



wwPDB EM Validation Summary Report ⓘ

Jul 9, 2024 – 09:34 pm BST

PDB ID : 7YXX
EMDB ID : EMD-14368
Title : Cryo-EM structure of USP9X
Authors : Deme, J.C.; Halabelian, L.; Arrowsmith, C.H.; Lea, S.M.; Structural Genomics Consortium (SGC)
Deposited on : 2022-02-16
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
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)	:	2.37.1

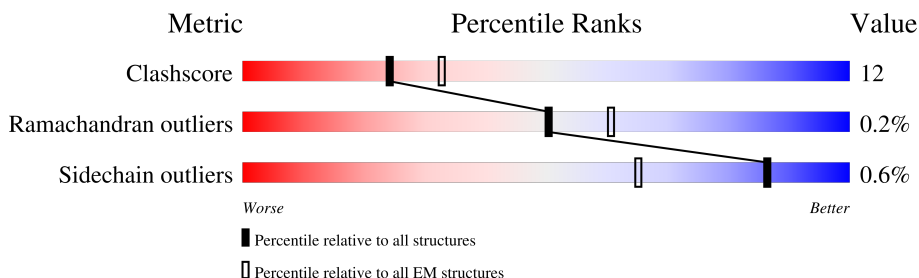
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	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 $\leq 5\%$. 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	2579	<div> <div>22%</div> <div>49%</div> <div>18%</div> <div>32%</div> </div>
1	B	2579	<div> <div>33%</div> <div>50%</div> <div>18%</div> <div>32%</div> </div>
1	C	2579	<div> <div>34%</div> <div>48%</div> <div>19%</div> <div>32%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 42357 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 Probable ubiquitin carboxyl-terminal hydrolase FAF-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1754	Total 14155	C 9062	N 2426	O 2571	S 96	1	0
1	B	1754	Total 14155	C 9062	N 2426	O 2571	S 96	1	0
1	C	1741	Total 14047	C 8997	N 2407	O 2547	S 96	1	0

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q93008
A	-16	HIS	-	expression tag	UNP Q93008
A	-15	HIS	-	expression tag	UNP Q93008
A	-14	HIS	-	expression tag	UNP Q93008
A	-13	HIS	-	expression tag	UNP Q93008
A	-12	HIS	-	expression tag	UNP Q93008
A	-11	HIS	-	expression tag	UNP Q93008
A	-10	SER	-	expression tag	UNP Q93008
A	-9	SER	-	expression tag	UNP Q93008
A	-8	GLY	-	expression tag	UNP Q93008
A	-7	ARG	-	expression tag	UNP Q93008
A	-6	GLU	-	expression tag	UNP Q93008
A	-5	ASN	-	expression tag	UNP Q93008
A	-4	LEU	-	expression tag	UNP Q93008
A	-3	TYR	-	expression tag	UNP Q93008
A	-2	PHE	-	expression tag	UNP Q93008
A	-1	GLN	-	expression tag	UNP Q93008
A	0	GLY	-	expression tag	UNP Q93008
A	2555	ASP	-	expression tag	UNP Q93008
A	2556	TYR	-	expression tag	UNP Q93008
A	2557	LYS	-	expression tag	UNP Q93008
A	2558	ASP	-	expression tag	UNP Q93008
A	2559	ASP	-	expression tag	UNP Q93008
A	2560	ASP	-	expression tag	UNP Q93008

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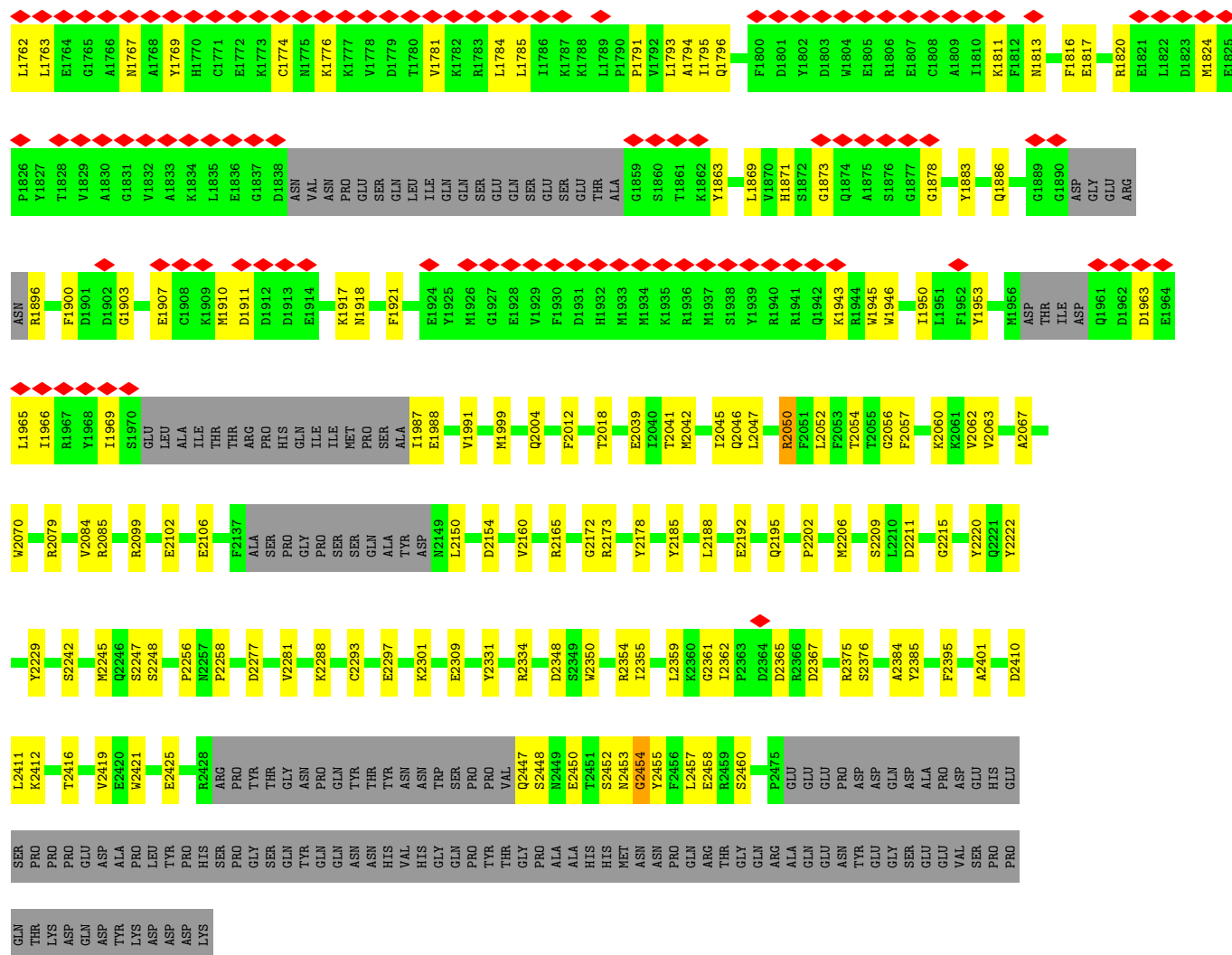
Chain	Residue	Modelled	Actual	Comment	Reference
A	2561	LYS	-	expression tag	UNP Q93008
B	-17	MET	-	initiating methionine	UNP Q93008
B	-16	HIS	-	expression tag	UNP Q93008
B	-15	HIS	-	expression tag	UNP Q93008
B	-14	HIS	-	expression tag	UNP Q93008
B	-13	HIS	-	expression tag	UNP Q93008
B	-12	HIS	-	expression tag	UNP Q93008
B	-11	HIS	-	expression tag	UNP Q93008
B	-10	SER	-	expression tag	UNP Q93008
B	-9	SER	-	expression tag	UNP Q93008
B	-8	GLY	-	expression tag	UNP Q93008
B	-7	ARG	-	expression tag	UNP Q93008
B	-6	GLU	-	expression tag	UNP Q93008
B	-5	ASN	-	expression tag	UNP Q93008
B	-4	LEU	-	expression tag	UNP Q93008
B	-3	TYR	-	expression tag	UNP Q93008
B	-2	PHE	-	expression tag	UNP Q93008
B	-1	GLN	-	expression tag	UNP Q93008
B	0	GLY	-	expression tag	UNP Q93008
B	2555	ASP	-	expression tag	UNP Q93008
B	2556	TYR	-	expression tag	UNP Q93008
B	2557	LYS	-	expression tag	UNP Q93008
B	2558	ASP	-	expression tag	UNP Q93008
B	2559	ASP	-	expression tag	UNP Q93008
B	2560	ASP	-	expression tag	UNP Q93008
B	2561	LYS	-	expression tag	UNP Q93008
C	-17	MET	-	initiating methionine	UNP Q93008
C	-16	HIS	-	expression tag	UNP Q93008
C	-15	HIS	-	expression tag	UNP Q93008
C	-14	HIS	-	expression tag	UNP Q93008
C	-13	HIS	-	expression tag	UNP Q93008
C	-12	HIS	-	expression tag	UNP Q93008
C	-11	HIS	-	expression tag	UNP Q93008
C	-10	SER	-	expression tag	UNP Q93008
C	-9	SER	-	expression tag	UNP Q93008
C	-8	GLY	-	expression tag	UNP Q93008
C	-7	ARG	-	expression tag	UNP Q93008
C	-6	GLU	-	expression tag	UNP Q93008
C	-5	ASN	-	expression tag	UNP Q93008
C	-4	LEU	-	expression tag	UNP Q93008
C	-3	TYR	-	expression tag	UNP Q93008
C	-2	PHE	-	expression tag	UNP Q93008

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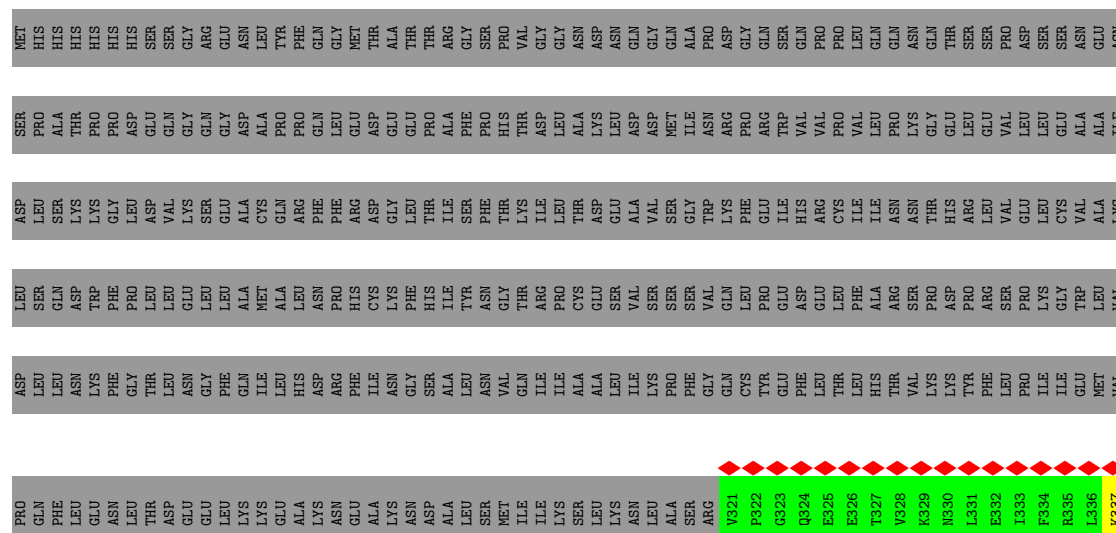
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLN	-	expression tag	UNP Q93008
C	0	GLY	-	expression tag	UNP Q93008
C	2555	ASP	-	expression tag	UNP Q93008
C	2556	TYR	-	expression tag	UNP Q93008
C	2557	LYS	-	expression tag	UNP Q93008
C	2558	ASP	-	expression tag	UNP Q93008
C	2559	ASP	-	expression tag	UNP Q93008
C	2560	ASP	-	expression tag	UNP Q93008
C	2561	LYS	-	expression tag	UNP Q93008



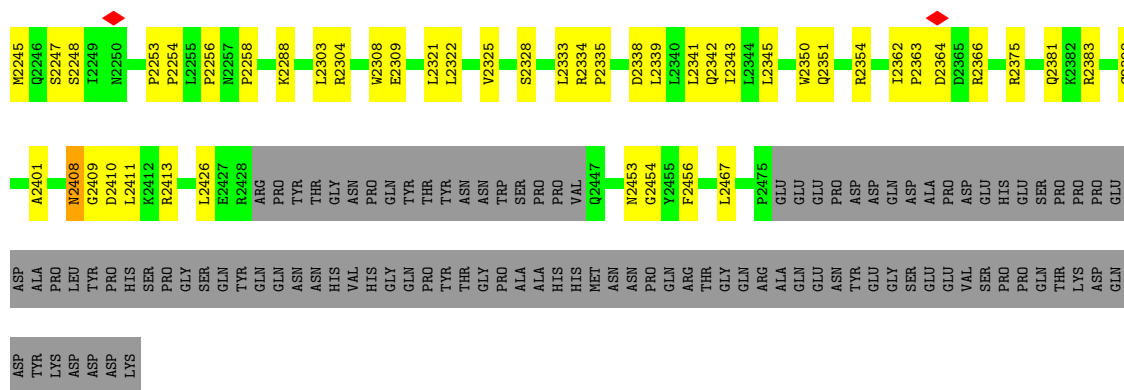


● Molecule 1: Probable ubiquitin carboxyl-terminal hydrolase FAF-X

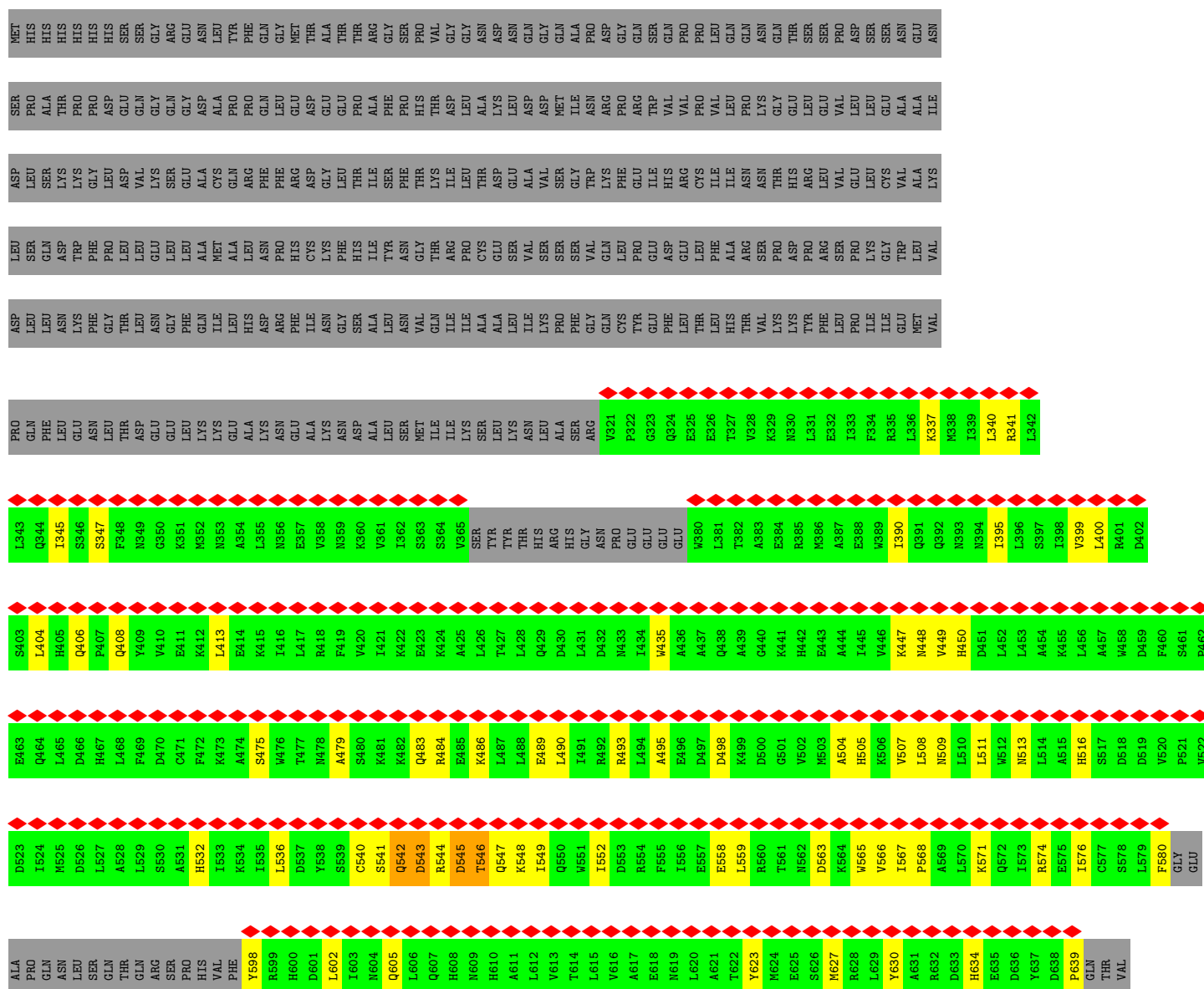


S1128	H1064	SER	ALA	LYS	L823	M763	K703	ARG	ALA	D523	E463	S403	L343
M1129	A1065	CYS	ASP	HIS	K824	D764	L704	LEU	PRO	I524	Q464	L404	Q344
T1130	K1066	LEU	ASP	LEU	A825	D765	M705	SER	GLN	M525	L465	H405	I345
L1131	LEU	GLY	ARG	SER	S826	L766	G706	ARG	ASN	D526	D466	Q406	S346
R1132	GLY	VAL	LEU	VAL	Y827	E767	D707	TYR	SER	L527	H467	P407	S347
N1133	GLU	ILE	ILE	VAL	D828	L768	E708			A528	L468	Q408	F348
M1134	SER	MET	GLY	ARG	T829	I769	P709	H650	ARG	L529	F469	Q408	N349
F1135	LEU		GLN	PHE	L830	G770	D710	V651	GLN	S530	D470	V410	G350
L1136	LEU	PRO	LEU	ARG	L830	G770	D710	Q652	ARG	A531	D470	V410	K351
P1137	SER	ASN	ASN	ASN	C831	L771	L711	E653	SER	C471	E411	E411	M352
M1138	SER	LEU	GLN	GLY	VAL	D772	D712	Q655	HIS	I533	F472	K412	M352
A1139	L1076	LEU	LEU	ASP	GLY	Y773	P713	Q655	VAL	K334	K473	L413	N353
D1140	D1077	SER	SER	ASP	ASP	W775	D714	E656	PHE	A474	K474	E414	A354
M1141		LYS	LEU	LYS	LYS	R776	I715	R657	Y598	I535	S475	K415	L355
E1142	F1080	ASP	ILE	ASP	ASP	R776	N716	R657	R599	I535	S475	K415	L355
T1143	F1081	THR	THR	LEU	SER	V777	K717	L658	H600	L336	W476	I416	N356
L1144	G1082	ALA	ALA	GLU	VAL	V778	D718	N659	D601	D537	T477	L417	E357
P1145	P1083	LYS	LYS	VAL	ASN	I779	F719	F660	L602	Y538	W478	R418	V358
R1146	S1084	LEU	LEU	TRP	C842	I779	F719	L661	L602	S539	A479	F419	N359
G1146	Q1087	THR	THR	SER	A843	Q780	F720	R662	I603	C540	S480	V420	K360
A1147	V1088	GLN	GLN	HIS	R844	S781	F720	L661	N604	S541	K481	I421	V361
Y1148	L1089	ILE	ILE	THR	Q845	N782	E721	F663	Q605	Q542	K482	K422	I362
M1150	Y1090	ASN	SER	ASN	E846	D783	S722	L664	L606	D543	Q483	E423	S363
A1151	T1092	ASN	THR	THR	E847	D784	W724	L665	Q607	R544	K484	K424	S364
L1152	E1093	ASP	ASP	THR	W848	I785	V724	K666	H608	D545	E485	A425	V365
K1153	I1094	THR	MET	ILE	R849	A786	L725	D667	N609	T546	K486	L426	SER
Y1095	V1094	ARG	PRO	GLY	N850	S787	Q726	Q669	H610	Q547	L487	T427	TYR
A1155	Y1096	ARG	PRO	ARG		R788	D728	Q669	A611	K548	L428	L428	THR
K1156		ASP	ASP	ARG		A789	P729	W671	L612	I549	Q429	HIS	HIS
L1157	A1097	SER	SER	CYS		I790	S730	L672	V613	Q550	L490	D430	ARG
L1158	L1098	SER	SER	ILE	L854	D791	L731	C673	T614	W551	I491	L431	HIS
L1159	L1099	ASP	ASP	LEU	V856	L792	L732	A674	L615	I552	R492	D432	ASN
T1160		SER	SER	ASN	L857	L793	L733	P675	V616	D553	R493	D432	PRO
A1161	M1100	THR	THR	LYS	R858	K794	E734	Q676	A617	R554	L494	I434	GLU
I1162	P1101	GLY	GLY	ALA	E859	E795	N735	A677	E618	F555	A495	W435	GLU
G1163	ALA	ALA	PRO	ASN	Y860	I796	G736	K678	N619	I556	E496	A436	GLU
Y1164	PRO	R1041	GLY	ALA	I861	Y797	M737	Q679	L620	E557	D497	A437	GLU
G1165	LEU	V1042	ASN	HIS	N862	T798	K738	I680	A621	E558	D498	Q438	W380
VAL	ALA	L1043	GLY	THR	E863	N799	C739	W681	Y623	L559	K439	A439	L381
ARG	ASP	M1044	ASN	ILE	C864	L800	F740	K682	M624	R560	G440	A383	T382
ALA	ASP	K1045	HIS	GLY	D865	G801	E741	C683	E625	T561	D500	E384	A383
VAL	S1110	L1046	TYR	LEU	S866	P802	R742	C683	S626	G501	H441	R385	E384
GLN	D1112	M1047	SER	PHE	ASP	R803	F743	A685	M627	M503	E443	M386	R385
CYS	F1113	P1048	GLY	GLY	TYR	L804	F744	E686	R628	A504	A444	A387	M386
PRO	Q1114	P1049	PRO	GLY	HIS	Q805	K745	E886	L629	H505	I445	E388	E388
GLU	F1115	D1050	ASN	GLY	GLU	V806	A746	N687	L629	K506	V446	W389	W389
GLY	H1116	S1051	PRO	LEU	ARG	N807	V747	A688	Y630	I567	K447	I390	I390
VAL		T1052	VAL	ASP	THR	Q808	I747	V689	A631	V507	L508	Q391	Q391
GLU	K1119	T1053	GLY	ILE	LEU	V809	N748	Y690	R632	P568	L508	Q392	Q392
GLY	S1120	I1054	PRO	PRO	PRO	W810	C749	R690	D633	A569	N509	Q392	Q392
ASN		E1055	MET	MET	MET	I811	R750	L691	L570	H450	N393	N393	N393
PRO	L1123	K1056	ARG	SER	ARG	H812	E751	C692	H634	L511	L510	H450	N394
THR	P1124	L1057	ALA	SER	ALA	E813	G752	D693	D636	D451	L512	L452	I395
GLN	L1125	R1058	PHE	THR	PHE	D814	K753	R694	E635	L453	N513	L453	L396
ILE	V1126	A1059	ARG	ARG	GLY	F815	L754	E695	A696	L454	A454	K455	I398
		I1060	GLY	GLY		I816	V755	C697	D638	L456	L454	K455	I398
		L1062	GLY	GLY		Q817	A756	F698	P639	H516	L456	L456	I399
		L1062	GLY	GLY		S818	R757	K699	THR	S517	L457	L457	V399
		L1063	GLY	GLY		C819	R758	W700	VAL	D518	L458	L458	L400
						F820	R759	Y701		D519	L459	L459	R401
						D821	A760	S702		V520	L460	L460	D402
						R822	Y761			P521	L461	L461	D402
							M762						





● Molecule 1: Probable ubiquitin carboxyl-terminal hydrolase FAF-X







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	330000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.330	Depositor
Minimum map value	-0.608	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.221	Depositor
Map size (Å)	372.73602, 372.73602, 372.73602	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	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		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/14461	0.47	0/19559
1	B	0.26	0/14461	0.47	0/19559
1	C	0.26	0/14351	0.47	0/19411
All	All	0.26	0/43273	0.47	0/58529

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	14155	0	14051	332	0
1	B	14155	0	14051	327	0
1	C	14047	0	13957	348	0
All	All	42357	0	42059	1000	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 1000 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2413:ARG:O	1:C:2416:THR:HG22	1.31	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1521:ASP:O	1:C:1524:THR:HG22	1.38	1.20
1:B:540:CYS:HB2	1:B:544:ARG:HA	1.29	1.07
1:C:1789:LEU:HB3	1:C:1863:TYR:OH	1.58	1.02
1:A:1265:THR:HA	1:A:1268:TYR:CD2	2.02	0.95

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	1721/2579 (67%)	1631 (95%)	86 (5%)	4 (0%)	47	77
1	B	1721/2579 (67%)	1631 (95%)	90 (5%)	0	100	100
1	C	1708/2579 (66%)	1614 (94%)	88 (5%)	6 (0%)	34	66
All	All	5150/7737 (67%)	4876 (95%)	264 (5%)	10 (0%)	50	77

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	ARG
1	A	2454	GLY
1	C	2365	ASP
1	C	546	THR
1	C	1348	ARG

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1544/2286 (68%)	1532 (99%)	12 (1%)	81	89
1	B	1544/2286 (68%)	1536 (100%)	8 (0%)	88	93
1	C	1532/2286 (67%)	1522 (99%)	10 (1%)	84	90
All	All	4620/6858 (67%)	4590 (99%)	30 (1%)	86	91

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	544	ARG
1	C	1357	LEU
1	B	794	LYS
1	C	2050	ARG
1	C	545	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1813	ASN
1	C	1653	HIS
1	B	1947	ASN
1	C	2221	GLN
1	C	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

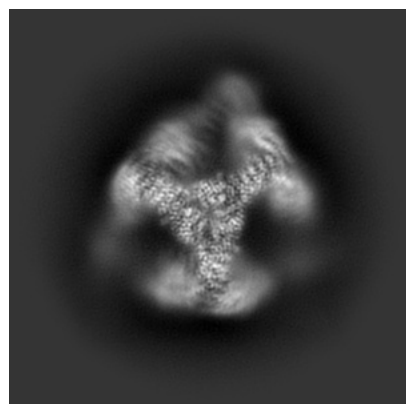
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14368. These allow visual inspection of the internal detail of the map and identification of artifacts.

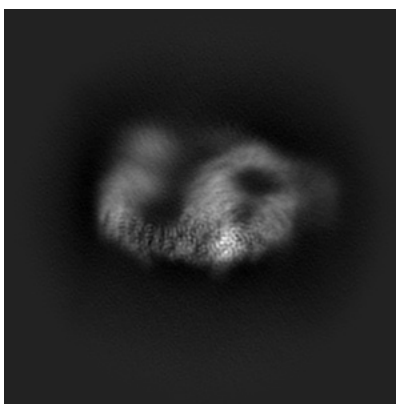
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

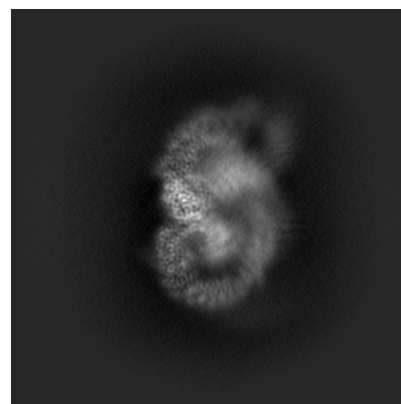
6.1.1 Primary map



X

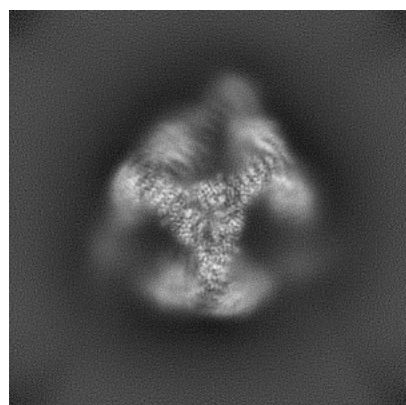


Y

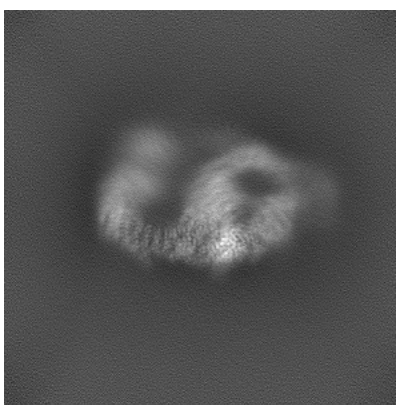


Z

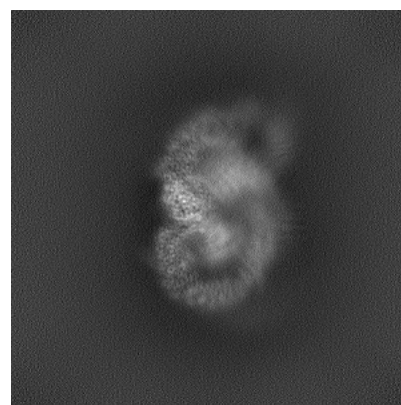
6.1.2 Raw map



X



Y

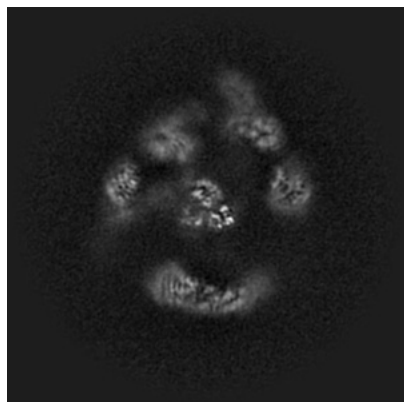


Z

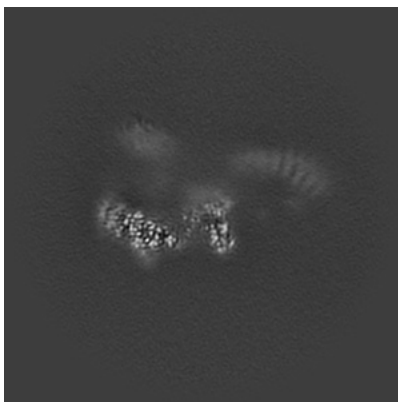
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

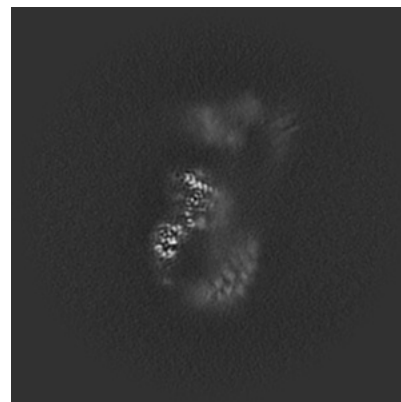
6.2.1 Primary map



X Index: 224

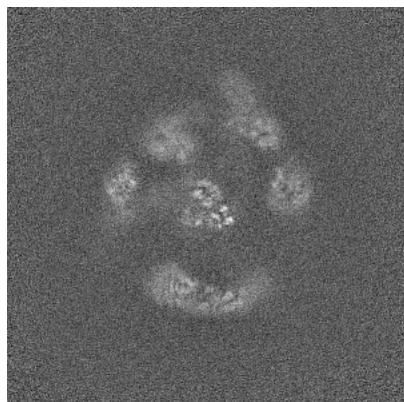


Y Index: 224

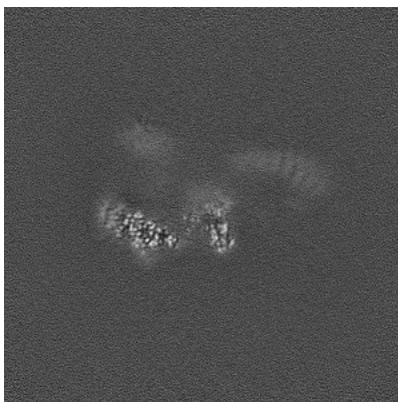


Z Index: 224

6.2.2 Raw map



X Index: 224



Y Index: 224

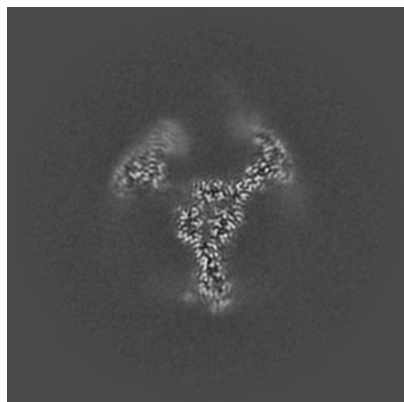


Z Index: 224

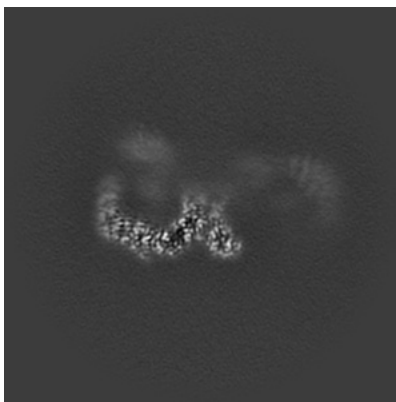
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

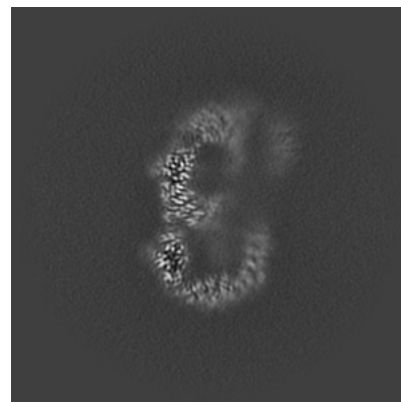
6.3.1 Primary map



X Index: 196

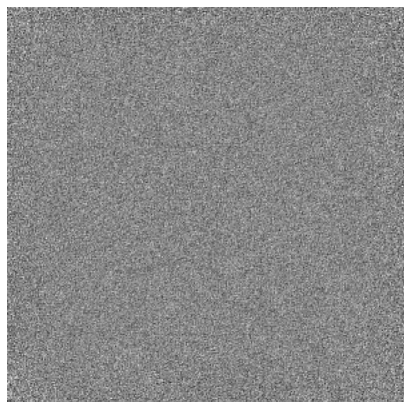


Y Index: 237

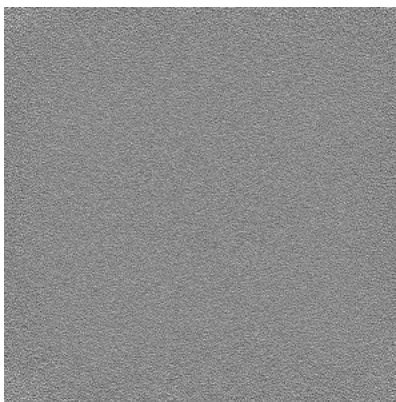


Z Index: 248

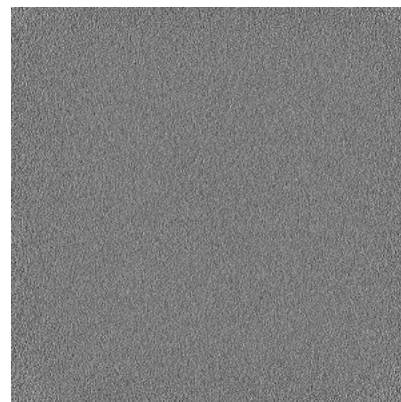
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

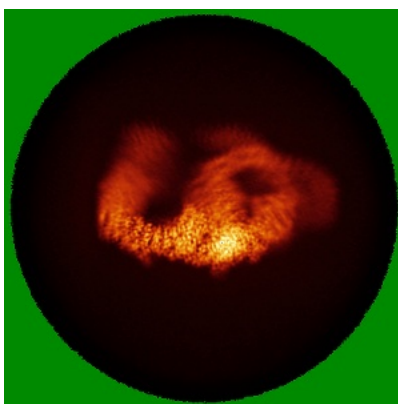
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

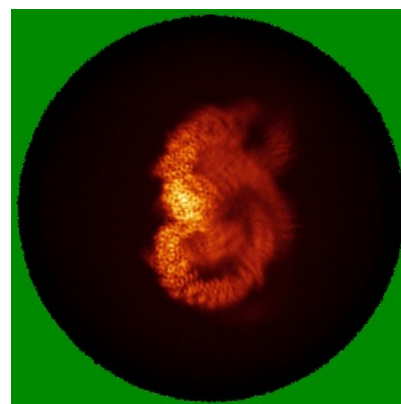
6.4.1 Primary map



X

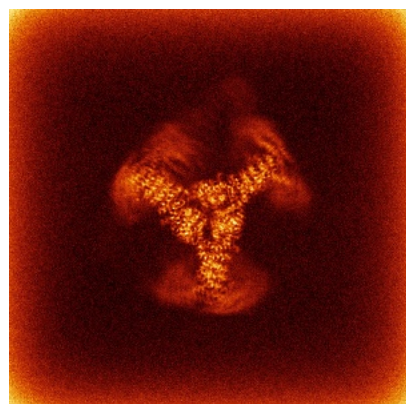


Y

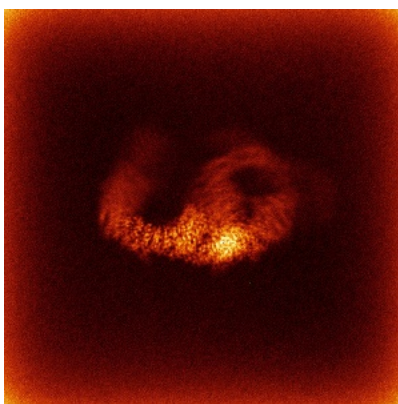


Z

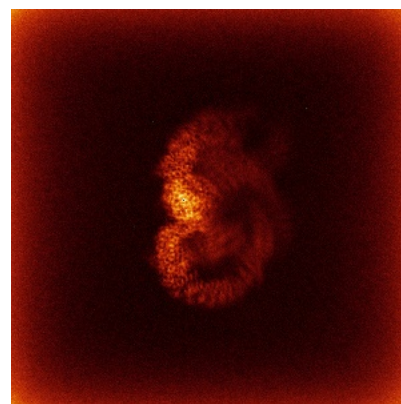
6.4.2 Raw map



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.

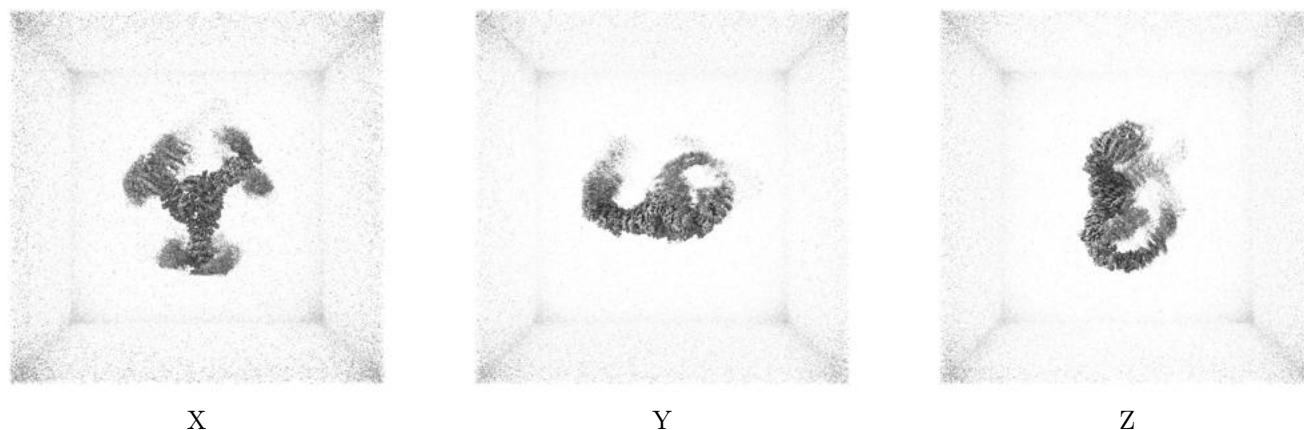
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.221. 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



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.

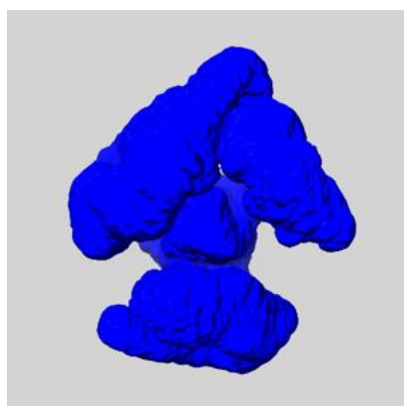
6.6 Mask visualisation [i](#)

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

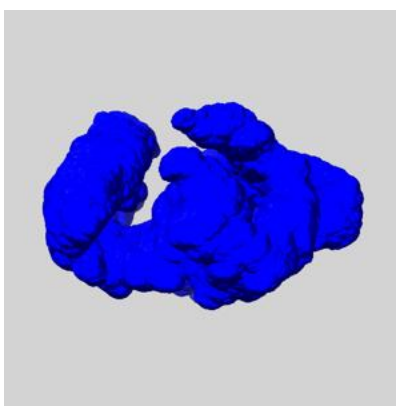
A mask typically either:

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

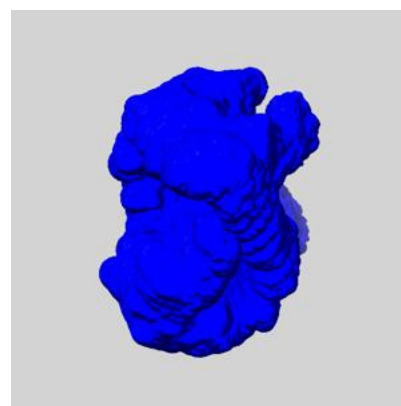
6.6.1 emd_14368_msk_1.map [i](#)



X



Y

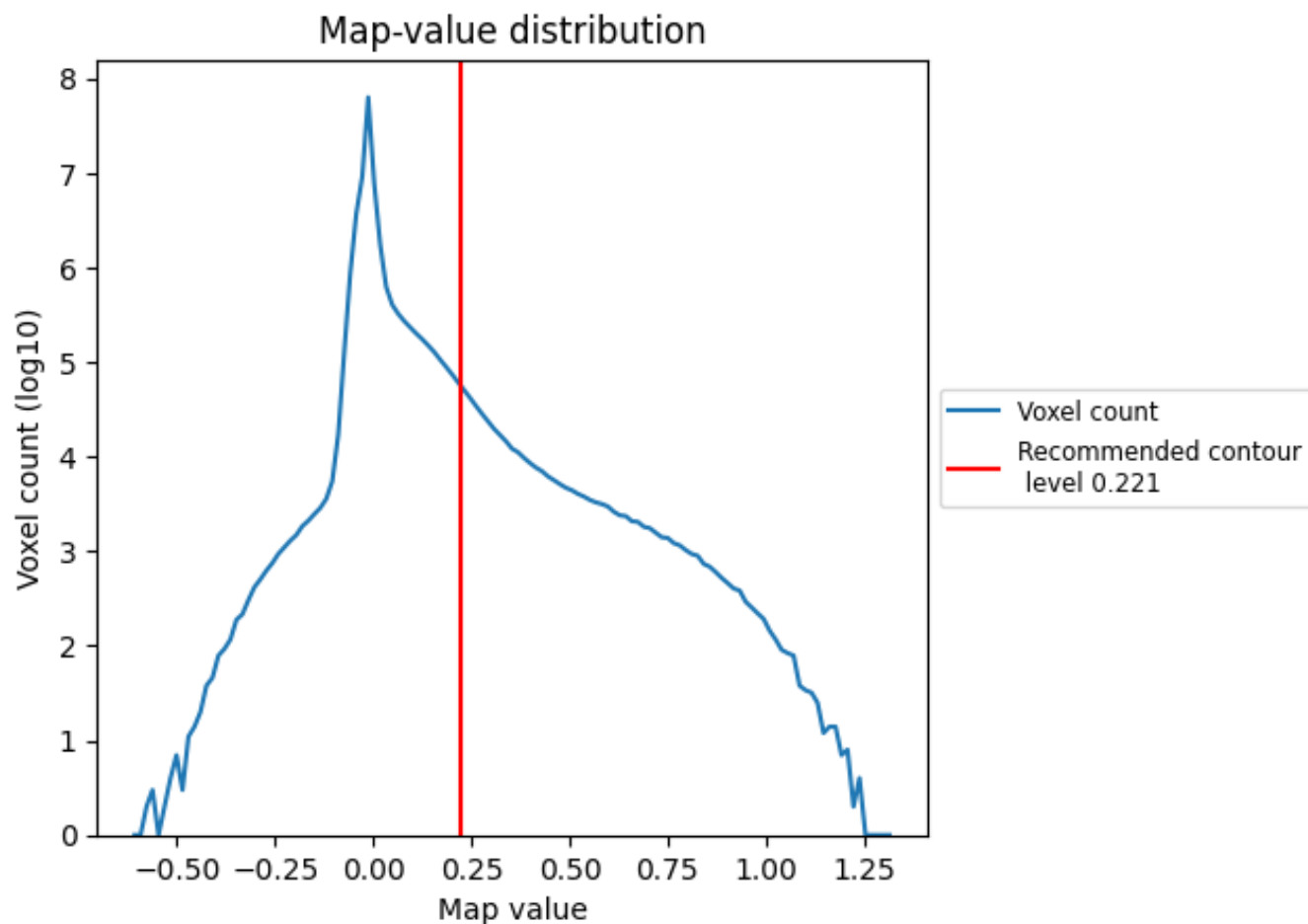


Z

7 Map analysis [i](#)

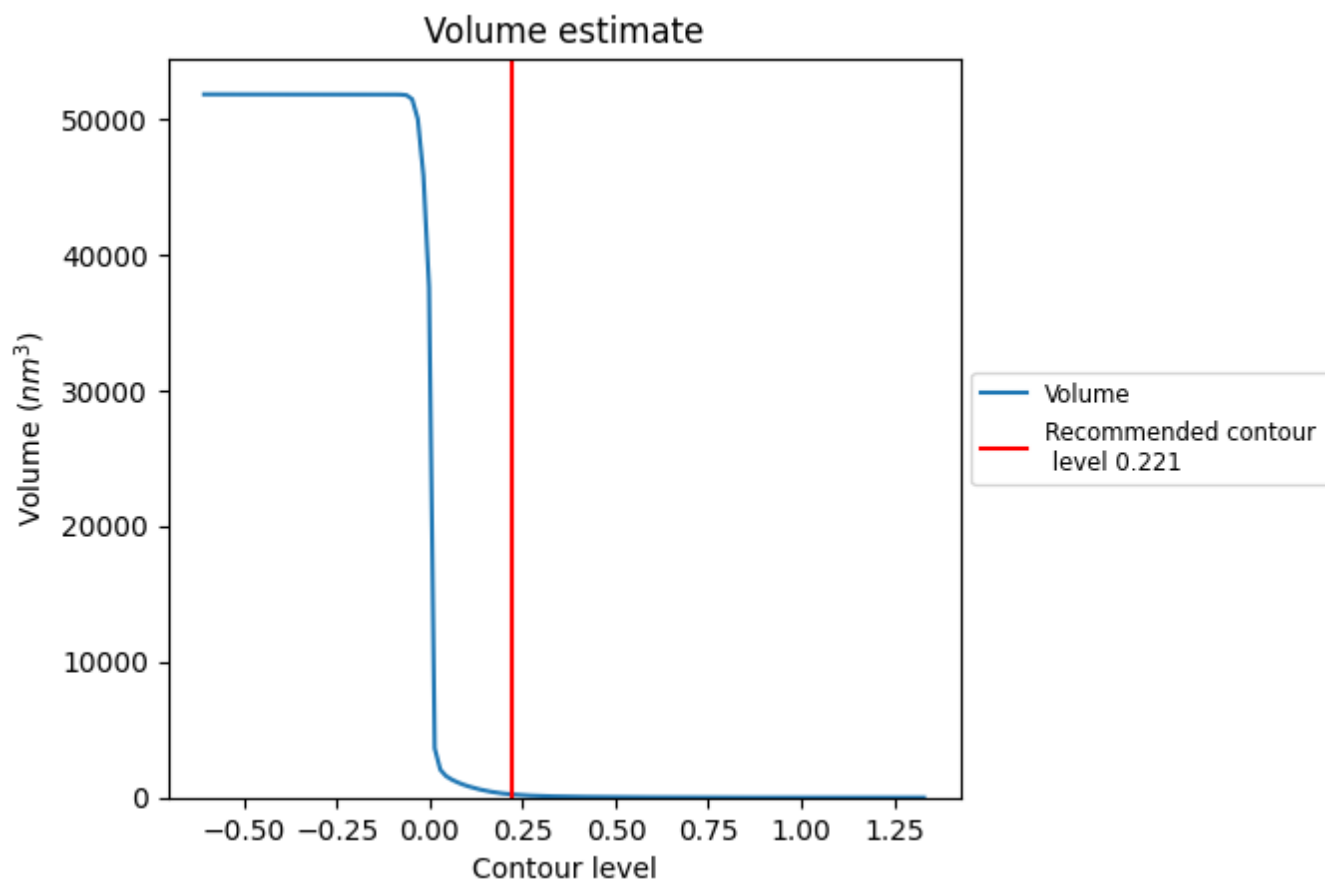
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

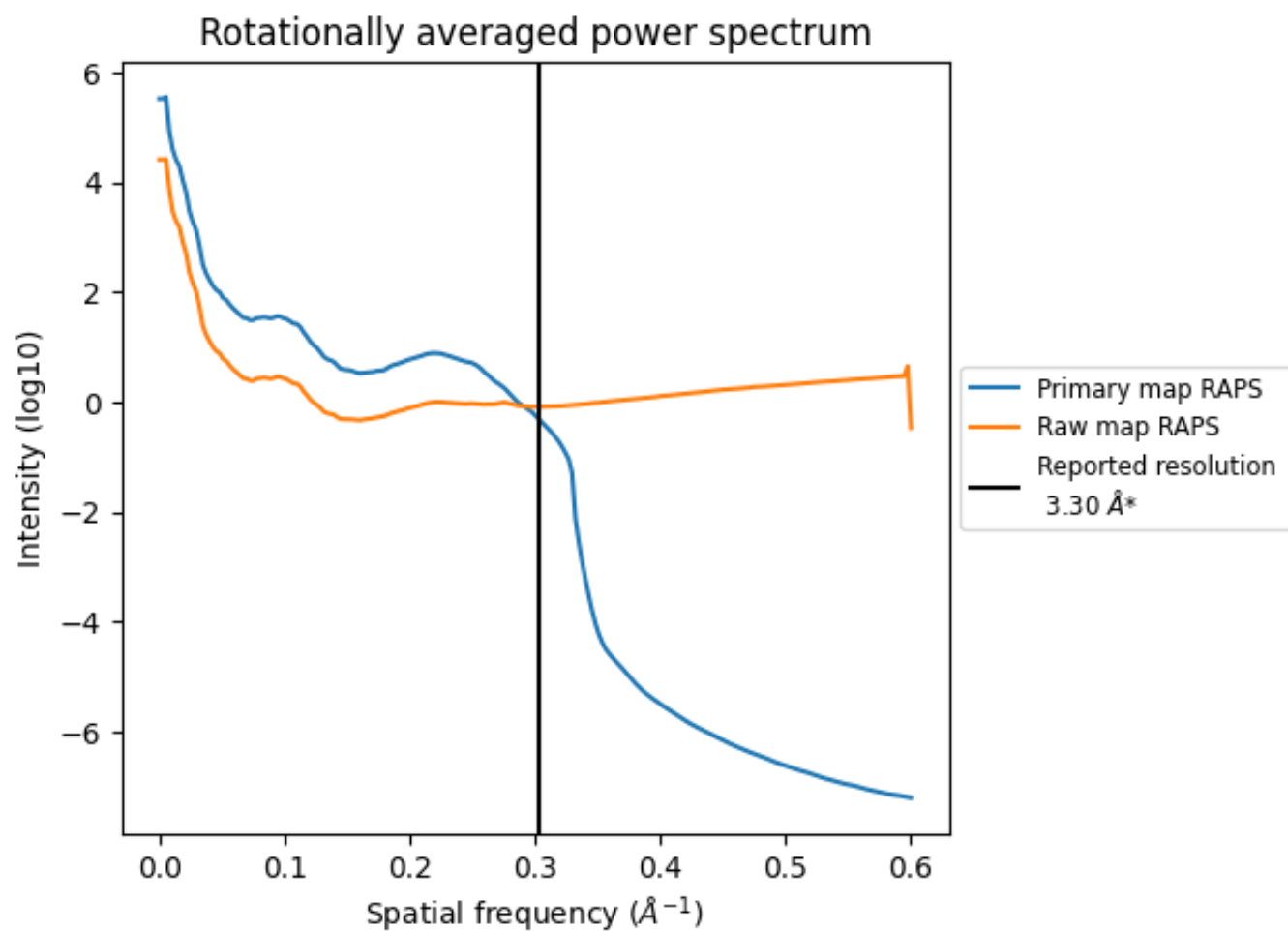
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 235 nm³; this corresponds to an approximate mass of 212 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 ⓘ

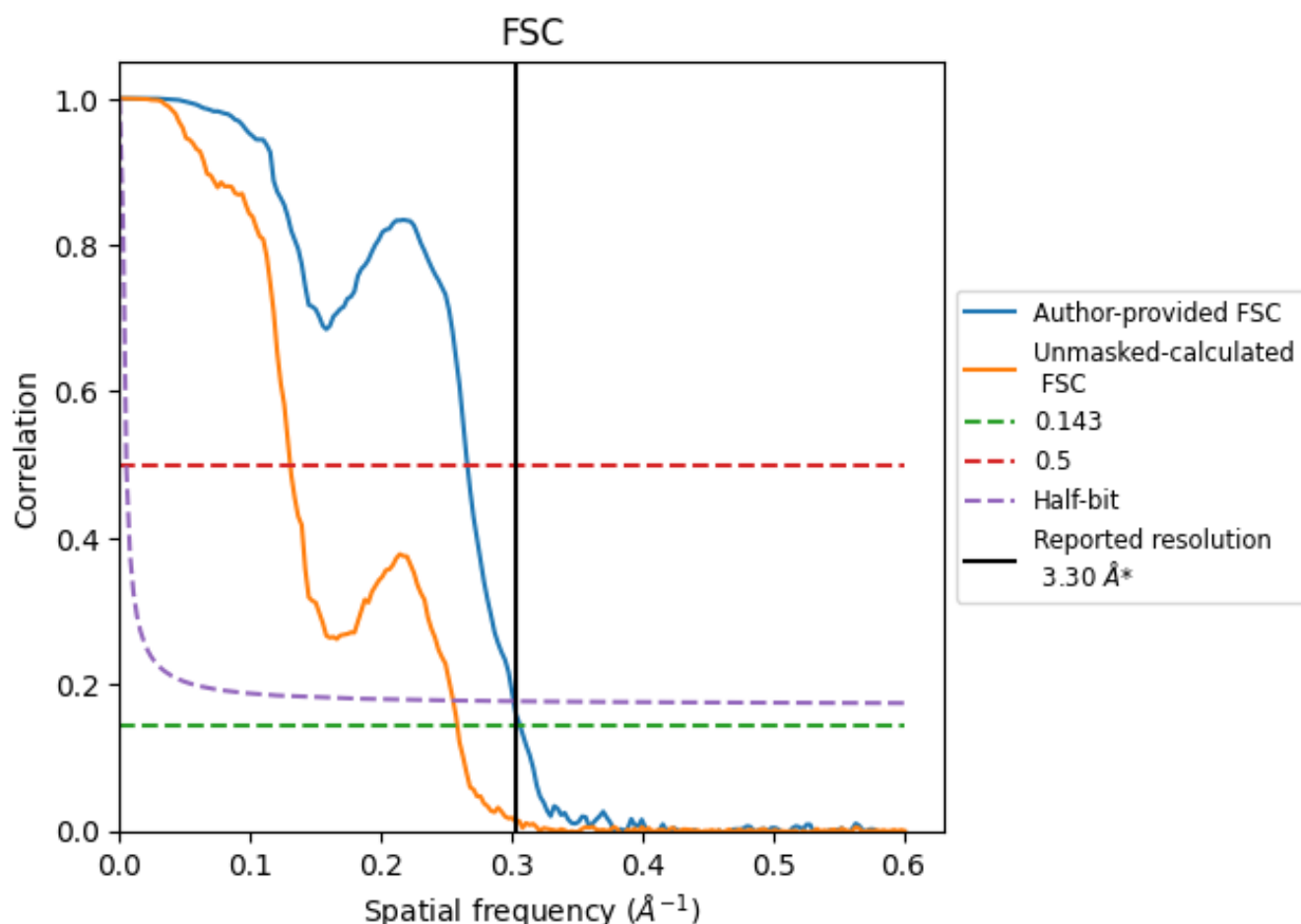


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

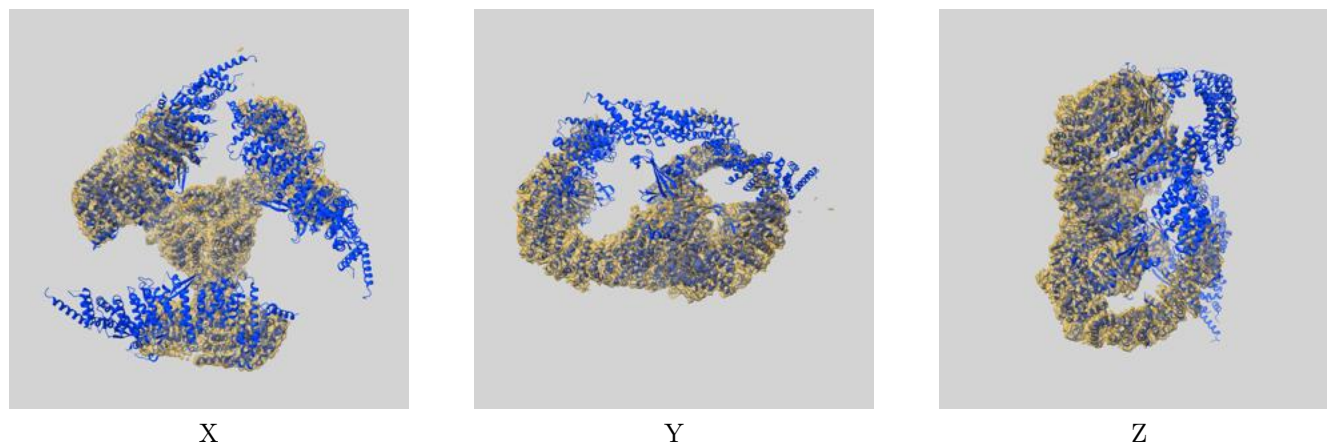
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.76	3.32
Unmasked-calculated*	3.87	7.65	3.92

*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 3.87 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

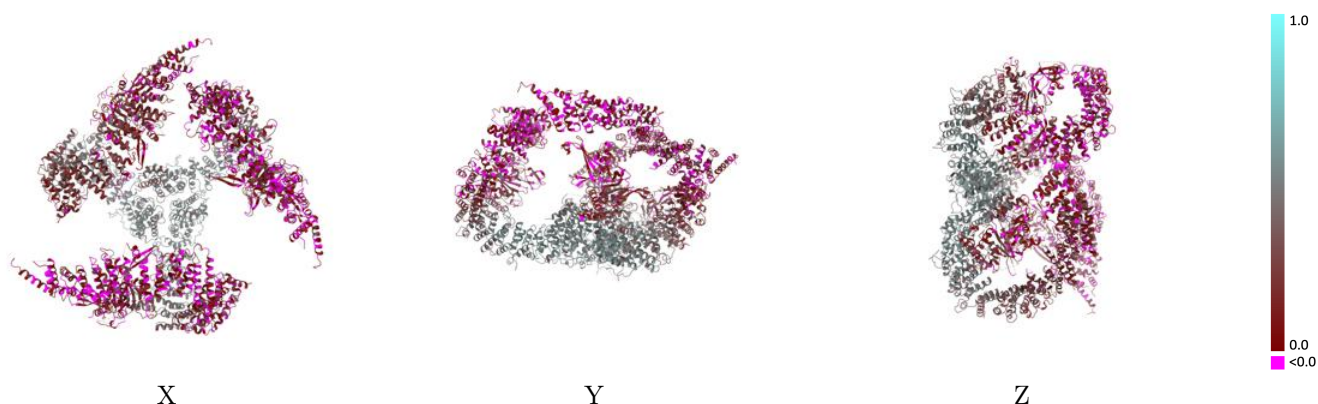
This section contains information regarding the fit between EMDB map EMD-14368 and PDB model 7YXX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



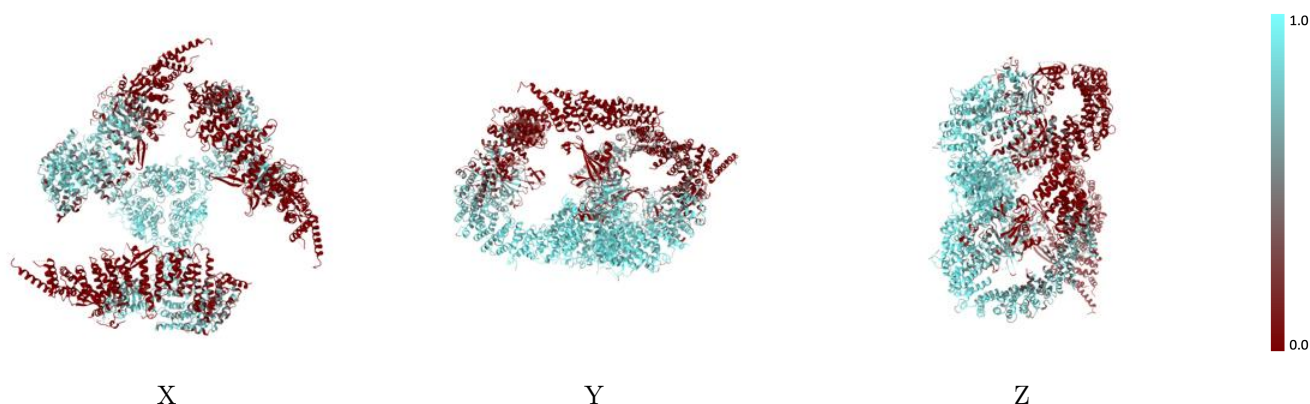
The images above show the 3D surface view of the map at the recommended contour level 0.221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



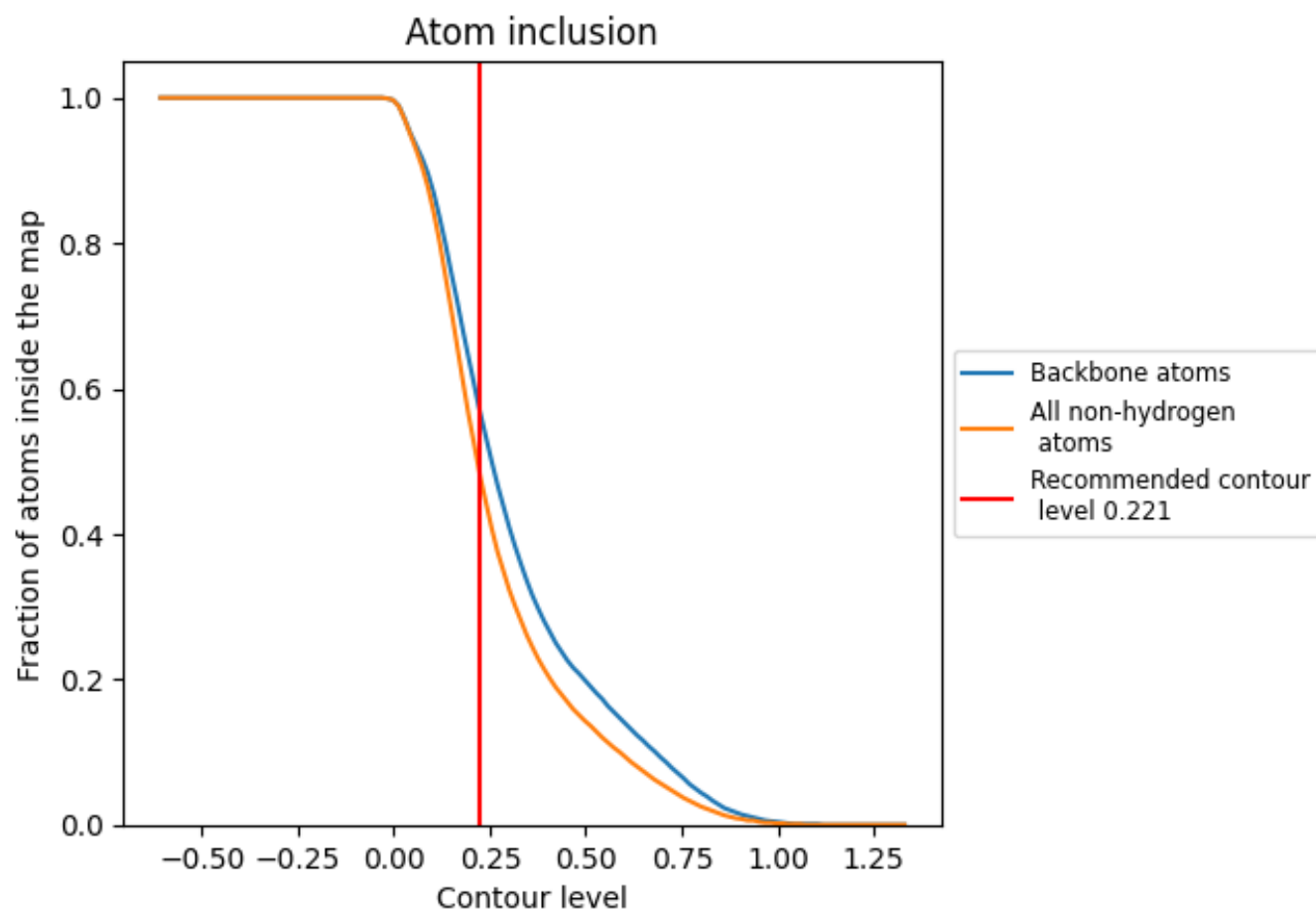
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.221).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4900	<div></div> 0.2580
A	<div></div> 0.5790	<div></div> 0.3010
B	<div></div> 0.4570	<div></div> 0.2330
C	<div></div> 0.4330	<div></div> 0.2400

