WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Mar 14, 2024 – 05:03 PM EDT

PDB ID	:	8UXW
EMDB ID	:	EMD-42787
Title	:	Arp2/3 branch junction complex, ADP state
Authors	:	Chavali, S.S.; Chou, S.Z.; Sindelar, C.V.
Deposited on	:	2023-11-11
Resolution	:	2.70 Å(reported)

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

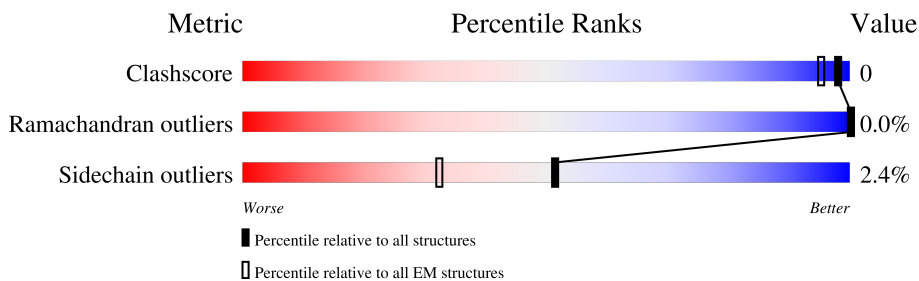|		
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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		0
Ramachandran outliers		0.0%
Sidechain outliers		2.4%

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	427	89%　　　　　5%　6%
2	B	390	93%　　　　　6%　••
3	C	377	90%　　　　　6%　•
4	D	317	92%　　　　　7%　•
5	E	174	10% 93%　　　　　5% ••
6	F	168	90%　　　　　9%　•
7	G	152	92%　　　　　7%　••
8	H	377	94%　　　　　• ••

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Mol	Chain	Length	Quality of chain
8	I	377	11% ... 93% ... 5% .
8	M	377	7% ... 93% ... 5% .
8	N	377	... 92% ... 5% ..
8	O	377	... 92% ... 6% .
8	P	377	... 93% ... 5% .
8	Q	377	... 93% ... 5% .
8	R	377	... 95% ... ..

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 77479 atoms, of which 38450 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	400	Total	C	H	N	O	S	0	0
			6226	2002	3065	540	608	11		

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	387	Total	C	H	N	O	S	0	0
			6153	1969	3073	530	566	15		

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	362	Total	C	H	N	O	S	0	0
			5576	1785	2751	501	532	7		

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	316	Total	C	H	N	O	S	0	0
			5153	1652	2563	445	482	11		

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	172	Total	C	H	N	O	S	0	0
			2746	889	1361	237	251	8		

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	168	Total	C	H	N	O	S	0	0
			2781	877	1404	234	258	8		

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	151	Total	C	H	N	O	S	0	0
			2362	746	1179	202	233	2		

- Molecule 8 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	370	Total	C	H	N	O	S	0	0
			5760	1833	2867	488	551	21		
8	I	370	Total	C	H	N	O	S	0	0
			5760	1833	2867	488	551	21		
8	M	370	Total	C	H	N	O	S	0	0
			5760	1833	2867	488	551	21		
8	N	370	Total	C	H	N	O	S	0	0
			5758	1833	2865	488	551	21		
8	O	370	Total	C	H	N	O	S	0	0
			5760	1833	2867	488	551	21		
8	P	370	Total	C	H	N	O	S	0	0
			5760	1833	2867	488	551	21		
8	Q	370	Total	C	H	N	O	S	0	0
			5760	1833	2867	488	551	21		
8	R	370	Total	C	H	N	O	S	0	0
			5760	1833	2867	488	551	21		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).
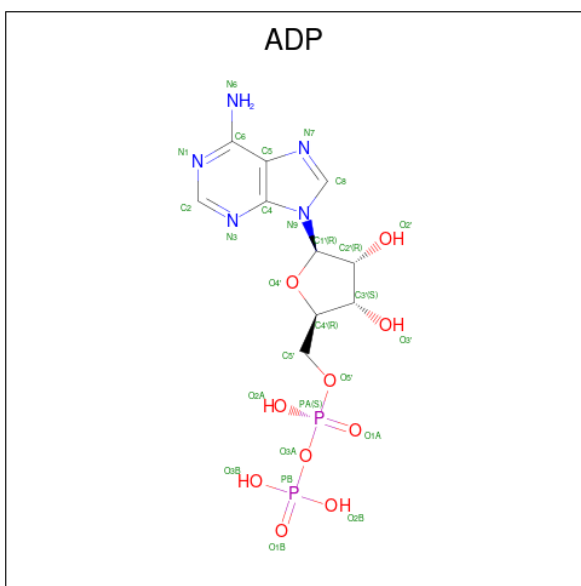
Mol	Chain	Residues	Atoms						AltConf
9	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	H	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	I	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	M	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	N	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	O	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	P	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	Q	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	R	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total 1	Mg 1	0
10	B	1	Total 1	Mg 1	0
10	H	1	Total 1	Mg 1	0
10	I	1	Total 1	Mg 1	0
10	M	1	Total 1	Mg 1	0
10	N	1	Total 1	Mg 1	0
10	O	1	Total 1	Mg 1	0
10	P	1	Total 1	Mg 1	0
10	Q	1	Total 1	Mg 1	0
10	R	1	Total 1	Mg 1	0

- Molecule 11 is **ADENOSINE-5'-TRIPHOSPHATE** (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).
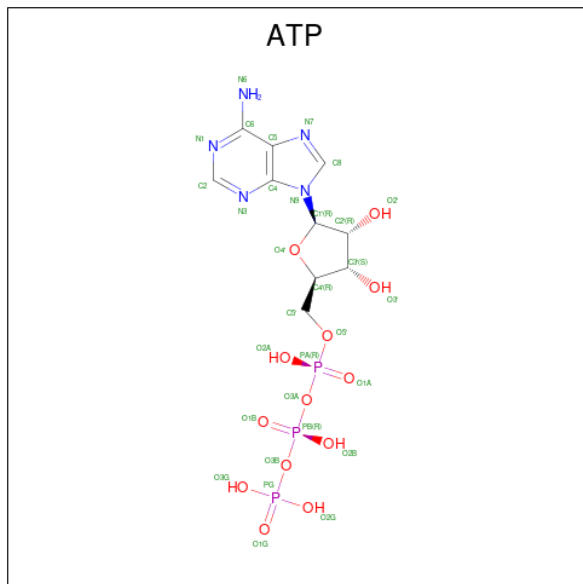
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
11	B	1	43	10	12	5	13	3	0

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: Actin-related protein 3

Chain A:
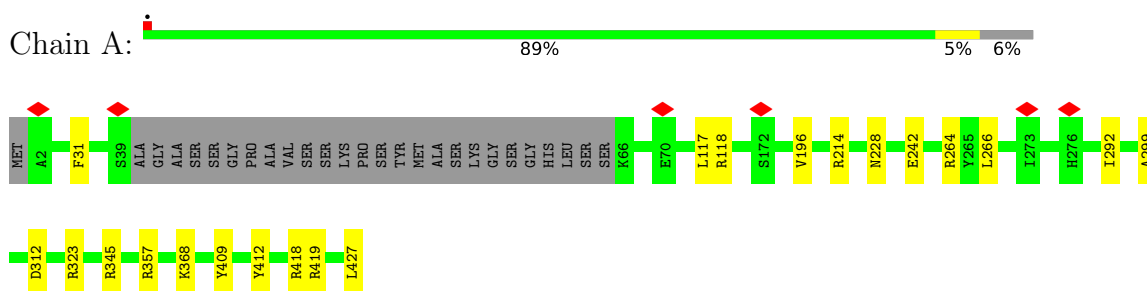
- Molecule 2: Actin-related protein 2

Chain B:
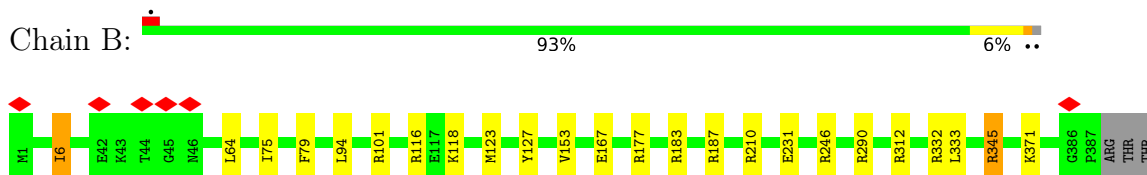
- Molecule 3: Actin-related protein 2/3 complex subunit 1
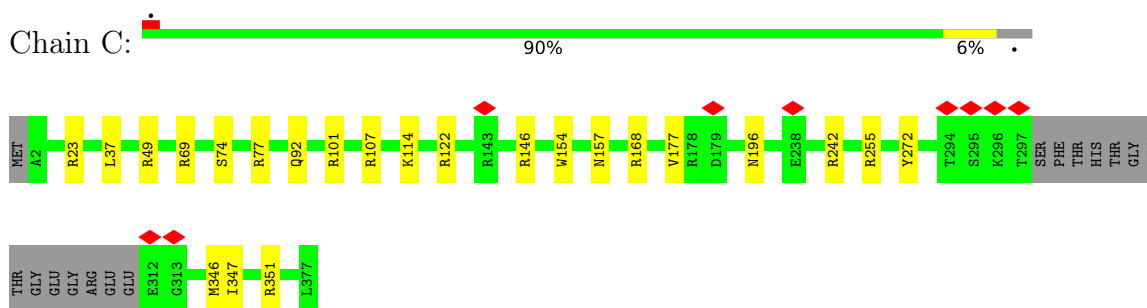
Chain C:

- Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:

R306 R316 A317

- Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:

MET P2 L11 T12 D13 R30 Y34 E38 S39 Q40 R52 R58 R68 R83 R90 D91 A92 E93 H94 N103 S109 ALA G111 L122 S123 P124 Q125 D126 I129 T132 R144 T152 E153 R167 L174
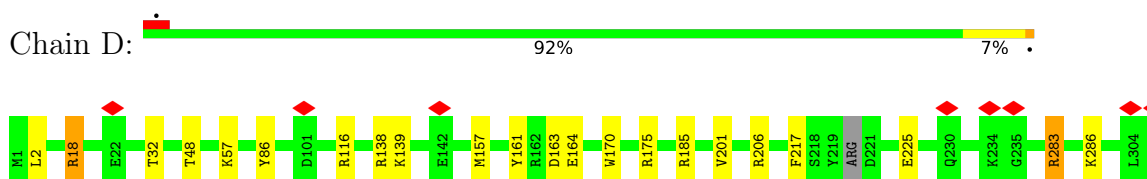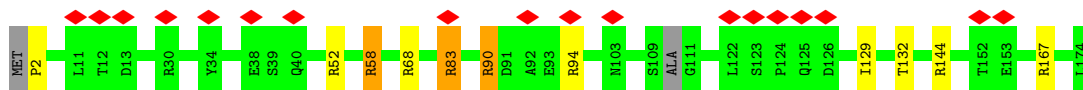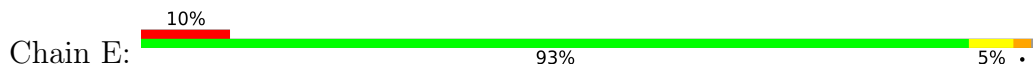
- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:

M1 R6 T15 L16 T17 S26 E31 R42 R71 R75 F101 L104 R105 R106 M139 R156 A157 R158 L159 V160 F168
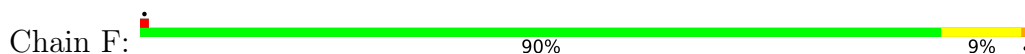
- Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:

MET T2 F3 R4 E13 T17 R25 R44 Q70 R73 Y112 R113 I142 V143 R144 L152

- Molecule 8: Actin, alpha skeletal muscle

Chain H:

MET CYS ASP GLU ASP GLU THR T6 R62 E72 M82 W86 R95 R116 I122 R147 R183 R196 R210 R254 F255 R256 R290 R312 K315 R335 R372 F375

- Molecule 8: Actin, alpha skeletal muscle

Chain I:

MET CYS ASP GLU ASP GLU THR T6 N12 G23 D24 D25 R28 V45 G48 D51 V54 R62 D80 E83 K84 I85 R95 V96 A97 E100 R116 E125 M132 G146 R147 V152 E167 A170 H173 R183 T194 E195

R196 R206 R210 S232 R254 C285 D286 I287 D288 A295 D311 R312 T324 M325 K326 I327 K328 S348 L349 S350 Q354 M355 W356 I357 T358 K359 Q360 E361 E364 A365 G366 R372 K373 C374 F375

- Molecule 8: Actin, alpha skeletal muscle

Chain M:

MET CYS ASP GLU ASP GLU THR T6 K18 R28 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 S60 K61 R62 L65 L94 R95 N111 R116 N128 R147 R196 R206 R210 D211 E214 K215 L216 A231 S232 L236 P243

D244 I248 T249 I250 R254 F255 R256 R290 M305 R335 I357 Q360 D363 E364 R372 F375

• Molecule 8: Actin, alpha skeletal muscle

Chain N:

92% 5%

MET CYS ASP GLU ASP GLU THR T6 D25 R28 G46 M47 G48 Q49 K50 V54 R62 R95 R116 R147 T148 T149 I165 Y166 E167 R177 R183 R196 R206 R210 D222 S233 S234 S235 N252 E253 R254 F255 R256 C257 R290

R312 R335 F375

• Molecule 8: Actin, alpha skeletal muscle

Chain O:

92% 6%

MET CYS ASP GLU ASP GLU THR T6 N12 G13 S14 R28 M47 G48 R62 R95 R177 R183 M190 R196 V209 R210 L242 R254 P258 R290 Y306 R312 T324 R335 R372 F375

• Molecule 8: Actin, alpha skeletal muscle

Chain P:

93% 5%

MET CYS ASP GLU ASP GLU THR T6 R28 R39 M47 G48 R62 I71 R95 R147 T148 T149 E167 R177 T194 E195 R196 T202 R206 R210 L236 R254 R290 N297 K315 L320 R335 F375

• Molecule 8: Actin, alpha skeletal muscle

Chain Q:

93% 5%

MET CYS ASP GLU ASP GLU THR T6 V9 R28 R39 M44 Y53 V54 K61 R62 T106 N111 Y166 R177 T194 E195 R196 R210 R254 F255 R256 I330 R335 F375

• Molecule 8: Actin, alpha skeletal muscle

Chain R:

95%

MET CYS ASP GLU ASP GLU THR T6 R39 M47 R62 R116 M123 R177 R183 R206 R210 S233 S234 R256 R335 Q354 R372 F375

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	400000	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 $(e^-/\text{Å}^2)$	51.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.623	Depositor
Minimum map value	-1.936	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	344.576, 344.576, 344.576	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.673, 0.673, 0.673	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, HIC, MG

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	0.67	0/3235	1.03	8/4384 (0.2%)
2	B	0.66	0/3147	1.08	12/4257 (0.3%)
3	C	0.64	0/2902	1.08	13/3963 (0.3%)
4	D	0.66	0/2647	1.04	7/3575 (0.2%)
5	E	0.71	0/1422	1.02	9/1924 (0.5%)
6	F	0.66	0/1398	1.13	8/1879 (0.4%)
7	G	0.62	0/1202	1.06	7/1640 (0.4%)
8	H	0.64	0/2943	1.04	15/3984 (0.4%)
8	I	0.66	0/2943	1.03	10/3984 (0.3%)
8	M	0.66	0/2943	1.01	12/3984 (0.3%)
8	N	0.64	0/2943	1.03	16/3984 (0.4%)
8	O	0.62	0/2943	1.08	15/3984 (0.4%)
8	P	0.63	0/2943	1.04	11/3984 (0.3%)
8	Q	0.62	0/2943	1.06	13/3984 (0.3%)
8	R	0.64	0/2943	1.06	12/3984 (0.3%)
All	All	0.65	0/39497	1.05	168/53494 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
3	C	0	1
4	D	0	1
6	F	0	1
7	G	0	1
8	H	0	2
8	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	M	0	1
8	N	0	2
8	O	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	183	ARG	NE-CZ-NH2	12.87	126.73	120.30
2	B	210	ARG	NE-CZ-NH2	12.67	126.64	120.30
8	O	183	ARG	NE-CZ-NH2	11.43	126.02	120.30
8	M	210	ARG	NE-CZ-NH2	10.57	125.59	120.30
8	H	210	ARG	NE-CZ-NH2	9.06	124.83	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	TYR	Sidechain
1	A	412	TYR	Sidechain
2	B	127	TYR	Sidechain
3	C	122	ARG	Sidechain
4	D	86	TYR	Sidechain

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	3161	3065	3063	1	0
2	B	3080	3073	3073	2	0
3	C	2825	2751	2747	1	0
4	D	2590	2563	2562	3	0
5	E	1385	1361	1360	1	0
6	F	1377	1404	1404	3	0
7	G	1183	1179	1178	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2893	2867	2865	2	0
8	I	2893	2867	2865	0	0
8	M	2893	2867	2865	1	0
8	N	2893	2865	2863	2	0
8	O	2893	2867	2865	3	0
8	P	2893	2867	2865	1	0
8	Q	2893	2867	2865	1	0
8	R	2893	2867	2865	0	0
9	A	27	12	12	0	0
9	H	27	12	12	0	0
9	I	27	12	12	0	0
9	M	27	12	12	0	0
9	N	27	12	12	0	0
9	O	27	12	12	0	0
9	P	27	12	12	0	0
9	Q	27	12	12	0	0
9	R	27	12	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	P	1	0	0	0	0
10	Q	1	0	0	0	0
10	R	1	0	0	0	0
11	B	31	12	12	0	0
All	All	39029	38450	38425	21	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 0.

The worst 5 of 21 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)
6:F:15:THR:HG21	7:G:112:TYR:OH	1.88	0.73
8:P:149:THR:HG22	8:P:167:GLU:H	1.59	0.68
8:O:190:MET:HG2	8:O:209:VAL:HG11	1.81	0.62
8:O:190:MET:CG	8:O:209:VAL:HG11	2.33	0.58
4:D:201:VAL:HG21	4:D:217:PHE:CB	2.39	0.52

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	396/427 (93%)	387 (98%)	9 (2%)	0	100	100
2	B	385/390 (99%)	373 (97%)	12 (3%)	0	100	100
3	C	358/377 (95%)	340 (95%)	18 (5%)	0	100	100
4	D	312/317 (98%)	303 (97%)	9 (3%)	0	100	100
5	E	168/174 (97%)	165 (98%)	3 (2%)	0	100	100
6	F	166/168 (99%)	160 (96%)	6 (4%)	0	100	100
7	G	149/152 (98%)	146 (98%)	3 (2%)	0	100	100
8	H	367/377 (97%)	357 (97%)	10 (3%)	0	100	100
8	I	367/377 (97%)	352 (96%)	15 (4%)	0	100	100
8	M	367/377 (97%)	355 (97%)	12 (3%)	0	100	100
8	N	367/377 (97%)	356 (97%)	10 (3%)	1 (0%)	41	66
8	O	367/377 (97%)	355 (97%)	12 (3%)	0	100	100
8	P	367/377 (97%)	358 (98%)	9 (2%)	0	100	100
8	Q	367/377 (97%)	358 (98%)	9 (2%)	0	100	100
8	R	367/377 (97%)	359 (98%)	8 (2%)	0	100	100
All	All	4870/5021 (97%)	4724 (97%)	145 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	N	257	CYS

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	344/364 (94%)	335 (97%)	9 (3%)	46	75
2	B	329/335 (98%)	319 (97%)	10 (3%)	41	70
3	C	305/317 (96%)	297 (97%)	8 (3%)	46	75
4	D	285/287 (99%)	272 (95%)	13 (5%)	27	54
5	E	149/150 (99%)	146 (98%)	3 (2%)	55	81
6	F	157/157 (100%)	152 (97%)	5 (3%)	39	68
7	G	133/134 (99%)	129 (97%)	4 (3%)	41	70
8	H	312/319 (98%)	309 (99%)	3 (1%)	76	91
8	I	312/319 (98%)	301 (96%)	11 (4%)	36	65
8	M	312/319 (98%)	306 (98%)	6 (2%)	57	82
8	N	312/319 (98%)	309 (99%)	3 (1%)	76	91
8	O	312/319 (98%)	306 (98%)	6 (2%)	57	82
8	P	312/319 (98%)	302 (97%)	10 (3%)	39	68
8	Q	312/319 (98%)	305 (98%)	7 (2%)	52	79
8	R	312/319 (98%)	310 (99%)	2 (1%)	86	95
All	All	4198/4296 (98%)	4098 (98%)	100 (2%)	51	77

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	54	VAL
8	M	357	ILE
8	R	234	SER
8	I	85	ILE
8	I	312	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
8	I	161	HIS
8	N	173	HIS
8	O	173	HIS
8	P	173	HIS
8	Q	173	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
8	HIC	N	73	8	8,11,12	0.38	0	6,14,16	0.69	0
8	HIC	O	73	8	8,11,12	0.38	0	6,14,16	0.80	0
8	HIC	H	73	8	8,11,12	0.53	0	6,14,16	0.69	0
8	HIC	Q	73	8	8,11,12	0.55	0	6,14,16	0.74	0
8	HIC	M	73	8	8,11,12	0.39	0	6,14,16	0.63	0
8	HIC	P	73	8	8,11,12	0.38	0	6,14,16	0.63	0
8	HIC	R	73	8	8,11,12	0.42	0	6,14,16	0.71	0
8	HIC	I	73	8	8,11,12	0.59	0	6,14,16	0.64	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
8	HIC	N	73	8	-	0/5/6/8	0/1/1/1
8	HIC	O	73	8	-	0/5/6/8	0/1/1/1
8	HIC	H	73	8	-	0/5/6/8	0/1/1/1
8	HIC	Q	73	8	-	0/5/6/8	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HIC	M	73	8	-	0/5/6/8	0/1/1/1
8	HIC	P	73	8	-	0/5/6/8	0/1/1/1
8	HIC	R	73	8	-	0/5/6/8	0/1/1/1
8	HIC	I	73	8	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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	$\#|Z| > 2$
9	ADP	I	802	10	24,29,29	0.96	0	29,45,45	1.80	9 (31%)
9	ADP	R	802	10	24,29,29	1.08	1 (4%)	29,45,45	1.46	6 (20%)
9	ADP	A	901	10	24,29,29	1.07	2 (8%)	29,45,45	1.67	8 (27%)
9	ADP	Q	802	10	24,29,29	1.10	2 (8%)	29,45,45	1.36	6 (20%)
9	ADP	P	802	10	24,29,29	1.11	3 (12%)	29,45,45	1.69	8 (27%)
9	ADP	M	802	10	24,29,29	1.08	1 (4%)	29,45,45	1.56	7 (24%)
9	ADP	H	802	10	24,29,29	1.01	1 (4%)	29,45,45	1.76	7 (24%)
11	ATP	B	902	10	26,33,33	1.05	1 (3%)	31,52,52	1.43	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
9	ADP	O	802	10	24,29,29	1.03	1 (4%)	29,45,45	1.47	6 (20%)
9	ADP	N	802	10	24,29,29	1.19	3 (12%)	29,45,45	1.69	6 (20%)

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
9	ADP	I	802	10	-	1/12/32/32	0/3/3/3
9	ADP	R	802	10	-	2/12/32/32	0/3/3/3
9	ADP	A	901	10	-	1/12/32/32	0/3/3/3
9	ADP	Q	802	10	-	2/12/32/32	0/3/3/3
9	ADP	P	802	10	-	1/12/32/32	0/3/3/3
9	ADP	M	802	10	-	1/12/32/32	0/3/3/3
9	ADP	H	802	10	-	1/12/32/32	0/3/3/3
11	ATP	B	902	10	-	1/18/38/38	0/3/3/3
9	ADP	O	802	10	-	0/12/32/32	0/3/3/3
9	ADP	N	802	10	-	5/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	802	ADP	O4'-C1'	2.83	1.45	1.41
9	Q	802	ADP	O4'-C1'	2.35	1.44	1.41
9	P	802	ADP	O4'-C1'	2.26	1.44	1.41
9	A	901	ADP	PB-O3B	-2.21	1.46	1.54
9	M	802	ADP	O4'-C1'	2.14	1.44	1.41

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	802	ADP	C4-C5-N7	4.58	114.17	109.40
9	A	901	ADP	C4-C5-N7	4.52	114.11	109.40
9	H	802	ADP	C4-C5-N7	4.50	114.09	109.40
9	I	802	ADP	C4-C5-N7	4.48	114.07	109.40
11	B	902	ATP	C4-C5-N7	4.43	114.02	109.40

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	N	802	ADP	C5'-O5'-PA-O3A
9	N	802	ADP	C3'-C4'-C5'-O5'
9	Q	802	ADP	C3'-C4'-C5'-O5'
9	N	802	ADP	O4'-C4'-C5'-O5'
9	R	802	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP I 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP R 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP Q 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP P 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP M 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP H 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 902

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP O 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP N 802

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-42787. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map
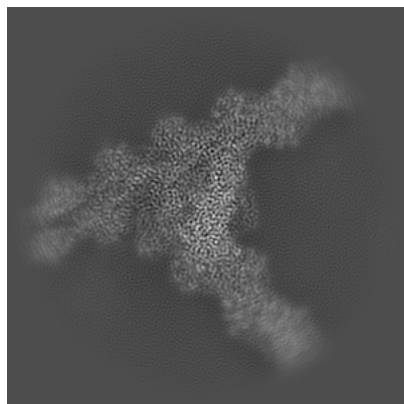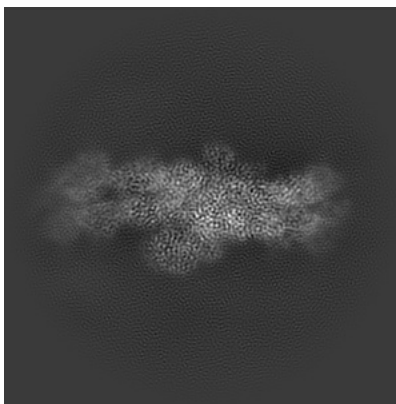
X
Y
Z

6.1.2 Raw map

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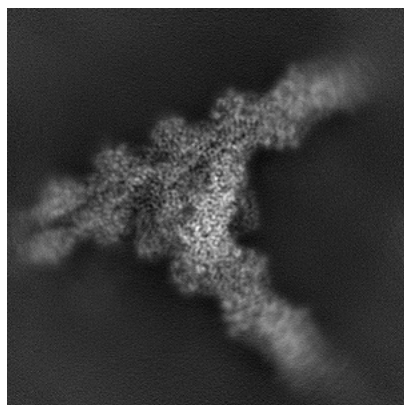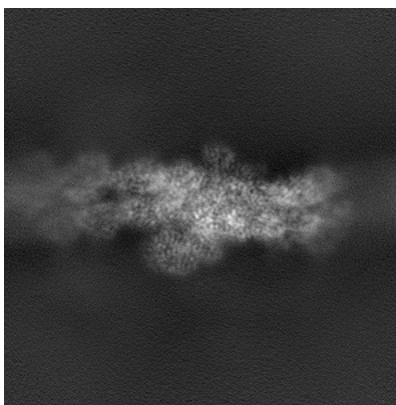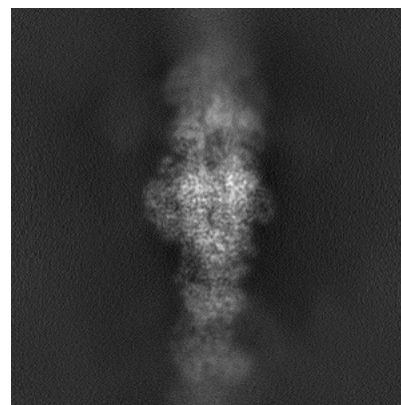
The images above show the map projected in three orthogonal directions.

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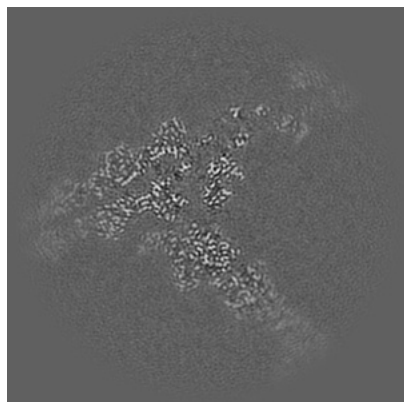
6.2.1 Primary map
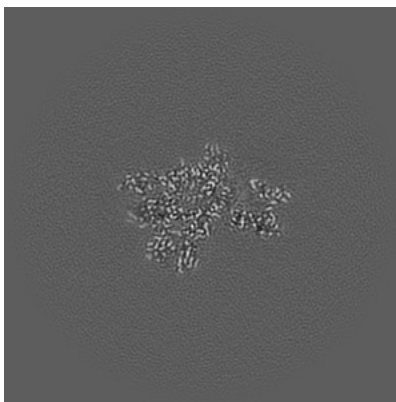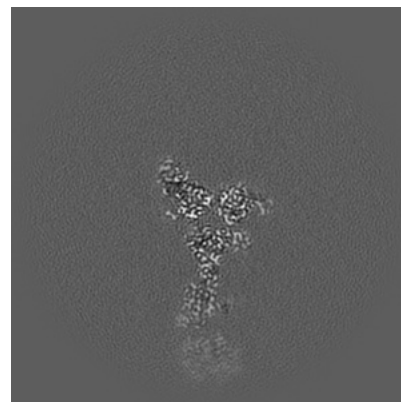
| X Index: 256 | Y Index: 256 | Z Index: 256 |

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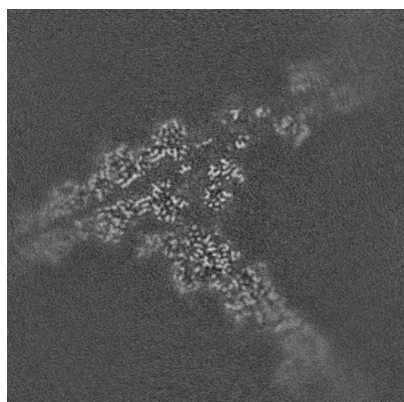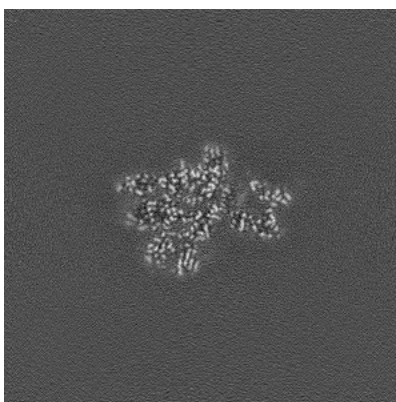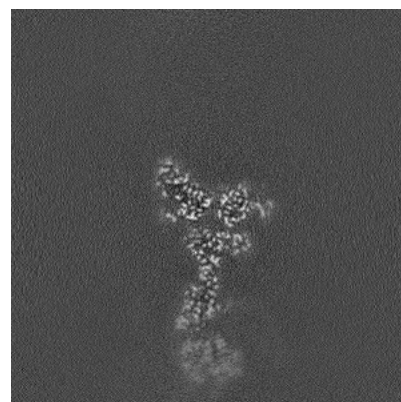
| X Index: 256 | Y Index: 256 | Z Index: 256 |

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

6.3   Largest variance slices ⓘ

6.3.1   Primary map
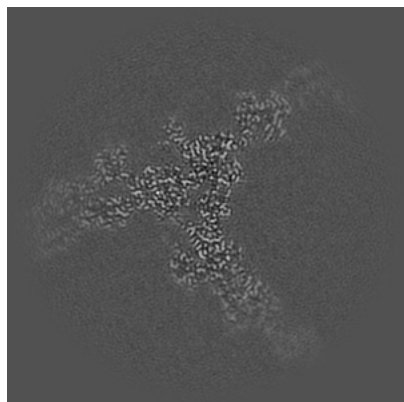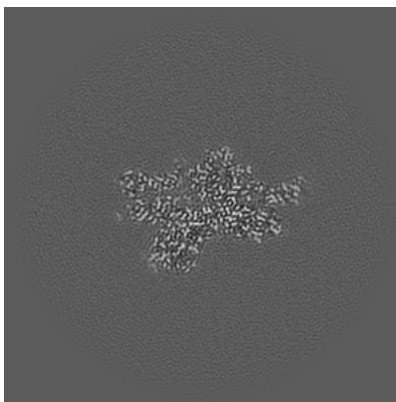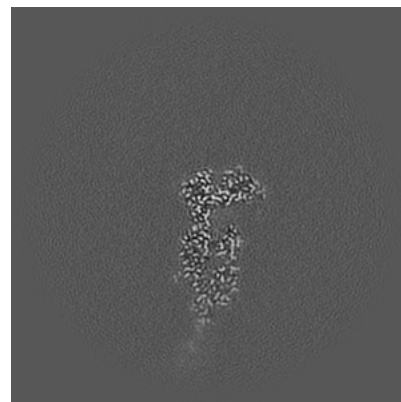
X Index: 244   Y Index: 266   Z Index: 294

6.3.2   Raw map
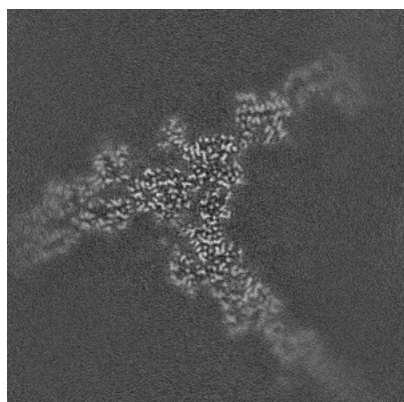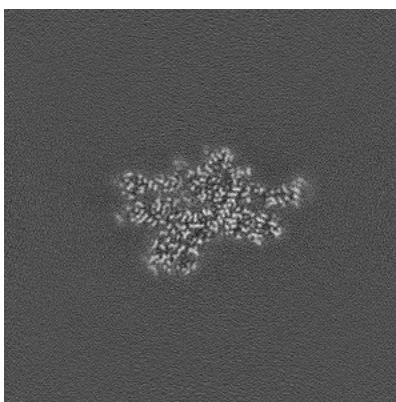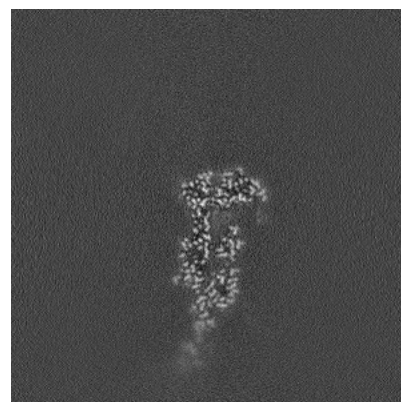
X Index: 244   Y Index: 266   Z Index: 293

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

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

6.4.1　Primary map
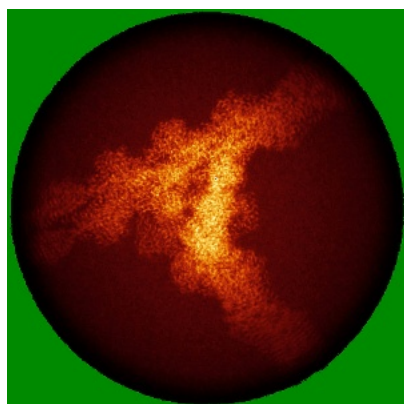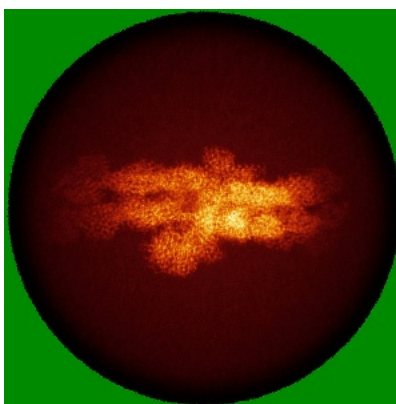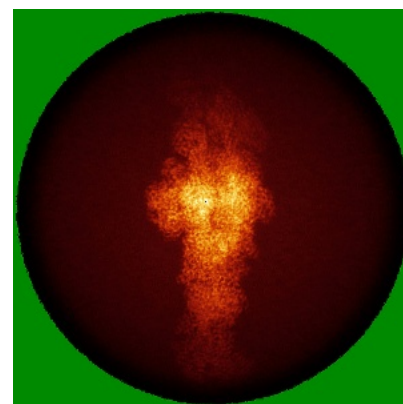
X　　　　　　　　　　　　Y　　　　　　　　　　　　Z

6.4.2　Raw map

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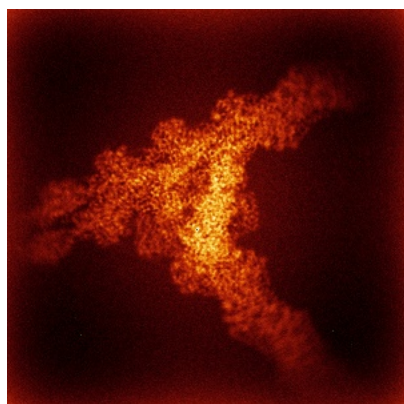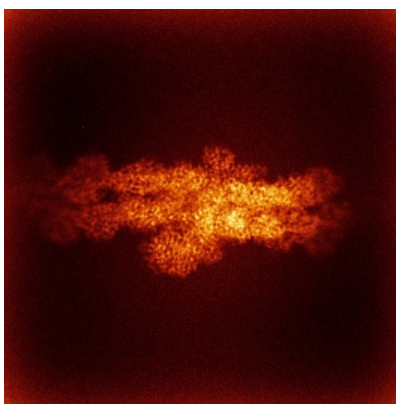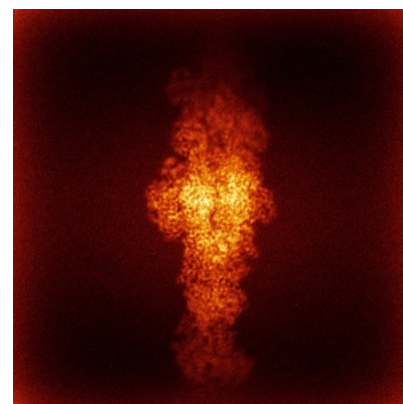
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
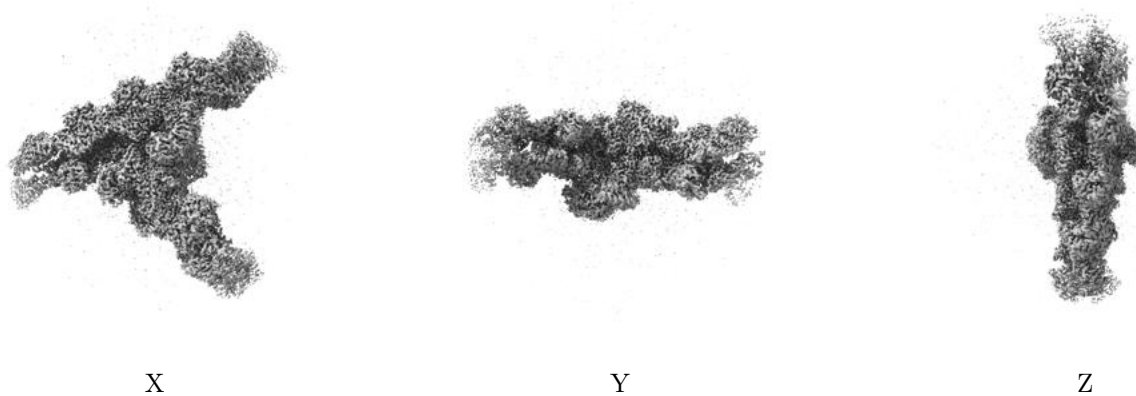
The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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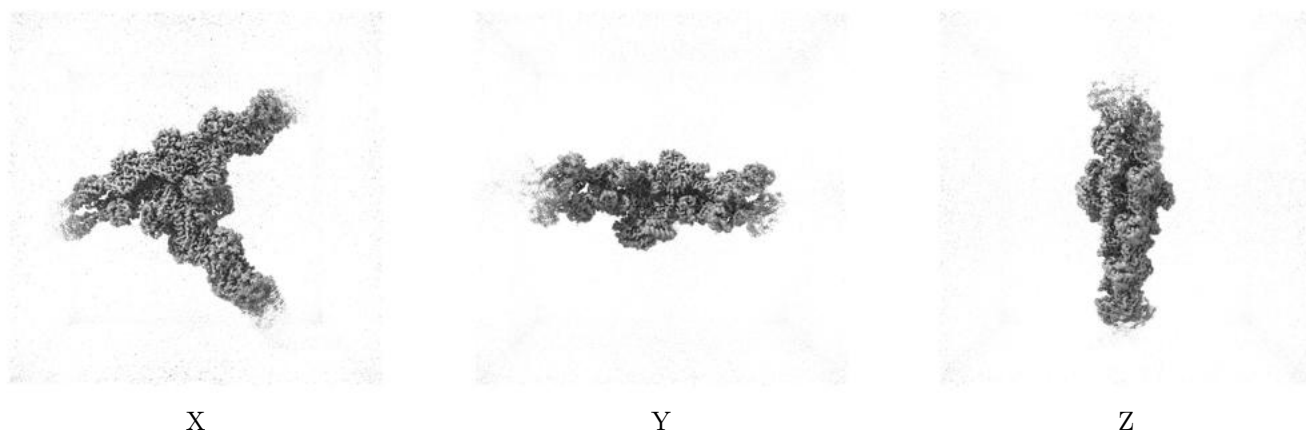
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

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

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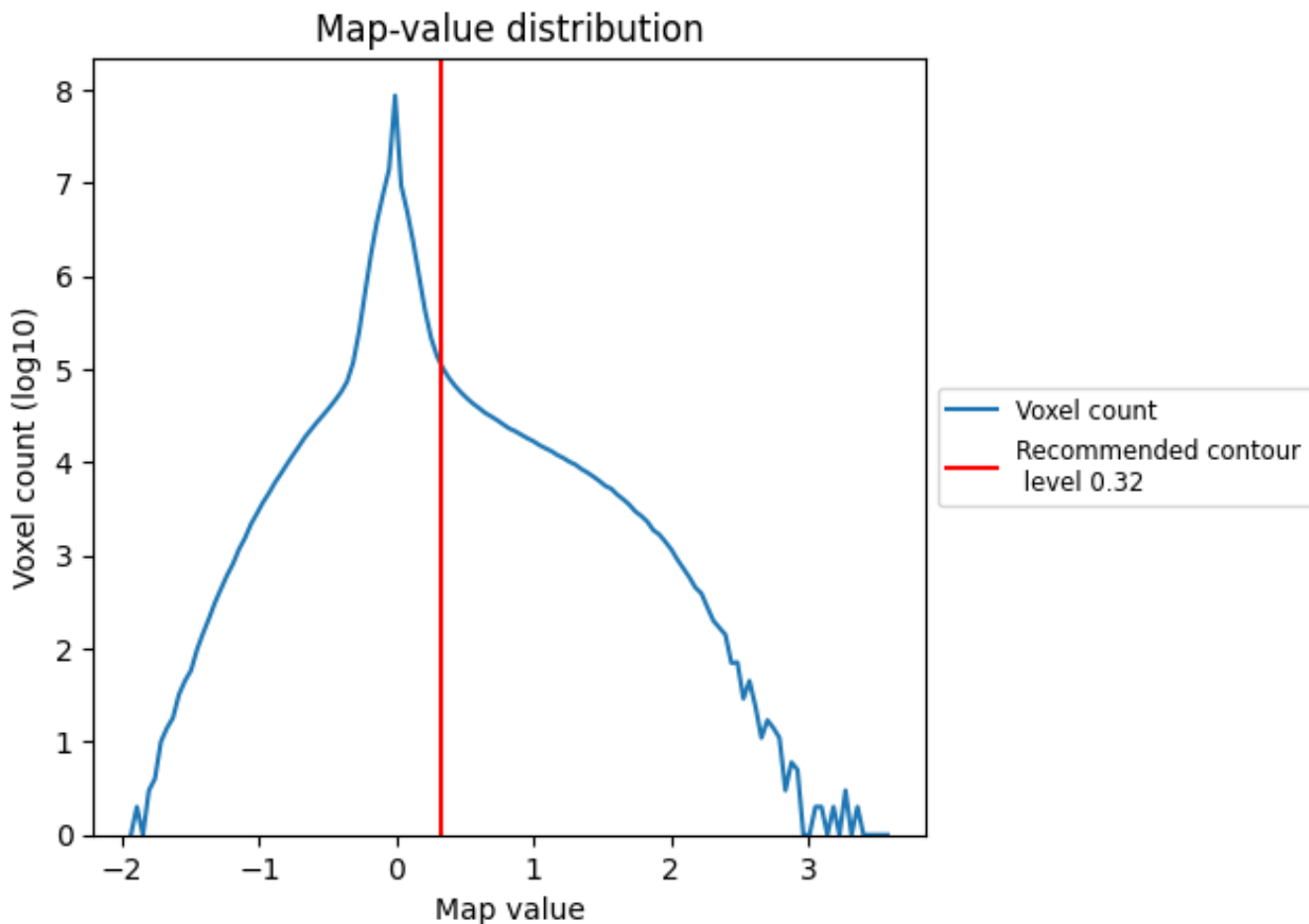
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
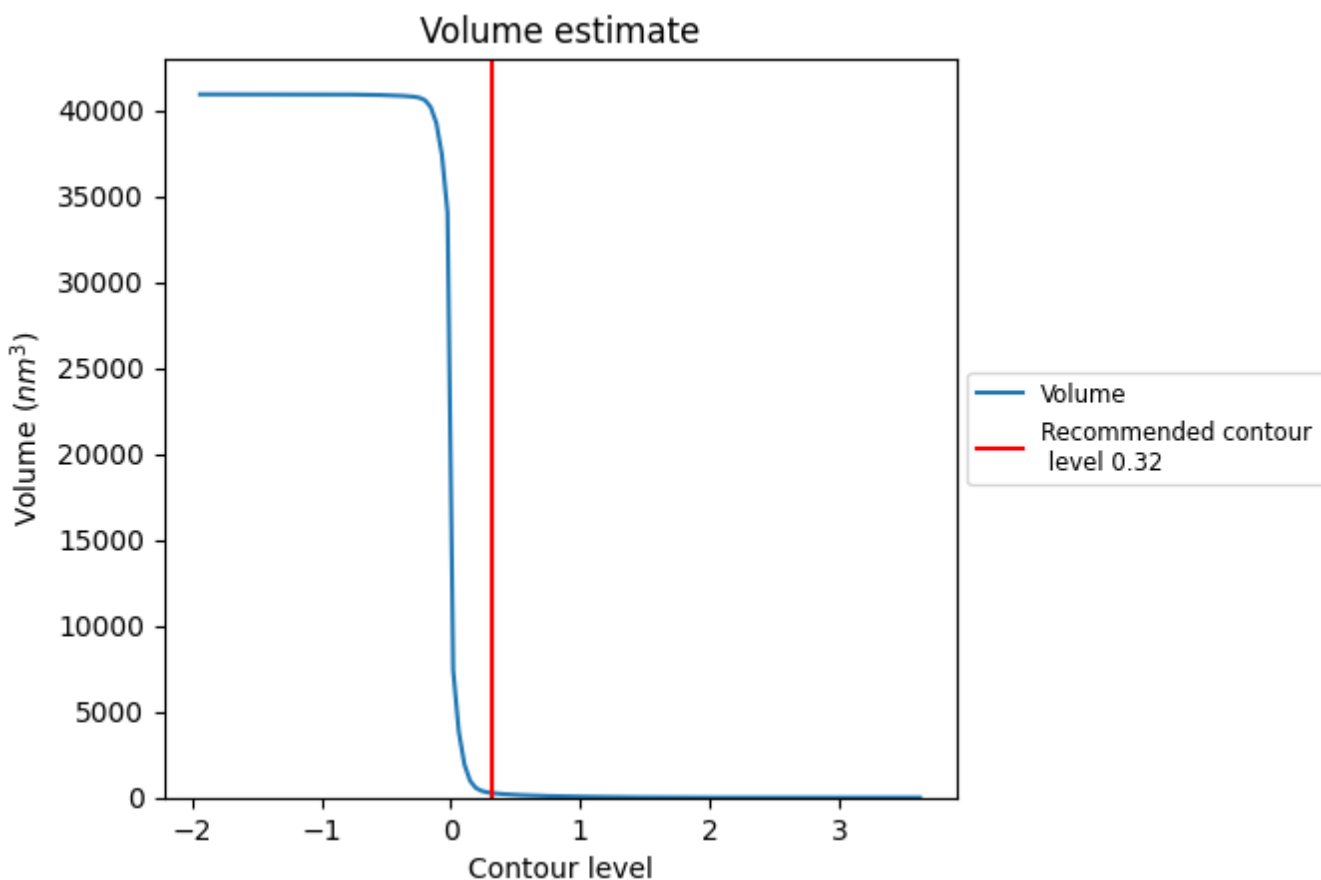
The volume at the recommended contour level is 263 nm^3; this corresponds to an approximate mass of 237 kDa.

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 ⓘ
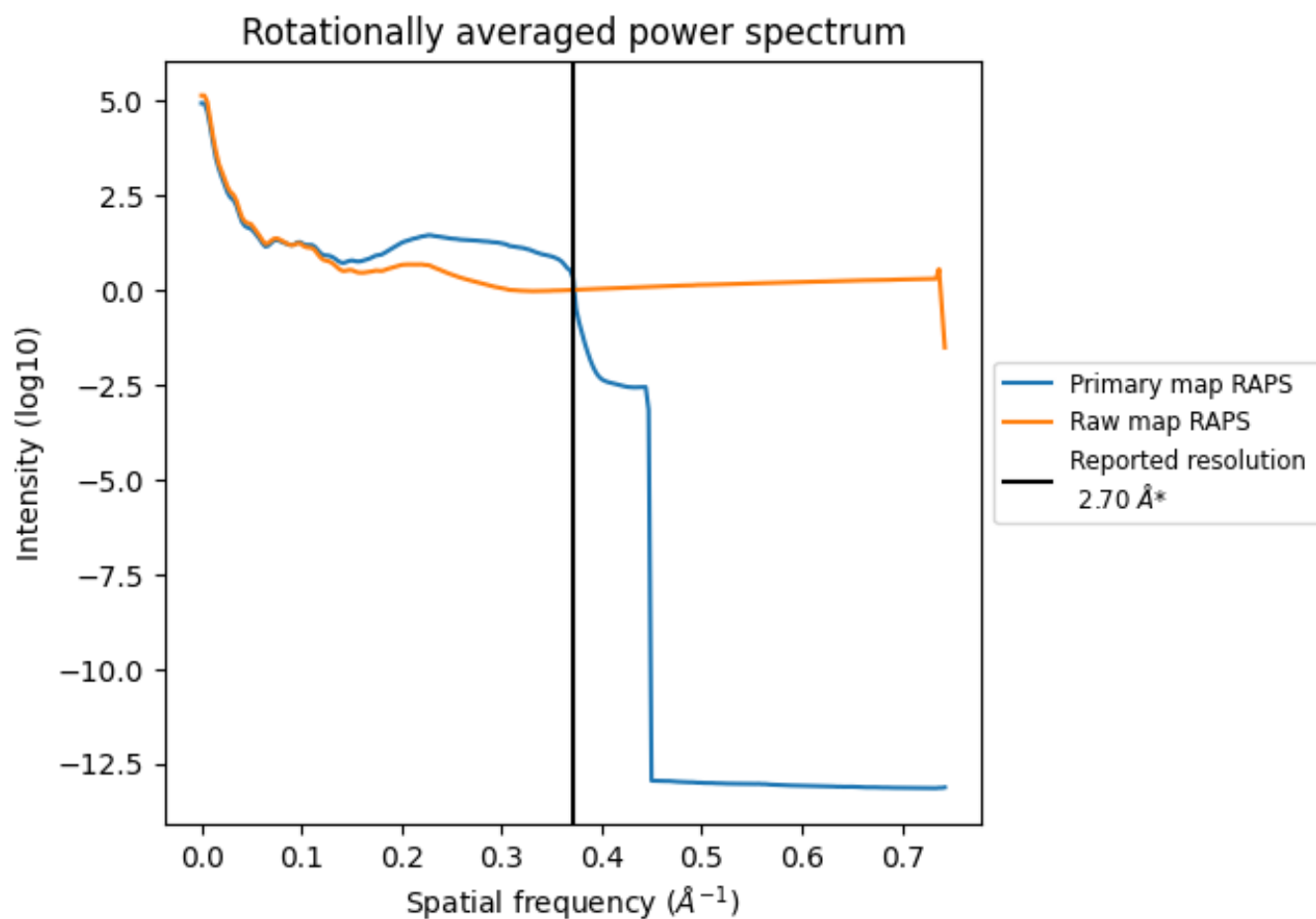
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8　Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1　FSC ⓘ
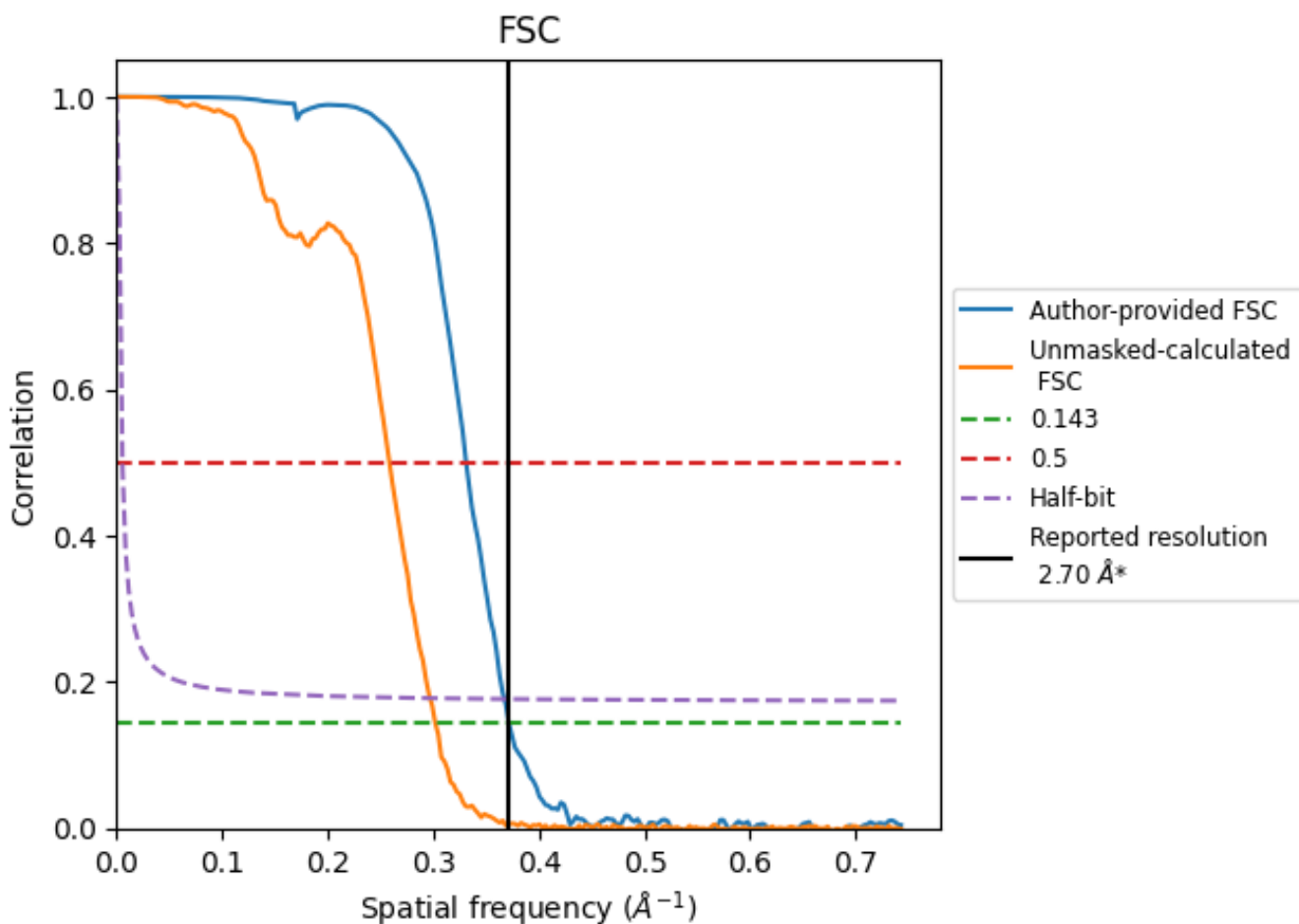
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.02	2.72
Unmasked-calculated*	3.31	3.87	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.7 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-42787 and PDB model 8UXW. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)

| X | Y | Z |
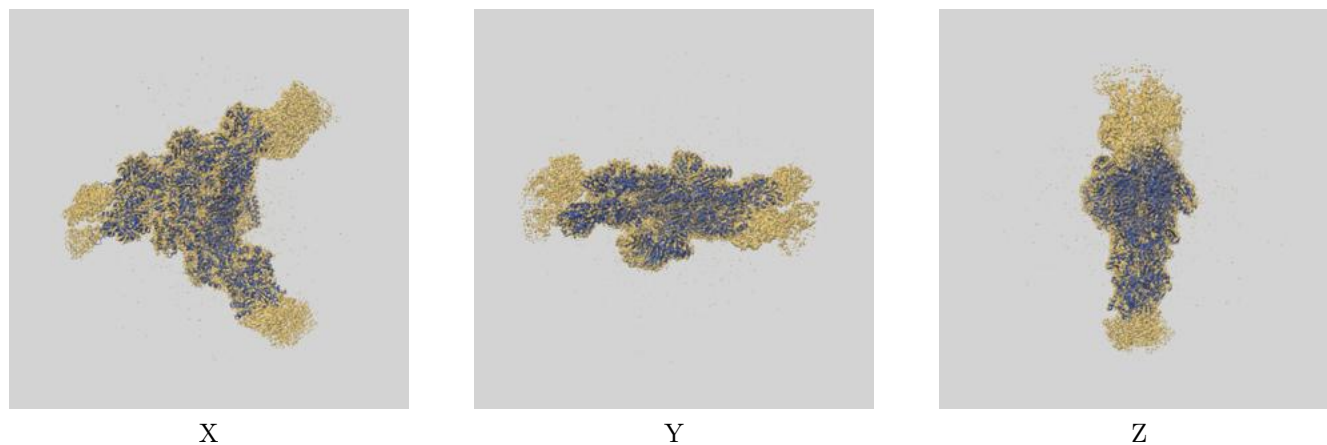
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X	Y	Z
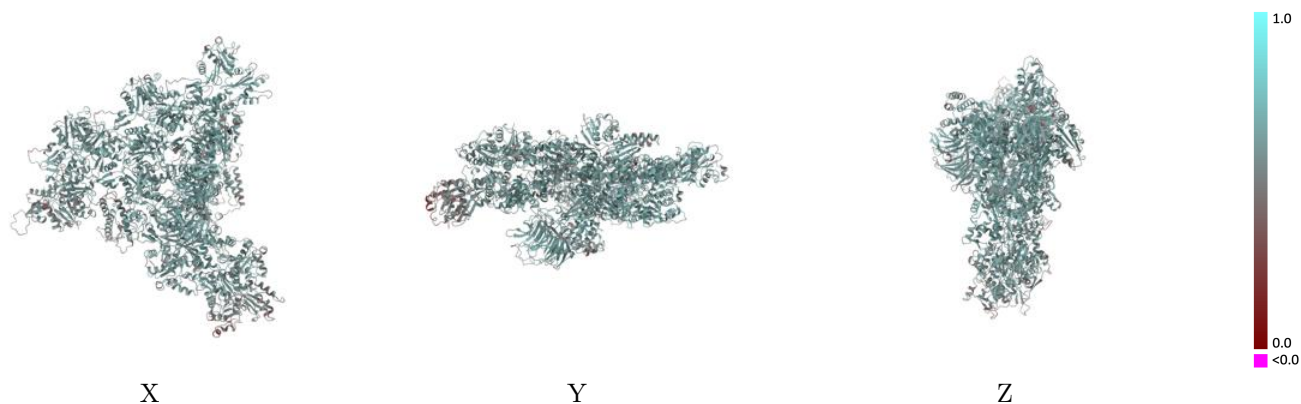
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
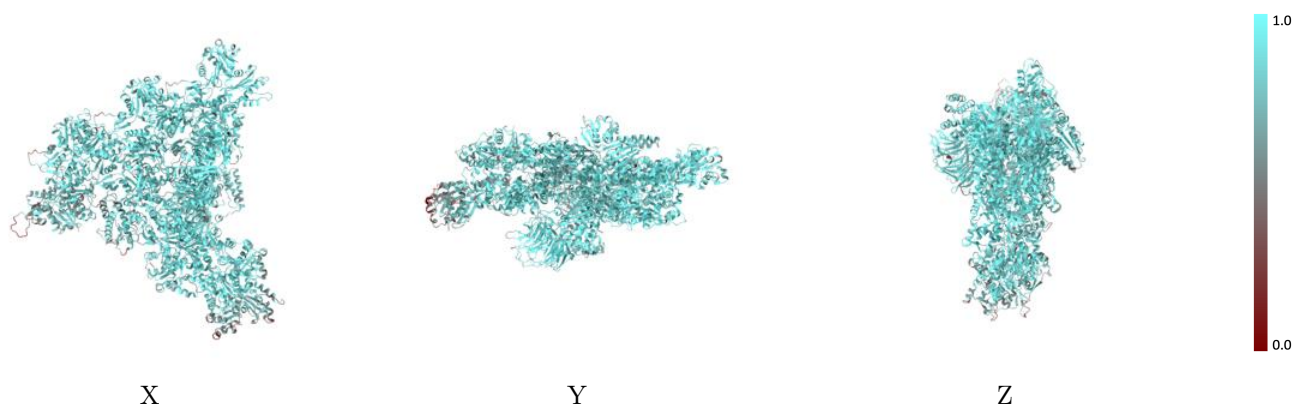
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).

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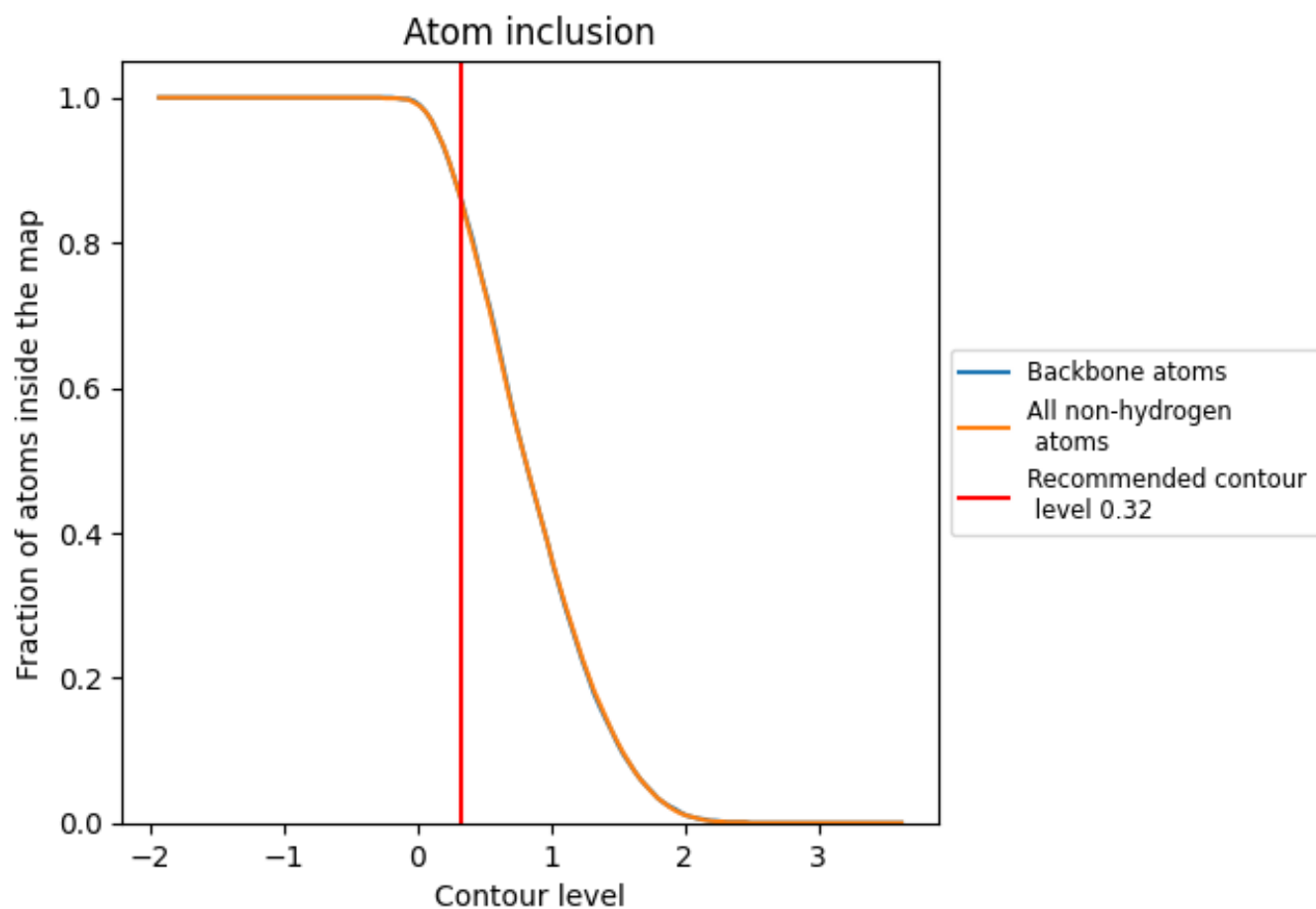
At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.5850
A	0.8960	0.6000
B	0.8990	0.6010
C	0.9050	0.6030
D	0.8660	0.5840
E	0.7410	0.5300
F	0.9440	0.6230
G	0.8470	0.5680
H	0.8730	0.5800
I	0.7070	0.4950
M	0.7560	0.5470
N	0.8430	0.5700
O	0.9370	0.6230
P	0.9210	0.6120
Q	0.9460	0.6280
R	0.8950	0.5950

1.0

0.0
<0.0