
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ

6.2.1   Primary map

X Index: 200   Y Index: 200   Z Index: 200
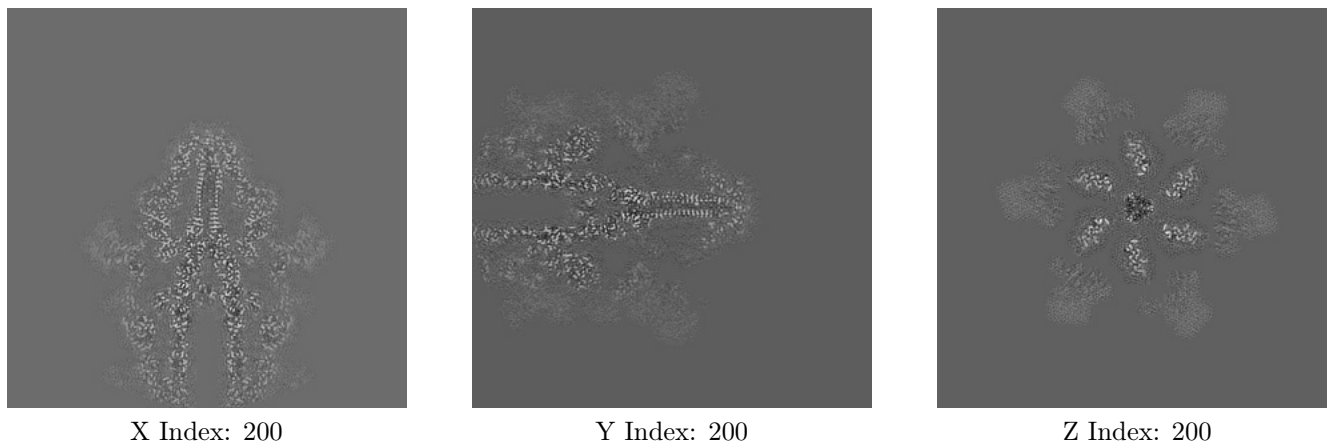
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
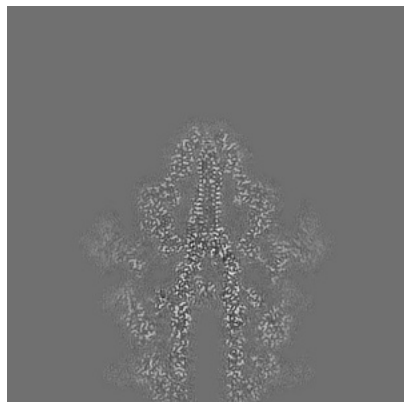
6.3.1   Primary map
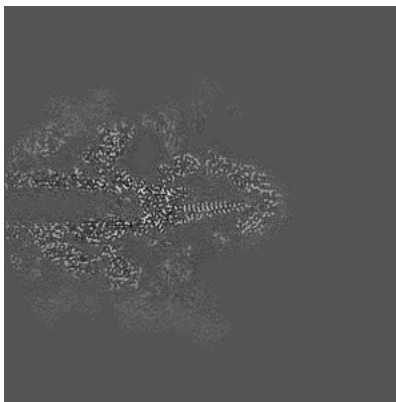
X Index: 198   Y Index: 210   Z Index: 110
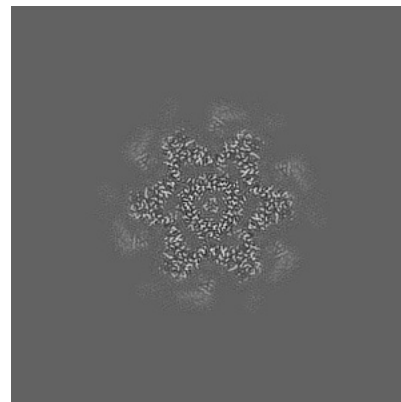
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views ⓘ
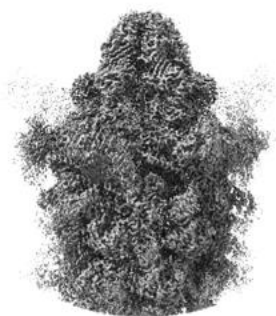
6.4.1   Primary map

X   Y   Z
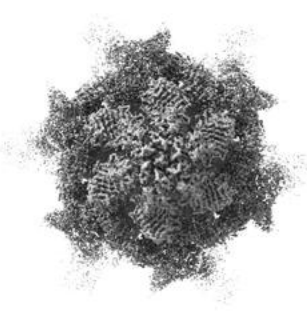
The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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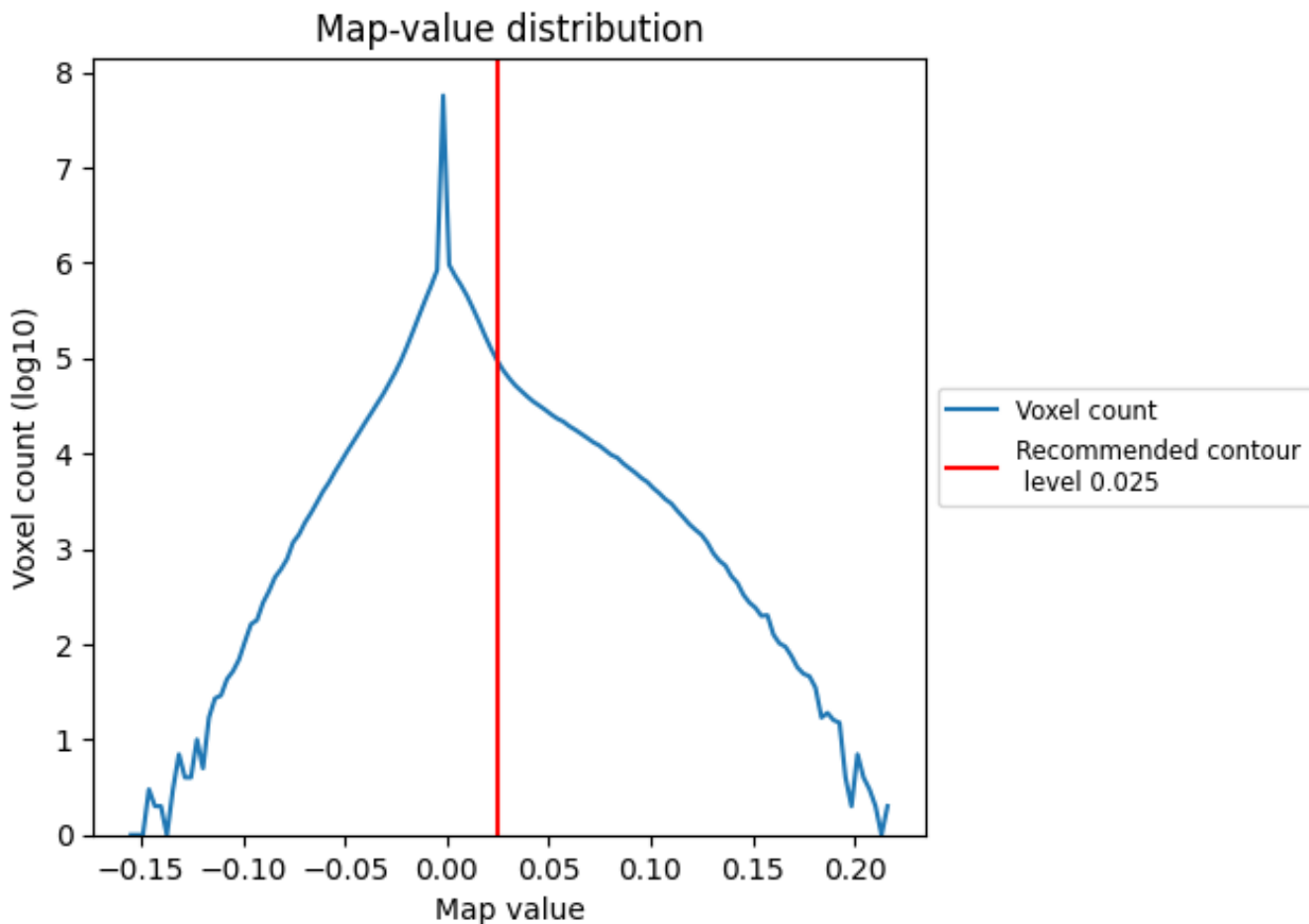
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate   ⓘ
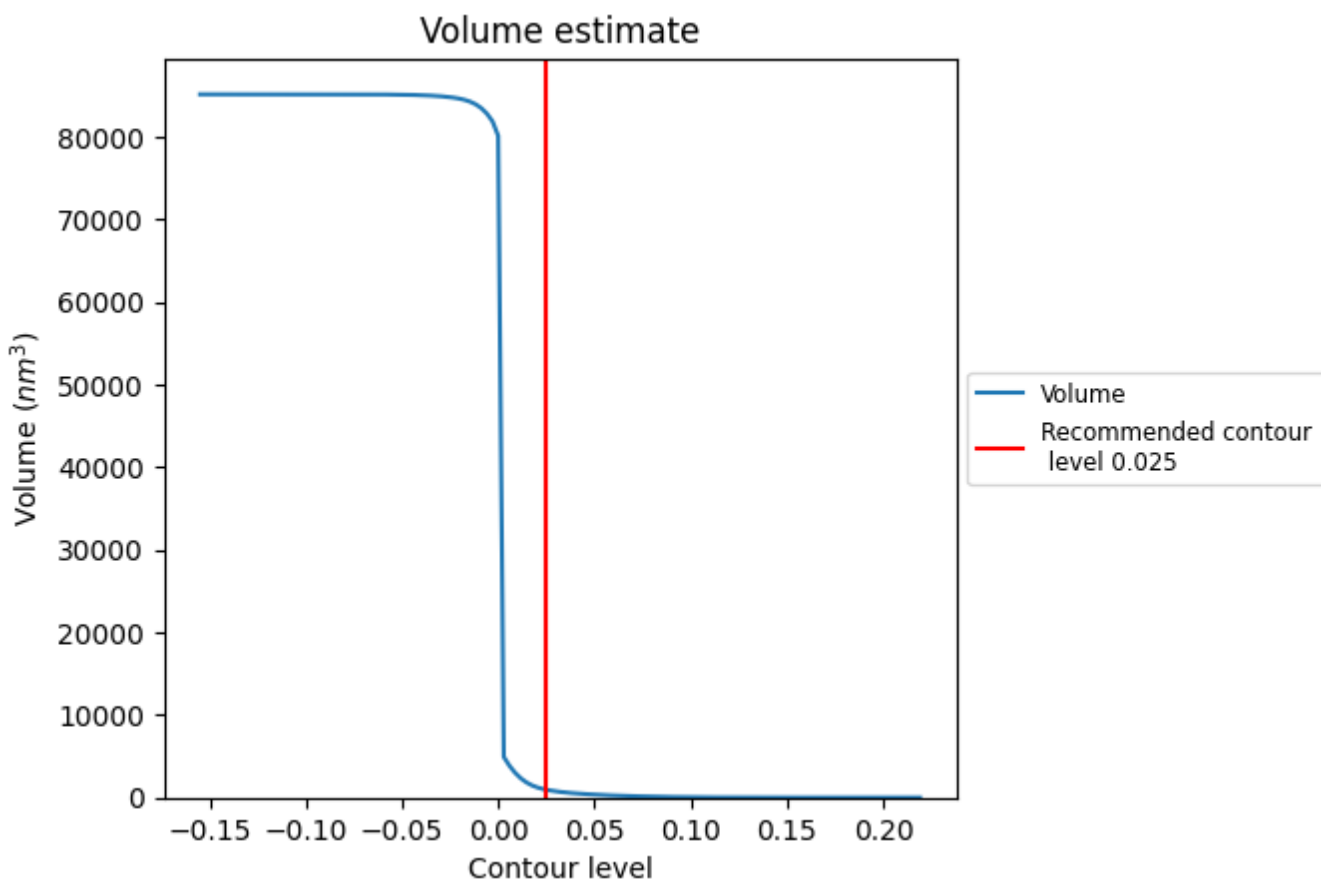
Volume estimate

The volume at the recommended contour level is 948 nm^3; this corresponds to an approximate mass of 856 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 ⓘ
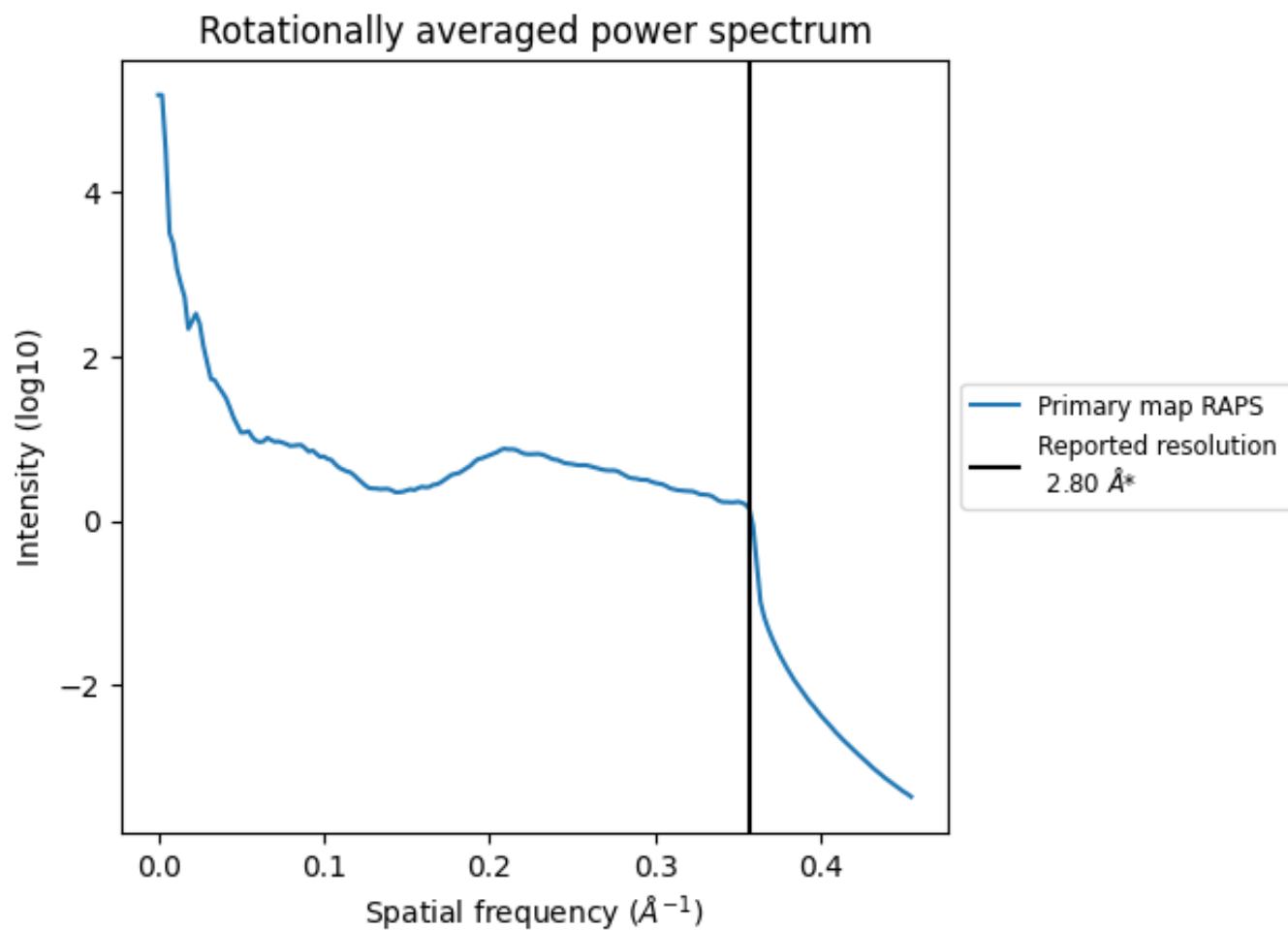
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation (i)

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-11745 and PDB model 7AEF. Per-residue inclusion information can be found in section 3 on page 9.

9.1   Map-model overlay ⓘ

X   Y   Z
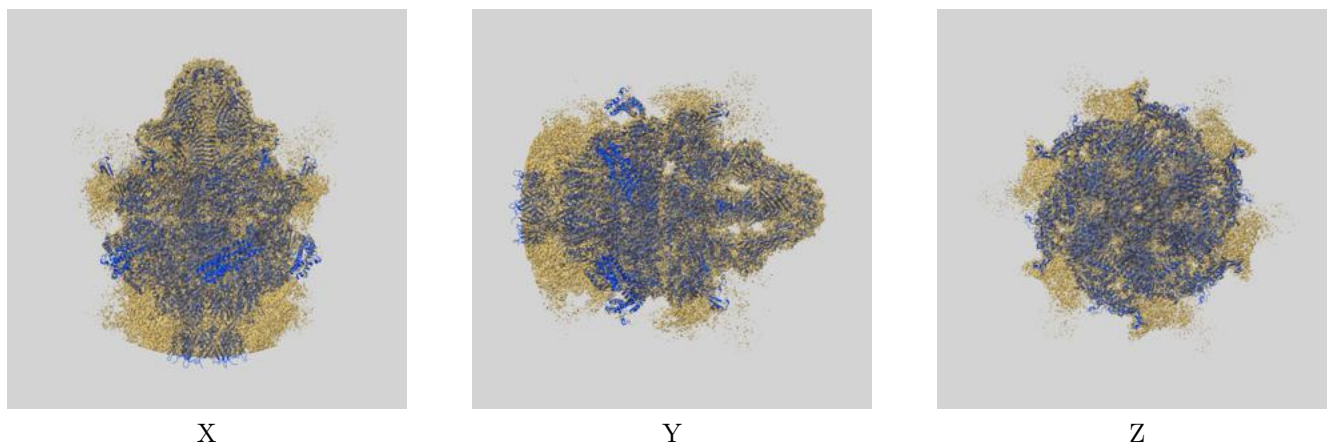
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model (i)

X   Y   Z
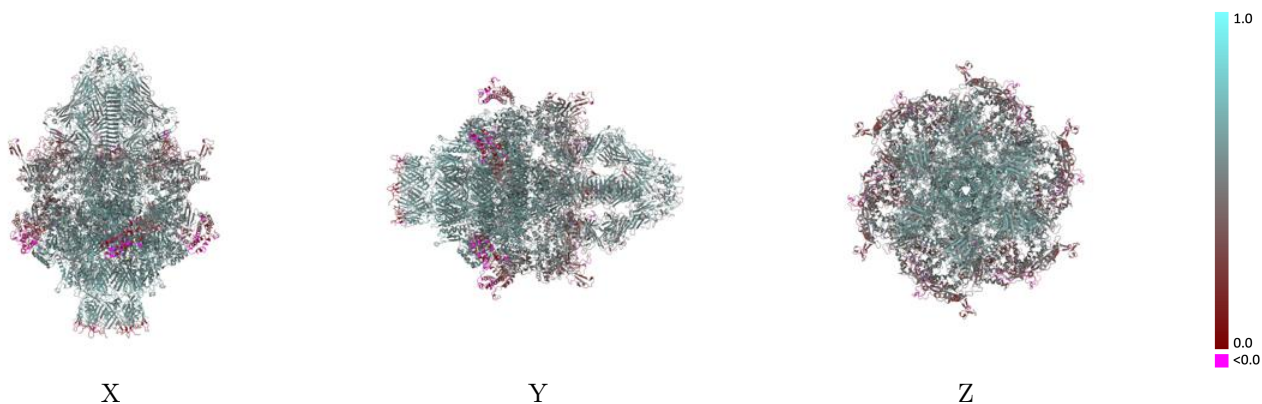
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)

X   Y   Z
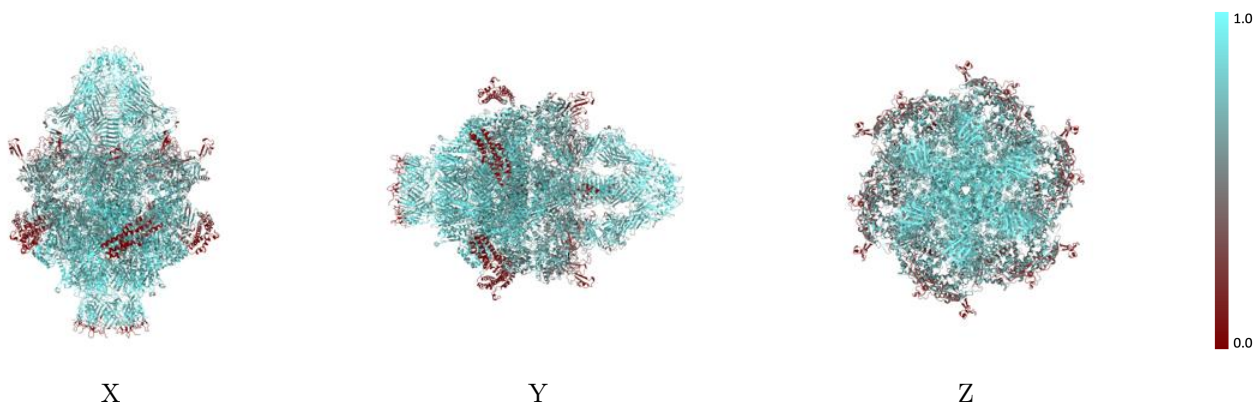
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion ⓘ
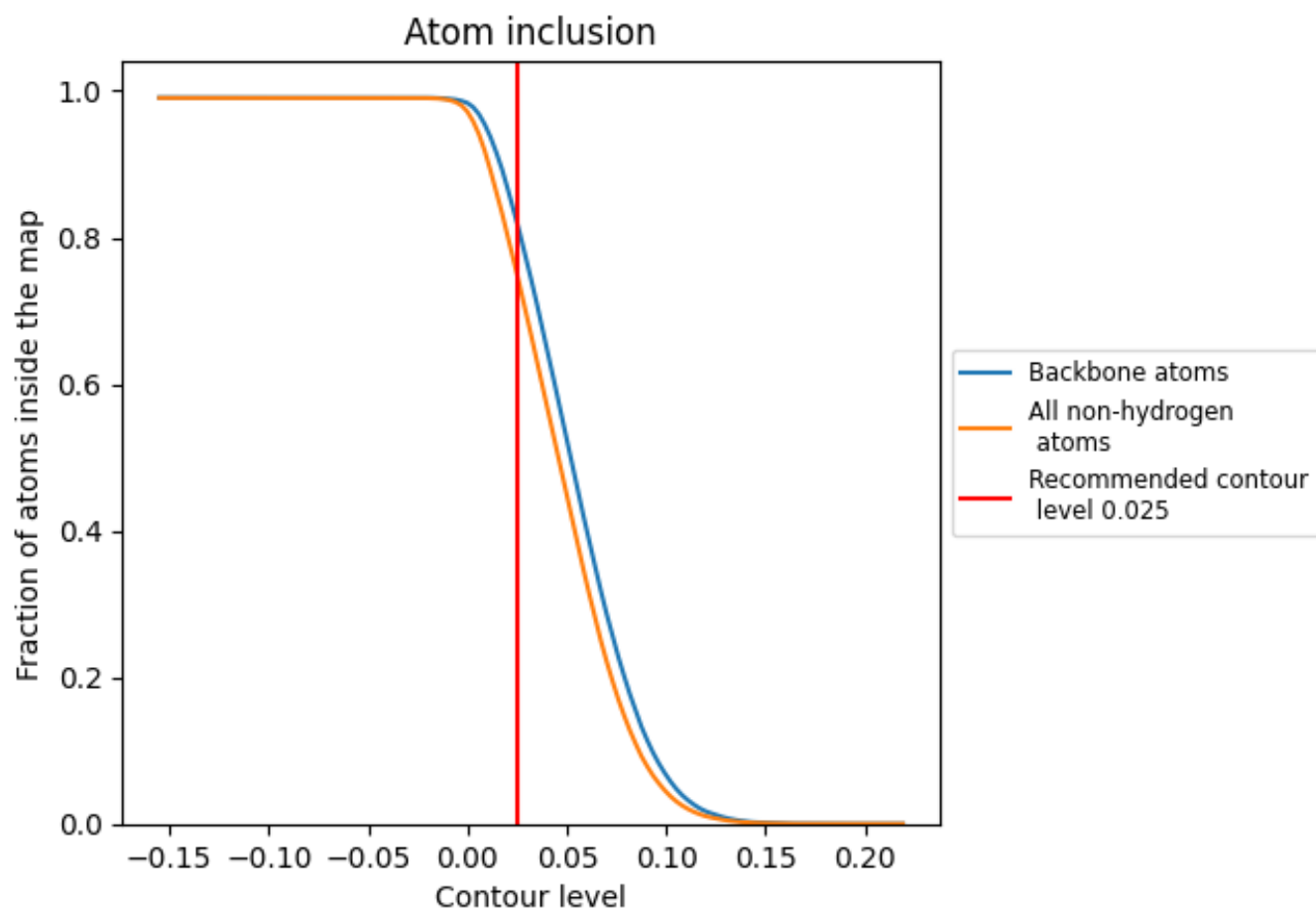
At the recommended contour level, 82% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7503	0.5290
A	0.6794	0.5040
B	0.6611	0.5020
C	0.6773	0.5040
D	0.6670	0.5010
E	0.6844	0.5050
F	0.6666	0.5000
G	0.7750	0.5410
H	0.7816	0.5400
I	0.7501	0.5140
J	0.7231	0.4740
K	0.7522	0.5180
L	0.7214	0.4740
M	0.9227	0.6340
N	0.9172	0.6300
O	0.9233	0.6320
P	0.9161	0.6340
Q	0.9178	0.6330
R	0.9145	0.6300
S	0.8742	0.5930
T	0.8524	0.5840
U	0.8723	0.5890
V	0.8543	0.5850
W	0.8751	0.5910
X	0.8505	0.5850
Y	0.8972	0.6160
Z	0.9006	0.6190
a	0.8904	0.6150
b	0.8963	0.6190
c	0.8955	0.6160
d	0.8997	0.6210
e	0.6401	0.4800
f	0.6481	0.4780
g	0.6437	0.4810
h	0.6451	0.4790

1.0

0.0
<0.0

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

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Chain	Atom inclusion	Q-score
i	0.6383	0.4800
j	0.6435	0.4780
k	0.6480	0.4770
l	0.6463	0.4760
m	0.6427	0.4710
n	0.6516	0.4690
o	0.6463	0.4710
p	0.6463	0.4780
q	0.9244	0.6240
r	0.9235	0.6200
s	0.9228	0.6240
t	0.8106	0.6230
u	0.8137	0.6180
v	0.8075	0.6160