



# wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 01:40 AM UTC

PDB ID : 6ROW / pdb\_00006row  
EMDB ID : EMD-4975  
Title : Haemonchus galactose containing glycoprotein complex  
Authors : Scarff, C.A.; Thompson, R.F.; Newlands, G.F.J.; Jamson, H.; Kennaway, C.; da Silva, V.J.; Rabelo, E.M.; Song, C.F.; Trinick, J.; Smith, W.D.; Muench, S.P.  
Deposited on : 2019-05-13  
Resolution : 4.50 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](mailto: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>.

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

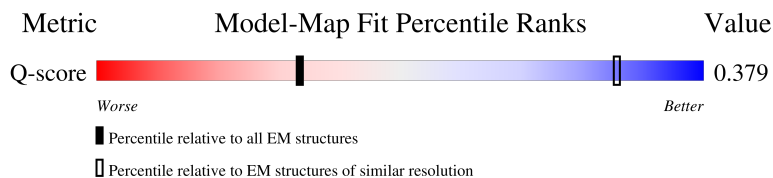
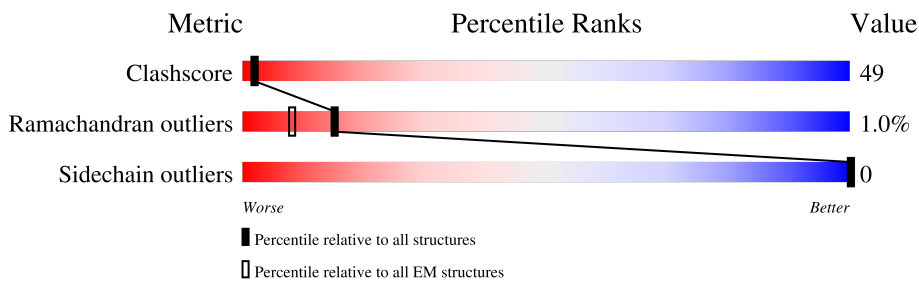
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 ( 4.00 - 5.00 )

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  $\geq 3$ , 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	755	
1	B	755	
1	C	755	
1	D	755	

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Mol	Chain	Length	Quality of chain
2	E	369	 56% 25% 19%
2	F	369	 59% 20% 21%
3	G	253	 63% . . 32%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 43049 atoms, of which 20156 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 Putative zinc metallopeptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	596	9475	3063	4638	824	919	31	0	0
1	B	619	9828	3187	4817	845	946	33	0	0
1	C	583	9290	3010	4556	801	893	30	0	0
1	D	566	8988	2910	4413	777	860	28	0	0

- Molecule 2 is a protein called Parasite pepsinogen.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
2	E	299	2133	860	676	299	298	0	0
2	F	293	2093	844	664	293	292	0	0

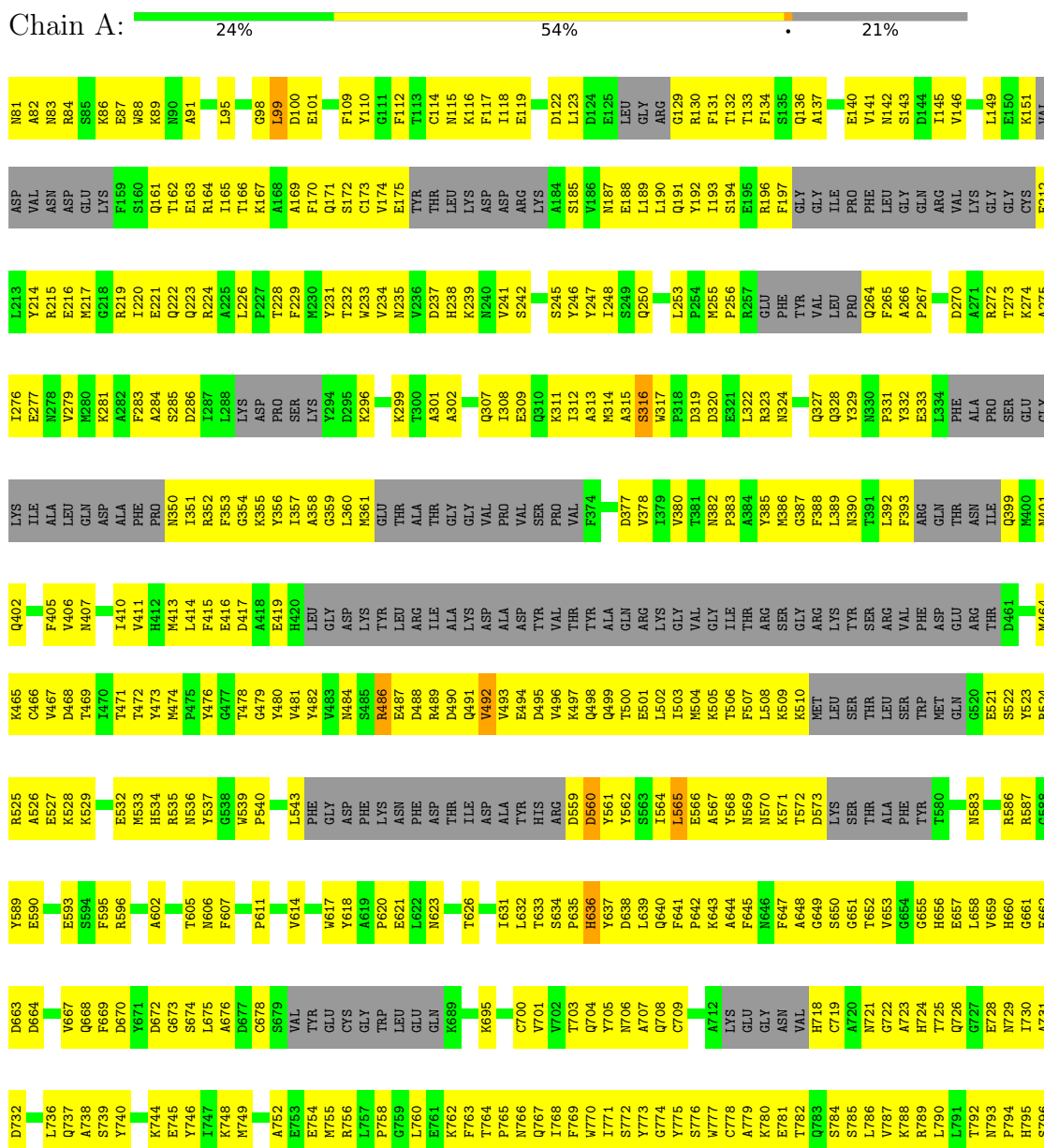
- Molecule 3 is a protein called Cysteine Protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	G	173	1242	504	392	173	173	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: Putative zinc metallopeptidase



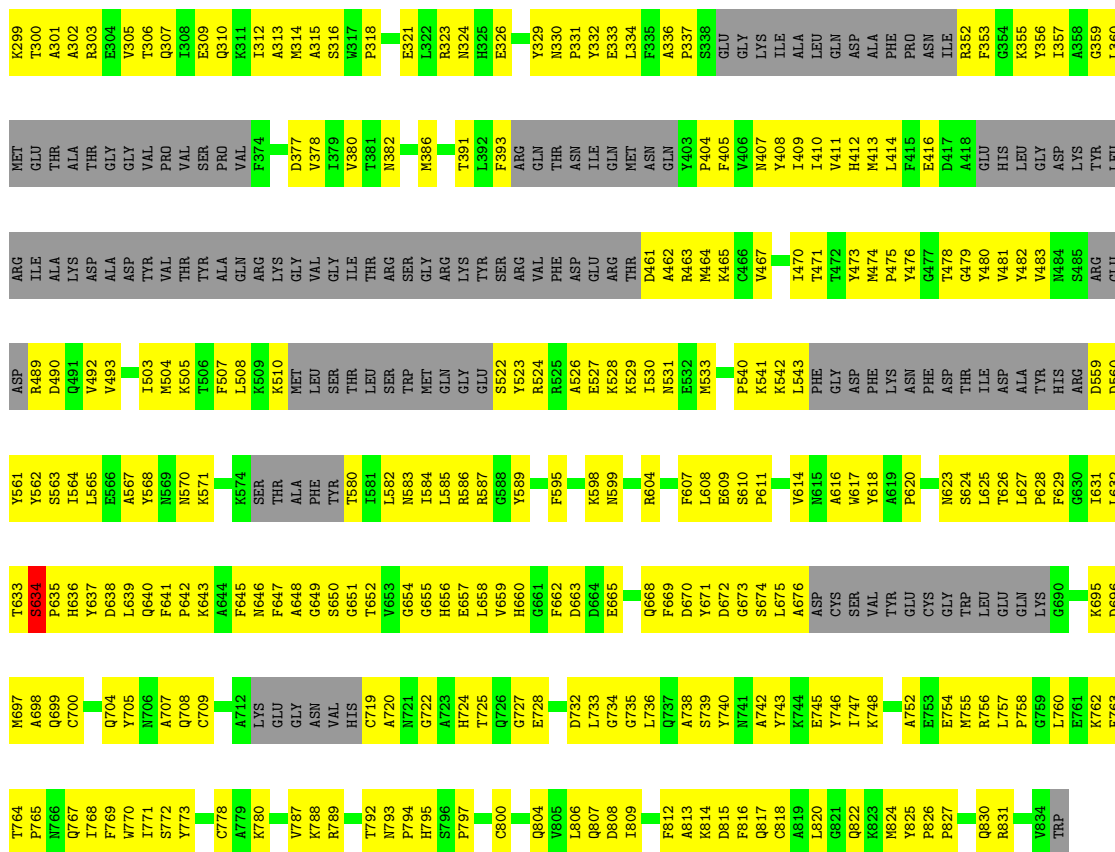


N81	VAL	T273	G340	ASN	ASP	E527	G588	L658	G722	S784	N81	S160	N81
S85	ASP	K274	LYS	GLN	A462	K528	Y689	V659	A723	S785	A82	Q161	S85
K86	VAL	A775	ILE	TYR	R463	K529	E590	H660	H724	L786	N83	T162	K86
E87	ASN	T276	LEU	PRO	M464	E531	N591	G661	T725	L790	S85	E216	E87
W88	ASP	E277	ALA	PHE	V467	E532	E592	D663	Q726	L791	W88	M217	W88
K89	GLU	N278	LEU	VAL	V467	E533	S594	D664	E728	T792	K89	N218	K89
N90	LYS	W279	GLN	M407	V467	E534	F596	E665	N729	N793	N90	R219	N90
A91	PHE	M280	ASP	Y408	V467	E535	H534	E666	N730	H795	A91	I220	A91
A92	S160	A284	PHE	Y410	V467	E536	H535	E667	A731	H795	A92	Q222	A92
N93	Q161	R289	ALA	V411	V467	E537	H536	E668	D732	N799	N93	Q223	N93
T94	T162	PRO	ASN	M412	V467	E538	H537	E669	L733	N799	T94	Q224	T94
L95	E163	ASP	ILE	M413	V467	E539	H538	E670	L733	N799	L95	R224	L95
L96	R164	PRO	ARG	L414	V467	E540	H539	E671	L733	N799	L96	A225	L96
F97	I166	SER	ARG	L414	V467	E541	H540	E672	L733	N799	F97	A226	F97
G98	K167	LYS	P353	F415	G477	K541	F607	E673	Q737	R800	G98	T227	G98
L99	T228	GLY	G354	E416	G477	K542	L608	E674	A738	R801	L99	T228	L99
D100	K168	LYS	K355	F417	G477	K543	L609	E675	A739	R802	D100	T229	D100
E101	A169	M230	Y356	D417	G477	K544	L610	E676	S739	R803	E101	F229	E101
S102	F170	Y231	L357	GLU	V481	G545	S610	E677	Y740	R804	S102	M230	S102
V103	Q171	M232	G358	HIS	V482	G546	P611	E678	N741	R805	V103	Y231	V103
D104	S172	W233	ASP	LEU	V483	G547	A612	E679	A742	R806	D104	W233	D104
P105	C173	V234	LEU	LEU	V484	G548	V614	E680	Y743	R807	P105	V234	P105
C106	V174	M235	GLY	GLY	V485	G549	V615	E681	K744	R808	C106	M235	C106
E107	E175	V236	LYS	LYS	V486	G550	W617	E682	E745	R809	E107	V236	E107
D108	Y176	D237	ALA	TYR	E487	G551	A619	E683	I747	R810	D108	D237	D108
F109	T177	H238	THR	LEU	V488	G552	A620	E684	LYS	R811	F109	H238	F109
Y110	K179	K239	GLY	ARG	V489	G553	A621	E685	MET	R812	Y110	K239	Y110
G111	L179	E240	GLY	ILE	V490	G554	E621	E686	LYS	R813	G111	E240	G111
G112	L189	M241	VAL	ALA	V491	G555	N623	E687	GLY	R814	G112	M241	G112
G113	L190	Q242	ALA	ALA	V492	G556	N624	E688	ALA	R815	G113	Q242	G113
Q191	Q191	T251	GLN	ASP	D493	G557	S624	E689	GLU	R816	Q191	T251	Q191
Y192	Y192	T252	ASP	ASP	D494	G558	L625	E690	GLU	R817	Y192	T252	Y192
ARG	ARG	L253	PRO	ALA	D495	G559	L626	E691	GLU	R818	ARG	L253	ARG
ARG	ARG	P254	VAL	VAL	D496	G560	L627	E692	GLU	R819	ARG	P254	ARG
F131	E195	M255	GLY	GLY	D497	G561	L628	E693	GLY	R820	F131	M255	F131
T132	R196	P256	THR	ILE	D498	G562	L629	E694	THR	R821	T132	P256	T132
T133	F197	R257	THR	ILE	D499	G563	L630	E695	THR	R822	T133	R257	T133
F134	G198	E258	THR	THR	T500	G564	L631	E696	GLY	R823	F134	E258	F134
G198	G198	F259	THR	THR	E501	G565	L632	E697	ILE	R824	G198	F259	G198
Q136	G199	F260	THR	THR	E502	G566	L633	E698	LEU	R825	Q136	F260	Q136
I200	I200	Y261	SER	GLN	E503	G567	L634	E699	THR	R826	I200	Y261	I200
P201	P201	W261	LEU	GLY	E504	G568	L635	E700	THR	R827	P201	W261	P201
F202	F202	L262	ASN	ARG	E505	G569	L636	E701	THR	R828	F202	L262	F202
L263	L263	P263	THR	LYS	E506	G570	L637	E702	THR	R829	L263	P263	L263
GLY	GLY	Q264	THR	TYR	E507	G571	L638	E703	THR	R830	GLY	Q264	GLY
GLN	GLN	F265	LEU	TYR	E508	G572	L639	E704	THR	R831	GLN	F265	GLN
ARG	ARG	A266	SER	SER	E509	G573	L640	E705	THR	R832	ARG	A266	ARG
VAL	VAL	P267	VAL	VAL	E510	G574	L641	E706	THR	R833	VAL	P267	VAL
LYS	LYS	E268	THR	THR	E511	G575	L642	E707	THR	R834	LYS	E268	LYS
LYS	LYS	L269	ASN	ASN	E512	G576	L643	E708	THR	R835	LYS	L269	LYS
GLY	GLY	D270	ASN	THR	E513	G577	L644	E709	THR	R836	GLY	D270	GLY
CYS	CYS	A271	ILE	THR	E514	G578	L645	E710	THR	R837	CYS	A271	CYS
GLU	GLU	R272	ILE	THR	E515	G579	L646	E711	THR	R838	GLU	R272	GLU
GLU	GLU	R273	MET	THR	E516	G580	L647	E712	THR	R839	GLU	R273	GLU
GLY	GLY	T274	THR	THR	E517	G581	L648	E713	THR	R840	GLY	T274	GLY
ILE	ILE	I275	THR	THR	E518	G582	L649	E714	THR	R841	ILE	I275	ILE
PRO	PRO	E276	THR	THR	E519	G583	L650	E715	THR	R842	PRO	E276	PRO
ASP	ASP	R277	THR	THR	E520	G584	L651	E716	THR	R843	ASP	R277	ASP
GLY	GLY	T278	THR	THR	E521	G585	L652	E717	THR	R844	GLY	T278	GLY
GLY	GLY	W279	THR	THR	E522	G586	L653	E718	THR	R845	GLY	W279	GLY
M280	M280	R280	THR	THR	E523	G587	L654	E719	THR	R846	M280	R280	M280
F283	F283	E281	THR	THR	E524	G588	L655	E720	THR	R847	F283	E281	F283
A284	A284	R282	THR	THR	E525	G589	L656	E721	THR	R848	A284	R282	A284
SER	SER	D283	THR	THR	E526	G590	L657	E722	THR	R849	SER	D283	SER
ASP	ASP	T284	THR	THR	E527	G591	L658	E723	THR	R850	ASP	T284	ASP
ILE	ILE	W285	THR	THR	E528	G592	L659	E724	THR	R851	ILE	W285	ILE
LYS	LYS	R286	THR	THR	E529	G593	L660	E725	THR	R852	LYS	R286	LYS
ASP	ASP	D287	THR	THR	E530	G594	L661	E726	THR	R853	ASP	D287	ASP
LEU	LEU	I288	THR	THR	E531	G595	L662	E727	THR	R854	LEU	I288	LEU
LYS	LYS	E289	THR	THR	E532	G596	L663	E728	THR	R855	LYS	E289	LYS
ASP	ASP	R290	THR	THR	E533	G597	L664	E729	THR	R856	ASP	R290	ASP
GLY	GLY	W291	THR	THR	E534	G598	L665	E730	THR	R857	GLY	W291	GLY
GLY	GLY	I292	THR	THR	E535	G599	L666	E731	THR	R858	GLY	I292	GLY
CYS	CYS	A293	THR	THR	E536	G600	L667	E732	THR	R859	CYS	A293	CYS
GLU	GLU	R294	THR	THR	E537	G601	L668	E733	THR	R860	GLU	R294	GLU
GLY	GLY	E295	THR	THR	E538	G602	L669	E734	THR	R861	GLY	E295	GLY
GLY	GLY	W296	THR	THR	E539	G603	L670	E735	THR	R862	GLY	W296	GLY
GLY	GLY	I297	THR	THR	E540	G604	L671	E736	THR	R863	GLY	I297	GLY
GLY	GLY	R298	THR	THR	E541	G605	L672	E737	THR	R864	GLY	R298	GLY
CYS	CYS	E299	THR	THR	E542	G606	L673	E738	THR	R865	CYS	E299	CYS
GLU	GLU	W299	THR	THR	E543	G607	L674	E739	THR	R866	GLU	W299	GLU
GLU	GLU	I299	THR	THR	E544	G608	L675	E740	THR	R867	GLU	I299	GLU

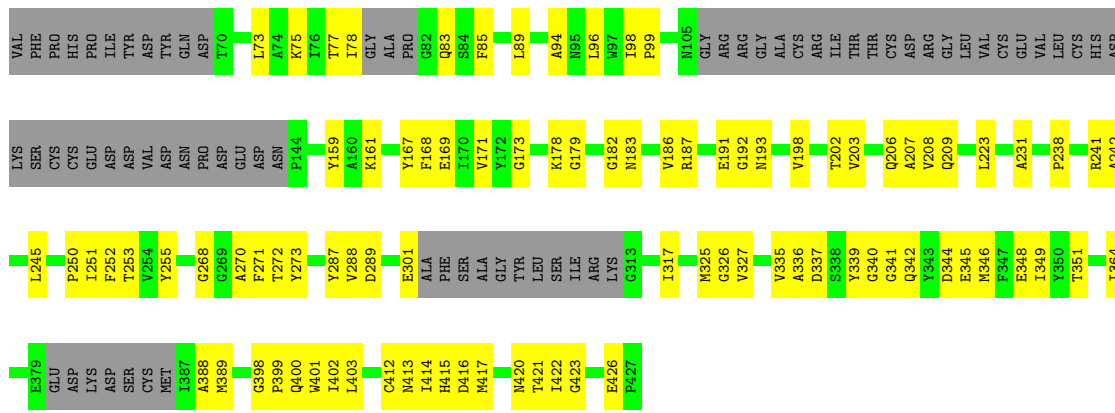
• Molecule 1: Putative zinc metallopeptidase



N81	S160	Q223	N81	S160	Q223	N81	S160	Q223	N81	S160	Q223	N81	S160	Q223
A82	Q161	R224	A82	Q161	R224	A82	Q161	R224	A82	Q161	R224	A82	Q161	R224
N83	T162	A225	N83	T162	A225	N83	T162	A225	N83	T162	A225	N83	T162	A225
R84	E163	L226	R84	E163	L226	R84	E163	L226	R84	E163	L226	R84	E163	L226
S85	R164	P227	S85	R164	P227	S85	R164	P227	S85	R164	P227	S85	R164	P227
W88	I165	T228	W88	I165	T228	W88	I165	T228	W88	I165	T228	W88	I165	T228
F97	T166	F229	F97	T166	F229	F97	T166	F229	F97	T166	F229	F97	T166	F229
G98	K167	M230	G98	K167	M230	G98	K167	M230	G98	K167	M230	G98	K167	M230
L99	Q171	T232	L99	Q171	T232	L99	Q171	T232	L99	Q171	T232	L99	Q171	T232
D100	C173	V236	D100	C173	V236	D100	C173	V236	D100	C173	V236	D100	C173	V236
E101	P174	D237	E101	P174	D237	E101	P174	D237	E101	P174	D237	E101	P174	D237
F109	E175	H238	F109	E175	H238	F109	E175	H238	F109	E175	H238	F109	E175	H238
G111	VAL	V241	G111	VAL	V241	G111	VAL	V241	G111	VAL	V241	G111	VAL	V241
G112	LEU	Y246	G112	LEU	Y246	G112	LEU	Y246	G112	LEU	Y246	G112	LEU	Y246
G113	ASP	Y247	G113	ASP	Y247	G113	ASP	Y247	G113	ASP	Y247	G113	ASP	Y247
G114	ASP	Q250	G114	ASP	Q250	G114	ASP	Q250	G114	ASP	Q250	G114	ASP	Q250
N115	ARG	E258	N115	ARG	E258	N115	ARG	E258	N115	ARG	E258	N115	ARG	E258
D122	ALA	V261	D122	ALA	V261	D122	ALA	V261	D122	ALA	V261	D122	ALA	V261
LEU	LEU	L262	LEU	LEU	L262	LEU	LEU	L262	LEU	LEU	L262	LEU	LEU	L262
ASP	ASP	P263	ASP	ASP	P263	ASP	ASP	P263	ASP	ASP	P263	ASP	ASP	P263
GLU	GLU	F265	GLU	GLU	F265	GLU	GLU	F265	GLU	GLU	F265	GLU	GLU	F265
GLY	GLY	A266	GLY	GLY	A266	GLY	GLY	A266	GLY	GLY	A266	GLY	GLY	A266
GLY	GLY	P267	GLY	GLY	P267	GLY	GLY	P267	GLY	GLY	P267	GLY	GLY	P267



• Molecule 2: Parasite pepsinogen

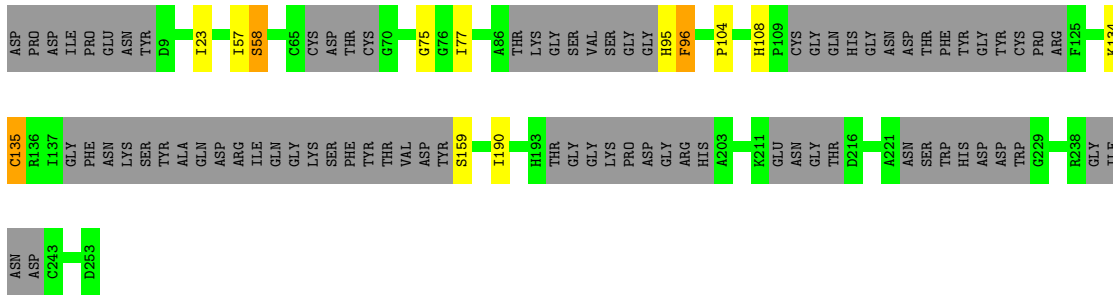


• Molecule 2: Parasite pepsinogen





● Molecule 3: Cysteine Protease



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110863	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 ( $e^-/\text{\AA}^2$ )	62.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	387.66003, 387.66003, 387.66003	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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	0.88	0/4938	0.97	10/6653 (0.2%)
1	B	0.88	4/5122 (0.1%)	0.98	10/6903 (0.1%)
1	C	0.81	1/4835 (0.0%)	0.90	7/6513 (0.1%)
1	D	0.82	0/4674	1.04	11/6304 (0.2%)
2	E	0.31	0/1452	0.56	0/2003
2	F	0.47	0/1424	0.71	0/1965
3	G	1.20	0/841	1.88	9/1154 (0.8%)
All	All	0.82	5/23286 (0.0%)	0.99	47/31495 (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
1	A	0	5
1	B	0	4
1	C	0	6
1	D	0	1
All	All	0	16

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	PRO	N-CD	-13.90	1.28	1.47
1	C	816	PHE	CA-CB	-9.87	1.36	1.52
1	B	115	ASN	C-O	-9.64	1.12	1.24
1	B	540	PRO	N-CD	8.89	1.60	1.47
1	B	314	MET	CA-C	-6.36	1.38	1.52

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	96	PHE	N-CA-C	-11.46	93.68	110.64
3	G	58	SER	N-CA-C	-10.97	93.84	110.30
3	G	96	PHE	CB-CA-C	9.85	121.91	109.80
3	G	135	CYS	N-CA-C	-9.62	96.38	110.42
1	B	262	LEU	N-CA-C	9.37	130.52	109.81

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	VAL	Peptide
1	A	486	ARG	Peptide
1	A	560	ASP	Peptide
1	A	676	ALA	Peptide
1	A	826	PRO	Peptide

## 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	4837	4638	4636	544	0
1	B	5011	4817	4815	581	0
1	C	4734	4556	4555	507	0
1	D	4575	4413	4413	404	0
2	E	1457	676	676	63	0
2	F	1429	664	663	42	0
3	G	850	392	389	3	0
All	All	22893	20156	20147	2127	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 49.

The worst 5 of 2127 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:B:540:PRO:HA	1:B:607:PHE:CZ	1.47	1.48

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HD3	1:A:329:TYR:CE2	1.64	1.33
1:A:234:VAL:HG23	1:A:245:SER:O	1.20	1.29
1:D:760:LEU:HD11	1:D:763:PHE:CE2	1.67	1.29
1:A:474:MET:CE	1:A:586:ARG:HD2	1.64	1.27

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	564/755 (75%)	375 (66%)	188 (33%)	1 (0%)	43	77
1	B	589/755 (78%)	385 (65%)	196 (33%)	8 (1%)	9	39
1	C	551/755 (73%)	364 (66%)	181 (33%)	6 (1%)	11	45
1	D	536/755 (71%)	378 (70%)	153 (28%)	5 (1%)	14	49
2	E	289/369 (78%)	217 (75%)	72 (25%)	0	100	100
2	F	283/369 (77%)	198 (70%)	81 (29%)	4 (1%)	9	39
3	G	155/253 (61%)	121 (78%)	29 (19%)	5 (3%)	3	21
All	All	2967/4011 (74%)	2038 (69%)	900 (30%)	29 (1%)	15	47

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	817	GLN
1	C	820	LEU
2	F	168	PHE
3	G	104	PRO
1	C	107	GLU

### 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	521/655 (80%)	521 (100%)	0	100	100
1	B	538/655 (82%)	538 (100%)	0	100	100
1	C	510/655 (78%)	510 (100%)	0	100	100
1	D	492/655 (75%)	492 (100%)	0	100	100
All	All	2061/2620 (79%)	2061 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	536	ASN
1	C	793	ASN
1	C	783	GLN
1	C	795	HIS
1	A	804	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

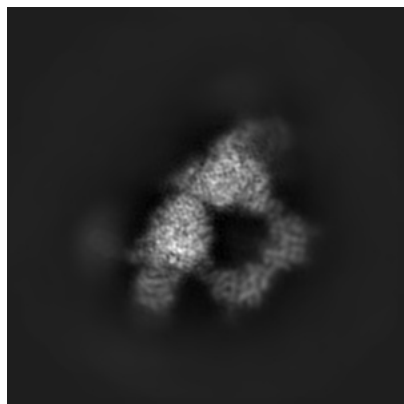
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4975. These allow visual inspection of the internal detail of the map and identification of artifacts.

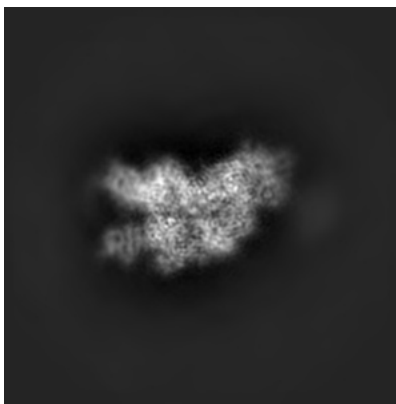
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

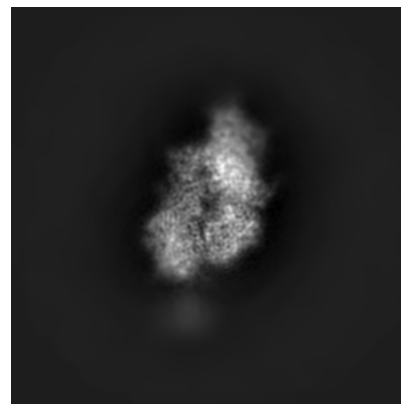
#### 6.1.1 Primary map



X

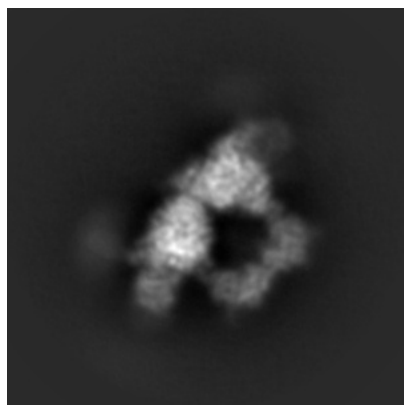


Y

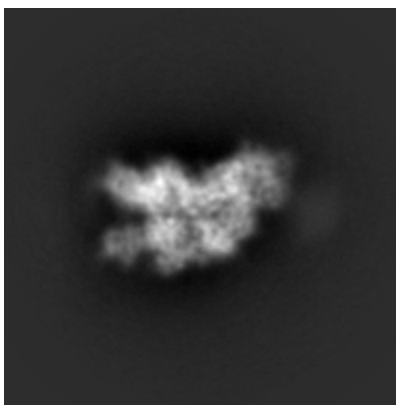


Z

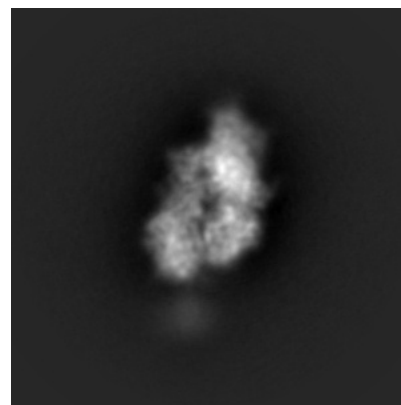
#### 6.1.2 Raw map



X



Y

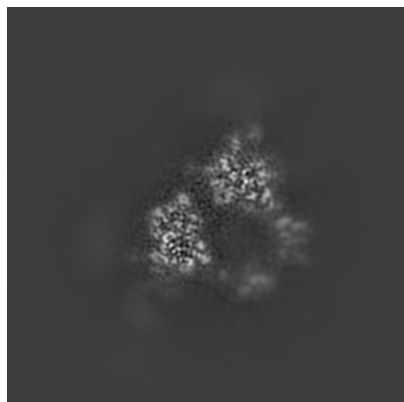


Z

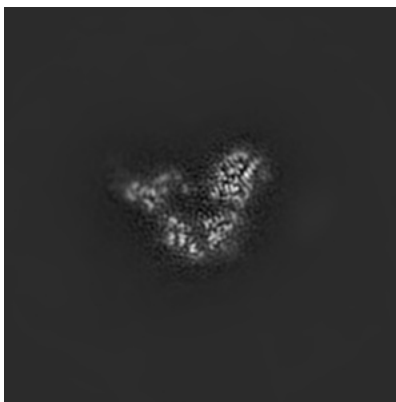
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

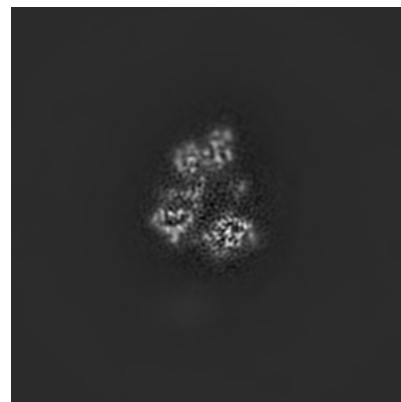
### 6.2.1 Primary map



X Index: 182

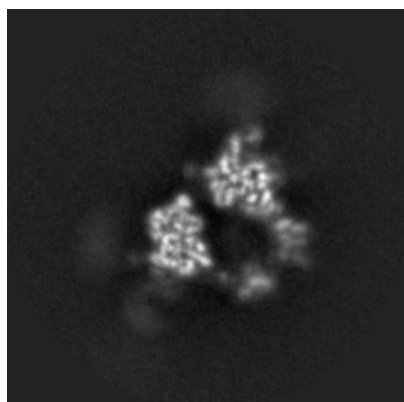


Y Index: 182

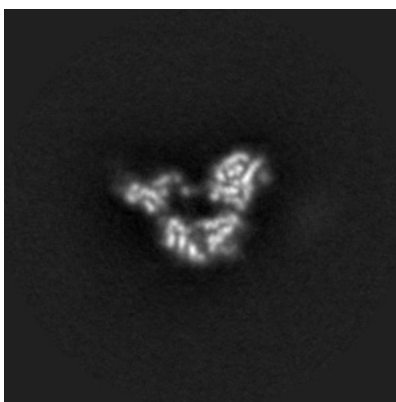


Z Index: 182

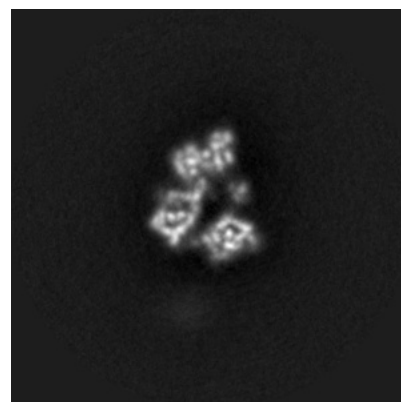
### 6.2.2 Raw map



X Index: 182



Y Index: 182

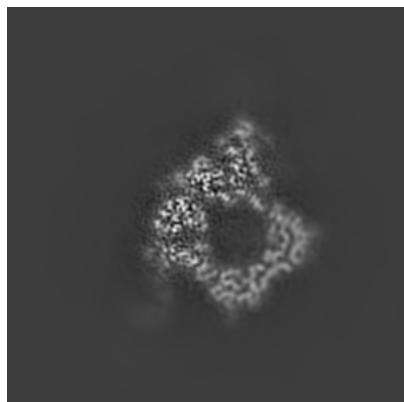


Z Index: 182

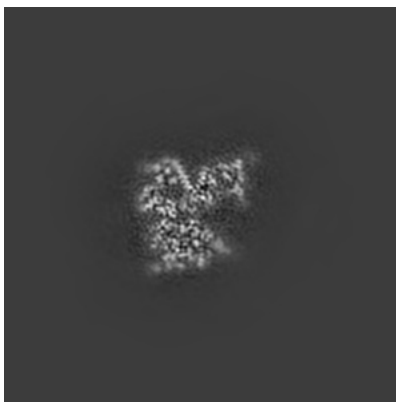
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

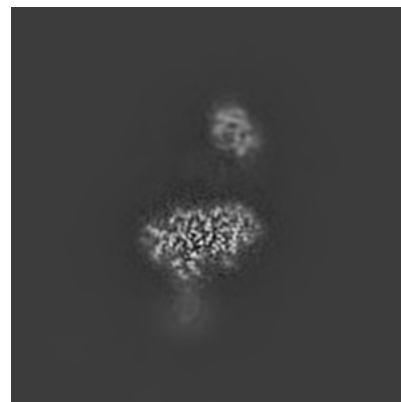
### 6.3.1 Primary map



X Index: 199

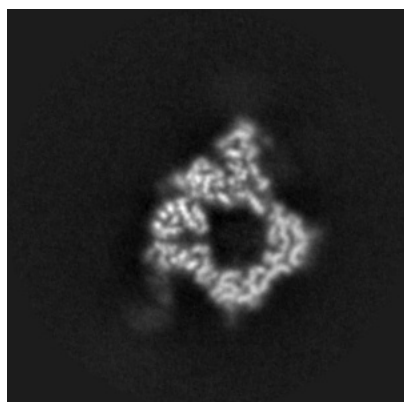


Y Index: 166

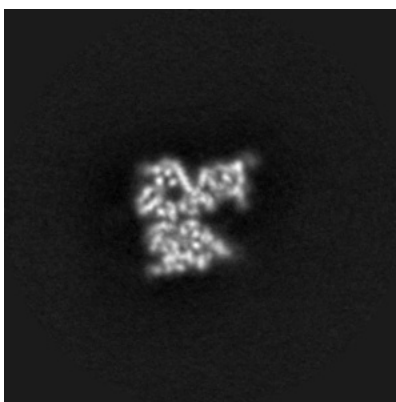


Z Index: 143

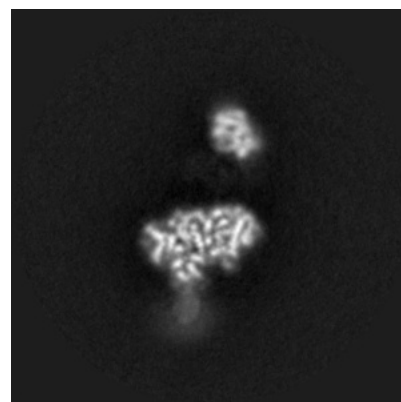
### 6.3.2 Raw map



X Index: 198



Y Index: 166

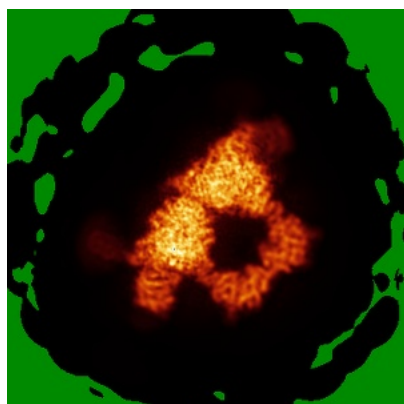


Z Index: 142

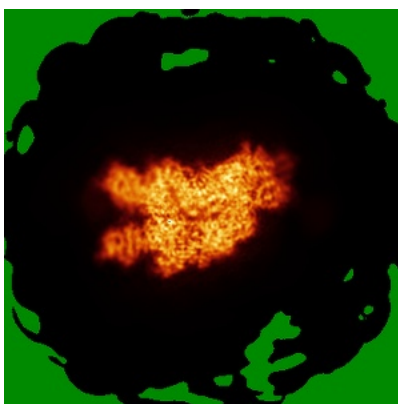
The images above show the largest variance slices of the map in three orthogonal directions.

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

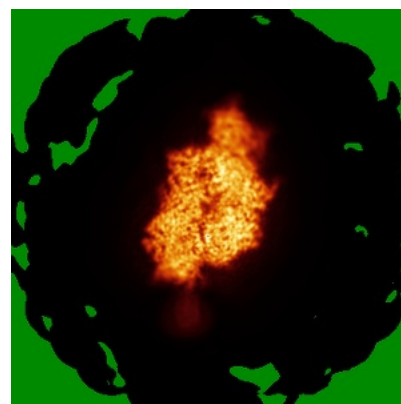
### 6.4.1 Primary map



X



Y

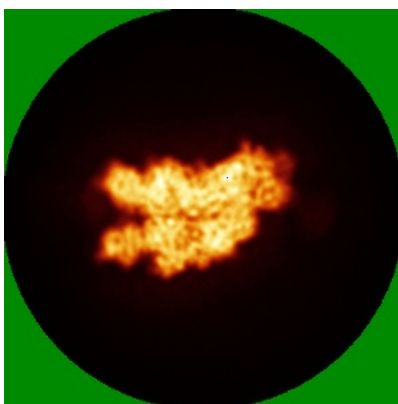


Z

### 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.

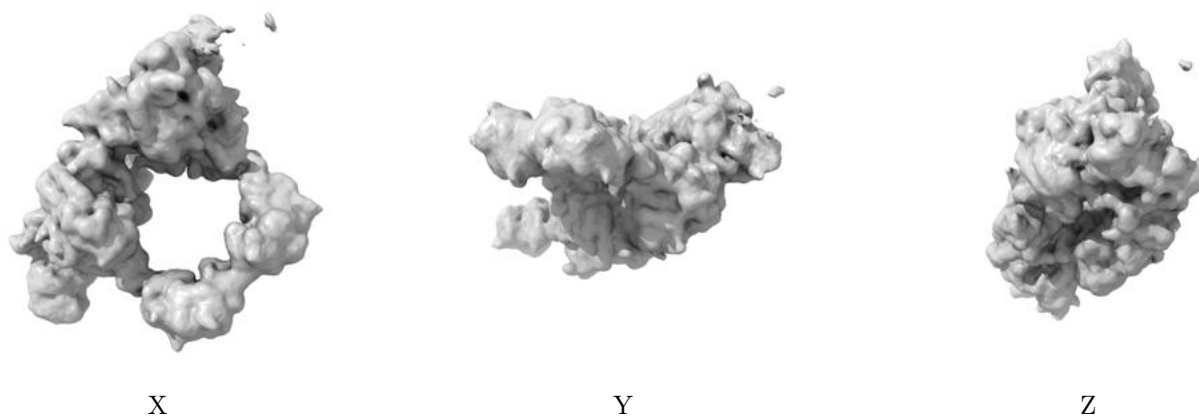
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

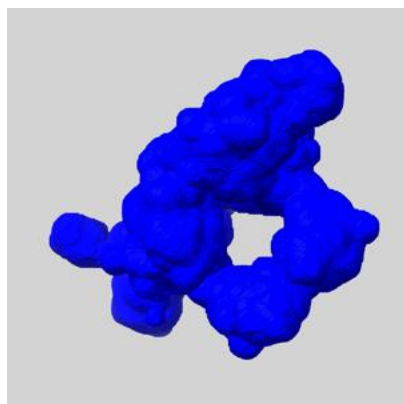
## 6.6 Mask visualisation [i](#)

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

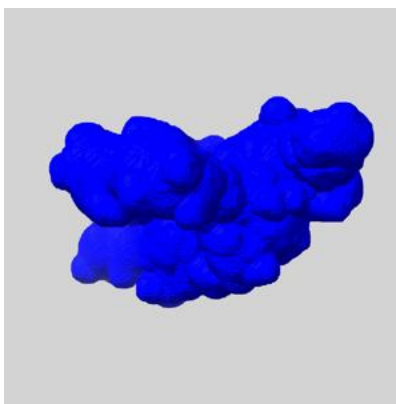
A mask typically either:

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

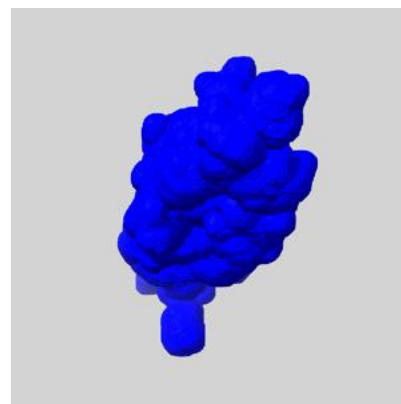
### 6.6.1 emd\_4975\_msk\_1.map [i](#)



X



Y

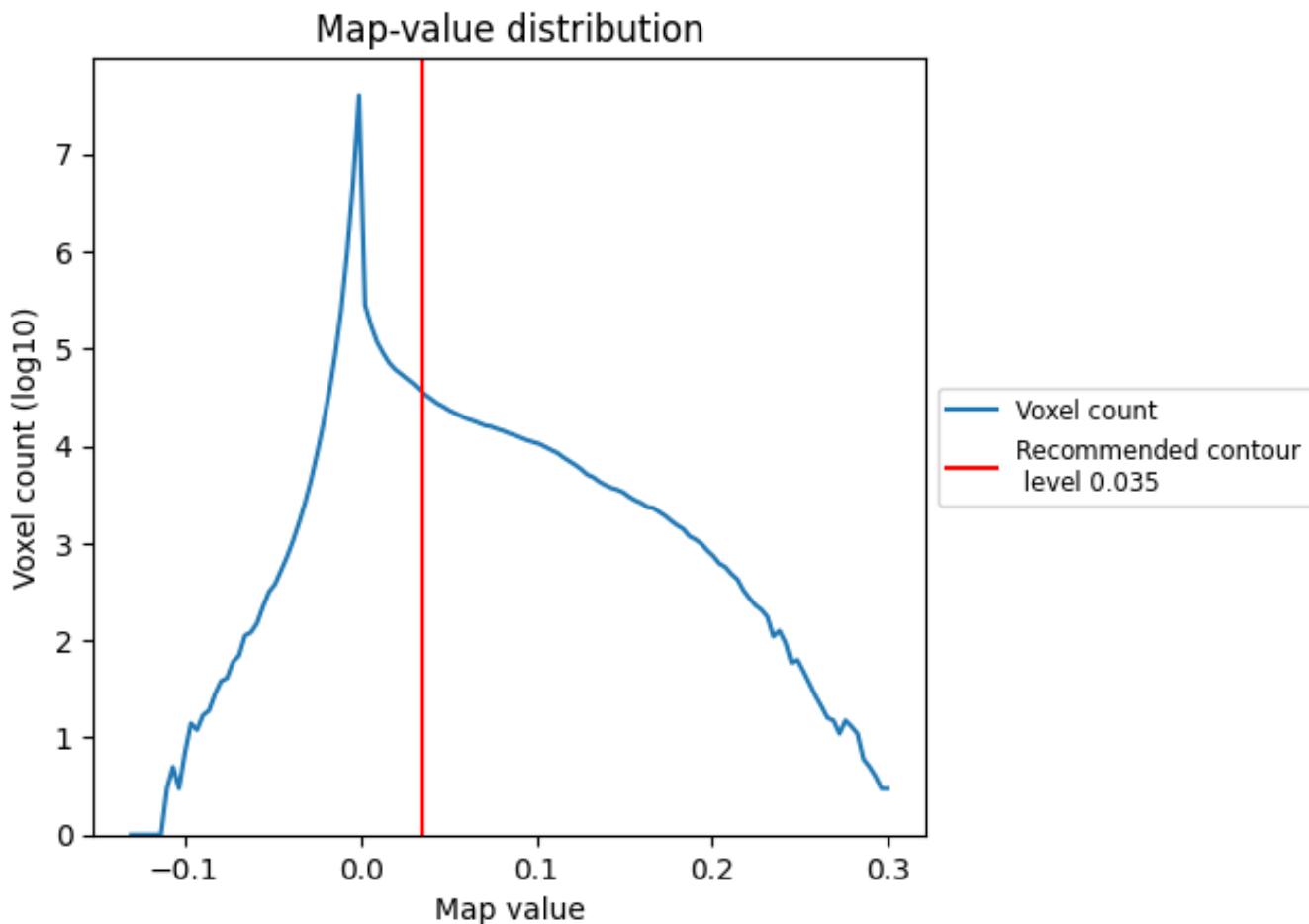


Z

## 7 Map analysis [i](#)

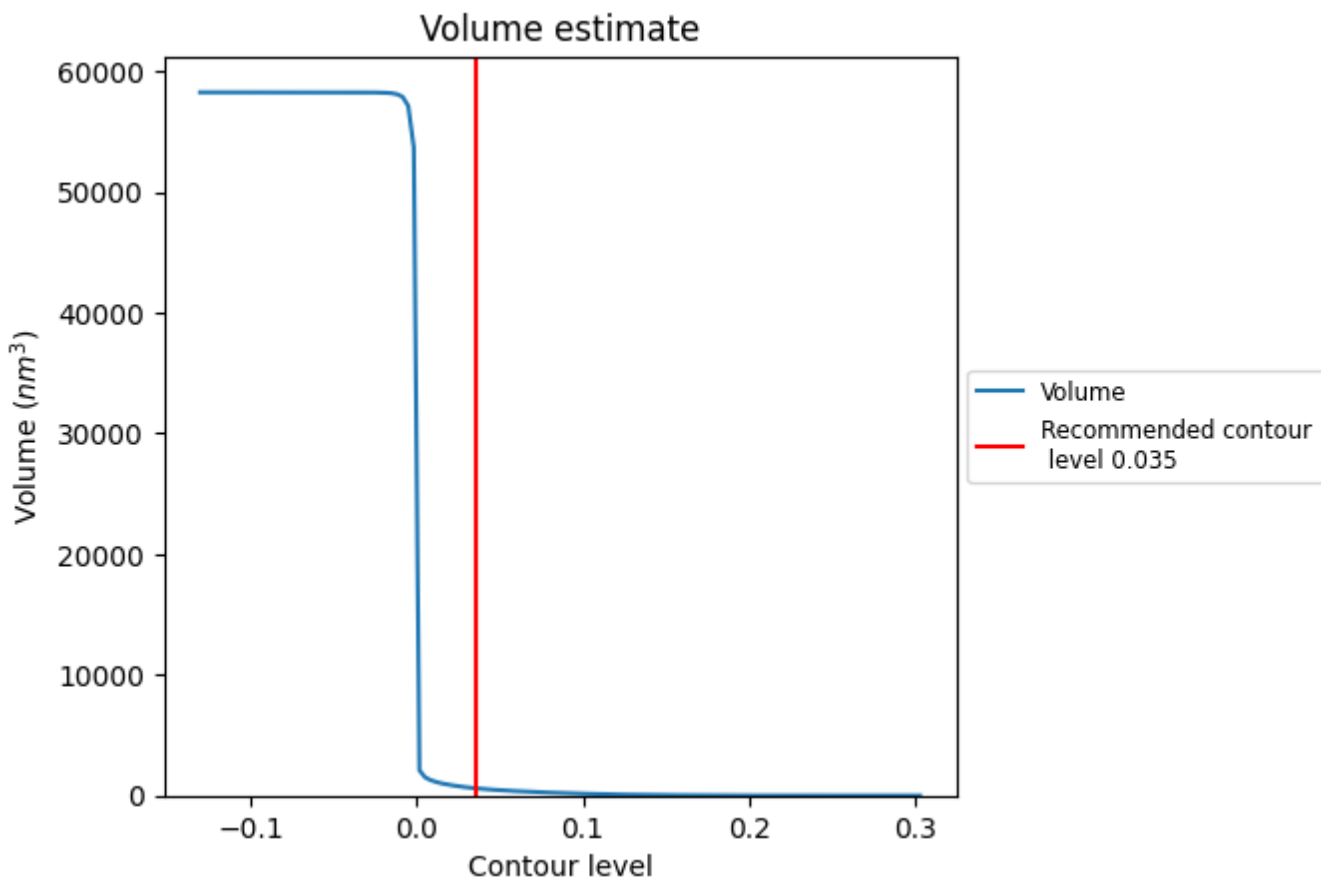
This section contains the results of statistical analysis of the map.

### 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.

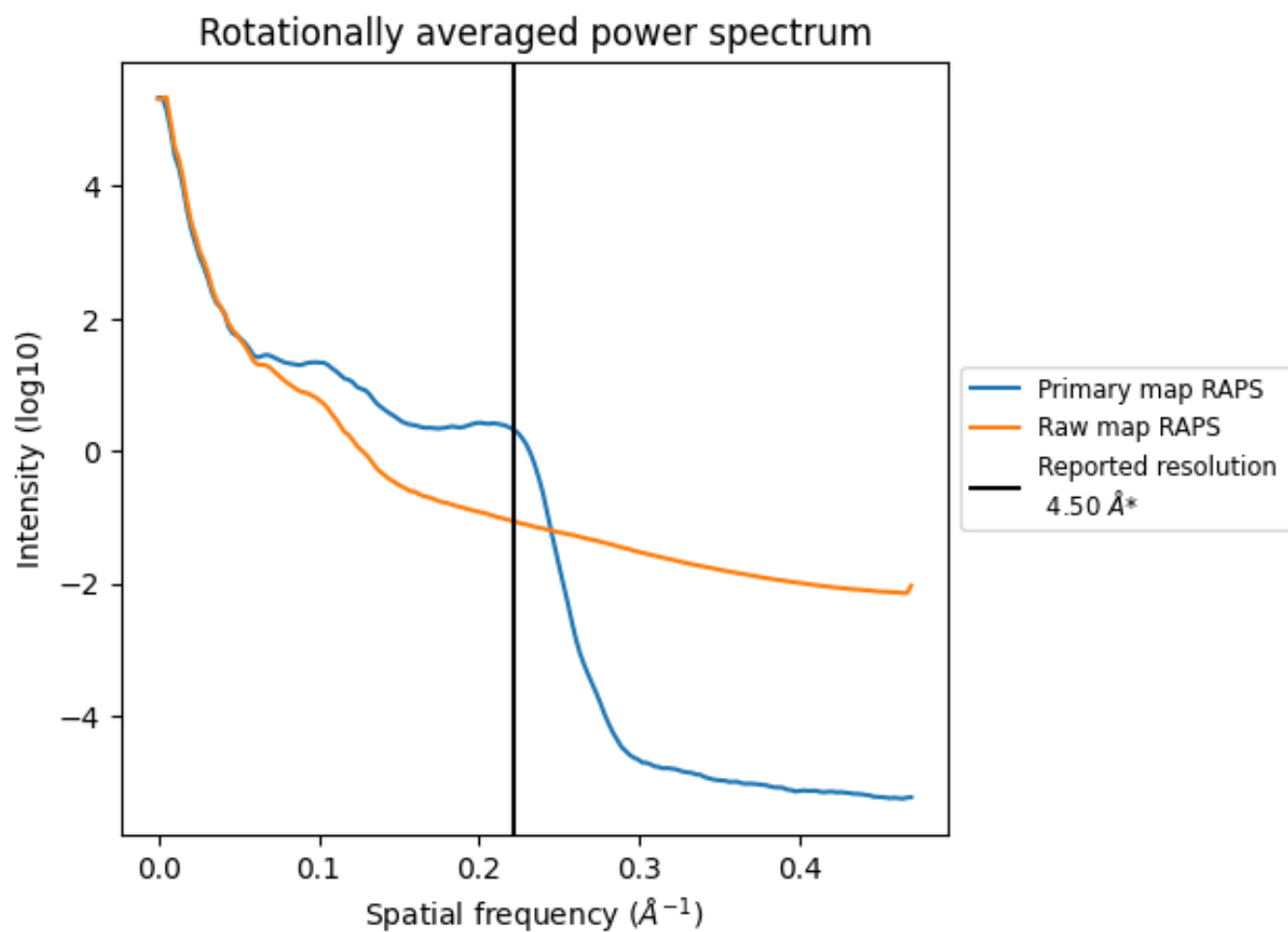
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 607 nm<sup>3</sup>; this corresponds to an approximate mass of 548 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 i

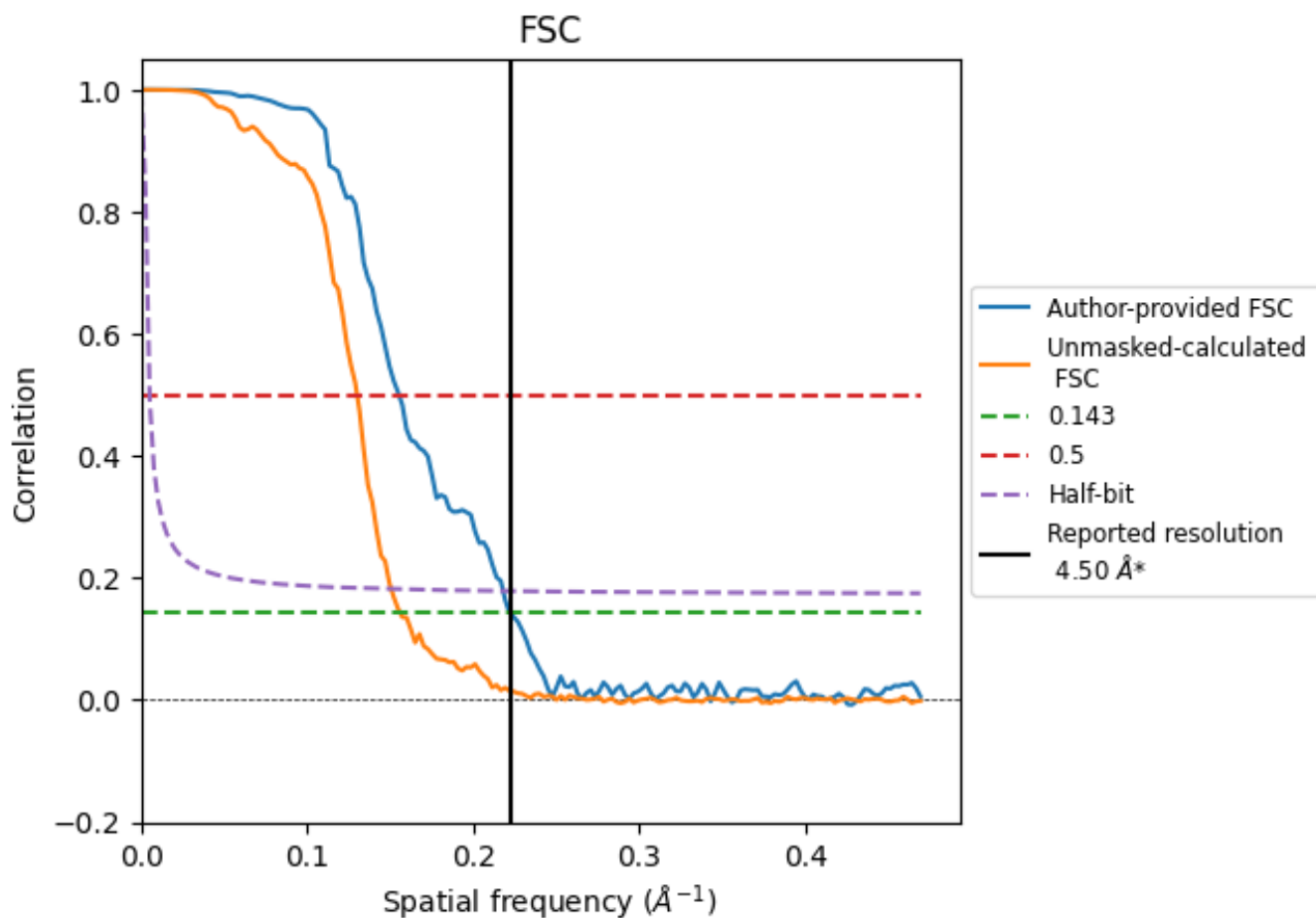


\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

## 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 0.222 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

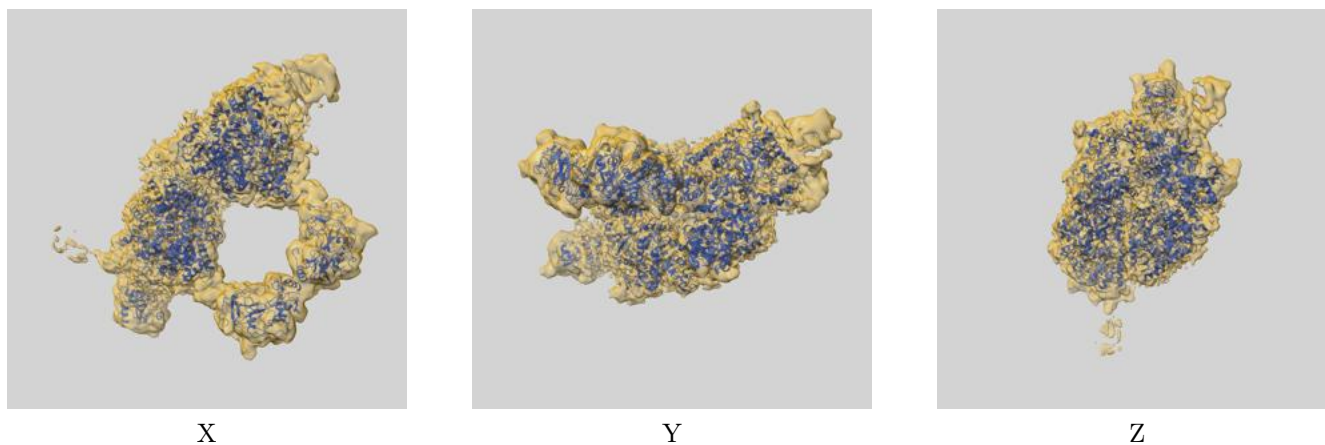
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.44	4.59
Unmasked-calculated*	6.41	7.69	6.64

\*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 6.41 differs from the reported value 4.5 by more than 10 %

## 9 Map-model fit [i](#)

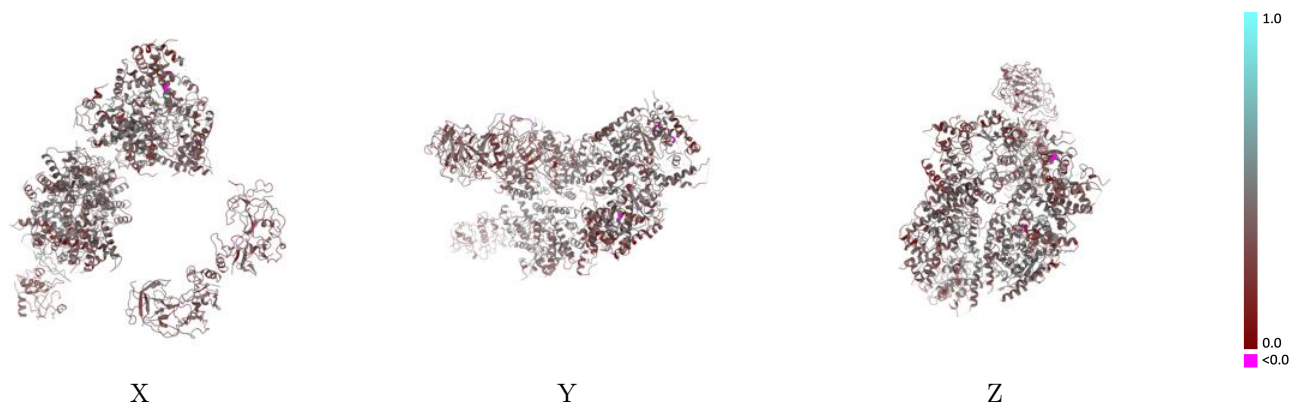
This section contains information regarding the fit between EMDB map EMD-4975 and PDB model 6ROW. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



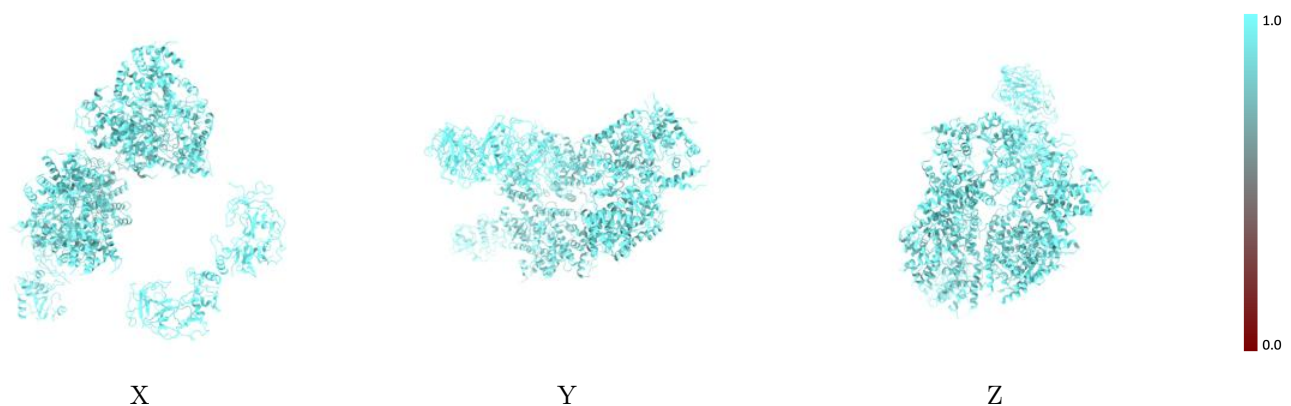
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



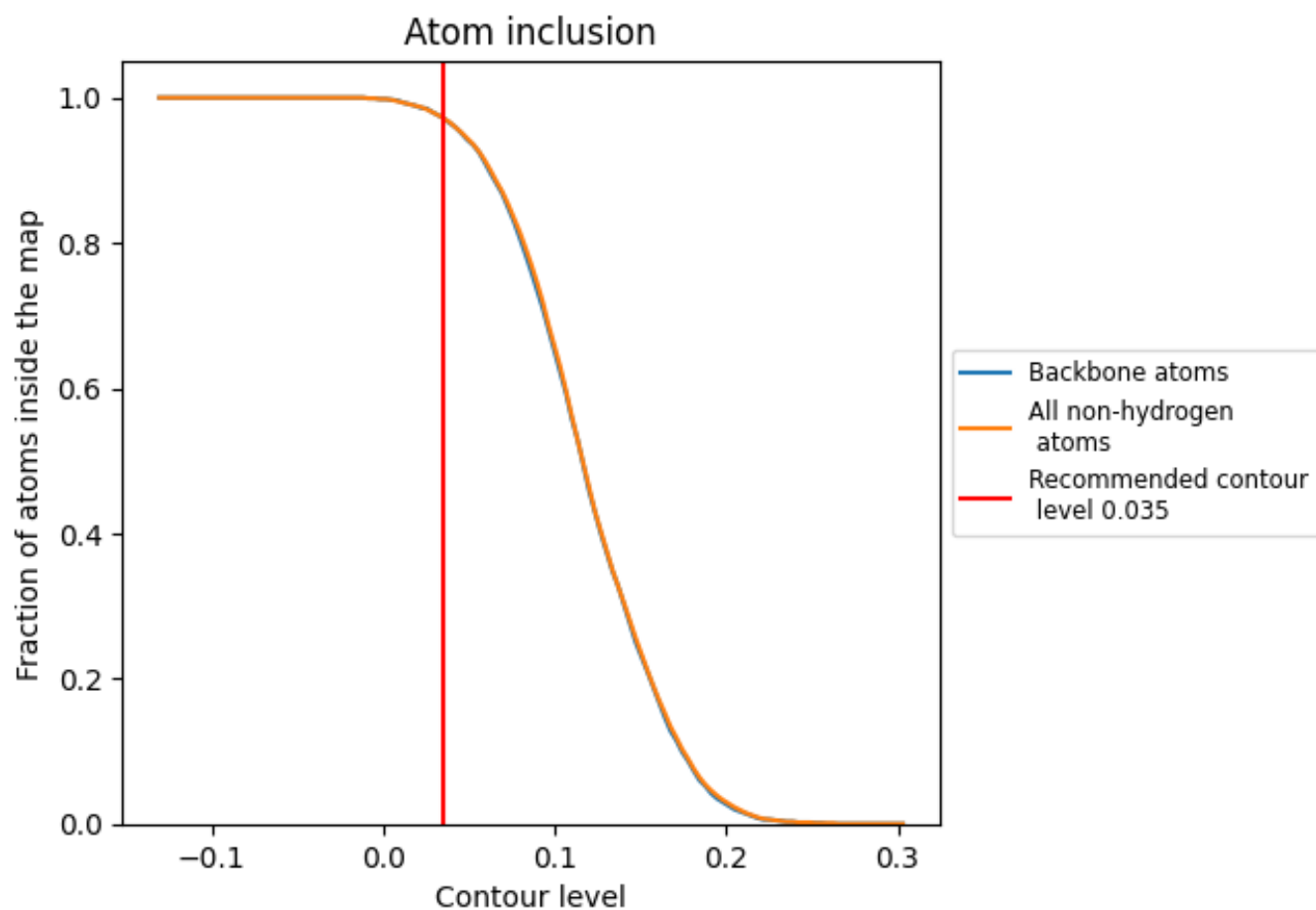
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9720	 0.3790
A	 0.9760	 0.4040
B	 0.9660	 0.3870
C	 0.9730	 0.3890
D	 0.9620	 0.3650
E	 1.0000	 0.3610
F	 1.0000	 0.3400
G	 0.9980	 0.2980

